Supplemental data for

Assessment of a composite CC2/DFT procedure for calculating 0–0 excitation energies of organic molecules

Baswanth Oruganti[†], Changfeng Fang[†] and Bo Durbeej*

Division of Theoretical Chemistry, IFM, Linköping University, Linköping, Sweden

---

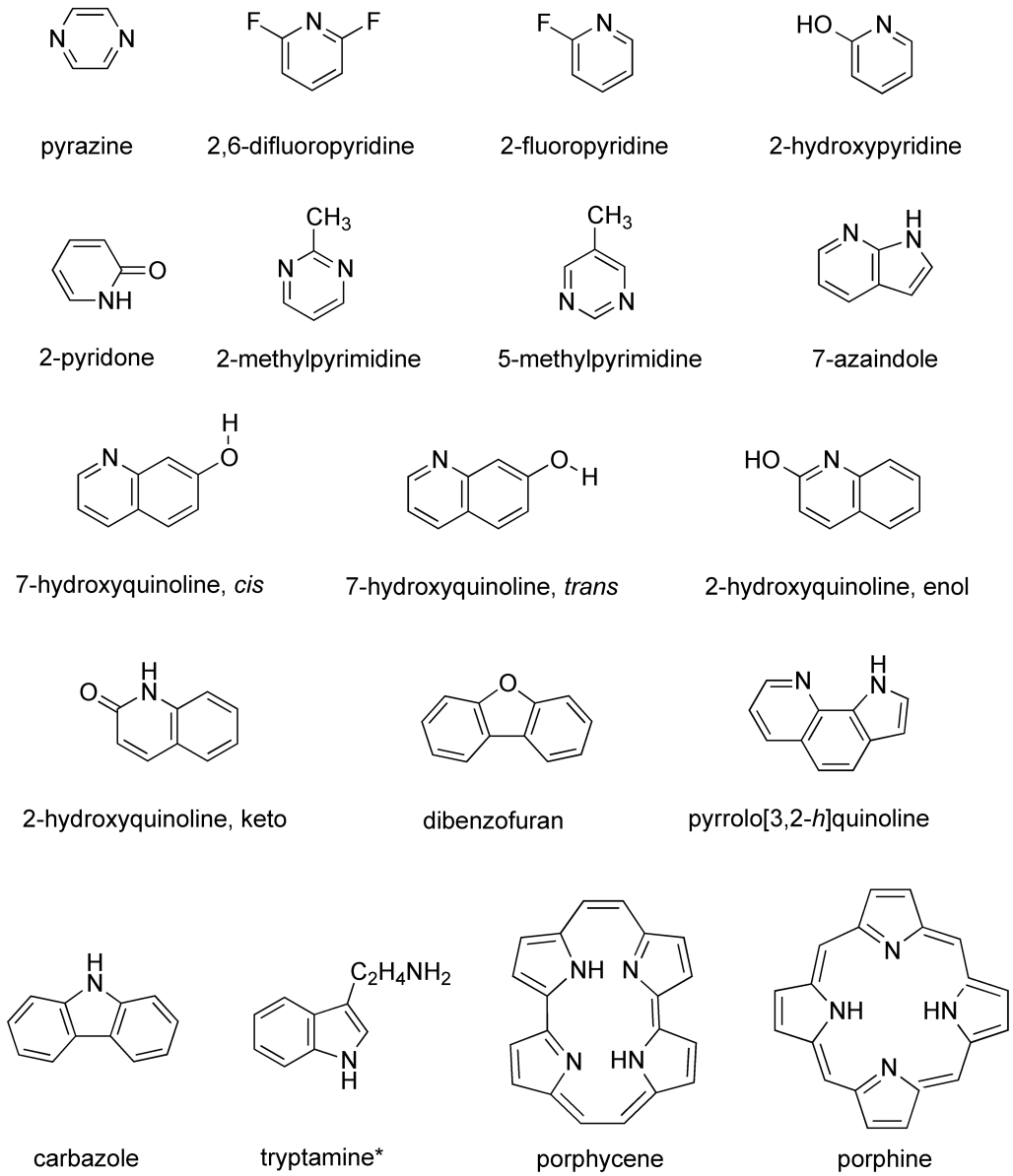
[†]These authors contributed equally to the work.

*Corresponding author. E-mail: bodur@ifm.liu.se. Tel: +46-(0)13-282497.

Table of Contents

Figure S1	page S3
Figure S2	page S5
Figure S3	page S6
Figure S4	page S8
Figure S5	page S9
Figure S6	page S10
Figure S7	page S11
Table S1	page S12
Table S2	page S13
Table S3	page S16
Table S4	page S20
Atomic coordinates of optimized ground- and excited-state geometries	page S21
BP86 geometries	page S21
B3LYP geometries	page S88
PBE0 geometries	page S155
M06-2X geometries	page S222
M06-HF geometries	page S290
CAM-B3LYP geometries	page S357
ωB97X-D geometries	page S424
CIS geometries	page S491
CC2 geometries	page S559

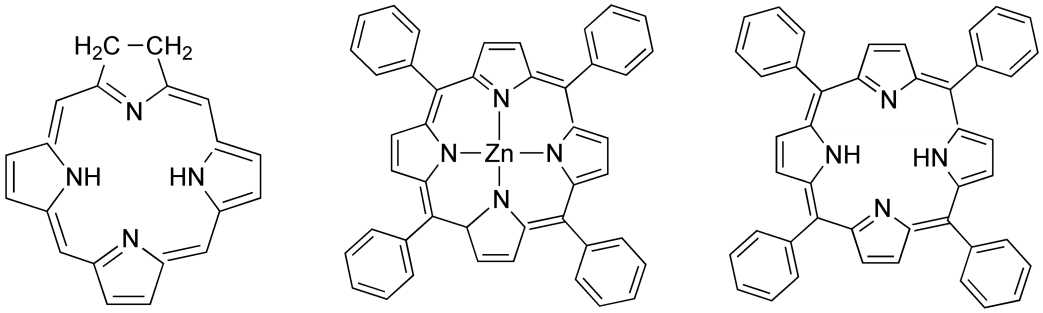
Group I



*Different tryptamine isomers are shown in Figure S2.

Figure S1. Chemical structures of the molecules in group I of the benchmark set (continued on page S4).

Group I continued



chlorin Zn-tetraphenylporphine tetraphenylporphine

Figure S1. Continued.

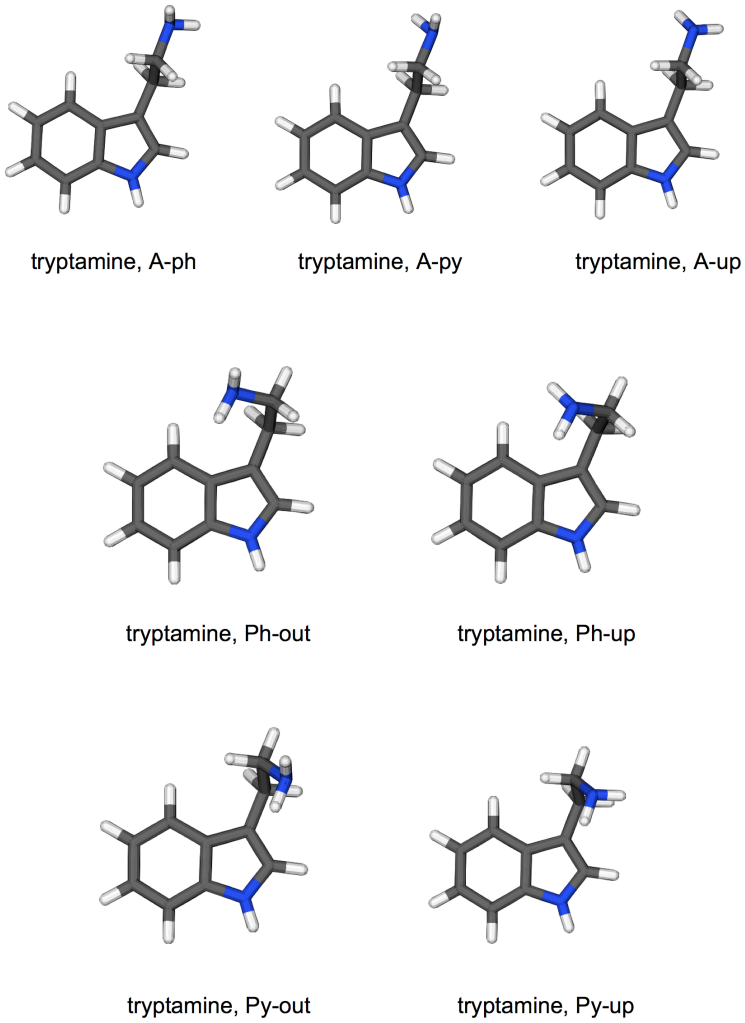
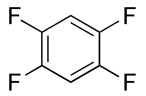
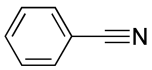
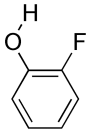


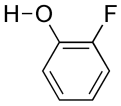
Figure S2. Different tryptamine isomers.

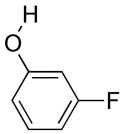
Group II

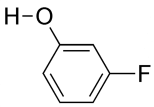

tetrafluorobenzene

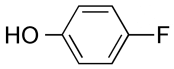

benzonitrile

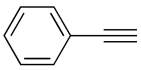

o-fluorophenol, *cis*

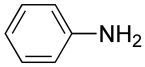

o-fluorophenol, *trans*

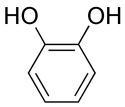

m-fluorophenol, *cis*

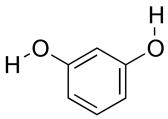

m-fluorophenol, *trans*

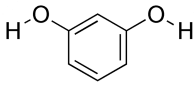

p-fluorophenol

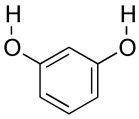

phenylacetylene

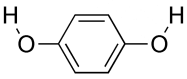

aniline

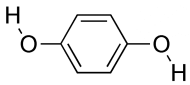

catechol

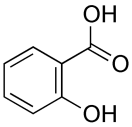

resorcinol, isomer 1

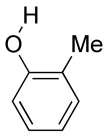

resorcinol, isomer 2

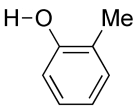

resorcinol, isomer 3

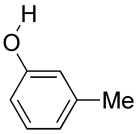

hydroquinone, *cis*

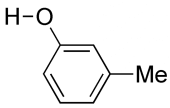

hydroquinone, *trans*

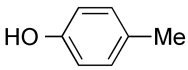

salicylic acid

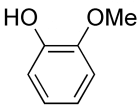

o-cresol, *cis*

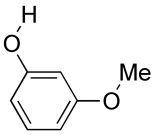

o-cresol, *trans*


m-cresol, *cis*


m-cresol, *trans*


p-cresol


o-methoxyphenol


m-methoxyphenol, isomer 1

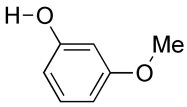
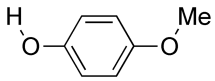
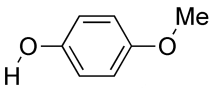

m-methoxyphenol, isomer 2

Figure S3. Chemical structures of the molecules in group II of the benchmark set (continued on page S7).

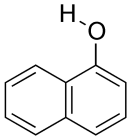
Group II continued



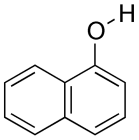
p-methoxyphenol, *cis*



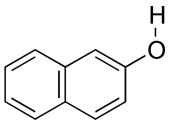
p-methoxyphenol, *trans*



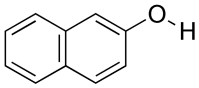
1-naphthol, *cis*



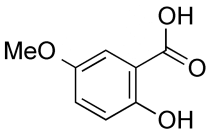
1-naphthol, *trans*



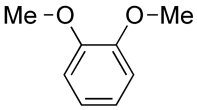
2-naphthol, *cis*



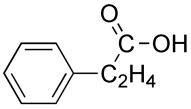
2-naphthol, *trans*



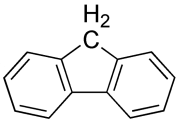
5-methoxysalicylic acid



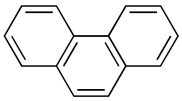
m-dimethoxybenzene, *trans*



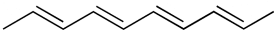
3P-propionic acid*



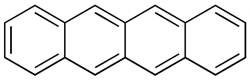
fluorene



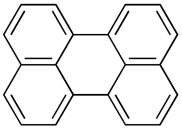
phenanthrene



2,4,6,8-decatetraene



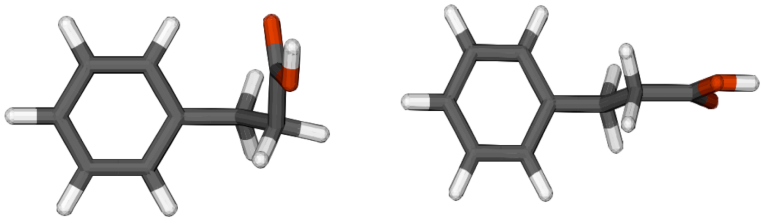
tetracene



perylene

*Different 3P-propionic acid isomers are shown in Figure S4.

Figure S3. Continued.



3P-propionic acid, *gauche* 3P-propionic acid, *anti*

Figure S4. Different 3P-propionic acid isomers.

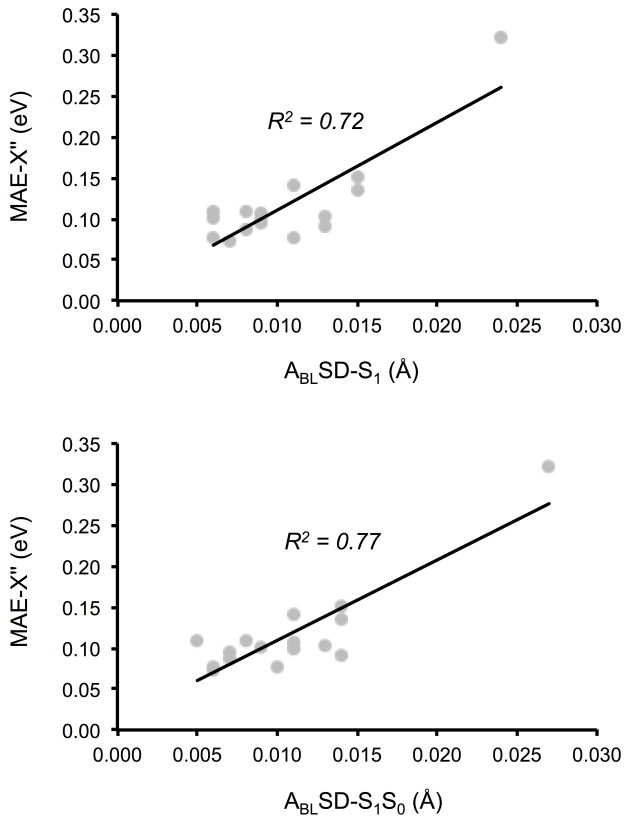


Figure S5. MAE-X'' values as functions of $A_{BL}SD\text{-}S_1$ and $A_{BL}SD\text{-}S_1S_0$ values (see Table S4) for selected states in the benchmark set.

Comments on Figure S5

In order to make possible trends more easily discernible, the analysis in Figure S5 only includes states in the benchmark set whose MAE-X'' values are larger than a specific threshold value. This threshold value was defined as the average MAE for the eight ΔE_{00}(CC2/X'') schemes in Figure 3, and amounts to 0.078 eV.

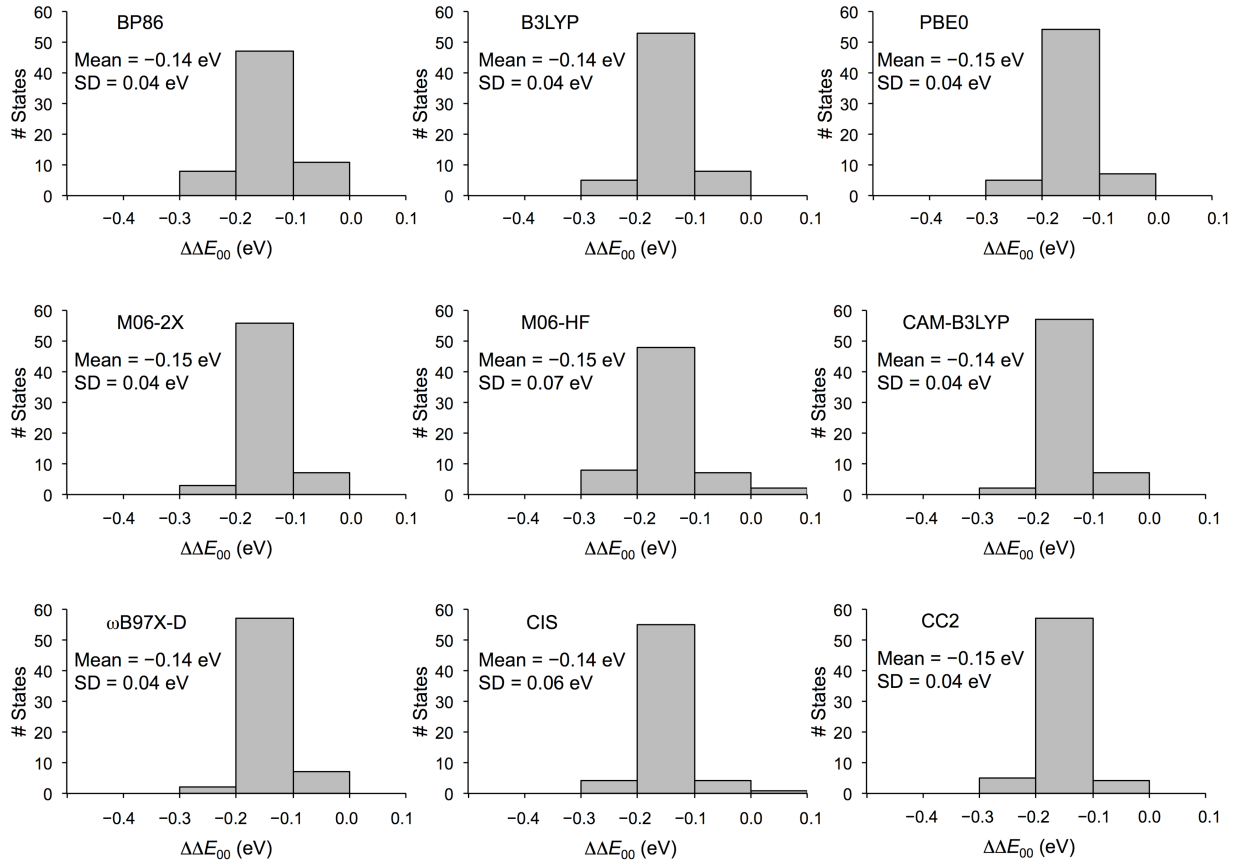


Figure S6. Histograms of calculated $\Delta\Delta E_{00}$ energy differences at different levels of theory.

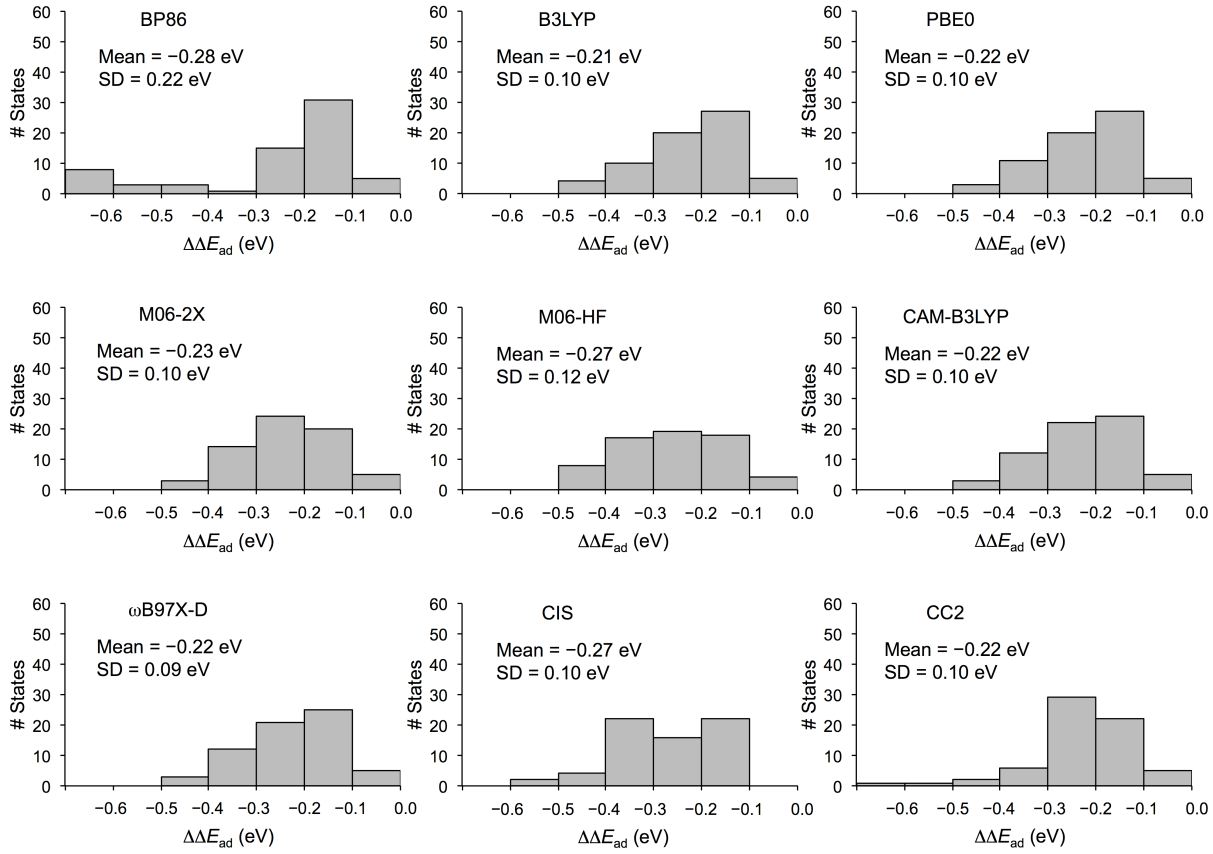


Figure S7. Histograms of calculated $\Delta\Delta E_{ad}$ energy differences at different levels of theory.

Table S1. Comparison of MAE and MaxAE values for the ΔE_{00}(CC2/X') and ΔE_{00}(CC2/X'') schemes relative to the ΔE_{00}(CC2) energies reported in this work and by Hättig (eV).

	Relative to ΔE_{00}(CC2) energies of this work		Relative to ΔE_{00}(CC2) energies of Hättig[a]	
Scheme	MAE	MaxAE	MAE	MaxAE
ΔE_{00}(CC2/X')				
ΔE_{00}(CC2/BP86')	0.04	0.15	0.03	0.08
ΔE_{00}(CC2/B3LYP')	0.03	0.18	0.02	0.08
ΔE_{00}(CC2/PBE0')	0.03	0.11	0.02	0.09
ΔE_{00}(CC2/M06-2X')	0.04	0.09	0.02	0.13
ΔE_{00}(CC2/M06-HF')	0.04	0.22	0.04	0.20
ΔE_{00}(CC2/CAM-B3LYP')	0.03	0.10	0.02	0.12
ΔE_{00}(CC2/ωB97X-D')	0.03	0.11	0.02	0.14
ΔE_{00}(CC2/CIS')	0.04	0.23	0.03	0.19
ΔE_{00}(CC2/X'')				
ΔE_{00}(CC2/BP86'')	0.12	0.79	0.14	0.79
ΔE_{00}(CC2/B3LYP'')	0.06	0.41	0.08	0.54
ΔE_{00}(CC2/PBE0'')	0.06	0.34	0.07	0.54
ΔE_{00}(CC2/M06-2X'')	0.06	0.35	0.08	0.50
ΔE_{00}(CC2/M06-HF'')	0.08	0.28	0.10	0.47
ΔE_{00}(CC2/CAM-B3LYP'')	0.07	0.35	0.08	0.51
ΔE_{00}(CC2/ωB97X-D'')	0.07	0.34	0.08	0.50
ΔE_{00}(CC2/CIS'')	0.11	0.33	0.11	0.50

[a]Taken from Ref. [25].

Table S2. Calculated ΔE_{ve} energies and $\Delta\Delta E_{ad}$ and $\Delta\Delta E_{00}$ energy differences for all states in group I of the benchmark set (eV).[a]

			Method and statistics[b]										
Label/Molecule	State	ΔE	BP86	B3LYP	PBE0	M06-2X	M06-HF	CB3LYP	ωB97X-D	CIS	CC2	SD	MaxAD
1/pyrazine	1^1A_u	ΔE_{ve}	3.58	3.96	4.02	4.00	3.82	4.20	4.17	5.18	4.27	0.42	1.60
		$\Delta\Delta E_{ad}$	-0.24	-0.14	-0.13	-0.12	-0.13	-0.13	-0.13	-0.13	-0.13	0.04	0.12
		$\Delta\Delta E_{00}$	-0.21	-0.21	-0.21	-0.20	-0.21	-0.21	-0.22	-0.23	-0.23	0.01	0.03
2/2,6-difluoropyridine	1^1B_2	ΔE_{ve}	5.10	5.41	5.52	5.64	5.86	5.56	5.55	6.40	5.24	0.35	1.30
		$\Delta\Delta E_{ad}$	-0.20	-0.21	-0.22	-0.24	-0.24	-0.22	-0.23	-0.23	-0.34	0.04	0.13
		$\Delta\Delta E_{00}$	-0.18	-0.17	-0.17	-0.16	-0.18	-0.15	-0.16	-0.15	-0.11	0.02	0.07
3/2-fluoropyridine	$2^1A'$	ΔE_{ve}	5.16	5.45	5.56	5.67	5.89	5.60	5.59	6.35	5.27	0.33	1.19
		$\Delta\Delta E_{ad}$	-0.18	-0.19	-0.20	-0.21	-0.22	-0.20	-0.20	-0.21	-0.38	0.06	0.20
		$\Delta\Delta E_{00}$	-0.15	-0.20	-0.20	-0.20	-0.09	-0.19	-0.19	-0.17	-0.13	0.04	0.11
4/2-hydroxypyridine	$2^1A'$	ΔE_{ve}	4.74	5.09	5.21	5.37	5.61	5.29	5.28	6.13	5.00	0.37	1.39
		$\Delta\Delta E_{ad}$	-0.21	-0.20	-0.21	-0.23	-0.25	-0.22	-0.22	-0.24	-0.30	0.03	0.10
		$\Delta\Delta E_{00}$	-0.18	-0.16	-0.16	-0.16	-0.18	-0.15	-0.16	-0.15	-0.13	0.02	0.06
5/2-pyridone	$2^1A'$	ΔE_{ve}	4.03	4.36	4.47	4.66	4.87	4.62	4.61	5.57	4.43	0.40	1.54
		$\Delta\Delta E_{ad}$	-0.53	-0.40	-0.38	-0.36	-0.43	-0.37	-0.37	-0.46	-0.63	0.09	0.27
		$\Delta\Delta E_{00}$	-0.09	-0.06	-0.15	-0.16	-0.16	-0.15	-0.16	-0.15	-0.24	0.05	0.18
6/2-methylpyrimidine	$1^1A''$	ΔE_{ve}	3.73	4.19	4.29	4.38	4.38	4.48	4.46	5.85	4.42	0.54	2.12
		$\Delta\Delta E_{ad}$	-0.45	-0.44	-0.45	-0.46	-0.49	-0.45	-0.46	-0.52	-0.48	0.02	0.08
		$\Delta\Delta E_{00}$	-0.13	-0.14	-0.14	-0.16	-0.17	-0.15	-0.15	-0.17	-0.10	0.02	0.07
7/5-methylpyrimidine	$1^1A''$	ΔE_{ve}	3.76	4.23	4.33	4.41	4.40	4.52	4.50	5.86	4.47	0.53	2.10
		$\Delta\Delta E_{ad}$	-0.45	-0.44	-0.44	-0.45	-0.48	-0.45	-0.46	-0.51	-0.46	0.02	0.08
		$\Delta\Delta E_{00}$	-0.13	-0.14	-0.14	-0.16	-0.17	-0.15	-0.15	-0.17	-0.17	0.01	0.05
8/7-azaindole	$2^1A'$	ΔE_{ve}	4.20	4.63	4.77	5.12	5.36	5.06	5.05	5.77	4.82	0.42	1.57
		$\Delta\Delta E_{ad}$	-0.41	-0.40	-0.40	-0.43	-0.34	-0.41	-0.41	-0.33	-0.28	0.05	0.15
		$\Delta\Delta E_{00}$	-0.12	-0.12	-0.13	-0.15	-0.18	-0.14	-0.14	-0.16	-0.14	0.02	0.06
9/7-hydroxyquinoline	$2^1A'$	ΔE_{ve}	3.68	4.13	4.25	4.54	4.92	4.49	4.49	5.42	4.26	0.47	1.75
		$\Delta\Delta E_{ad}$	-0.19	-0.22	-0.22	-0.22	-0.27	-0.22	-0.21	-0.31	-0.19	0.04	0.13
		$\Delta\Delta E_{00}$	-0.12	-0.14	-0.14	-0.16	-0.17	-0.15	-0.16	-0.17	-0.14	0.02	0.05
10/7-hydroxyquinoline	2^1A	ΔE_{ve}	3.63	4.06	4.18	4.48	4.87	4.43	4.43	5.35	4.19	0.46	1.72
		$\Delta\Delta E_{ad}$	-0.61	-0.43	-0.45	-0.23	-0.27	-0.22	-0.22	-0.32	-0.20	0.13	0.42
		$\Delta\Delta E_{00}$	-0.10	-0.12	-0.12	-0.16	-0.01	-0.15	-0.15	-0.13	-0.13	0.04	0.15
11/2-hydroxyquinoline	$2^1A'$	ΔE_{ve}	3.82	4.22	4.34	4.59	4.95	4.54	4.54	5.47	4.30	0.44	1.65
		$\Delta\Delta E_{ad}$	-0.20	-0.22	-0.22	-0.23	-0.29	-0.22	-0.22	-0.36	-0.20	0.05	0.17
		$\Delta\Delta E_{00}$	-0.15	-0.15	-0.16	-0.17	-0.16	-0.16	-0.16	-0.17	-0.11	0.02	0.06

Table S2. Continued.

			Method and statistics[b]										
Label/Molecule	State	ΔE	BP86	B3LYP	PBE0	M06-2X	M06-HF	CB3LYP	ωB97X-D	CIS	CC2	SD	MaxAD
12/2-hydroxyquinoline	$2^1A'$	ΔE_{ve}	3.61	4.01	4.13	4.41	4.76	4.38	4.38	5.35	4.11	0.47	1.75
		$\Delta\Delta E_{ad}$	-0.23	-0.24	-0.24	-0.30	-0.41	-0.28	-0.28	-0.37	-0.25	0.06	0.19
		$\Delta\Delta E_{00}$	-0.13	-0.15	-0.15	-0.14	-0.13	-0.14	-0.14	-0.14	-0.11	0.01	0.04
13/dibenzofuran	2^1A_1	ΔE_{ve}	4.02	4.47	4.61	4.89	5.19	4.85	4.86	5.75	4.55	0.45	1.72
		$\Delta\Delta E_{ad}$	-0.11	-0.12	-0.12	-0.13	-0.09	-0.12	-0.12	-0.13	-0.14	0.01	0.05
		$\Delta\Delta E_{00}$	-0.20	-0.21	-0.21	-0.22	-0.23	-0.21	-0.21	-0.11	-0.16	0.03	0.12
14/pyrrolo[3,2-*h*]quinoline	$2^1A'$	ΔE_{ve}	3.46	3.90	4.04	4.38	4.82	4.34	4.37	5.14	4.11	0.47	1.69
		$\Delta\Delta E_{ad}$	-0.24	-0.27	-0.27	-0.27	-0.27	-0.26	-0.26	-0.29	-0.19	0.03	0.11
		$\Delta\Delta E_{00}$	-0.12	-0.13	-0.14	-0.16	-0.19	-0.16	-0.16	-0.18	-0.14	0.02	0.07
15/carbazole	2^1A_1	ΔE_{ve}	3.66	4.07	4.20	4.48	4.80	4.46	4.48	5.35	4.18	0.45	1.69
		$\Delta\Delta E_{ad}$	-0.11	-0.12	-0.12	-0.13	-0.15	-0.12	-0.12	-0.28	-0.15	0.05	0.17
		$\Delta\Delta E_{00}$	-0.17	-0.14	-0.14	-0.15	-0.17	-0.14	-0.15	-0.16	-0.12	0.01	0.05
16/tryptamine	2^1A	ΔE_{ve}	4.11	4.62	4.74	5.04	5.34	4.99	5.00	5.73	4.82	0.43	1.62
		$\Delta\Delta E_{ad}$	-0.78	-0.32	-0.32	-0.33	-0.33	-0.31	-0.31	-0.32	-0.19	0.15	0.59
		$\Delta\Delta E_{00}$	-0.18	-0.15	-0.15	-0.15	-0.16	-0.15	-0.14	-0.15	-0.21	0.02	0.06
17/tryptamine	2^1A	ΔE_{ve}	4.04	4.59	4.72	5.03	5.34	4.99	4.99	5.72	4.82	0.45	1.69
		$\Delta\Delta E_{ad}$	-0.70	-0.33	-0.33	-0.34	-0.34	-0.32	-0.32	-0.32	-0.21	0.13	0.49
		$\Delta\Delta E_{00}$	-0.18	-0.15	-0.15	-0.15	-0.16	-0.15	-0.14	-0.15	-0.20	0.02	0.06
18/tryptamine	2^1A	ΔE_{ve}	3.90	4.55	4.69	5.02	5.34	4.98	4.98	5.73	4.82	0.48	1.83
		$\Delta\Delta E_{ad}$	-0.55	-0.34	-0.34	-0.34	-0.34	-0.31	-0.32	-0.32	-0.21	0.08	0.34
		$\Delta\Delta E_{00}$	-0.18	-0.15	-0.15	-0.15	-0.15	-0.15	-0.14	-0.15	-0.20	0.02	0.06
19/tryptamine	2^1A	ΔE_{ve}	3.99	4.61	4.74	5.04	5.35	5.00	5.00	5.73	4.82	0.46	1.74
		$\Delta\Delta E_{ad}$	-0.90	-0.32	-0.32	-0.33	-0.33	-0.31	-0.31	-0.32	-0.19	0.19	0.71
		$\Delta\Delta E_{00}$	-0.15	-0.15	-0.15	-0.16	-0.17	-0.15	-0.15	-0.16	-0.20	0.02	0.05
20/tryptamine	2^1A	ΔE_{ve}	3.79	4.52	4.65	5.00	5.34	4.96	4.96	5.71	4.82	0.50	1.92
		$\Delta\Delta E_{ad}$	-0.70	-0.37	-0.37	-0.36	-0.38	-0.34	-0.34	-0.32	-0.26	0.12	0.43
		$\Delta\Delta E_{00}$	-0.15	-0.14	-0.14	-0.15	-0.16	-0.14	-0.14	-0.15	-0.20	0.02	0.06
21/tryptamine	2^1A	ΔE_{ve}	3.94	4.60	4.73	5.04	5.35	4.99	5.00	5.73	4.82	0.47	1.79
		$\Delta\Delta E_{ad}$	-0.84	-0.32	-0.32	-0.34	-0.33	-0.31	-0.31	-0.31	-0.24	0.17	0.60
		$\Delta\Delta E_{00}$	-0.14	-0.15	-0.15	-0.15	-0.16	-0.15	-0.14	-0.15	-0.18	0.01	0.05
22/tryptamine	2^1A	ΔE_{ve}	3.92	4.60	4.73	5.04	5.34	5.00	5.00	5.74	4.82	0.47	1.82
		$\Delta\Delta E_{ad}$	-0.71	-0.33	-0.33	-0.33	-0.32	-0.30	-0.30	-0.31	-0.19	0.14	0.53
		$\Delta\Delta E_{00}$	-0.17	-0.16	-0.16	-0.15	-0.17	-0.15	-0.13	-0.15	-0.20	0.02	0.07
23/porphycene	$2^1A'$	ΔE_{ve}	2.11	2.24	2.29	2.26	2.16	2.19	2.14	2.83	2.24	0.21	0.72

Table S2. Continued.

Label/Molecule	State	ΔE	Method and statistics[b]										
			BP86	B3LYP	PBE0	M06-2X	M06-HF	CB3LYP	ωB97X-D	CIS	CC2	SD	MaxAD
		$\Delta\Delta E_{ad}$	-0.07	-0.05	-0.05	-0.05	-0.11	-0.04	-0.04	-0.29	-0.04	0.08	0.25
		$\Delta\Delta E_{00}$	-0.15	-0.10	-0.09	-0.08	-0.01	-0.07	-0.09	-0.04	-0.13	0.04	0.14
24/porphine	1^1B_{1u}	ΔE_{ve}	2.15	2.28	2.34	2.29	2.59	2.22	2.16	2.96	2.29	0.24	0.81
		$\Delta\Delta E_{ad}$	-0.03	-0.02	-0.02	-0.01	-0.14	-0.01	-0.01	-0.34	-0.03	0.10	0.33
		$\Delta\Delta E_{00}$	-0.08	-0.07	-0.07	-0.03	0.10	-0.02	-0.01	0.11	-0.12	0.08	0.23
25/chlorin	1^1B_2	ΔE_{ve}	2.19	2.28	2.32	2.25	2.10	2.20	2.16	3.03	2.27	0.26	0.93
		$\Delta\Delta E_{ad}$	-0.01	-0.01	-0.01	-0.02	-0.04	-0.03	-0.03	-0.42	0.00	0.13	0.42
		$\Delta\Delta E_{00}$	-0.09	-0.07	-0.07	-0.03	0.06	-0.02	-0.02	-0.03	-0.12	0.05	0.18
26/Zn-tetraphenylporphine	1^1B_2	ΔE_{ve}	2.12	2.30	2.34	2.33	2.24	2.30	2.25	2.64	2.34	0.13	0.52
		$\Delta\Delta E_{ad}$	-0.08	-0.04	-0.05	-0.03	-0.02	-0.03	-0.03	-0.12	-0.04	0.03	0.10
		$\Delta\Delta E_{00}$	-0.06	-0.06	-0.06	-0.07	-0.02	-0.06	-0.05	0.03	-0.06	0.03	0.10
27/tetraphenylporphine	1^1B	ΔE_{ve}	1.97	2.16	2.20	2.16	2.35	2.12	2.07	2.95	2.08	0.27	0.98
		$\Delta\Delta E_{ad}$	-0.04	-0.04	-0.04	-0.03	-0.03	-0.03	-0.03	-0.35	-0.04	0.10	0.32
		$\Delta\Delta E_{00}$	-0.06	-0.05	-0.04	-0.03	0.00	0.00	-0.02	0.11	-0.05	0.05	0.17

[a]$\Delta\Delta E_{ad} = \Delta E_{ad} - \Delta E_{ve}$ and $\Delta\Delta E_{00} = \Delta E_{00} - \Delta E_{ad}$. [b]Standard deviation (SD) and maximum absolute deviation (MaxAD) for calculations with the nine methods.

Table S3. Calculated ΔE_{ve} energies and $\Delta\Delta E_{ad}$ and $\Delta\Delta E_{00}$ energy differences for all states in group II of the benchmark set (eV).[a]

			Method and statistics[b]										
Label/Molecule	State	ΔE	BP86	B3LYP	PBE0	M06-2X	M06-HF	CB3LYP	ωB97X-D	CIS	CC2	SD	MaxAD
1/tetrafluorobenzene	1^1B_1	ΔE_{ve}	4.84	5.19	5.31	5.46	5.70	5.37	5.36	6.31	5.06	0.40	1.47
		$\Delta\Delta E_{ad}$	-0.37	-0.34	-0.36	-0.36	-0.46	-0.32	-0.31	-0.27	-0.31	0.05	0.19
		$\Delta\Delta E_{00}$	-0.13	-0.13	-0.12	-0.12	-0.11	-0.12	-0.12	-0.12	-0.18	0.02	0.07
2/benzonitrile	1^1B_2	ΔE_{ve}	4.80	5.12	5.25	5.41	5.66	5.34	5.34	6.07	5.07	0.34	1.26
		$\Delta\Delta E_{ad}$	-0.15	-0.15	-0.15	-0.14	-0.14	-0.14	-0.14	-0.13	-0.19	0.01	0.05
		$\Delta\Delta E_{00}$	-0.16	-0.15	-0.16	-0.17	-0.10	-0.14	-0.15	-0.16	-0.15	0.02	0.07
3/*o*-fluorophenol	2^1A	ΔE_{ve}	4.84	5.16	5.28	5.43	5.66	5.35	5.34	6.17	5.07	0.36	1.33
		$\Delta\Delta E_{ad}$	-0.15	-0.31	-0.28	-0.26	-0.18	-0.24	-0.22	-0.14	-0.24	0.05	0.18
		$\Delta\Delta E_{00}$	-0.19	-0.12	-0.11	-0.11	-0.20	-0.11	-0.10	-0.09	-0.15	0.04	0.10
4/*o*-fluorophenol	2^1A	ΔE_{ve}	4.81	5.13	5.26	5.40	5.63	5.32	5.31	6.15	5.04	0.36	1.33
		$\Delta\Delta E_{ad}$	-0.28	-0.24	-0.25	-0.26	-0.34	-0.23	-0.21	-0.20	-0.25	0.04	0.14
		$\Delta\Delta E_{00}$	-0.10	-0.12	-0.12	-0.11	-0.13	-0.11	-0.12	-0.12	-0.16	0.02	0.07
5/*m*-fluorophenol	2^1A	ΔE_{ve}	4.84	5.16	5.28	5.42	5.64	5.34	5.34	6.18	5.07	0.36	1.34
		$\Delta\Delta E_{ad}$	-0.19	-0.18	-0.19	-0.20	-0.18	-0.18	-0.17	-0.17	-0.22	0.02	0.05
		$\Delta\Delta E_{00}$	-0.13	-0.13	-0.13	-0.13	-0.20	-0.12	-0.13	-0.13	-0.16	0.02	0.08
6/*m*-fluorophenol	$2^1A'$	ΔE_{ve}	4.85	5.17	5.30	5.43	5.66	5.36	5.35	6.19	5.08	0.36	1.34
		$\Delta\Delta E_{ad}$	-0.15	-0.15	-0.16	-0.16	-0.17	-0.16	-0.16	-0.16	-0.20	0.02	0.05
		$\Delta\Delta E_{00}$	-0.21	-0.19	-0.19	-0.18	-0.19	-0.17	-0.17	-0.17	-0.16	0.01	0.05
7/*p*-fluorophenol	$2^1A'$	ΔE_{ve}	4.56	4.91	5.01	5.18	5.44	5.10	5.09	5.96	4.83	0.38	1.40
		$\Delta\Delta E_{ad}$	-0.16	-0.17	-0.18	-0.19	-0.20	-0.19	-0.19	-0.20	-0.21	0.02	0.05
		$\Delta\Delta E_{00}$	-0.19	-0.19	-0.18	-0.17	-0.19	-0.17	-0.17	-0.17	-0.14	0.01	0.05
8/phenylacetylene	1^1B_2	ΔE_{ve}	4.62	4.99	5.13	5.32	5.59	5.27	5.27	5.83	5.01	0.33	1.21
		$\Delta\Delta E_{ad}$	-0.15	-0.14	-0.14	-0.14	-0.13	-0.14	-0.14	-0.34	-0.18	0.06	0.21
		$\Delta\Delta E_{00}$	-0.16	-0.16	-0.16	-0.17	-0.17	-0.15	-0.15	-0.18	-0.17	0.01	0.03
9/aniline	$1^1A''$	ΔE_{ve}	4.39	4.75	4.87	5.05	5.25	4.98	4.99	5.84	4.82	0.37	1.44
		$\Delta\Delta E_{ad}$	-0.23	-0.21	-0.22	-0.23	-0.27	-0.22	-0.22	-0.22	-0.24	0.02	0.05
		$\Delta\Delta E_{00}$	-0.21	-0.21	-0.21	-0.21	-0.21	-0.19	-0.19	-0.20	-0.17	0.01	0.04
10/catechol	2^1A	ΔE_{ve}	4.69	5.01	5.13	5.29	5.53	5.21	5.20	6.04	4.96	0.36	1.35
		$\Delta\Delta E_{ad}$	-0.16	-0.17	-0.17	-0.19	-0.21	-0.18	-0.18	-0.18	-0.32	0.05	0.16
		$\Delta\Delta E_{00}$	-0.20	-0.20	-0.20	-0.20	-0.21	-0.19	-0.18	-0.18	-0.15	0.02	0.06
11/resorcinol	2^1A	ΔE_{ve}	4.72	5.05	5.17	5.31	5.53	5.24	5.24	6.09	4.99	0.36	1.37
		$\Delta\Delta E_{ad}$	-0.17	-0.16	-0.17	-0.20	-0.18	-0.17	-0.17	-0.17	-0.24	0.02	0.08
		$\Delta\Delta E_{00}$	-0.14	-0.13	-0.12	-0.12	-0.21	-0.12	-0.12	-0.13	-0.17	0.03	0.09

Table S3. Continued.

			Method and statistics[b]										
Label/Molecule	State	ΔE	BP86	B3LYP	PBE0	M06-2X	M06-HF	CB3LYP	ωB97X-D	CIS	CC2	SD	MaxAD
12/resorcinol	1^1B_2	ΔE_{ve}	4.73	5.06	5.19	5.33	5.56	5.26	5.26	6.10	4.98	0.37	1.37
		$\Delta\Delta E_{ad}$	-0.13	-0.13	-0.14	-0.15	-0.16	-0.15	-0.15	-0.14	-0.21	0.02	0.08
		$\Delta\Delta E_{00}$	-0.20	-0.19	-0.18	-0.18	-0.20	-0.17	-0.17	-0.17	-0.17	0.01	0.03
13/resorcinol	$1^1A''$	ΔE_{ve}	4.71	5.03	5.15	5.28	5.49	5.21	5.21	6.05	4.93	0.36	1.35
		$\Delta\Delta E_{ad}$	-0.24	-0.23	-0.24	-0.24	-0.39	-0.22	-0.21	-0.19	-0.27	0.05	0.20
		$\Delta\Delta E_{00}$	-0.15	-0.13	-0.12	-0.12	-0.11	-0.11	-0.11	-0.11	-0.15	0.01	0.04
14/hydroquinone	2^1A_1	ΔE_{ve}	4.29	4.66	4.76	4.95	5.22	4.86	4.85	5.76	4.62	0.39	1.46
		$\Delta\Delta E_{ad}$	-0.16	-0.18	-0.19	-0.21	-0.23	-0.20	-0.20	-0.23	-0.22	0.02	0.07
		$\Delta\Delta E_{00}$	-0.19	-0.19	-0.18	-0.18	-0.19	-0.17	-0.16	-0.17	-0.15	0.01	0.05
15/hydroquinone	1^1B_u	ΔE_{ve}	4.29	4.65	4.75	4.94	5.21	4.85	4.84	5.74	4.60	0.39	1.45
		$\Delta\Delta E_{ad}$	-0.16	-0.18	-0.19	-0.20	-0.23	-0.20	-0.20	-0.22	-0.21	0.02	0.06
		$\Delta\Delta E_{00}$	-0.20	-0.19	-0.18	-0.17	-0.19	-0.17	-0.17	-0.16	-0.14	0.02	0.06
16/salicylic acid	$2^1A'$	ΔE_{ve}	3.74	4.21	4.34	4.64	4.94	4.54	4.54	5.61	4.32	0.49	1.87
		$\Delta\Delta E_{ad}$	-0.30	-0.28	-0.29	-0.32	-0.47	-0.29	-0.27	-0.30	-0.53	0.09	0.26
		$\Delta\Delta E_{00}$	-0.23	-0.20	-0.22	-0.20	-0.16	-0.19	-0.18	-0.14	-0.12	0.03	0.11
17/*o*-cresol	2^1A	ΔE_{ve}	4.78	5.10	5.21	5.35	5.59	5.29	5.28	6.06	5.01	0.35	1.28
		$\Delta\Delta E_{ad}$	-0.19	-0.19	-0.18	-0.17	-0.17	-0.17	-0.17	-0.16	-0.20	0.01	0.04
		$\Delta\Delta E_{00}$	-0.14	-0.15	-0.15	-0.14	-0.19	-0.14	-0.14	-0.13	-0.16	0.02	0.06
18/*o*-cresol	2^1A	ΔE_{ve}	4.78	5.09	5.21	5.35	5.58	5.28	5.27	6.06	5.02	0.34	1.28
		$\Delta\Delta E_{ad}$	-0.21	-0.20	-0.21	-0.20	-0.18	-0.20	-0.19	-0.18	-0.22	0.01	0.04
		$\Delta\Delta E_{00}$	-0.08	-0.14	-0.14	-0.13	-0.21	-0.14	-0.14	-0.15	-0.16	0.03	0.12
19/*m*-cresol	2^1A	ΔE_{ve}	4.71	5.04	5.15	5.29	5.52	5.23	5.23	6.02	4.97	0.35	1.31
		$\Delta\Delta E_{ad}$	-0.16	-0.16	-0.16	-0.17	-0.17	-0.16	-0.16	-0.16	-0.20	0.01	0.04
		$\Delta\Delta E_{00}$	-0.15	-0.15	-0.15	-0.15	-0.19	-0.15	-0.16	-0.16	-0.16	0.01	0.05
20/*m*-cresol	$2^1A'$	ΔE_{ve}	4.71	5.04	5.15	5.30	5.53	5.23	5.23	6.03	4.96	0.35	1.31
		$\Delta\Delta E_{ad}$	-0.14	-0.15	-0.15	-0.16	-0.17	-0.15	-0.15	-0.15	-0.19	0.01	0.04
		$\Delta\Delta E_{00}$	-0.18	-0.18	-0.17	-0.18	-0.19	-0.16	-0.16	-0.15	-0.16	0.01	0.04
21/*p*-cresol	2^1A	ΔE_{ve}	4.63	4.95	5.05	5.19	5.43	5.13	5.13	5.93	4.89	0.35	1.30
		$\Delta\Delta E_{ad}$	-0.16	-0.17	-0.18	-0.19	-0.23	-0.18	-0.18	-0.20	-0.20	0.02	0.07
		$\Delta\Delta E_{00}$	-0.09	-0.16	-0.16	-0.14	-0.14	-0.15	-0.15	-0.14	-0.16	0.02	0.07
22/*o*-methoxyphenol	2^1A	ΔE_{ve}	4.69	5.02	5.14	5.29	5.53	5.21	5.20	6.06	4.93	0.37	1.37
		$\Delta\Delta E_{ad}$	-0.25	-0.23	-0.23	-0.24	-0.34	-0.21	-0.20	-0.20	-0.25	0.04	0.14
		$\Delta\Delta E_{00}$	-0.11	-0.15	-0.14	-0.14	-0.13	-0.14	-0.14	-0.15	-0.18	0.02	0.07
23/*m*-methoxyphenol	2^1A	ΔE_{ve}	4.69	5.02	5.14	5.27	5.49	5.21	5.21	6.06	4.91	0.37	1.38

Table S3. Continued.

			Method and statistics[b]										
Label/Molecule	State	ΔE	BP86	B3LYP	PBE0	M06-2X	M06-HF	CB3LYP	ωB97X-D	CIS	CC2	SD	MaxAD
		$\Delta\Delta E_{ad}$	-0.21	-0.20	-0.21	-0.21	-0.40	-0.19	-0.19	-0.19	-0.25	0.06	0.21
		$\Delta\Delta E_{00}$	-0.14	-0.14	-0.13	-0.13	-0.12	-0.13	-0.12	-0.14	-0.16	0.01	0.04
24/*m*-methoxyphenol	2^1A	ΔE_{ve}	4.70	5.04	5.16	5.30	5.54	5.24	5.23	6.10	4.93	0.38	1.40
		$\Delta\Delta E_{ad}$	-0.15	-0.15	-0.16	-0.20	-0.18	-0.16	-0.16	-0.17	-0.21	0.02	0.06
		$\Delta\Delta E_{00}$	-0.14	-0.15	-0.14	-0.12	-0.20	-0.14	-0.14	-0.14	-0.17	0.02	0.08
25/*p*-methoxyphenol	2^1A	ΔE_{ve}	4.26	4.65	4.76	4.95	5.23	4.86	4.86	5.79	4.60	0.41	1.53
		$\Delta\Delta E_{ad}$	-0.16	-0.18	-0.18	-0.20	-0.26	-0.20	-0.20	-0.24	-0.22	0.03	0.10
		$\Delta\Delta E_{00}$	-0.15	-0.15	-0.15	-0.17	-0.14	-0.16	-0.17	-0.13	-0.15	0.01	0.04
26/*p*-methoxyphenol	2^1A	ΔE_{ve}	4.25	4.63	4.74	4.93	5.21	4.85	4.84	5.76	4.58	0.40	1.50
		$\Delta\Delta E_{ad}$	-0.16	-0.17	-0.18	-0.20	-0.25	-0.19	-0.19	-0.22	-0.21	0.03	0.10
		$\Delta\Delta E_{00}$	-0.14	-0.16	-0.16	-0.17	-0.10	-0.16	-0.15	-0.13	-0.15	0.02	0.07
27/1-naphthol	2^1A	ΔE_{ve}	3.60	4.04	4.16	4.54	4.89	4.48	4.48	5.23	4.32	0.45	1.63
		$\Delta\Delta E_{ad}$	-0.26	-0.30	-0.31	-0.39	-0.40	-0.37	-0.37	-0.40	-0.20	0.07	0.20
		$\Delta\Delta E_{00}$	-0.07	-0.08	-0.07	-0.08	-0.17	-0.09	-0.08	-0.11	-0.14	0.03	0.10
28/1-naphthol	2^1A′	ΔE_{ve}	3.77	4.19	4.31	4.64	4.92	4.59	4.59	5.30	4.37	0.41	1.52
		$\Delta\Delta E_{ad}$	-0.24	-0.28	-0.29	-0.34	-0.29	-0.34	-0.33	-0.36	-0.16	0.06	0.21
		$\Delta\Delta E_{00}$	-0.15	-0.17	-0.17	-0.19	-0.23	-0.19	-0.19	-0.22	-0.13	0.03	0.10
29/2-naphthol	2^1A′	ΔE_{ve}	3.78	4.16	4.27	4.52	4.87	4.48	4.48	5.33	4.27	0.42	1.56
		$\Delta\Delta E_{ad}$	-0.17	-0.21	-0.21	-0.23	-0.28	-0.22	-0.22	-0.36	-0.18	0.05	0.19
		$\Delta\Delta E_{00}$	-0.12	-0.14	-0.16	-0.17	-0.16	-0.17	-0.17	-0.19	-0.12	0.02	0.07
30/2-naphthol	2^1A′	ΔE_{ve}	3.71	4.09	4.20	4.46	4.81	4.41	4.42	5.25	4.21	0.41	1.54
		$\Delta\Delta E_{ad}$	-0.16	-0.20	-0.21	-0.23	-0.28	-0.23	-0.22	-0.36	-0.18	0.06	0.20
		$\Delta\Delta E_{00}$	-0.12	-0.14	-0.15	-0.17	-0.15	-0.16	-0.16	-0.17	-0.11	0.02	0.07
31/5-methoxysalicylic acid	2^1A′	ΔE_{ve}	3.24	3.74	3.87	4.22	4.59	4.10	4.10	5.30	3.89	0.54	2.07
		$\Delta\Delta E_{ad}$	-0.19	-0.23	-0.25	-0.30	-0.45	-0.28	-0.27	-0.37	-0.33	0.07	0.26
		$\Delta\Delta E_{00}$	-0.15	-0.15	-0.15	-0.16	-0.16	-0.14	-0.14	-0.13	-0.15	0.01	0.04
32/*m*-dimethoxybenzene	2^1A′	ΔE_{ve}	4.63	4.97	5.10	5.26	5.51	5.18	5.17	6.07	4.91	0.39	1.44
		$\Delta\Delta E_{ad}$	-0.24	-0.22	-0.23	-0.25	-0.36	-0.22	-0.22	-0.24	-0.29	0.04	0.14
		$\Delta\Delta E_{00}$	-0.18	-0.16	-0.16	-0.15	-0.14	-0.16	-0.16	-0.15	-0.19	0.02	0.05
33/3P-propionic acid	2^1A	ΔE_{ve}	4.83	5.33	5.45	5.54	5.74	5.50	5.50	6.16	5.20	0.34	1.33
		$\Delta\Delta E_{ad}$	-1.02	-0.11	-0.11	-0.13	-0.15	-0.13	-0.14	-0.13	-0.18	0.28	0.90
		$\Delta\Delta E_{00}$	-0.11	-0.18	-0.17	-0.16	-0.16	-0.14	-0.13	-0.12	-0.15	0.02	0.07
34/3P-propionic acid	1^1A″	ΔE_{ve}	4.91	5.33	5.45	5.54	5.74	5.50	5.49	6.16	5.20	0.33	1.25
		$\Delta\Delta E_{ad}$	-0.52	-0.13	-0.13	-0.14	-0.15	-0.13	-0.14	-0.13	-0.18	0.12	0.40

Table S3. Continued.

			Method and statistics[b]										
Label/Molecule	State	ΔE	BP86	B3LYP	PBE0	M06-2X	M06-HF	CB3LYP	ωB97X-D	CIS	CC2	SD	MaxAD
		$\Delta\Delta E_{00}$	-0.16	-0.16	-0.16	-0.16	-0.15	-0.14	-0.14	-0.12	-0.16	0.01	0.04
35/fluorene	1^1B_2	ΔE_{ve}	4.19	4.55	4.68	4.92	5.23	4.88	4.92	5.37	4.67	0.34	1.18
		$\Delta\Delta E_{ad}$	-0.12	-0.16	-0.18	-0.25	-0.32	-0.27	-0.28	-0.37	-0.14	0.08	0.25
		$\Delta\Delta E_{00}$	-0.20	-0.17	-0.16	-0.15	-0.15	-0.14	-0.14	-0.13	-0.16	0.02	0.08
36/phenanthrene	2^1A_1	ΔE_{ve}	3.60	3.98	4.11	4.37	4.74	4.35	4.36	5.07	4.08	0.40	1.47
		$\Delta\Delta E_{ad}$	-0.12	-0.13	-0.14	-0.17	-0.25	-0.17	-0.17	-0.21	-0.16	0.04	0.13
		$\Delta\Delta E_{00}$	-0.13	-0.12	-0.12	-0.13	-0.14	-0.12	-0.12	-0.21	-0.11	0.03	0.09
37/2,4,6,8-decatetraene	1^1B_u	ΔE_{ve}	3.64	3.94	4.03	4.34	4.78	4.33	4.34	5.18	4.59	0.43	1.53
		$\Delta\Delta E_{ad}$	-0.15	-0.23	-0.24	-0.35	-0.49	-0.35	-0.36	-0.50	-0.31	0.11	0.35
		$\Delta\Delta E_{00}$	-0.13	-0.12	-0.12	-0.11	-0.11	-0.12	-0.11	-0.12	-0.11	0.01	0.02
38/tetracene	1^1B_{1u}	ΔE_{ve}	2.15	2.47	2.56	2.92	3.41	2.91	2.96	3.73	2.97	0.45	1.59
		$\Delta\Delta E_{ad}$	-0.13	-0.18	-0.18	-0.26	-0.39	-0.25	-0.25	-0.37	-0.17	0.08	0.26
		$\Delta\Delta E_{00}$	-0.10	-0.13	-0.15	-0.19	-0.21	-0.18	-0.20	-0.25	-0.23	0.04	0.14
39/perylene	1^1B	ΔE_{ve}	2.53	2.82	2.91	3.24	3.70	3.22	3.26	3.92	3.16	0.40	1.39
		$\Delta\Delta E_{ad}$	-0.12	-0.17	-0.18	-0.26	-0.38	-0.26	-0.26	-0.37	-0.22	0.08	0.26
		$\Delta\Delta E_{00}$	-0.06	-0.03	-0.05	-0.04	-0.04	-0.03	-0.04	-0.04	-0.04	0.01	0.03

[a]$\Delta\Delta E_{ad} = \Delta E_{ad} - \Delta E_{ve}$ and $\Delta\Delta E_{00} = \Delta E_{00} - \Delta E_{ad}$. [b]Standard deviation (SD) and maximum absolute deviation (MaxAD) for calculations with the nine methods.

Table S4. $<A_{BL}SD\text{-}S_1>$, $<A_{BL}SD\text{-}S_1S_0>$ and $<A_{BL}SD\text{-}S_0>$ values for bonds between heavy atoms for selected states in groups I and II of the benchmark set (Å).[a]

Group(s)[b]	$<A_{BL}SD\text{-}S_1>$	$<A_{BL}SD\text{-}S_1S_0>$	$<A_{BL}SD\text{-}S_0>$
I	0.013	0.013	0.007
II	0.009	0.009	0.007
I–II	0.011	0.010	0.007

[a]Average ASDs for excited-state bond lengths ($<A_{BL}SD\text{-}S_1>$), for excited-state bond lengths relative to ground-state bond lengths ($<A_{BL}SD\text{-}S_1S_0>$), and for ground-state bond lengths ($<A_{BL}SD\text{-}S_0>$) with calculations performed using the BP86, B3LYP, PBE0, M06-2X, M06-HF, CAM-B3LYP, ωB97X-D, CIS and CC2 methods. [b]From group I, the states considered in the analysis are the S_1 states of pyrazine, 2,6-difluoropyridine, 2-pyridone, 2-methylpyrimidine, 7-azaindole, 7-hydroxyquinoline (*cis*), dibenzofuran, pyrrolo[3,2-*h*]quinoline, carbazole, tryptamine (A-ph) and porphycene. From group II, the states considered in the analysis are the S_1 states of tetrafluorobenzene, benzonitrile, *o*-fluorophenol (*cis*), phenylacetylene, aniline, catechol, resorcinol (isomer 1), hydroquinone (*cis*), salicylic acid, *o*-cresol (*cis*), *o*-methoxyphenol, 1-naphthol (*cis*), 5-methoxysalicylic acid, *m*-dimethoxybenzene (*trans*), 3P-propionic acid (*gauche*), fluorene, phenanthrene, 2,4,6,8-decatetraene, tetracene and perylene.

Comments on Table S4

The similarity between the methods (BP86, B3LYP, PBE0, M06-2X, M06-HF, CAM-B3LYP, ωB97X-D, CIS and CC2) in their descriptions of the excited states in the benchmark set was quantified geometrically in the following way. First, for a representative subset of excited states (see footnote [b]), SDs were computed for the estimates of each excited-state bond length, as well as for the estimates of each excited-state bond length relative to the corresponding ground-state bond length. Throughout, only bonds between heavy atoms were considered. Then, by averaging the resulting SDs over all bonds in the excited state in question, average bond-length SDs denoted $A_{BL}SD\text{-}S_1$ and $A_{BL}SD\text{-}S_1S_0$, respectively, were obtained for that excited state. Finally, by averaging the $A_{BL}SD\text{-}S_1$ and $A_{BL}SD\text{-}S_1S_0$ values over all excited states considered, 'similarity measures' denoted $<A_{BL}SD\text{-}S_1>$ and $<A_{BL}SD\text{-}S_1S_0>$, respectively, were obtained. These are the values given in Table S4. Notably, their smallness (0.011 and 0.010 Å for the full subset of excited states) are indicative of a large degree of similarity between the descriptions of the excited states by the methods, which helps explain why also the estimates of $\Delta\Delta E_{ad}$ are similar.

Atomic coordinates of optimized ground- and excited-state geometries

BP86/TZVP geometries – Group I

pyrazine S_0

C	1.136741	-0.700091	0.000000
C	1.136741	0.700091	0.000000
N	0.000000	1.415836	0.000000
C	-1.136741	0.700091	0.000000
C	-1.136741	-0.700091	0.000000
N	0.000000	-1.415836	0.000000
H	-2.075256	-1.263288	0.000000
H	2.075256	-1.263288	0.000000
H	2.075256	1.263288	0.000000
H	-2.075256	1.263288	0.000000

pyrazine S_1

C	-1.194537	0.711534	0.000000
C	-1.143270	-0.791758	0.000000
N	0.045994	-1.339174	0.000000
C	1.194537	-0.711534	0.000000
C	1.143270	0.791758	0.000000
N	-0.045994	1.339174	0.000000
H	2.054296	1.386842	0.000000
H	-2.144173	1.242961	0.000000
H	-2.054296	-1.386842	0.000000
H	2.144173	-1.242961	0.000000

2,6-difluoropyridine S_0

C	1.122223	0.000000	-0.881003
N	0.000000	0.000000	-1.580445
C	-1.122223	0.000000	-0.881003
C	-1.210941	0.000000	0.511558
C	0.000000	0.000000	1.210052
C	1.210941	0.000000	0.511558
F	-2.262310	0.000000	-1.606181
H	-2.179095	0.000000	1.010283
H	0.000000	0.000000	2.301497
H	2.179095	0.000000	1.010283
F	2.262310	0.000000	-1.606181

2,6-difluoropyridine S_1

C	-1.108049	0.000000	-0.338787
N	0.000000	0.000000	-1.116400
C	1.108049	0.000000	-0.338787
C	1.204198	0.000000	1.075616
C	0.000000	0.000000	1.854217
C	-1.204198	0.000000	1.075616
F	2.264104	0.000000	-1.030409
H	2.195547	0.000000	1.529601
H	0.000000	0.000000	2.939434
H	-2.195547	0.000000	1.529601
F	-2.264104	0.000000	-1.030409

2-fluoropyridine S_0

C	-1.322697	0.506378	0.000000
N	-1.378282	-0.809808	0.000000
C	-0.198302	-1.462325	0.000000
C	1.037487	-0.813803	0.000000
C	1.051633	0.587518	0.000000
C	-0.158188	1.281127	0.000000
H	-0.261117	-2.554215	0.000000
H	1.963751	-1.389807	0.000000
H	1.995960	1.135691	0.000000
H	-0.212925	2.369854	0.000000
F	-2.517331	1.149381	0.000000

2-fluoropyridine S_1

C	-1.326387	0.498671	0.000000
N	-1.439048	-0.845692	0.000000
C	-0.219221	-1.482539	0.000000
C	1.040544	-0.807114	0.000000
C	1.107080	0.618887	0.000000
C	-0.156124	1.303235	0.000000
H	-0.256008	-2.573252	0.000000
H	1.952830	-1.405795	0.000000
H	2.052744	1.155366	0.000000
H	-0.244051	2.388791	0.000000
F	-2.512370	1.149433	0.000000

2-hydroxypyridine S_0

C	-0.987526	0.759336	0.000000
C	-0.980023	-0.647264	0.000000
N	0.129751	-1.390420	0.000000

C	1.311177	-0.742977	0.000000
C	1.425935	0.646491	0.000000
C	0.244763	1.404775	0.000000
O	-2.169982	-1.309237	0.000000
H	2.199908	-1.381029	0.000000
H	2.407328	1.122038	0.000000
H	0.287381	2.496152	0.000000
H	-1.932498	1.303031	0.000000
H	-1.936215	-2.260895	0.000000

2-hydroxypyridine S_1

C	-1.021693	0.778762	0.000000
C	-0.969554	-0.616073	0.000000
N	0.097208	-1.449809	0.000000
C	1.303659	-0.777410	0.000000
C	1.396848	0.640959	0.000000
C	0.258656	1.465932	0.000000
O	-2.161910	-1.320034	0.000000
H	2.201421	-1.396173	0.000000
H	2.395256	1.085665	0.000000
H	0.326107	2.550868	0.000000
H	-1.978760	1.298088	0.000000
H	-1.847238	-2.260775	0.000000

2-pyridone S_0

C	-1.255560	0.727076	0.000000
N	-1.139695	-0.693862	0.000000
C	0.032294	-1.395488	0.000000
C	1.232287	-0.733907	0.000000
C	1.213893	0.691964	0.000000
C	0.034842	1.394353	0.000000
H	-2.033284	-1.185810	0.000000
H	-0.055318	-2.482848	0.000000
H	2.166357	-1.292818	0.000000
H	2.163020	1.234449	0.000000
H	0.012725	2.484345	0.000000
O	-2.371562	1.252558	0.000000

2-pyridone S_1

C	-1.356335	0.100156	0.000000
N	-0.735684	-1.103967	0.000000
C	0.649837	-1.265576	0.000000
C	1.433611	-0.076395	0.000000

C	0.836795	1.159264	0.000000
C	-0.621783	1.273714	0.000000
H	-1.365197	-1.907608	0.000000
H	1.034962	-2.279803	0.000000
H	2.520070	-0.176679	0.000000
H	1.445526	2.064217	0.000000
H	-1.140285	2.227827	0.000000
O	-2.701516	-0.015161	0.000000

2-methylpyrimidine S_0

C	0.000122	1.975040	0.000000
C	-1.183179	1.231325	0.000000
N	-1.194446	-0.108706	0.000000
C	0.010225	-0.722325	0.000000
N	1.208566	-0.101620	0.000000
C	1.186866	1.241463	0.000000
H	-2.162031	1.723264	0.000000
H	2.162610	1.739118	0.000000
H	-0.004416	3.066081	0.000000
C	0.005379	-2.225763	0.000000
H	1.031864	-2.610222	0.000000
H	-0.530785	-2.603827	0.883900
H	-0.530785	-2.603827	-0.883900

2-methylpyrimidine S_1

C	-0.018858	2.029709	0.000000
C	-1.169082	1.270719	0.000000
N	-1.189313	-0.089862	0.000000
C	0.017607	-0.789122	0.000000
N	1.089680	-0.059136	0.000000
C	1.224301	1.299739	0.000000
H	-2.154939	1.747376	0.000000
H	2.222721	1.724372	0.000000
H	-0.036952	3.119174	0.000000
C	0.016291	-2.277144	0.000000
H	1.039967	-2.671670	0.000000
H	-0.520711	-2.652083	0.886434
H	-0.520711	-2.652083	-0.886434

5-methylpyrimidine S_0

C	0.879602	0.857605	0.000000
C	-0.364866	0.212339	0.000000
C	-0.302884	-1.190745	0.000000

N	0.849372	-1.877217	0.000000
C	1.970446	-1.136444	0.000000
N	2.052048	0.202174	0.000000
H	2.917407	-1.684694	0.000000
H	-1.222210	-1.788937	0.000000
H	0.936253	1.952854	0.000000
C	-1.669157	0.965077	0.000000
H	-1.498635	2.051164	0.000000
H	-2.273688	0.718401	-0.886916
H	-2.273688	0.718401	0.886916

5-methylpyrimidine S_1

C	0.861160	0.852296	0.000000
C	-0.383415	0.252388	0.000000
C	-0.352328	-1.206926	0.000000
N	0.881128	-1.763930	0.000000
C	2.045812	-1.189799	0.000000
N	2.051015	0.197330	0.000000
H	2.974080	-1.754994	0.000000
H	-1.222214	-1.857196	0.000000
H	0.940503	1.945626	0.000000
C	-1.685431	0.987362	0.000000
H	-1.526048	2.074947	0.000000
H	-2.292137	0.731453	-0.887061
H	-2.292137	0.731453	0.887061

7-azaindole S_0

N	-0.637571	1.854213	0.000000
C	-0.679511	0.473966	0.000000
C	0.675768	0.007402	0.000000
C	1.518202	1.169427	0.000000
C	0.685344	2.268532	0.000000
C	0.851846	-1.386156	0.000000
C	-0.293259	-2.183689	0.000000
C	-1.573117	-1.589901	0.000000
N	-1.791715	-0.264286	0.000000
H	-2.467982	-2.219282	0.000000
H	1.849073	-1.832587	0.000000
H	-0.212143	-3.272119	0.000000
H	-1.458869	2.449906	0.000000
H	2.604262	1.197604	0.000000
H	0.929692	3.326970	0.000000

7-azaindole S_1

N	-0.599324	1.887010	0.000000
C	-0.653417	0.435413	0.000000
C	0.645217	-0.018078	0.000000
C	1.505701	1.175265	0.000000
C	0.663380	2.329672	0.000000
C	0.895504	-1.426687	0.000000
C	-0.308488	-2.197892	0.000000
C	-1.566653	-1.604025	0.000000
N	-1.834543	-0.239381	0.000000
H	-2.457209	-2.239496	0.000000
H	1.890965	-1.863250	0.000000
H	-0.255094	-3.289060	0.000000
H	-1.440955	2.462362	0.000000
H	2.593310	1.204377	0.000000
H	0.921617	3.383791	0.000000

7-hydroxyquinoline, *cis* S_0

N	0.473337	1.984315	0.000000
C	0.440268	0.614229	0.000000
C	-0.793479	-0.128534	0.000000
C	-2.003173	0.608711	0.000000
C	-1.955890	1.989373	0.000000
C	-0.688076	2.623904	0.000000
C	1.672429	-0.088711	0.000000
C	1.685676	-1.473717	0.000000
C	0.470596	-2.212648	0.000000
C	-0.736999	-1.550379	0.000000
H	-0.631037	3.718356	0.000000
H	-1.671173	-2.118359	0.000000
H	0.524371	-3.302566	0.000000
O	2.839694	-2.217607	0.000000
H	2.594777	0.498826	0.000000
H	-2.958032	0.075399	0.000000
H	-2.866518	2.591054	0.000000
H	3.603230	-1.611636	0.000000

7-hydroxyquinoline, *cis* S_1

N	0.508803	1.987365	0.000000
C	0.421489	0.636200	0.000000
C	-0.784317	-0.130827	0.000000
C	-2.027462	0.605165	0.000000
C	-1.939475	2.010291	0.000000
C	-0.700495	2.652588	0.000000

C	1.650216	-0.105402	0.000000
C	1.669321	-1.530941	0.000000
C	0.485455	-2.285183	0.000000
C	-0.709522	-1.556392	0.000000
H	-0.637934	3.743122	0.000000
H	-1.653624	-2.110103	0.000000
H	0.514941	-3.372798	0.000000
O	2.863854	-2.182389	0.000000
H	2.586100	0.464333	0.000000
H	-2.985730	0.085798	0.000000
H	-2.850947	2.614085	0.000000
H	3.589326	-1.524903	0.000000

7-hydroxyquinoline, *trans* S_0

N	0.523191	2.057576	0.000000
C	0.488120	0.685727	0.000000
C	-0.750764	-0.051395	0.000000
C	-1.959310	0.689799	0.000000
C	-1.907032	2.069089	0.000000
C	-0.635293	2.699385	0.000000
C	1.718098	-0.016025	0.000000
C	1.728144	-1.400899	0.000000
C	0.508913	-2.133892	0.000000
C	-0.700929	-1.470723	0.000000
H	-0.575595	3.793838	0.000000
H	-1.635594	-2.037829	0.000000
H	0.537483	-3.228252	0.000000
O	2.944934	-2.039226	0.000000
H	2.649659	0.550723	0.000000
H	-2.915894	0.159515	0.000000
H	-2.815176	2.674581	0.000000
H	2.797027	-3.001971	0.000000

7-hydroxyquinoline, *trans* S_1

N	0.372242	1.980247	-0.000001
C	0.523576	0.657087	-0.000001
C	-0.761534	-0.061573	-0.000002
C	-1.951866	0.714301	0.000000
C	-1.935829	2.123749	0.000001
C	-0.703902	2.770227	-0.000001
C	1.755112	-0.030073	-0.000001
C	1.736858	-1.437379	0.000000
C	0.542420	-2.161936	-0.000001
C	-0.695178	-1.472058	-0.000001

H	-0.549992	3.848524	0.000000
H	-1.632762	-2.029422	-0.000001
H	0.561597	-3.254698	0.000000
O	2.967225	-2.050467	0.000001
H	2.699823	0.508617	0.000000
H	-2.908920	0.188908	0.000001
H	-2.846296	2.720646	0.000003
H	2.827408	-3.014677	0.000002

2-hydroxyquinoline, enol S_0

C	0.436651	1.912871	0.000000
C	0.491862	0.494504	0.000000
C	-0.730653	-0.263113	0.000000
C	-1.966269	0.437406	0.000000
C	-1.987543	1.820359	0.000000
C	-0.782209	2.565966	0.000000
C	1.707527	-0.242774	0.000000
C	1.674956	-1.617476	0.000000
C	0.399240	-2.263754	0.000000
N	-0.751076	-1.631402	0.000000
O	0.311532	-3.631254	0.000000
H	1.371843	2.479882	0.000000
H	-0.820345	3.657229	0.000000
H	-2.944305	2.347636	0.000000
H	-2.884849	-0.152050	0.000000
H	2.662110	0.290235	0.000000
H	2.598636	-2.203043	0.000000
H	1.212894	-4.001224	0.000000

2-hydroxyquinoline, enol S_1

C	0.422191	1.889184	0.000000
C	0.520478	0.483228	0.000000
C	-0.709274	-0.260517	0.000000
C	-1.955471	0.449215	0.000000
C	-2.021773	1.861989	0.000000
C	-0.833972	2.579551	0.000000
C	1.757040	-0.233384	0.000000
C	1.705600	-1.657608	0.000000
C	0.433599	-2.257228	0.000000
N	-0.760317	-1.627183	0.000000
O	0.287962	-3.614183	0.000000
H	1.342651	2.480590	0.000000
H	-0.837578	3.671204	0.000000
H	-2.987918	2.367744	0.000000

H	-2.864192	-0.156863	0.000000
H	2.706644	0.301116	0.000000
H	2.614773	-2.261713	0.000000
H	1.179548	-4.015122	0.000000

2-hydroxyquinoline, keto S_0

N	0.561446	1.713477	0.000000
C	0.608135	0.331682	0.000000
C	-0.622025	-0.385187	0.000000
C	-1.844111	0.376019	0.000000
C	-1.842704	1.737590	0.000000
C	-0.600353	2.509746	0.000000
C	1.831982	-0.365596	0.000000
C	1.833526	-1.756792	0.000000
C	0.625645	-2.479665	0.000000
C	-0.584594	-1.796142	0.000000
H	-1.530025	-2.344564	0.000000
H	0.641716	-3.570720	0.000000
H	2.786073	-2.290712	0.000000
H	2.772624	0.190974	0.000000
H	-2.791351	-0.171666	0.000000
H	-2.764364	2.319980	0.000000
O	-0.516402	3.740285	0.000000
H	1.434799	2.241310	0.000000

2-hydroxyquinoline, keto S_1

N	0.538592	1.720435	0.000000
C	0.593069	0.312068	0.000000
C	-0.664701	-0.385980	0.000000
C	-1.843833	0.358475	0.000000
C	-1.850630	1.789420	0.000000
C	-0.614963	2.426720	0.000000
C	1.816512	-0.344827	0.000000
C	1.848682	-1.754708	0.000000
C	0.635009	-2.472531	0.000000
C	-0.588365	-1.826560	0.000000
H	-1.520080	-2.395812	0.000000
H	0.661939	-3.565087	0.000000
H	2.804859	-2.277579	0.000000
H	2.747219	0.229498	0.000000
H	-2.802413	-0.163679	0.000000
H	-2.765524	2.372576	0.000000
O	-0.416068	3.748636	0.000000
H	1.420695	2.228946	0.000000

dibenzofuran S_0

C	1.729100	0.000000	-1.367760
C	0.726408	0.000000	-0.385839
C	1.104014	0.000000	0.977017
C	2.427642	0.000000	1.404042
C	3.408991	0.000000	0.405810
C	3.065556	0.000000	-0.959978
C	-0.726408	0.000000	-0.385839
C	-1.104014	0.000000	0.977017
O	0.000000	0.000000	1.813402
C	-1.729100	0.000000	-1.367760
C	-3.065556	0.000000	-0.959978
C	-3.408991	0.000000	0.405810
C	-2.427642	0.000000	1.404042
H	-2.681217	0.000000	2.464910
H	-4.461938	0.000000	0.694695
H	-3.858559	0.000000	-1.710351
H	-1.472103	0.000000	-2.429082
H	1.472103	0.000000	-2.429082
H	3.858559	0.000000	-1.710351
H	4.461938	0.000000	0.694695
H	2.681217	0.000000	2.464910

dibenzofuran S_1

C	0.000000	1.746522	-1.539553
C	0.000000	0.717569	-0.567768
C	0.000000	1.115446	0.801066
C	0.000000	2.426595	1.265606
C	0.000000	3.448073	0.264882
C	0.000000	3.098957	-1.089951
C	0.000000	-0.717569	-0.567768
C	0.000000	-1.115446	0.801066
O	0.000000	0.000000	1.621991
C	0.000000	-1.746522	-1.539553
C	0.000000	-3.098957	-1.089951
C	0.000000	-3.448073	0.264882
C	0.000000	-2.426595	1.265606
H	0.000000	-2.651891	2.331764
H	0.000000	-4.496308	0.562695
H	0.000000	-3.893630	-1.839706
H	0.000000	-1.521443	-2.606319
H	0.000000	1.521443	-2.606319
H	0.000000	3.893630	-1.839706

H	0.000000	4.496308	0.562695
H	0.000000	2.651891	2.331764

pyrrolo[3,2-*h*]quinoline S_0

C	0.130960	-0.692703	0.000000
N	0.055343	-2.053518	0.000000
C	1.203035	-2.726128	0.000000
C	2.477026	-2.113304	0.000000
C	2.555135	-0.729839	0.000000
C	1.369084	0.042001	0.000000
H	1.121214	-3.818410	0.000000
H	3.377101	-2.730888	0.000000
H	3.524741	-0.223874	0.000000
C	-1.058132	0.080527	0.000000
C	-1.064495	1.497380	0.000000
C	0.179715	2.190832	0.000000
C	1.358428	1.476182	0.000000
H	0.196630	3.283134	0.000000
H	2.318325	1.999117	0.000000
C	-2.439953	1.903130	0.000000
C	-3.203318	0.750162	0.000000
N	-2.362992	-0.348124	0.000000
H	-2.631402	-1.327124	0.000000
H	-2.824571	2.919141	0.000000
H	-4.281866	0.622308	0.000000

pyrrolo[3,2-*h*]quinoline S_1

C	0.159611	-0.701294	0.000000
N	-0.002491	-2.058953	0.000000
C	1.201315	-2.746471	0.000000
C	2.453326	-2.143902	0.000000
C	2.593078	-0.734852	0.000000
C	1.359489	0.018354	0.000000
H	1.115336	-3.836331	0.000000
H	3.341845	-2.780743	0.000000
H	3.563942	-0.241991	0.000000
C	-1.032117	0.109063	0.000000
C	-1.075847	1.562283	0.000000
C	0.147521	2.247099	0.000000
C	1.316229	1.471931	0.000000
H	0.199272	3.336084	0.000000
H	2.279398	1.991591	0.000000
C	-2.472871	1.922163	0.000000
C	-3.193464	0.756652	0.000000

N	-2.294891	-0.341560	0.000000
H	-2.505982	-1.339586	0.000000
H	-2.887226	2.925806	0.000000
H	-4.265485	0.584656	0.000000

carbazole S_0

C	1.136766	0.000000	-0.904103
N	0.000000	0.000000	-1.704322
C	-1.136766	0.000000	-0.904103
C	-0.725723	0.000000	0.462792
C	0.725723	0.000000	0.462792
C	-1.703175	0.000000	1.470120
C	-3.052064	0.000000	1.110249
C	-3.436972	0.000000	-0.245648
C	-2.487832	0.000000	-1.270441
C	2.487832	0.000000	-1.270441
C	3.436972	0.000000	-0.245648
C	3.052064	0.000000	1.110249
C	1.703175	0.000000	1.470120
H	-2.793752	0.000000	-2.319194
H	-4.498461	0.000000	-0.502402
H	-3.820302	0.000000	1.885918
H	-1.412841	0.000000	2.523231
H	1.412841	0.000000	2.523231
H	3.820302	0.000000	1.885918
H	4.498461	0.000000	-0.502402
H	2.793752	0.000000	-2.319194
H	0.000000	0.000000	-2.717681

carbazole S_1

C	1.152087	0.000000	-0.837701
N	0.000000	0.000000	-1.623315
C	-1.152087	0.000000	-0.837701
C	-0.721521	0.000000	0.528155
C	0.721521	0.000000	0.528155
C	-1.718987	0.000000	1.529529
C	-3.082373	0.000000	1.125711
C	-3.474349	0.000000	-0.216292
C	-2.484598	0.000000	-1.247902
C	2.484598	0.000000	-1.247902
C	3.474349	0.000000	-0.216292
C	3.082373	0.000000	1.125711
C	1.718987	0.000000	1.529529
H	-2.761418	0.000000	-2.303633

H	-4.531959	0.000000	-0.479996
H	-3.853612	0.000000	1.900041
H	-1.458384	0.000000	2.588274
H	1.458384	0.000000	2.588274
H	3.853612	0.000000	1.900041
H	4.531959	0.000000	-0.479996
H	2.761418	0.000000	-2.303633
H	0.000000	0.000000	-2.641687

tryptamine, A-ph S_0

C	-2.137641	0.128895	0.890611
N	-1.256383	0.117171	1.963965
C	0.040530	0.043549	1.488431
C	-0.039271	0.002469	0.061111
C	-1.438474	0.059402	-0.297232
C	1.262466	0.014463	2.173050
C	2.427109	-0.056214	1.408943
C	2.375076	-0.093250	-0.002554
C	1.157847	-0.064180	-0.679987
C	-2.015935	0.009871	-1.682426
C	-2.020620	-1.404153	-2.294212
N	-2.504215	-1.358798	-3.684882
H	1.306079	0.046778	3.264436
H	3.396476	-0.080603	1.911184
H	3.307488	-0.144255	-0.568879
H	1.133260	-0.089075	-1.772023
H	-1.522132	0.180956	2.939445
H	-3.209625	0.192865	1.060852
H	-1.451216	0.671442	-2.360702
H	-3.050971	0.394102	-1.664815
H	-2.604179	-2.074053	-1.628570
H	-0.990227	-1.793124	-2.307730
H	-3.494196	-1.097814	-3.705118
H	-2.438656	-2.284065	-4.115528

tryptamine, A-ph S_1

C	-2.216695	0.086047	0.956564
N	-1.264778	0.122930	1.979584
C	0.024036	0.059296	1.468574
C	-0.091887	0.032540	0.046386
C	-1.485835	0.066680	-0.248819
C	1.255870	-0.005090	2.151954
C	2.435796	-0.080647	1.334567
C	2.350551	-0.094858	-0.056516

C	1.114246	-0.051010	-0.746421
C	-2.094245	0.012675	-1.623362
C	-2.024583	-1.410300	-2.187841
N	-2.509602	-1.556141	-3.555296
H	1.312677	0.029559	3.240806
H	3.415456	-0.131300	1.815214
H	3.276609	-0.142588	-0.638649
H	1.095216	0.020056	-1.836395
H	-1.481319	0.132237	2.968501
H	-3.256209	0.338862	1.149501
H	-1.561083	0.697133	-2.308536
H	-3.147953	0.337922	-1.587591
H	-2.600324	-2.134803	-1.589144
H	-0.994626	-1.801034	-2.200394
H	-2.803517	-0.746118	-4.104025
H	-2.515232	-2.459668	-4.031335

tryptamine, A-py S_0

C	-2.131185	0.108799	0.867612
N	-1.260687	0.112513	1.949328
C	0.041326	0.046177	1.487459
C	-0.023946	-0.006852	0.059395
C	-1.420031	0.034852	-0.312897
C	1.256166	0.032643	2.185004
C	2.429619	-0.033490	1.434216
C	2.392709	-0.081892	0.022630
C	1.182243	-0.069164	-0.667275
C	-1.996087	-0.020440	-1.698770
C	-1.970402	-1.428304	-2.322934
N	-2.577085	-1.399252	-3.665631
H	1.287650	0.073232	3.276524
H	3.393705	-0.045896	1.946891
H	3.331401	-0.130067	-0.533504
H	1.170688	-0.106004	-1.759259
H	-1.536939	0.179790	2.921681
H	-3.205392	0.165394	1.025513
H	-1.438971	0.669095	-2.359873
H	-3.039408	0.333050	-1.693851
H	-2.571154	-2.104033	-1.693031
H	-0.930895	-1.815055	-2.302132
H	-1.992547	-0.849179	-4.301689
H	-2.620867	-2.343527	-4.056296

tryptamine, A-py S_1

C	-2.198011	0.097370	0.871474
N	-1.283151	0.131660	1.927795
C	0.022777	0.060513	1.463314
C	-0.042322	0.031304	0.038021
C	-1.424652	0.071711	-0.306945
C	1.229048	-0.008614	2.190532
C	2.437010	-0.091771	1.416009
C	2.401536	-0.108503	0.022790
C	1.190945	-0.060091	-0.711043
C	-1.983775	0.017489	-1.702280
C	-1.900896	-1.407108	-2.260713
N	-2.336700	-1.553935	-3.644587
H	1.246954	0.028035	3.280645
H	3.398625	-0.146298	1.931422
H	3.347616	-0.162050	-0.525663
H	1.211245	0.009419	-1.801091
H	-1.534811	0.144436	2.908321
H	-3.242484	0.355722	1.026551
H	-1.423087	0.697784	-2.369388
H	-3.036461	0.347919	-1.704922
H	-2.501414	-2.127419	-1.681661
H	-0.873045	-1.802804	-2.235239
H	-2.605268	-0.743734	-4.205902
H	-2.329769	-2.458658	-4.118338

tryptamine, A-up S_0

C	-2.130030	0.122014	0.878796
N	-1.256912	0.095595	1.958170
C	0.043763	0.034999	1.491834
C	-0.024593	0.017451	0.063268
C	-1.421253	0.076813	-0.305080
C	1.260041	-0.001781	2.185986
C	2.431235	-0.056282	1.430825
C	2.391072	-0.070893	0.018636
C	1.179259	-0.034215	-0.667955
C	-1.992296	0.036248	-1.693123
C	-1.991811	-1.379430	-2.328521
N	-2.507972	-1.469706	-3.699897
H	1.294301	0.011826	3.278061
H	3.396417	-0.086769	1.940656
H	3.328189	-0.111967	-0.540628
H	1.165342	-0.045603	-1.760483
H	-1.530702	0.136583	2.932711
H	-3.203477	0.178593	1.042083
H	-1.423904	0.715978	-2.354090

H	-3.029286	0.414882	-1.680650
H	-2.586563	-2.055129	-1.692352
H	-0.966298	-1.781791	-2.323097
H	-1.954550	-0.880895	-4.328432
H	-3.468732	-1.118610	-3.743481

tryptamine, A-up S_1

C	-2.208150	0.034654	0.947945
N	-1.268762	0.026559	1.983129
C	0.026735	0.016420	1.485387
C	-0.072426	0.073162	0.062811
C	-1.463300	0.100626	-0.247215
C	1.251681	-0.067605	2.178962
C	2.441987	-0.073380	1.373299
C	2.372919	-0.005421	-0.017095
C	1.143946	0.058134	-0.718524
C	-2.054621	0.118151	-1.630131
C	-1.952615	-1.267234	-2.277167
N	-2.418792	-1.339765	-3.656971
H	1.295416	-0.097849	3.268550
H	3.416866	-0.135891	1.862210
H	3.306283	-0.001935	-0.589416
H	1.136049	0.195274	-1.802318
H	-1.496726	-0.026259	2.968106
H	-3.254077	0.257950	1.142716
H	-1.525879	0.851350	-2.266557
H	-3.114371	0.422412	-1.588568
H	-2.522190	-2.036000	-1.729972
H	-0.915660	-1.638549	-2.299645
H	-2.402308	-2.213209	-4.185962
H	-2.720785	-0.503675	-4.160354

tryptamine, Ph-out S_0

C	0.011451	0.007133	0.075691
C	0.051646	0.063444	1.504867
C	1.254347	0.077452	2.223368
C	2.441033	0.038771	1.491881
C	2.428230	-0.014157	0.079744
C	1.231089	-0.029240	-0.632892
N	-1.258619	0.100707	1.945735
H	1.266337	0.119171	3.315252
H	3.396662	0.049374	2.020330
H	3.377095	-0.042371	-0.460363
H	1.231223	-0.085445	-1.723485

C	-1.380432	0.018452	-0.319642
C	-2.111531	0.080434	0.850739
H	-1.550850	0.174202	2.913043
H	-3.188644	0.123208	0.993086
C	-1.940945	-0.038701	-1.714923
H	-1.292968	0.531324	-2.401476
C	-2.103353	-1.464348	-2.277591
H	-2.929640	0.449797	-1.729171
H	-2.573739	-1.395054	-3.272870
N	-0.797444	-2.120163	-2.443863
H	-2.807583	-2.020596	-1.621963
H	-0.352503	-2.246452	-1.529967
H	-0.915891	-3.052833	-2.846318

tryptamine, Ph-out S_1

C	-0.082018	0.007914	0.055796
C	-0.001433	0.085892	1.469545
C	1.213125	-0.012609	2.192473
C	2.399584	-0.166373	1.404589
C	2.359626	-0.226784	0.018560
C	1.132500	-0.202963	-0.729327
N	-1.298425	0.229058	1.943893
H	1.249739	0.065705	3.279224
H	3.364380	-0.237506	1.913623
H	3.304256	-0.296633	-0.530149
H	1.181244	0.190099	-1.757389
C	-1.471634	0.077528	-0.286070
C	-2.207171	0.224336	0.894486
H	-1.540059	0.352189	2.919805
H	-3.269088	0.374099	1.063459
C	-2.041764	-0.056773	-1.673696
H	-1.514685	0.596801	-2.390885
C	-2.013276	-1.495927	-2.216292
H	-3.095417	0.264108	-1.696454
H	-2.449742	-1.601381	-3.228201
N	-0.688201	-2.062879	-2.261300
H	-2.602266	-2.181028	-1.574516
H	0.113534	-1.596023	-1.743464
H	-0.557818	-3.006733	-2.628497

tryptamine, Ph-up S_0

C	-2.085183	0.014536	0.818790
N	-1.245584	0.005275	1.923847
C	0.069848	0.032539	1.499515

C	0.046425	0.052332	0.068880
C	-1.338892	0.039957	-0.343983
C	1.263649	0.047022	2.232733
C	2.459042	0.087141	1.516041
C	2.463950	0.113690	0.103063
C	1.274812	0.097034	-0.622346
C	-1.874337	0.015274	-1.748486
C	-2.144086	-1.411757	-2.298199
N	-0.994657	-2.316552	-2.394683
H	1.262161	0.030054	3.325275
H	3.407807	0.099950	2.056400
H	3.418944	0.150102	-0.425441
H	1.295031	0.121678	-1.714486
H	-1.551650	0.009321	2.889739
H	-3.164460	0.010552	0.950421
H	-1.166861	0.528479	-2.423130
H	-2.816877	0.588926	-1.798430
H	-2.592758	-1.325438	-3.302331
H	-2.900285	-1.898117	-1.659214
H	-0.543140	-2.411196	-1.480482
H	-0.289249	-1.931171	-3.028435

tryptamine, Ph-up S_1

C	-2.201460	0.162441	0.903261
N	-1.300475	0.132577	1.958984
C	0.003323	0.054565	1.488418
C	-0.065030	0.057683	0.071728
C	-1.453633	0.107291	-0.277459
C	1.215037	-0.052089	2.214805
C	2.411076	-0.125484	1.429673
C	2.382634	-0.104969	0.042218
C	1.160696	-0.071522	-0.713541
C	-2.010551	0.038545	-1.675223
C	-1.936354	-1.364819	-2.300953
N	-0.595020	-1.889926	-2.368004
H	1.241883	-0.036724	3.304555
H	3.373820	-0.199423	1.942181
H	3.332687	-0.115551	-0.501471
H	1.205321	0.381786	-1.716634
H	-1.552568	0.188226	2.938424
H	-3.268211	0.274109	1.071363
H	-1.498818	0.748362	-2.348757
H	-3.073128	0.329225	-1.687374
H	-2.362575	-1.423052	-3.321015
H	-2.509419	-2.103054	-1.705408

H	0.189212	-1.431752	-1.816799
H	-0.434786	-2.806836	-2.787882

tryptamine, Py-out S_0

C	0.525253	0.457812	0.215756
C	0.601121	0.528236	1.642554
C	1.819395	0.489954	2.333091
C	2.985605	0.380239	1.576042
C	2.938346	0.314137	0.165601
C	1.724472	0.352504	-0.517664
N	-0.695701	0.635715	2.112159
H	1.858985	0.545397	3.423685
H	3.952243	0.347453	2.082992
H	3.871825	0.233047	-0.395435
H	1.704625	0.303248	-1.608929
C	-0.872404	0.533922	-0.148236
C	-1.573909	0.639764	1.036590
H	-0.963204	0.721052	3.085609
H	-2.645622	0.723704	1.197947
C	-1.457773	0.472449	-1.531178
H	-0.891051	1.135717	-2.207317
C	-1.469611	-0.946727	-2.133235
H	-2.494913	0.843967	-1.508051
H	-0.422951	-1.304142	-2.230803
N	-2.328707	-1.831733	-1.331338
H	-1.889887	-0.893493	-3.151143
H	-2.332611	-2.776198	-1.723815
H	-1.943506	-1.906025	-0.384862

tryptamine, Py-out S_1

C	0.572597	0.510209	0.158535
C	0.598476	0.432777	1.597129
C	1.789664	0.394470	2.333219
C	3.014170	0.449255	1.604074
C	3.014258	0.532007	0.206047
C	1.825395	0.557462	-0.542464
N	-0.710437	0.367379	2.028631
H	1.781940	0.335085	3.423545
H	3.961839	0.419192	2.145353
H	3.972174	0.573061	-0.320628
H	1.861151	0.633011	-1.631645
C	-0.783711	0.486223	-0.229210
C	-1.622417	0.279911	0.935040
H	-0.967747	0.185994	2.991669

H	-2.571769	0.829745	1.056920
C	-1.319690	0.449979	-1.634555
H	-0.613035	0.907515	-2.342566
C	-1.597170	-0.988083	-2.126571
H	-2.256459	1.029459	-1.721813
H	-0.656209	-1.553375	-2.276719
N	-2.320312	-1.737273	-1.130976
H	-2.141915	-1.059873	-3.083691
H	-2.560821	-2.717176	-1.286166
H	-2.269984	-1.316965	-0.153167

tryptamine, Py-up S_0

C	-2.124936	0.225857	0.890332
N	-1.246453	0.202484	1.965782
C	0.049095	0.090654	1.493926
C	-0.027888	0.038290	0.066780
C	-1.424766	0.129296	-0.296485
C	1.267253	0.034716	2.183353
C	2.431821	-0.076063	1.424148
C	2.383321	-0.126142	0.013174
C	1.169625	-0.069897	-0.668832
C	-2.003041	0.071831	-1.679579
C	-2.039638	-1.360803	-2.281835
N	-2.859144	-2.344831	-1.568908
H	1.307888	0.076551	3.274473
H	3.398473	-0.123016	1.929912
H	3.315672	-0.209876	-0.549243
H	1.149454	-0.106935	-1.760590
H	-1.512173	0.280498	2.940315
H	-3.194542	0.327290	1.056735
H	-1.422354	0.723707	-2.357452
H	-3.031282	0.473832	-1.667886
H	-1.012478	-1.756589	-2.336610
H	-2.406516	-1.299232	-3.319913
H	-3.835016	-2.035576	-1.535814
H	-2.543855	-2.416424	-0.596893

tryptamine, Py-up S_1

C	-2.260694	0.459295	0.957006
N	-1.311625	0.439170	1.979658
C	-0.049381	0.134841	1.491357
C	-0.168982	0.010440	0.073930
C	-1.547943	0.227009	-0.244675
C	1.158672	-0.062296	2.193008

C	2.312963	-0.372340	1.396974
C	2.227482	-0.482135	0.010517
C	1.010283	-0.313764	-0.695273
C	-2.164291	0.250885	-1.617745
C	-2.171081	-1.124977	-2.344357
N	-2.084305	-2.222413	-1.428162
H	1.221719	0.056795	3.275306
H	3.274566	-0.527807	1.891140
H	3.136989	-0.705878	-0.555755
H	1.002632	-0.318895	-1.787111
H	-1.522193	0.564411	2.962589
H	-3.248300	0.885547	1.114629
H	-1.643559	0.956564	-2.286059
H	-3.205257	0.602903	-1.551545
H	-1.291860	-1.261324	-3.003429
H	-3.041744	-1.289525	-3.000876
H	-2.083325	-3.194322	-1.735081
H	-1.762246	-1.962555	-0.477131

porphycene S_0

C	-3.447292	1.920092	0.000000
C	-2.421788	0.915125	0.000000
N	-1.216520	1.563133	0.000000
C	-1.401995	2.924102	0.000000
C	-2.822253	3.152616	0.000000
C	-0.370377	3.886216	0.000000
C	1.018408	3.735940	0.000000
C	1.841182	2.584641	0.000000
H	-0.221601	1.162087	0.000000
N	1.408428	1.284814	0.000000
C	3.297121	2.614936	0.000000
C	3.720801	1.310356	0.000000
C	2.518127	0.498362	0.000000
C	2.421788	-0.915125	0.000000
C	3.447292	-1.920092	0.000000
C	2.822253	-3.152616	0.000000
C	1.401995	-2.924102	0.000000
N	1.216520	-1.563133	0.000000
C	0.370377	-3.886216	0.000000
C	-1.018408	-3.735940	0.000000
C	-1.841182	-2.584641	0.000000
C	-3.297121	-2.614936	0.000000
C	-3.720801	-1.310356	0.000000
C	-2.518127	-0.498362	0.000000
N	-1.408428	-1.284814	0.000000

H	0.221601	-1.162087	0.000000
H	3.294523	-4.132071	0.000000
H	4.516438	-1.725409	0.000000
H	0.731988	-4.918244	0.000000
H	-1.579890	-4.675090	0.000000
H	-3.911918	-3.513212	0.000000
H	-4.745038	-0.944241	0.000000
H	-4.516438	1.725409	0.000000
H	-3.294523	4.132070	0.000000
H	-0.731988	4.918245	0.000000
H	1.579890	4.675090	0.000000
H	3.911918	3.513212	0.000000
H	4.745038	0.944241	0.000000

porphycene S_1

C	-3.471614	1.912772	0.000000
C	-2.456791	0.909704	0.000000
N	-1.240205	1.557904	0.000000
C	-1.422649	2.917867	0.000000
C	-2.837814	3.148529	0.000000
C	-0.384720	3.887583	0.000000
C	0.997947	3.750931	0.000000
C	1.852315	2.608220	0.000000
H	-0.261406	1.150965	0.000000
N	1.425882	1.297647	0.000000
C	3.288462	2.643497	0.000000
C	3.731607	1.323646	0.000000
C	2.562116	0.508217	0.000000
C	2.456791	-0.909704	0.000000
C	3.471614	-1.912772	0.000000
C	2.837814	-3.148529	0.000000
C	1.422649	-2.917867	0.000000
N	1.240205	-1.557904	0.000000
C	0.384720	-3.887583	0.000000
C	-0.997947	-3.750931	0.000000
C	-1.852315	-2.608220	0.000000
C	-3.288462	-2.643497	0.000000
C	-3.731607	-1.323646	0.000000
C	-2.562116	-0.508217	0.000000
N	-1.425882	-1.297647	0.000000
H	0.261406	-1.150965	0.000000
H	3.307085	-4.129362	0.000000
H	4.541387	-1.723306	0.000000
H	0.753653	-4.916778	0.000000
H	-1.548395	-4.696973	0.000000

H	-3.902700	-3.542194	0.000000
H	-4.762070	-0.976243	0.000000
H	-4.541387	1.723306	0.000000
H	-3.307085	4.129362	0.000000
H	-0.753653	4.916778	0.000000
H	1.548395	4.696973	0.000000
H	3.902699	3.542194	0.000000
H	4.762070	0.976243	0.000000

porphine S_0

N	0.000000	-2.030802	0.000000
N	2.123919	0.000000	0.000000
C	1.089600	-2.862419	0.000000
C	0.681164	-4.266630	0.000000
C	2.429949	-2.446695	0.000000
C	2.906854	-1.133327	0.000000
C	4.274586	-0.688651	0.000000
H	1.355839	-5.121063	0.000000
H	3.190924	-3.230154	0.000000
H	5.135567	-1.352518	0.000000
H	1.099723	0.000000	0.000000
N	0.000000	2.030802	0.000000
N	-2.123919	0.000000	0.000000
C	1.089600	2.862419	0.000000
C	-1.089600	2.862419	0.000000
C	-1.089600	-2.862419	0.000000
C	0.681164	4.266630	0.000000
C	-0.681164	4.266630	0.000000
C	-0.681164	-4.266630	0.000000
C	2.429949	2.446695	0.000000
C	-2.429949	2.446695	0.000000
C	-2.429949	-2.446695	0.000000
C	2.906854	1.133327	0.000000
C	-2.906854	1.133327	0.000000
C	-2.906854	-1.133327	0.000000
C	4.274586	0.688651	0.000000
C	-4.274586	0.688651	0.000000
C	-4.274586	-0.688651	0.000000
H	1.355839	5.121063	0.000000
H	-1.355839	5.121063	0.000000
H	-1.355839	-5.121063	0.000000
H	3.190924	3.230154	0.000000
H	-3.190924	3.230154	0.000000
H	-3.190924	-3.230154	0.000000
H	5.135567	1.352518	0.000000

H	-5.135567	1.352518	0.000000
H	-5.135567	-1.352518	0.000000
H	-1.099723	0.000000	0.000000

porphine S_1

N	0.000000	-2.055470	0.000000
N	2.120716	0.000000	0.000000
C	1.095084	-2.892891	0.000000
C	0.685657	-4.287710	0.000000
C	2.436608	-2.454601	0.000000
C	2.906466	-1.136040	0.000000
C	4.274376	-0.690076	0.000000
H	1.357874	-5.143810	0.000000
H	3.205544	-3.230517	0.000000
H	5.135854	-1.353319	0.000000
H	1.098278	0.000000	0.000000
N	0.000000	2.055470	0.000000
N	-2.120716	0.000000	0.000000
C	1.095084	2.892891	0.000000
C	-1.095084	2.892891	0.000000
C	-1.095084	-2.892891	0.000000
C	0.685657	4.287710	0.000000
C	-0.685657	4.287710	0.000000
C	-0.685657	-4.287710	0.000000
C	2.436608	2.454601	0.000000
C	-2.436608	2.454601	0.000000
C	-2.436608	-2.454601	0.000000
C	2.906466	1.136040	0.000000
C	-2.906466	1.136040	0.000000
C	-2.906466	-1.136040	0.000000
C	4.274376	0.690076	0.000000
C	-4.274376	0.690076	0.000000
C	-4.274376	-0.690076	0.000000
H	1.357874	5.143810	0.000000
H	-1.357874	5.143810	0.000000
H	-1.357874	-5.143810	0.000000
H	3.205544	3.230517	0.000000
H	-3.205544	3.230517	0.000000
H	-3.205544	-3.230517	0.000000
H	5.135854	1.353319	0.000000
H	-5.135854	1.353319	0.000000
H	-5.135854	-1.353319	0.000000
H	-1.098278	0.000000	0.000000

chlorin S_0

C	0.000000	-4.268309	0.929314
C	0.000000	-2.907547	1.384049
N	0.000000	-2.114507	0.248658
C	0.000000	-2.887333	-0.886102
C	0.000000	-4.257158	-0.449585
C	0.000000	-2.432628	2.693763
C	0.000000	-1.090461	3.114148
N	0.000000	0.000000	2.281450
C	0.000000	1.090461	3.114148
C	0.000000	0.682947	4.513052
C	0.000000	-0.682947	4.513052
C	0.000000	2.432628	2.693763
C	0.000000	2.907547	1.384049
N	0.000000	2.114507	0.248658
C	0.000000	2.887333	-0.886102
C	0.000000	4.257158	-0.449585
C	0.000000	4.268309	0.929314
C	0.000000	2.423006	-2.212239
C	0.000000	1.107241	-2.669059
C	0.000000	0.769964	-4.160752
C	0.000000	-0.769964	-4.160752
C	0.000000	-1.107241	-2.669059
N	0.000000	0.000000	-1.883996
C	0.000000	-2.423006	-2.212239
H	-0.884872	1.196079	-4.658474
H	0.000000	3.205499	-2.974765
H	0.000000	5.112938	-1.120118
H	0.000000	1.356526	5.368397
H	0.000000	-1.356526	5.368397
H	-0.884872	-1.196079	-4.658474
H	0.000000	3.194243	3.476950
H	0.000000	-3.194243	3.476950
H	0.000000	-3.205499	-2.974765
H	0.000000	5.135026	1.585780
H	0.000000	-5.135026	1.585780
H	0.000000	-5.112938	-1.120118
H	0.884872	-1.196079	-4.658474
H	0.884872	1.196079	-4.658474
H	0.000000	-1.092797	0.276726
H	0.000000	1.092797	0.276726

chlorin S_1

C	0.000000	-4.278537	0.929959
C	0.000000	-2.915209	1.382410

N	0.000000	-2.122743	0.246517
C	0.000000	-2.902570	-0.890697
C	0.000000	-4.269444	-0.453570
C	0.000000	-2.438802	2.698589
C	0.000000	-1.092916	3.119258
N	0.000000	0.000000	2.283378
C	0.000000	1.092916	3.119258
C	0.000000	0.682681	4.520981
C	0.000000	-0.682681	4.520981
C	0.000000	2.438802	2.698589
C	0.000000	2.915209	1.382410
N	0.000000	2.122743	0.246517
C	0.000000	2.902570	-0.890697
C	0.000000	4.269444	-0.453570
C	0.000000	4.278537	0.929959
C	0.000000	2.432572	-2.219318
C	0.000000	1.108812	-2.670828
C	0.000000	0.768859	-4.156761
C	0.000000	-0.768859	-4.156761
C	0.000000	-1.108812	-2.670828
N	0.000000	0.000000	-1.877846
C	0.000000	-2.432572	-2.219318
H	-0.883866	1.196009	-4.657772
H	0.000000	3.210512	-2.986117
H	0.000000	5.126600	-1.122203
H	0.000000	1.357267	5.375250
H	0.000000	-1.357267	5.375250
H	-0.883866	-1.196009	-4.657772
H	0.000000	3.200022	3.481427
H	0.000000	-3.200022	3.481427
H	0.000000	-3.210512	-2.986117
H	0.000000	5.143871	1.587875
H	0.000000	-5.143871	1.587875
H	0.000000	-5.126600	-1.122203
H	0.883866	-1.196009	-4.657772
H	0.883866	1.196009	-4.657772
H	0.000000	-1.101182	0.270019
H	0.000000	1.101182	0.270019

Zn-tetraphenylporphine S_0

C	-3.709343	4.333997	1.125859
C	-3.513648	3.513648	0.000000
C	-4.333997	3.709340	-1.125860
C	-5.321407	4.699931	-1.126751
C	-5.508376	5.508373	-0.000002

C	-4.699935	5.321406	1.126748
C	-2.454158	2.454158	0.000001
C	-1.108851	2.880059	-0.012094
N	0.000000	2.056199	0.033806
C	1.108851	2.880059	-0.012094
C	0.683602	4.260857	-0.103504
C	-0.683602	4.260857	-0.103504
C	2.454158	2.454158	0.000001
C	3.513648	3.513648	0.000000
C	4.333997	3.709340	-1.125860
C	5.321407	4.699931	-1.126751
C	5.508376	5.508373	-0.000002
C	4.699935	5.321406	1.126748
C	3.709343	4.333997	1.125859
C	-2.880059	1.108851	0.012097
N	-2.056199	0.000000	-0.033805
C	-2.880059	-1.108851	0.012097
C	-4.260857	-0.683602	0.103506
C	-4.260857	0.683602	0.103506
C	-2.454158	-2.454158	0.000001
C	-3.513648	-3.513648	0.000000
C	-4.333997	-3.709340	-1.125860
C	-5.321407	-4.699931	-1.126751
C	-5.508376	-5.508373	-0.000002
C	-4.699935	-5.321406	1.126748
C	-3.709343	-4.333997	1.125859
C	2.880059	1.108851	0.012097
N	2.056199	0.000000	-0.033805
C	2.880059	-1.108851	0.012097
C	4.260857	-0.683602	0.103506
C	4.260857	0.683602	0.103506
C	2.454158	-2.454158	0.000001
C	3.513648	-3.513648	0.000000
C	4.333997	-3.709340	-1.125860
C	5.321407	-4.699931	-1.126751
C	5.508376	-5.508373	-0.000002
C	4.699935	-5.321406	1.126748
C	3.709343	-4.333997	1.125859
C	1.108851	-2.880059	-0.012094
N	0.000000	-2.056199	0.033806
C	-1.108851	-2.880059	-0.012094
C	-0.683602	-4.260857	-0.103504
C	0.683602	-4.260857	-0.103504
H	1.348047	-5.116906	-0.177248
H	5.116906	-1.348047	0.177251
H	1.348047	5.116906	-0.177248

H	-1.348047	5.116906	-0.177248
H	-1.348047	-5.116906	-0.177248
H	5.116906	1.348047	0.177251
H	-5.116906	1.348047	0.177251
H	-5.116906	-1.348047	0.177251
H	4.185472	3.082819	-2.008303
H	5.944428	4.842351	-2.012785
H	6.280700	6.280697	-0.000003
H	4.842356	5.944428	2.012781
H	3.082823	4.185474	2.008303
H	4.185472	-3.082819	-2.008303
H	5.944428	-4.842351	-2.012785
H	6.280700	-6.280697	-0.000003
H	4.842356	-5.944428	2.012781
H	3.082823	-4.185474	2.008303
H	-4.185472	-3.082819	-2.008303
H	-5.944428	-4.842351	-2.012785
H	-6.280700	-6.280697	-0.000003
H	-4.842356	-5.944428	2.012781
H	-3.082823	-4.185474	2.008303
H	-4.185472	3.082819	-2.008303
H	-5.944428	4.842351	-2.012785
H	-6.280700	6.280697	-0.000003
H	-4.842356	5.944428	2.012781
H	-3.082823	4.185474	2.008303
Zn	0.000000	0.000000	0.000000

Zn-tetraphenylporphine S_1

C	-3.550612	4.555748	0.941506
C	-3.515152	3.510252	-0.004376
C	-4.510981	3.478908	-1.003032
C	-5.498473	4.464534	-1.061442
C	-5.522476	5.495836	-0.113875
C	-4.546744	5.535059	0.888724
C	-2.459364	2.463751	0.040576
C	-1.111489	2.875676	-0.020619
N	0.000000	2.060197	0.146253
C	1.111489	2.875676	-0.020619
C	0.683837	4.226144	-0.307362
C	-0.683837	4.226144	-0.307362
C	2.459364	2.463751	0.040576
C	3.515152	3.510252	-0.004376
C	4.510981	3.478908	-1.003032
C	5.498473	4.464534	-1.061442
C	5.522476	5.495836	-0.113875

C	4.546744	5.535059	0.888724
C	3.550612	4.555748	0.941506
C	-2.885365	1.109247	0.134211
N	-2.068373	0.000000	-0.025504
C	-2.885365	-1.109247	0.134211
C	-4.230609	-0.688393	0.413416
C	-4.230609	0.688393	0.413416
C	-2.459364	-2.463751	0.040576
C	-3.515152	-3.510252	-0.004376
C	-4.510981	-3.478908	-1.003032
C	-5.498473	-4.464534	-1.061442
C	-5.522476	-5.495836	-0.113875
C	-4.546744	-5.535059	0.888724
C	-3.550612	-4.555748	0.941506
C	2.885365	1.109247	0.134211
N	2.068373	0.000000	-0.025504
C	2.885365	-1.109247	0.134211
C	4.230609	-0.688393	0.413416
C	4.230609	0.688393	0.413416
C	2.459364	-2.463751	0.040576
C	3.515152	-3.510252	-0.004376
C	4.510981	-3.478908	-1.003032
C	5.498473	-4.464534	-1.061442
C	5.522476	-5.495836	-0.113875
C	4.546744	-5.535059	0.888724
C	3.550612	-4.555748	0.941506
C	1.111489	-2.875676	-0.020619
N	0.000000	-2.060197	0.146253
C	-1.111489	-2.875676	-0.020619
C	-0.683837	-4.226144	-0.307362
C	0.683837	-4.226144	-0.307362
H	1.347637	-5.058568	-0.520838
H	5.065531	-1.352603	0.614674
H	1.347637	5.058568	-0.520838
H	-1.347637	5.058568	-0.520838
H	-1.347637	-5.058568	-0.520838
H	5.065531	1.352603	0.614674
H	-5.065531	1.352603	0.614674
H	-5.065531	-1.352603	0.614674
H	4.489180	2.681052	-1.748287
H	6.250164	4.431109	-1.853486
H	6.298191	6.263523	-0.156249
H	4.564124	6.329153	1.638815
H	2.798339	4.580635	1.732682
H	4.489180	-2.681052	-1.748287
H	6.250164	-4.431109	-1.853486

H	6.298191	-6.263523	-0.156249
H	4.564124	-6.329153	1.638815
H	2.798339	-4.580635	1.732682
H	-4.489180	-2.681052	-1.748287
H	-6.250164	-4.431109	-1.853486
H	-6.298191	-6.263523	-0.156249
H	-4.564124	-6.329153	1.638815
H	-2.798339	-4.580635	1.732682
H	-4.489180	2.681052	-1.748287
H	-6.250164	4.431109	-1.853486
H	-6.298191	6.263523	-0.156249
H	-4.564124	6.329153	1.638815
H	-2.798339	4.580635	1.732682
Zn	0.000000	0.000000	0.056494

tetraphenylporphine S_0

C	-0.691018	4.280797	0.142043
C	-1.135974	2.914295	0.014677
N	0.000000	2.130387	-0.049416
C	1.135974	2.914295	0.014676
C	0.691019	4.280797	0.142043
C	2.476387	2.457809	-0.024448
C	2.876525	1.092437	-0.074537
N	2.045874	0.000000	-0.010549
C	2.876525	-1.092437	-0.074536
C	4.278102	-0.683720	-0.217519
C	4.278102	0.683720	-0.217519
C	2.476387	-2.457809	-0.024447
C	1.135974	-2.914295	0.014677
N	0.000000	-2.130387	-0.049416
C	-1.135974	-2.914295	0.014676
C	-0.691019	-4.280797	0.142043
C	0.691018	-4.280797	0.142043
C	-2.476387	-2.457809	-0.024448
C	-2.876525	-1.092437	-0.074537
N	-2.045874	0.000000	-0.010549
C	-2.876525	1.092437	-0.074536
C	-4.278102	0.683720	-0.217519
C	-4.278102	-0.683720	-0.217519
C	-2.476387	2.457809	-0.024447
H	-5.136818	-1.355700	-0.327257
C	-3.544947	-3.510406	0.000637
H	-1.356611	-5.144933	0.238508
H	0.000000	-1.101120	-0.084406
H	5.136819	-1.355700	-0.327256

H	5.136818	1.355700	-0.327257
H	-5.136819	1.355700	-0.327256
C	3.544947	-3.510406	0.000639
C	3.544947	3.510406	0.000637
C	-3.544947	3.510406	0.000639
H	1.356610	-5.144933	0.238509
H	1.356611	5.144933	0.238508
H	-1.356610	5.144933	0.238509
H	0.000000	1.101120	-0.084406
C	3.689769	-4.427467	-1.067065
C	4.691722	-5.412370	-1.038194
C	5.565066	-5.501459	0.060145
C	5.431125	-4.597191	1.128643
C	4.431688	-3.610281	1.098908
H	3.014278	-4.352901	-1.934059
H	4.793796	-6.111622	-1.883580
H	6.349777	-6.274320	0.082941
H	6.107711	-4.662450	1.995815
H	4.323720	-2.907474	1.940044
C	-3.689768	-4.427467	-1.067068
C	-4.691721	-5.412370	-1.038199
C	-5.565065	-5.501460	0.060139
C	-5.431125	-4.597193	1.128638
C	-4.431689	-3.610282	1.098904
H	-3.014276	-4.352900	-1.934062
H	-4.793795	-6.111621	-1.883585
H	-6.349776	-6.274320	0.082935
H	-6.107711	-4.662452	1.995810
H	-4.323720	-2.907476	1.940041
C	-3.689769	4.427467	-1.067065
C	-4.691722	5.412370	-1.038194
C	-5.565066	5.501459	0.060145
C	-5.431125	4.597191	1.128643
C	-4.431688	3.610281	1.098908
H	-3.014278	4.352901	-1.934059
H	-4.793796	6.111622	-1.883580
H	-6.349777	6.274320	0.082941
H	-6.107711	4.662450	1.995815
H	-4.323720	2.907474	1.940044
C	3.689768	4.427467	-1.067068
C	4.691721	5.412370	-1.038199
C	5.565065	5.501460	0.060139
C	5.431125	4.597193	1.128638
C	4.431689	3.610282	1.098904
H	3.014276	4.352900	-1.934062
H	4.793795	6.111621	-1.883585

H	6.349776	6.274320	0.082935
H	6.107711	4.662452	1.995810
H	4.323720	2.907476	1.940041

tetraphenylporphine S_1

C	-4.263962	-0.691863	0.299069
C	-2.913960	-1.138779	0.054113
N	-2.135718	0.000000	-0.070800
C	-2.913960	1.138778	0.054106
C	-4.263963	0.691864	0.299062
C	-2.465510	2.482554	-0.036975
C	-1.096033	2.894134	-0.155954
N	0.000000	2.065925	-0.029641
C	1.096033	2.894135	-0.155949
C	0.688346	4.267966	-0.420197
C	-0.688346	4.267965	-0.420198
C	2.465510	2.482555	-0.036963
C	2.913960	1.138779	0.054113
N	2.135718	0.000000	-0.070800
C	2.913960	-1.138778	0.054106
C	4.263963	-0.691864	0.299062
C	4.263962	0.691863	0.299069
C	2.465510	-2.482554	-0.036975
C	1.096033	-2.894134	-0.155954
N	0.000000	-2.065925	-0.029641
C	-1.096033	-2.894135	-0.155949
C	-0.688346	-4.267966	-0.420197
C	0.688346	-4.267965	-0.420198
C	-2.465510	-2.482555	-0.036963
H	1.357606	-5.114843	-0.608520
C	3.511413	-3.546437	0.002380
H	5.116391	-1.355036	0.478488
H	1.110698	0.000000	-0.154571
H	1.357607	5.114843	-0.608517
H	-1.357606	5.114843	-0.608520
H	-1.357607	-5.114843	-0.608517
C	3.511414	3.546437	0.002398
C	-3.511413	3.546437	0.002380
C	-3.511414	-3.546437	0.002398
H	5.116390	1.355033	0.478500
H	-5.116391	1.355036	0.478488
H	-5.116390	-1.355033	0.478500
H	-1.110698	0.000000	-0.154571
C	4.562711	3.580444	-0.948009
C	5.543348	4.585095	-0.901981

C	5.499389	5.572877	0.097833
C	4.462803	5.551440	1.049405
C	3.476692	4.554104	0.999218
H	4.590385	2.818819	-1.743054
H	6.344146	4.599982	-1.658661
H	6.270124	6.359108	0.134802
H	4.424850	6.316143	1.841758
H	2.672336	4.534957	1.751013
C	4.562707	-3.580441	-0.948031
C	5.543343	-4.585094	-0.902011
C	5.499386	-5.572880	0.097800
C	4.462804	-5.551444	1.049376
C	3.476694	-4.554107	0.999196
H	4.590379	-2.818814	-1.743074
H	6.344139	-4.599979	-1.658694
H	6.270120	-6.359111	0.134762
H	4.424853	-6.316151	1.841726
H	2.672341	-4.534962	1.750994
C	-4.562711	-3.580444	-0.948009
C	-5.543348	-4.585095	-0.901981
C	-5.499389	-5.572877	0.097833
C	-4.462803	-5.551440	1.049405
C	-3.476692	-4.554104	0.999218
H	-4.590385	-2.818819	-1.743054
H	-6.344146	-4.599982	-1.658661
H	-6.270124	-6.359108	0.134802
H	-4.424850	-6.316143	1.841758
H	-2.672336	-4.534957	1.751013
C	-4.562707	3.580441	-0.948031
C	-5.543343	4.585094	-0.902011
C	-5.499386	5.572880	0.097800
C	-4.462804	5.551444	1.049376
C	-3.476694	4.554107	0.999196
H	-4.590379	2.818814	-1.743074
H	-6.344139	4.599979	-1.658694
H	-6.270120	6.359111	0.134762
H	-4.424853	6.316151	1.841726
H	-2.672341	4.534962	1.750994

BP86/TZVP geometries – Group II

tetrafluorobenzene S_0

C	-1.200749	0.699908	0.000000
C	-1.200749	-0.699908	0.000000
C	0.000000	-1.406578	0.000000

C	1.200749	-0.699908	0.000000
C	1.200749	0.699908	0.000000
C	0.000000	1.406578	0.000000
F	-2.375441	-1.366172	0.000000
H	0.000000	-2.496729	0.000000
F	2.375441	-1.366172	0.000000
F	2.375441	1.366172	0.000000
H	0.000000	2.496729	0.000000
F	-2.375441	1.366172	0.000000

tetrafluorobenzene S_1

C	1.172990	-0.712093	0.110382
C	1.172990	0.712093	0.110382
C	0.000000	1.473170	0.300645
C	-1.172990	0.712093	0.110382
C	-1.172990	-0.712093	0.110382
C	0.000000	-1.473170	0.300645
F	2.333101	1.334912	-0.221015
H	0.000000	2.519151	0.618745
F	-2.333101	1.334912	-0.221015
F	-2.333101	-1.334912	-0.221015
H	0.000000	-2.519151	0.618745
F	2.333101	-1.334912	-0.221015

benzonitrile S_0

C	0.000000	0.000000	-1.066347
C	-1.220721	0.000000	-0.361575
C	-1.213243	0.000000	1.033840
C	0.000000	0.000000	1.732710
C	1.213243	0.000000	1.033840
C	1.220721	0.000000	-0.361575
H	-2.161362	0.000000	-0.914349
H	-2.159392	0.000000	1.578562
H	0.000000	0.000000	2.824687
H	2.159392	0.000000	1.578562
H	2.161362	0.000000	-0.914349
C	0.000000	0.000000	-2.498254
N	0.000000	0.000000	-3.665743

benzonitrile S_1

C	0.000000	0.000000	-1.120467
C	-1.235788	0.000000	-0.376924
C	-1.220250	0.000000	1.055562

C	0.000000	0.000000	1.772932
C	1.220250	0.000000	1.055562
C	1.235788	0.000000	-0.376924
H	-2.182937	0.000000	-0.915769
H	-2.171096	0.000000	1.589976
H	0.000000	0.000000	2.862614
H	2.171096	0.000000	1.589976
H	2.182937	0.000000	-0.915769
C	0.000000	0.000000	-2.518310
N	0.000000	0.000000	-3.702458

o-fluorophenol, *cis* S_0

C	0.327737	1.462676	0.000000
C	-0.879085	0.779392	0.000000
C	-0.956585	-0.621240	0.000000
C	0.239871	-1.347723	0.000000
C	1.466494	-0.676138	0.000000
C	1.517649	0.722926	0.000000
F	-2.070405	1.466106	0.000000
O	-2.157485	-1.279392	0.000000
H	0.186518	-2.437779	0.000000
H	2.391615	-1.255457	0.000000
H	2.476886	1.242460	0.000000
H	0.325083	2.553821	0.000000
H	-2.868282	-0.609673	0.000000

o-fluorophenol, *cis* S_1

C	0.327542	1.523969	0.000000
C	-0.899997	0.793763	0.000000
C	-0.946891	-0.622470	0.000000
C	0.242864	-1.414869	0.000000
C	1.476357	-0.696394	0.000000
C	1.502323	0.725616	0.000000
F	-2.101472	1.457172	0.000000
O	-2.149892	-1.270584	0.000000
H	0.175838	-2.500124	0.000000
H	2.420212	-1.241629	0.000000
H	2.472276	1.227571	0.000000
H	0.341306	2.610680	0.000000
H	-2.860455	-0.592724	0.000000

o-fluorophenol, *trans* S_0

C	0.293369	1.272884	0.000000

C	-0.954164	0.623235	0.000000
C	-0.968349	-0.778431	0.000000
C	0.227641	-1.505777	0.000000
C	1.456653	-0.840558	0.000000
C	1.486067	0.560256	0.000000
O	-2.080357	1.403423	0.000000
H	-1.930340	-1.300577	0.000000
H	0.191359	-2.596674	0.000000
H	2.391833	-1.402415	0.000000
H	2.426232	1.114466	0.000000
F	0.320123	2.630245	0.000000
H	-2.860077	0.819923	0.000000

o-fluorophenol, *trans* S_1

C	0.829251	1.060149	0.137700
C	-0.588126	0.976929	0.087976
C	-1.265299	-0.282880	0.066631
C	-0.463601	-1.436480	-0.099158
C	0.945166	-1.344372	-0.053419
C	1.614597	-0.128902	0.236839
O	-1.274851	2.149249	-0.030217
H	-2.305551	-0.363556	0.407494
H	-0.932982	-2.413783	-0.228545
H	1.537323	-2.247002	-0.240714
H	2.689647	-0.080901	0.407705
F	1.414614	2.191452	-0.411713
H	-2.200218	1.920097	-0.280579

m-fluorophenol, *cis* S_0

C	0.310209	1.418041	0.000000
C	-0.934874	0.792199	0.000000
C	-0.974052	-0.610417	0.000000
C	0.216528	-1.353330	0.000000
C	1.441766	-0.685328	0.000000
C	1.510532	0.714190	0.000000
O	-2.155420	-1.311772	0.000000
F	0.341216	2.781001	0.000000
H	0.161780	-2.442396	0.000000
H	2.366756	-1.265277	0.000000
H	2.459876	1.249389	0.000000
H	-1.845038	1.396616	0.000000
H	-2.899278	-0.682916	0.000000

m-fluorophenol, *cis* S_1

C	1.221006	-0.067249	-0.692560
C	-0.067546	0.038406	-0.105612
C	-0.024381	0.042279	1.328710
C	1.162206	0.033008	2.099195
C	2.433427	0.102647	1.439945
C	2.435518	-0.034957	0.032412
O	-1.200145	-0.051340	2.027965
F	1.296662	-0.238641	-2.044728
H	1.081217	-0.131675	3.175325
H	3.361666	0.179405	2.001771
H	3.370148	-0.103568	-0.529834
H	-0.903626	0.486351	-0.661770
H	-1.910792	-0.254666	1.379130

m-fluorophenol, *trans* S_0

C	0.270424	1.313194	0.000000
C	-0.956250	0.633905	0.000000
C	-0.991036	-0.769758	0.000000
C	0.207718	-1.489769	0.000000
C	1.443844	-0.836340	0.000000
C	1.437847	0.558394	0.000000
O	-2.092370	1.406534	0.000000
H	-1.950073	-1.295347	0.000000
H	0.177123	-2.581071	0.000000
H	2.388063	-1.380502	0.000000
F	2.629810	1.218414	0.000000
H	0.304931	2.402509	0.000000
H	-2.870033	0.819846	0.000000

m-fluorophenol, *trans* S_1

C	1.095027	-0.017330	0.000000
C	0.328400	1.182257	0.000000
C	-1.093381	1.224460	0.000000
C	-1.832028	-0.009727	0.000000
C	-1.089643	-1.226044	0.000000
C	0.320265	-1.211420	0.000000
O	1.056264	2.345737	0.000000
H	-1.607009	2.189355	0.000000
H	-2.919176	-0.018146	0.000000
H	-1.596677	-2.192503	0.000000
F	0.981361	-2.402096	0.000000
H	2.181447	-0.011910	0.000000
H	0.434001	3.101516	0.000000

p-fluorophenol S_0

C	0.273901	1.325969	0.000000
C	-0.957087	0.653338	0.000000
C	-0.987487	-0.748986	0.000000
C	0.206098	-1.479675	0.000000
C	1.415408	-0.791666	0.000000
C	1.467226	0.601339	0.000000
O	-2.097887	1.425743	0.000000
H	-1.944759	-1.278679	0.000000
H	0.199982	-2.570436	0.000000
F	2.583074	-1.500143	0.000000
H	2.433577	1.107460	0.000000
H	0.282852	2.416857	0.000000
H	-2.874918	0.838869	0.000000

p-fluorophenol S_1

C	1.276428	0.686366	0.000000
C	0.030312	1.360117	0.000000
C	-1.239007	0.717377	0.000000
C	-1.257867	-0.713204	0.000000
C	-0.006877	-1.371265	0.000000
C	1.258411	-0.745324	0.000000
O	0.095692	2.731125	0.000000
H	-2.162098	1.300796	0.000000
H	-2.179141	-1.291810	0.000000
F	-0.027604	-2.726267	0.000000
H	2.165598	-1.345540	0.000000
H	2.201284	1.260071	0.000000
H	-0.818434	3.083151	0.000000

phenylacetylene S_0

C	1.216684	0.000000	-0.014491
C	0.000000	0.000000	-0.731782
C	-1.216684	0.000000	-0.014491
C	-1.211212	0.000000	1.381094
C	0.000000	0.000000	2.083602
C	1.211212	0.000000	1.381094
C	0.000000	0.000000	-2.158837
C	0.000000	0.000000	-3.374760
H	-2.158918	0.000000	-0.565143
H	-2.158775	0.000000	1.924222
H	0.000000	0.000000	3.175653

H	2.158775	0.000000	1.924222
H	2.158918	0.000000	-0.565143
H	0.000000	0.000000	-4.445257

phenylacetylene S_1

C	1.247661	0.000000	-0.036145
C	0.000000	0.000000	-0.750713
C	-1.247661	0.000000	-0.036145
C	-1.232432	0.000000	1.401107
C	0.000000	0.000000	2.089744
C	1.232432	0.000000	1.401107
C	0.000000	0.000000	-2.143479
C	0.000000	0.000000	-3.379952
H	-2.184741	0.000000	-0.591169
H	-2.172532	0.000000	1.952725
H	0.000000	0.000000	3.182199
H	2.172532	0.000000	1.952725
H	2.184741	0.000000	-0.591169
H	0.000000	0.000000	-4.450836

aniline S_0

C	0.928070	0.025211	0.000000
C	0.206799	0.033620	1.211415
C	-1.189124	0.043569	1.205438
C	-1.901204	0.049527	0.000000
C	-1.189124	0.043569	-1.205438
C	0.206799	0.033620	-1.211415
H	0.749662	0.033301	2.161019
H	-2.992438	0.056486	0.000000
H	-1.725845	0.046876	2.157210
H	-1.725845	0.046876	-2.157210
H	0.749662	0.033301	-2.161019
N	2.325992	0.079001	0.000000
H	2.778304	-0.262474	-0.844037
H	2.778304	-0.262474	0.844037

aniline S_1

C	0.878818	-0.033600	0.000000
C	0.229327	-0.008781	1.248675
C	-1.214493	0.046412	1.240085
C	-1.882284	0.071950	0.000000
C	-1.214493	0.046412	-1.240085
C	0.229327	-0.008781	-1.248675

H	0.801662	-0.030720	2.178027
H	-2.976002	0.113760	0.000000
H	-1.775135	0.067822	2.173794
H	-1.775135	0.067822	-2.173794
H	0.801662	-0.030720	-2.178027
N	2.285115	-0.087302	0.000000
H	2.805810	-0.107147	-0.873379
H	2.805810	-0.107147	0.873379

catechol S_0

C	0.472952	1.286986	0.000000
C	-0.753381	0.623139	0.000000
C	-0.804125	-0.785965	0.000000
C	0.386742	-1.514733	0.000000
C	1.618180	-0.848052	0.000000
C	1.665149	0.549185	0.000000
O	-1.990964	1.249117	0.000000
O	-2.010148	-1.438882	0.000000
H	0.329997	-2.604718	0.000000
H	2.542956	-1.427770	0.000000
H	2.622982	1.071922	0.000000
H	0.497496	2.381240	0.000000
H	-1.868460	2.214081	0.000000
H	-2.709376	-0.755549	0.000000

catechol S_1

C	0.477478	1.354865	0.000000
C	-0.767106	0.626268	0.000000
C	-0.807272	-0.787276	0.000000
C	0.390878	-1.581922	0.000000
C	1.610607	-0.861179	0.000000
C	1.650704	0.559774	0.000000
O	-1.993046	1.263667	0.000000
O	-2.007031	-1.448750	0.000000
H	0.329644	-2.667107	0.000000
H	2.556115	-1.406337	0.000000
H	2.625408	1.052143	0.000000
H	0.502433	2.444264	0.000000
H	-1.847954	2.227342	0.000000
H	-2.720858	-0.775752	0.000000

resorcinol, isomer 1 S_0

C	0.076388	1.155736	0.000000

C	-1.145853	0.470836	0.000000
C	-1.176887	-0.930850	0.000000
C	0.032265	-1.636445	0.000000
C	1.259915	-0.974591	0.000000
C	1.272984	0.429184	0.000000
O	-2.287213	1.240800	0.000000
H	-2.132088	-1.463126	0.000000
H	0.012882	-2.728360	0.000000
H	2.204613	-1.518768	0.000000
O	2.502055	1.047039	0.000000
H	0.072712	2.248969	0.000000
H	-3.059777	0.647684	0.000000
H	2.368005	2.011882	0.000000

resorcinol, isomer 1 S_1

C	0.003164	1.081988	0.041215
C	-1.194667	0.310641	-0.014303
C	-1.208776	-1.109594	-0.037623
C	0.001273	-1.855450	0.073625
C	1.217710	-1.114928	0.023946
C	1.201886	0.303445	0.042839
O	-2.366808	1.027631	-0.062339
H	-2.165887	-1.627652	-0.159857
H	-0.002390	-2.942586	0.083478
H	2.183399	-1.615872	-0.067635
O	2.423316	0.929196	-0.021390
H	-0.025678	2.105644	0.430531
H	-3.116598	0.401966	-0.030009
H	2.261050	1.861691	-0.282826

resorcinol, isomer 2 S_0

C	1.206694	0.000000	-0.551383
C	0.000000	0.000000	-1.258141
C	-1.206694	0.000000	-0.551383
C	-1.216761	0.000000	0.853683
C	0.000000	0.000000	1.540460
C	1.216761	0.000000	0.853683
O	-2.363168	0.000000	-1.297186
O	2.363168	0.000000	-1.297186
H	-2.163656	0.000000	1.400580
H	0.000000	0.000000	2.632513
H	2.163656	0.000000	1.400580
H	0.000000	0.000000	-2.348317
H	-3.124012	0.000000	-0.689191

H	3.124012	0.000000	-0.689191

resorcinol, isomer 2 S_1

C	1.203985	0.000000	-0.331008
C	0.000000	0.000000	-1.092165
C	-1.203985	0.000000	-0.331008
C	-1.221365	0.000000	1.089832
C	0.000000	0.000000	1.834686
C	1.221365	0.000000	1.089832
O	-2.374490	0.000000	-1.053833
O	2.374490	0.000000	-1.053833
H	-2.183288	0.000000	1.611562
H	0.000000	0.000000	2.921840
H	2.183288	0.000000	1.611562
H	0.000000	0.000000	-2.178541
H	-3.125032	0.000000	-0.429005
H	3.125032	0.000000	-0.429005

resorcinol, isomer 3 S_0

C	1.212768	0.000000	-0.291046
C	0.000000	0.000000	-0.996783
C	-1.212768	0.000000	-0.291046
C	-1.220016	0.000000	1.109784
C	0.000000	0.000000	1.790771
C	1.220016	0.000000	1.109784
O	-2.431779	0.000000	-0.930590
O	2.431779	0.000000	-0.930590
H	-2.172978	0.000000	1.639424
H	0.000000	0.000000	2.882889
H	2.172978	0.000000	1.639424
H	0.000000	0.000000	-2.092995
H	2.284851	0.000000	-1.893275
H	-2.284851	0.000000	-1.893275

resorcinol, isomer 3 S_1

C	-0.035949	-0.302229	1.191467
C	-0.145130	-1.085589	0.000000
C	-0.035949	-0.302229	-1.191467
C	0.013837	1.117548	-1.208182
C	-0.053878	1.857697	0.000000
C	0.013837	1.117548	1.208182
O	0.090115	-0.926566	-2.408007
O	0.090115	-0.926566	2.408007

H	0.141429	1.612652	-2.173456
H	-0.079779	2.945363	0.000000
H	0.141429	1.612652	2.173456
H	-0.745853	-2.015938	0.000000
H	0.280162	-1.873074	2.228345
H	0.280162	-1.873074	-2.228345

hydroquinone, *cis* S_0

C	-0.700473	0.000000	1.098584
C	0.700473	0.000000	1.098584
C	1.405113	0.000000	-0.110980
C	0.696785	0.000000	-1.321985
C	-0.696785	0.000000	-1.321985
C	-1.405113	0.000000	-0.110980
O	2.784137	0.000000	-0.180499
O	-2.784137	0.000000	-0.180499
H	1.253258	0.000000	-2.260754
H	-1.253258	0.000000	-2.260754
H	-1.239283	0.000000	2.051095
H	1.239283	0.000000	2.051095
H	-3.141561	0.000000	0.724828
H	3.141561	0.000000	0.724828

hydroquinone, *cis* S_1

C	0.714308	0.000000	-1.134790
C	-0.714308	0.000000	-1.134790
C	-1.376979	0.000000	0.122181
C	-0.714438	0.000000	1.371619
C	0.714438	0.000000	1.371619
C	1.376979	0.000000	0.122181
O	-2.747440	0.000000	0.167851
O	2.747440	0.000000	0.167851
H	-1.297964	0.000000	2.290345
H	1.297964	0.000000	2.290345
H	1.285138	0.000000	-2.065791
H	-1.285138	0.000000	-2.065791
H	3.083959	0.000000	-0.750644
H	-3.083959	0.000000	-0.750644

hydroquinone, *trans* S_0

C	0.022536	1.399812	0.000000
C	-1.203917	0.724564	0.000000
C	-1.218799	-0.678010	0.000000

C	-0.022536	-1.399812	0.000000
C	1.203917	-0.724564	0.000000
C	1.218799	0.678010	0.000000
O	-2.353677	1.489219	0.000000
H	-2.171758	-1.216326	0.000000
H	-0.029968	-2.491016	0.000000
O	2.353677	-1.489219	0.000000
H	2.171758	1.216326	0.000000
H	0.029968	2.491016	0.000000
H	-3.123006	0.892997	0.000000
H	3.123006	-0.892997	0.000000

hydroquinone, *trans* S_1

C	1.271591	0.683445	0.000000
C	0.037850	1.376373	0.000000
C	-1.234094	0.744713	0.000000
C	-1.271591	-0.683445	0.000000
C	-0.037850	-1.376373	0.000000
C	1.234094	-0.744713	0.000000
O	0.122646	2.744789	0.000000
H	-2.150696	1.338357	0.000000
H	-2.204212	-1.244732	0.000000
O	-0.122646	-2.744789	0.000000
H	2.150696	-1.338357	0.000000
H	2.204212	1.244732	0.000000
H	-0.786419	3.106532	0.000000
H	0.786419	-3.106532	0.000000

salicylic acid S_0

C	1.110815	1.607987	0.000000
C	1.139976	0.200295	0.000000
C	-0.091951	-0.520069	0.000000
C	-1.312503	0.191433	0.000000
C	-1.325545	1.579430	0.000000
C	-0.104995	2.281456	0.000000
O	2.339350	-0.413767	0.000000
C	-0.040690	-1.981872	0.000000
O	-1.250606	-2.602696	0.000000
O	1.009351	-2.643953	0.000000
H	-2.245144	-0.373926	0.000000
H	2.061086	2.144001	0.000000
H	-2.272378	2.121176	0.000000
H	-0.108845	3.373968	0.000000
H	2.149897	-1.399836	0.000000

H	-1.057816	-3.563628	0.000000

salicylic acid S_1

C	0.996462	1.918583	0.000000
C	0.962728	0.506598	0.000000
C	-0.286253	-0.205877	0.000000
C	-1.444381	0.551644	0.000000
C	-1.413418	2.004888	0.000000
C	-0.212707	2.678118	0.000000
O	2.098171	-0.190389	0.000000
C	-0.227959	-1.674748	0.000000
O	-1.427748	-2.337899	0.000000
O	0.888465	-2.328070	0.000000
H	-2.411583	0.045365	0.000000
H	1.973770	2.404161	0.000000
H	-2.361149	2.545619	0.000000
H	-0.172570	3.767671	0.000000
H	1.751458	-1.259112	0.000000
H	-1.202707	-3.289604	0.000000

o-cresol, *cis* S_0

C	1.975343	0.515940	0.000000
C	0.733206	1.157665	0.000000
C	-0.469713	0.435828	0.000000
C	-0.392889	-0.973500	0.000000
C	0.845267	-1.628252	0.000000
C	2.025454	-0.882801	0.000000
C	-1.811133	1.129704	0.000000
O	-1.520076	-1.767439	0.000000
H	0.861487	-2.719647	0.000000
H	2.987676	-1.399462	0.000000
H	2.895451	1.103082	0.000000
H	0.686991	2.250381	0.000000
H	-2.307989	-1.194395	0.000000
H	-2.412530	0.876132	0.891632
H	-1.684014	2.220641	0.000000
H	-2.412530	0.876132	-0.891632

o-cresol, *cis* S_1

C	1.862687	-0.024492	-0.784016
C	0.627567	0.154466	-1.457803
C	-0.605671	0.120107	-0.710837
C	-0.468708	0.076565	0.716150

C	0.772288	-0.014391	1.405974
C	1.956278	-0.115440	0.624096
C	-1.896980	-0.099905	-1.430928
O	-1.575445	0.104681	1.521541
H	0.787303	0.098013	2.489871
H	2.928264	-0.235857	1.102469
H	2.777756	-0.099241	-1.378078
H	0.599736	0.237489	-2.544681
H	-2.360265	0.276184	0.951974
H	-2.780822	-0.202048	-0.775687
H	-2.118054	0.726616	-2.132402
H	-1.856514	-1.022238	-2.055234

o-cresol, *trans* S_0

C	2.425523	0.000022	0.029247
C	1.244809	-0.000031	-0.724862
C	0.021988	-0.000002	-0.021561
C	-0.007166	0.000061	1.378894
C	1.188590	0.000113	2.104556
C	2.411814	0.000088	1.429769
C	1.253404	-0.000114	-2.231584
O	-1.130378	-0.000052	-0.781061
H	-0.969324	0.000086	1.901786
H	1.157215	0.000158	3.196146
H	3.350418	0.000136	1.986979
H	3.381424	0.000003	-0.502025
H	-1.897272	-0.000048	-0.180581
H	2.283267	-0.000072	-2.614672
H	0.732255	-0.882631	-2.635478
H	0.732139	0.882282	-2.635583

o-cresol, *trans* S_1

C	2.427985	0.281573	-0.002517
C	1.206011	0.139252	-0.763407
C	0.005188	-0.000124	-0.015160
C	-0.058852	-0.105939	1.415168
C	1.181125	-0.093200	2.111301
C	2.391971	0.091191	1.395386
C	1.255960	-0.026309	-2.244764
O	-1.163568	-0.102310	-0.725951
H	-1.005375	0.076933	1.934831
H	1.203911	-0.183076	3.198095
H	3.330905	0.099945	1.956097
H	3.372240	0.447446	-0.521106

H	-1.853916	-0.418602	-0.100366
H	1.838398	-0.928442	-2.529872
H	0.259377	-0.103650	-2.696382
H	1.787331	0.825312	-2.711373

m-cresol, *cis* S_0

C	1.159709	-0.005281	2.099258
C	2.378039	0.008493	1.420544
C	2.422807	0.019291	0.020407
C	1.235711	0.014417	-0.726935
C	0.008981	0.002515	-0.041973
C	-0.030912	-0.007876	1.358350
C	1.263137	0.002010	-2.237924
O	-1.213939	-0.018132	2.064373
H	1.110476	-0.011093	3.189146
H	3.308757	0.013946	1.992509
H	3.385736	0.032730	-0.495435
H	-0.928456	0.002710	-0.610032
H	-1.954276	-0.018335	1.431365
H	2.266718	0.237237	-2.619281
H	0.981076	-0.987949	-2.633167
H	0.558737	0.734687	-2.661256

m-cresol, *cis* S_1

C	1.162168	0.013115	2.141002
C	2.412701	0.087388	1.451483
C	2.412231	0.043524	0.037249
C	1.223309	-0.010646	-0.751226
C	-0.040941	0.013525	-0.067807
C	-0.017019	0.009399	1.360071
C	1.266313	-0.047885	-2.242973
O	-1.201833	-0.042066	2.050118
H	1.092675	-0.143679	3.217762
H	3.351169	0.125946	2.002725
H	3.371418	0.067135	-0.489188
H	-0.956737	0.297196	-0.600787
H	-1.915277	-0.217661	1.398167
H	2.293353	0.038936	-2.625263
H	0.833727	-0.986925	-2.644328
H	0.665023	0.772069	-2.687064

m-cresol, *trans* S_0

C	-1.196757	-1.102431	0.000000

C	0.203770	-1.215989	0.000000
C	0.978794	-0.046946	0.000000
C	0.368496	1.212763	0.000000
C	-1.030623	1.321015	0.000000
C	-1.803914	0.157477	0.000000
C	0.875773	-2.570029	0.000000
O	1.196931	2.314087	0.000000
H	-1.508134	2.305735	0.000000
H	-2.893359	0.237535	0.000000
H	-1.812636	-2.004692	0.000000
H	2.070184	-0.099053	0.000000
H	0.645793	3.117042	0.000000
H	0.135757	-3.382433	0.000000
H	1.517506	-2.697779	-0.886316
H	1.517506	-2.697779	0.886316

m-cresol, *trans* S_1

C	-1.207069	-1.059183	0.000000
C	0.205306	-1.245611	0.000000
C	1.035124	-0.068629	0.000000
C	0.395963	1.198264	0.000000
C	-1.013965	1.386954	0.000000
C	-1.833440	0.215339	0.000000
C	0.827644	-2.602530	0.000000
O	1.232758	2.287297	0.000000
H	-1.441076	2.392721	0.000000
H	-2.919690	0.294592	0.000000
H	-1.842105	-1.950052	0.000000
H	2.123473	-0.122140	0.000000
H	0.682498	3.097475	0.000000
H	0.068803	-3.398208	0.000000
H	1.481128	-2.755636	-0.883431
H	1.481128	-2.755636	0.883431

p-cresol S_0

C	0.712530	0.008458	-1.197831
C	-0.682364	0.010982	-1.207207
C	-1.385613	0.000723	0.005496
C	-0.678518	-0.014765	1.214514
C	0.720881	-0.017126	1.203734
C	1.445277	-0.003676	0.003072
O	-2.762808	0.001193	-0.057291
C	2.956387	0.021973	-0.004336
H	-1.218516	-0.028629	2.166757

H	1.257666	-0.032079	2.156318
H	1.246936	0.013828	-2.152063
H	-1.241474	0.017366	-2.144585
H	-3.114866	-0.008452	0.850655
H	3.368406	-0.657140	-0.766560
H	3.341552	1.031514	-0.226210
H	3.366083	-0.278794	0.970838

p-cresol S_1

C	0.735912	-0.095589	-1.241099
C	-0.693564	-0.040969	-1.252064
C	-1.358902	-0.017108	-0.003740
C	-0.695530	-0.002134	1.256124
C	0.732813	-0.004752	1.242780
C	1.434511	-0.032916	0.001413
O	-2.729791	0.013177	-0.049574
C	2.926815	0.042856	-0.000237
H	-1.260248	-0.138962	2.181982
H	1.295096	0.008083	2.177153
H	1.296936	-0.125755	-2.175313
H	-1.270862	0.069256	-2.169744
H	-3.058880	0.147408	0.864137
H	3.356509	-0.507125	-0.853040
H	3.263570	1.094080	-0.099754
H	3.357165	-0.344170	0.936267

o-methoxyphenol S_0

C	2.043074	-0.089256	0.000000
C	0.881933	0.701181	0.000000
C	-0.370325	0.084892	0.000000
C	-0.471717	-1.326321	0.000000
C	0.686731	-2.101612	0.000000
C	1.943955	-1.481703	0.000000
O	-1.596141	0.724625	0.000000
O	-1.704445	-1.925565	0.000000
H	0.587431	-3.188571	0.000000
H	2.845933	-2.096494	0.000000
H	3.020782	0.395705	0.000000
H	0.964042	1.788873	0.000000
C	-1.600320	2.154667	0.000000
H	-2.365428	-1.203533	0.000000
H	-2.655381	2.452805	0.000000
H	-1.105062	2.555152	0.900847
H	-1.105062	2.555152	-0.900847

o-methoxyphenol S_1

C	2.486573	0.008773	0.043460
C	1.385618	-0.396760	-0.745577
C	0.108827	-0.388116	-0.084668
C	0.015096	-0.165226	1.318233
C	1.176184	0.026249	2.132635
C	2.387156	0.219904	1.440790
O	-1.101448	-0.276832	-0.749564
O	-1.204987	0.088519	1.878620
H	1.116361	-0.056670	3.219236
H	3.285413	0.514960	1.990873
H	3.463679	0.140028	-0.433891
H	1.535105	-0.860005	-1.725401
C	-1.092923	0.203129	-2.130170
H	-1.871305	-0.002923	1.153016
H	-2.148845	0.235695	-2.421013
H	-0.639718	1.203289	-2.191671
H	-0.542226	-0.494021	-2.776829

m-methoxyphenol, isomer 1 S_0

C	0.935618	1.457561	0.000000
C	-0.262351	0.723164	0.000000
C	-0.232040	-0.680477	0.000000
C	1.008068	-1.342475	0.000000
C	2.206725	-0.622422	0.000000
C	2.151603	0.775643	0.000000
H	-1.154794	-1.264864	0.000000
O	1.093836	-2.717612	0.000000
H	3.155438	-1.159702	0.000000
H	3.083147	1.345842	0.000000
H	0.887638	2.546928	0.000000
O	-1.418341	1.464457	0.000000
H	0.193293	-3.088452	0.000000
C	-2.661682	0.761561	0.000000
H	-3.439853	1.534070	0.000000
H	-2.773153	0.133388	-0.901266
H	-2.773153	0.133388	0.901266

m-methoxyphenol, isomer 1 S_1

C	1.172234	-0.023551	-0.628328
C	-0.025441	-0.048161	0.130176
C	-0.054213	-0.089513	1.560044

C	1.245264	0.000377	2.155945
C	2.458574	0.008869	1.420472
C	2.444583	-0.089334	0.008248
H	-0.866890	-0.602305	2.098053
O	1.352736	0.181988	3.514698
H	3.392171	0.129793	1.974958
H	3.365239	-0.142327	-0.569031
H	1.083210	0.069315	-1.712799
O	-1.167954	0.050071	-0.632018
H	0.464382	0.455819	3.837926
C	-2.443284	0.028396	0.025686
H	-3.161162	0.437753	-0.694988
H	-2.727100	-1.008353	0.274168
H	-2.424041	0.641164	0.939531

m-methoxyphenol, isomer 2 S_0

C	0.350334	2.173580	0.000000
C	-0.842867	1.457304	0.000000
C	-0.800017	0.049706	0.000000
C	0.428308	-0.623639	0.000000
C	1.617761	0.121687	0.000000
C	1.591032	1.520923	0.000000
O	-2.018307	-0.580947	0.000000
C	-2.027468	-2.011036	0.000000
O	2.791782	-0.600282	0.000000
H	0.498630	-1.710545	0.000000
H	2.522334	2.094107	0.000000
H	0.320695	3.265342	0.000000
H	-1.811955	1.957139	0.000000
H	-3.085103	-2.300323	0.000000
H	-1.536657	-2.419282	-0.900355
H	-1.536657	-2.419282	0.900355
H	3.538145	0.025556	0.000000

m-methoxyphenol, isomer 2 S_1

C	1.244598	-0.078145	-0.720224
C	0.047721	-0.040239	0.066272
C	0.111435	-0.054314	1.481084
C	1.338637	-0.022433	2.211043
C	2.512712	0.026202	1.399539
C	2.478829	0.038540	-0.016782
O	-1.119848	-0.031258	2.099653
C	-1.172272	0.033576	3.530653
O	3.705992	0.100695	2.084751

H	1.422919	-0.290464	3.263875
H	3.418945	0.148666	-0.568013
H	1.209221	-0.072991	-1.806694
H	-0.936446	0.024819	-0.400609
H	-2.223918	0.214311	3.781309
H	-0.847370	-0.921728	3.975779
H	-0.542070	0.851173	3.913346
H	4.436047	0.073591	1.436918

p-methoxyphenol, *cis* S_0

C	-0.320710	0.736713	0.000000
C	-1.560547	0.072247	0.000000
C	-1.619873	-1.317105	0.000000
C	-0.436788	-2.073816	0.000000
C	0.797194	-1.418101	0.000000
C	0.861048	-0.015954	0.000000
O	-0.562918	-3.449465	0.000000
O	-0.377773	2.113402	0.000000
C	0.862157	2.819626	0.000000
H	1.838101	0.467313	0.000000
H	-2.474276	0.669180	0.000000
H	-2.580598	-1.834745	0.000000
H	1.726816	-1.995892	0.000000
H	0.599610	3.884422	0.000000
H	1.460411	2.592518	0.900474
H	1.460411	2.592518	-0.900474
H	0.327734	-3.842841	0.000000

p-methoxyphenol, *cis* S_1

C	1.325430	-0.031152	-0.609225
C	0.041116	-0.047853	-0.000334
C	-0.027165	-0.005861	1.426431
C	1.184183	-0.006863	2.148210
C	2.470533	-0.012276	1.542927
C	2.540771	-0.020876	0.114180
O	1.080813	0.009665	3.515767
O	1.281219	-0.042438	-1.982554
C	2.500486	0.033093	-2.734457
H	3.506079	-0.028925	-0.387558
H	-0.847747	-0.051434	-0.627845
H	-0.971325	0.094531	1.959739
H	3.365608	-0.173107	2.148898
H	2.199362	0.003576	-3.787387
H	3.032915	0.972066	-2.517714

H	3.151713	-0.824907	-2.505439
H	1.979539	0.132744	3.883362

p-methoxyphenol, *trans* S_0

C	-0.662984	1.314440	0.000000
C	-1.901717	0.675185	0.000000
C	-1.975928	-0.726978	0.000000
C	-0.796299	-1.476293	0.000000
C	0.449790	-0.837913	0.000000
C	0.523530	0.563899	0.000000
O	-3.174320	-1.414640	0.000000
H	1.353459	-1.447760	0.000000
O	1.694476	1.290542	0.000000
H	-0.596758	2.403777	0.000000
H	-2.818060	1.273916	0.000000
H	-3.902546	-0.768496	0.000000
H	-0.859205	-2.565799	0.000000
C	2.919095	0.557258	0.000000
H	3.717251	1.309382	0.000000
H	3.015103	-0.075269	0.900356
H	3.015103	-0.075269	-0.900356

p-methoxyphenol, *trans* S_1

C	0.123524	-0.019430	-1.401273
C	-1.295399	-0.018280	-1.222791
C	-1.793320	0.014796	0.105194
C	-0.974858	0.058908	1.255619
C	0.444439	0.038228	1.079718
C	0.945772	0.010349	-0.242084
O	-3.145866	0.017938	0.333295
H	1.103511	0.064562	1.944410
O	2.289783	0.001517	-0.529104
H	0.589022	-0.046560	-2.384594
H	-1.972135	-0.184635	-2.064260
H	-3.597170	0.082093	-0.532280
H	-1.432735	0.168949	2.237421
C	3.243720	-0.030546	0.541779
H	4.227626	-0.025178	0.060014
H	3.134448	0.855772	1.186037
H	3.120427	-0.944173	1.143600

1-naphthol, *cis* S_0

C	0.836377	1.526706	0.017846

C	0.533412	0.125746	0.006488
C	-0.853546	-0.269358	-0.010806
C	-1.869081	0.724769	-0.016167
C	-1.529634	2.064344	-0.004852
C	-0.177585	2.470860	0.012188
C	1.531331	-0.887676	0.011439
C	1.193311	-2.227885	0.000126
C	-0.168168	-2.617168	-0.016794
C	-1.162307	-1.658843	-0.022078
O	2.128900	1.993000	0.034587
H	-2.214167	-1.956453	-0.035167
H	-0.427768	-3.677899	-0.025653
H	1.976919	-2.988144	0.004208
H	2.595529	-0.627937	0.024320
H	-2.915769	0.413050	-0.029306
H	-2.310742	2.827624	-0.008994
H	0.090630	3.528534	0.021177
H	2.742369	1.236740	0.037434

1-naphthol, *cis* S_1

C	0.859861	1.481730	0.015066
C	0.529611	0.086792	-0.073572
C	-0.842836	-0.245448	-0.006985
C	-1.799905	0.825712	-0.023722
C	-1.443544	2.189371	-0.029884
C	-0.099162	2.533957	-0.018973
C	1.542596	-0.930647	-0.120938
C	1.117539	-2.295755	-0.029565
C	-0.228088	-2.621893	0.058427
C	-1.240817	-1.623856	0.047290
O	2.144604	1.850289	0.171406
H	-2.297060	-1.885487	0.102656
H	-0.518338	-3.672827	0.133004
H	1.867312	-3.089840	-0.037313
H	2.570589	-0.708574	-0.421763
H	-2.860064	0.558222	-0.038013
H	-2.215607	2.958923	-0.056382
H	0.249915	3.566445	0.012446
H	2.663395	1.022878	0.316795

1-naphthol, *trans* S_0

C	-0.721390	-0.544613	0.000000
C	-0.677830	-1.967010	0.000000
C	0.526200	-2.644609	0.000000

C	1.748778	-1.928940	0.000000
C	1.748879	-0.546390	0.000000
C	0.524630	0.174605	0.000000
H	-1.622109	-2.517894	0.000000
H	0.538869	-3.736919	0.000000
H	2.695251	-2.473965	0.000000
H	2.686767	0.010350	0.000000
C	-1.950004	0.174544	0.000000
C	-1.947421	1.554834	0.000000
C	-0.730203	2.277506	0.000000
C	0.480801	1.604404	0.000000
H	-2.890427	-0.381195	0.000000
H	-2.889841	2.106747	0.000000
H	-0.746778	3.371896	0.000000
O	1.694183	2.253127	0.000000
H	1.531656	3.213512	0.000000

1-naphthol, *trans* S_1

C	-0.930155	-0.393383	0.000000
C	-1.324727	-1.766630	0.000000
C	-0.318967	-2.781227	0.000000
C	1.025754	-2.445765	0.000000
C	1.451522	-1.082461	0.000000
C	0.455973	-0.056270	0.000000
H	-2.384100	-2.024594	0.000000
H	-0.617867	-3.831776	0.000000
H	1.781597	-3.234744	0.000000
H	2.508142	-0.824087	0.000000
C	-1.892064	0.665361	0.000000
C	-1.542411	2.036506	0.000000
C	-0.201195	2.381965	0.000000
C	0.776436	1.338169	0.000000
H	-2.951232	0.393453	0.000000
H	-2.318657	2.802371	0.000000
H	0.124351	3.426467	0.000000
O	2.094433	1.661227	0.000000
H	2.187489	2.634490	0.000000

2-naphthol, *cis* S_0

C	0.602132	2.019601	0.000000
C	0.627600	0.598914	0.000000
C	-0.617493	-0.123897	0.000000
C	-1.833355	0.616100	0.000000
C	-1.822458	1.998243	0.000000

C	-0.596158	2.708916	0.000000
C	1.842898	-0.143283	0.000000
C	1.842947	-1.520800	0.000000
C	0.611263	-2.228690	0.000000
C	-0.592959	-1.545320	0.000000
H	-1.541190	-2.093479	0.000000
H	1.552092	2.561172	0.000000
H	-0.602344	3.800890	0.000000
H	-2.765404	2.549783	0.000000
H	-2.782039	0.072405	0.000000
H	2.791637	0.399820	0.000000
H	2.772622	-2.092380	0.000000
O	0.704749	-3.601373	0.000000
H	-0.194550	-3.976612	0.000000

2-naphthol, *cis* S_1

C	0.602628	2.008413	0.000000
C	0.640231	0.585782	0.000000
C	-0.625023	-0.114368	0.000000
C	-1.843128	0.609429	0.000000
C	-1.848481	2.033622	0.000000
C	-0.632602	2.711517	0.000000
C	1.855712	-0.155447	0.000000
C	1.899188	-1.568081	0.000000
C	0.663622	-2.233078	0.000000
C	-0.578573	-1.536124	0.000000
H	-1.512317	-2.110055	0.000000
H	1.541908	2.565879	0.000000
H	-0.616607	3.804135	0.000000
H	-2.792634	2.579312	0.000000
H	-2.786769	0.058218	0.000000
H	2.795414	0.402708	0.000000
H	2.830998	-2.129583	0.000000
O	0.665621	-3.597270	0.000000
H	-0.259178	-3.915000	0.000000

2-naphthol, *trans* S_0

C	0.514694	2.021392	0.000000
C	0.545244	0.599838	0.000000
C	-0.697333	-0.129908	0.000000
C	-1.916660	0.607112	0.000000
C	-1.910409	1.988324	0.000000
C	-0.686022	2.704706	0.000000
C	1.761431	-0.136101	0.000000

C	1.760509	-1.516066	0.000000
C	0.531481	-2.229634	0.000000
C	-0.673403	-1.548535	0.000000
H	-1.608191	-2.113053	0.000000
H	1.462381	2.567043	0.000000
H	-0.697231	3.796671	0.000000
H	-2.855187	2.536766	0.000000
H	-2.862394	0.058813	0.000000
H	2.709750	0.407643	0.000000
H	2.705727	-2.068655	0.000000
O	0.500407	-3.606234	0.000000
H	1.415216	-3.940122	0.000000

2-naphthol, *trans* S_1

C	0.514569	2.013151	0.000000
C	0.553178	0.590361	0.000000
C	-0.708647	-0.114882	0.000000
C	-1.927698	0.606779	0.000000
C	-1.935019	2.031514	0.000000
C	-0.722276	2.713391	0.000000
C	1.771269	-0.146468	0.000000
C	1.814420	-1.559338	0.000000
C	0.575661	-2.226723	0.000000
C	-0.665030	-1.536941	0.000000
H	-1.583652	-2.127212	0.000000
H	1.452993	2.572145	0.000000
H	-0.709613	3.806049	0.000000
H	-2.880751	2.574761	0.000000
H	-2.869701	0.053385	0.000000
H	2.710038	0.413355	0.000000
H	2.757843	-2.107733	0.000000
O	0.475635	-3.587933	0.000000
H	1.376780	-3.967651	0.000000

5-methoxysalicylic acid S_0

C	2.293537	-0.165828	0.000000
C	1.577297	-1.350334	0.000000
C	0.163186	-1.346481	0.000000
C	-0.517289	-0.133767	0.000000
C	0.204787	1.086945	0.000000
C	1.625975	1.076207	0.000000
O	-0.428880	-2.587227	0.000000
C	-1.857679	-2.627561	0.000000
C	-0.474879	2.380442	0.000000

O	-1.836029	2.319524	0.000000
O	2.371628	2.202656	0.000000
O	0.105917	3.477826	0.000000
H	-2.125640	-3.690641	0.000000
H	-2.276136	-2.144413	-0.900416
H	-2.276136	-2.144413	0.900416
H	-1.604901	-0.088026	0.000000
H	3.384514	-0.167845	0.000000
H	2.092496	-2.312942	0.000000
H	1.720152	2.965184	0.000000
H	-2.141902	3.250696	0.000000

5-methoxysalicylic acid S_1

C	2.184434	-0.137167	0.000000
C	1.747690	-1.468296	0.000000
C	0.360052	-1.694849	0.000000
C	-0.579672	-0.617535	0.000000
C	-0.146087	0.711962	0.000000
C	1.273234	0.939722	0.000000
O	-0.032130	-3.003194	0.000000
C	-1.430646	-3.346815	0.000000
C	-1.046698	1.861210	0.000000
O	-2.397761	1.563894	0.000000
O	1.733827	2.199347	0.000000
O	-0.645758	3.074811	0.000000
H	-1.456661	-4.441491	0.000000
H	-1.928775	-2.960356	-0.901648
H	-1.928775	-2.960356	0.901648
H	-1.651620	-0.814410	0.000000
H	3.248996	0.102602	0.000000
H	2.439406	-2.308966	0.000000
H	0.873930	2.797287	0.000000
H	-2.844932	2.433379	0.000000

m-dimethoxybenzene, *trans* S_0

C	0.000000	-0.135184	0.711983
C	0.000000	-0.135184	-0.711983
C	0.000000	1.082545	-1.398050
C	0.000000	2.299441	-0.695600
C	0.000000	2.299441	0.695600
C	0.000000	1.082545	1.398050
O	0.000000	-1.371152	-1.302558
H	0.000000	1.092312	-2.488169
H	0.000000	3.239239	-1.250886

H	0.000000	3.239239	1.250886
H	0.000000	1.092312	2.488169
O	0.000000	-1.371152	1.302558
C	0.000000	-1.415431	2.730111
H	0.000000	-2.480230	2.991977
H	0.900239	-0.935165	3.152134
H	-0.900239	-0.935165	3.152134
C	0.000000	-1.415431	-2.730111
H	0.000000	-2.480230	-2.991977
H	-0.900239	-0.935165	-3.152134
H	0.900239	-0.935165	-3.152134

m-dimethoxybenzene, *trans* S_1

C	-0.142696	-1.075503	-1.451846
C	-0.375533	0.138575	-0.710118
C	-0.375533	0.138575	0.710118
C	-0.142696	-1.075503	1.451846
C	0.284088	-2.193693	0.706303
C	0.284088	-2.193693	-0.706303
O	-0.397135	1.374908	-1.311289
C	0.049974	1.479080	-2.680343
O	-0.397135	1.374908	1.311289
C	0.049974	1.479080	2.680343
H	-0.464329	-1.188220	2.491967
H	0.573228	-3.110266	1.230892
H	0.573228	-3.110266	-1.230892
H	-0.464329	-1.188220	-2.491967
H	0.011230	2.550094	-2.910401
H	1.075640	1.097387	-2.793486
H	-0.621377	0.930077	-3.358767
H	0.011230	2.550094	2.910401
H	-0.621377	0.930077	3.358767
H	1.075640	1.097387	2.793486

3P-propionic acid, *gauche* S_0

C	-1.040556	0.911483	-1.176587
C	-0.388392	0.669179	0.044961
C	-1.054543	-0.094354	1.018498
C	-2.334918	-0.603833	0.775404
C	-2.971955	-0.357155	-0.445420
C	-2.320232	0.403857	-1.422521
C	1.007418	1.207867	0.291516
C	2.124358	0.281955	-0.229822
C	2.339323	-0.947807	0.630593

O	2.079663	-1.047832	1.815311
O	2.919712	-1.962255	-0.081536
H	1.939710	-0.032074	-1.267757
H	3.088847	0.821110	-0.235008
H	1.161966	1.373087	1.368417
H	1.113832	2.184053	-0.207503
H	-0.557601	-0.291899	1.971070
H	-2.838128	-1.192896	1.545794
H	-3.973178	-0.751260	-0.633297
H	-2.812452	0.608576	-2.376207
H	-0.542750	1.514748	-1.941961
H	3.059887	-2.694570	0.556064

3P-propionic acid, *gauche* S_1

C	-1.275543	1.198949	-1.160431
C	-0.400956	0.581292	-0.205526
C	-0.924573	-0.445729	0.666178
C	-2.252683	-0.794442	0.595752
C	-3.102527	-0.173203	-0.358983
C	-2.600021	0.830971	-1.238518
C	1.011084	1.033806	-0.050270
C	2.152922	-0.000320	-0.270308
C	2.213706	-1.133298	0.770431
O	1.738559	-0.931264	1.965179
O	3.540461	-1.710048	0.632159
H	2.113011	-0.408904	-1.294188
H	3.071037	0.612147	-0.226825
H	1.092589	1.343583	1.009936
H	1.179501	1.921987	-0.676052
H	-0.201162	-0.882738	1.371911
H	-2.661465	-1.553663	1.263764
H	-4.151581	-0.467769	-0.426402
H	-3.269487	1.293389	-1.965062
H	-0.870792	1.965858	-1.822491
H	3.597929	-2.280625	1.419758

3P-propionic acid, *anti* S_0

C	1.471008	-0.449292	0.000000
C	0.547020	0.780187	0.000000
C	2.941487	-0.087266	0.000000
H	1.277305	-1.090371	0.876346
H	1.277305	-1.090371	-0.876346
C	-0.916689	0.390321	0.000000
H	0.775185	1.400213	0.880484

H	0.775185	1.400213	-0.880484
C	-1.609082	0.191046	1.206148
C	-2.951972	-0.200616	1.208958
C	-3.627861	-0.399568	0.000000
C	-2.951972	-0.200616	-1.208958
C	-1.609082	0.191046	-1.206148
H	-1.090826	0.354289	2.155685
H	-3.473769	-0.344805	2.157907
H	-4.677458	-0.701410	0.000000
H	-3.473769	-0.344805	-2.157907
H	-1.090826	0.354289	-2.155685
O	3.728979	-1.209464	0.000000
O	3.407053	1.036460	0.000000
H	4.655617	-0.888159	0.000000

3P-propionic acid, *anti* S_1

C	1.478108	-0.561142	0.000000
C	0.549475	0.689780	0.000000
C	2.898422	-0.047965	0.000000
H	1.237479	-1.190831	0.885145
H	1.237479	-1.190831	-0.885145
C	-0.892084	0.352300	0.000000
H	0.806535	1.289177	0.884935
H	0.806535	1.289177	-0.884935
C	-1.610791	0.173314	1.236435
C	-2.945231	-0.158419	1.237189
C	-3.628885	-0.327718	0.000000
C	-2.945231	-0.158419	-1.237189
C	-1.610791	0.173314	-1.236435
H	-1.063841	0.304750	2.169863
H	-3.487471	-0.295789	2.173327
H	-4.686844	-0.594745	0.000000
H	-3.487471	-0.295789	-2.173327
H	-1.063841	0.304750	-2.169863
O	3.824859	-1.159603	0.000000
O	3.284902	1.191969	0.000000
H	4.681525	-0.695961	0.000000

fluorine S_0

C	0.000000	0.000000	-1.799774
C	0.000000	1.185985	-0.855157
C	0.000000	0.735034	0.487206
C	0.000000	-0.735034	0.487206
C	0.000000	1.656632	1.542545

C	0.000000	3.024524	1.246352
C	0.000000	3.469297	-0.084207
C	0.000000	2.549684	-1.143617
H	0.000000	2.903408	-2.178124
H	0.000000	4.540763	-0.296392
H	0.000000	3.754318	2.059176
H	0.000000	1.318860	2.581746
C	0.000000	-1.656632	1.542545
C	0.000000	-3.024524	1.246352
C	0.000000	-3.469297	-0.084207
C	0.000000	-2.549684	-1.143617
C	0.000000	-1.185985	-0.855157
H	0.000000	-1.318860	2.581746
H	0.000000	-3.754318	2.059176
H	0.000000	-4.540763	-0.296392
H	0.000000	-2.903408	-2.178124
H	-0.885019	0.000000	-2.459631
H	0.885019	0.000000	-2.459631

fluorine S_1

C	0.000000	0.000000	-1.867837
C	0.000000	1.169744	-0.918856
C	0.000000	0.713845	0.444094
C	0.000000	-0.713845	0.444094
C	0.000000	1.618911	1.537773
C	0.000000	2.997499	1.242876
C	0.000000	3.443785	-0.099773
C	0.000000	2.550420	-1.195288
H	0.000000	2.927638	-2.218996
H	0.000000	4.519575	-0.293074
H	0.000000	3.732638	2.049262
H	0.000000	1.255193	2.565755
C	0.000000	-1.618911	1.537773
C	0.000000	-2.997499	1.242876
C	0.000000	-3.443785	-0.099773
C	0.000000	-2.550420	-1.195288
C	0.000000	-1.169744	-0.918856
H	0.000000	-1.255193	2.565755
H	0.000000	-3.732638	2.049262
H	0.000000	-4.519575	-0.293074
H	0.000000	-2.927638	-2.218996
H	-0.883100	0.000000	-2.547694
H	0.883100	0.000000	-2.547694

phenanthrene S_0

C	0.729369	0.000000	-0.353670
C	-0.729369	0.000000	-0.353670
C	-1.426405	0.000000	0.897974
C	-0.682667	0.000000	2.126108
C	0.682667	0.000000	2.126108
C	1.426405	0.000000	0.897974
C	-1.501116	0.000000	-1.542365
C	-2.844260	0.000000	0.908866
H	-1.238085	0.000000	3.067854
H	1.238085	0.000000	3.067854
C	1.501116	0.000000	-1.542365
C	2.887874	0.000000	-1.506018
C	3.568855	0.000000	-0.271171
C	2.844260	0.000000	0.908866
H	1.002857	0.000000	-2.512896
H	3.454232	0.000000	-2.439976
H	4.660711	0.000000	-0.247913
H	3.359448	0.000000	1.873297
C	-3.568855	0.000000	-0.271171
C	-2.887874	0.000000	-1.506018
H	-1.002857	0.000000	-2.512896
H	-3.454232	0.000000	-2.439976
H	-4.660711	0.000000	-0.247913
H	-3.359448	0.000000	1.873297

phenanthrene S_1

C	0.716817	0.000000	-0.376275
C	-0.716817	0.000000	-0.376275
C	-1.441516	0.000000	0.888488
C	-0.702332	0.000000	2.094681
C	0.702332	0.000000	2.094681
C	1.441516	0.000000	0.888488
C	-1.499512	0.000000	-1.574802
C	-2.857430	0.000000	0.891211
H	-1.242833	0.000000	3.044739
H	1.242833	0.000000	3.044739
C	1.499512	0.000000	-1.574802
C	2.902542	0.000000	-1.535197
C	3.592248	0.000000	-0.313329
C	2.857430	0.000000	0.891211
H	1.004956	0.000000	-2.545973
H	3.461193	0.000000	-2.473862
H	4.682950	0.000000	-0.292581
H	3.378297	0.000000	1.851939

C	-3.592248	0.000000	-0.313329
C	-2.902542	0.000000	-1.535197
H	-1.004956	0.000000	-2.545973
H	-3.461193	0.000000	-2.473862
H	-4.682950	0.000000	-0.292581
H	-3.378297	0.000000	1.851939

2,4,6,8-decatetraene S_0

C	-2.601171	-5.034927	0.000000
C	-2.488572	-3.542433	0.000000
C	-1.325475	-2.848691	0.000000
C	-1.225999	-1.410938	0.000000
C	-0.050800	-0.715576	0.000000
C	0.050800	0.715576	0.000000
C	1.225999	1.410938	0.000000
C	1.325475	2.848691	0.000000
C	2.488572	3.542433	0.000000
C	2.601171	5.034927	0.000000
H	-0.380326	-3.407830	0.000000
H	-2.168103	-0.847893	0.000000
H	0.890251	-1.280647	0.000000
H	-0.890251	1.280647	0.000000
H	2.168103	0.847893	0.000000
H	0.380326	3.407830	0.000000
H	3.430549	2.979420	0.000000
H	-3.430549	-2.979420	0.000000
H	1.612224	5.516875	0.000000
H	3.157514	5.395836	0.882858
H	3.157514	5.395836	-0.882858
H	-1.612224	-5.516875	0.000000
H	-3.157514	-5.395836	0.882858
H	-3.157514	-5.395836	-0.882858

2,4,6,8-decatetraene S_1

C	-2.597285	-5.053147	0.000000
C	-2.535838	-3.566384	0.000000
C	-1.362268	-2.832307	0.000000
C	-1.270063	-1.417725	0.000000
C	-0.054632	-0.702091	0.000000
C	0.054632	0.702091	0.000000
C	1.270063	1.417725	0.000000
C	1.362268	2.832307	0.000000
C	2.535838	3.566384	0.000000
C	2.597285	5.053147	0.000000

H	-0.414760	-3.389237	0.000000
H	-2.204039	-0.841669	0.000000
H	0.875442	-1.285252	0.000000
H	-0.875442	1.285252	0.000000
H	2.204039	0.841669	0.000000
H	0.414760	3.389237	0.000000
H	3.490023	3.024549	0.000000
H	-3.490023	-3.024549	0.000000
H	1.592856	5.503178	0.000000
H	3.146284	5.444935	0.880083
H	3.146284	5.444935	-0.880083
H	-1.592856	-5.503178	0.000000
H	-3.146284	-5.444935	0.880083
H	-3.146284	-5.444935	-0.880083

tetracene S_0

C	3.717924	1.412143	0.000000
C	2.456948	0.728329	0.000000
C	2.456948	-0.728329	0.000000
C	3.717924	-1.412143	0.000000
C	4.900754	-0.715477	0.000000
C	4.900754	0.715477	0.000000
C	1.237451	1.410929	0.000000
C	0.000000	0.729086	0.000000
C	0.000000	-0.729086	0.000000
C	1.237451	-1.410929	0.000000
C	-1.237451	1.410929	0.000000
C	-2.456948	0.728329	0.000000
C	-2.456948	-0.728329	0.000000
C	-1.237451	-1.410929	0.000000
C	-3.717924	1.412143	0.000000
C	-4.900754	0.715477	0.000000
C	-4.900754	-0.715477	0.000000
C	-3.717924	-1.412143	0.000000
H	-3.716259	-2.505536	0.000000
H	-5.853071	-1.250374	0.000000
H	-5.853071	1.250374	0.000000
H	-3.716259	2.505536	0.000000
H	-1.237471	-2.505220	0.000000
H	-1.237471	2.505220	0.000000
H	1.237471	-2.505220	0.000000
H	1.237471	2.505220	0.000000
H	3.716259	-2.505536	0.000000
H	5.853071	-1.250374	0.000000
H	5.853071	1.250374	0.000000

H	3.716259	2.505536	0.000000

tetracene S_1

C	3.723567	1.404860	0.000000
C	2.481694	0.724335	0.000000
C	2.481694	-0.724335	0.000000
C	3.723567	-1.404860	0.000000
C	4.936185	-0.701765	0.000000
C	4.936185	0.701765	0.000000
C	1.237928	1.403860	0.000000
C	0.000000	0.726429	0.000000
C	0.000000	-0.726429	0.000000
C	1.237928	-1.403860	0.000000
C	-1.237928	1.403860	0.000000
C	-2.481694	0.724335	0.000000
C	-2.481694	-0.724335	0.000000
C	-1.237928	-1.403860	0.000000
C	-3.723567	1.404860	0.000000
C	-4.936185	0.701765	0.000000
C	-4.936185	-0.701765	0.000000
C	-3.723567	-1.404860	0.000000
H	-3.725670	-2.498055	0.000000
H	-5.881080	-1.248832	0.000000
H	-5.881080	1.248832	0.000000
H	-3.725670	2.498055	0.000000
H	-1.239150	-2.498341	0.000000
H	-1.239150	2.498341	0.000000
H	1.239150	-2.498341	0.000000
H	1.239150	2.498341	0.000000
H	3.725670	-2.498055	0.000000
H	5.881080	-1.248832	0.000000
H	5.881080	1.248832	0.000000
H	3.725670	2.498055	0.000000

perylene S_0

C	0.021956	1.481761	-2.434445
C	0.011903	0.737528	-1.251351
C	0.012741	1.440221	0.000000
C	0.034039	2.881388	0.000000
C	0.043358	3.582016	-1.235351
C	0.037644	2.888932	-2.429853
C	0.043633	3.582010	1.235354
C	0.038180	2.888923	2.429854
C	0.022415	1.481753	2.434445

C	0.012019	0.737525	1.251350
C	-0.011903	-0.737528	-1.251351
C	-0.012741	-1.440221	0.000000
C	-0.012019	-0.737525	1.251350
C	-0.034039	-2.881388	0.000000
C	-0.043633	-3.582010	1.235354
C	-0.038180	-2.888923	2.429854
C	-0.022415	-1.481753	2.434445
C	-0.021956	-1.481761	-2.434445
C	-0.037644	-2.888932	-2.429853
C	-0.043358	-3.582016	-1.235351
H	0.056964	4.674670	1.221679
H	0.046501	3.427793	3.379874
H	0.020100	0.973374	3.399025
H	-0.056964	-4.674670	1.221679
H	-0.046501	-3.427793	3.379874
H	-0.020100	-0.973374	3.399025
H	-0.056673	-4.674676	-1.221675
H	-0.045696	-3.427805	-3.379873
H	-0.019441	-0.973390	-3.399028
H	0.056673	4.674676	-1.221675
H	0.045696	3.427805	-3.379873
H	0.019441	0.973390	-3.399028

perylene S_1

C	-0.006797	1.475809	-2.461927
C	-0.006547	0.723014	-1.248933
C	0.010499	1.430046	0.000002
C	0.008759	2.868081	-0.000002
C	0.009395	3.565038	-1.237625
C	-0.001623	2.868449	-2.447970
C	0.009655	3.565045	1.237613
C	-0.001079	2.868461	2.447967
C	-0.006323	1.475824	2.461932
C	-0.006419	0.723017	1.248942
C	0.006547	-0.723014	-1.248933
C	-0.010499	-1.430046	0.000002
C	0.006419	-0.723017	1.248942
C	-0.008759	-2.868081	-0.000002
C	-0.009655	-3.565045	1.237613
C	0.001079	-2.868461	2.447967
C	0.006323	-1.475824	2.461932
C	0.006797	-1.475809	-2.461927
C	0.001623	-2.868449	-2.447970
C	-0.009395	-3.565038	-1.237625

H	0.014010	4.657751	1.228120
H	-0.004749	3.418325	3.391812
H	-0.028624	0.960490	3.421482
H	-0.014010	-4.657751	1.228120
H	0.004749	-3.418325	3.391812
H	0.028624	-0.960490	3.421482
H	-0.013732	-4.657744	-1.228137
H	0.005578	-3.418305	-3.391819
H	0.029441	-0.960464	-3.421464
H	0.013732	4.657744	-1.228137
H	-0.005578	3.418305	-3.391819
H	-0.029441	0.960464	-3.421464

B3LYP/TZVP geometries – Group I

pyrazine S_0

C	1.131190	-0.696330	0.000000
C	1.131190	0.696330	0.000000
N	0.000000	1.402180	0.000000
C	-1.131190	0.696330	0.000000
C	-1.131190	-0.696330	0.000000
N	0.000000	-1.402180	0.000000
H	-2.062100	-1.253940	0.000000
H	2.062100	-1.253940	0.000000
H	2.062100	1.253940	0.000000
H	-2.062100	1.253940	0.000000

pyrazine S_1

C	-1.210743	0.677974	0.000000
C	-1.115368	-0.746154	0.000000
N	0.020130	-1.350897	0.000000
C	1.210743	-0.677974	0.000000
C	1.115368	0.746154	0.000000
N	-0.020130	1.350897	0.000000
H	2.040304	1.318591	0.000000
H	-2.157658	1.189742	0.000000
H	-2.040304	-1.318591	0.000000
H	2.157658	-1.189742	0.000000

2,6-difluoropyridine S_0

C	1.116540	0.000000	-0.876120
N	0.000000	0.000000	-1.567360

C	-1.116540	0.000000	-0.876120
C	-1.203790	0.000000	0.508170
C	0.000000	0.000000	1.203840
C	1.203790	0.000000	0.508170
F	-2.248090	0.000000	-1.594690
H	-2.164990	0.000000	1.001360
H	0.000000	0.000000	2.286500
H	2.164990	0.000000	1.001360
F	2.248090	0.000000	-1.594690

2,6-difluoropyridine S_1

C	-1.103893	0.000000	-0.336229
N	0.000000	0.000000	-1.100834
C	1.103893	0.000000	-0.336229
C	1.196771	0.000000	1.072742
C	0.000000	0.000000	1.846564
C	-1.196771	0.000000	1.072742
F	2.247435	0.000000	-1.018323
H	2.180417	0.000000	1.522185
H	0.000000	0.000000	2.922810
H	-2.180417	0.000000	1.522185
F	-2.247435	0.000000	-1.018323

2-fluoropyridine S_0

C	-1.315853	0.503722	0.000000
N	-1.366748	-0.802315	0.000000
C	-0.196489	-1.454306	0.000000
C	1.031560	-0.809659	0.000000
C	1.045457	0.584268	0.000000
C	-0.157408	1.272923	0.000000
H	-0.258754	-2.536633	0.000000
H	1.949878	-1.381146	0.000000
H	1.982074	1.127628	0.000000
H	-0.213370	2.352400	0.000000
F	-2.500357	1.143110	0.000000

2-fluoropyridine S_1

C	-1.321412	0.492354	0.000000
N	-1.436379	-0.843123	0.000000
C	-0.222770	-1.469195	0.000000
C	1.032234	-0.795732	0.000000
C	1.108078	0.618532	0.000000
C	-0.153099	1.286990	0.000000

H	-0.249096	-2.551238	0.000000
H	1.932017	-1.397666	0.000000
H	2.044535	1.151359	0.000000
H	-0.250928	2.363071	0.000000
F	-2.483190	1.144640	0.000000

2-hydroxypyridine S_0

C	-0.979745	0.752737	0.000000
C	-0.971189	-0.646252	0.000000
N	0.132525	-1.378349	0.000000
C	1.307882	-0.736636	0.000000
C	1.420295	0.644346	0.000000
C	0.243771	1.397052	0.000000
O	-2.155791	-1.302427	0.000000
H	2.190061	-1.367992	0.000000
H	2.393261	1.117298	0.000000
H	0.285225	2.479714	0.000000
H	-1.918681	1.289069	0.000000
H	-1.947613	-2.248560	0.000000

2-hydroxypyridine S_1

C	-1.003650	0.769010	0.000000
C	-0.968870	-0.634010	0.000000
N	0.117070	-1.450530	0.000000
C	1.299510	-0.773490	0.000000
C	1.394870	0.643760	0.000000
C	0.252200	1.462530	0.000000
O	-2.136490	-1.297400	0.000000
H	2.198250	-1.376730	0.000000
H	2.384980	1.083950	0.000000
H	0.312160	2.538970	0.000000
H	-1.957780	1.276520	0.000000
H	-1.892250	-2.242580	0.000000

2-pyridone S_0

C	-1.248580	0.717660	0.000000
N	-1.136580	-0.688950	0.000000
C	0.033150	-1.386450	0.000000
C	1.224060	-0.732630	0.000000
C	1.206220	0.691100	0.000000
C	0.037050	1.387730	0.000000
H	-2.021220	-1.179140	0.000000
H	-0.054060	-2.464810	0.000000

H	2.151220	-1.286170	0.000000
H	2.147790	1.228840	0.000000
H	0.013300	2.468720	0.000000
O	-2.352350	1.244110	0.000000

2-pyridone S_1

C	-1.367970	0.102400	0.000000
N	-0.732940	-1.119770	0.000000
C	0.634630	-1.256190	0.000000
C	1.420460	-0.075740	0.000000
C	0.832890	1.162830	0.000000
C	-0.616660	1.265490	0.000000
H	-1.348740	-1.922210	0.000000
H	1.036340	-2.256140	0.000000
H	2.497150	-0.184600	0.000000
H	1.436620	2.059480	0.000000
H	-1.132720	2.212420	0.000000
O	-2.659060	0.012020	0.000000

2-methylpyrimidine S_0

C	0.000134	1.965897	0.000000
C	-1.175835	1.226533	0.000000
N	-1.182269	-0.104064	0.000000
C	0.010461	-0.717842	0.000000
N	1.196513	-0.096938	0.000000
C	1.179438	1.236938	0.000000
H	-2.146217	1.713674	0.000000
H	2.146662	1.729909	0.000000
H	-0.004483	3.047398	0.000000
C	0.004978	-2.217575	0.000000
H	1.022884	-2.600221	0.000000
H	-0.526138	-2.591854	0.877751
H	-0.526138	-2.591854	-0.877751

2-methylpyrimidine S_1

C	-0.013510	2.014240	0.000000
C	-1.170020	1.280130	0.000000
N	-1.154980	-0.093600	0.000000
C	0.013780	-0.784090	0.000000
N	1.092080	-0.070360	0.000000
C	1.207090	1.296040	0.000000
H	-2.148980	1.742930	0.000000
H	2.193220	1.728900	0.000000

H	-0.025940	3.096510	0.000000
C	0.012880	-2.272160	0.000000
H	1.030880	-2.657990	0.000000
H	-0.518250	-2.640280	0.881210
H	-0.518250	-2.640280	-0.881210

5-methylpyrimidine S_0

C	0.875259	0.852142	0.000000
C	-0.360891	0.210967	0.000000
C	-0.300073	-1.183018	0.000000
N	0.845885	-1.861596	0.000000
C	1.962118	-1.131811	0.000000
N	2.037392	0.196864	0.000000
H	2.900451	-1.675458	0.000000
H	-1.210932	-1.776272	0.000000
H	0.933628	1.937292	0.000000
C	-1.663399	0.960735	0.000000
H	-1.495038	2.038255	0.000000
H	-2.262200	0.715941	-0.880517
H	-2.262200	0.715941	0.880517

5-methylpyrimidine S_1

C	0.846500	0.858370	0.000000
C	-0.377980	0.242810	0.000000
C	-0.349130	-1.191800	0.000000
N	0.883900	-1.765670	0.000000
C	2.035390	-1.182870	0.000000
N	2.034000	0.172120	0.000000
H	2.962350	-1.737440	0.000000
H	-1.218410	-1.828680	0.000000
H	0.933000	1.939050	0.000000
C	-1.679340	0.982080	0.000000
H	-1.519170	2.060820	0.000000
H	-2.275560	0.725610	-0.881320
H	-2.275560	0.725610	0.881320

7-azaindole S_0

N	-0.634970	1.846100	0.000000
C	-0.676370	0.472580	0.000000
C	0.667750	0.006920	0.000000
C	1.509400	1.166440	0.000000
C	0.683460	2.256530	0.000000
C	0.845260	-1.378550	0.000000

C	-0.291770	-2.174100	0.000000
C	-1.564960	-1.583440	0.000000
N	-1.777710	-0.267220	0.000000
H	-2.452080	-2.208010	0.000000
H	1.835160	-1.820180	0.000000
H	-0.210460	-3.253650	0.000000
H	-1.448720	2.438020	0.000000
H	2.587050	1.192430	0.000000
H	0.928980	3.306130	0.000000

7-azaindole S_1

N	-0.600874	1.877305	0.000000
C	-0.654691	0.442294	0.000000
C	0.647573	-0.011575	0.000000
C	1.494489	1.157693	0.000000
C	0.655160	2.313806	0.000000
C	0.888831	-1.413823	0.000000
C	-0.306364	-2.187238	0.000000
C	-1.555062	-1.598962	0.000000
N	-1.809995	-0.234370	0.000000
H	-2.441145	-2.223042	0.000000
H	1.876195	-1.847621	0.000000
H	-0.249492	-3.268751	0.000000
H	-1.434217	2.449421	0.000000
H	2.572812	1.186955	0.000000
H	0.916789	3.357928	0.000000

7-hydroxyquinoline, *cis* S_0

N	0.463212	1.972567	0.000000
C	0.435680	0.610714	0.000000
C	-0.788385	-0.125810	0.000000
C	-1.993589	0.607913	0.000000
C	-1.947687	1.978618	0.000000
C	-0.685515	2.611187	0.000000
C	1.664141	-0.089125	0.000000
C	1.677260	-1.462936	0.000000
C	0.467731	-2.199223	0.000000
C	-0.731647	-1.542420	0.000000
H	-0.629875	3.696176	0.000000
H	-1.657675	-2.105932	0.000000
H	0.522076	-3.279986	0.000000
O	2.825296	-2.202769	0.000000
H	2.579248	0.492010	0.000000
H	-2.940507	0.079394	0.000000

H	-2.850440	2.575490	0.000000
H	3.590677	-1.615858	0.000000

7-hydroxyquinoline, *cis* S_1

N	0.493129	1.973576	0.000000
C	0.424420	0.632217	0.000000
C	-0.787155	-0.132513	0.000000
C	-2.008391	0.599837	0.000000
C	-1.928527	2.003748	0.000000
C	-0.698486	2.643401	0.000000
C	1.638730	-0.096813	0.000000
C	1.661854	-1.523983	0.000000
C	0.487107	-2.268646	0.000000
C	-0.711881	-1.550243	0.000000
H	-0.633518	3.723955	0.000000
H	-1.645161	-2.102975	0.000000
H	0.519372	-3.347391	0.000000
O	2.843084	-2.168678	0.000000
H	2.567698	0.464288	0.000000
H	-2.961138	0.088459	0.000000
H	-2.835372	2.596920	0.000000
H	3.574235	-1.535151	0.000000

7-hydroxyquinoline, *trans* S_0

N	0.513612	2.044862	0.000000
C	0.483463	0.681009	0.000000
C	-0.746073	-0.049464	0.000000
C	-1.949929	0.689066	0.000000
C	-1.898376	2.058175	0.000000
C	-0.631762	2.686080	0.000000
C	1.708642	-0.018818	0.000000
C	1.717999	-1.392709	0.000000
C	0.504371	-2.122427	0.000000
C	-0.696620	-1.463138	0.000000
H	-0.573027	3.771046	0.000000
H	-1.623580	-2.025042	0.000000
H	0.532433	-3.207328	0.000000
O	2.927117	-2.030529	0.000000
H	2.633591	0.541074	0.000000
H	-2.898796	0.163990	0.000000
H	-2.798330	2.659315	0.000000
H	2.795245	-2.985141	0.000000

7-hydroxyquinoline, *trans* S_1

N	0.374425	1.966977	0.000107
C	0.522214	0.653656	0.000026
C	-0.756709	-0.066200	0.000014
C	-1.950595	0.714155	-0.000011
C	-1.920914	2.105646	0.000010
C	-0.697727	2.764388	0.000020
C	1.739091	-0.035915	-0.000019
C	1.726812	-1.433810	-0.000021
C	0.537859	-2.149485	0.000000
C	-0.684800	-1.458839	0.000018
H	-0.556966	3.834453	-0.000004
H	-1.614337	-2.015066	0.000048
H	0.550250	-3.233088	0.000016
O	2.950816	-2.043061	-0.000045
H	2.676084	0.499874	-0.000031
H	-2.901380	0.197142	-0.000072
H	-2.825321	2.698768	-0.000022
H	2.831198	-2.999613	-0.000034

2-hydroxyquinoline, enol S_0

C	0.432526	1.905024	0.000000
C	0.487973	0.492120	0.000000
C	-0.724642	-0.259177	0.000000
C	-1.955863	0.436940	0.000000
C	-1.977975	1.810115	0.000000
C	-0.777659	2.553229	0.000000
C	1.699019	-0.242477	0.000000
C	1.666814	-1.607096	0.000000
C	0.396947	-2.251909	0.000000
N	-0.739995	-1.621145	0.000000
O	0.315142	-3.610786	0.000000
H	1.359345	2.467868	0.000000
H	-0.816333	3.635372	0.000000
H	-2.926793	2.332878	0.000000
H	-2.866754	-0.147319	0.000000
H	2.645736	0.285706	0.000000
H	2.581258	-2.189230	0.000000
H	1.201253	-3.990112	0.000000

2-hydroxyquinoline, enol S_1

C	0.425898	1.880509	0.000000
C	0.521875	0.485994	0.000000
C	-0.710898	-0.259207	0.000000

C	-1.949244	0.444793	0.000000
C	-2.011955	1.851312	0.000000
C	-0.829088	2.561884	0.000000
C	1.742155	-0.232709	0.000000
C	1.696365	-1.646695	0.000000
C	0.437175	-2.248627	0.000000
N	-0.748406	-1.610408	0.000000
O	0.292665	-3.591098	0.000000
H	1.335464	2.470679	0.000000
H	-0.833793	3.644580	0.000000
H	-2.967980	2.356199	0.000000
H	-2.851007	-0.154336	0.000000
H	2.685581	0.295425	0.000000
H	2.599767	-2.242334	0.000000
H	1.165416	-4.005941	0.000000

2-hydroxyquinoline, keto S_0

N	0.559580	1.707510	0.000000
C	0.604000	0.328810	0.000000
C	-0.616210	-0.383390	0.000000
C	-1.837040	0.377280	0.000000
C	-1.835800	1.727350	0.000000
C	-0.592950	2.494530	0.000000
C	1.821660	-0.364500	0.000000
C	1.824330	-1.747780	0.000000
C	0.622780	-2.467180	0.000000
C	-0.580280	-1.786970	0.000000
H	-1.517450	-2.331920	0.000000
H	0.638610	-3.549490	0.000000
H	2.769320	-2.277440	0.000000
H	2.754700	0.187770	0.000000
H	-2.776740	-0.165420	0.000000
H	-2.748940	2.306590	0.000000
O	-0.515180	3.714290	0.000000
H	1.425630	2.229980	0.000000

2-hydroxyquinoline, keto S_1

N	0.557295	1.679745	0.000000
C	0.606723	0.320103	0.000000
C	-0.666018	-0.381303	0.000000
C	-1.862653	0.366466	0.000000
C	-1.860503	1.772967	0.000000
C	-0.631591	2.473534	0.000000
C	1.834263	-0.363953	0.000000

C	1.860816	-1.758543	0.000000
C	0.642773	-2.453594	0.000000
C	-0.588512	-1.786036	0.000000
H	-1.506730	-2.359696	0.000000
H	0.649298	-3.536814	0.000000
H	2.801075	-2.290980	0.000000
H	2.755285	0.207812	0.000000
H	-2.802533	-0.170102	0.000000
H	-2.767479	2.356084	0.000000
O	-0.430746	3.695973	0.000000
H	1.409238	2.228347	0.000000

dibenzofuran S_0

C	1.721087	0.000000	-1.358801
C	0.724932	0.000000	-0.381673
C	1.099164	0.000000	0.971297
C	2.415730	0.000000	1.395052
C	3.392158	0.000000	0.403408
C	3.050334	0.000000	-0.954816
C	-0.724932	0.000000	-0.381673
C	-1.099164	0.000000	0.971297
O	0.000000	0.000000	1.799541
C	-1.721087	0.000000	-1.358801
C	-3.050334	0.000000	-0.954816
C	-3.392158	0.000000	0.403408
C	-2.415730	0.000000	1.395052
H	-2.666382	0.000000	2.447340
H	-4.436524	0.000000	0.689334
H	-3.836321	0.000000	-1.699443
H	-1.465889	0.000000	-2.411303
H	1.465889	0.000000	-2.411303
H	3.836321	0.000000	-1.699443
H	4.436524	0.000000	0.689334
H	2.666382	0.000000	2.447340

dibenzofuran S_1

C	0.000000	1.735158	-1.532005
C	0.000000	0.712569	-0.568164
C	0.000000	1.108004	0.801527
C	0.000000	2.412280	1.256919
C	0.000000	3.427404	0.264658
C	0.000000	3.079716	-1.086254
C	0.000000	-0.712569	-0.568164
C	0.000000	-1.108004	0.801527

O	0.000000	0.000000	1.607013
C	0.000000	-1.735158	-1.532005
C	0.000000	-3.079716	-1.086254
C	0.000000	-3.427404	0.264658
C	0.000000	-2.412280	1.256919
H	0.000000	-2.637285	2.314292
H	0.000000	-4.467151	0.559150
H	0.000000	-3.867781	-1.829560
H	0.000000	-1.513015	-2.590358
H	0.000000	1.513015	-2.590358
H	0.000000	3.867781	-1.829560
H	0.000000	4.467151	0.559150
H	0.000000	2.637285	2.314292

pyrrolo[3,2-*h*]quinoline S_0

C	0.132211	-0.688029	0.000000
N	0.062551	-2.040871	0.000000
C	1.198020	-2.711778	0.000000
C	2.466188	-2.101586	0.000000
C	2.542608	-0.727647	0.000000
C	1.361267	0.039596	0.000000
H	1.117684	-3.794682	0.000000
H	3.358540	-2.714137	0.000000
H	3.504025	-0.226030	0.000000
C	-1.054331	0.080678	0.000000
C	-1.058746	1.485548	0.000000
C	0.180699	2.177830	0.000000
C	1.350860	1.469633	0.000000
H	0.196617	3.261126	0.000000
H	2.302376	1.988556	0.000000
C	-2.429528	1.891669	0.000000
C	-3.187236	0.747945	0.000000
N	-2.353214	-0.346638	0.000000
H	-2.623502	-1.316099	0.000000
H	-2.809512	2.900198	0.000000
H	-4.257565	0.624720	0.000000

pyrrolo[3,2-*h*]quinoline S_1

C	0.154831	-0.699743	0.000000
N	0.011790	-2.040886	0.000000
C	1.203468	-2.734803	0.000000
C	2.443980	-2.135667	0.000000
C	2.574115	-0.728896	0.000000
C	1.357422	0.021956	0.000000

H	1.113310	-3.814359	0.000000
H	3.328742	-2.761299	0.000000
H	3.537815	-0.241030	0.000000
C	-1.029763	0.102235	0.000000
C	-1.067059	1.551347	0.000000
C	0.143268	2.230976	0.000000
C	1.314790	1.459779	0.000000
H	0.194319	3.310977	0.000000
H	2.266938	1.979280	0.000000
C	-2.459716	1.911279	0.000000
C	-3.175518	0.755088	0.000000
N	-2.290400	-0.340180	0.000000
H	-2.513596	-1.325699	0.000000
H	-2.868637	2.907739	0.000000
H	-4.240110	0.591910	0.000000

carbazole S_0

C	1.131414	0.000000	-0.899123
N	0.000000	0.000000	-1.697447
C	-1.131414	0.000000	-0.899123
C	-0.723937	0.000000	0.457912
C	0.723937	0.000000	0.457912
C	-1.694804	0.000000	1.460909
C	-3.036212	0.000000	1.104934
C	-3.419430	0.000000	-0.243509
C	-2.475717	0.000000	-1.262040
C	2.475717	0.000000	-1.262040
C	3.419430	0.000000	-0.243509
C	3.036212	0.000000	1.104934
C	1.694804	0.000000	1.460909
H	-2.779047	0.000000	-2.302156
H	-4.472335	0.000000	-0.497445
H	-3.797580	0.000000	1.874708
H	-1.406314	0.000000	2.505214
H	1.406314	0.000000	2.505214
H	3.797580	0.000000	1.874708
H	4.472335	0.000000	-0.497445
H	2.779047	0.000000	-2.302156
H	0.000000	0.000000	-2.702320

carbazole S_1

C	1.144511	0.000000	-0.836430
N	0.000000	0.000000	-1.613816
C	-1.144511	0.000000	-0.836430

C	-0.716813	0.000000	0.528938
C	0.716813	0.000000	0.528938
C	-1.708787	0.000000	1.521762
C	-3.064785	0.000000	1.119765
C	-3.454684	0.000000	-0.216484
C	-2.469182	0.000000	-1.239805
C	2.469182	0.000000	-1.239805
C	3.454684	0.000000	-0.216484
C	3.064785	0.000000	1.119765
C	1.708787	0.000000	1.521762
H	-2.744040	0.000000	-2.287029
H	-4.503396	0.000000	-0.478114
H	-3.829729	0.000000	1.887404
H	-1.452596	0.000000	2.572406
H	1.452596	0.000000	2.572406
H	3.829729	0.000000	1.887404
H	4.503396	0.000000	-0.478114
H	2.744040	0.000000	-2.287029
H	0.000000	0.000000	-2.623638

tryptamine, A-ph S_0

C	-2.127843	0.129408	0.886846
N	-1.251512	0.122161	1.956721
C	0.038582	0.045009	1.481507
C	-0.040221	-0.003149	0.065371
C	-1.436296	0.052848	-0.291117
C	1.255996	0.018232	2.161125
C	2.412852	-0.056469	1.402100
C	2.360381	-0.100798	-0.002278
C	1.149583	-0.074634	-0.673489
C	-2.013016	0.004943	-1.673152
C	-2.008473	-1.399678	-2.292335
N	-2.507253	-1.353384	-3.670296
H	1.299691	0.055574	3.243353
H	3.374756	-0.078942	1.899336
H	3.284578	-0.155009	-0.564358
H	1.124185	-0.105641	-1.756242
H	-1.515234	0.190573	2.923637
H	-3.191417	0.195273	1.053540
H	-1.459437	0.670660	-2.341463
H	-3.042905	0.376815	-1.651116
H	-2.576453	-2.074845	-1.635382
H	-0.983752	-1.776649	-2.319848
H	-3.489584	-1.100443	-3.688689
H	-2.424619	-2.259475	-4.116401

tryptamine, A-ph S_1

C	-2.182810	0.168181	0.922039
N	-1.294304	0.137456	1.922572
C	0.036331	0.054503	1.436572
C	-0.039887	0.040993	0.050360
C	-1.442055	0.109966	-0.300173
C	1.233327	-0.025787	2.173605
C	2.415132	-0.112372	1.361093
C	2.369555	-0.124587	-0.016735
C	1.138993	-0.052440	-0.739406
C	-2.026931	0.049791	-1.654068
C	-1.992622	-1.384658	-2.252704
N	-2.513705	-1.369719	-3.615031
H	1.270171	-0.016973	3.252359
H	3.377465	-0.170806	1.855919
H	3.298692	-0.190022	-0.570199
H	1.113519	-0.020181	-1.818440
H	-1.531416	0.187132	2.901964
H	-3.243711	0.255965	1.084317
H	-1.460661	0.688733	-2.336168
H	-3.062296	0.402820	-1.642522
H	-2.532682	-2.059563	-1.575274
H	-0.953844	-1.716238	-2.280258
H	-3.526301	-1.341886	-3.630738
H	-2.217392	-2.187928	-4.131754

tryptamine, A-py S_0

C	-2.120738	0.106325	0.863909
N	-1.254967	0.113781	1.941846
C	0.040205	0.046598	1.479969
C	-0.024171	-0.010720	0.062983
C	-1.417284	0.028579	-0.307069
C	1.250672	0.035602	2.172291
C	2.416375	-0.031990	1.426310
C	2.378867	-0.085193	0.021808
C	1.174725	-0.075396	-0.661718
C	-1.992270	-0.025391	-1.689981
C	-1.964531	-1.425482	-2.317554
N	-2.556982	-1.393417	-3.658928
H	1.282295	0.079507	3.254671
H	3.373134	-0.042097	1.933652
H	3.309311	-0.134738	-0.530309
H	1.162459	-0.116124	-1.744406

H	-1.529009	0.183506	2.905815
H	-3.186529	0.163049	1.018782
H	-1.442629	0.662530	-2.343692
H	-3.027743	0.322592	-1.681155
H	-2.564093	-2.098789	-1.700143
H	-0.935272	-1.810740	-2.297911
H	-1.983971	-0.843258	-4.290098
H	-2.617945	-2.326347	-4.049961

tryptamine, A-py S_1

C	-2.177862	0.121775	0.886729
N	-1.304927	0.103843	1.901648
C	0.034128	0.047134	1.435871
C	-0.020770	0.035980	0.048555
C	-1.417142	0.082983	-0.322853
C	1.221873	-0.012128	2.190159
C	2.416586	-0.076687	1.395355
C	2.392512	-0.086833	0.016773
C	1.172017	-0.033701	-0.724052
C	-1.986471	0.022564	-1.681704
C	-1.899557	-1.406615	-2.295079
N	-2.528594	-1.420042	-3.607533
H	1.242921	-0.001904	3.269322
H	3.372329	-0.119344	1.904441
H	3.331216	-0.135486	-0.522173
H	1.162847	0.000494	-1.803345
H	-1.558477	0.144799	2.877164
H	-3.243008	0.186459	1.031193
H	-1.433822	0.698591	-2.342402
H	-3.034721	0.326692	-1.686692
H	-2.443021	-2.098190	-1.647998
H	-0.846565	-1.713208	-2.291750
H	-1.943740	-0.982894	-4.309943
H	-2.737842	-2.361901	-3.912584

tryptamine, A-up S_0

C	-2.120095	0.121139	0.875951
N	-1.251604	0.100541	1.951468
C	0.042075	0.036473	1.484935
C	-0.025713	0.010959	0.067393
C	-1.419433	0.068185	-0.298422
C	1.254071	0.002734	2.173815
C	2.417354	-0.056121	1.423426
C	2.376284	-0.078877	0.018228

C	1.170735	-0.045873	-0.661954
C	-1.990720	0.031500	-1.683129
C	-1.979496	-1.372615	-2.326567
N	-2.497659	-1.450177	-3.691198
H	1.288658	0.022429	3.256780
H	3.375234	-0.083844	1.927932
H	3.304983	-0.123393	-0.537140
H	1.155928	-0.063985	-1.745220
H	-1.522947	0.147114	2.917610
H	-3.185081	0.179338	1.035994
H	-1.434569	0.716401	-2.333702
H	-3.022378	0.397627	-1.664268
H	-2.563057	-2.053397	-1.701588
H	-0.959635	-1.763878	-2.330130
H	-1.954522	-0.869588	-4.320750
H	-3.457174	-1.124782	-3.736221

tryptamine, A-up S_1

C	-2.173958	0.114759	0.891325
N	-1.295565	0.072478	1.904747
C	0.039676	0.030814	1.436140
C	-0.017669	0.056499	0.048354
C	-1.416070	0.123847	-0.317029
C	1.230240	-0.044297	2.186059
C	2.423249	-0.088588	1.389734
C	2.395781	-0.066021	0.011298
C	1.174869	0.004046	-0.726270
C	-1.974830	0.101536	-1.671123
C	-1.973467	-1.372000	-2.273901
N	-2.477060	-1.468491	-3.617648
H	1.252225	-0.055010	3.265302
H	3.380166	-0.143533	1.895426
H	3.333514	-0.102735	-0.530651
H	1.165969	0.051802	-1.805263
H	-1.546051	0.094846	2.881374
H	-3.237820	0.181379	1.044683
H	-1.372663	0.714986	-2.345513
H	-3.003946	0.469081	-1.688174
H	-2.574228	-2.007401	-1.623145
H	-0.947322	-1.737971	-2.243984
H	-1.929316	-0.956940	-4.297091
H	-3.454504	-1.225165	-3.711429

tryptamine, Ph-out S_0

C	0.013860	0.003439	0.084204
C	0.052172	0.068843	1.502061
C	1.249915	0.087684	2.216436
C	2.429407	0.044623	1.490952
C	2.417255	-0.017565	0.086047
C	1.226961	-0.037974	-0.620978
N	-1.251620	0.109380	1.942006
H	1.261013	0.136494	3.299054
H	3.377270	0.058837	2.014838
H	3.358335	-0.049278	-0.449229
H	1.228250	-0.100602	-1.701875
C	-1.374712	0.011906	-0.309925
C	-2.098786	0.082218	0.850249
H	-1.542366	0.187466	2.900504
H	-3.167599	0.126152	0.988507
C	-1.935078	-0.045533	-1.702039
H	-1.296623	0.525030	-2.382278
C	-2.099101	-1.462555	-2.271615
H	-2.917181	0.436484	-1.711125
H	-2.571646	-1.384670	-3.254963
N	-0.805058	-2.123660	-2.452461
H	-2.792015	-2.021242	-1.623388
H	-0.356953	-2.285344	-1.557056
H	-0.920729	-3.026022	-2.898715

tryptamine, Ph-out S_1

C	0.009011	0.026555	0.079442
C	0.039781	0.100260	1.466740
C	1.211203	0.062997	2.246547
C	2.422586	-0.024708	1.479577
C	2.424288	-0.098222	0.103381
C	1.218162	-0.092172	-0.663988
N	-1.305257	0.177741	1.908057
H	1.210714	0.138377	3.323395
H	3.368147	-0.036627	2.008823
H	3.372744	-0.164375	-0.416120
H	1.229616	-0.084529	-1.743162
C	-1.382799	0.056871	-0.317511
C	-2.160874	0.151499	0.880469
H	-1.573506	0.264703	2.876719
H	-3.227664	0.229495	1.005528
C	-1.962337	-0.052725	-1.674183
H	-1.351673	0.500114	-2.391872
C	-2.067241	-1.516839	-2.191516
H	-2.969631	0.372678	-1.674784

H	-2.700105	-1.496997	-3.082334
N	-0.765555	-2.037295	-2.574182
H	-2.595360	-2.110325	-1.430528
H	-0.119439	-2.083651	-1.791987
H	-0.839821	-2.958705	-2.987301

tryptamine, Ph-up S_0

C	-2.073203	0.016153	0.818151
N	-1.239319	0.012750	1.920098
C	0.069593	0.036792	1.496064
C	0.048016	0.048045	0.076237
C	-1.334029	0.032573	-0.335073
C	1.258442	0.055265	2.225115
C	2.446716	0.090326	1.513974
C	2.452216	0.107909	0.107723
C	1.270030	0.087257	-0.612261
C	-1.869962	0.009207	-1.736562
C	-2.138624	-1.407310	-2.295054
N	-0.991846	-2.302390	-2.411813
H	1.256133	0.044899	3.308778
H	3.387759	0.106048	2.049722
H	3.399413	0.139809	-0.416513
H	1.291002	0.103742	-1.695284
H	-1.543571	0.021609	2.877642
H	-3.144216	0.013545	0.945877
H	-1.173181	0.526259	-2.404533
H	-2.807791	0.573493	-1.779599
H	-2.591640	-1.311361	-3.286325
H	-2.881875	-1.899062	-1.661018
H	-0.539317	-2.430827	-1.513585
H	-0.297100	-1.925103	-3.046702

tryptamine, Ph-up S_1

C	-2.170745	0.170094	0.871959
N	-1.313186	0.163400	1.908038
C	0.025775	0.097134	1.465275
C	-0.006460	0.079348	0.073775
C	-1.395133	0.123313	-0.317939
C	1.199342	0.011091	2.238035
C	2.409179	-0.066198	1.471777
C	2.411145	-0.085794	0.093443
C	1.207020	-0.036308	-0.674470
C	-1.949363	0.008260	-1.666349
C	-1.987748	-1.511694	-2.191884

N	-0.722671	-2.090223	-2.498057
H	1.199252	0.042441	3.317334
H	3.354225	-0.113934	2.000042
H	3.360529	-0.138100	-0.426957
H	1.235297	0.115902	-1.744273
H	-1.581767	0.232595	2.877003
H	-3.237135	0.250178	1.001650
H	-1.365052	0.571714	-2.396372
H	-2.983753	0.361119	-1.697053
H	-2.609230	-1.507296	-3.089786
H	-2.491296	-2.106092	-1.430403
H	-0.063446	-2.123261	-1.726510
H	-0.271120	-1.698081	-3.313189

tryptamine, Py-out S_0

C	0.527079	0.455386	0.224129
C	0.603413	0.533970	1.639613
C	1.817945	0.499986	2.323928
C	2.975828	0.386851	1.571122
C	2.926650	0.312072	0.168068
C	1.718417	0.345581	-0.507853
N	-0.686205	0.643967	2.109736
H	1.858645	0.561507	3.405167
H	3.935577	0.357626	2.072109
H	3.851352	0.228046	-0.389540
H	1.697075	0.289343	-1.589600
C	-0.867857	0.528400	-0.136655
C	-1.560464	0.642054	1.038542
H	-0.950752	0.735691	3.074596
H	-2.623653	0.725657	1.197858
C	-1.452555	0.466256	-1.516414
H	-0.891617	1.127560	-2.184897
C	-1.463715	-0.943622	-2.126167
H	-2.481269	0.834027	-1.492205
H	-0.428100	-1.302328	-2.221193
N	-2.321686	-1.838010	-1.345603
H	-1.875254	-0.880425	-3.137140
H	-2.362306	-2.758418	-1.767671
H	-1.946527	-1.951175	-0.409911

tryptamine, Py-out S_1

C	0.533090	0.491979	0.217325
C	0.608856	0.552037	1.601861
C	1.805248	0.483736	2.342966

C	2.986047	0.360840	1.534578
C	2.941472	0.302910	0.157971
C	1.711601	0.360530	-0.568359
N	-0.721786	0.658572	2.084786
H	1.842657	0.543801	3.420043
H	3.947782	0.310974	2.031625
H	3.870496	0.210533	-0.391893
H	1.688289	0.357029	-1.647828
C	-0.869711	0.561964	-0.135551
C	-1.609576	0.661449	1.083476
H	-0.959818	0.730457	3.062522
H	-2.671837	0.742199	1.239424
C	-1.455916	0.485982	-1.487556
H	-0.878449	1.123392	-2.164761
C	-1.426632	-0.952439	-2.078807
H	-2.492226	0.829571	-1.480810
H	-0.380098	-1.278393	-2.119747
N	-2.300690	-1.845146	-1.327599
H	-1.800469	-0.894704	-3.102697
H	-2.474946	-2.702093	-1.838002
H	-1.893393	-2.095190	-0.432978

tryptamine, Py-up S_0

C	-2.115612	0.241338	0.897573
N	-1.238766	0.224781	1.966782
C	0.047776	0.099400	1.492044
C	-0.033333	0.031151	0.076707
C	-1.427989	0.125524	-0.280550
C	1.263615	0.044154	2.172746
C	2.417372	-0.080686	1.415727
C	2.363303	-0.146466	0.012375
C	1.153912	-0.091860	-0.659726
C	-2.009791	0.071141	-1.659532
C	-2.025763	-1.344721	-2.282972
N	-2.831437	-2.346975	-1.592787
H	1.308232	0.097767	3.254221
H	3.378023	-0.126932	1.913667
H	3.285029	-0.241135	-0.548337
H	1.129067	-0.141848	-1.741719
H	-1.498854	0.315529	2.932925
H	-3.175938	0.348489	1.063097
H	-1.447266	0.735420	-2.325846
H	-3.035468	0.454027	-1.637753
H	-1.002889	-1.724504	-2.344256
H	-2.390155	-1.269066	-3.311297

H	-3.806346	-2.068184	-1.559834
H	-2.518202	-2.456725	-0.634367

tryptamine, Py-up S_1

C	-2.159519	0.273977	0.972689
N	-1.254966	0.269848	1.964144
C	0.063839	0.137597	1.466369
C	-0.031146	0.067659	0.082027
C	-1.437987	0.158367	-0.252497
C	1.268082	0.054791	2.192117
C	2.437379	-0.099688	1.373456
C	2.373342	-0.169758	-0.001624
C	1.137168	-0.094923	-0.713724
C	-2.030035	0.086461	-1.589625
C	-1.980200	-1.366252	-2.239581
N	-2.847813	-2.358835	-1.673506
H	1.317842	0.121227	3.268478
H	3.403649	-0.165714	1.859492
H	3.293145	-0.286410	-0.562601
H	1.104677	-0.106944	-1.793118
H	-1.476553	0.371032	2.942922
H	-3.214325	0.404064	1.146737
H	-1.458812	0.719357	-2.277129
H	-3.068803	0.426305	-1.590009
H	-0.948791	-1.714395	-2.181854
H	-2.235661	-1.239187	-3.293150
H	-3.832632	-2.149511	-1.768458
H	-2.633361	-2.589439	-0.712639

porphycene S_0

C	-3.442066	1.919138	0.000000
C	-2.431354	0.909832	0.000000
N	-1.230305	1.549126	0.000000
C	-1.398277	2.903302	0.000000
C	-2.810639	3.138971	0.000000
C	-0.367067	3.854952	0.000000
C	1.014569	3.706048	0.000000
C	1.838275	2.563995	0.000000
H	-0.271073	1.135135	0.000000
N	1.421343	1.270995	0.000000
C	3.290391	2.604247	0.000000
C	3.720097	1.312861	0.000000
C	2.526054	0.495821	0.000000
C	2.431354	-0.909832	0.000000

C	3.442066	-1.919138	0.000000
C	2.810639	-3.138971	0.000000
C	1.398277	-2.903302	0.000000
N	1.230305	-1.549126	0.000000
C	0.367067	-3.854952	0.000000
C	-1.014569	-3.706048	0.000000
C	-1.838275	-2.563995	0.000000
C	-3.290391	-2.604247	0.000000
C	-3.720097	-1.312861	0.000000
C	-2.526054	-0.495821	0.000000
N	-1.421343	-1.270995	0.000000
H	0.271073	-1.135135	0.000000
H	3.272364	-4.113737	0.000000
H	4.504292	-1.735673	0.000000
H	0.722814	-4.879329	0.000000
H	-1.567268	-4.639674	0.000000
H	-3.893197	-3.499896	0.000000
H	-4.738198	-0.956087	0.000000
H	-4.504292	1.735673	0.000000
H	-3.272364	4.113737	0.000000
H	-0.722814	4.879329	0.000000
H	1.567268	4.639674	0.000000
H	3.893197	3.499896	0.000000
H	4.738198	0.956087	0.000000

porphycene S_1

C	-3.464211	1.907721	0.000000
C	-2.458483	0.900268	0.000000
N	-1.246401	1.544545	0.000000
C	-1.417904	2.893983	0.000000
C	-2.829331	3.130117	0.000000
C	-0.381666	3.858427	0.000000
C	0.992265	3.718181	0.000000
C	1.844686	2.576541	0.000000
H	-0.292992	1.129233	0.000000
N	1.431337	1.283867	0.000000
C	3.285668	2.625234	0.000000
C	3.730515	1.327340	0.000000
C	2.559735	0.506164	0.000000
C	2.458483	-0.900268	0.000000
C	3.464211	-1.907721	0.000000
C	2.829331	-3.130117	0.000000
C	1.417904	-2.893983	0.000000
N	1.246401	-1.544545	0.000000
C	0.381666	-3.858427	0.000000

C	-0.992265	-3.718181	0.000000
C	-1.844686	-2.576541	0.000000
C	-3.285668	-2.625234	0.000000
C	-3.730515	-1.327340	0.000000
C	-2.559735	-0.506164	0.000000
N	-1.431337	-1.283867	0.000000
H	0.292992	-1.129233	0.000000
H	3.289575	-4.105574	0.000000
H	4.526407	-1.725050	0.000000
H	0.745000	-4.879788	0.000000
H	-1.538778	-4.655871	0.000000
H	-3.884292	-3.523687	0.000000
H	-4.752736	-0.983555	0.000000
H	-4.526407	1.725050	0.000000
H	-3.289575	4.105574	0.000000
H	-0.745000	4.879788	0.000000
H	1.538778	4.655871	0.000000
H	3.884292	3.523687	0.000000
H	4.752736	0.983555	0.000000

porphine S_0

N	0.000000	-2.030709	0.000000
N	2.110481	0.000000	0.000000
C	1.084273	-2.851109	0.000000
C	0.676043	-4.250323	0.000000
C	2.416609	-2.435225	0.000000
C	2.887581	-1.127867	0.000000
C	4.248970	-0.683967	0.000000
H	1.345099	-5.097723	0.000000
H	3.172808	-3.210538	0.000000
H	5.103904	-1.341346	0.000000
H	1.097850	0.000000	0.000000
N	0.000000	2.030709	0.000000
N	-2.110481	0.000000	0.000000
C	1.084273	2.851109	0.000000
C	-1.084273	2.851109	0.000000
C	-1.084273	-2.851109	0.000000
C	0.676043	4.250323	0.000000
C	-0.676043	4.250323	0.000000
C	-0.676043	-4.250323	0.000000
C	2.416609	2.435225	0.000000
C	-2.416609	2.435225	0.000000
C	-2.416609	-2.435225	0.000000
C	2.887581	1.127867	0.000000
C	-2.887581	1.127867	0.000000

C	-2.887581	-1.127867	0.000000
C	4.248970	0.683967	0.000000
C	-4.248970	0.683967	0.000000
C	-4.248970	-0.683967	0.000000
H	1.345099	5.097723	0.000000
H	-1.345099	5.097723	0.000000
H	-1.345099	-5.097723	0.000000
H	3.172808	3.210538	0.000000
H	-3.172808	3.210538	0.000000
H	-3.172808	-3.210538	0.000000
H	5.103904	1.341346	0.000000
H	-5.103904	1.341346	0.000000
H	-5.103904	-1.341346	0.000000
H	-1.097850	0.000000	0.000000

porphine S_1

N	0.000000	-2.051382	0.000000
N	2.108175	0.000000	0.000000
C	1.088102	-2.876572	0.000000
C	0.679059	-4.269031	0.000000
C	2.422587	-2.442733	0.000000
C	2.888683	-1.130453	0.000000
C	4.249831	-0.685479	0.000000
H	1.346177	-5.117615	0.000000
H	3.184594	-3.212359	0.000000
H	5.105274	-1.342006	0.000000
H	1.097073	0.000000	0.000000
N	0.000000	2.051382	0.000000
N	-2.108175	0.000000	0.000000
C	1.088102	2.876572	0.000000
C	-1.088102	2.876572	0.000000
C	-1.088102	-2.876572	0.000000
C	0.679059	4.269031	0.000000
C	-0.679059	4.269031	0.000000
C	-0.679059	-4.269031	0.000000
C	2.422587	2.442733	0.000000
C	-2.422587	2.442733	0.000000
C	-2.422587	-2.442733	0.000000
C	2.888683	1.130453	0.000000
C	-2.888683	1.130453	0.000000
C	-2.888683	-1.130453	0.000000
C	4.249831	0.685479	0.000000
C	-4.249831	0.685479	0.000000
C	-4.249831	-0.685479	0.000000
H	1.346177	5.117615	0.000000

H	-1.346177	5.117615	0.000000
H	-1.346177	-5.117615	0.000000
H	3.184594	3.212359	0.000000
H	-3.184594	3.212359	0.000000
H	-3.184594	-3.212359	0.000000
H	5.105274	1.342006	0.000000
H	-5.105274	1.342006	0.000000
H	-5.105274	-1.342006	0.000000
H	-1.097073	0.000000	0.000000

chlorin S_0

C	0.000000	-4.241934	0.924571
C	0.000000	-2.887393	1.378189
N	0.000000	-2.100583	0.245634
C	0.000000	-2.868583	-0.881126
C	0.000000	-4.232159	-0.444738
C	0.000000	-2.419200	2.680512
C	0.000000	-1.084507	3.103738
N	0.000000	0.000000	2.281976
C	0.000000	1.084507	3.103738
C	0.000000	0.678390	4.496335
C	0.000000	-0.678390	4.496335
C	0.000000	2.419200	2.680512
C	0.000000	2.887393	1.378189
N	0.000000	2.100583	0.245634
C	0.000000	2.868583	-0.881126
C	0.000000	4.232159	-0.444738
C	0.000000	4.241934	0.924571
C	0.000000	2.410053	-2.202294
C	0.000000	1.102495	-2.657894
C	0.000000	0.767686	-4.144875
C	0.000000	-0.767686	-4.144875
C	0.000000	-1.102495	-2.657894
N	0.000000	0.000000	-1.883136
C	0.000000	-2.410053	-2.202294
H	-0.878261	1.189276	-4.638165
H	0.000000	3.187395	-2.956936
H	0.000000	5.082275	-1.108217
H	0.000000	1.346115	5.344854
H	0.000000	-1.346115	5.344854
H	-0.878261	-1.189276	-4.638165
H	0.000000	3.176711	3.455028
H	0.000000	-3.176711	3.455028
H	0.000000	-3.187395	-2.956936
H	0.000000	5.102262	1.575077

H	0.000000	-5.102262	1.575077
H	0.000000	-5.082275	-1.108217
H	0.878261	-1.189276	-4.638165
H	0.878261	1.189276	-4.638165
H	0.000000	-1.090065	0.269046
H	0.000000	1.090065	0.269046

chlorin S_1

C	0.000000	-4.251183	0.925033
C	0.000000	-2.894544	1.375701
N	0.000000	-2.108276	0.244158
C	0.000000	-2.883114	-0.886642
C	0.000000	-4.243480	-0.448987
C	0.000000	-2.424161	2.686709
C	0.000000	-1.087297	3.106004
N	0.000000	0.000000	2.281869
C	0.000000	1.087297	3.106004
C	0.000000	0.676738	4.504246
C	0.000000	-0.676738	4.504246
C	0.000000	2.424161	2.686709
C	0.000000	2.894544	1.375701
N	0.000000	2.108276	0.244158
C	0.000000	2.883114	-0.886642
C	0.000000	4.243480	-0.448987
C	0.000000	4.251183	0.925033
C	0.000000	2.419512	-2.209796
C	0.000000	1.104018	-2.659419
C	0.000000	0.766610	-4.141058
C	0.000000	-0.766610	-4.141058
C	0.000000	-1.104018	-2.659419
N	0.000000	0.000000	-1.876353
C	0.000000	-2.419512	-2.209796
H	-0.877606	1.189211	-4.636540
H	0.000000	3.192141	-2.968816
H	0.000000	5.095193	-1.110391
H	0.000000	1.345726	5.351542
H	0.000000	-1.345726	5.351542
H	-0.877606	-1.189211	-4.636540
H	0.000000	3.180674	3.461327
H	0.000000	-3.180674	3.461327
H	0.000000	-3.192141	-2.968816
H	0.000000	5.110026	1.577161
H	0.000000	-5.110026	1.577161
H	0.000000	-5.095193	-1.110391
H	0.877606	-1.189211	-4.636540

H	0.877606	1.189211	-4.636540
H	0.000000	-1.097884	0.263558
H	0.000000	1.097884	0.263558

Zn-tetraphenylporphine S_0

C	-3.779874	4.232037	1.158443
C	-3.501430	3.501412	-0.000032
C	-4.232204	3.779989	-1.158353
C	-5.215025	4.764690	-1.159309
C	-5.484719	5.484714	0.000227
C	-4.764550	5.214861	1.159652
C	-2.441866	2.441839	-0.000133
C	-1.104244	2.866313	-0.010264
N	0.000000	2.051969	0.021629
C	1.104244	2.866313	-0.010264
C	0.678537	4.243785	-0.075062
C	-0.678537	4.243785	-0.075062
C	2.441866	2.441839	-0.000133
C	3.501430	3.501412	-0.000032
C	4.232204	3.779989	-1.158353
C	5.215025	4.764690	-1.159309
C	5.484719	5.484714	0.000227
C	4.764550	5.214861	1.159652
C	3.779874	4.232037	1.158443
C	-2.866376	1.104234	0.009992
N	-2.052048	0.000000	-0.022056
C	-2.866376	-1.104234	0.009992
C	-4.243844	-0.678537	0.075036
C	-4.243844	0.678537	0.075036
C	-2.441866	-2.441839	-0.000133
C	-3.501430	-3.501412	-0.000032
C	-4.232204	-3.779989	-1.158353
C	-5.215025	-4.764690	-1.159309
C	-5.484719	-5.484714	0.000227
C	-4.764550	-5.214861	1.159652
C	-3.779874	-4.232037	1.158443
C	2.866376	1.104234	0.009992
N	2.052048	0.000000	-0.022056
C	2.866376	-1.104234	0.009992
C	4.243844	-0.678537	0.075036
C	4.243844	0.678537	0.075036
C	2.441866	-2.441839	-0.000133
C	3.501430	-3.501412	-0.000032
C	4.232204	-3.779989	-1.158353
C	5.215025	-4.764690	-1.159309

C	5.484719	-5.484714	0.000227
C	4.764550	-5.214861	1.159652
C	3.779874	-4.232037	1.158443
C	1.104244	-2.866313	-0.010264
N	0.000000	-2.051969	0.021629
C	-1.104244	-2.866313	-0.010264
C	-0.678537	-4.243785	-0.075062
C	0.678537	-4.243785	-0.075062
H	1.335287	-5.095916	-0.126255
H	5.095970	-1.335287	0.126360
H	1.335287	5.095916	-0.126255
H	-1.335287	5.095916	-0.126255
H	-1.335287	-5.095916	-0.126255
H	5.095970	1.335287	0.126360
H	-5.095970	1.335287	0.126360
H	-5.095970	-1.335287	0.126360
H	4.023112	3.223126	-2.063733
H	5.768240	4.970454	-2.067829
H	6.250654	6.250662	0.000322
H	4.970205	5.767968	2.068262
H	3.222895	4.022804	2.063718
H	4.023112	-3.223126	-2.063733
H	5.768240	-4.970454	-2.067829
H	6.250654	-6.250662	0.000322
H	4.970205	-5.767968	2.068262
H	3.222895	-4.022804	2.063718
H	-4.023112	-3.223126	-2.063733
H	-5.768240	-4.970454	-2.067829
H	-6.250654	-6.250662	0.000322
H	-4.970205	-5.767968	2.068262
H	-3.222895	-4.022804	2.063718
H	-4.023112	3.223126	-2.063733
H	-5.768240	4.970454	-2.067829
H	-6.250654	6.250662	0.000322
H	-4.970205	5.767968	2.068262
H	-3.222895	4.022804	2.063718
Zn	0.000000	0.000000	-0.000071

Zn-tetraphenylporphine S_1

C	3.616394	4.411814	-1.059599
C	3.501486	3.505601	0.001335
C	4.400940	3.613777	1.069044
C	5.378473	4.601946	1.079409
C	5.483415	5.494853	0.016722
C	4.600430	5.394358	-1.053833

C	2.449504	2.450309	-0.004786
C	1.106788	2.867221	0.025948
N	0.000000	2.052632	-0.072020
C	-1.106788	2.867221	0.025948
C	-0.679327	4.232732	0.202276
C	0.679327	4.232732	0.202276
C	-2.449504	2.450309	-0.004786
C	-3.501486	3.505601	0.001335
C	-4.400940	3.613777	1.069044
C	-5.378473	4.601946	1.079409
C	-5.483415	5.494853	0.016722
C	-4.600430	5.394358	-1.053833
C	-3.616394	4.411814	-1.059599
C	2.883747	1.104192	-0.043847
N	2.070297	0.000000	0.055621
C	2.883747	-1.104192	-0.043847
C	4.245524	-0.681983	-0.220828
C	4.245524	0.681983	-0.220828
C	2.449504	-2.450309	-0.004786
C	3.501486	-3.505601	0.001335
C	4.400940	-3.613777	1.069044
C	5.378473	-4.601946	1.079409
C	5.483415	-5.494853	0.016722
C	4.600430	-5.394358	-1.053833
C	3.616394	-4.411814	-1.059599
C	-2.883747	1.104192	-0.043847
N	-2.070297	0.000000	0.055621
C	-2.883747	-1.104192	-0.043847
C	-4.245524	-0.681983	-0.220828
C	-4.245524	0.681983	-0.220828
C	-2.449504	-2.450309	-0.004786
C	-3.501486	-3.505601	0.001335
C	-4.400940	-3.613777	1.069044
C	-5.378473	-4.601946	1.079409
C	-5.483415	-5.494853	0.016722
C	-4.600430	-5.394358	-1.053833
C	-3.616394	-4.411814	-1.059599
C	-1.106788	-2.867221	0.025948
N	0.000000	-2.052632	-0.072020
C	1.106788	-2.867221	0.025948
C	0.679327	-4.232732	0.202276
C	-0.679327	-4.232732	0.202276
H	-1.333166	-5.077310	0.337609
H	-5.089749	-1.336527	-0.353864
H	-1.333166	5.077310	0.337609
H	1.333166	5.077310	0.337609

H	1.333166	-5.077310	0.337609
H	-5.089749	1.336527	-0.353864
H	5.089749	1.336527	-0.353864
H	5.089749	-1.336527	-0.353864
H	-4.320647	2.924121	1.900163
H	-6.057008	4.676660	1.920706
H	-6.247682	6.262375	0.023018
H	-4.678941	6.079828	-1.889142
H	-2.934987	4.333861	-1.897683
H	-4.320647	-2.924121	1.900163
H	-6.057008	-4.676660	1.920706
H	-6.247682	-6.262375	0.023018
H	-4.678941	-6.079828	-1.889142
H	-2.934987	-4.333861	-1.897683
H	4.320647	-2.924121	1.900163
H	6.057008	-4.676660	1.920706
H	6.247682	-6.262375	0.023018
H	4.678941	-6.079828	-1.889142
H	2.934987	-4.333861	-1.897683
H	4.320647	2.924121	1.900163
H	6.057008	4.676660	1.920706
H	6.247682	6.262375	0.023018
H	4.678941	6.079828	-1.889142
H	2.934987	4.333861	-1.897683
Zn	0.000000	0.000000	-0.007261

tetraphenylporphine S_0

C	-4.239366	-0.684673	0.081020
C	-2.881471	-1.131378	0.009403
N	-2.102185	-0.001001	-0.028014
C	-2.882527	1.128664	0.009266
C	-4.240004	0.680696	0.080926
C	-2.434935	2.454487	-0.008132
C	-1.088242	2.859020	-0.030647
N	-0.000944	2.037733	0.007909
C	1.085574	2.860050	-0.030519
C	0.672867	4.255105	-0.113982
C	-0.676864	4.254454	-0.114090
C	2.432658	2.456800	-0.007929
C	2.881471	1.131378	0.009403
N	2.102185	0.001001	-0.028014
C	2.882527	-1.128664	0.009266
C	4.240004	-0.680696	0.080926
C	4.239366	0.684673	0.081020
C	2.434935	-2.454487	-0.008132

C	1.088242	-2.859020	-0.030647
N	0.000944	-2.037733	0.007909
C	-1.085574	-2.860050	-0.030519
C	-0.672867	-4.255105	-0.113982
C	0.676864	-4.254454	-0.114090
C	-2.432658	-2.456800	-0.007929
H	1.337741	-5.102813	-0.177685
C	3.491488	-3.516925	0.001231
H	5.095029	-1.332460	0.134787
H	1.090174	0.000507	-0.041562
H	1.332899	5.104129	-0.177496
H	-1.337741	5.102813	-0.177685
H	-1.332899	-5.104129	-0.177496
C	3.488222	3.520203	0.001600
C	-3.491488	3.516925	0.001231
C	-3.488222	-3.520203	0.001600
H	5.093743	1.337274	0.134980
H	-5.095029	1.332460	0.134787
H	-5.093743	-1.337274	0.134980
H	-1.090174	-0.000507	-0.041562
C	4.240004	3.791433	-1.145042
C	5.218833	4.780105	-1.135750
C	5.463836	5.510592	0.022688
C	4.723008	5.247476	1.170651
C	3.742287	4.260911	1.159368
H	4.048567	3.227943	-2.050258
H	5.787605	4.981216	-2.035649
H	6.226360	6.279882	0.030690
H	4.909032	5.809287	2.078121
H	3.168199	4.057542	2.055160
C	4.243133	-3.787640	-1.145605
C	5.222821	-4.775462	-1.136481
C	5.468822	-5.505594	0.021969
C	4.728135	-5.242982	1.170137
C	3.746554	-4.257261	1.159024
H	4.050923	-3.224421	-2.050827
H	5.791480	-4.976209	-2.036533
H	6.231988	-6.274250	0.029796
H	4.914917	-5.804530	2.077612
H	3.172559	-4.054283	2.054964
C	-4.240004	-3.791433	-1.145042
C	-5.218833	-4.780105	-1.135750
C	-5.463836	-5.510592	0.022688
C	-4.723008	-5.247476	1.170651
C	-3.742287	-4.260911	1.159368
H	-4.048567	-3.227943	-2.050258

H	-5.787605	-4.981216	-2.035649
H	-6.226360	-6.279882	0.030690
H	-4.909032	-5.809287	2.078121
H	-3.168199	-4.057542	2.055160
C	-4.243133	3.787640	-1.145605
C	-5.222821	4.775462	-1.136481
C	-5.468822	5.505594	0.021969
C	-4.728135	5.242982	1.170137
C	-3.746554	4.257261	1.159024
H	-4.050923	3.224421	-2.050827
H	-5.791480	4.976209	-2.036533
H	-6.231988	6.274250	0.029796
H	-4.914917	5.804530	2.077612
H	-3.172559	4.054283	2.054964

tetraphenylporphine S_1

C	4.236136	0.681076	0.180332
C	2.887081	1.131690	0.018359
N	2.107765	-0.000990	-0.070934
C	2.885715	-1.134736	0.016540
C	4.235332	-0.686056	0.178944
C	2.441526	-2.464363	-0.029048
C	1.088456	-2.882327	-0.095476
N	-0.001137	-2.058959	-0.008775
C	-1.091718	-2.881160	-0.093785
C	-0.681376	-4.258495	-0.270363
C	0.676324	-4.259195	-0.271723
C	-2.444298	-2.461823	-0.025830
C	-2.887081	-1.131690	0.018359
N	-2.107765	0.000990	-0.070934
C	-2.885715	1.134736	0.016540
C	-4.235332	0.686056	0.178944
C	-4.236136	-0.681076	0.180332
C	-2.441526	2.464363	-0.029048
C	-1.088456	2.882327	-0.095476
N	0.001137	2.058959	-0.008775
C	1.091718	2.881160	-0.093785
C	0.681376	4.258495	-0.270363
C	-0.676324	4.259195	-0.271723
C	2.444298	2.461823	-0.025830
H	-1.332587	5.103423	-0.398956
C	-3.492067	3.522837	-0.000963
H	-5.085100	1.335507	0.297570
H	-1.097587	0.000270	-0.108890
H	-1.338844	-5.101988	-0.396347

H	1.332587	-5.103423	-0.398956
H	1.338844	5.101988	-0.396347
C	-3.495407	-3.519566	0.006560
C	3.492067	-3.522837	-0.000963
C	3.495407	3.519566	0.006560
H	-5.086751	-1.329179	0.300168
H	5.085100	-1.335507	0.297570
H	5.086751	1.329179	0.300168
H	1.097587	-0.000270	-0.108890
C	-4.408095	-3.662686	-1.044514
C	-5.384496	-4.652740	-1.009092
C	-5.470533	-5.512180	0.081455
C	-4.569877	-5.378539	1.134351
C	-3.588436	-4.395064	1.094822
H	-4.339949	-3.000861	-1.899152
H	-6.075700	-4.754402	-1.837124
H	-6.232635	-6.281336	0.110467
H	-4.632668	-6.039830	1.990191
H	-2.890570	-4.293331	1.916621
C	-4.401241	3.664786	-1.055227
C	-5.377438	4.655154	-1.024521
C	-5.466914	5.516050	0.064587
C	-4.569778	5.383608	1.120656
C	-3.588436	4.399816	1.085815
H	-4.330538	3.001556	-1.908559
H	-6.065914	4.755768	-1.854951
H	-6.229003	6.285341	0.090097
H	-4.635319	6.046036	1.975407
H	-2.893433	4.298938	1.910145
C	4.408095	3.662686	-1.044514
C	5.384496	4.652740	-1.009092
C	5.470533	5.512180	0.081455
C	4.569877	5.378539	1.134351
C	3.588436	4.395064	1.094822
H	4.339949	3.000861	-1.899152
H	6.075700	4.754402	-1.837124
H	6.232635	6.281336	0.110467
H	4.632668	6.039830	1.990191
H	2.890570	4.293331	1.916621
C	4.401241	-3.664786	-1.055227
C	5.377438	-4.655154	-1.024521
C	5.466914	-5.516050	0.064587
C	4.569778	-5.383608	1.120656
C	3.588436	-4.399816	1.085815
H	4.330538	-3.001556	-1.908559
H	6.065914	-4.755768	-1.854951

H	6.229003	-6.285341	0.090097
H	4.635319	-6.046036	1.975407
H	2.893433	-4.298938	1.910145

B3LYP/TZVP geometries – Group II

tetrafluorobenzene S_0

C	-1.192398	0.694468	0.000000
C	-1.192398	-0.694468	0.000000
C	0.000000	-1.398216	0.000000
C	1.192398	-0.694468	0.000000
C	1.192398	0.694468	0.000000
C	0.000000	1.398216	0.000000
F	-2.359921	-1.355953	0.000000
H	0.000000	-2.479402	0.000000
F	2.359921	-1.355953	0.000000
F	2.359921	1.355953	0.000000
H	0.000000	2.479402	0.000000
F	-2.359921	1.355953	0.000000

tetrafluorobenzene S_1

C	1.168103	-0.708304	0.108065
C	1.168103	0.708304	0.108065
C	0.000000	1.466015	0.294052
C	-1.168103	0.708304	0.108065
C	-1.168103	-0.708304	0.108065
C	0.000000	-1.466015	0.294052
F	2.319321	1.324056	-0.202901
H	0.000000	2.506153	0.593745
F	-2.319321	1.324056	-0.202901
F	-2.319321	-1.324056	-0.202901
H	0.000000	-2.506153	0.593745
F	2.319321	-1.324056	-0.202901

benzonitrile S_0

C	0.000000	0.000000	-1.059057
C	-1.212896	0.000000	-0.359273
C	-1.206428	0.000000	1.028569
C	0.000000	0.000000	1.723227
C	1.206428	0.000000	1.028569
C	1.212896	0.000000	-0.359273
H	-2.146132	0.000000	-0.906795

H	-2.144559	0.000000	1.568929
H	0.000000	0.000000	2.806120
H	2.144559	0.000000	1.568929
H	2.146132	0.000000	-0.906795
C	0.000000	0.000000	-2.489663
N	0.000000	0.000000	-3.643479

benzonitrile S_1

C	0.000000	0.000000	-1.112255
C	-1.227644	0.000000	-0.374040
C	-1.214824	0.000000	1.048450
C	0.000000	0.000000	1.766409
C	1.214824	0.000000	1.048450
C	1.227644	0.000000	-0.374040
H	-2.167519	0.000000	-0.907475
H	-2.158378	0.000000	1.577156
H	0.000000	0.000000	2.846625
H	2.158378	0.000000	1.577156
H	2.167519	0.000000	-0.907475
C	0.000000	0.000000	-2.511850
N	0.000000	0.000000	-3.677113

o-fluorophenol, *cis* S_0

C	0.327530	1.454460	0.000000
C	-0.873209	0.776204	0.000000
C	-0.950353	-0.614253	0.000000
C	0.237851	-1.337947	0.000000
C	1.458694	-0.671895	0.000000
C	1.510513	0.719211	0.000000
F	-2.053212	1.462092	0.000000
O	-2.144268	-1.269846	0.000000
H	0.184001	-2.418884	0.000000
H	2.375763	-1.247111	0.000000
H	2.462403	1.233417	0.000000
H	0.325114	2.536619	0.000000
H	-2.860819	-0.622086	0.000000

o-fluorophenol, *cis* S_1

C	1.226623	-0.248620	-0.731540
C	0.003677	-0.077853	-0.095699
C	-0.006181	-0.028244	1.339440
C	1.178483	0.037109	2.089015
C	2.401595	0.103414	1.413309

C	2.415655	-0.024768	0.021881
F	-1.003611	0.810513	-0.703213
O	-1.174299	-0.138285	1.990015
H	1.126172	-0.102752	3.162725
H	3.326349	0.215018	1.961933
H	3.352890	0.088821	-0.514088
H	1.284283	-0.388740	-1.803852
H	-1.876257	-0.245614	1.320014

o-fluorophenol, *trans* S_0

C	0.291050	1.262950	0.000000
C	-0.947280	0.617210	0.000000
C	-0.962540	-0.775670	0.000000
C	0.228060	-1.498100	0.000000
C	1.449790	-0.836200	0.000000
C	1.478050	0.557170	0.000000
O	-2.068640	1.392760	0.000000
H	-1.916020	-1.294430	0.000000
H	0.193150	-2.580270	0.000000
H	2.377450	-1.393670	0.000000
H	2.410180	1.107900	0.000000
F	0.316950	2.612150	0.000000
H	-2.850210	0.828200	0.000000

o-fluorophenol, *trans* S_1

C	0.819463	1.038468	0.112157
C	-0.589079	0.974265	0.089922
C	-1.274712	-0.287516	0.089429
C	-0.470036	-1.427345	-0.081862
C	0.941536	-1.339511	-0.067194
C	1.619066	-0.128198	0.164170
O	-1.259802	2.126367	-0.087680
H	-2.295093	-0.361963	0.454740
H	-0.930016	-2.401661	-0.193087
H	1.516885	-2.247048	-0.215461
H	2.687751	-0.068138	0.304761
F	1.402882	2.216372	-0.199485
H	-2.168875	1.905909	-0.370411

m-fluorophenol, *cis* S_0

C	0.310040	1.410270	0.000000
C	-0.928180	0.788660	0.000000
C	-0.967970	-0.605260	0.000000

C	0.215220	-1.344410	0.000000
C	1.434810	-0.681590	0.000000
C	1.502810	0.710690	0.000000
O	-2.144130	-1.300900	0.000000
F	0.341150	2.763970	0.000000
H	0.159970	-2.424760	0.000000
H	2.351900	-1.257670	0.000000
H	2.444680	1.241940	0.000000
H	-1.830640	1.388580	0.000000
H	-2.889660	-0.689520	0.000000

m-fluorophenol, *cis* S_1

C	1.223835	-0.054051	-0.688316
C	-0.053977	0.026849	-0.103688
C	-0.025102	0.039089	1.325686
C	1.163040	0.031172	2.088986
C	2.427202	0.104882	1.440042
C	2.431608	-0.037782	0.033235
O	-1.184698	-0.021016	2.015626
F	1.300293	-0.158986	-2.033556
H	1.078616	-0.105651	3.159251
H	3.347105	0.147523	2.000566
H	3.357280	-0.123665	-0.522234
H	-0.905143	0.395368	-0.667317
H	-1.904699	-0.243732	1.401669

m-fluorophenol, *trans* S_0

C	0.268819	1.303777	0.000000
C	-0.950166	0.628236	0.000000
C	-0.984389	-0.766467	0.000000
C	0.208134	-1.482428	0.000000
C	1.436416	-0.831346	0.000000
C	1.429712	0.554668	0.000000
O	-2.080957	1.394757	0.000000
H	-1.935149	-1.287904	0.000000
H	0.178205	-2.564703	0.000000
H	2.373499	-1.370145	0.000000
F	2.613243	1.210466	0.000000
H	0.302520	2.384205	0.000000
H	-2.859888	0.826894	0.000000

m-fluorophenol, *trans* S_1

C	1.085193	-0.016489	0.000000

C	0.327151	1.183343	0.000000
C	-1.092029	1.215065	0.000000
C	-1.825305	-0.008317	0.000000
C	-1.086606	-1.221458	0.000000
C	0.318361	-1.200882	0.000000
O	1.042726	2.331041	0.000000
H	-1.602956	2.170701	0.000000
H	-2.903387	-0.015990	0.000000
H	-1.586575	-2.180968	0.000000
F	0.973125	-2.382200	0.000000
H	2.162756	-0.012217	0.000000
H	0.446397	3.092519	0.000000

p-fluorophenol S_0

C	0.271848	1.316786	0.000000
C	-0.950929	0.647401	0.000000
C	-0.981116	-0.745693	0.000000
C	0.207032	-1.471417	0.000000
C	1.407987	-0.787344	0.000000
C	1.459176	0.596921	0.000000
O	-2.086605	1.414425	0.000000
H	-1.930099	-1.271046	0.000000
H	0.202442	-2.553247	0.000000
F	2.568417	-1.490678	0.000000
H	2.417553	1.098966	0.000000
H	0.279176	2.398645	0.000000
H	-2.864902	0.846270	0.000000

p-fluorophenol S_1

C	1.266995	0.681414	0.000000
C	0.027239	1.360909	0.000000
C	-1.236741	0.710964	0.000000
C	-1.251157	-0.708016	0.000000
C	-0.006474	-1.366420	0.000000
C	1.251811	-0.738823	0.000000
O	0.092905	2.709849	0.000000
H	-2.152539	1.287568	0.000000
H	-2.163574	-1.284115	0.000000
F	-0.026576	-2.707767	0.000000
H	2.152147	-1.333105	0.000000
H	2.183342	1.251768	0.000000
H	-0.800682	3.081368	0.000000

phenylacetylene S_0

C	1.208805	0.000000	-0.014088
C	0.000000	0.000000	-0.726252
C	-1.208805	0.000000	-0.014088
C	-1.204287	0.000000	1.374004
C	0.000000	0.000000	2.072345
C	1.204287	0.000000	1.374004
C	0.000000	0.000000	-2.152937
C	0.000000	0.000000	-3.356489
H	-2.143698	0.000000	-0.559315
H	-2.143918	0.000000	1.912691
H	0.000000	0.000000	3.155347
H	2.143918	0.000000	1.912691
H	2.143698	0.000000	-0.559315
H	0.000000	0.000000	-4.418618

phenylacetylene S_1

C	1.235902	0.000000	-0.032094
C	0.000000	0.000000	-0.756783
C	-1.235902	0.000000	-0.032094
C	-1.223681	0.000000	1.392543
C	0.000000	0.000000	2.091188
C	1.223681	0.000000	1.392543
C	0.000000	0.000000	-2.148788
C	0.000000	0.000000	-3.366302
H	-2.168808	0.000000	-0.576644
H	-2.159397	0.000000	1.934138
H	0.000000	0.000000	3.173262
H	2.159397	0.000000	1.934138
H	2.168808	0.000000	-0.576644
H	0.000000	0.000000	-4.428461

aniline S_0

C	0.921128	0.026253	0.000000
C	0.205060	0.034152	1.204062
C	-1.183441	0.043209	1.198540
C	-1.891316	0.048505	0.000000
C	-1.183441	0.043209	-1.198540
C	0.205060	0.034152	-1.204062
H	0.743388	0.034816	2.145661
H	-2.973607	0.055079	0.000000
H	-1.716115	0.046732	2.142191
H	-1.716115	0.046732	-2.142191
H	0.743388	0.034816	-2.145661

N	2.315491	0.074478	0.000000
H	2.765264	-0.261062	-0.837404
H	2.765264	-0.261062	0.837404

aniline S_1

C	0.891430	-0.033620	0.000000
C	0.225580	-0.008070	1.246210
C	-1.201660	0.046090	1.236700
C	-1.871920	0.071230	0.000000
C	-1.201660	0.046090	-1.236700
C	0.225580	-0.008070	-1.246210
H	0.791900	-0.029740	2.168640
H	-2.955960	0.111990	0.000000
H	-1.759390	0.067210	2.161880
H	-1.759390	0.067210	-2.161880
H	0.791900	-0.029740	-2.168640
N	2.263040	-0.086800	0.000000
H	2.780270	-0.106900	-0.864400
H	2.780270	-0.106900	0.864400

catechol S_0

C	0.471928	1.279334	0.000000
C	-0.747855	0.620678	0.000000
C	-0.798623	-0.778566	0.000000
C	0.384195	-1.504141	0.000000
C	1.610060	-0.843197	0.000000
C	1.657371	0.545627	0.000000
O	-1.974916	1.250721	0.000000
O	-1.996699	-1.430878	0.000000
H	0.326755	-2.585038	0.000000
H	2.526678	-1.419003	0.000000
H	2.607687	1.063422	0.000000
H	0.497166	2.364282	0.000000
H	-1.861325	2.206887	0.000000
H	-2.702420	-0.770128	0.000000

catechol S_1

C	0.476371	1.347593	0.000000
C	-0.761018	0.626151	0.000000
C	-0.804866	-0.783260	0.000000
C	0.388807	-1.572288	0.000000
C	1.602468	-0.858466	0.000000
C	1.644492	0.557707	0.000000

O	-1.974226	1.257189	0.000000
O	-1.991875	-1.432114	0.000000
H	0.326724	-2.648350	0.000000
H	2.539601	-1.399809	0.000000
H	2.611458	1.044675	0.000000
H	0.500593	2.427675	-0.000001
H	-1.848797	2.213563	0.000001
H	-2.709731	-0.780266	0.000000

resorcinol, isomer 1 S_0

C	0.074720	1.147540	0.000000
C	-1.139910	0.465360	0.000000
C	-1.170470	-0.927470	0.000000
C	0.033120	-1.628670	0.000000
C	1.253150	-0.968820	0.000000
C	1.264940	0.426710	0.000000
O	-2.276130	1.229440	0.000000
H	-2.117610	-1.455950	0.000000
H	0.014750	-2.711880	0.000000
H	2.191010	-1.507540	0.000000
O	2.485870	1.044010	0.000000
H	0.069770	2.231870	0.000000
H	-3.050070	0.654650	0.000000
H	2.366860	2.000740	0.000000

resorcinol, isomer 1 S_1

C	-0.001111	1.067394	0.046271
C	-1.193576	0.306634	-0.010189
C	-1.203649	-1.108777	-0.038098
C	0.001304	-1.849321	0.084556
C	1.211282	-1.109752	0.017523
C	1.195807	0.302854	0.038991
O	-2.354369	1.014036	-0.050779
H	-2.150493	-1.622657	-0.171684
H	-0.000240	-2.927299	0.087124
H	2.168665	-1.604153	-0.086404
O	2.404083	0.923022	-0.008545
H	-0.027035	2.100925	0.369783
H	-3.107659	0.410166	-0.011387
H	2.267984	1.853048	-0.247513

resorcinol, isomer 2 S_0

C	1.199870	0.000000	-0.546160

C	0.000000	0.000000	-1.248540
C	-1.199870	0.000000	-0.546160
C	-1.210110	0.000000	0.850420
C	0.000000	0.000000	1.533780
C	1.210110	0.000000	0.850420
O	-2.350850	0.000000	-1.286440
O	2.350850	0.000000	-1.286440
H	-2.149430	0.000000	1.392680
H	0.000000	0.000000	2.617170
H	2.149430	0.000000	1.392680
H	0.000000	0.000000	-2.330050
H	-3.113540	0.000000	-0.696920
H	3.113540	0.000000	-0.696920

resorcinol, isomer 2 S_1

C	1.198928	0.000000	-0.328275
C	0.000000	0.000000	-1.080665
C	-1.198928	0.000000	-0.328275
C	-1.215145	0.000000	1.088139
C	0.000000	0.000000	1.828539
C	1.215145	0.000000	1.088139
O	-2.357588	0.000000	-1.042079
O	2.357588	0.000000	-1.042079
H	-2.168823	0.000000	1.604854
H	0.000000	0.000000	2.906575
H	2.168823	0.000000	1.604854
H	0.000000	0.000000	-2.158130
H	-3.112764	0.000000	-0.440342
H	3.112764	0.000000	-0.440342

resorcinol, isomer 3 S_0

C	1.205164	0.000000	-0.288427
C	0.000000	0.000000	-0.990132
C	-1.205164	0.000000	-0.288427
C	-1.212839	0.000000	1.103533
C	0.000000	0.000000	1.781683
C	1.212839	0.000000	1.103533
O	-2.416386	0.000000	-0.926044
O	2.416386	0.000000	-0.926044
H	-2.158307	0.000000	1.628269
H	0.000000	0.000000	2.864776
H	2.158307	0.000000	1.628269
H	0.000000	0.000000	-2.076800
H	2.285868	0.000000	-1.880854

H	-2.285868	0.000000	-1.880854

resorcinol, isomer 3 S_1

C	-0.025730	-0.302925	1.189319
C	-0.110620	-1.076912	0.000000
C	-0.025730	-0.302925	-1.189319
C	0.021034	1.110128	-1.201902
C	-0.066715	1.849063	0.000000
C	0.021034	1.110128	1.201902
O	0.061516	-0.919109	-2.396383
O	0.061516	-0.919109	2.396383
H	0.155231	1.600428	-2.158206
H	-0.078858	2.927334	0.000000
H	0.155231	1.600428	2.158206
H	-0.640368	-2.031691	0.000000
H	0.272436	-1.855047	2.249631
H	0.272436	-1.855047	-2.249631

hydroquinone, *cis* S_0

C	-0.696953	0.000000	1.092428
C	0.696953	0.000000	1.092428
C	1.396255	0.000000	-0.108957
C	0.692887	0.000000	-1.312779
C	-0.692887	0.000000	-1.312779
C	-1.396255	0.000000	-0.108957
O	2.768757	0.000000	-0.177005
O	-2.768757	0.000000	-0.177005
H	1.245549	0.000000	-2.243246
H	-1.245549	0.000000	-2.243246
H	-1.231506	0.000000	2.036617
H	1.231506	0.000000	2.036617
H	-3.137003	0.000000	0.713232
H	3.137003	0.000000	0.713232

hydroquinone, *cis* S_1

C	0.708634	0.000000	-1.131995
C	-0.708634	0.000000	-1.131995
C	-1.375030	0.000000	0.119751
C	-0.708799	0.000000	1.362428
C	0.708799	0.000000	1.362428
C	1.375030	0.000000	0.119751
O	-2.727422	0.000000	0.165749
O	2.727422	0.000000	0.165749

H	-1.287896	0.000000	2.273269
H	1.287896	0.000000	2.273269
H	1.274725	0.000000	-2.054647
H	-1.274725	0.000000	-2.054647
H	3.082155	0.000000	-0.733787
H	-3.082155	0.000000	-0.733787

hydroquinone, *trans* S_0

C	0.020550	1.391060	0.000000
C	-1.197370	0.718710	0.000000
C	-1.211860	-0.674830	0.000000
C	-0.020550	-1.391060	0.000000
C	1.197370	-0.718710	0.000000
C	1.211860	0.674830	0.000000
O	-2.343130	1.478040	0.000000
H	-2.156550	-1.209360	0.000000
H	-0.025930	-2.473470	0.000000
O	2.343130	-1.478040	0.000000
H	2.156550	1.209360	0.000000
H	0.025930	2.473470	0.000000
H	-3.113960	0.899770	0.000000
H	3.113960	-0.899770	0.000000

hydroquinone, *trans* S_1

C	1.262903	0.679146	0.000000
C	0.035137	1.374403	0.000000
C	-1.230899	0.737909	0.000000
C	-1.262903	-0.679146	0.000000
C	-0.035137	-1.374403	0.000000
C	1.230899	-0.737909	0.000000
O	0.118582	2.724879	0.000000
H	-2.140739	1.324248	0.000000
H	-2.186410	-1.238299	0.000000
O	-0.118582	-2.724879	0.000000
H	2.140739	-1.324248	0.000000
H	2.186410	1.238299	0.000000
H	-0.771428	3.103170	0.000000
H	0.771428	-3.103170	0.000000

salicylic acid S_0

C	1.102298	1.599491	0.000000
C	1.134246	0.200350	0.000000
C	-0.085249	-0.518596	0.000000

C	-1.300507	0.187187	0.000000
C	-1.318658	1.567037	0.000000
C	-0.107025	2.267998	0.000000
O	2.335855	-0.398219	0.000000
C	-0.044055	-1.980565	0.000000
O	-1.251085	-2.582019	0.000000
O	0.986210	-2.644565	0.000000
H	-2.224492	-0.374359	0.000000
H	2.043961	2.132349	0.000000
H	-2.259529	2.101067	0.000000
H	-0.112879	3.351415	0.000000
H	2.189639	-1.370531	0.000000
H	-1.088731	-3.538040	0.000000

salicylic acid S_1

C	0.994817	1.911512	0.000000
C	0.958670	0.506775	0.000000
C	-0.291123	-0.222380	0.000000
C	-1.445925	0.539946	0.000000
C	-1.401626	1.978205	0.000000
C	-0.203963	2.662882	0.000000
O	2.086995	-0.176106	0.000000
C	-0.232739	-1.664944	0.000000
O	-1.430006	-2.315303	0.000000
O	0.857445	-2.321401	0.000000
H	-2.407450	0.044741	0.000000
H	1.965709	2.389234	0.000000
H	-2.340181	2.517626	0.000000
H	-0.173814	3.742930	0.000000
H	1.800014	-1.195395	0.000000
H	-1.226245	-3.261376	0.000000

o-cresol, *cis* S_0

C	1.965208	0.512912	0.000000
C	0.730122	1.150860	0.000000
C	-0.466391	0.433086	0.000000
C	-0.389713	-0.966856	0.000000
C	0.840862	-1.617667	0.000000
C	2.015306	-0.877710	0.000000
C	-1.802954	1.129994	0.000000
O	-1.509251	-1.759793	0.000000
H	0.856035	-2.700017	0.000000
H	2.969562	-1.390047	0.000000
H	2.877596	1.095491	0.000000

H	0.686300	2.234342	0.000000
H	-2.301515	-1.212019	0.000000
H	-2.398814	0.877808	0.884438
H	-1.673539	2.211817	0.000000
H	-2.398814	0.877808	-0.884438

o-cresol, *cis* S_1

C	1.855686	-0.032451	-0.782592
C	0.623916	0.127544	-1.454438
C	-0.598108	0.096934	-0.712651
C	-0.472701	0.077249	0.712939
C	0.768792	-0.003882	1.396309
C	1.945256	-0.106216	0.623416
C	-1.890890	-0.094873	-1.433079
O	-1.561907	0.112214	1.508562
H	0.780771	0.101272	2.471502
H	2.909804	-0.210390	1.099991
H	2.764479	-0.104374	-1.368860
H	0.596145	0.189030	-2.533431
H	-2.353065	0.287627	0.972675
H	-2.753156	-0.260702	-0.779306
H	-2.133895	0.765733	-2.069642
H	-1.831707	-0.964205	-2.108985

o-cresol, *trans* S_0

C	2.418630	0.000505	0.029960
C	1.243460	0.000078	-0.718310
C	0.028340	0.000172	-0.018880
C	-0.000813	-0.000243	1.372720
C	1.189190	-0.000381	2.094380
C	2.405230	0.000320	1.423300
C	1.251410	-0.000447	-2.222520
O	-1.119640	0.000780	-0.772880
H	-0.954510	-0.000254	1.892130
H	1.158440	-0.000760	3.177240
H	3.336480	0.000417	1.976010
H	3.367520	0.000915	-0.495560
H	-1.887380	0.000865	-0.190010
H	2.273360	-0.000449	-2.603130
H	0.734680	-0.877050	-2.621810
H	0.734310	0.875530	-2.622670

o-cresol, *trans* S_1

C	2.424982	0.254835	-0.005114
C	1.211059	0.116214	-0.754587
C	0.006667	-0.009186	-0.014758
C	-0.050399	-0.094040	1.412951
C	1.178705	-0.072061	2.104950
C	2.388998	0.089433	1.391588
C	1.253067	-0.017185	-2.236648
O	-1.143306	-0.109910	-0.717826
H	-0.994119	0.053435	1.925251
H	1.199822	-0.141011	3.184140
H	3.318949	0.100647	1.948256
H	3.363081	0.399080	-0.521724
H	-1.844915	-0.418976	-0.119741
H	1.844189	-0.896625	-2.534699
H	0.262260	-0.102350	-2.677244
H	1.759648	0.847701	-2.684816

m-cresol, *cis* S_0

C	1.158489	-0.004290	2.087516
C	2.370500	0.010220	1.413993
C	2.415801	0.020061	0.021277
C	1.236154	0.013651	-0.721538
C	0.015619	0.000947	-0.041062
C	-0.024413	-0.008529	1.350245
C	1.262830	0.002001	-2.229252
O	-1.201918	-0.019807	2.050796
H	1.108498	-0.009716	3.168366
H	3.293454	0.016479	1.981341
H	3.371655	0.033753	-0.488375
H	-0.913771	-0.000292	-0.604225
H	-1.944535	-0.021109	1.436371
H	2.260706	0.225270	-2.607879
H	0.971576	-0.976988	-2.620839
H	0.571655	0.737719	-2.646785

m-cresol, *cis* S_1

C	1.162746	0.013464	2.125661
C	2.407108	0.082778	1.447435
C	2.408494	0.033544	0.035603
C	1.221281	-0.003846	-0.745680
C	-0.032223	0.012296	-0.070350
C	-0.019109	0.008932	1.353585
C	1.266569	-0.034077	-2.235541
O	-1.184668	-0.034294	2.036789

H	1.089515	-0.107562	3.197433
H	3.336783	0.110967	1.995817
H	3.359470	0.038157	-0.485550
H	-0.950206	0.235323	-0.604427
H	-1.909429	-0.207239	1.415500
H	2.285200	0.061918	-2.613024
H	0.845962	-0.968431	-2.634199
H	0.664787	0.777440	-2.669113

m-cresol, *trans* S_0

C	-1.144261	-1.134826	0.000000
C	-1.195511	0.261064	0.000000
C	0.000000	0.979262	0.000000
C	1.224155	0.318363	0.000000
C	1.270983	-1.075247	0.000000
C	0.081102	-1.792647	0.000000
C	-2.514960	0.991712	0.000000
O	2.355256	1.092340	0.000000
H	2.225630	-1.591059	0.000000
H	0.112604	-2.875549	0.000000
H	-2.064127	-1.706921	0.000000
H	-0.003090	2.062830	0.000000
H	3.134720	0.525537	0.000000
H	-3.353406	0.294723	0.000000
H	-2.611713	1.632815	0.879954
H	-2.611713	1.632815	-0.879954

m-cresol, *trans* S_1

C	-1.204120	-1.058551	0.000000
C	0.203853	-1.237453	0.000000
C	1.025509	-0.070949	0.000000
C	0.396018	1.196629	0.000000
C	-1.012198	1.375042	0.000000
C	-1.827053	0.213748	0.000000
C	0.826940	-2.592109	0.000000
O	1.220622	2.269440	0.000000
H	-1.436629	2.371587	0.000000
H	-2.904072	0.292831	0.000000
H	-1.833018	-1.941672	0.000000
H	2.104662	-0.124270	0.000000
H	0.697193	3.083058	0.000000
H	0.074857	-3.382350	0.000000
H	1.471957	-2.739982	-0.877653
H	1.471957	-2.739982	0.877653

p-cresol S_0

C	0.710913	0.011299	-1.189862
C	-0.676185	0.013268	-1.198070
C	-1.374801	0.000369	0.007436
C	-0.672412	-0.016639	1.208340
C	0.720012	-0.018389	1.197571
C	1.439430	-0.002586	0.004225
O	-2.744765	0.000620	-0.053927
C	2.947477	0.021659	-0.004989
H	-1.207449	-0.031666	2.152664
H	1.251460	-0.034277	2.142539
H	1.240245	0.018830	-2.136474
H	-1.231293	0.021584	-2.127318
H	-3.108157	-0.010510	0.838558
H	3.353746	-0.664109	-0.751844
H	3.329256	1.019909	-0.239849
H	3.354082	-0.263986	0.966299

p-cresol S_1

C	0.732469	-0.083614	-1.235125
C	-0.685517	-0.031740	-1.243001
C	-1.355970	-0.012778	-0.000919
C	-0.685426	-0.004286	1.251197
C	0.731492	-0.016384	1.238125
C	1.431889	-0.034016	0.001512
O	-2.706584	0.014531	-0.047680
C	2.919870	0.041662	-0.000792
H	-1.247610	-0.084991	2.173344
H	1.288783	-0.011797	2.164706
H	1.287010	-0.107211	-2.162620
H	-1.261580	0.040555	-2.154027
H	-3.057776	0.121545	0.848364
H	3.343660	-0.497566	-0.852027
H	3.250989	1.086110	-0.089149
H	3.345851	-0.354642	0.923380

o-methoxyphenol S_0

C	2.035437	-0.092276	0.000000
C	0.881241	0.694589	0.000000
C	-0.365491	0.085197	0.000000
C	-0.466432	-1.316651	0.000000
C	0.683410	-2.089115	0.000000

C	1.935560	-1.475996	0.000000
O	-1.579963	0.729023	0.000000
O	-1.691002	-1.916005	0.000000
H	0.582734	-3.166867	0.000000
H	2.829141	-2.087111	0.000000
H	3.005634	0.387620	0.000000
H	0.966035	1.772533	0.000000
C	-1.595613	2.149882	0.000000
H	-2.360328	-1.217440	0.000000
H	-2.643882	2.439731	0.000000
H	-1.108240	2.551443	0.893210
H	-1.108240	2.551443	-0.893210

o-methoxyphenol S_1

C	2.486015	0.054379	0.059853
C	1.384672	-0.285627	-0.746620
C	0.112572	-0.284997	-0.091524
C	0.018815	-0.153878	1.317564
C	1.180249	-0.039029	2.138143
C	2.388593	0.177444	1.464234
O	-1.084036	-0.127331	-0.738215
O	-1.183879	0.063781	1.893189
H	1.107512	-0.148301	3.211002
H	3.281982	0.429624	2.024856
H	3.454152	0.212327	-0.405441
H	1.518457	-0.652874	-1.756430
C	-1.093311	0.135135	-2.151952
H	-1.867003	0.028004	1.198247
H	-2.137470	0.293120	-2.409576
H	-0.504316	1.022136	-2.387964
H	-0.704446	-0.723923	-2.701286

m-methoxyphenol, isomer 1 S_0

C	0.929644	1.446124	0.000000
C	-0.260246	0.714306	0.000000
C	-0.226388	-0.680859	0.000000
C	1.007853	-1.336192	0.000000
C	2.197494	-0.618948	0.000000
C	2.140625	0.771564	0.000000
H	-1.138787	-1.263360	0.000000
O	1.094213	-2.703489	0.000000
H	3.139147	-1.150507	0.000000
H	3.063189	1.339125	0.000000
H	0.879607	2.526391	0.000000

O	-1.411252	1.447117	0.000000
H	0.210218	-3.086925	0.000000
C	-2.656193	0.765817	0.000000
H	-3.419697	1.540450	0.000000
H	-2.774713	0.144694	-0.893589
H	-2.774713	0.144694	0.893589

m-methoxyphenol, isomer 1 S_1

C	1.167831	-0.010217	-0.620398
C	-0.029338	-0.030484	0.131460
C	-0.047764	-0.071810	1.554284
C	1.243360	-0.012275	2.151429
C	2.449143	0.004756	1.416989
C	2.435216	-0.099463	0.008339
H	-0.877355	-0.512982	2.099839
O	1.354442	0.110024	3.500692
H	3.372975	0.134371	1.967176
H	3.347425	-0.128311	-0.565908
H	1.078510	0.086497	-1.695174
O	-1.158971	0.046395	-0.618232
H	0.492525	0.389109	3.853992
C	-2.433255	0.026382	0.022398
H	-3.153541	0.314258	-0.739608
H	-2.669002	-0.979105	0.381746
H	-2.463891	0.732856	0.853717

m-methoxyphenol, isomer 2 S_0

C	0.347796	2.163089	0.000000
C	-0.836005	1.447270	0.000000
C	-0.790768	0.047711	0.000000
C	0.432510	-0.616998	0.000000
C	1.613189	0.127172	0.000000
C	1.583759	1.516910	0.000000
O	-1.998871	-0.583640	0.000000
C	-2.026238	-2.004140	0.000000
O	2.782680	-0.587141	0.000000
H	0.506706	-1.694212	0.000000
H	2.505758	2.087522	0.000000
H	0.315423	3.245743	0.000000
H	-1.798460	1.940322	0.000000
H	-3.078066	-2.281036	0.000000
H	-1.544870	-2.414815	-0.892797
H	-1.544870	-2.414815	0.892797
H	3.530317	0.021066	0.000000

m-methoxyphenol, isomer 2 S_1

C	1.241283	-0.075080	-0.711957
C	0.054054	-0.023632	0.073641
C	0.112578	-0.039228	1.485656
C	1.341796	-0.028697	2.200602
C	2.508722	0.010265	1.397540
C	2.474334	0.031933	-0.014829
O	-1.098636	-0.026994	2.099724
C	-1.166154	0.028423	3.522117
O	3.692052	0.054102	2.071625
H	1.424482	-0.202897	3.260804
H	3.406296	0.137513	-0.560936
H	1.202316	-0.050777	-1.788959
H	-0.922595	0.036788	-0.387929
H	-2.223322	0.104279	3.764379
H	-0.754198	-0.879737	3.969426
H	-0.633087	0.900575	3.907248
H	4.425211	0.023166	1.443747

p-methoxyphenol, *cis* S_0

C	-0.313609	0.729314	0.000000
C	-1.547316	0.070448	0.000000
C	-1.609110	-1.310920	0.000000
C	-0.434525	-2.065180	0.000000
C	0.792142	-1.416661	0.000000
C	0.858293	-0.021317	0.000000
O	-0.561812	-3.433472	0.000000
O	-0.366356	2.098137	0.000000
C	0.856137	2.816505	0.000000
H	1.828394	0.454696	0.000000
H	-2.452030	0.664558	0.000000
H	-2.562590	-1.822977	0.000000
H	1.712744	-1.991259	0.000000
H	0.584258	3.869826	0.000000
H	1.451667	2.598747	0.892855
H	1.451667	2.598747	-0.892855
H	0.312046	-3.839172	0.000000

p-methoxyphenol, *cis* S_1

C	1.329716	-0.026500	-0.612259
C	0.051279	-0.049823	0.003310
C	-0.017780	-0.004341	1.417798

C	1.186395	-0.008001	2.143825
C	2.468512	-0.015483	1.535468
C	2.540411	-0.014042	0.118975
O	1.082360	0.007168	3.493632
O	1.290810	-0.032892	-1.961725
C	2.495711	0.029328	-2.724890
H	3.497719	-0.024696	-0.377456
H	-0.829727	-0.050626	-0.619869
H	-0.955119	0.081043	1.947286
H	3.356908	-0.155286	2.138862
H	2.183531	0.018050	-3.765791
H	3.043114	0.949070	-2.510210
H	3.128659	-0.836379	-2.519725
H	1.961031	0.133393	3.879770

p-methoxyphenol, *trans* S_0

C	-0.657814	1.303408	0.000000
C	-1.891863	0.671487	0.000000
C	-1.968915	-0.721596	0.000000
C	-0.799163	-1.468937	0.000000
C	0.442474	-0.837450	0.000000
C	0.520062	0.555130	0.000000
O	-3.163476	-1.401444	0.000000
H	1.335988	-1.445472	0.000000
O	1.686973	1.272984	0.000000
H	-0.588938	2.383485	0.000000
H	-2.798856	1.267443	0.000000
H	-3.892919	-0.772189	0.000000
H	-0.864755	-2.549240	0.000000
C	2.912887	0.559998	0.000000
H	3.697323	1.313743	0.000000
H	3.015491	-0.065685	0.892753
H	3.015491	-0.065685	-0.892753

p-methoxyphenol, *trans* S_1

C	0.122542	-0.030406	-1.391944
C	-1.284650	-0.017985	-1.219491
C	-1.789010	0.016935	0.101626
C	-0.969427	0.056168	1.248261
C	0.438898	0.027991	1.079329
C	0.949497	-0.000730	-0.238686
O	-3.124487	0.026380	0.325452
H	1.090491	0.057238	1.937674
O	2.271131	-0.012879	-0.515082

H	0.586493	-0.064602	-2.365898
H	-1.956913	-0.139362	-2.059533
H	-3.590337	0.079180	-0.520594
H	-1.428032	0.141115	2.222139
C	3.233109	-0.022090	0.539914
H	4.203484	-0.035864	0.050783
H	3.141025	0.875088	1.155171
H	3.116975	-0.911867	1.161580

1-naphthol, *cis* S_0

C	0.830778	1.518341	0.014542
C	0.529571	0.123860	-0.000199
C	-0.847439	-0.268502	-0.006766
C	-1.859102	0.721825	-0.016029
C	-1.522355	2.051526	-0.017084
C	-0.174763	2.455267	0.000476
C	1.523619	-0.886856	-0.012039
C	1.185870	-2.216808	-0.013905
C	-0.170471	-2.604224	-0.008687
C	-1.156959	-1.652255	-0.007627
O	2.117817	1.981796	0.029571
H	-2.200061	-1.947108	-0.009261
H	-0.428012	-3.656187	-0.009614
H	1.961785	-2.972050	-0.024400
H	2.577294	-0.628291	-0.032130
H	-2.897260	0.413126	-0.023237
H	-2.296625	2.808821	-0.026122
H	0.091239	3.504181	0.009520
H	2.735083	1.253549	0.152987

1-naphthol, *cis* S_1

C	0.864608	1.470969	0.013458
C	0.534546	0.086925	-0.056302
C	-0.845334	-0.246412	0.005272
C	-1.794141	0.809533	-0.014731
C	-1.432097	2.174443	-0.025156
C	-0.102825	2.515261	-0.027172
C	1.516220	-0.935258	-0.116428
C	1.099757	-2.297633	-0.042571
C	-0.234674	-2.619992	0.041898
C	-1.232474	-1.610791	0.048636
O	2.138702	1.865494	0.136227
H	-2.280902	-1.869354	0.105337
H	-0.533615	-3.659634	0.098148

H	1.847410	-3.080613	-0.061772
H	2.558969	-0.715461	-0.312879
H	-2.846108	0.548771	-0.021136
H	-2.199114	2.936465	-0.051165
H	0.242726	3.539690	-0.012795
H	2.698346	1.087585	0.293109

1-naphthol, *trans* S_0

C	-0.717152	-0.541694	0.000000
C	-0.673678	-1.958384	0.000000
C	0.522475	-2.630055	0.000000
C	1.739860	-1.916536	0.000000
C	1.739205	-0.543881	0.000000
C	0.518983	0.173680	0.000000
H	-1.609108	-2.506065	0.000000
H	0.536186	-3.713284	0.000000
H	2.678349	-2.457193	0.000000
H	2.668902	0.008284	0.000000
C	-1.941334	0.174705	0.000000
C	-1.939122	1.544660	0.000000
C	-0.726207	2.265000	0.000000
C	0.474939	1.596907	0.000000
H	-2.874085	-0.376061	0.000000
H	-2.873790	2.091864	0.000000
H	-0.743247	3.350016	0.000000
O	1.682081	2.242613	0.000000
H	1.536755	3.195414	0.000000

1-naphthol, *trans* S_1

C	-0.936455	-0.392063	0.000000
C	-1.312111	-1.754762	0.000000
C	-0.315076	-2.771392	0.000000
C	1.018152	-2.434929	0.000000
C	1.429474	-1.071080	0.000000
C	0.452588	-0.049696	0.000000
H	-2.362215	-2.016646	0.000000
H	-0.615482	-3.811895	0.000000
H	1.774591	-3.210637	0.000000
H	2.478437	-0.815321	0.000000
C	-1.891254	0.653582	0.000000
C	-1.530588	2.023834	0.000000
C	-0.203644	2.369803	0.000000
C	0.778540	1.332003	0.000000
H	-2.942992	0.391184	0.000000

H	-2.300887	2.783599	0.000000
H	0.115039	3.406352	0.000000
O	2.089649	1.653489	0.000000
H	2.198555	2.613647	0.000000

2-naphthol, *cis* S_0

C	0.597839	2.011210	0.000000
C	0.622792	0.595891	0.000000
C	-0.613032	-0.121136	0.000000
C	-1.824052	0.615608	0.000000
C	-1.813310	1.988026	0.000000
C	-0.591825	2.695628	0.000000
C	1.833260	-0.143904	0.000000
C	1.832148	-1.511755	0.000000
C	0.605567	-2.215811	0.000000
C	-0.588950	-1.537857	0.000000
H	-1.528796	-2.081628	0.000000
H	1.539310	2.549013	0.000000
H	-0.598242	3.778547	0.000000
H	-2.748132	2.535457	0.000000
H	-2.764996	0.077004	0.000000
H	2.774509	0.393734	0.000000
H	2.753574	-2.079384	0.000000
O	0.697996	-3.581451	0.000000
H	-0.185668	-3.967183	0.000000

2-naphthol, *cis* S_1

C	0.599340	1.996000	0.000000
C	0.640930	0.586950	0.000000
C	-0.622680	-0.115660	0.000000
C	-1.831380	0.609010	0.000000
C	-1.840250	2.026230	0.000000
C	-0.632100	2.698660	0.000000
C	1.847950	-0.152270	0.000000
C	1.882370	-1.560790	0.000000
C	0.661080	-2.225020	0.000000
C	-0.579000	-1.525010	0.000000
H	-1.504450	-2.093840	0.000000
H	1.528660	2.552980	0.000000
H	-0.613420	3.782250	0.000000
H	-2.777320	2.566310	0.000000
H	-2.768360	0.063580	0.000000
H	2.782780	0.396360	0.000000
H	2.806760	-2.118660	0.000000

O	0.663270	-3.577140	0.000000
H	-0.244170	-3.909930	0.000000

2-naphthol, *trans* S_0

C	0.510481	2.013336	0.000000
C	0.541332	0.596903	0.000000
C	-0.691805	-0.127559	0.000000
C	-1.906779	0.605783	0.000000
C	-1.901205	1.977117	0.000000
C	-0.681766	2.691124	0.000000
C	1.752654	-0.135913	0.000000
C	1.752115	-1.506413	0.000000
C	0.528680	-2.216430	0.000000
C	-0.666894	-1.541131	0.000000
H	-1.593131	-2.102116	0.000000
H	1.449484	2.555535	0.000000
H	-0.693806	3.774023	0.000000
H	-2.838069	2.521083	0.000000
H	-2.844581	0.062227	0.000000
H	2.693149	0.402956	0.000000
H	2.689260	-2.054092	0.000000
O	0.500490	-3.586072	0.000000
H	1.400400	-3.930361	0.000000

2-naphthol, *trans* S_1

C	0.510978	2.000496	0.000000
C	0.555084	0.591716	0.000000
C	-0.704368	-0.116459	0.000000
C	-1.914086	0.604557	0.000000
C	-1.926332	2.022094	0.000000
C	-0.722187	2.699251	0.000000
C	1.764613	-0.141861	0.000000
C	1.800770	-1.550969	0.000000
C	0.577000	-2.217919	0.000000
C	-0.661407	-1.525704	0.000000
H	-1.571243	-2.112224	0.000000
H	1.438737	2.559756	0.000000
H	-0.707517	3.782631	0.000000
H	-2.865289	2.558453	0.000000
H	-2.848753	0.056374	0.000000
H	2.697795	0.408980	0.000000
H	2.736985	-2.093795	0.000000
O	0.477959	-3.566497	0.000000
H	1.361262	-3.958870	0.000000

5-methoxysalicylic acid S_0

C	2.279780	-0.164394	0.000000
C	1.565936	-1.340646	0.000000
C	0.160258	-1.333561	0.000000
C	-0.509522	-0.125925	0.000000
C	0.211058	1.088164	0.000000
C	1.619559	1.072602	0.000000
O	-0.435085	-2.564133	0.000000
C	-1.853625	-2.620977	0.000000
C	-0.477836	2.377093	0.000000
O	-1.826261	2.301338	0.000000
O	2.375646	2.186101	0.000000
O	0.085819	3.465456	0.000000
H	-2.110355	-3.677785	0.000000
H	-2.274097	-2.146960	-0.892771
H	-2.274097	-2.146960	0.892771
H	-1.587239	-0.077631	0.000000
H	3.361685	-0.168032	0.000000
H	2.075011	-2.296120	0.000000
H	1.770597	2.959688	0.000000
H	-2.157211	3.212682	0.000000

5-methoxysalicylic acid S_1

C	2.174052	-0.136324	0.000000
C	1.733492	-1.459629	0.000000
C	0.347569	-1.685523	0.000000
C	-0.588475	-0.610699	0.000000
C	-0.156310	0.713008	0.000000
C	1.269670	0.934231	0.000000
O	-0.035848	-2.974678	0.000000
C	-1.421059	-3.336976	0.000000
C	-1.042153	1.851002	0.000000
O	-2.380359	1.557057	0.000000
O	1.731254	2.179714	0.000000
O	-0.653398	3.051565	0.000000
H	-1.433628	-4.423143	0.000000
H	-1.920998	-2.961554	-0.894437
H	-1.920998	-2.961554	0.894437
H	-1.649771	-0.807837	0.000000
H	3.229848	0.100650	0.000000
H	2.414730	-2.296979	0.000000
H	0.912808	2.788990	0.000000
H	-2.838375	2.409458	0.000000

m-dimethoxybenzene, *trans* S_0

C	0.000000	-0.707606	-0.169392
C	0.000000	0.707606	-0.169392
C	0.000000	1.389445	1.040586
C	0.000000	0.691067	2.251548
C	0.000000	-0.691067	2.251548
C	0.000000	-1.389445	1.040586
O	0.000000	1.297647	-1.396297
H	0.000000	2.470089	1.052254
H	0.000000	1.241980	3.183477
H	0.000000	-1.241980	3.183477
H	0.000000	-2.470089	1.052254
O	0.000000	-1.297647	-1.396297
C	0.000000	-2.714599	-1.460796
H	0.000000	-2.962496	-2.519934
H	0.892653	-3.139859	-0.990712
H	-0.892653	-3.139859	-0.990712
C	0.000000	2.714599	-1.460796
H	0.000000	2.962496	-2.519934
H	-0.892653	3.139859	-0.990712
H	0.892653	3.139859	-0.990712

m-dimethoxybenzene, *trans* S_1

C	-0.110813	-1.073075	-1.446202
C	-0.291626	0.146196	-0.708836
C	-0.291626	0.146196	0.708836
C	-0.110813	-1.073075	1.446202
C	0.279095	-2.198155	0.704635
C	0.279095	-2.198155	-0.704635
O	-0.281915	1.367146	-1.297859
C	0.008156	1.471878	-2.695261
O	-0.281915	1.367146	1.297859
C	0.008156	1.471878	2.695261
H	-0.390750	-1.158926	2.488528
H	0.552504	-3.111448	1.223580
H	0.552504	-3.111448	-1.223580
H	-0.390750	-1.158926	-2.488528
H	0.028690	2.538475	-2.905018
H	0.973509	1.022259	-2.933628
H	-0.773762	0.998090	-3.292747
H	0.028690	2.538475	2.905018
H	-0.773762	0.998090	3.292747
H	0.973509	1.022259	2.933628

3P-propionic acid, *gauche* S_0

C	-1.039750	0.903712	-1.170395
C	-0.392391	0.662737	0.044709
C	-1.058573	-0.091079	1.014127
C	-2.334200	-0.592474	0.773092
C	-2.966251	-0.347747	-0.441594
C	-2.314285	0.403665	-1.414583
C	1.001474	1.198140	0.289798
C	2.117799	0.277196	-0.226782
C	2.336617	-0.950610	0.626138
O	2.056658	-1.062116	1.793220
O	2.944072	-1.942186	-0.071231
H	1.936712	-0.034553	-1.256420
H	3.073036	0.814279	-0.230038
H	1.153168	1.368405	1.356685
H	1.107203	2.164455	-0.208741
H	-0.568724	-0.289117	1.959564
H	-2.835709	-1.173042	1.538199
H	-3.960558	-0.735248	-0.627525
H	-2.800641	0.606121	-2.361388
H	-0.544259	1.497488	-1.931514
H	3.088612	-2.678046	0.544690

3P-propionic acid, *gauche* S_1

C	-0.690643	0.240762	-1.096931
C	-0.362209	0.550006	0.261196
C	-1.352555	0.372907	1.272814
C	-2.659640	-0.058395	0.937907
C	-2.973858	-0.347118	-0.414274
C	-1.996786	-0.195382	-1.430900
C	0.971853	1.111877	0.626118
C	2.166265	0.500764	-0.120053
C	2.313616	-0.976892	0.146697
O	1.970962	-1.549253	1.154833
O	2.945703	-1.616562	-0.876087
H	2.114584	0.673163	-1.195143
H	3.086290	0.990622	0.220142
H	1.123774	1.001714	1.701223
H	0.975254	2.195168	0.422024
H	-1.086025	0.552348	2.305596
H	-3.408399	-0.180409	1.707813
H	-3.967637	-0.687727	-0.673864
H	-2.249532	-0.413329	-2.459293

H	0.042704	0.381225	-1.877784
H	3.036287	-2.545498	-0.612034

3P-propionic acid, *anti* S_0

C	1.466946	-0.447881	0.000000
C	0.542642	0.775377	0.000000
C	2.931929	-0.085962	0.000000
H	1.278300	-1.082931	0.870291
H	1.278300	-1.082931	-0.870291
C	-0.917669	0.385911	0.000000
H	0.766819	1.390877	0.873201
H	0.766819	1.390877	-0.873201
C	-1.606526	0.188999	1.199093
C	-2.942566	-0.198665	1.201922
C	-3.615141	-0.395545	0.000000
C	-2.942566	-0.198665	-1.201922
C	-1.606526	0.188999	-1.199093
H	-1.093529	0.349119	2.141390
H	-3.459931	-0.341523	2.143081
H	-4.656375	-0.693771	0.000000
H	-3.459931	-0.341523	-2.143081
H	-1.093529	0.349119	-2.141390
O	3.716274	-1.194574	0.000000
O	3.391039	1.027953	0.000000
H	4.638057	-0.891940	0.000000

3P-propionic acid, *anti* S_1

C	1.470453	-0.434134	0.000000
C	0.557256	0.809392	0.000000
C	2.937461	-0.083436	0.000000
H	1.269040	-1.062553	0.872001
H	1.269040	-1.062553	-0.872001
C	-0.888972	0.444348	0.000000
H	0.795644	1.414351	0.878706
H	0.795644	1.414351	-0.878706
C	-1.581965	0.235261	1.231940
C	-2.928978	-0.215972	1.232329
C	-3.596845	-0.437548	0.000000
C	-2.928978	-0.215972	-1.232329
C	-1.581965	0.235261	-1.231940
H	-1.072387	0.427146	2.167215
H	-3.444376	-0.389708	2.166608
H	-4.624447	-0.776068	0.000000
H	-3.444376	-0.389708	-2.166608

H	-1.072387	0.427146	-2.167215
O	3.711669	-1.199919	0.000000
O	3.405673	1.027478	0.000000
H	4.636422	-0.906004	0.000000

fluorine S_0

C	0.000000	0.000000	-1.793872
C	0.000000	1.181917	-0.850043
C	0.000000	0.733675	0.483084
C	0.000000	-0.733675	0.483084
C	0.000000	1.648576	1.532983
C	0.000000	3.009378	1.240168
C	0.000000	3.452371	-0.082385
C	0.000000	2.538054	-1.135946
H	0.000000	2.889427	-2.161680
H	0.000000	4.515033	-0.292308
H	0.000000	3.732389	2.046878
H	0.000000	1.312945	2.563283
C	0.000000	-1.648576	1.532983
C	0.000000	-3.009378	1.240168
C	0.000000	-3.452371	-0.082385
C	0.000000	-2.538054	-1.135946
C	0.000000	-1.181917	-0.850043
H	0.000000	-1.312945	2.563283
H	0.000000	-3.732389	2.046878
H	0.000000	-4.515033	-0.292308
H	0.000000	-2.889427	-2.161680
H	-0.878756	0.000000	-2.447089
H	0.878756	0.000000	-2.447089

fluorine S_1

C	0.000000	0.000000	-1.866771
C	0.000000	1.182508	-0.917552
C	0.000000	0.700554	0.451385
C	0.000000	-0.700554	0.451385
C	0.000000	1.642723	1.536167
C	0.000000	2.985260	1.230840
C	0.000000	3.442324	-0.106494
C	0.000000	2.526870	-1.186759
H	0.000000	2.894164	-2.206442
H	0.000000	4.506590	-0.305009
H	0.000000	3.717344	2.029915
H	0.000000	1.299947	2.562744
C	0.000000	-1.642723	1.536167

C	0.000000	-2.985260	1.230840
C	0.000000	-3.442324	-0.106494
C	0.000000	-2.526870	-1.186759
C	0.000000	-1.182508	-0.917552
H	0.000000	-1.299947	2.562744
H	0.000000	-3.717344	2.029915
H	0.000000	-4.506590	-0.305009
H	0.000000	-2.894164	-2.206442
H	-0.877962	0.000000	-2.523247
H	0.877962	0.000000	-2.523247

phenanthrene S_0

C	0.727341	0.000000	-0.351684
C	-0.727341	0.000000	-0.351684
C	-1.419262	0.000000	0.891197
C	-0.677222	0.000000	2.115797
C	0.677222	0.000000	2.115797
C	1.419262	0.000000	0.891197
C	-1.496301	0.000000	-1.534662
C	-2.830169	0.000000	0.903080
H	-1.226910	0.000000	3.050105
H	1.226910	0.000000	3.050105
C	1.496301	0.000000	-1.534662
C	2.874044	0.000000	-1.497775
C	3.550999	0.000000	-0.268753
C	2.830169	0.000000	0.903080
H	1.004654	0.000000	-2.497663
H	3.436197	0.000000	-2.423647
H	4.633768	0.000000	-0.244989
H	3.341408	0.000000	1.859083
C	-3.550999	0.000000	-0.268753
C	-2.874044	0.000000	-1.497775
H	-1.004654	0.000000	-2.497663
H	-3.436197	0.000000	-2.423647
H	-4.633768	0.000000	-0.244989
H	-3.341408	0.000000	1.859083

phenanthrene S_1

C	0.713217	0.000000	-0.383114
C	-0.713217	0.000000	-0.383114
C	-1.436114	0.000000	0.883912
C	-0.696837	0.000000	2.082271
C	0.696837	0.000000	2.082271
C	1.436114	0.000000	0.883912

C	-1.495344	0.000000	-1.569583
C	-2.842263	0.000000	0.886818
H	-1.230773	0.000000	3.025350
H	1.230773	0.000000	3.025350
C	1.495344	0.000000	-1.569583
C	2.887605	0.000000	-1.526705
C	3.573540	0.000000	-0.305314
C	2.842263	0.000000	0.886818
H	1.010172	0.000000	-2.534943
H	3.444545	0.000000	-2.455649
H	4.655053	0.000000	-0.283683
H	3.358557	0.000000	1.839679
C	-3.573540	0.000000	-0.305314
C	-2.887605	0.000000	-1.526705
H	-1.010172	0.000000	-2.534943
H	-3.444545	0.000000	-2.455649
H	-4.655053	0.000000	-0.283683
H	-3.358557	0.000000	1.839679

2,4,6,8-decatetraene S_0

C	-2.590146	-5.015583	0.000000
C	-2.472178	-3.525678	0.000000
C	-1.318151	-2.841467	0.000000
C	-1.216689	-1.402081	0.000000
C	-0.052563	-0.716434	0.000000
C	0.052563	0.716434	0.000000
C	1.216689	1.402081	0.000000
C	1.318151	2.841467	0.000000
C	2.472178	3.525678	0.000000
C	2.590146	5.015583	0.000000
H	-0.380493	-3.394393	0.000000
H	-2.151360	-0.845092	0.000000
H	0.880810	-1.276260	0.000000
H	-0.880810	1.276260	0.000000
H	2.151360	0.845092	0.000000
H	0.380493	3.394393	0.000000
H	3.405713	2.966697	0.000000
H	-3.405713	-2.966697	0.000000
H	1.611067	5.496329	0.000000
H	3.144424	5.368422	0.876487
H	3.144424	5.368422	-0.876487
H	-1.611067	-5.496329	0.000000
H	-3.144424	-5.368422	0.876487
H	-3.144424	-5.368422	-0.876487

2,4,6,8-decatetraene S_1

C	-2.584166	-5.029821	0.000000
C	-2.520962	-3.545308	0.000000
C	-1.356446	-2.816426	0.000000
C	-1.265625	-1.409746	0.000000
C	-0.054368	-0.696186	0.000000
C	0.054368	0.696186	0.000000
C	1.265625	1.409746	0.000000
C	1.356446	2.816426	0.000000
C	2.520962	3.545308	0.000000
C	2.584166	5.029821	0.000000
H	-0.416770	-3.367636	0.000000
H	-2.191338	-0.838635	0.000000
H	0.867045	-1.275098	0.000000
H	-0.867045	1.275098	0.000000
H	2.191338	0.838635	0.000000
H	0.416770	3.367636	0.000000
H	3.467531	3.009116	0.000000
H	-3.467531	-3.009116	0.000000
H	1.587863	5.476560	0.000000
H	3.127439	5.415218	0.874700
H	3.127439	5.415218	-0.874700
H	-1.587863	-5.476560	0.000000
H	-3.127439	-5.415218	0.874700
H	-3.127439	-5.415218	-0.874700

tetracene S_0

C	3.701544	1.405132	0.000000
C	2.442975	0.724011	0.000000
C	2.442975	-0.724011	0.000000
C	3.701544	-1.405132	0.000000
C	4.874449	-0.713560	0.000000
C	4.874449	0.713560	0.000000
C	1.232042	1.402578	0.000000
C	0.000000	0.724150	0.000000
C	0.000000	-0.724150	0.000000
C	1.232042	-1.402578	0.000000
C	-1.232042	1.402578	0.000000
C	-2.442975	0.724011	0.000000
C	-2.442975	-0.724011	0.000000
C	-1.232042	-1.402578	0.000000
C	-3.701544	1.405132	0.000000
C	-4.874449	0.713560	0.000000
C	-4.874449	-0.713560	0.000000

C	-3.701544	-1.405132	0.000000
H	-3.701580	-2.489194	0.000000
H	-5.819069	-1.243525	0.000000
H	-5.819069	1.243525	0.000000
H	-3.701580	2.489194	0.000000
H	-1.232320	-2.487392	0.000000
H	-1.232320	2.487392	0.000000
H	1.232320	-2.487392	0.000000
H	1.232320	2.487392	0.000000
H	3.701580	-2.489194	0.000000
H	5.819069	-1.243525	0.000000
H	5.819069	1.243525	0.000000
H	3.701580	2.489194	0.000000

tetracene S_1

C	3.704126	1.396660	0.000000
C	2.470095	0.720289	0.000000
C	2.470095	-0.720289	0.000000
C	3.704126	-1.396660	0.000000
C	4.908836	-0.697940	0.000000
C	4.908836	0.697940	0.000000
C	1.230157	1.397218	0.000000
C	0.000000	0.724565	0.000000
C	0.000000	-0.724565	0.000000
C	1.230157	-1.397218	0.000000
C	-1.230157	1.397218	0.000000
C	-2.470095	0.720289	0.000000
C	-2.470095	-0.720289	0.000000
C	-1.230157	-1.397218	0.000000
C	-3.704126	1.396660	0.000000
C	-4.908836	0.697940	0.000000
C	-4.908836	-0.697940	0.000000
C	-3.704126	-1.396660	0.000000
H	-3.707608	-2.480602	0.000000
H	-5.845949	-1.240319	0.000000
H	-5.845949	1.240319	0.000000
H	-3.707608	2.480602	0.000000
H	-1.231749	-2.482172	0.000000
H	-1.231749	2.482172	0.000000
H	1.231749	-2.482172	0.000000
H	1.231749	2.482172	0.000000
H	3.707608	-2.480602	0.000000
H	5.845949	-1.240319	0.000000
H	5.845949	1.240319	0.000000
H	3.707608	2.480602	0.000000

perylene S_0

C	0.020203	1.475614	-2.420285
C	0.010956	0.737097	-1.246515
C	0.014120	1.436211	0.000003
C	0.034599	2.867787	0.000001
C	0.043306	3.565836	-1.230100
C	0.036337	2.877860	-2.415522
C	0.044411	3.565824	1.230101
C	0.038550	2.877835	2.415522
C	0.022112	1.475592	2.420285
C	0.011532	0.737089	1.246518
C	-0.010956	-0.737097	-1.246515
C	-0.014120	-1.436211	0.000003
C	-0.011532	-0.737089	1.246518
C	-0.034599	-2.867787	0.000001
C	-0.044411	-3.565824	1.230101
C	-0.038550	-2.877835	2.415522
C	-0.022112	-1.475592	2.420285
C	-0.020203	-1.475614	-2.420285
C	-0.036337	-2.877860	-2.415522
C	-0.043306	-3.565836	-1.230100
H	0.057810	4.649271	1.217298
H	0.046783	3.411504	3.358082
H	0.019053	0.974748	3.377800
H	-0.057810	-4.649271	1.217298
H	-0.046783	-3.411504	3.358082
H	-0.019053	-0.974748	3.377800
H	-0.056663	-4.649285	-1.217298
H	-0.043529	-3.411540	-3.358085
H	-0.016132	-0.974781	-3.377802
H	0.056663	4.649285	-1.217298
H	0.043529	3.411540	-3.358085
H	0.016132	0.974781	-3.377802

perylene S_1

C	-0.006753	1.469981	-2.449088
C	-0.006337	0.719704	-1.241674
C	0.010227	1.421963	-0.000003
C	0.008344	2.854711	0.000000
C	0.009416	3.546975	-1.230625
C	-0.001625	2.853779	-2.434092
C	0.009735	3.546971	1.230621
C	-0.000983	2.853769	2.434094

C	-0.006209	1.469976	2.449085
C	-0.006198	0.719702	1.241669
C	0.006337	-0.719704	-1.241674
C	-0.010227	-1.421963	-0.000003
C	0.006198	-0.719702	1.241669
C	-0.008344	-2.854711	0.000000
C	-0.009735	-3.546971	1.230621
C	0.000983	-2.853769	2.434094
C	0.006209	-1.469976	2.449085
C	0.006753	-1.469981	-2.449088
C	0.001625	-2.853779	-2.434092
C	-0.009416	-3.546975	-1.230625
H	0.014119	4.630425	1.222967
H	-0.004716	3.399248	3.369976
H	-0.029103	0.961720	3.401205
H	-0.014119	-4.630425	1.222967
H	0.004716	-3.399248	3.369976
H	0.029103	-0.961720	3.401205
H	-0.013768	-4.630429	-1.222966
H	0.005696	-3.399257	-3.369973
H	0.030023	-0.961732	-3.401201
H	0.013768	4.630429	-1.222966
H	-0.005696	3.399257	-3.369973
H	-0.030023	0.961732	-3.401201

PBE0/TZVP geometries – Group I

pyrazine S_0

C	1.126134	-0.694452	0.000000
C	1.126134	0.694452	0.000000
N	0.000000	1.399102	0.000000
C	-1.126134	0.694452	0.000000
C	-1.126134	-0.694452	0.000000
N	0.000000	-1.399102	0.000000
H	-2.058237	-1.251875	0.000000
H	2.058237	-1.251875	0.000000
H	2.058237	1.251875	0.000000
H	-2.058237	1.251875	0.000000

pyrazine S_1

C	-1.203528	0.671715	0.000000
C	-1.112033	-0.738801	0.000000
N	0.022663	-1.349694	0.000000

C	1.203528	-0.671715	0.000000
C	1.112033	0.738801	0.000000
N	-0.022663	1.349694	0.000000
H	2.040861	1.307501	0.000000
H	-2.155920	1.178163	0.000000
H	-2.040861	-1.307501	0.000000
H	2.155920	-1.178163	0.000000

2,6-difluoropyridine S_0

C	1.113061	0.000000	-0.875147
N	0.000000	0.000000	-1.564782
C	-1.113061	0.000000	-0.875147
C	-1.200692	0.000000	0.506061
C	0.000000	0.000000	1.199144
C	1.200692	0.000000	0.506061
F	-2.234451	0.000000	-1.588469
H	-2.162993	0.000000	0.999120
H	0.000000	0.000000	2.282929
H	2.162993	0.000000	0.999120
F	2.234451	0.000000	-1.588469

2,6-difluoropyridine S_1

C	-1.097439	0.000000	-0.336019
N	0.000000	0.000000	-1.102521
C	1.097439	0.000000	-0.336019
C	1.189848	0.000000	1.070506
C	0.000000	0.000000	1.845793
C	-1.189848	0.000000	1.070506
F	2.233651	0.000000	-1.008800
H	2.177089	0.000000	1.515674
H	0.000000	0.000000	2.923302
H	-2.177089	0.000000	1.515674
F	-2.233651	0.000000	-1.008800

2-fluoropyridine S_0

C	-1.314008	0.502542	0.000000
N	-1.364532	-0.800561	0.000000
C	-0.198251	-1.448323	0.000000
C	1.028277	-0.807381	0.000000
C	1.042141	0.583012	0.000000
C	-0.157572	1.270181	0.000000
H	-0.260078	-2.532245	0.000000
H	1.946942	-1.380429	0.000000

H	1.979956	1.127040	0.000000
H	-0.214360	2.350872	0.000000
F	-2.488525	1.135282	0.000000

2-fluoropyridine S_1

C	-1.318346	0.488620	0.000000
N	-1.436568	-0.842857	0.000000
C	-0.226257	-1.460918	0.000000
C	1.026949	-0.790788	0.000000
C	1.107126	0.618741	0.000000
C	-0.151828	1.281314	0.000000
H	-0.248483	-2.544802	0.000000
H	1.925450	-1.397247	0.000000
H	2.044818	1.151954	0.000000
H	-0.254254	2.358534	0.000000
F	-2.468617	1.137438	0.000000

2-hydroxypyridine S_0

C	-0.978518	0.751041	0.000000
C	-0.970229	-0.644635	0.000000
N	0.129491	-1.375535	0.000000
C	1.299659	-0.736047	0.000000
C	1.415214	0.641254	0.000000
C	0.242406	1.392599	0.000000
O	-2.145579	-1.297639	0.000000
H	2.182513	-1.368554	0.000000
H	2.389726	1.112663	0.000000
H	0.283878	2.476306	0.000000
H	-1.918340	1.287712	0.000000
H	-1.930221	-2.239164	0.000000

2-hydroxypyridine S_1

C	-0.999611	0.767337	0.000000
C	-0.965848	-0.633713	0.000000
N	0.114671	-1.450545	0.000000
C	1.288954	-0.773948	0.000000
C	1.386970	0.640083	0.000000
C	0.249752	1.460652	0.000000
O	-2.124548	-1.289903	0.000000
H	2.190760	-1.375145	0.000000
H	2.379812	1.076655	0.000000
H	0.311076	2.538010	0.000000
H	-1.957009	1.271199	0.000000

H	-1.874978	-2.230683	0.000000

2-pyridone S_0

C	-1.244899	0.712984	0.000000
N	-1.131631	-0.684404	0.000000
C	0.031385	-1.379856	0.000000
C	1.221392	-0.730701	0.000000
C	1.202855	0.688754	0.000000
C	0.035841	1.382805	0.000000
H	-2.015551	-1.172933	0.000000
H	-0.057463	-2.459320	0.000000
H	2.148266	-1.286371	0.000000
H	2.144832	1.227827	0.000000
H	0.010319	2.464818	0.000000
O	-2.345346	1.236406	0.000000

2-pyridone S_1

C	-1.367913	0.101128	0.000000
N	-0.730170	-1.121149	0.000000
C	0.628223	-1.252082	0.000000
C	1.413183	-0.076254	0.000000
C	0.829114	1.163614	0.000000
C	-0.612721	1.262953	0.000000
H	-1.345900	-1.921959	0.000000
H	1.035558	-2.251429	0.000000
H	2.490498	-0.187851	0.000000
H	1.435481	2.059456	0.000000
H	-1.133377	2.208757	0.000000
O	-2.641975	0.014806	0.000000

2-methylpyrimidine S_0

C	0.000128	1.959302	0.000000
C	-1.171868	1.219899	0.000000
N	-1.179285	-0.106166	0.000000
C	0.010343	-0.715192	0.000000
N	1.193397	-0.099013	0.000000
C	1.175499	1.230223	0.000000
H	-2.143798	1.707184	0.000000
H	2.144259	1.723390	0.000000
H	-0.004446	3.041855	0.000000
C	0.005196	-2.208431	0.000000
H	1.024323	-2.589825	0.000000
H	-0.526879	-2.581613	0.878165

H	-0.526879	-2.581613	-0.878165

2-methylpyrimidine S_1

C	-0.012877	2.007060	0.000000
C	-1.165366	1.272768	0.000000
N	-1.148803	-0.094803	0.000000
C	0.012548	-0.782303	0.000000
N	1.086460	-0.068972	0.000000
C	1.202574	1.289092	0.000000
H	-2.145505	1.735710	0.000000
H	2.190170	1.722112	0.000000
H	-0.025973	3.090351	0.000000
C	0.012907	-2.263525	0.000000
H	1.031771	-2.647625	0.000000
H	-0.518952	-2.629938	0.881268
H	-0.518952	-2.629938	-0.881268

5-methylpyrimidine S_0

C	0.872535	0.848742	0.000000
C	-0.361084	0.210516	0.000000
C	-0.298555	-1.179770	0.000000
N	0.843233	-1.856443	0.000000
C	1.953973	-1.126983	0.000000
N	2.031236	0.196873	0.000000
H	2.893852	-1.671279	0.000000
H	-1.210866	-1.773578	0.000000
H	0.929822	1.935565	0.000000
C	-1.656822	0.957165	0.000000
H	-1.486624	2.035083	0.000000
H	-2.255351	0.712044	-0.881144
H	-2.255351	0.712044	0.881144

5-methylpyrimidine S_1

C	0.843962	0.854247	0.000000
C	-0.378215	0.241626	0.000000
C	-0.347752	-1.187875	0.000000
N	0.879498	-1.756034	0.000000
C	2.028181	-1.177102	0.000000
N	2.026096	0.170190	0.000000
H	2.955693	-1.733140	0.000000
H	-1.218281	-1.825613	0.000000
H	0.929290	1.936188	0.000000
C	-1.672554	0.978203	0.000000

H	-1.510687	2.057067	0.000000
H	-2.267620	0.721127	-0.881792
H	-2.267620	0.721127	0.881792

7-azaindole S_0

N	-0.632061	1.837346	0.000000
C	-0.672317	0.470767	0.000000
C	0.667225	0.006998	0.000000
C	1.505646	1.162983	0.000000
C	0.678152	2.247926	0.000000
C	0.843617	-1.374964	0.000000
C	-0.291402	-2.166367	0.000000
C	-1.559854	-1.574491	0.000000
N	-1.772450	-0.263758	0.000000
H	-2.448261	-2.199298	0.000000
H	1.833985	-1.817648	0.000000
H	-0.212552	-3.246905	0.000000
H	-1.445658	2.427222	0.000000
H	2.584115	1.191021	0.000000
H	0.921835	3.299168	0.000000

7-azaindole S_1

N	-0.599782	1.866400	0.000000
C	-0.652662	0.442854	0.000000
C	0.650229	-0.011677	0.000000
C	1.489583	1.151316	0.000000
C	0.649749	2.305007	0.000000
C	0.889039	-1.410118	0.000000
C	-0.304967	-2.177539	0.000000
C	-1.549395	-1.587266	0.000000
N	-1.803354	-0.228238	0.000000
H	-2.436448	-2.212569	0.000000
H	1.876877	-1.846194	0.000000
H	-0.252863	-3.260417	0.000000
H	-1.434454	2.435021	0.000000
H	2.569464	1.182302	0.000000
H	0.908994	3.351137	0.000000

7-hydroxyquinoline, *cis* S_0

N	0.464538	1.965196	0.000000
C	0.434314	0.608647	0.000000
C	-0.784805	-0.125478	0.000000
C	-1.987607	0.605227	0.000000

C	-1.941318	1.972773	0.000000
C	-0.680605	2.601053	0.000000
C	1.659848	-0.088981	0.000000
C	1.674431	-1.460162	0.000000
C	0.466783	-2.193949	0.000000
C	-0.729528	-1.538282	0.000000
H	-0.623773	3.687392	0.000000
H	-1.657477	-2.101156	0.000000
H	0.521346	-3.276011	0.000000
O	2.814421	-2.193785	0.000000
H	2.574724	0.495128	0.000000
H	-2.935055	0.074914	0.000000
H	-2.844170	2.571500	0.000000
H	3.573935	-1.604017	0.000000

7-hydroxyquinoline, *cis* S_1

N	0.493973	1.967057	0.000000
C	0.423643	0.631098	0.000000
C	-0.784854	-0.133670	0.000000
C	-2.000488	0.596029	0.000000
C	-1.919620	1.996816	0.000000
C	-0.690944	2.634014	0.000000
C	1.632214	-0.096210	0.000000
C	1.657123	-1.521071	0.000000
C	0.485606	-2.265522	0.000000
C	-0.709851	-1.547783	0.000000
H	-0.626624	3.716048	0.000000
H	-1.645584	-2.099068	0.000000
H	0.518882	-3.345433	0.000000
O	2.831601	-2.157163	0.000000
H	2.561890	0.467103	0.000000
H	-2.954893	0.084688	0.000000
H	-2.826740	2.591711	0.000000
H	3.554667	-1.518634	0.000000

7-hydroxyquinoline, *trans* S_0

N	0.514148	2.037999	0.000000
C	0.482015	0.679487	0.000000
C	-0.742270	-0.049122	0.000000
C	-1.944151	0.685762	0.000000
C	-1.892797	2.051756	0.000000
C	-0.627963	2.675939	0.000000
C	1.704749	-0.017430	0.000000
C	1.716278	-1.388641	0.000000

C	0.504805	-2.116284	0.000000
C	-0.693550	-1.458972	0.000000
H	-0.568545	3.762283	0.000000
H	-1.622088	-2.020791	0.000000
H	0.532522	-3.202580	0.000000
O	2.915662	-2.023160	0.000000
H	2.629693	0.545024	0.000000
H	-2.893306	0.158447	0.000000
H	-2.793134	2.654322	0.000000
H	2.777912	-2.974020	0.000000

7-hydroxyquinoline, *trans* S_1

N	0.370956	1.958655	0.000076
C	0.520856	0.650847	0.000025
C	-0.752411	-0.066193	0.000014
C	-1.945218	0.712047	0.000008
C	-1.914966	2.097565	0.000006
C	-0.693172	2.756874	0.000014
C	1.734405	-0.035926	-0.000008
C	1.725245	-1.430463	-0.000012
C	0.537949	-2.143938	-0.000012
C	-0.679485	-1.454098	0.000010
H	-0.552943	3.828434	-0.000019
H	-1.611395	-2.009322	0.000020
H	0.549334	-3.228850	-0.000010
O	2.939990	-2.035338	-0.000026
H	2.671648	0.502019	-0.000014
H	-2.896441	0.193197	-0.000020
H	-2.819786	2.692801	-0.000023
H	2.815434	-2.988331	-0.000030

2-hydroxyquinoline, enol S_0

C	0.432072	1.898172	0.000000
C	0.485431	0.489033	0.000000
C	-0.721913	-0.260743	0.000000
C	-1.950148	0.434000	0.000000
C	-1.972162	1.804020	0.000000
C	-0.774932	2.545671	0.000000
C	1.693968	-0.242665	0.000000
C	1.661154	-1.604085	0.000000
C	0.393401	-2.246318	0.000000
N	-0.740717	-1.617050	0.000000
O	0.313136	-3.595203	0.000000
H	1.361065	2.459935	0.000000

H	-0.813120	3.629033	0.000000
H	-2.922314	2.326983	0.000000
H	-2.861438	-0.152137	0.000000
H	2.641388	0.287024	0.000000
H	2.576483	-2.187357	0.000000
H	1.198648	-3.968314	0.000000

2-hydroxyquinoline, enol S_1

C	0.426409	1.873367	0.000000
C	0.521945	0.482903	0.000000
C	-0.709971	-0.260099	0.000000
C	-1.944789	0.441858	0.000000
C	-2.008043	1.844149	0.000000
C	-0.825213	2.551368	0.000000
C	1.736989	-0.233957	0.000000
C	1.691955	-1.642821	0.000000
C	0.433297	-2.241261	0.000000
N	-0.748760	-1.604606	0.000000
O	0.289833	-3.573340	0.000000
H	1.337492	2.463686	0.000000
H	-0.829482	3.635547	0.000000
H	-2.964269	2.351090	0.000000
H	-2.846025	-0.160767	0.000000
H	2.681126	0.296059	0.000000
H	2.595388	-2.240708	0.000000
H	1.162109	-3.982448	0.000000

2-hydroxyquinoline, keto S_0

N	0.556279	1.700781	0.000000
C	0.600286	0.329280	0.000000
C	-0.614419	-0.382051	0.000000
C	-1.831951	0.375436	0.000000
C	-1.828947	1.722321	0.000000
C	-0.588306	2.485009	0.000000
C	1.815325	-0.360999	0.000000
C	1.818440	-1.740635	0.000000
C	0.621019	-2.459599	0.000000
C	-0.579017	-1.781362	0.000000
H	-1.517673	-2.325917	0.000000
H	0.637545	-3.542813	0.000000
H	2.764769	-2.269756	0.000000
H	2.748705	0.192337	0.000000
H	-2.772363	-0.167979	0.000000
H	-2.741691	2.303993	0.000000

O	-0.509683	3.700185	0.000000
H	1.421703	2.221790	0.000000

2-hydroxyquinoline, keto S_1

N	0.554091	1.672357	0.000000
C	0.603879	0.320373	0.000000
C	-0.665325	-0.379588	0.000000
C	-1.857946	0.365740	0.000000
C	-1.854623	1.767674	0.000000
C	-0.626898	2.463772	0.000000
C	1.829369	-0.360511	0.000000
C	1.856310	-1.750927	0.000000
C	0.640016	-2.444852	0.000000
C	-0.587864	-1.781187	0.000000
H	-1.507365	-2.355232	0.000000
H	0.647342	-3.529441	0.000000
H	2.797604	-2.284142	0.000000
H	2.750570	0.213376	0.000000
H	-2.798552	-0.172362	0.000000
H	-2.761103	2.353998	0.000000
O	-0.424736	3.680607	0.000000
H	1.405231	2.220354	0.000000

dibenzofuran S_0

C	1.716742	0.000000	-1.356753
C	0.722429	0.000000	-0.382976
C	1.091932	0.000000	0.966963
C	2.405193	0.000000	1.392365
C	3.379770	0.000000	0.404307
C	3.041597	0.000000	-0.951130
C	-0.722429	0.000000	-0.382976
C	-1.091932	0.000000	0.966963
O	0.000000	0.000000	1.789095
C	-1.716742	0.000000	-1.356753
C	-3.041597	0.000000	-0.951130
C	-3.379770	0.000000	0.404307
C	-2.405193	0.000000	1.392365
H	-2.654661	0.000000	2.446191
H	-4.424971	0.000000	0.692235
H	-3.830059	0.000000	-1.694934
H	-1.461996	0.000000	-2.410650
H	1.461996	0.000000	-2.410650
H	3.830059	0.000000	-1.694934
H	4.424971	0.000000	0.692235

H	2.654661	0.000000	2.446191

dibenzofuran S_1

C	0.000000	1.731144	-1.530458
C	0.000000	0.710166	-0.571212
C	0.000000	1.100487	0.796557
C	0.000000	2.401354	1.253978
C	0.000000	3.414620	0.266918
C	0.000000	3.070340	-1.081967
C	0.000000	-0.710166	-0.571212
C	0.000000	-1.100487	0.796557
O	0.000000	0.000000	1.594841
C	0.000000	-1.731144	-1.530458
C	0.000000	-3.070340	-1.081967
C	0.000000	-3.414620	0.266918
C	0.000000	-2.401354	1.253978
H	0.000000	-2.624000	2.313199
H	0.000000	-4.455117	0.563421
H	0.000000	-3.861683	-1.823687
H	0.000000	-1.510739	-2.590459
H	0.000000	1.510739	-2.590459
H	0.000000	3.861683	-1.823687
H	0.000000	4.455117	0.563421
H	0.000000	2.624000	2.313199

pyrrolo[3,2-*h*]quinoline S_0

C	0.132262	-0.685787	0.000000
N	0.058712	-2.033195	0.000000
C	1.190291	-2.702051	0.000000
C	2.456675	-2.096136	0.000000
C	2.534168	-0.725393	0.000000
C	1.355789	0.039829	0.000000
H	1.108523	-3.786230	0.000000
H	3.348899	-2.710854	0.000000
H	3.496589	-0.222828	0.000000
C	-1.050989	0.082211	0.000000
C	-1.055754	1.482624	0.000000
C	0.180617	2.173515	0.000000
C	1.347313	1.465837	0.000000
H	0.196948	3.257980	0.000000
H	2.300952	1.983513	0.000000
C	-2.422733	1.885759	0.000000
C	-3.174775	0.741565	0.000000
N	-2.342395	-0.345190	0.000000

H	-2.608849	-1.314859	0.000000
H	-2.805950	2.894356	0.000000
H	-4.246281	0.615334	0.000000

pyrrolo[3,2-*h*]quinoline S_1

C	0.154273	-0.697847	0.000000
N	0.007041	-2.030666	0.000000
C	1.192461	-2.724074	0.000000
C	2.431590	-2.129513	0.000000
C	2.565112	-0.725923	0.000000
C	1.354855	0.023687	0.000000
H	1.101370	-3.804937	0.000000
H	3.315183	-2.758664	0.000000
H	3.531183	-0.239548	0.000000
C	-1.023919	0.105274	0.000000
C	-1.063802	1.550161	0.000000
C	0.143141	2.228639	0.000000
C	1.311267	1.455741	0.000000
H	0.195518	3.309680	0.000000
H	2.265790	1.974155	0.000000
C	-2.452893	1.904572	0.000000
C	-3.160784	0.745372	0.000000
N	-2.278428	-0.339397	0.000000
H	-2.494703	-1.325879	0.000000
H	-2.867636	2.899868	0.000000
H	-4.226629	0.579298	0.000000

carbazole S_0

C	1.125756	0.000000	-0.895871
N	0.000000	0.000000	-1.689701
C	-1.125756	0.000000	-0.895871
C	-0.721481	0.000000	0.457399
C	0.721481	0.000000	0.457399
C	-1.689966	0.000000	1.457939
C	-3.027505	0.000000	1.101472
C	-3.408143	0.000000	-0.244145
C	-2.466814	0.000000	-1.259850
C	2.466814	0.000000	-1.259850
C	3.408143	0.000000	-0.244145
C	3.027505	0.000000	1.101472
C	1.689966	0.000000	1.457939
H	-2.770016	0.000000	-2.301178
H	-4.462063	0.000000	-0.499275
H	-3.790568	0.000000	1.871238

H	-1.400844	0.000000	2.503375
H	1.400844	0.000000	2.503375
H	3.790568	0.000000	1.871238
H	4.462063	0.000000	-0.499275
H	2.770016	0.000000	-2.301178
H	0.000000	0.000000	-2.693468

carbazole S_1

C	1.139114	0.000000	-0.831873
N	0.000000	0.000000	-1.603322
C	-1.139114	0.000000	-0.831873
C	-0.714360	0.000000	0.530385
C	0.714360	0.000000	0.530385
C	-1.704621	0.000000	1.519105
C	-3.055770	0.000000	1.114956
C	-3.443561	0.000000	-0.218894
C	-2.459922	0.000000	-1.237526
C	2.459922	0.000000	-1.237526
C	3.443561	0.000000	-0.218894
C	3.055770	0.000000	1.114956
C	1.704621	0.000000	1.519105
H	-2.732883	0.000000	-2.286530
H	-4.493291	0.000000	-0.481592
H	-3.823120	0.000000	1.882039
H	-1.449482	0.000000	2.571365
H	1.449482	0.000000	2.571365
H	3.823120	0.000000	1.882039
H	4.493291	0.000000	-0.481592
H	2.732883	0.000000	-2.286530
H	0.000000	0.000000	-2.612175

tryptamine, A-ph S_0

C	-2.127038	0.135325	0.886958
N	-1.251803	0.124520	1.947828
C	0.030456	0.043190	1.472101
C	-0.050655	-0.003552	0.060600
C	-1.442020	0.057749	-0.291740
C	1.246579	0.011221	2.148117
C	2.397665	-0.067318	1.387520
C	2.342357	-0.109850	-0.013510
C	1.133522	-0.078368	-0.680438
C	-2.016941	0.007658	-1.666771
C	-1.990148	-1.389573	-2.280800
N	-2.477186	-1.351140	-3.652127

H	1.293381	0.047610	3.231375
H	3.361783	-0.094096	1.882925
H	3.266297	-0.167025	-0.578001
H	1.103829	-0.107531	-1.764561
H	-1.511652	0.191754	2.914818
H	-3.191568	0.203800	1.056179
H	-1.471270	0.682155	-2.334721
H	-3.052257	0.366661	-1.643471
H	-2.550666	-2.071379	-1.622022
H	-0.958065	-1.751023	-2.297494
H	-3.458289	-1.099112	-3.674725
H	-2.393721	-2.259298	-4.090669

tryptamine, A-ph S_1

C	-2.184844	0.178720	0.923247
N	-1.293311	0.141690	1.914289
C	0.025099	0.054882	1.427634
C	-0.055422	0.047068	0.041929
C	-1.450302	0.120742	-0.299486
C	1.218965	-0.037534	2.155866
C	2.394659	-0.130635	1.340202
C	2.344354	-0.136656	-0.033963
C	1.115952	-0.050923	-0.750027
C	-2.034698	0.052860	-1.647287
C	-1.963795	-1.371685	-2.235936
N	-2.466501	-1.371568	-3.595907
H	1.260619	-0.038925	3.235876
H	3.359318	-0.199429	1.831595
H	3.272457	-0.207054	-0.590773
H	1.086106	-0.008520	-1.830241
H	-1.524178	0.189892	2.894360
H	-3.245606	0.273034	1.091684
H	-1.479846	0.704261	-2.329525
H	-3.077544	0.386030	-1.634394
H	-2.492960	-2.057320	-1.557889
H	-0.915067	-1.678155	-2.248379
H	-3.477517	-1.330102	-3.617727
H	-2.183368	-2.208291	-4.087821

tryptamine, A-py S_0

C	-2.119623	0.112629	0.863156
N	-1.255133	0.117369	1.932428
C	0.032433	0.045153	1.470330
C	-0.034037	-0.012583	0.058115

C	-1.422408	0.032341	-0.308280
C	1.241568	0.029830	2.159292
C	2.401657	-0.042344	1.411968
C	2.361553	-0.095558	0.010836
C	1.159378	-0.081411	-0.668561
C	-1.994954	-0.024231	-1.684317
C	-1.946645	-1.417009	-2.306068
N	-2.535436	-1.394539	-3.637892
H	1.276158	0.073911	3.242719
H	3.360577	-0.056213	1.917825
H	3.291909	-0.148511	-0.543468
H	1.142694	-0.122046	-1.752614
H	-1.525585	0.187236	2.896358
H	-3.186491	0.172491	1.020071
H	-1.452433	0.672028	-2.336897
H	-3.035744	0.310907	-1.675980
H	-2.535672	-2.096707	-1.683315
H	-0.910114	-1.786793	-2.280662
H	-1.974831	-0.827683	-4.263357
H	-2.568909	-2.325878	-4.032577

tryptamine, A-py S_1

C	-2.179596	0.133778	0.886664
N	-1.303854	0.109399	1.892315
C	0.023401	0.047882	1.426050
C	-0.035491	0.042132	0.039346
C	-1.424752	0.094891	-0.323366
C	1.208152	-0.024054	2.171949
C	2.396866	-0.096219	1.373988
C	2.368319	-0.100640	-0.001036
C	1.149892	-0.033254	-0.735526
C	-1.992550	0.026146	-1.676535
C	-1.876700	-1.394822	-2.274700
N	-2.498524	-1.429032	-3.580680
H	1.234025	-0.023584	3.252430
H	3.355076	-0.149716	1.879791
H	3.306306	-0.155055	-0.542948
H	1.136247	0.010318	-1.816040
H	-1.551460	0.149305	2.868511
H	-3.244931	0.204925	1.036829
H	-1.447938	0.710691	-2.337333
H	-3.046489	0.313798	-1.683594
H	-2.408691	-2.091348	-1.620972
H	-0.815906	-1.681276	-2.260198
H	-1.928035	-0.963298	-4.275017

H	-2.653456	-2.378587	-3.890828

tryptamine, A-up S_0

C	-2.118769	0.126410	0.874768
N	-1.252009	0.103015	1.941887
C	0.034266	0.035033	1.475485
C	-0.035055	0.009751	0.062655
C	-1.423895	0.071931	-0.299879
C	1.244657	-0.002435	2.161370
C	2.402615	-0.064691	1.409955
C	2.359504	-0.086910	0.008093
C	1.156199	-0.050080	-0.668328
C	-1.992389	0.032902	-1.678010
C	-1.960934	-1.363563	-2.315382
N	-2.470538	-1.448919	-3.672360
H	1.281785	0.016904	3.245410
H	3.362476	-0.095767	1.913224
H	3.288336	-0.134022	-0.549198
H	1.137503	-0.067574	-1.752967
H	-1.520141	0.149027	2.907918
H	-3.184909	0.187009	1.036581
H	-1.442778	0.726100	-2.327203
H	-3.029069	0.387496	-1.659043
H	-2.535173	-2.051557	-1.687455
H	-0.934641	-1.741928	-2.311056
H	-1.934115	-0.858178	-4.296323
H	-3.431685	-1.132043	-3.716901

tryptamine, A-up S_1

C	-2.175326	0.125327	0.890343
N	-1.295596	0.076615	1.894494
C	0.029234	0.031325	1.426742
C	-0.030504	0.063287	0.039985
C	-1.421543	0.135431	-0.318601
C	1.215795	-0.054789	2.169655
C	2.403619	-0.104616	1.371045
C	2.373304	-0.075733	-0.003640
C	1.154779	0.007277	-0.735926
C	-1.978141	0.102900	-1.669202
C	-1.946844	-1.358680	-2.254953
N	-2.440781	-1.478601	-3.594050
H	1.241613	-0.075621	3.250009
H	3.362517	-0.169290	1.874217
H	3.310892	-0.116788	-0.547683

H	1.142156	0.062759	-1.816042
H	-1.541273	0.094531	2.871665
H	-3.239643	0.196058	1.048001
H	-1.381742	0.727237	-2.341281
H	-3.012656	0.458389	-1.686952
H	-2.534549	-2.004056	-1.599110
H	-0.912558	-1.706846	-2.214502
H	-1.902773	-0.948125	-4.265488
H	-3.418758	-1.240071	-3.685506

tryptamine, Ph-out S_0

C	0.006192	0.001563	0.075229
C	0.045212	0.060623	1.488777
C	1.240979	0.073310	2.201076
C	2.415768	0.030209	1.475205
C	2.402467	-0.025783	0.073301
C	1.214839	-0.039773	-0.631046
N	-1.251431	0.101814	1.928009
H	1.253810	0.117301	3.284996
H	3.365366	0.039457	1.998576
H	3.344117	-0.057919	-0.463326
H	1.212213	-0.098665	-1.713764
C	-1.377550	0.014612	-0.316317
C	-2.096587	0.080400	0.844262
H	-1.539500	0.174157	2.886725
H	-3.166736	0.124275	0.983870
C	-1.935121	-0.042366	-1.701909
H	-1.296448	0.531343	-2.381110
C	-2.082902	-1.456069	-2.260549
H	-2.920125	0.434978	-1.712161
H	-2.547112	-1.388951	-3.249965
N	-0.787918	-2.098720	-2.416247
H	-2.780600	-2.013391	-1.613916
H	-0.344047	-2.220496	-1.513188
H	-0.889912	-3.017800	-2.827317

tryptamine, Ph-out S_1

C	0.000351	0.030168	0.065029
C	0.030876	0.089942	1.452752
C	1.197674	0.042891	2.227377
C	2.405896	-0.043848	1.460823
C	2.407495	-0.103329	0.087401
C	1.205321	-0.083140	-0.677600
N	-1.303629	0.166935	1.891082

H	1.198445	0.097451	3.306866
H	3.352560	-0.065611	1.990090
H	3.357077	-0.168077	-0.432586
H	1.215494	-0.061998	-1.758525
C	-1.383117	0.065815	-0.327157
C	-2.159234	0.152119	0.869704
H	-1.568856	0.246556	2.860346
H	-3.226984	0.231492	0.997547
C	-1.959855	-0.048626	-1.678585
H	-1.345573	0.499082	-2.399156
C	-2.051747	-1.509975	-2.171756
H	-2.968084	0.376292	-1.683456
H	-2.682036	-1.508163	-3.066493
N	-0.748408	-2.016988	-2.533972
H	-2.581195	-2.096329	-1.403723
H	-0.101908	-2.005158	-1.750733
H	-0.805571	-2.963381	-2.886065

tryptamine, Ph-up S_0

C	-2.073107	0.018643	0.813707
N	-1.240183	0.010143	1.906798
C	0.061424	0.030657	1.482439
C	0.037797	0.046326	0.067344
C	-1.339867	0.037129	-0.340193
C	1.249161	0.041773	2.208036
C	2.432224	0.073403	1.495400
C	2.435252	0.095016	0.092466
C	1.254767	0.082008	-0.623302
C	-1.872759	0.011479	-1.735219
C	-2.117131	-1.404383	-2.280144
N	-0.962224	-2.277196	-2.365482
H	1.249668	0.028213	3.292782
H	3.375604	0.083260	2.029624
H	3.382697	0.124261	-0.433876
H	1.271485	0.102053	-1.707809
H	-1.540981	0.015351	2.864413
H	-3.145347	0.017583	0.943694
H	-1.177299	0.534535	-2.401703
H	-2.815897	0.567826	-1.780090
H	-2.559569	-1.326783	-3.278939
H	-2.865013	-1.897293	-1.650218
H	-0.519288	-2.369617	-1.458700
H	-0.267764	-1.894758	-2.995967

tryptamine, Ph-up S_1

C	-2.171070	0.178957	0.863687
N	-1.313446	0.162608	1.891094
C	0.016225	0.093813	1.449504
C	-0.017176	0.088657	0.059335
C	-1.399059	0.136084	-0.326889
C	1.185264	-0.006802	2.216524
C	2.389664	-0.091604	1.448311
C	2.390217	-0.098251	0.073342
C	1.189259	-0.026262	-0.690434
C	-1.951807	0.005582	-1.670096
C	-1.960327	-1.507566	-2.161612
N	-0.688735	-2.070564	-2.443589
H	1.187621	0.004657	3.297479
H	3.336156	-0.154872	1.974687
H	3.339783	-0.156253	-0.448303
H	1.215307	0.139119	-1.759881
H	-1.578016	0.225303	2.860832
H	-3.238279	0.261509	0.996552
H	-1.370198	0.570689	-2.403040
H	-2.989810	0.350657	-1.702033
H	-2.576497	-1.533709	-3.064815
H	-2.464562	-2.097721	-1.394582
H	-0.036609	-2.053066	-1.664884
H	-0.240246	-1.671354	-3.256096

tryptamine, Py-out S_0

C	0.516560	0.452942	0.216189
C	0.591089	0.524095	1.627476
C	1.802349	0.483149	2.311531
C	2.956463	0.370393	1.559906
C	2.908476	0.302817	0.159714
C	1.704227	0.343411	-0.515165
N	-0.692036	0.635126	2.095070
H	1.843160	0.539234	3.394173
H	3.916990	0.335735	2.061695
H	3.834519	0.218599	-0.397897
H	1.681215	0.292624	-1.598532
C	-0.872498	0.532939	-0.144301
C	-1.562180	0.640881	1.030313
H	-0.955559	0.721084	3.059699
H	-2.626902	0.726418	1.188997
C	-1.452544	0.471534	-1.518367
H	-0.894996	1.137684	-2.185880
C	-1.449583	-0.935108	-2.114065

H	-2.485390	0.830572	-1.493849
H	-0.407606	-1.279560	-2.210744
N	-2.285968	-1.820471	-1.319502
H	-1.865812	-0.885750	-3.125164
H	-2.286996	-2.756616	-1.704035
H	-1.916959	-1.881734	-0.377244

tryptamine, Py-out S_1

C	0.516702	0.492750	0.206090
C	0.592536	0.543025	1.590858
C	1.783418	0.461753	2.326833
C	2.960767	0.335684	1.518657
C	2.915655	0.287746	0.145242
C	1.690228	0.359921	-0.578408
N	-0.727002	0.654524	2.070476
H	1.822209	0.506489	3.405991
H	3.923379	0.275507	2.015261
H	3.845408	0.193001	-0.405223
H	1.665649	0.365857	-1.659434
C	-0.877240	0.572662	-0.142043
C	-1.614840	0.668843	1.075632
H	-0.961664	0.722714	3.048420
H	-2.677571	0.756553	1.234333
C	-1.459508	0.493016	-1.489773
H	-0.887565	1.138663	-2.165515
C	-1.403172	-0.939726	-2.062892
H	-2.501671	0.821715	-1.483920
H	-0.347690	-1.243716	-2.099646
N	-2.254933	-1.829356	-1.299891
H	-1.777526	-0.902830	-3.088982
H	-2.370728	-2.715426	-1.773853
H	-1.854850	-2.019379	-0.388222

tryptamine, Py-up S_0

C	-2.117453	0.242093	0.888958
N	-1.245278	0.219145	1.952039
C	0.034949	0.092457	1.480546
C	-0.043716	0.030067	0.069432
C	-1.432262	0.130669	-0.288081
C	1.247151	0.031012	2.161474
C	2.397434	-0.094478	1.406248
C	2.345184	-0.154799	0.005859
C	1.140151	-0.093781	-0.665728
C	-2.008804	0.075628	-1.661727

C	-2.010026	-1.337182	-2.268754
N	-2.788037	-2.333449	-1.558357
H	1.291406	0.080435	3.244269
H	3.358585	-0.145764	1.905361
H	3.268431	-0.250612	-0.554392
H	1.114268	-0.139541	-1.749262
H	-1.504789	0.305096	2.917728
H	-3.179310	0.350814	1.053621
H	-1.449555	0.744711	-2.327126
H	-3.038466	0.450339	-1.640332
H	-0.980390	-1.701418	-2.336836
H	-2.383890	-1.279555	-3.295956
H	-3.763800	-2.062469	-1.518867
H	-2.463264	-2.409800	-0.601228

tryptamine, Py-up S_1

C	-2.164526	0.280184	0.960026
N	-1.262872	0.263987	1.946069
C	0.047187	0.129405	1.454045
C	-0.044793	0.071462	0.069664
C	-1.442378	0.169404	-0.263446
C	1.244119	0.033804	2.177559
C	2.411350	-0.121371	1.360733
C	2.349913	-0.179027	-0.011420
C	1.119259	-0.089301	-0.723253
C	-2.028976	0.090319	-1.599131
C	-1.958639	-1.353466	-2.220971
N	-2.793526	-2.351631	-1.627252
H	1.293051	0.083536	3.256195
H	3.377386	-0.197891	1.848132
H	3.271452	-0.296647	-0.571401
H	1.086996	-0.091980	-1.804258
H	-1.483484	0.356757	2.925150
H	-3.220131	0.414088	1.134549
H	-1.459806	0.731712	-2.282606
H	-3.071211	0.423167	-1.600804
H	-0.917754	-1.681107	-2.172702
H	-2.226612	-1.253750	-3.275972
H	-3.779626	-2.141607	-1.697272
H	-2.557858	-2.540415	-0.662721

porphycene S_0

C	-3.423792	1.906944	0.000000
C	-2.407499	0.908372	0.000000

N	-1.214753	1.547662	0.000000
C	-1.390882	2.893911	0.000000
C	-2.799895	3.126509	0.000000
C	-0.367241	3.848742	0.000000
C	1.010099	3.698220	0.000000
C	1.824965	2.554115	0.000000
H	-0.243845	1.141892	0.000000
N	1.403542	1.268318	0.000000
C	3.271531	2.592042	0.000000
C	3.696145	1.301484	0.000000
C	2.501962	0.494063	0.000000
C	2.407499	-0.908372	0.000000
C	3.423792	-1.906944	0.000000
C	2.799895	-3.126509	0.000000
C	1.390882	-2.893911	0.000000
N	1.214753	-1.547662	0.000000
C	0.367241	-3.848742	0.000000
C	-1.010099	-3.698220	0.000000
C	-1.824965	-2.554115	0.000000
C	-3.271531	-2.592042	0.000000
C	-3.696145	-1.301484	0.000000
C	-2.501962	-0.494063	0.000000
N	-1.403542	-1.268318	0.000000
H	0.243845	-1.141892	0.000000
H	3.264724	-4.101300	0.000000
H	4.485888	-1.715051	0.000000
H	0.726390	-4.873137	0.000000
H	-1.568963	-4.629549	0.000000
H	-3.876448	-3.487833	0.000000
H	-4.713554	-0.938627	0.000000
H	-4.485888	1.715051	0.000000
H	-3.264724	4.101300	0.000000
H	-0.726390	4.873137	0.000000
H	1.568963	4.629549	0.000000
H	3.876448	3.487833	0.000000
H	4.713554	0.938627	0.000000

porphycene S_1

C	-3.445589	1.894645	0.000000
C	-2.433354	0.898415	0.000000
N	-1.229934	1.544740	0.000000
C	-1.411247	2.885191	0.000000
C	-2.819483	3.117317	0.000000
C	-0.381315	3.854182	0.000000
C	0.986529	3.710887	0.000000

C	1.829189	2.563958	0.000000
H	-0.264090	1.138806	0.000000
N	1.411039	1.281163	0.000000
C	3.266870	2.610725	0.000000
C	3.705644	1.315253	0.000000
C	2.531935	0.503813	0.000000
C	2.433354	-0.898415	0.000000
C	3.445589	-1.894645	0.000000
C	2.819483	-3.117317	0.000000
C	1.411247	-2.885191	0.000000
N	1.229934	-1.544740	0.000000
C	0.381315	-3.854182	0.000000
C	-0.986529	-3.710887	0.000000
C	-1.829189	-2.563958	0.000000
C	-3.266870	-2.610725	0.000000
C	-3.705644	-1.315253	0.000000
C	-2.531935	-0.503813	0.000000
N	-1.411039	-1.281163	0.000000
H	0.264090	-1.138806	0.000000
H	3.283420	-4.092492	0.000000
H	4.507500	-1.702683	0.000000
H	0.747729	-4.875621	0.000000
H	-1.540379	-4.645648	0.000000
H	-3.867112	-3.509689	0.000000
H	-4.726730	-0.964217	0.000000
H	-4.507500	1.702683	0.000000
H	-3.283420	4.092492	0.000000
H	-0.747729	4.875621	0.000000
H	1.540379	4.645648	0.000000
H	3.867112	3.509689	0.000000
H	4.726730	0.964217	0.000000

porphine S_0

N	0.000000	-2.016480	0.000000
N	2.103984	0.000000	0.000000
C	1.077905	-2.836149	0.000000
C	0.674788	-4.231517	0.000000
C	2.408516	-2.425812	0.000000
C	2.877898	-1.121493	0.000000
C	4.236666	-0.682365	0.000000
H	1.346608	-5.078384	0.000000
H	3.164256	-3.203168	0.000000
H	5.091158	-1.342467	0.000000
H	1.090982	0.000000	0.000000
N	0.000000	2.016480	0.000000

N	-2.103984	0.000000	0.000000
C	1.077905	2.836149	0.000000
C	-1.077905	2.836149	0.000000
C	-1.077905	-2.836149	0.000000
C	0.674788	4.231517	0.000000
C	-0.674788	4.231517	0.000000
C	-0.674788	-4.231517	0.000000
C	2.408516	2.425812	0.000000
C	-2.408516	2.425812	0.000000
C	-2.408516	-2.425812	0.000000
C	2.877898	1.121493	0.000000
C	-2.877898	1.121493	0.000000
C	-2.877898	-1.121493	0.000000
C	4.236666	0.682365	0.000000
C	-4.236666	0.682365	0.000000
C	-4.236666	-0.682365	0.000000
H	1.346608	5.078384	0.000000
H	-1.346608	5.078384	0.000000
H	-1.346608	-5.078384	0.000000
H	3.164256	3.203168	0.000000
H	-3.164256	3.203168	0.000000
H	-3.164256	-3.203168	0.000000
H	5.091158	1.342467	0.000000
H	-5.091158	1.342467	0.000000
H	-5.091158	-1.342467	0.000000
H	-1.090982	0.000000	0.000000

porphine S_1

N	0.000000	-2.037392	0.000000
N	2.101308	0.000000	0.000000
C	1.081358	-2.861417	0.000000
C	0.677408	-4.250920	0.000000
C	2.413961	-2.433311	0.000000
C	2.878604	-1.123997	0.000000
C	4.237106	-0.683835	0.000000
H	1.347327	-5.098959	0.000000
H	3.175616	-3.204897	0.000000
H	5.092100	-1.343107	0.000000
H	1.089910	0.000000	0.000000
N	0.000000	2.037392	0.000000
N	-2.101308	0.000000	0.000000
C	1.081358	2.861417	0.000000
C	-1.081358	2.861417	0.000000
C	-1.081358	-2.861417	0.000000
C	0.677408	4.250920	0.000000

C	-0.677408	4.250920	0.000000
C	-0.677408	-4.250920	0.000000
C	2.413961	2.433311	0.000000
C	-2.413961	2.433311	0.000000
C	-2.413961	-2.433311	0.000000
C	2.878604	1.123997	0.000000
C	-2.878604	1.123997	0.000000
C	-2.878604	-1.123997	0.000000
C	4.237106	0.683835	0.000000
C	-4.237106	0.683835	0.000000
C	-4.237106	-0.683835	0.000000
H	1.347327	5.098959	0.000000
H	-1.347327	5.098959	0.000000
H	-1.347327	-5.098959	0.000000
H	3.175616	3.204897	0.000000
H	-3.175616	3.204897	0.000000
H	-3.175616	-3.204897	0.000000
H	5.092100	1.343107	0.000000
H	-5.092100	1.343107	0.000000
H	-5.092100	-1.343107	0.000000
H	-1.089910	0.000000	0.000000

chlorin S_0

C	0.000000	-4.229941	0.921136
C	0.000000	-2.877953	1.370182
N	0.000000	-2.094379	0.244080
C	0.000000	-2.858814	-0.876594
C	0.000000	-4.219962	-0.444860
C	0.000000	-2.411340	2.669160
C	0.000000	-1.078173	3.087409
N	0.000000	0.000000	2.266546
C	0.000000	1.078173	3.087409
C	0.000000	0.677231	4.475939
C	0.000000	-0.677231	4.475939
C	0.000000	2.411340	2.669160
C	0.000000	2.877953	1.370182
N	0.000000	2.094379	0.244080
C	0.000000	2.858814	-0.876594
C	0.000000	4.219962	-0.444860
C	0.000000	4.229941	0.921136
C	0.000000	2.402247	-2.194781
C	0.000000	1.096064	-2.644952
C	0.000000	0.763222	-4.123749
C	0.000000	-0.763222	-4.123749
C	0.000000	-1.096064	-2.644952

N	0.000000	0.000000	-1.868955
C	0.000000	-2.402247	-2.194781
H	-0.878961	1.187160	-4.615607
H	0.000000	3.179153	-2.951417
H	0.000000	5.069475	-1.111223
H	0.000000	1.347730	5.323915
H	0.000000	-1.347730	5.323915
H	-0.878961	-1.187160	-4.615607
H	0.000000	3.168545	3.445606
H	0.000000	-3.168545	3.445606
H	0.000000	-3.179153	-2.951417
H	0.000000	5.089927	1.574267
H	0.000000	-5.089927	1.574267
H	0.000000	-5.069475	-1.111223
H	0.878961	-1.187160	-4.615607
H	0.878961	1.187160	-4.615607
H	0.000000	-1.083636	0.268296
H	0.000000	1.083636	0.268296

chlorin S_1

C	0.000000	-4.239184	0.921465
C	0.000000	-2.885201	1.367273
N	0.000000	-2.102457	0.242318
C	0.000000	-2.873779	-0.882447
C	0.000000	-4.231592	-0.449217
C	0.000000	-2.415830	2.675329
C	0.000000	-1.080958	3.088295
N	0.000000	0.000000	2.265272
C	0.000000	1.080958	3.088295
C	0.000000	0.675223	4.483261
C	0.000000	-0.675223	4.483261
C	0.000000	2.415830	2.675329
C	0.000000	2.885201	1.367273
N	0.000000	2.102457	0.242318
C	0.000000	2.873779	-0.882447
C	0.000000	4.231592	-0.449217
C	0.000000	4.239184	0.921465
C	0.000000	2.411874	-2.202303
C	0.000000	1.097482	-2.645443
C	0.000000	0.762012	-4.118867
C	0.000000	-0.762012	-4.118867
C	0.000000	-1.097482	-2.645443
N	0.000000	0.000000	-1.861130
C	0.000000	-2.411874	-2.202303
H	-0.878271	1.187276	-4.612777

H	0.000000	3.183568	-2.963820
H	0.000000	5.082846	-1.113333
H	0.000000	1.347007	5.329999
H	0.000000	-1.347007	5.329999
H	-0.878271	-1.187276	-4.612777
H	0.000000	3.171603	3.452238
H	0.000000	-3.171603	3.452238
H	0.000000	-3.183568	-2.963820
H	0.000000	5.097523	1.576430
H	0.000000	-5.097523	1.576430
H	0.000000	-5.082846	-1.113333
H	0.878271	-1.187276	-4.612777
H	0.878271	1.187276	-4.612777
H	0.000000	-1.091797	0.262315
H	0.000000	1.091797	0.262315

Zn-tetraphenylporphine S_0

C	-3.681346	4.292963	1.118720
C	-3.484166	3.484174	-0.000006
C	-4.292941	3.681354	-1.118743
C	-5.272900	4.663784	-1.119857
C	-5.461961	5.461987	-0.000023
C	-4.663767	5.272930	1.119818
C	-2.431481	2.431483	0.000000
C	-1.096873	2.853082	-0.007404
N	0.000000	2.040898	0.033415
C	1.096873	2.853082	-0.007404
C	0.677417	4.226549	-0.088676
C	-0.677417	4.226549	-0.088676
C	2.431481	2.431483	0.000000
C	3.484166	3.484174	-0.000006
C	4.292941	3.681354	-1.118743
C	5.272900	4.663784	-1.119857
C	5.461961	5.461987	-0.000023
C	4.663767	5.272930	1.119818
C	3.681346	4.292963	1.118720
C	-2.853083	1.096875	0.007416
N	-2.040899	0.000000	-0.033378
C	-2.853083	-1.096875	0.007416
C	-4.226548	-0.677417	0.088704
C	-4.226548	0.677417	0.088704
C	-2.431481	-2.431483	0.000000
C	-3.484166	-3.484174	-0.000006
C	-4.292941	-3.681354	-1.118743
C	-5.272900	-4.663784	-1.119857

C	-5.461961	-5.461987	-0.000023
C	-4.663767	-5.272930	1.119818
C	-3.681346	-4.292963	1.118720
C	2.853083	1.096875	0.007416
N	2.040899	0.000000	-0.033378
C	2.853083	-1.096875	0.007416
C	4.226548	-0.677417	0.088704
C	4.226548	0.677417	0.088704
C	2.431481	-2.431483	0.000000
C	3.484166	-3.484174	-0.000006
C	4.292941	-3.681354	-1.118743
C	5.272900	-4.663784	-1.119857
C	5.461961	-5.461987	-0.000023
C	4.663767	-5.272930	1.119818
C	3.681346	-4.292963	1.118720
C	1.096873	-2.853082	-0.007404
N	0.000000	-2.040898	0.033415
C	-1.096873	-2.853082	-0.007404
C	-0.677417	-4.226549	-0.088676
C	0.677417	-4.226549	-0.088676
H	1.338948	-5.076009	-0.155651
H	5.076008	-1.338947	0.155686
H	1.338948	5.076009	-0.155651
H	-1.338948	5.076009	-0.155651
H	-1.338948	-5.076009	-0.155651
H	5.076008	1.338947	0.155686
H	-5.076008	1.338947	0.155686
H	-5.076008	-1.338947	0.155686
H	4.142833	3.061031	-1.995761
H	5.888845	4.807862	-2.000882
H	6.228741	6.228777	-0.000029
H	4.807844	5.888885	2.000837
H	3.061028	4.142858	1.995745
H	4.142833	-3.061031	-1.995761
H	5.888845	-4.807862	-2.000882
H	6.228741	-6.228777	-0.000029
H	4.807844	-5.888885	2.000837
H	3.061028	-4.142858	1.995745
H	-4.142833	-3.061031	-1.995761
H	-5.888845	-4.807862	-2.000882
H	-6.228741	-6.228777	-0.000029
H	-4.807844	-5.888885	2.000837
H	-3.061028	-4.142858	1.995745
H	-4.142833	3.061031	-1.995761
H	-5.888845	4.807862	-2.000882
H	-6.228741	6.228777	-0.000029

H	-4.807844	5.888885	2.000837
H	-3.061028	4.142858	1.995745
Zn	0.000000	0.000000	0.000030

Zn-tetraphenylporphine S_1

C	-3.564123	4.462570	0.991647
C	-3.486248	3.484512	-0.002615
C	-4.424414	3.511822	-1.037936
C	-5.403680	4.491701	-1.082644
C	-5.471879	5.457077	-0.086404
C	-4.550399	5.437130	0.951758
C	-2.437866	2.440249	0.031873
C	-1.099216	2.854589	-0.002606
N	0.000000	2.044292	0.115216
C	1.099216	2.854589	-0.002606
C	0.678054	4.212426	-0.212969
C	-0.678054	4.212426	-0.212969
C	2.437866	2.440249	0.031873
C	3.486248	3.484512	-0.002615
C	4.424414	3.511822	-1.037936
C	5.403680	4.491701	-1.082644
C	5.471879	5.457077	-0.086404
C	4.550399	5.437130	0.951758
C	3.564123	4.462570	0.991647
C	-2.867337	1.096573	0.087674
N	-2.056954	0.000000	-0.021416
C	-2.867337	-1.096573	0.087674
C	-4.222064	-0.681107	0.287648
C	-4.222064	0.681107	0.287648
C	-2.437866	-2.440249	0.031873
C	-3.486248	-3.484512	-0.002615
C	-4.424414	-3.511822	-1.037936
C	-5.403680	-4.491701	-1.082644
C	-5.471879	-5.457077	-0.086404
C	-4.550399	-5.437130	0.951758
C	-3.564123	-4.462570	0.991647
C	2.867337	1.096573	0.087674
N	2.056954	0.000000	-0.021416
C	2.867337	-1.096573	0.087674
C	4.222064	-0.681107	0.287648
C	4.222064	0.681107	0.287648
C	2.437866	-2.440249	0.031873
C	3.486248	-3.484512	-0.002615
C	4.424414	-3.511822	-1.037936
C	5.403680	-4.491701	-1.082644

C	5.471879	-5.457077	-0.086404
C	4.550399	-5.437130	0.951758
C	3.564123	-4.462570	0.991647
C	1.099216	-2.854589	-0.002606
N	0.000000	-2.044292	0.115216
C	-1.099216	-2.854589	-0.002606
C	-0.678054	-4.212426	-0.212969
C	0.678054	-4.212426	-0.212969
H	1.336932	-5.050521	-0.375342
H	5.061410	-1.340873	0.438661
H	1.336932	5.050521	-0.375342
H	-1.336932	5.050521	-0.375342
H	-1.336932	-5.050521	-0.375342
H	5.061410	1.340873	0.438661
H	-5.061410	1.340873	0.438661
H	-5.061410	-1.340873	0.438661
H	4.368227	2.762699	-1.819949
H	6.114427	4.504316	-1.901789
H	6.240563	6.221223	-0.118819
H	4.601812	6.181534	1.738881
H	2.850846	4.442477	1.808186
H	4.368227	-2.762699	-1.819949
H	6.114427	-4.504316	-1.901789
H	6.240563	-6.221223	-0.118819
H	4.601812	-6.181534	1.738881
H	2.850846	-4.442477	1.808186
H	-4.368227	-2.762699	-1.819949
H	-6.114427	-4.504316	-1.901789
H	-6.240563	-6.221223	-0.118819
H	-4.601812	-6.181534	1.738881
H	-2.850846	-4.442477	1.808186
H	-4.368227	2.762699	-1.819949
H	-6.114427	4.504316	-1.901789
H	-6.240563	6.221223	-0.118819
H	-4.601812	6.181534	1.738881
H	-2.850846	4.442477	1.808186
Zn	0.000000	0.000000	0.046575

tetraphenylporphine S_0

C	-0.681404	4.226342	0.089943
C	-1.122883	2.872292	0.000276
N	0.000000	2.096302	-0.047398
C	1.122883	2.872292	0.000277
C	0.681405	4.226342	0.089944
C	2.444926	2.424435	-0.016160

C	2.844275	1.079839	-0.041290
N	2.023673	0.000000	0.004583
C	2.844275	-1.079839	-0.041291
C	4.234579	-0.673908	-0.142343
C	4.234579	0.673908	-0.142341
C	2.444926	-2.424435	-0.016161
C	1.122883	-2.872292	0.000276
N	0.000000	-2.096302	-0.047398
C	-1.122883	-2.872292	0.000277
C	-0.681405	-4.226342	0.089944
C	0.681404	-4.226342	0.089943
C	-2.444926	-2.424435	-0.016160
C	-2.844275	-1.079839	-0.041290
N	-2.023673	0.000000	0.004583
C	-2.844275	1.079839	-0.041291
C	-4.234579	0.673908	-0.142343
C	-4.234579	-0.673908	-0.142341
C	-2.444926	2.424435	-0.016161
H	-5.080640	-1.338675	-0.222302
C	-3.502579	-3.471939	0.001203
H	-1.338427	-5.078334	0.159853
H	0.000000	-1.083915	-0.062643
H	5.080639	-1.338675	-0.222306
H	5.080640	1.338675	-0.222302
H	-5.080639	1.338675	-0.222306
C	3.502579	-3.471940	0.001200
C	3.502579	3.471939	0.001203
C	-3.502579	3.471940	0.001200
H	1.338427	-5.078334	0.159852
H	1.338427	5.078334	0.159853
H	-1.338427	5.078334	0.159852
H	0.000000	1.083915	-0.062643
C	3.700163	-4.305404	-1.099209
C	4.687840	-5.280047	-1.080655
C	5.490036	-5.439036	0.040920
C	5.300137	-4.616168	1.142724
C	4.315090	-3.639288	1.122192
H	3.078642	-4.176939	-1.978876
H	4.833446	-5.914587	-1.948115
H	6.261190	-6.201269	0.056055
H	5.919869	-4.736255	2.024658
H	4.164805	-2.998475	1.984215
C	-3.700164	-4.305404	-1.099205
C	-4.687842	-5.280048	-1.080649
C	-5.490037	-5.439035	0.040927
C	-5.300137	-4.616165	1.142729

C	-4.315090	-3.639286	1.122195
H	-3.078644	-4.176941	-1.978873
H	-4.833448	-5.914588	-1.948109
H	-6.261191	-6.201267	0.056063
H	-5.919869	-4.736251	2.024663
H	-4.164804	-2.998472	1.984217
C	-3.700163	4.305404	-1.099209
C	-4.687840	5.280047	-1.080655
C	-5.490036	5.439036	0.040920
C	-5.300137	4.616168	1.142724
C	-4.315090	3.639288	1.122192
H	-3.078642	4.176939	-1.978876
H	-4.833446	5.914587	-1.948115
H	-6.261190	6.201269	0.056055
H	-5.919869	4.736255	2.024658
H	-4.164805	2.998475	1.984215
C	3.700164	4.305404	-1.099205
C	4.687842	5.280048	-1.080649
C	5.490037	5.439035	0.040927
C	5.300137	4.616165	1.142729
C	4.315090	3.639286	1.122195
H	3.078644	4.176941	-1.978873
H	4.833448	5.914588	-1.948109
H	6.261191	6.201267	0.056063
H	5.919869	4.736251	2.024663
H	4.164804	2.998472	1.984217

tetraphenylporphine S_1

C	-4.218748	-0.682299	0.192192
C	-2.877588	-1.126033	-0.011443
N	-2.105613	-0.000007	-0.124412
C	-2.877588	1.126011	-0.011392
C	-4.218740	0.682262	0.192262
C	-2.433204	2.451361	-0.064121
C	-1.082549	2.862193	-0.155256
N	0.000001	2.042059	-0.058374
C	1.082543	2.862211	-0.155306
C	0.677734	4.231980	-0.360725
C	-0.677782	4.231972	-0.360671
C	2.433193	2.451377	-0.064183
C	2.877588	1.126033	-0.011443
N	2.105613	0.000007	-0.124412
C	2.877588	-1.126011	-0.011392
C	4.218740	-0.682262	0.192262
C	4.218748	0.682299	0.192192

C	2.433204	-2.451361	-0.064121
C	1.082549	-2.862193	-0.155256
N	-0.000001	-2.042059	-0.058374
C	-1.082543	-2.862211	-0.155306
C	-0.677734	-4.231980	-0.360725
C	0.677782	-4.231972	-0.360671
C	-2.433193	-2.451377	-0.064183
H	1.339602	-5.070600	-0.509117
C	3.469565	-3.507959	0.000601
H	5.062405	-1.335863	0.343188
H	1.095688	0.000009	-0.177372
H	1.339532	5.070619	-0.509198
H	-1.339602	5.070600	-0.509117
H	-1.339532	-5.070619	-0.509198
C	3.469573	3.507969	0.000440
C	-3.469565	3.507959	0.000601
C	-3.469573	-3.507969	0.000440
H	5.062426	1.335899	0.343042
H	-5.062405	1.335863	0.343188
H	-5.062426	-1.335899	0.343042
H	-1.095688	-0.000009	-0.177372
C	4.464755	3.609983	-0.973578
C	5.429168	4.604717	-0.899198
C	5.420163	5.509291	0.153625
C	4.436489	5.416534	1.129775
C	3.467348	4.428903	1.050975
H	4.466101	2.911595	-1.803297
H	6.187574	4.676122	-1.671237
H	6.175834	6.284754	0.212595
H	4.425810	6.115046	1.959365
H	2.702103	4.354364	1.815579
C	4.464752	-3.610048	-0.973408
C	5.429168	-4.604773	-0.898952
C	5.420181	-5.509253	0.153955
C	4.436513	-5.416411	1.130103
C	3.467363	-4.428795	1.051219
H	4.466098	-2.911695	-1.803155
H	6.187584	-4.676221	-1.670977
H	6.175866	-6.284696	0.213006
H	4.425850	-6.114844	1.959758
H	2.702133	-4.354191	1.815833
C	-4.464755	-3.609983	-0.973578
C	-5.429168	-4.604717	-0.899198
C	-5.420163	-5.509291	0.153625
C	-4.436489	-5.416534	1.129775
C	-3.467348	-4.428903	1.050975

H	-4.466101	-2.911595	-1.803297
H	-6.187574	-4.676122	-1.671237
H	-6.175834	-6.284754	0.212595
H	-4.425810	-6.115046	1.959365
H	-2.702103	-4.354364	1.815579
C	-4.464752	3.610048	-0.973408
C	-5.429168	4.604773	-0.898952
C	-5.420181	5.509253	0.153955
C	-4.436513	5.416411	1.130103
C	-3.467363	4.428795	1.051219
H	-4.466098	2.911695	-1.803155
H	-6.187584	4.676221	-1.670977
H	-6.175866	6.284696	0.213006
H	-4.425850	6.114844	1.959758
H	-2.702133	4.354191	1.815833

PBE0/TZVP geometries – Group II

tetrafluorobenzene S_0

C	-1.190569	0.693080	0.000000
C	-1.190569	-0.693080	0.000000
C	0.000000	-1.393702	0.000000
C	1.190569	-0.693080	0.000000
C	1.190569	0.693080	0.000000
C	0.000000	1.393702	0.000000
F	-2.349344	-1.348845	0.000000
H	0.000000	-2.476201	0.000000
F	2.349344	-1.348845	0.000000
F	2.349344	1.348845	0.000000
H	0.000000	2.476201	0.000000
F	-2.349344	1.348845	0.000000

tetrafluorobenzene S_1

C	1.161456	-0.707271	0.105386
C	1.161456	0.707271	0.105386
C	0.000000	1.462488	0.314329
C	-1.161456	0.707271	0.105386
C	-1.161456	-0.707271	0.105386
C	0.000000	-1.462488	0.314329
F	2.300105	1.314967	-0.219340
H	0.000000	2.504076	0.611703
F	-2.300105	1.314967	-0.219340
F	-2.300105	-1.314967	-0.219340

H	0.000000	-2.504076	0.611703
F	2.300105	-1.314967	-0.219340

benzonitrile S_0

C	0.000000	0.000000	-1.054789
C	-1.210328	0.000000	-0.358801
C	-1.203810	0.000000	1.025861
C	0.000000	0.000000	1.718460
C	1.203810	0.000000	1.025861
C	1.210328	0.000000	-0.358801
H	-2.143839	0.000000	-0.908514
H	-2.142957	0.000000	1.566939
H	0.000000	0.000000	2.802614
H	2.142957	0.000000	1.566939
H	2.143839	0.000000	-0.908514
C	0.000000	0.000000	-2.482239
N	0.000000	0.000000	-3.635007

benzonitrile S_1

C	0.000000	0.000000	-1.107956
C	-1.223762	0.000000	-0.373179
C	-1.211418	0.000000	1.045377
C	0.000000	0.000000	1.762912
C	1.211418	0.000000	1.045377
C	1.223762	0.000000	-0.373179
H	-2.164485	0.000000	-0.908237
H	-2.156736	0.000000	1.573858
H	0.000000	0.000000	2.844369
H	2.156736	0.000000	1.573858
H	2.164485	0.000000	-0.908237
C	0.000000	0.000000	-2.505761
N	0.000000	0.000000	-3.669200

o-fluorophenol, *cis* S_0

C	0.324607	1.450080	0.000000
C	-0.874044	0.773986	0.000000
C	-0.950202	-0.614542	0.000000
C	0.236138	-1.334966	0.000000
C	1.453711	-0.670123	0.000000
C	1.505014	0.717384	0.000000
F	-2.044628	1.452179	0.000000
O	-2.136738	-1.263738	0.000000
H	0.182366	-2.417224	0.000000

H	2.372013	-1.245725	0.000000
H	2.457812	1.232544	0.000000
H	0.321199	2.533552	0.000000
H	-2.847238	-0.613427	0.000000

o-fluorophenol, *cis* S_1

C	1.228719	-0.254498	-0.733628
C	0.002845	-0.062411	-0.092903
C	-0.008573	-0.025175	1.344372
C	1.173559	0.029728	2.090224
C	2.389748	0.109779	1.410100
C	2.403078	-0.016180	0.017596
F	-0.963397	0.789098	-0.689034
O	-1.172376	-0.113667	1.987729
H	1.124792	-0.131938	3.162432
H	3.318151	0.221958	1.955197
H	3.343297	0.103951	-0.515362
H	1.282738	-0.406396	-1.805215
H	-1.867201	-0.244248	1.318432

o-fluorophenol, *trans* S_0

C	0.289693	1.262096	0.000000
C	-0.945994	0.618329	0.000000
C	-0.960431	-0.770800	0.000000
C	0.226093	-1.492271	0.000000
C	1.444554	-0.832947	0.000000
C	1.472827	0.556509	0.000000
O	-2.060146	1.387671	0.000000
H	-1.914966	-1.289869	0.000000
H	0.190456	-2.575420	0.000000
H	2.372849	-1.391185	0.000000
H	2.405689	1.107811	0.000000
F	0.314831	2.600190	0.000000
H	-2.835466	0.819886	0.000000

o-fluorophenol, *trans* S_1

C	0.818909	1.036675	0.110395
C	-0.587028	0.973139	0.090501
C	-1.273182	-0.284027	0.106787
C	-0.470979	-1.416661	-0.083271
C	0.937503	-1.329545	-0.071157
C	1.615875	-0.127053	0.181898
O	-1.251475	2.115149	-0.110315

H	-2.292380	-0.357286	0.479847
H	-0.929883	-2.391614	-0.208625
H	1.511076	-2.236714	-0.239263
H	2.685539	-0.068156	0.323856
F	1.394878	2.202367	-0.206901
H	-2.158882	1.883726	-0.373752

m-fluorophenol, *cis* S_0

C	0.307724	1.408000	0.000000
C	-0.926696	0.785370	0.000000
C	-0.967108	-0.605169	0.000000
C	0.214013	-1.341420	0.000000
C	1.429397	-0.679127	0.000000
C	1.497568	0.709137	0.000000
O	-2.134665	-1.294653	0.000000
F	0.337570	2.749536	0.000000
H	0.158709	-2.422760	0.000000
H	2.347636	-1.255306	0.000000
H	2.439942	1.241204	0.000000
H	-1.829884	1.386241	0.000000
H	-2.874206	-0.681053	0.000000

m-fluorophenol, *cis* S_1

C	1.218995	-0.054117	-0.683368
C	-0.053805	0.043026	-0.101164
C	-0.022790	0.038286	1.323866
C	1.163971	0.029834	2.083714
C	2.423758	0.128900	1.438894
C	2.423956	-0.038833	0.037735
O	-1.172759	-0.039254	2.009260
F	1.296074	-0.173842	-2.015505
H	1.078534	-0.132803	3.152105
H	3.345234	0.175316	1.998770
H	3.348238	-0.152098	-0.518560
H	-0.906148	0.414371	-0.663519
H	-1.887899	-0.238786	1.387721

m-fluorophenol, *trans* S_0

C	0.268213	1.301922	0.000000
C	-0.948484	0.629029	0.000000
C	-0.982723	-0.762306	0.000000
C	0.206536	-1.476353	0.000000
C	1.432261	-0.828478	0.000000

C	1.426676	0.554548	0.000000
O	-2.072228	1.388928	0.000000
H	-1.934652	-1.284400	0.000000
H	0.175850	-2.559975	0.000000
H	2.370290	-1.368094	0.000000
F	2.600730	1.204297	0.000000
H	0.302297	2.383554	0.000000
H	-2.844766	0.817337	0.000000

m-fluorophenol, *trans* S_1

C	1.084426	-0.016187	0.000000
C	0.328299	1.180033	0.000000
C	-1.088071	1.211666	0.000000
C	-1.821809	-0.005646	0.000000
C	-1.083179	-1.214371	0.000000
C	0.319473	-1.196692	0.000000
O	1.036264	2.319997	0.000000
H	-1.597033	2.170127	0.000000
H	-2.901137	-0.013174	0.000000
H	-1.582668	-2.175818	0.000000
F	0.965971	-2.368793	0.000000
H	2.163177	-0.011061	0.000000
H	0.435137	3.074067	0.000000

p-fluorophenol S_0

C	0.271157	1.313721	0.000000
C	-0.950172	0.647862	0.000000
C	-0.978920	-0.742249	0.000000
C	0.205511	-1.466706	0.000000
C	1.405772	-0.786464	0.000000
C	1.454938	0.595357	0.000000
O	-2.077926	1.408414	0.000000
H	-1.928974	-1.268625	0.000000
H	0.199990	-2.549883	0.000000
F	2.555770	-1.483790	0.000000
H	2.414623	1.097870	0.000000
H	0.278808	2.396937	0.000000
H	-2.850597	0.837547	0.000000

p-fluorophenol S_1

C	1.264933	0.679778	0.000000
C	0.028084	1.357868	0.000000
C	-1.233485	0.710932	0.000000

C	-1.248535	-0.703085	0.000000
C	-0.006662	-1.360396	0.000000
C	1.249590	-0.735524	0.000000
O	0.092157	2.696837	0.000000
H	-2.149900	1.290008	0.000000
H	-2.161337	-1.281175	0.000000
F	-0.027693	-2.690680	0.000000
H	2.149671	-1.332670	0.000000
H	2.181413	1.252743	0.000000
H	-0.801538	3.060958	0.000000

phenylacetylene S_0

C	1.206133	0.000000	-0.013854
C	0.000000	0.000000	-0.722235
C	-1.206133	0.000000	-0.013854
C	-1.201625	0.000000	1.371055
C	0.000000	0.000000	2.067412
C	1.201625	0.000000	1.371055
C	0.000000	0.000000	-2.146073
C	0.000000	0.000000	-3.349504
H	-2.141170	0.000000	-0.561429
H	-2.142280	0.000000	1.910379
H	0.000000	0.000000	3.151640
H	2.142280	0.000000	1.910379
H	2.141170	0.000000	-0.561429
H	0.000000	0.000000	-4.413561

phenylacetylene S_1

C	1.232251	0.000000	-0.031173
C	0.000000	0.000000	-0.752683
C	-1.232251	0.000000	-0.031173
C	-1.220655	0.000000	1.389054
C	0.000000	0.000000	2.087415
C	1.220655	0.000000	1.389054
C	0.000000	0.000000	-2.143191
C	0.000000	0.000000	-3.359681
H	-2.165603	0.000000	-0.577910
H	-2.157950	0.000000	1.930660
H	0.000000	0.000000	3.170663
H	2.157950	0.000000	1.930660
H	2.165603	0.000000	-0.577910
H	0.000000	0.000000	-4.423788

aniline S_0

C	0.920600	0.027617	0.000000
C	0.205937	0.035555	1.200842
C	-1.179209	0.042901	1.195237
C	-1.885834	0.047624	0.000000
C	-1.179209	0.042901	-1.195237
C	0.205937	0.035555	-1.200842
H	0.744895	0.036602	2.143446
H	-2.969291	0.052977	0.000000
H	-1.712183	0.046105	2.140145
H	-1.712183	0.046105	-2.140145
H	0.744895	0.036602	-2.143446
N	2.307859	0.075778	0.000000
H	2.753898	-0.263155	-0.836679
H	2.753898	-0.263155	0.836679

aniline S_1

C	0.889519	-0.033948	0.000000
C	0.226010	-0.008578	1.244196
C	-1.195501	0.045719	1.234415
C	-1.863138	0.071172	0.000000
C	-1.195501	0.045719	-1.234415
C	0.226010	-0.008578	-1.244196
H	0.794446	-0.030353	2.166392
H	-2.948159	0.112516	0.000000
H	-1.754914	0.067063	2.159703
H	-1.754914	0.067063	-2.159703
H	0.794446	-0.030353	-2.166392
N	2.250658	-0.086059	0.000000
H	2.765514	-0.105701	-0.864341
H	2.765514	-0.105701	0.864341

catechol S_0

C	0.467969	1.275646	0.000000
C	-0.748718	0.618218	0.000000
C	-0.798854	-0.778580	0.000000
C	0.382068	-1.501011	0.000000
C	1.604518	-0.840770	0.000000
C	1.651034	0.544542	0.000000
O	-1.968069	1.240578	0.000000
O	-1.990478	-1.422100	0.000000
H	0.324838	-2.583205	0.000000
H	2.522614	-1.416530	0.000000
H	2.602130	1.063455	0.000000

H	0.492555	2.361930	0.000000
H	-1.853845	2.193774	0.000000
H	-2.687762	-0.755947	0.000000

catechol S_1

C	0.471773	1.346249	0.000000
C	-0.759807	0.623577	0.000000
C	-0.803054	-0.783328	0.000000
C	0.386542	-1.571456	0.000000
C	1.594070	-0.856238	0.000000
C	1.635078	0.556840	0.000000
O	-1.966091	1.245537	0.000000
O	-1.983891	-1.422210	0.000000
H	0.324565	-2.648786	0.000000
H	2.534120	-1.395336	0.000000
H	2.604097	1.042854	0.000000
H	0.495493	2.427660	0.000000
H	-1.839944	2.199034	0.000000
H	-2.692951	-0.764397	0.000000

resorcinol, isomer 1 S_0

C	0.075855	1.145705	0.000000
C	-1.136511	0.466702	0.000000
C	-1.167597	-0.922489	0.000000
C	0.032205	-1.622083	0.000000
C	1.249515	-0.965713	0.000000
C	1.262670	0.426331	0.000000
O	-2.264811	1.224742	0.000000
H	-2.115703	-1.451159	0.000000
H	0.013024	-2.706317	0.000000
H	2.188049	-1.505107	0.000000
O	2.474682	1.039293	0.000000
H	0.070721	2.230941	0.000000
H	-3.032582	0.646926	0.000000
H	2.350482	1.992216	0.000000

resorcinol, isomer 1 S_1

C	0.000339	1.066031	0.066045
C	-1.188015	0.309232	-0.003906
C	-1.197212	-1.103236	-0.034600
C	-0.000515	-1.845977	0.117007
C	1.204250	-1.107477	0.012815
C	1.191412	0.301851	0.034655

O	-2.341042	1.008679	-0.057537
H	-2.142480	-1.614204	-0.202277
H	-0.003701	-2.925057	0.123081
H	2.159816	-1.600067	-0.128527
O	2.391196	0.915278	-0.030401
H	-0.022277	2.102349	0.384614
H	-3.087311	0.400107	-0.029161
H	2.246532	1.848610	-0.232158

resorcinol, isomer 2 S_0

C	1.197141	0.000000	-0.547096
C	0.000000	0.000000	-1.247071
C	-1.197141	0.000000	-0.547096
C	-1.207061	0.000000	0.845809
C	0.000000	0.000000	1.526388
C	1.207061	0.000000	0.845809
O	-2.340664	0.000000	-1.280616
O	2.340664	0.000000	-1.280616
H	-2.146894	0.000000	1.389053
H	0.000000	0.000000	2.610732
H	2.146894	0.000000	1.389053
H	0.000000	0.000000	-2.329451
H	-3.096721	0.000000	-0.687688
H	3.096721	0.000000	-0.687688

resorcinol, isomer 2 S_1

C	1.194403	0.000000	-0.330223
C	0.000000	0.000000	-1.081365
C	-1.194403	0.000000	-0.330223
C	-1.210070	0.000000	1.083197
C	0.000000	0.000000	1.823451
C	1.210070	0.000000	1.083197
O	-2.346487	0.000000	-1.035591
O	2.346487	0.000000	-1.035591
H	-2.165902	0.000000	1.599323
H	0.000000	0.000000	2.902859
H	2.165902	0.000000	1.599323
H	0.000000	0.000000	-2.160254
H	-3.093829	0.000000	-0.428596
H	3.093829	0.000000	-0.428596

resorcinol, isomer 3 S_0

C	1.202655	0.000000	-0.288374

C	0.000000	0.000000	-0.987787
C	-1.202655	0.000000	-0.288374
C	-1.209998	0.000000	1.100373
C	0.000000	0.000000	1.776090
C	1.209998	0.000000	1.100373
O	-2.404401	0.000000	-0.923328
O	2.404401	0.000000	-0.923328
H	-2.156786	0.000000	1.625191
H	0.000000	0.000000	2.860537
H	2.156786	0.000000	1.625191
H	0.000000	0.000000	-2.075816
H	2.267230	0.000000	-1.874135
H	-2.267230	0.000000	-1.874135

resorcinol, isomer 3 S_1

C	-0.025230	-0.303377	1.184060
C	-0.125095	-1.076036	0.000000
C	-0.025230	-0.303377	-1.184060
C	0.024883	1.106292	-1.195806
C	-0.083305	1.846572	0.000000
C	0.024883	1.106292	1.195806
O	0.071148	-0.915065	-2.381934
O	0.071148	-0.915065	2.381934
H	0.184290	1.593224	-2.151929
H	-0.091240	2.925952	0.000000
H	0.184290	1.593224	2.151929
H	-0.666938	-2.025965	0.000000
H	0.252898	-1.851799	2.226500
H	0.252898	-1.851799	-2.226500

hydroquinone, *cis* S_0

C	-0.695123	0.000000	1.088014
C	0.695123	0.000000	1.088014
C	1.394034	0.000000	-0.109667
C	0.691135	0.000000	-1.309866
C	-0.691135	0.000000	-1.309866
C	-1.394034	0.000000	-0.109667
O	2.756974	0.000000	-0.175391
O	-2.756974	0.000000	-0.175391
H	1.244772	0.000000	-2.241258
H	-1.244772	0.000000	-2.241258
H	-1.229758	0.000000	2.033710
H	1.229758	0.000000	2.033710
H	-3.117541	0.000000	0.714748

H	3.117541	0.000000	0.714748

hydroquinone, *cis* S_1

C	0.706134	0.000000	-1.128515
C	-0.706134	0.000000	-1.128515
C	-1.370313	0.000000	0.120519
C	-0.706389	0.000000	1.360853
C	0.706389	0.000000	1.360853
C	1.370313	0.000000	0.120519
O	-2.712924	0.000000	0.164078
O	2.712924	0.000000	0.164078
H	-1.288244	0.000000	2.271539
H	1.288244	0.000000	2.271539
H	1.273921	0.000000	-2.051975
H	-1.273921	0.000000	-2.051975
H	3.059081	0.000000	-0.735728
H	-3.059081	0.000000	-0.735728

hydroquinone, *trans* S_0

C	0.021432	1.386731	0.000000
C	-1.194634	0.718528	0.000000
C	-1.208690	-0.671299	0.000000
C	-0.021432	-1.386731	0.000000
C	1.194634	-0.718528	0.000000
C	1.208690	0.671299	0.000000
O	-2.332575	1.471642	0.000000
H	-2.154571	-1.205959	0.000000
H	-0.027501	-2.470129	0.000000
O	2.332575	-1.471642	0.000000
H	2.154571	1.205959	0.000000
H	0.027501	2.470129	0.000000
H	-3.096896	0.890104	0.000000
H	3.096896	-0.890104	0.000000

hydroquinone, *trans* S_1

C	1.260738	0.675264	0.000000
C	0.036115	1.369834	0.000000
C	-1.227968	0.736942	0.000000
C	-1.260738	-0.675264	0.000000
C	-0.036115	-1.369834	0.000000
C	1.227968	-0.736942	0.000000
O	0.118586	2.710597	0.000000
H	-2.138012	1.325861	0.000000

H	-2.184631	-1.236442	0.000000
O	-0.118586	-2.710597	0.000000
H	2.138012	-1.325861	0.000000
H	2.184631	1.236442	0.000000
H	-0.771487	3.081835	0.000000
H	0.771487	-3.081835	0.000000

salicylic acid S_0

C	1.101102	1.593830	0.000000
C	1.132280	0.197228	0.000000
C	-0.085953	-0.515232	0.000000
C	-1.298201	0.186945	0.000000
C	-1.315833	1.563718	0.000000
C	-0.105434	2.260709	0.000000
O	2.320976	-0.405299	0.000000
C	-0.042154	-1.972912	0.000000
O	-1.237846	-2.573655	0.000000
O	0.989200	-2.629085	0.000000
H	-2.222562	-0.377261	0.000000
H	2.044270	2.126589	0.000000
H	-2.256955	2.099644	0.000000
H	-0.109969	3.345463	0.000000
H	2.156755	-1.374860	0.000000
H	-1.069676	-3.525820	0.000000

salicylic acid S_1

C	0.994460	1.906665	0.000000
C	0.958581	0.505006	0.000000
C	-0.294461	-0.216671	0.000000
C	-1.447605	0.542775	0.000000
C	-1.398773	1.974635	0.000000
C	-0.201026	2.656410	0.000000
O	2.066833	-0.186203	0.000000
C	-0.230925	-1.650542	0.000000
O	-1.406117	-2.311589	0.000000
O	0.864947	-2.294182	0.000000
H	-2.410643	0.046808	0.000000
H	1.967397	2.383505	0.000000
H	-2.336449	2.518470	0.000000
H	-0.171123	3.737760	0.000000
H	1.743971	-1.224004	0.000000
H	-1.188488	-3.251897	0.000000

o-cresol, *cis* S_0

C	1.959621	0.511754	0.000000
C	0.727346	1.147950	0.000000
C	-0.465295	0.431383	0.000000
C	-0.390875	-0.965507	0.000000
C	0.837263	-1.614378	0.000000
C	2.008632	-0.875659	0.000000
C	-1.797443	1.120498	0.000000
O	-1.505925	-1.746022	0.000000
H	0.852184	-2.698004	0.000000
H	2.963865	-1.388842	0.000000
H	2.873234	1.094562	0.000000
H	0.681700	2.232758	0.000000
H	-2.288207	-1.187959	0.000000
H	-2.392471	0.867014	0.885611
H	-1.671158	2.203450	0.000000
H	-2.392471	0.867014	-0.885611

o-cresol, *cis* S_1

C	1.851122	-0.044231	-0.779357
C	0.622869	0.096372	-1.454749
C	-0.593182	0.064017	-0.711754
C	-0.470256	0.075622	0.709446
C	0.767442	0.016253	1.395704
C	1.941025	-0.090966	0.625251
C	-1.888543	-0.080322	-1.422385
O	-1.556226	0.120883	1.492031
H	0.774522	0.123344	2.471762
H	2.908090	-0.180481	1.102583
H	2.762708	-0.119435	-1.363287
H	0.593366	0.132245	-2.536085
H	-2.340580	0.247527	0.939435
H	-2.742361	-0.308431	-0.774134
H	-2.149472	0.823809	-1.991692
H	-1.831103	-0.895695	-2.160358

o-cresol, *trans* S_0

C	2.414841	0.000015	0.029394
C	1.243567	-0.000039	-0.717390
C	0.030124	-0.000011	-0.022245
C	0.001158	0.000065	1.366295
C	1.187341	0.000114	2.086952
C	2.400976	0.000087	1.419033
C	1.249248	-0.000110	-2.213767

O	-1.107489	-0.000067	-0.771915
H	-0.953831	0.000094	1.885486
H	1.155768	0.000173	3.170741
H	3.332578	0.000134	1.972742
H	3.364048	-0.000010	-0.497627
H	-1.871045	-0.000057	-0.188643
H	2.270823	-0.000058	-2.596311
H	0.730360	-0.876631	-2.611348
H	0.730239	0.876301	-2.611427

o-cresol, *trans* S_1

C	2.421052	0.267766	-0.006760
C	1.211808	0.117698	-0.753138
C	0.009411	-0.008873	-0.016790
C	-0.049898	-0.092488	1.406932
C	1.175994	-0.074690	2.096170
C	2.383391	0.090023	1.385088
C	1.251415	-0.022034	-2.227484
O	-1.130423	-0.110947	-0.716995
H	-0.996703	0.048633	1.918688
H	1.198915	-0.151725	3.176147
H	3.314227	0.092012	1.943188
H	3.360205	0.412581	-0.524000
H	-1.831262	-0.397641	-0.113532
H	1.847933	-0.899410	-2.521932
H	0.259230	-0.115204	-2.665917
H	1.753393	0.844298	-2.679687

m-cresol, *cis* S_0

C	1.157568	-0.004873	2.082239
C	2.366392	0.009183	1.409943
C	2.411927	0.019591	0.020810
C	1.234573	0.014027	-0.719122
C	0.017381	0.002082	-0.040455
C	-0.023838	-0.008101	1.347942
C	1.260582	0.002126	-2.219355
O	-1.193170	-0.018861	2.041961
H	1.107574	-0.010680	3.164338
H	3.290268	0.014775	1.978157
H	3.368054	0.032952	-0.491052
H	-0.912382	0.001775	-0.605704
H	-1.929440	-0.019430	1.424400
H	2.257607	0.231990	-2.598200
H	0.975908	-0.980047	-2.609182

H	0.563296	0.732862	-2.636771

m-cresol, *cis* S_1

C	1.163158	0.009973	2.120456
C	2.403789	0.085993	1.444649
C	2.402340	0.035007	0.035989
C	1.218170	-0.003395	-0.742735
C	-0.031048	0.011026	-0.069903
C	-0.016704	0.005393	1.350320
C	1.264984	-0.032997	-2.225942
O	-1.173442	-0.038564	2.028302
H	1.087502	-0.111172	3.193414
H	3.335345	0.114699	1.992169
H	3.353254	0.037345	-0.488512
H	-0.953208	0.220627	-0.605051
H	-1.894297	-0.189336	1.402252
H	2.285223	0.060278	-2.601740
H	0.841611	-0.966457	-2.624608
H	0.665602	0.780950	-2.659118

m-cresol, *trans* S_0

C	-1.188078	-1.096578	0.000000
C	0.200779	-1.208254	0.000000
C	0.969468	-0.048996	0.000000
C	0.365746	1.201077	0.000000
C	-1.021798	1.307711	0.000000
C	-1.789148	0.153640	0.000000
C	0.869038	-2.551977	0.000000
O	1.181302	2.289686	0.000000
H	-1.496131	2.285119	0.000000
H	-2.870787	0.233424	0.000000
H	-1.799684	-1.992222	0.000000
H	2.053091	-0.100832	0.000000
H	0.645504	3.087323	0.000000
H	0.134738	-3.358828	0.000000
H	1.505523	-2.675884	-0.880536
H	1.505523	-2.675884	0.880536

m-cresol, *trans* S_1

C	-1.198090	-1.054429	0.000000
C	0.205867	-1.233725	0.000000
C	1.025711	-0.072357	0.000000
C	0.397165	1.191824	0.000000

C	-1.007904	1.370706	0.000000
C	-1.821084	0.213845	0.000000
C	0.823348	-2.583893	0.000000
O	1.213423	2.258015	0.000000
H	-1.431538	2.369288	0.000000
H	-2.899506	0.292122	0.000000
H	-1.826372	-1.939914	0.000000
H	2.106283	-0.125088	0.000000
H	0.685327	3.065253	0.000000
H	0.068218	-3.372541	0.000000
H	1.467816	-2.732045	-0.878122
H	1.467816	-2.732045	0.878122

p-cresol S_0

C	0.710248	0.013307	-1.186798
C	-0.673290	0.015142	-1.195583
C	-1.372119	0.000524	0.006535
C	-0.670167	-0.017896	1.204429
C	0.718600	-0.019475	1.193950
C	1.436954	-0.001970	0.004160
O	-2.731774	0.000692	-0.053137
C	2.937503	0.021241	-0.004313
H	-1.205588	-0.034234	2.150044
H	1.251331	-0.036517	2.139727
H	1.241144	0.022226	-2.134026
H	-1.228967	0.024646	-2.125945
H	-3.088349	-0.012243	0.838971
H	3.343735	-0.672822	-0.744353
H	3.319330	1.017502	-0.249307
H	3.342969	-0.254747	0.970947

p-cresol S_1

C	0.731845	-0.083731	-1.233612
C	-0.681302	-0.028374	-1.242110
C	-1.350002	-0.008978	-0.002108
C	-0.681891	-0.000870	1.247695
C	0.730317	-0.021672	1.235705
C	1.427054	-0.037251	0.001025
O	-2.690141	0.019732	-0.047496
C	2.907700	0.039762	-0.000195
H	-1.247694	-0.057203	2.171168
H	1.290968	-0.016142	2.161911
H	1.290274	-0.107357	-2.160438
H	-1.260777	0.032972	-2.153263

H	-3.035088	0.100649	0.850214
H	3.332275	-0.486286	-0.859882
H	3.234557	1.087299	-0.073706
H	3.333455	-0.367169	0.920384

o-methoxyphenol S_0

C	2.023520	-0.086516	0.000000
C	0.870458	0.695927	0.000000
C	-0.371361	0.084796	0.000000
C	-0.470370	-1.314323	0.000000
C	0.678997	-2.081870	0.000000
C	1.926594	-1.467002	0.000000
O	-1.578508	0.721432	0.000000
O	-1.687452	-1.906644	0.000000
H	0.580331	-3.161079	0.000000
H	2.822638	-2.076709	0.000000
H	2.993840	0.395841	0.000000
H	0.951599	1.775805	0.000000
C	-1.582249	2.130933	0.000000
H	-2.349627	-1.204440	0.000000
H	-2.627683	2.434451	0.000000
H	-1.090363	2.529699	0.893500
H	-1.090363	2.529699	-0.893500

o-methoxyphenol S_1

C	2.466707	0.069305	0.052764
C	1.374233	-0.294477	-0.748976
C	0.108154	-0.281123	-0.091233
C	0.016898	-0.163905	1.315882
C	1.177765	-0.068342	2.133253
C	2.373283	0.179211	1.455668
O	-1.079619	-0.089335	-0.725952
O	-1.176824	0.060962	1.884453
H	1.108441	-0.183116	3.206698
H	3.266099	0.446982	2.012917
H	3.430213	0.257872	-0.414589
H	1.506635	-0.659418	-1.760870
C	-1.077325	0.130508	-2.131265
H	-1.849962	0.043173	1.183249
H	-2.112666	0.328486	-2.401520
H	-0.447675	0.983334	-2.393858
H	-0.725797	-0.760125	-2.658540

m-methoxyphenol, isomer 1 S_0

C	0.926270	1.445577	0.000000
C	-0.262269	0.717863	0.000000
C	-0.230991	-0.673952	0.000000
C	0.998574	-1.331680	0.000000
C	2.186875	-0.617579	0.000000
C	2.132421	0.769490	0.000000
H	-1.146685	-1.254464	0.000000
O	1.078881	-2.689066	0.000000
H	3.128246	-1.152105	0.000000
H	3.057349	1.335729	0.000000
H	0.877764	2.527153	0.000000
O	-1.405610	1.445049	0.000000
H	0.194247	-3.063638	0.000000
C	-2.633193	0.756311	0.000000
H	-3.408808	1.520301	0.000000
H	-2.746536	0.132505	-0.893927
H	-2.746536	0.132505	0.893927

m-methoxyphenol, isomer 1 S_1

C	1.165844	-0.018485	-0.616203
C	-0.030791	-0.039903	0.130340
C	-0.054659	-0.090578	1.548203
C	1.231657	-0.003221	2.142410
C	2.436114	0.014451	1.412643
C	2.429407	-0.124933	0.009374
H	-0.877827	-0.549152	2.093575
O	1.338472	0.136279	3.480525
H	3.355026	0.180798	1.964628
H	3.343750	-0.152400	-0.563503
H	1.076021	0.101867	-1.690440
O	-1.151087	0.046771	-0.615352
H	0.464925	0.367830	3.826327
C	-2.407306	0.033984	0.033298
H	-3.137490	0.336653	-0.715043
H	-2.652521	-0.972370	0.387954
H	-2.421224	0.732407	0.874003

m-methoxyphenol, isomer 2 S_0

C	0.346206	2.154346	0.000000
C	-0.836910	1.444142	0.000000
C	-0.795438	0.047674	0.000000
C	0.423126	-0.618551	0.000000
C	1.603972	0.119876	0.000000

C	1.577426	1.506888	0.000000
O	-1.995342	-0.578889	0.000000
C	-2.007939	-1.988114	0.000000
O	2.763519	-0.590894	0.000000
H	0.494694	-1.697559	0.000000
H	2.501898	2.076003	0.000000
H	0.316758	3.238389	0.000000
H	-1.799472	1.939724	0.000000
H	-3.056677	-2.280341	0.000000
H	-1.521341	-2.395343	-0.892988
H	-1.521341	-2.395343	0.892988
H	3.506853	0.018003	0.000000

m-methoxyphenol, isomer 2 S_1

C	1.241534	-0.129749	-0.704470
C	0.059095	-0.029530	0.077431
C	0.111050	-0.057788	1.486166
C	1.332013	-0.092725	2.203247
C	2.493784	0.001174	1.407176
C	2.461468	0.037808	-0.002423
O	-1.091926	-0.007454	2.092611
C	-1.143893	0.043345	3.503861
O	3.665787	0.081762	2.075408
H	1.412648	-0.296668	3.259957
H	3.388422	0.218977	-0.541588
H	1.206336	-0.120086	-1.782974
H	-0.913843	0.098325	-0.383364
H	-2.195258	0.156919	3.760991
H	-0.761341	-0.881587	3.946148
H	-0.573957	0.893432	3.889509
H	4.393214	0.083848	1.444215

p-methoxyphenol, *cis* S_0

C	-0.317387	0.733443	0.000000
C	-1.546278	0.072613	0.000000
C	-1.605102	-1.305397	0.000000
C	-0.432279	-2.057090	0.000000
C	0.789493	-1.405427	0.000000
C	0.852705	-0.013625	0.000000
O	-0.553797	-3.415554	0.000000
O	-0.369568	2.092695	0.000000
C	0.850545	2.791826	0.000000
H	1.823137	0.465559	0.000000
H	-2.453171	0.665882	0.000000

H	-2.558596	-1.820201	0.000000
H	1.712951	-1.978063	0.000000
H	0.594978	3.850307	0.000000
H	1.445834	2.567948	0.893151
H	1.445834	2.567948	-0.893151
H	0.320698	-3.812845	0.000000

p-methoxyphenol, *cis* S_1

C	1.326589	-0.022174	-0.614479
C	0.051925	-0.043089	0.001166
C	-0.015443	0.000354	1.411142
C	1.188267	-0.004963	2.133200
C	2.466254	-0.010612	1.523699
C	2.536848	-0.011958	0.112110
O	1.088911	0.008213	3.473061
O	1.287494	-0.027650	-1.953885
C	2.489383	0.023330	-2.699229
H	3.493979	-0.017282	-0.388191
H	-0.829539	-0.043935	-0.623791
H	-0.952575	0.069490	1.945728
H	3.358545	-0.123911	2.129492
H	2.190845	0.014134	-3.745266
H	3.045006	0.939008	-2.481168
H	3.115627	-0.847636	-2.488404
H	1.971413	0.098666	3.851818

p-methoxyphenol, *trans* S_0

C	-0.655728	1.302548	0.000000
C	-1.884967	0.669004	0.000000
C	-1.960068	-0.721223	0.000000
C	-0.789607	-1.462251	0.000000
C	0.447191	-0.829254	0.000000
C	0.521894	0.560095	0.000000
O	-3.144768	-1.397536	0.000000
H	1.343842	-1.435618	0.000000
O	1.680282	1.273610	0.000000
H	-0.589219	2.384119	0.000000
H	-2.794231	1.264073	0.000000
H	-3.869869	-0.767759	0.000000
H	-0.852622	-2.544005	0.000000
C	2.889150	0.554394	0.000000
H	3.684970	1.297614	0.000000
H	2.986870	-0.073915	0.893027
H	2.986870	-0.073915	-0.893027

p-methoxyphenol, *trans* S_1

C	0.123794	-0.045683	-1.390538
C	-1.277616	-0.011043	-1.215602
C	-1.777954	0.022239	0.103582
C	-0.957280	0.055058	1.246877
C	0.445794	0.028933	1.075042
C	0.951064	-0.010647	-0.241529
O	-3.102712	0.037495	0.327937
H	1.102181	0.060641	1.931703
O	2.262430	-0.029791	-0.517182
H	0.588368	-0.083944	-2.365557
H	-1.955890	-0.086337	-2.057903
H	-3.564619	0.054910	-0.518145
H	-1.417003	0.113830	2.223501
C	3.207221	-0.017498	0.536519
H	4.184599	-0.042234	0.059530
H	3.111690	0.892631	1.134399
H	3.086723	-0.894249	1.178068

1-naphthol, *cis* S_0

C	0.830530	1.515713	0.016065
C	0.527547	0.125192	0.001400
C	-0.843446	-0.266021	-0.007509
C	-1.854136	0.719773	-0.016254
C	-1.517993	2.046444	-0.014625
C	-0.174047	2.449825	0.003035
C	1.520280	-0.881405	-0.006860
C	1.184534	-2.208601	-0.010636
C	-0.168405	-2.595719	-0.010042
C	-1.152661	-1.645978	-0.010523
O	2.108755	1.970926	0.033768
H	-2.197357	-1.939888	-0.014680
H	-0.426217	-3.648837	-0.012522
H	1.962094	-2.963876	-0.018209
H	2.576261	-0.624707	-0.020276
H	-2.892879	0.408833	-0.024742
H	-2.293317	2.804432	-0.022992
H	0.092677	3.499835	0.012288
H	2.717792	1.234069	0.123311

1-naphthol, *cis* S_1

C	0.862804	1.466575	0.017341

C	0.532170	0.087939	-0.063223
C	-0.843219	-0.245548	0.005986
C	-1.788079	0.807624	-0.018949
C	-1.426621	2.170073	-0.028562
C	-0.100970	2.510332	-0.028020
C	1.512532	-0.927358	-0.127970
C	1.099990	-2.286678	-0.045707
C	-0.230355	-2.609800	0.047177
C	-1.227294	-1.604525	0.053956
O	2.129150	1.848470	0.154545
H	-2.276577	-1.863775	0.117962
H	-0.527261	-3.650862	0.110074
H	1.849061	-3.069956	-0.065556
H	2.553581	-0.707080	-0.342804
H	-2.841285	0.545900	-0.029331
H	-2.194592	2.932799	-0.057986
H	0.246084	3.535652	-0.011563
H	2.670881	1.060207	0.312609

1-naphthol, *trans* S_0

C	-0.714631	-0.539245	0.000000
C	-0.672094	-1.952245	0.000000
C	0.521512	-2.622310	0.000000
C	1.736007	-1.910475	0.000000
C	1.734565	-0.540896	0.000000
C	0.516620	0.172710	0.000000
H	-1.609245	-2.499529	0.000000
H	0.535112	-3.706757	0.000000
H	2.675866	-2.451187	0.000000
H	2.664165	0.014554	0.000000
C	-1.936158	0.174213	0.000000
C	-1.932566	1.541100	0.000000
C	-0.722451	2.259306	0.000000
C	0.476503	1.592688	0.000000
H	-2.869602	-0.377807	0.000000
H	-2.868127	2.089275	0.000000
H	-0.739225	3.345613	0.000000
O	1.675578	2.230696	0.000000
H	1.528182	3.180285	0.000000

1-naphthol, *trans* S_1

C	-0.933731	-0.391293	0.000000
C	-1.307945	-1.748668	0.000000
C	-0.314291	-2.762966	0.000000

C	1.015358	-2.426910	0.000000
C	1.424705	-1.066608	0.000000
C	0.450939	-0.050085	0.000000
H	-2.359523	-2.009649	0.000000
H	-0.614509	-3.804445	0.000000
H	1.772630	-3.203033	0.000000
H	2.474527	-0.808333	0.000000
C	-1.885124	0.651168	0.000000
C	-1.524854	2.018286	0.000000
C	-0.201442	2.362813	0.000000
C	0.778014	1.326604	0.000000
H	-2.937700	0.387382	0.000000
H	-2.295605	2.779095	0.000000
H	0.117716	3.400578	0.000000
O	2.080276	1.643784	0.000000
H	2.184880	2.601351	0.000000

2-naphthol, *cis* S_0

C	0.596761	2.004599	0.000000
C	0.620281	0.593076	0.000000
C	-0.610164	-0.121713	0.000000
C	-1.818691	0.611973	0.000000
C	-1.808331	1.981300	0.000000
C	-0.590053	2.687777	0.000000
C	1.828301	-0.143551	0.000000
C	1.827577	-1.508142	0.000000
C	0.604157	-2.212232	0.000000
C	-0.587498	-1.534475	0.000000
H	-1.529517	-2.077127	0.000000
H	1.540231	2.541535	0.000000
H	-0.596365	3.771883	0.000000
H	-2.744572	2.528740	0.000000
H	-2.760096	0.071620	0.000000
H	2.769920	0.396096	0.000000
H	2.749954	-2.076725	0.000000
O	0.695591	-3.567443	0.000000
H	-0.187498	-3.947182	0.000000

2-naphthol, *cis* S_1

C	0.598017	1.987444	0.000000
C	0.639236	0.583307	0.000000
C	-0.621076	-0.115669	0.000000
C	-1.826468	0.605818	0.000000
C	-1.836369	2.018378	0.000000

C	-0.629747	2.687844	0.000000
C	1.842845	-0.152989	0.000000
C	1.879115	-1.556806	0.000000
C	0.660225	-2.219185	0.000000
C	-0.576907	-1.519805	0.000000
H	-1.503729	-2.088950	0.000000
H	1.528710	2.544380	0.000000
H	-0.610448	3.772489	0.000000
H	-2.773654	2.559672	0.000000
H	-2.763075	0.057691	0.000000
H	2.777116	0.398698	0.000000
H	2.803865	-2.115689	0.000000
O	0.659736	-3.560903	0.000000
H	-0.247379	-3.885714	0.000000

2-naphthol, *trans* S_0

C	0.509987	2.006505	0.000000
C	0.538739	0.593827	0.000000
C	-0.689344	-0.127863	0.000000
C	-1.901512	0.602940	0.000000
C	-1.895721	1.971186	0.000000
C	-0.679138	2.683510	0.000000
C	1.747188	-0.136401	0.000000
C	1.746262	-1.503652	0.000000
C	0.525833	-2.213230	0.000000
C	-0.666558	-1.537530	0.000000
H	-1.594689	-2.097858	0.000000
H	1.451158	2.547552	0.000000
H	-0.690585	3.767605	0.000000
H	-2.833764	2.515569	0.000000
H	-2.839916	0.057873	0.000000
H	2.688346	0.403966	0.000000
H	2.684850	-2.051604	0.000000
O	0.499715	-3.572526	0.000000
H	1.399161	-3.909868	0.000000

2-naphthol, *trans* S_1

C	0.510247	1.992357	0.000000
C	0.553455	0.588134	0.000000
C	-0.703263	-0.116030	0.000000
C	-1.909574	0.602537	0.000000
C	-1.922372	2.015841	0.000000
C	-0.719303	2.689624	0.000000
C	1.759567	-0.143302	0.000000

C	1.796813	-1.548205	0.000000
C	0.574883	-2.212845	0.000000
C	-0.660619	-1.520531	0.000000
H	-1.571559	-2.108072	0.000000
H	1.439814	2.551308	0.000000
H	-0.703571	3.774314	0.000000
H	-2.861594	2.554036	0.000000
H	-2.844309	0.051719	0.000000
H	2.692737	0.410341	0.000000
H	2.733943	-2.092015	0.000000
O	0.475997	-3.551259	0.000000
H	1.358709	-3.937944	0.000000

5-methoxysalicylic acid S_0

C	2.273824	-0.164666	0.000000
C	1.562979	-1.338928	0.000000
C	0.160302	-1.336593	0.000000
C	-0.509798	-0.132650	0.000000
C	0.208524	1.077304	0.000000
C	1.612952	1.069055	0.000000
O	-0.430768	-2.558853	0.000000
C	-1.838084	-2.598683	0.000000
C	-0.478336	2.362548	0.000000
O	-1.816244	2.289227	0.000000
O	2.354652	2.180265	0.000000
O	0.087951	3.445890	0.000000
H	-2.112394	-3.652158	0.000000
H	-2.255013	-2.118798	-0.893017
H	-2.255013	-2.118798	0.893017
H	-1.589602	-0.084132	0.000000
H	3.357045	-0.166672	0.000000
H	2.074116	-2.294949	0.000000
H	1.734582	2.941981	0.000000
H	-2.141655	3.199611	0.000000

5-methoxysalicylic acid S_1

C	2.168051	-0.137447	0.000000
C	1.729513	-1.458555	0.000000
C	0.345742	-1.686637	0.000000
C	-0.590941	-0.618702	0.000000
C	-0.159878	0.702005	0.000000
C	1.263706	0.929182	0.000000
O	-0.031919	-2.967846	0.000000
C	-1.406968	-3.315279	0.000000

C	-1.037212	1.837236	0.000000
O	-2.364444	1.557457	0.000000
O	1.707169	2.169056	0.000000
O	-0.640007	3.030964	0.000000
H	-1.434029	-4.402367	0.000000
H	-1.907399	-2.936250	-0.894488
H	-1.907399	-2.936250	0.894488
H	-1.653970	-0.817462	0.000000
H	3.224502	0.102590	0.000000
H	2.411052	-2.297343	0.000000
H	0.868843	2.764208	0.000000
H	-2.812358	2.412216	0.000000

m-dimethoxybenzene, *trans* S_0

C	0.000000	-0.705967	-0.179561
C	0.000000	0.705967	-0.179561
C	0.000000	1.386159	1.027173
C	0.000000	0.689390	2.235185
C	0.000000	-0.689390	2.235185
C	0.000000	-1.386159	1.027173
O	0.000000	1.292295	-1.398009
H	0.000000	2.468469	1.037540
H	0.000000	1.240764	3.168243
H	0.000000	-1.240764	3.168243
H	0.000000	-2.468469	1.037540
O	0.000000	-1.292295	-1.398009
C	0.000000	-2.698578	-1.446479
H	0.000000	-2.963242	-2.502607
H	0.892946	-3.120100	-0.970733
H	-0.892946	-3.120100	-0.970733
C	0.000000	2.698578	-1.446479
H	0.000000	2.963242	-2.502607
H	-0.892946	3.120100	-0.970733
H	0.892946	3.120100	-0.970733

m-dimethoxybenzene, *trans* S_1

C	-0.131453	-1.060624	-1.442117
C	-0.294373	0.157231	-0.707340
C	-0.294373	0.157231	0.707340
C	-0.131453	-1.060624	1.442117
C	0.291495	-2.170585	0.703328
C	0.291495	-2.170585	-0.703328
O	-0.252116	1.370736	-1.289008
C	0.003818	1.451832	-2.681004

O	-0.252116	1.370736	1.289008
C	0.003818	1.451832	2.681004
H	-0.411610	-1.148198	2.485165
H	0.592052	-3.077737	1.221337
H	0.592052	-3.077737	-1.221337
H	-0.411610	-1.148198	-2.485165
H	0.062947	2.514976	-2.906122
H	0.943987	0.960020	-2.942095
H	-0.811656	1.004788	-3.256813
H	0.062947	2.514976	2.906122
H	-0.811656	1.004788	3.256813
H	0.943987	0.960020	2.942095

3P-propionic acid, *gauche* S_0

C	-1.028387	0.902608	-1.164992
C	-0.384109	0.664720	0.048129
C	-1.045378	-0.090545	1.014408
C	-2.315417	-0.596202	0.772122
C	-2.945486	-0.354185	-0.440371
C	-2.297278	0.398372	-1.410374
C	1.002303	1.199137	0.291506
C	2.102621	0.279064	-0.231840
C	2.310009	-0.944496	0.617351
O	2.019190	-1.052418	1.779276
O	2.915454	-1.930983	-0.068682
H	1.913064	-0.032013	-1.261470
H	3.064908	0.805061	-0.240084
H	1.157761	1.359882	1.360631
H	1.105848	2.169554	-0.201398
H	-0.551984	-0.286901	1.960100
H	-2.815915	-1.180064	1.537094
H	-3.938993	-0.746354	-0.627772
H	-2.784032	0.598957	-2.358738
H	-0.532145	1.499132	-1.925452
H	3.047976	-2.662348	0.550568

3P-propionic acid, *gauche* S_1

C	-0.679614	0.242153	-1.094323
C	-0.355569	0.549002	0.260421
C	-1.341730	0.369715	1.269680
C	-2.646055	-0.062184	0.934883
C	-2.956757	-0.350571	-0.414403
C	-1.982983	-0.194560	-1.428616
C	0.972279	1.108698	0.626256

C	2.151981	0.502786	-0.126130
C	2.296170	-0.968412	0.146051
O	1.948154	-1.530476	1.152118
O	2.920088	-1.609010	-0.864244
H	2.090772	0.668486	-1.202781
H	3.080218	0.986167	0.201649
H	1.126618	0.985928	1.701164
H	0.973170	2.194695	0.433882
H	-1.072892	0.548272	2.303645
H	-3.395898	-0.186762	1.705105
H	-3.950419	-0.694922	-0.675326
H	-2.236502	-0.409584	-2.458827
H	0.055740	0.384826	-1.875220
H	3.003239	-2.534257	-0.594983

3P-propionic acid, *anti* S_0

C	1.453460	-0.447142	0.000000
C	0.542608	0.774464	0.000000
C	2.912102	-0.090008	0.000000
H	1.262138	-1.082744	0.870596
H	1.262138	-1.082744	-0.870596
C	-0.910640	0.388462	0.000000
H	0.769602	1.389721	0.874033
H	0.769602	1.389721	-0.874033
C	-1.596512	0.190022	1.196301
C	-2.928469	-0.199501	1.199136
C	-3.598905	-0.397069	0.000000
C	-2.928469	-0.199501	-1.199136
C	-1.596512	0.190022	-1.196301
H	-1.081441	0.351372	2.138828
H	-3.446190	-0.343781	2.141267
H	-4.640666	-0.697789	0.000000
H	-3.446190	-0.343781	-2.141267
H	-1.081441	0.351372	-2.138828
O	3.691011	-1.189709	0.000000
O	3.367499	1.022353	0.000000
H	4.608111	-0.882419	0.000000

3P-propionic acid, *anti* S_1

C	1.452878	-0.431716	0.000000
C	0.557474	0.811826	0.000000
C	2.914922	-0.090205	0.000000
H	1.247521	-1.060107	0.872382
H	1.247521	-1.060107	-0.872382

C	-0.883604	0.452221	0.000000
H	0.799114	1.415945	0.879808
H	0.799114	1.415945	-0.879808
C	-1.571586	0.241718	1.229238
C	-2.910914	-0.220266	1.229838
C	-3.575319	-0.442595	0.000000
C	-2.910914	-0.220266	-1.229838
C	-1.571586	0.241718	-1.229238
H	-1.060515	0.439000	2.164337
H	-3.425765	-0.400370	2.164726
H	-4.603371	-0.784290	0.000000
H	-3.425765	-0.400370	-2.164726
H	-1.060515	0.439000	-2.164337
O	3.680254	-1.199569	0.000000
O	3.382352	1.017617	0.000000
H	4.601330	-0.903974	0.000000

fluorine S_0

C	0.000000	0.000000	-1.785581
C	0.000000	1.176468	-0.847418
C	0.000000	0.731139	0.482365
C	0.000000	-0.731139	0.482365
C	0.000000	1.643626	1.529811
C	0.000000	3.000640	1.236130
C	0.000000	3.441491	-0.083719
C	0.000000	2.529496	-1.134405
H	0.000000	2.880168	-2.161609
H	0.000000	4.505283	-0.294328
H	0.000000	3.725336	2.042961
H	0.000000	1.307338	2.561251
C	0.000000	-1.643626	1.529811
C	0.000000	-3.000640	1.236130
C	0.000000	-3.441491	-0.083719
C	0.000000	-2.529496	-1.134405
C	0.000000	-1.176468	-0.847418
H	0.000000	-1.307338	2.561251
H	0.000000	-3.725336	2.042961
H	0.000000	-4.505283	-0.294328
H	0.000000	-2.880168	-2.161609
H	-0.879997	0.000000	-2.438238
H	0.879997	0.000000	-2.438238

fluorine S_1

C	0.000000	0.000000	-1.858368

C	0.000000	1.176864	-0.914642
C	0.000000	0.698166	0.450535
C	0.000000	-0.698166	0.450535
C	0.000000	1.637271	1.532832
C	0.000000	2.976066	1.226570
C	0.000000	3.430811	-0.107794
C	0.000000	2.518069	-1.185053
H	0.000000	2.884379	-2.206316
H	0.000000	4.496356	-0.306779
H	0.000000	3.709817	2.025792
H	0.000000	1.293785	2.560593
C	0.000000	-1.637271	1.532832
C	0.000000	-2.976066	1.226570
C	0.000000	-3.430811	-0.107794
C	0.000000	-2.518069	-1.185053
C	0.000000	-1.176864	-0.914642
H	0.000000	-1.293785	2.560593
H	0.000000	-3.709817	2.025792
H	0.000000	-4.496356	-0.306779
H	0.000000	-2.884379	-2.206316
H	-0.879111	0.000000	-2.514390
H	0.879111	0.000000	-2.514390

phenanthrene S_0

C	0.724812	0.000000	-0.349696
C	-0.724812	0.000000	-0.349696
C	-1.414316	0.000000	0.888276
C	-0.675822	0.000000	2.110785
C	0.675822	0.000000	2.110785
C	1.414316	0.000000	0.888276
C	-1.489756	0.000000	-1.530481
C	-2.821386	0.000000	0.900885
H	-1.227590	0.000000	3.045355
H	1.227590	0.000000	3.045355
C	1.489756	0.000000	-1.530481
C	2.864404	0.000000	-1.494380
C	3.540385	0.000000	-0.268525
C	2.821386	0.000000	0.900885
H	0.995895	0.000000	-2.494084
H	3.426528	0.000000	-2.421674
H	4.624344	0.000000	-0.244990
H	3.332162	0.000000	1.858622
C	-3.540385	0.000000	-0.268525
C	-2.864404	0.000000	-1.494380
H	-0.995895	0.000000	-2.494084

H	-3.426528	0.000000	-2.421674
H	-4.624344	0.000000	-0.244990
H	-3.332162	0.000000	1.858622

phenanthrene S_1

C	0.710975	0.000000	-0.382214
C	-0.710975	0.000000	-0.382214
C	-1.431580	0.000000	0.880302
C	-0.695014	0.000000	2.076191
C	0.695014	0.000000	2.076191
C	1.431580	0.000000	0.880302
C	-1.489606	0.000000	-1.565260
C	-2.833840	0.000000	0.884374
H	-1.231098	0.000000	3.019631
H	1.231098	0.000000	3.019631
C	1.489606	0.000000	-1.565260
C	2.878229	0.000000	-1.522806
C	3.563400	0.000000	-0.303734
C	2.833840	0.000000	0.884374
H	1.002982	0.000000	-2.531649
H	3.435537	0.000000	-2.452984
H	4.646156	0.000000	-0.282261
H	3.348954	0.000000	1.839448
C	-3.563400	0.000000	-0.303734
C	-2.878229	0.000000	-1.522806
H	-1.002982	0.000000	-2.531649
H	-3.435537	0.000000	-2.452984
H	-4.646156	0.000000	-0.282261
H	-3.348954	0.000000	1.839448

2,4,6,8-decatetraene S_0

C	-2.582387	-4.997683	0.000000
C	-2.464962	-3.514345	0.000000
C	-1.311692	-2.834007	0.000000
C	-1.212712	-1.397908	0.000000
C	-0.050358	-0.715216	0.000000
C	0.050358	0.715216	0.000000
C	1.212712	1.397908	0.000000
C	1.311692	2.834007	0.000000
C	2.464962	3.514345	0.000000
C	2.582387	4.997683	0.000000
H	-0.373717	-3.388677	0.000000
H	-2.148252	-0.839996	0.000000
H	0.884245	-1.274966	0.000000

H	-0.884245	1.274966	0.000000
H	2.148252	0.839996	0.000000
H	0.373717	3.388677	0.000000
H	3.397863	2.951895	0.000000
H	-3.397863	-2.951895	0.000000
H	1.601374	5.477255	0.000000
H	3.135382	5.350772	0.877318
H	3.135382	5.350772	-0.877318
H	-1.601374	-5.477255	0.000000
H	-3.135382	-5.350772	0.877318
H	-3.135382	-5.350772	-0.877318

2,4,6,8-decatetraene S_1

C	-2.574353	-5.011548	0.000000
C	-2.514422	-3.533284	0.000000
C	-1.351843	-2.806801	0.000000
C	-1.263537	-1.403885	0.000000
C	-0.053591	-0.694160	0.000000
C	0.053591	0.694160	0.000000
C	1.263537	1.403885	0.000000
C	1.351843	2.806801	0.000000
C	2.514422	3.533284	0.000000
C	2.574353	5.011548	0.000000
H	-0.411020	-3.358591	0.000000
H	-2.190152	-0.831870	0.000000
H	0.868509	-1.274334	0.000000
H	-0.868509	1.274334	0.000000
H	2.190152	0.831870	0.000000
H	0.411020	3.358591	0.000000
H	3.461429	2.995339	0.000000
H	-3.461429	-2.995339	0.000000
H	1.575814	5.454950	0.000000
H	3.117023	5.397594	0.875124
H	3.117023	5.397594	-0.875124
H	-1.575814	-5.454950	0.000000
H	-3.117023	-5.397594	0.875124
H	-3.117023	-5.397594	-0.875124

tetracene S_0

C	3.690030	1.401692	0.000000
C	2.435629	0.721136	0.000000
C	2.435629	-0.721136	0.000000
C	3.690030	-1.401692	0.000000
C	4.860410	-0.711836	0.000000

C	4.860410	0.711836	0.000000
C	1.228324	1.399020	0.000000
C	0.000000	0.721282	0.000000
C	0.000000	-0.721282	0.000000
C	1.228324	-1.399020	0.000000
C	-1.228324	1.399020	0.000000
C	-2.435629	0.721136	0.000000
C	-2.435629	-0.721136	0.000000
C	-1.228324	-1.399020	0.000000
C	-3.690030	1.401692	0.000000
C	-4.860410	0.711836	0.000000
C	-4.860410	-0.711836	0.000000
C	-3.690030	-1.401692	0.000000
H	-3.688642	-2.487012	0.000000
H	-5.805864	-1.242789	0.000000
H	-5.805864	1.242789	0.000000
H	-3.688642	2.487012	0.000000
H	-1.228695	-2.485176	0.000000
H	-1.228695	2.485176	0.000000
H	1.228695	-2.485176	0.000000
H	1.228695	2.485176	0.000000
H	3.688642	-2.487012	0.000000
H	5.805864	-1.242789	0.000000
H	5.805864	1.242789	0.000000
H	3.688642	2.487012	0.000000

tetracene S_1

C	3.692823	1.392958	0.000000
C	2.463023	0.717487	0.000000
C	2.463023	-0.717487	0.000000
C	3.692823	-1.392958	0.000000
C	4.894664	-0.696318	0.000000
C	4.894664	0.696318	0.000000
C	1.226338	1.393520	0.000000
C	0.000000	0.722150	0.000000
C	0.000000	-0.722150	0.000000
C	1.226338	-1.393520	0.000000
C	-1.226338	1.393520	0.000000
C	-2.463023	0.717487	0.000000
C	-2.463023	-0.717487	0.000000
C	-1.226338	-1.393520	0.000000
C	-3.692823	1.392958	0.000000
C	-4.894664	0.696318	0.000000
C	-4.894664	-0.696318	0.000000
C	-3.692823	-1.392958	0.000000

H	-3.694615	-2.478223	0.000000
H	-5.832829	-1.239354	0.000000
H	-5.832829	1.239354	0.000000
H	-3.694615	2.478223	0.000000
H	-1.227913	-2.479867	0.000000
H	-1.227913	2.479867	0.000000
H	1.227913	-2.479867	0.000000
H	1.227913	2.479867	0.000000
H	3.694615	-2.478223	0.000000
H	5.832829	-1.239354	0.000000
H	5.832829	1.239354	0.000000
H	3.694615	2.478223	0.000000

perylene S_0

C	0.022671	1.469409	-2.413284
C	0.012315	0.734375	-1.242116
C	0.010789	1.431528	0.000008
C	0.033183	2.857320	-0.000001
C	0.042433	3.554770	-1.226204
C	0.037709	2.868647	-2.409226
C	0.042751	3.554780	1.226193
C	0.038312	2.868670	2.409221
C	0.023166	1.469431	2.413297
C	0.012455	0.734379	1.242139
C	-0.012315	-0.734375	-1.242116
C	-0.010789	-1.431528	0.000008
C	-0.012455	-0.734379	1.242139
C	-0.033183	-2.857320	-0.000001
C	-0.042751	-3.554780	1.226193
C	-0.038312	-2.868670	2.409221
C	-0.023166	-1.469431	2.413297
C	-0.022671	-1.469409	-2.413284
C	-0.037709	-2.868647	-2.409226
C	-0.042433	-3.554770	-1.226204
H	0.055933	4.639490	1.211538
H	0.046916	3.402964	3.352737
H	0.022062	0.966190	3.371354
H	-0.055933	-4.639490	1.211538
H	-0.046916	-3.402964	3.352737
H	-0.022062	-0.966190	3.371354
H	-0.055582	-4.639480	-1.211565
H	-0.046005	-3.402929	-3.352751
H	-0.021354	-0.966153	-3.371337
H	0.055582	4.639480	-1.211565
H	0.046005	3.402929	-3.352751

H	0.021354	0.966153	-3.371337

perylene S_1

C	-0.006669	1.463734	-2.441977
C	-0.006126	0.717289	-1.237131
C	0.011073	1.416938	0.000002
C	0.008161	2.844707	-0.000001
C	0.009487	3.535718	-1.226603
C	-0.001534	2.844327	-2.427655
C	0.009733	3.535724	1.226592
C	-0.001032	2.844336	2.427652
C	-0.006239	1.463746	2.441981
C	-0.006018	0.717291	1.237138
C	0.006126	-0.717289	-1.237131
C	-0.011073	-1.416938	0.000002
C	0.006018	-0.717291	1.237138
C	-0.008161	-2.844707	-0.000001
C	-0.009733	-3.535724	1.226592
C	0.001032	-2.844336	2.427652
C	0.006239	-1.463746	2.441981
C	0.006669	-1.463734	-2.441977
C	0.001534	-2.844327	-2.427655
C	-0.009487	-3.535718	-1.226603
H	0.013838	4.620522	1.217455
H	-0.004733	3.390374	3.364582
H	-0.029043	0.953505	3.394895
H	-0.013838	-4.620522	1.217455
H	0.004733	-3.390374	3.364582
H	0.029043	-0.953505	3.394895
H	-0.013570	-4.620516	-1.217469
H	0.005501	-3.390358	-3.364588
H	0.029777	-0.953482	-3.394879
H	0.013570	4.620516	-1.217469
H	-0.005501	3.390358	-3.364588
H	-0.029777	0.953482	-3.394879

M06-2X/TZVP geometries – Group I

pyrazine S_0

C	1.127391	-0.694999	0.000000
C	1.127391	0.694999	0.000000
N	0.000000	1.398730	0.000000
C	-1.127391	0.694999	0.000000

C	-1.127391	-0.694999	0.000000
N	0.000000	-1.398730	0.000000
H	-2.057378	-1.251526	0.000000
H	2.057378	-1.251526	0.000000
H	2.057378	1.251526	0.000000
H	-2.057378	1.251526	0.000000

pyrazine S_1

C	-1.181751	0.655882	0.000000
C	-1.135290	-0.733913	0.000000
N	0.045942	-1.360963	0.000000
C	1.181751	-0.655882	0.000000
C	1.135290	0.733913	0.000000
N	-0.045942	1.360963	0.000000
H	2.060333	1.295159	0.000000
H	-2.142420	1.153801	0.000000
H	-2.060333	-1.295159	0.000000
H	2.142420	-1.153801	0.000000

2,6-difluoropyridine S_0

C	1.112162	0.000000	-0.874080
N	0.000000	0.000000	-1.566005
C	-1.112162	0.000000	-0.874080
C	-1.200823	0.000000	0.506827
C	0.000000	0.000000	1.200616
C	1.200823	0.000000	0.506827
F	-2.235972	0.000000	-1.586179
H	-2.163574	0.000000	0.995019
H	0.000000	0.000000	2.282636
H	2.163574	0.000000	0.995019
F	2.235972	0.000000	-1.586179

2,6-difluoropyridine S_1

C	-1.096807	0.000000	-0.337179
N	0.000000	0.000000	-1.105924
C	1.096807	0.000000	-0.337179
C	1.188961	0.000000	1.072628
C	0.000000	0.000000	1.848425
C	-1.188961	0.000000	1.072628
F	2.233534	0.000000	-1.005160
H	2.177728	0.000000	1.511010
H	0.000000	0.000000	2.924193
H	-2.177728	0.000000	1.511010

F	-2.233534	0.000000	-1.005160

2-fluoropyridine S_0

C	-1.312961	0.501983	0.000000
N	-1.365191	-0.800542	0.000000
C	-0.197482	-1.449668	0.000000
C	1.028737	-0.807649	0.000000
C	1.043236	0.583845	0.000000
C	-0.156191	1.270854	0.000000
H	-0.259873	-2.531597	0.000000
H	1.945430	-1.380308	0.000000
H	1.980033	1.126341	0.000000
H	-0.218347	2.349480	0.000000
F	-2.487400	1.137251	0.000000

2-fluoropyridine S_1

C	-1.319221	0.488488	0.000000
N	-1.438034	-0.844579	0.000000
C	-0.227773	-1.461034	0.000000
C	1.028607	-0.790286	0.000000
C	1.109098	0.620571	0.000000
C	-0.149420	1.280385	0.000000
H	-0.248339	-2.543485	0.000000
H	1.924159	-1.398266	0.000000
H	2.045172	1.153354	0.000000
H	-0.258035	2.355537	0.000000
F	-2.466221	1.139304	0.000000

2-hydroxypyridine S_0

C	-0.977209	0.751209	0.000000
C	-0.966703	-0.644774	0.000000
N	0.131589	-1.375726	0.000000
C	1.303389	-0.734930	0.000000
C	1.416807	0.642527	0.000000
C	0.242897	1.394003	0.000000
O	-2.147225	-1.296303	0.000000
H	2.184783	-1.366074	0.000000
H	2.389360	1.113471	0.000000
H	0.284090	2.476017	0.000000
H	-1.918430	1.281678	0.000000
H	-1.943349	-2.241098	0.000000

2-hydroxypyridine S_1

C	-0.993774	0.767248	0.000000
C	-0.964841	-0.640011	0.000000
N	0.123840	-1.457542	0.000000
C	1.290719	-0.774495	0.000000
C	1.390117	0.643604	0.000000
C	0.247835	1.465056	0.000000
O	-2.122390	-1.284068	0.000000
H	2.195021	-1.369665	0.000000
H	2.382202	1.077548	0.000000
H	0.306131	2.540805	0.000000
H	-1.954219	1.262324	0.000000
H	-1.900640	-2.230803	0.000000

2-pyridone S_0

C	-1.246033	0.711123	0.000000
N	-1.134126	-0.685093	0.000000
C	0.034022	-1.381753	0.000000
C	1.221577	-0.733679	0.000000
C	1.202709	0.692197	0.000000
C	0.039389	1.385955	0.000000
H	-2.019260	-1.173433	0.000000
H	-0.056170	-2.459492	0.000000
H	2.147134	-1.287570	0.000000
H	2.143977	1.229093	0.000000
H	0.009622	2.466280	0.000000
O	-2.342840	1.236380	0.000000

2-pyridone S_1

C	-1.393354	0.112286	0.000000
N	-0.727810	-1.147519	0.000000
C	0.620864	-1.253574	0.000000
C	1.408569	-0.077236	0.000000
C	0.827769	1.176577	0.000000
C	-0.605235	1.270266	0.000000
H	-1.340569	-1.951477	0.000000
H	1.047398	-2.245022	0.000000
H	2.483208	-0.197634	0.000000
H	1.436294	2.067981	0.000000
H	-1.125835	2.215624	0.000000
O	-2.631299	0.029719	0.000000

2-methylpyrimidine S_0

C	0.000008	1.960750	0.000000
C	-1.172734	1.220868	0.000000
N	-1.177603	-0.105789	0.000000
C	0.011914	-0.715621	0.000000
N	1.193856	-0.097448	0.000000
C	1.176731	1.232610	0.000000
H	-2.143477	1.706264	0.000000
H	2.143741	1.725054	0.000000
H	-0.005198	3.041108	0.000000
C	0.004785	-2.213213	0.000000
H	1.022592	-2.593395	0.000000
H	-0.527313	-2.580594	0.878306
H	-0.527313	-2.580594	-0.878306

2-methylpyrimidine S_1

C	-0.005255	2.007870	0.000000
C	-1.180410	1.288758	0.000000
N	-1.116084	-0.087134	0.000000
C	0.009788	-0.786637	0.000000
N	1.107501	-0.078016	0.000000
C	1.191323	1.290691	0.000000
H	-2.162476	1.735891	0.000000
H	2.172756	1.735949	0.000000
H	-0.009767	3.090014	0.000000
C	0.006361	-2.274308	0.000000
H	1.027838	-2.646119	0.000000
H	-0.520787	-2.638485	0.882106
H	-0.520787	-2.638485	-0.882106

5-methylpyrimidine S_0

C	0.873726	0.850587	0.000000
C	-0.359111	0.211351	0.000000
C	-0.299502	-1.178907	0.000000
N	0.842529	-1.855963	0.000000
C	1.955864	-1.128521	0.000000
N	2.031875	0.196231	0.000000
H	2.893517	-1.672406	0.000000
H	-1.212246	-1.769298	0.000000
H	0.930940	1.935756	0.000000
C	-1.660120	0.957814	0.000000
H	-1.489415	2.033896	0.000000
H	-2.254028	0.709719	-0.881023
H	-2.254028	0.709719	0.881023

5-methylpyrimidine S_1

C	0.839453	0.871874	0.000000
C	-0.377645	0.234694	0.000000
C	-0.344698	-1.178206	0.000000
N	0.879421	-1.774462	0.000000
C	2.035877	-1.178505	0.000000
N	2.011756	0.146848	0.000000
H	2.965807	-1.728151	0.000000
H	-1.223156	-1.803794	0.000000
H	0.935825	1.948323	0.000000
C	-1.678097	0.975759	0.000000
H	-1.512384	2.052186	0.000000
H	-2.266084	0.716723	-0.882272
H	-2.266084	0.716723	0.882272

7-azaindole S_0

N	-0.632533	1.839626	0.000000
C	-0.671206	0.470376	0.000000
C	0.666089	0.006259	0.000000
C	1.507612	1.166164	0.000000
C	0.680964	2.249698	0.000000
C	0.843070	-1.376845	0.000000
C	-0.290525	-2.168763	0.000000
C	-1.561593	-1.575556	0.000000
N	-1.773408	-0.266002	0.000000
H	-2.448329	-2.199589	0.000000
H	1.832791	-1.817338	0.000000
H	-0.212649	-3.247379	0.000000
H	-1.448508	2.427663	0.000000
H	2.584153	1.192289	0.000000
H	0.924092	3.299398	0.000000

7-azaindole S_1

N	-0.604511	1.870716	0.000000
C	-0.659319	0.447950	0.000000
C	0.660529	-0.006058	0.000000
C	1.490428	1.141442	0.000000
C	0.647749	2.305667	0.000000
C	0.887557	-1.408835	0.000000
C	-0.304031	-2.179991	0.000000
C	-1.547869	-1.594960	0.000000
N	-1.793856	-0.221135	0.000000
H	-2.438127	-2.210534	0.000000

H	1.873627	-1.845568	0.000000
H	-0.247573	-3.260569	0.000000
H	-1.440952	2.438583	0.000000
H	2.568608	1.173149	0.000000
H	0.907748	3.350163	0.000000

7-hydroxyquinoline, *cis* S_0

N	0.462333	1.967683	0.000000
C	0.431775	0.607750	0.000000
C	-0.783492	-0.123740	0.000000
C	-1.989985	0.607175	0.000000
C	-1.944727	1.972781	0.000000
C	-0.680658	2.604009	0.000000
C	1.662211	-0.089005	0.000000
C	1.674461	-1.457049	0.000000
C	0.464921	-2.194887	0.000000
C	-0.730033	-1.540492	0.000000
H	-0.624603	3.688427	0.000000
H	-1.658228	-2.100070	0.000000
H	0.524473	-3.275167	0.000000
O	2.815353	-2.195929	0.000000
H	2.575755	0.494375	0.000000
H	-2.934564	0.074731	0.000000
H	-2.845472	2.571247	0.000000
H	3.580480	-1.611830	0.000000

7-hydroxyquinoline, *cis* S_1

N	0.490063	1.974270	0.000000
C	0.435927	0.634351	0.000000
C	-0.788356	-0.140460	0.000000
C	-1.993533	0.591895	0.000000
C	-1.918972	1.993372	0.000000
C	-0.685454	2.640028	0.000000
C	1.636030	-0.083925	0.000000
C	1.652056	-1.512985	0.000000
C	0.480310	-2.264805	0.000000
C	-0.720984	-1.556502	0.000000
H	-0.625768	3.720265	0.000000
H	-1.656437	-2.104298	0.000000
H	0.527056	-3.342603	0.000000
O	2.820960	-2.156579	0.000000
H	2.568385	0.471457	0.000000
H	-2.947510	0.081881	0.000000
H	-2.827511	2.582647	0.000000

H	3.553738	-1.527998	0.000000

7-hydroxyquinoline, *trans* S_0

N	0.512504	2.040395	0.000000
C	0.479797	0.678037	0.000000
C	-0.740811	-0.047621	0.000000
C	-1.946681	0.687965	0.000000
C	-1.895870	2.051735	0.000000
C	-0.627204	2.678714	0.000000
C	1.706621	-0.018424	0.000000
C	1.715574	-1.386872	0.000000
C	0.502569	-2.117799	0.000000
C	-0.694275	-1.460783	0.000000
H	-0.568613	3.763145	0.000000
H	-1.623121	-2.019102	0.000000
H	0.533612	-3.202159	0.000000
O	2.917287	-2.025067	0.000000
H	2.630916	0.542423	0.000000
H	-2.893086	0.158667	0.000000
H	-2.793961	2.654372	0.000000
H	2.784723	-2.977605	0.000000

7-hydroxyquinoline, *trans* S_1

N	0.533166	2.049502	0.000000
C	0.478227	0.711859	0.000000
C	-0.747272	-0.057574	0.000001
C	-1.951784	0.675102	0.000001
C	-1.875446	2.077544	0.000000
C	-0.643138	2.718866	0.000000
C	1.680157	-0.008988	0.000001
C	1.688997	-1.435041	0.000000
C	0.514602	-2.185844	0.000000
C	-0.686086	-1.472565	0.000000
H	-0.579174	3.798821	-0.000001
H	-1.623273	-2.017663	-0.000001
H	0.538730	-3.266977	-0.000001
O	2.903574	-1.989002	0.000000
H	2.624206	0.519664	0.000001
H	-2.906243	0.165796	0.000001
H	-2.783030	2.668336	0.000000
H	2.833768	-2.951815	0.000000

2-hydroxyquinoline, enol S_0

C	0.431488	1.900879	0.000000
C	0.483499	0.488742	0.000000
C	-0.720456	-0.257484	0.000000
C	-1.952613	0.436087	0.000000
C	-1.975010	1.804414	0.000000
C	-0.774024	2.547827	0.000000
C	1.696635	-0.243171	0.000000
C	1.664036	-1.602332	0.000000
C	0.391729	-2.245755	0.000000
N	-0.740332	-1.618708	0.000000
O	0.315669	-3.597519	0.000000
H	1.360561	2.459544	0.000000
H	-0.812645	3.629393	0.000000
H	-2.922996	2.327698	0.000000
H	-2.860743	-0.152374	0.000000
H	2.641189	0.288748	0.000000
H	2.574605	-2.189308	0.000000
H	1.199408	-3.976679	0.000000

2-hydroxyquinoline, enol S_1

C	0.437929	1.878281	0.000000
C	0.528434	0.487546	0.000000
C	-0.726896	-0.261672	0.000000
C	-1.961060	0.438646	0.000000
C	-2.012433	1.836154	0.000000
C	-0.813834	2.541587	0.000000
C	1.734506	-0.235151	0.000000
C	1.695994	-1.637365	0.000000
C	0.430175	-2.238792	0.000000
N	-0.752396	-1.602704	0.000000
O	0.296373	-3.568662	0.000000
H	1.346996	2.468065	0.000000
H	-0.823289	3.624692	0.000000
H	-2.959474	2.355618	0.000000
H	-2.860772	-0.163167	0.000000
H	2.676825	0.296539	0.000000
H	2.595543	-2.237152	0.000000
H	1.167370	-3.982442	0.000000

2-hydroxyquinoline, keto S_0

N	0.559205	1.703882	0.000000
C	0.600811	0.326474	0.000000
C	-0.611389	-0.382654	0.000000
C	-1.836508	0.377514	0.000000

C	-1.834894	1.720661	0.000000
C	-0.586162	2.486276	0.000000
C	1.817542	-0.362580	0.000000
C	1.820293	-1.742009	0.000000
C	0.621004	-2.461353	0.000000
C	-0.578717	-1.782145	0.000000
H	-1.517479	-2.323801	0.000000
H	0.637187	-3.542752	0.000000
H	2.764753	-2.271080	0.000000
H	2.747902	0.192768	0.000000
H	-2.773608	-0.168685	0.000000
H	-2.743474	2.306019	0.000000
O	-0.512475	3.698567	0.000000
H	1.426029	2.224918	0.000000

2-hydroxyquinoline, keto S_1

N	0.564140	1.672038	0.000000
C	0.613663	0.327322	0.000000
C	-0.665335	-0.380310	0.000000
C	-1.856872	0.365296	0.000000
C	-1.857994	1.763547	0.000000
C	-0.634509	2.475236	0.000000
C	1.839136	-0.361529	0.000000
C	1.856322	-1.748258	0.000000
C	0.632319	-2.446083	0.000000
C	-0.591179	-1.784933	0.000000
H	-1.512784	-2.352777	0.000000
H	0.643595	-3.528962	0.000000
H	2.792677	-2.286940	0.000000
H	2.759836	0.209997	0.000000
H	-2.794894	-0.174748	0.000000
H	-2.764923	2.346867	0.000000
O	-0.439083	3.682532	0.000000
H	1.415883	2.221713	0.000000

dibenzofuran S_0

C	1.717214	0.000000	-1.356906
C	0.725228	0.000000	-0.380878
C	1.094118	0.000000	0.967946
C	2.408881	0.000000	1.392985
C	3.382166	0.000000	0.403716
C	3.042981	0.000000	-0.952957
C	-0.725228	0.000000	-0.380878
C	-1.094118	0.000000	0.967946

O	0.000000	0.000000	1.790090
C	-1.717214	0.000000	-1.356906
C	-3.042981	0.000000	-0.952957
C	-3.382166	0.000000	0.403716
C	-2.408881	0.000000	1.392985
H	-2.656156	0.000000	2.445654
H	-4.426122	0.000000	0.690060
H	-3.829672	0.000000	-1.695999
H	-1.458993	0.000000	-2.408500
H	1.458993	0.000000	-2.408500
H	3.829672	0.000000	-1.695999
H	4.426122	0.000000	0.690060
H	2.656156	0.000000	2.445654

dibenzofuran S_1

C	0.000000	1.727845	-1.531333
C	0.000000	0.710703	-0.570267
C	0.000000	1.101399	0.804143
C	0.000000	2.406184	1.256139
C	0.000000	3.413615	0.266865
C	0.000000	3.067854	-1.087004
C	0.000000	-0.710703	-0.570267
C	0.000000	-1.101399	0.804143
O	0.000000	0.000000	1.598122
C	0.000000	-1.727845	-1.531333
C	0.000000	-3.067854	-1.087004
C	0.000000	-3.413615	0.266865
C	0.000000	-2.406184	1.256139
H	0.000000	-2.630859	2.313396
H	0.000000	-4.453665	0.559446
H	0.000000	-3.857660	-1.827832
H	0.000000	-1.502480	-2.588904
H	0.000000	1.502480	-2.588904
H	0.000000	3.857660	-1.827832
H	0.000000	4.453665	0.559446
H	0.000000	2.630859	2.313396

pyrrolo[3,2-*h*]quinoline S_0

C	0.136122	-0.683353	0.000000
N	0.058309	-2.032238	0.000000
C	1.187500	-2.703243	0.000000
C	2.457494	-2.096861	0.000000
C	2.536841	-0.727395	0.000000
C	1.356449	0.038707	0.000000

H	1.105088	-3.785457	0.000000
H	3.346426	-2.713068	0.000000
H	3.497551	-0.224674	0.000000
C	-1.051410	0.086428	0.000000
C	-1.056786	1.483043	0.000000
C	0.184373	2.176541	0.000000
C	1.349130	1.470341	0.000000
H	0.198973	3.259378	0.000000
H	2.302839	1.984388	0.000000
C	-2.427568	1.886134	0.000000
C	-3.177697	0.741375	0.000000
N	-2.342222	-0.346784	0.000000
H	-2.603950	-1.319147	0.000000
H	-2.810247	2.892935	0.000000
H	-4.247206	0.612949	0.000000

pyrrolo[3,2-*h*]quinoline S_1

C	0.152257	-0.701518	0.000000
N	0.012463	-2.022941	0.000000
C	1.197388	-2.729807	0.000000
C	2.432505	-2.134150	0.000000
C	2.561014	-0.725703	0.000000
C	1.362571	0.029102	0.000000
H	1.098708	-3.807263	0.000000
H	3.317692	-2.757569	0.000000
H	3.526890	-0.241381	0.000000
C	-1.024474	0.104096	0.000000
C	-1.061151	1.552713	0.000000
C	0.140847	2.231191	0.000000
C	1.319966	1.454688	0.000000
H	0.190959	3.310554	0.000000
H	2.272410	1.973758	0.000000
C	-2.457347	1.905743	0.000000
C	-3.162725	0.746869	0.000000
N	-2.281566	-0.340330	0.000000
H	-2.499446	-1.327756	0.000000
H	-2.871973	2.899174	0.000000
H	-4.226999	0.580528	0.000000

carbazole S_0

C	1.127714	0.000000	-0.895809
N	0.000000	0.000000	-1.693215
C	-1.127714	0.000000	-0.895809
C	-0.723829	0.000000	0.455919

C	0.723829	0.000000	0.455919
C	-1.690760	0.000000	1.458539
C	-3.028767	0.000000	1.103429
C	-3.410314	0.000000	-0.243656
C	-2.470297	0.000000	-1.259971
C	2.470297	0.000000	-1.259971
C	3.410314	0.000000	-0.243656
C	3.028767	0.000000	1.103429
C	1.690760	0.000000	1.458539
H	-2.771454	0.000000	-2.300146
H	-4.462885	0.000000	-0.497435
H	-3.790111	0.000000	1.872371
H	-1.398678	0.000000	2.501791
H	1.398678	0.000000	2.501791
H	3.790111	0.000000	1.872371
H	4.462885	0.000000	-0.497435
H	2.771454	0.000000	-2.300146
H	0.000000	0.000000	-2.697809

carbazole S_1

C	1.140401	0.000000	-0.836026
N	0.000000	0.000000	-1.605871
C	-1.140401	0.000000	-0.836026
C	-0.714381	0.000000	0.532861
C	0.714381	0.000000	0.532861
C	-1.703002	0.000000	1.520599
C	-3.055201	0.000000	1.117357
C	-3.444146	0.000000	-0.219726
C	-2.462840	0.000000	-1.238663
C	2.462840	0.000000	-1.238663
C	3.444146	0.000000	-0.219726
C	3.055201	0.000000	1.117357
C	1.703002	0.000000	1.520599
H	-2.735122	0.000000	-2.286263
H	-4.492581	0.000000	-0.480498
H	-3.821059	0.000000	1.883642
H	-1.446140	0.000000	2.571074
H	1.446140	0.000000	2.571074
H	3.821059	0.000000	1.883642
H	4.492581	0.000000	-0.480498
H	2.735122	0.000000	-2.286263
H	0.000000	0.000000	-2.615472

tryptamine, A-ph S_0

C	-2.144586	0.161512	0.904482
N	-1.258530	0.142527	1.961880
C	0.021277	0.046120	1.472629
C	-0.073166	-0.001486	0.064896
C	-1.469330	0.076023	-0.276058
C	1.247172	0.000206	2.136302
C	2.386462	-0.093370	1.361965
C	2.315869	-0.136738	-0.041287
C	1.100408	-0.091023	-0.693503
C	-2.038864	0.021426	-1.656361
C	-1.949354	-1.377034	-2.265913
N	-2.423464	-1.352783	-3.647744
H	1.305362	0.036911	3.217186
H	3.354821	-0.131054	1.844721
H	3.231964	-0.204893	-0.613724
H	1.052070	-0.118109	-1.776001
H	-1.508751	0.212759	2.932022
H	-3.205689	0.239940	1.080956
H	-1.509289	0.714244	-2.315779
H	-3.085627	0.339636	-1.637278
H	-2.493589	-2.077145	-1.618020
H	-0.904719	-1.695359	-2.270864
H	-3.412696	-1.133249	-3.678954
H	-2.305160	-2.256681	-4.088182

tryptamine, A-ph S_1

C	-2.195016	0.185697	0.919293
N	-1.303614	0.136517	1.915100
C	0.015101	0.058104	1.430782
C	-0.072081	0.076751	0.032729
C	-1.449589	0.150324	-0.306003
C	1.200050	-0.065705	2.141729
C	2.388911	-0.153474	1.322995
C	2.333939	-0.133875	-0.047871
C	1.103250	-0.019457	-0.756831
C	-2.024579	0.070100	-1.665335
C	-1.925859	-1.364151	-2.215055
N	-2.444698	-1.403286	-3.576529
H	1.242858	-0.100375	3.219893
H	3.348793	-0.238242	1.816098
H	3.256517	-0.201489	-0.610486
H	1.069647	0.044344	-1.835082
H	-1.536149	0.169959	2.896590
H	-3.253966	0.286843	1.086585
H	-1.472982	0.721224	-2.348053

H	-3.070683	0.388605	-1.662366
H	-2.434837	-2.044804	-1.519964
H	-0.871185	-1.646434	-2.233061
H	-3.453919	-1.313060	-3.582791
H	-2.217338	-2.281737	-4.025038

tryptamine, A-py S_0

C	-2.138916	0.135367	0.883051
N	-1.261393	0.133043	1.947326
C	0.023258	0.047825	1.469288
C	-0.059361	-0.010458	0.060920
C	-1.453487	0.048702	-0.291620
C	1.243984	0.020108	2.143410
C	2.391036	-0.065609	1.379765
C	2.332736	-0.119992	-0.023633
C	1.122090	-0.093200	-0.685758
C	-2.021114	-0.013600	-1.672572
C	-1.916011	-1.409620	-2.284528
N	-2.460217	-1.400369	-3.640846
H	1.292273	0.064159	3.224522
H	3.355522	-0.089168	1.871048
H	3.254296	-0.183055	-0.587842
H	1.084230	-0.132523	-1.768348
H	-1.520562	0.204805	2.915026
H	-3.202311	0.203400	1.049438
H	-1.491605	0.695454	-2.319156
H	-3.070608	0.286770	-1.669912
H	-2.509866	-2.099510	-1.681571
H	-0.873187	-1.749185	-2.225684
H	-1.890588	-0.819118	-4.245496
H	-2.460289	-2.331834	-4.037720

tryptamine, A-py S_1

C	-2.189966	0.145532	0.898130
N	-1.308038	0.113327	1.902000
C	0.016893	0.054833	1.429704
C	-0.057993	0.065833	0.031530
C	-1.432977	0.118244	-0.319899
C	1.198281	-0.043998	2.151950
C	2.394116	-0.116534	1.343074
C	2.351659	-0.104619	-0.028623
C	1.125373	-0.013987	-0.748645
C	-1.998863	0.034406	-1.681839
C	-1.876106	-1.397149	-2.237990

N	-2.455696	-1.449257	-3.573426
H	1.233293	-0.068805	3.230578
H	3.351230	-0.183118	1.844457
H	3.280650	-0.160710	-0.581844
H	1.099640	0.040384	-1.827594
H	-1.550545	0.144723	2.881102
H	-3.252617	0.224829	1.053497
H	-1.447199	0.707320	-2.346588
H	-3.050192	0.326015	-1.698015
H	-2.440805	-2.071903	-1.591208
H	-0.821225	-1.695592	-2.185518
H	-1.877293	-0.942866	-4.233953
H	-2.521711	-2.404528	-3.901780

tryptamine, A-up S_0

C	-2.137423	0.149943	0.893941
N	-1.258946	0.120244	1.956818
C	0.024809	0.038514	1.475668
C	-0.059034	0.010981	0.066617
C	-1.453129	0.087309	-0.283196
C	1.245750	-0.010869	2.148071
C	2.391500	-0.087847	1.381657
C	2.331879	-0.112700	-0.022490
C	1.121145	-0.063653	-0.682991
C	-2.016608	0.043834	-1.666406
C	-1.917469	-1.352486	-2.298674
N	-2.395878	-1.451759	-3.671866
H	1.295148	0.009890	3.229795
H	3.356228	-0.128199	1.871324
H	3.252463	-0.170931	-0.588711
H	1.082790	-0.081074	-1.766086
H	-1.516848	0.169668	2.926290
H	-3.200207	0.219042	1.063992
H	-1.485657	0.757324	-2.306254
H	-3.065216	0.355213	-1.651017
H	-2.480443	-2.059353	-1.685312
H	-0.878317	-1.688188	-2.273260
H	-1.867842	-0.836951	-4.280415
H	-3.367458	-1.170040	-3.734254

tryptamine, A-up S_1

C	-2.188567	0.151684	0.904333
N	-1.304045	0.091257	1.906027
C	0.019718	0.043439	1.432548

C	-0.055316	0.093591	0.035117
C	-1.431462	0.164447	-0.313958
C	1.201118	-0.077208	2.151223
C	2.396507	-0.133811	1.341351
C	2.353089	-0.086823	-0.029171
C	1.126510	0.028114	-0.746189
C	-1.988179	0.103167	-1.676262
C	-1.910038	-1.351445	-2.228719
N	-2.389274	-1.514756	-3.584845
H	1.235658	-0.131562	3.228822
H	3.353303	-0.218708	1.840412
H	3.281004	-0.134427	-0.585002
H	1.101739	0.102503	-1.824021
H	-1.545425	0.097012	2.885947
H	-3.250045	0.233997	1.065860
H	-1.406623	0.745550	-2.343907
H	-3.028684	0.437384	-1.694792
H	-2.485329	-2.006510	-1.571978
H	-0.869078	-1.677188	-2.175222
H	-1.852246	-0.959182	-4.239141
H	-3.363113	-1.252605	-3.675213

tryptamine, Ph-out S_0

C	-0.006446	0.003984	0.068710
C	0.038745	0.054388	1.479295
C	1.241037	0.055792	2.186593
C	2.409456	0.009845	1.453035
C	2.388423	-0.039061	0.047769
C	1.197407	-0.042731	-0.649010
N	-1.258354	0.098883	1.927085
H	1.258409	0.092333	3.268921
H	3.361439	0.010773	1.968611
H	3.325506	-0.074655	-0.492960
H	1.181428	-0.099654	-1.730802
C	-1.394754	0.026099	-0.317496
C	-2.109843	0.086072	0.842849
H	-1.541401	0.162099	2.888757
H	-3.178086	0.134018	0.985242
C	-1.947033	-0.026809	-1.708925
H	-1.301899	0.544738	-2.381048
C	-2.068798	-1.450552	-2.252780
H	-2.933975	0.441969	-1.724442
H	-2.498131	-1.409092	-3.256443
N	-0.750704	-2.070880	-2.353437
H	-2.768559	-2.008770	-1.615103

H	-0.342165	-2.180777	-1.430897
H	-0.816733	-2.993901	-2.764311

tryptamine, Ph-out S_1

C	-0.000758	0.029305	0.049116
C	0.034864	0.065821	1.451391
C	1.195778	0.032340	2.209430
C	2.420667	-0.014344	1.441924
C	2.417582	-0.053994	0.070717
C	1.212088	-0.046970	-0.688291
N	-1.300307	0.114351	1.885847
H	1.196678	0.056162	3.288935
H	3.363060	-0.021062	1.974147
H	3.362995	-0.091330	-0.455732
H	1.215016	-0.065617	-1.768592
C	-1.366781	0.060548	-0.341215
C	-2.156329	0.104943	0.858484
H	-1.568936	0.164054	2.857360
H	-3.223824	0.168456	0.985641
C	-1.932247	-0.021464	-1.707430
H	-1.276455	0.492350	-2.413582
C	-2.078584	-1.482297	-2.177956
H	-2.915701	0.455079	-1.726978
H	-2.643131	-1.478092	-3.112780
N	-0.768928	-2.055015	-2.438234
H	-2.674652	-2.028142	-1.432917
H	-0.183912	-2.050103	-1.607654
H	-0.843193	-3.010859	-2.762419

tryptamine, Ph-up S_0

C	-2.097227	0.054330	0.822079
N	-1.254562	0.040293	1.912837
C	0.046156	0.034402	1.475324
C	0.011782	0.042234	0.063369
C	-1.372139	0.053621	-0.333912
C	1.242777	0.025505	2.191867
C	2.418133	0.027796	1.468332
C	2.409570	0.041305	0.062181
C	1.223107	0.048184	-0.641728
C	-1.908349	0.016727	-1.730802
C	-2.073588	-1.414637	-2.269048
N	-0.857511	-2.212580	-2.334275
H	1.250643	0.016502	3.274875
H	3.365482	0.020577	1.992015

H	3.351207	0.047523	-0.471559
H	1.225600	0.061766	-1.725451
H	-1.546755	0.052069	2.873852
H	-3.167195	0.072290	0.958061
H	-1.237161	0.572384	-2.393627
H	-2.876662	0.523877	-1.767015
H	-2.507024	-1.374169	-3.271215
H	-2.788373	-1.946371	-1.636067
H	-0.422982	-2.270622	-1.419409
H	-0.181281	-1.783376	-2.955624

tryptamine, Ph-up S_1

C	-2.162293	0.126905	0.852581
N	-1.306948	0.098811	1.880455
C	0.028664	0.063706	1.444188
C	-0.007543	0.087011	0.043166
C	-1.374006	0.122836	-0.345418
C	1.190831	-0.016140	2.199723
C	2.412014	-0.045033	1.429403
C	2.410196	-0.020995	0.057438
C	1.204398	0.038235	-0.699622
C	-1.919582	0.024296	-1.708298
C	-2.012274	-1.469680	-2.172450
N	-0.756914	-2.153185	-2.348527
H	1.192306	-0.046423	3.278949
H	3.354922	-0.088798	1.959136
H	3.356249	-0.041856	-0.468802
H	1.214216	0.125897	-1.776554
H	-1.575746	0.119888	2.852762
H	-3.229841	0.186628	0.982135
H	-1.278184	0.558237	-2.413589
H	-2.922918	0.456768	-1.751760
H	-2.556207	-1.483553	-3.119193
H	-2.614739	-2.016673	-1.444823
H	-0.192261	-2.147476	-1.504659
H	-0.200679	-1.729795	-3.081151

tryptamine, Py-out S_0

C	0.499273	0.462319	0.211118
C	0.576419	0.518790	1.620059
C	1.791766	0.458137	2.301203
C	2.940319	0.339759	1.543971
C	2.887809	0.285323	0.140441
C	1.682487	0.346230	-0.529122

N	-0.707628	0.637120	2.092914
H	1.834653	0.503539	3.382396
H	3.901232	0.290560	2.040326
H	3.810090	0.196861	-0.419107
H	1.650419	0.307693	-1.611681
C	-0.891824	0.559589	-0.147279
C	-1.580857	0.659489	1.025085
H	-0.968583	0.711476	3.059999
H	-2.644231	0.746014	1.183215
C	-1.460175	0.492558	-1.528836
H	-0.906057	1.164323	-2.190579
C	-1.413843	-0.925284	-2.101434
H	-2.500188	0.824991	-1.513819
H	-0.365111	-1.244863	-2.176949
N	-2.232659	-1.813163	-1.281140
H	-1.828076	-0.914184	-3.111775
H	-2.220977	-2.756643	-1.648520
H	-1.854240	-1.850633	-0.340466

tryptamine, Py-out S_1

C	0.494475	0.504329	0.186270
C	0.570733	0.523906	1.584101
C	1.749964	0.414044	2.309509
C	2.943643	0.299136	1.502149
C	2.900180	0.281971	0.130987
C	1.674981	0.379336	-0.591732
N	-0.750722	0.634575	2.056937
H	1.784791	0.423033	3.388412
H	3.899654	0.225043	2.004516
H	3.827206	0.195969	-0.421679
H	1.650419	0.401854	-1.671633
C	-0.880442	0.601919	-0.164459
C	-1.633212	0.675970	1.054378
H	-0.990467	0.681026	3.036127
H	-2.695898	0.761316	1.205804
C	-1.453491	0.518935	-1.524852
H	-0.879369	1.161664	-2.198563
C	-1.383041	-0.926031	-2.053194
H	-2.495824	0.842375	-1.524354
H	-0.326583	-1.217337	-2.109081
N	-2.191588	-1.800150	-1.210541
H	-1.795706	-0.944290	-3.062791
H	-2.269402	-2.721928	-1.622650
H	-1.750311	-1.916673	-0.303671

tryptamine, Py-up S_0

C	-2.137729	0.266505	0.887946
N	-1.261434	0.230409	1.953013
C	0.018711	0.091070	1.475233
C	-0.064434	0.036030	0.067007
C	-1.454980	0.154567	-0.287093
C	1.235711	0.011181	2.151719
C	2.378864	-0.125305	1.389738
C	2.320157	-0.179218	-0.013639
C	1.113502	-0.099632	-0.678310
C	-2.020288	0.094987	-1.668384
C	-1.968163	-1.324666	-2.260239
N	-2.719334	-2.332709	-1.526093
H	1.283676	0.055260	3.232717
H	3.340780	-0.190348	1.882302
H	3.238648	-0.283526	-0.576560
H	1.076778	-0.138609	-1.760705
H	-1.517120	0.310801	2.921000
H	-3.197585	0.380477	1.053040
H	-1.469588	0.776647	-2.324748
H	-3.059718	0.436556	-1.654536
H	-0.928120	-1.655925	-2.309304
H	-2.340529	-1.300548	-3.286745
H	-3.699764	-2.077630	-1.476690
H	-2.379521	-2.386751	-0.571778

tryptamine, Py-up S_1

C	-2.190972	0.287049	0.919975
N	-1.301353	0.238725	1.918656
C	0.014224	0.107154	1.439997
C	-0.070137	0.088492	0.041318
C	-1.445477	0.200314	-0.302779
C	1.193435	-0.026554	2.158034
C	2.382571	-0.168476	1.347068
C	2.331022	-0.185555	-0.023255
C	1.104784	-0.060758	-0.739376
C	-2.019228	0.115297	-1.658853
C	-1.936497	-1.334336	-2.214993
N	-2.691390	-2.333892	-1.487113
H	1.232295	-0.024105	3.236945
H	3.338256	-0.265252	1.845809
H	3.252273	-0.293618	-0.581630
H	1.077523	-0.039003	-1.819349
H	-1.533620	0.300671	2.898853

H	-3.246718	0.424709	1.081556
H	-1.453091	0.765869	-2.333363
H	-3.062218	0.443390	-1.660538
H	-0.887282	-1.636267	-2.223776
H	-2.283583	-1.320645	-3.249645
H	-3.674022	-2.093624	-1.432964
H	-2.342273	-2.439955	-0.541663

porphycene S_0

C	-3.433333	1.913816	0.000000
C	-2.420290	0.908273	0.000000
N	-1.223806	1.540969	0.000000
C	-1.390824	2.889270	0.000000
C	-2.802337	3.128491	0.000000
C	-0.367084	3.844262	0.000000
C	1.010123	3.693444	0.000000
C	1.824149	2.548078	0.000000
H	-0.265910	1.120234	0.000000
N	1.410237	1.260317	0.000000
C	3.276580	2.593004	0.000000
C	3.707534	1.307155	0.000000
C	2.512574	0.492982	0.000000
C	2.420290	-0.908273	0.000000
C	3.433333	-1.913816	0.000000
C	2.802337	-3.128491	0.000000
C	1.390824	-2.889270	0.000000
N	1.223806	-1.540969	0.000000
C	0.367084	-3.844262	0.000000
C	-1.010123	-3.693444	0.000000
C	-1.824149	-2.548078	0.000000
C	-3.276580	-2.593004	0.000000
C	-3.707534	-1.307155	0.000000
C	-2.512574	-0.492982	0.000000
N	-1.410237	-1.260317	0.000000
H	0.265910	-1.120234	0.000000
H	3.256916	-4.106444	0.000000
H	4.494354	-1.723979	0.000000
H	0.727771	-4.866654	0.000000
H	-1.569758	-4.622690	0.000000
H	-3.871870	-3.493485	0.000000
H	-4.723249	-0.944237	0.000000
H	-4.494354	1.723979	0.000000
H	-3.256916	4.106444	0.000000
H	-0.727771	4.866654	0.000000
H	1.569758	4.622690	0.000000

H	3.871870	3.493485	0.000000
H	4.723249	0.944237	0.000000

porphycene S_1

C	-3.455786	1.901181	0.000000
C	-2.447377	0.897748	0.000000
N	-1.237958	1.540209	0.000000
C	-1.412807	2.879268	0.000000
C	-2.822197	3.119455	0.000000
C	-0.378883	3.853386	0.000000
C	0.983903	3.707359	0.000000
C	1.826698	2.552470	0.000000
H	-0.283232	1.119511	0.000000
N	1.416307	1.273212	0.000000
C	3.270740	2.610415	0.000000
C	3.716906	1.321794	0.000000
C	2.541464	0.501306	0.000000
C	2.447377	-0.897748	0.000000
C	3.455786	-1.901181	0.000000
C	2.822197	-3.119455	0.000000
C	1.412807	-2.879268	0.000000
N	1.237958	-1.540209	0.000000
C	0.378883	-3.853386	0.000000
C	-0.983903	-3.707359	0.000000
C	-1.826698	-2.552470	0.000000
C	-3.270740	-2.610415	0.000000
C	-3.716906	-1.321794	0.000000
C	-2.541464	-0.501306	0.000000
N	-1.416307	-1.273212	0.000000
H	0.283232	-1.119511	0.000000
H	3.275203	-4.098065	0.000000
H	4.516598	-1.710965	0.000000
H	0.747861	-4.872347	0.000000
H	-1.542591	-4.637747	0.000000
H	-3.859239	-3.515400	0.000000
H	-4.736386	-0.970805	0.000000
H	-4.516598	1.710965	0.000000
H	-3.275203	4.098065	0.000000
H	-0.747861	4.872347	0.000000
H	1.542591	4.637747	0.000000
H	3.859239	3.515400	0.000000
H	4.736386	0.970805	0.000000

porphine S_0

N	0.000000	-2.013446	0.000000
N	2.095889	0.000000	0.000000
C	1.077887	-2.833278	0.000000
C	0.673628	-4.233410	0.000000
C	2.409025	-2.427440	0.000000
C	2.872370	-1.121639	0.000000
C	4.234477	-0.681414	0.000000
H	1.348145	-5.076011	0.000000
H	3.164881	-3.203162	0.000000
H	5.085583	-1.343541	0.000000
H	1.081891	0.000000	0.000000
N	0.000000	2.013446	0.000000
N	-2.095889	0.000000	0.000000
C	1.077887	2.833278	0.000000
C	-1.077887	2.833278	0.000000
C	-1.077887	-2.833278	0.000000
C	0.673628	4.233410	0.000000
C	-0.673628	4.233410	0.000000
C	-0.673628	-4.233410	0.000000
C	2.409025	2.427440	0.000000
C	-2.409025	2.427440	0.000000
C	-2.409025	-2.427440	0.000000
C	2.872370	1.121639	0.000000
C	-2.872370	1.121639	0.000000
C	-2.872370	-1.121639	0.000000
C	4.234477	0.681414	0.000000
C	-4.234477	0.681414	0.000000
C	-4.234477	-0.681414	0.000000
H	1.348145	5.076011	0.000000
H	-1.348145	5.076011	0.000000
H	-1.348145	-5.076011	0.000000
H	3.164881	3.203162	0.000000
H	-3.164881	3.203162	0.000000
H	-3.164881	-3.203162	0.000000
H	5.085583	1.343541	0.000000
H	-5.085583	1.343541	0.000000
H	-5.085583	-1.343541	0.000000
H	-1.081891	0.000000	0.000000

porphine S_1

N	0.000000	-2.033010	0.000000
N	2.093361	0.000000	0.000000
C	1.080936	-2.856154	0.000000
C	0.674877	-4.253096	0.000000
C	2.414150	-2.435992	0.000000

C	2.873990	-1.124535	0.000000
C	4.235048	-0.683140	0.000000
H	1.347605	-5.096822	0.000000
H	3.174768	-3.207020	0.000000
H	5.086885	-1.344165	0.000000
H	1.081039	0.000000	0.000000
N	0.000000	2.033010	0.000000
N	-2.093361	0.000000	0.000000
C	1.080936	2.856154	0.000000
C	-1.080936	2.856154	0.000000
C	-1.080936	-2.856154	0.000000
C	0.674877	4.253096	0.000000
C	-0.674877	4.253096	0.000000
C	-0.674877	-4.253096	0.000000
C	2.414150	2.435992	0.000000
C	-2.414150	2.435992	0.000000
C	-2.414150	-2.435992	0.000000
C	2.873990	1.124535	0.000000
C	-2.873990	1.124535	0.000000
C	-2.873990	-1.124535	0.000000
C	4.235048	0.683140	0.000000
C	-4.235048	0.683140	0.000000
C	-4.235048	-0.683140	0.000000
H	1.347605	5.096822	0.000000
H	-1.347605	5.096822	0.000000
H	-1.347605	-5.096822	0.000000
H	3.174768	3.207020	0.000000
H	-3.174768	3.207020	0.000000
H	-3.174768	-3.207020	0.000000
H	5.086885	1.344165	0.000000
H	-5.086885	1.344165	0.000000
H	-5.086885	-1.344165	0.000000
H	-1.081039	0.000000	0.000000

chlorin S_0

C	0.000000	-4.226886	0.920417
C	0.000000	-2.871262	1.370412
N	0.000000	-2.085722	0.240222
C	0.000000	-2.853678	-0.876917
C	0.000000	-4.218745	-0.443109
C	0.000000	-2.412120	2.668714
C	0.000000	-1.077323	3.087317
N	0.000000	0.000000	2.266333
C	0.000000	1.077323	3.087317
C	0.000000	0.677036	4.478221

C	0.000000	-0.677036	4.478221
C	0.000000	2.412120	2.668714
C	0.000000	2.871262	1.370412
N	0.000000	2.085722	0.240222
C	0.000000	2.853678	-0.876917
C	0.000000	4.218745	-0.443109
C	0.000000	4.226886	0.920417
C	0.000000	2.403523	-2.198120
C	0.000000	1.096554	-2.640811
C	0.000000	0.764514	-4.124411
C	0.000000	-0.764514	-4.124411
C	0.000000	-1.096554	-2.640811
N	0.000000	0.000000	-1.861882
C	0.000000	-2.403523	-2.198120
H	-0.879634	1.188835	-4.609719
H	0.000000	3.179405	-2.953819
H	0.000000	5.065173	-1.110872
H	0.000000	1.349836	5.322229
H	0.000000	-1.349836	5.322229
H	-0.879634	-1.188835	-4.609719
H	0.000000	3.170864	3.442466
H	0.000000	-3.170864	3.442466
H	0.000000	-3.179405	-2.953819
H	0.000000	5.083065	1.576353
H	0.000000	-5.083065	1.576353
H	0.000000	-5.065173	-1.110872
H	0.879634	-1.188835	-4.609719
H	0.879634	1.188835	-4.609719
H	0.000000	-1.073781	0.258913
H	0.000000	1.073781	0.258913

chlorin S_1

C	0.000000	-4.233899	0.921079
C	0.000000	-2.877176	1.366770
N	0.000000	-2.092434	0.239738
C	0.000000	-2.868189	-0.884135
C	0.000000	-4.228433	-0.447848
C	0.000000	-2.414990	2.677644
C	0.000000	-1.080911	3.087100
N	0.000000	0.000000	2.264815
C	0.000000	1.080911	3.087100
C	0.000000	0.673325	4.488653
C	0.000000	-0.673325	4.488653
C	0.000000	2.414990	2.677644
C	0.000000	2.877176	1.366770

N	0.000000	2.092434	0.239738
C	0.000000	2.868189	-0.884135
C	0.000000	4.228433	-0.447848
C	0.000000	4.233899	0.921079
C	0.000000	2.413002	-2.206250
C	0.000000	1.097903	-2.643487
C	0.000000	0.763560	-4.122366
C	0.000000	-0.763560	-4.122366
C	0.000000	-1.097903	-2.643487
N	0.000000	0.000000	-1.856762
C	0.000000	-2.413002	-2.206250
H	-0.879225	1.189045	-4.609071
H	0.000000	3.183972	-2.966682
H	0.000000	5.077296	-1.112624
H	0.000000	1.347797	5.331144
H	0.000000	-1.347797	5.331144
H	-0.879225	-1.189045	-4.609071
H	0.000000	3.171957	3.451804
H	0.000000	-3.171957	3.451804
H	0.000000	-3.183972	-2.966682
H	0.000000	5.088211	1.579052
H	0.000000	-5.088211	1.579052
H	0.000000	-5.077296	-1.112624
H	0.879225	-1.189045	-4.609071
H	0.879225	1.189045	-4.609071
H	0.000000	-1.080827	0.254533
H	0.000000	1.080827	0.254533

Zn-tetraphenylporphine S_0

C	-3.667264	4.424181	1.007125
C	-3.493715	3.480094	-0.004287
C	-4.333529	3.524952	-1.117506
C	-5.325062	4.490148	-1.218469
C	-5.491435	5.425607	-0.205055
C	-4.660280	5.390070	0.907342
C	-2.433582	2.434997	0.082521
C	-1.099057	2.861557	0.072765
N	0.000000	2.055512	0.151298
C	1.099057	2.861557	0.072765
C	0.676854	4.235530	-0.070357
C	-0.676854	4.235530	-0.070357
C	2.433582	2.434997	0.082521
C	3.493715	3.480094	-0.004287
C	4.333529	3.524952	-1.117506
C	5.325062	4.490148	-1.218469

C	5.491435	5.425607	-0.205055
C	4.660280	5.390070	0.907342
C	3.667264	4.424181	1.007125
C	-2.855935	1.099237	0.125295
N	-2.047577	0.000000	0.091609
C	-2.855935	-1.099237	0.125295
C	-4.234367	-0.676849	0.213964
C	-4.234367	0.676849	0.213964
C	-2.433582	-2.434997	0.082521
C	-3.493715	-3.480094	-0.004287
C	-4.333529	-3.524952	-1.117506
C	-5.325062	-4.490148	-1.218469
C	-5.491435	-5.425607	-0.205055
C	-4.660280	-5.390070	0.907342
C	-3.667264	-4.424181	1.007125
C	2.855935	1.099237	0.125295
N	2.047577	0.000000	0.091609
C	2.855935	-1.099237	0.125295
C	4.234367	-0.676849	0.213964
C	4.234367	0.676849	0.213964
C	2.433582	-2.434997	0.082521
C	3.493715	-3.480094	-0.004287
C	4.333529	-3.524952	-1.117506
C	5.325062	-4.490148	-1.218469
C	5.491435	-5.425607	-0.205055
C	4.660280	-5.390070	0.907342
C	3.667264	-4.424181	1.007125
C	1.099057	-2.861557	0.072765
N	0.000000	-2.055512	0.151298
C	-1.099057	-2.861557	0.072765
C	-0.676854	-4.235530	-0.070357
C	0.676854	-4.235530	-0.070357
H	1.337689	-5.079198	-0.182585
H	5.082415	-1.337644	0.287044
H	1.337689	5.079198	-0.182585
H	-1.337689	5.079198	-0.182585
H	-1.337689	-5.079198	-0.182585
H	5.082415	1.337644	0.287044
H	-5.082415	1.337644	0.287044
H	-5.082415	-1.337644	0.287044
H	4.198163	2.795265	-1.907034
H	5.965042	4.514120	-2.091661
H	6.264766	6.179394	-0.282813
H	4.787827	6.113857	1.702564
H	3.021256	4.391901	1.876640
H	4.198163	-2.795265	-1.907034

H	5.965042	-4.514120	-2.091661
H	6.264766	-6.179394	-0.282813
H	4.787827	-6.113857	1.702564
H	3.021256	-4.391901	1.876640
H	-4.198163	-2.795265	-1.907034
H	-5.965042	-4.514120	-2.091661
H	-6.264766	-6.179394	-0.282813
H	-4.787827	-6.113857	1.702564
H	-3.021256	-4.391901	1.876640
H	-4.198163	2.795265	-1.907034
H	-5.965042	4.514120	-2.091661
H	-6.264766	6.179394	-0.282813
H	-4.787827	6.113857	1.702564
H	-3.021256	4.391901	1.876640
Zn	0.000000	0.000000	0.131686

Zn-tetraphenylporphine S_1

C	-3.622151	4.485861	0.956037
C	-3.496402	3.481808	-0.005327
C	-4.388739	3.466140	-1.079866
C	-5.377714	4.431286	-1.194167
C	-5.495694	5.425202	-0.230286
C	-4.616692	5.448470	0.845002
C	-2.440101	2.442241	0.090487
C	-1.101580	2.864246	0.078588
N	0.000000	2.056420	0.194078
C	1.101580	2.864246	0.078588
C	0.677839	4.229165	-0.121347
C	-0.677839	4.229165	-0.121347
C	2.440101	2.442241	0.090487
C	3.496402	3.481808	-0.005327
C	4.388739	3.466140	-1.079866
C	5.377714	4.431286	-1.194167
C	5.495694	5.425202	-0.230286
C	4.616692	5.448470	0.845002
C	3.622151	4.485861	0.956037
C	-2.871809	1.098597	0.144835
N	-2.062530	0.000000	0.070239
C	-2.871809	-1.098597	0.144835
C	-4.239895	-0.679745	0.295897
C	-4.239895	0.679745	0.295897
C	-2.440101	-2.442241	0.090487
C	-3.496402	-3.481808	-0.005327
C	-4.388739	-3.466140	-1.079866
C	-5.377714	-4.431286	-1.194167

C	-5.495694	-5.425202	-0.230286
C	-4.616692	-5.448470	0.845002
C	-3.622151	-4.485861	0.956037
C	2.871809	1.098597	0.144835
N	2.062530	0.000000	0.070239
C	2.871809	-1.098597	0.144835
C	4.239895	-0.679745	0.295897
C	4.239895	0.679745	0.295897
C	2.440101	-2.442241	0.090487
C	3.496402	-3.481808	-0.005327
C	4.388739	-3.466140	-1.079866
C	5.377714	-4.431286	-1.194167
C	5.495694	-5.425202	-0.230286
C	4.616692	-5.448470	0.845002
C	3.622151	-4.485861	0.956037
C	1.101580	-2.864246	0.078588
N	0.000000	-2.056420	0.194078
C	-1.101580	-2.864246	0.078588
C	-0.677839	-4.229165	-0.121347
C	0.677839	-4.229165	-0.121347
H	1.336684	-5.066851	-0.278862
H	5.082274	-1.340639	0.414300
H	1.336684	5.066851	-0.278862
H	-1.336684	5.066851	-0.278862
H	-1.336684	-5.066851	-0.278862
H	5.082274	1.340639	0.414300
H	-5.082274	1.340639	0.414300
H	-5.082274	-1.340639	0.414300
H	4.290338	2.692922	-1.832478
H	6.053759	4.410743	-2.039680
H	6.268881	6.178061	-0.317569
H	4.708877	6.215406	1.603919
H	2.940578	4.498114	1.798193
H	4.290338	-2.692922	-1.832478
H	6.053759	-4.410743	-2.039680
H	6.268881	-6.178061	-0.317569
H	4.708877	-6.215406	1.603919
H	2.940578	-4.498114	1.798193
H	-4.290338	-2.692922	-1.832478
H	-6.053759	-4.410743	-2.039680
H	-6.268881	-6.178061	-0.317569
H	-4.708877	-6.215406	1.603919
H	-2.940578	-4.498114	1.798193
H	-4.290338	2.692922	-1.832478
H	-6.053759	4.410743	-2.039680
H	-6.268881	6.178061	-0.317569

H	-4.708877	6.215406	1.603919
H	-2.940578	4.498114	1.798193
Zn	0.000000	0.000000	0.139726

tetraphenylporphine S_0

C	4.221725	0.689507	0.086161
C	2.869112	1.129263	-0.070713
N	2.096976	0.004297	-0.157282
C	2.873758	-1.117369	-0.069408
C	4.224497	-0.671904	0.087057
C	2.429345	-2.439308	-0.099108
C	1.085957	-2.834926	-0.169104
N	0.004184	-2.017328	-0.121052
C	-1.074148	-2.839378	-0.170421
C	-0.663939	-4.232424	-0.298452
C	0.681654	-4.229664	-0.297569
C	-2.419225	-2.449351	-0.101328
C	-2.869112	-1.129263	-0.070713
N	-2.096976	-0.004297	-0.157282
C	-2.873758	1.117369	-0.069408
C	-4.224497	0.671904	0.087057
C	-4.221725	-0.689507	0.086161
C	-2.429345	2.439308	-0.099108
C	-1.085957	2.834926	-0.169104
N	-0.004184	2.017328	-0.121052
C	1.074148	2.839378	-0.170421
C	0.663939	4.232424	-0.298452
C	-0.681654	4.229664	-0.297569
C	2.419225	2.449351	-0.101328
H	-1.349957	5.069251	-0.396553
C	-3.469767	3.502441	-0.002434
H	-5.070527	1.327813	0.205441
H	-1.084379	-0.002044	-0.206101
H	-1.328635	-5.074758	-0.398338
H	1.349957	-5.069251	-0.396553
H	1.328635	5.074758	-0.398338
C	-3.455367	-3.516844	-0.006399
C	3.469767	-3.502441	-0.002434
C	3.455367	3.516844	-0.006399
H	-5.065102	-1.348970	0.203649
H	5.070527	-1.327813	0.205441
H	5.065102	1.348970	0.203649
H	1.084379	0.002044	-0.206101
C	-4.421324	-3.683232	-0.998247
C	-5.379289	-4.682932	-0.888771

C	-5.384678	-5.527470	0.213948
C	-4.426896	-5.368390	1.207604
C	-3.469767	-4.370173	1.097325
H	-4.410186	-3.029183	-1.862278
H	-6.119311	-4.806049	-1.669671
H	-6.132088	-6.306161	0.299192
H	-4.427534	-6.019312	2.072907
H	-2.722501	-4.240243	1.871117
C	-4.437090	3.665777	-0.993421
C	-5.398982	4.661520	-0.882420
C	-5.406975	5.505115	0.221000
C	-4.447857	5.349053	1.213859
C	-3.486797	4.354766	1.102068
H	-4.423945	3.012479	-1.858000
H	-6.139988	4.782368	-1.662742
H	-6.157444	6.280727	0.307430
H	-4.450486	5.999265	2.079699
H	-2.738490	4.227158	1.875239
C	4.421324	3.683232	-0.998247
C	5.379289	4.682932	-0.888771
C	5.384678	5.527470	0.213948
C	4.426896	5.368390	1.207604
C	3.469767	4.370173	1.097325
H	4.410186	3.029183	-1.862278
H	6.119311	4.806049	-1.669671
H	6.132088	6.306161	0.299192
H	4.427534	6.019312	2.072907
H	2.722501	4.240243	1.871117
C	4.437090	-3.665777	-0.993421
C	5.398982	-4.661520	-0.882420
C	5.406975	-5.505115	0.221000
C	4.447857	-5.349053	1.213859
C	3.486797	-4.354766	1.102068
H	4.423945	-3.012479	-1.858000
H	6.139988	-4.782368	-1.662742
H	6.157444	-6.280727	0.307430
H	4.450486	-5.999265	2.079699
H	2.738490	-4.227158	1.875239

tetraphenylporphine S_1

C	4.218518	0.700379	0.139337
C	2.871518	1.139110	-0.064282
N	2.101825	0.008845	-0.177785
C	2.881410	-1.114301	-0.060655
C	4.224426	-0.663234	0.141769

C	2.442647	-2.440740	-0.100840
C	1.094769	-2.852942	-0.194380
N	0.008905	-2.036838	-0.116534
C	-1.069698	-2.862182	-0.198039
C	-0.656940	-4.241343	-0.378867
C	0.694387	-4.235635	-0.376284
C	-2.421281	-2.461635	-0.107224
C	-2.871518	-1.139110	-0.064282
N	-2.101825	-0.008845	-0.177785
C	-2.881410	1.114301	-0.060655
C	-4.224426	0.663234	0.141769
C	-4.218518	-0.700379	0.139337
C	-2.442647	2.440740	-0.100840
C	-1.094769	2.852942	-0.194380
N	-0.008905	2.036838	-0.116534
C	1.069698	2.862182	-0.198039
C	0.656940	4.241343	-0.378867
C	-0.694387	4.235635	-0.376284
C	2.421281	2.461635	-0.107224
H	-1.363509	5.069671	-0.508615
C	-3.480746	3.498608	0.003649
H	-5.067910	1.314704	0.295893
H	-1.091086	-0.004165	-0.235689
H	-1.318451	-5.081035	-0.513699
H	1.363509	-5.069671	-0.508615
H	1.318451	5.081035	-0.513699
C	-3.450861	-3.528320	-0.008116
C	3.480746	-3.498608	0.003649
C	3.450861	3.528320	-0.008116
H	-5.056337	-1.359658	0.291095
H	5.067910	-1.314704	0.295893
H	5.056337	1.359658	0.291095
H	1.091086	0.004165	-0.235689
C	-4.465347	-3.653604	-0.957886
C	-5.417958	-4.657609	-0.843984
C	-5.372863	-5.545685	0.222869
C	-4.367398	-5.428037	1.174834
C	-3.412345	-4.429539	1.057866
H	-4.493114	-2.966165	-1.794985
H	-6.193216	-4.750148	-1.594309
H	-6.117432	-6.326579	0.312425
H	-4.329261	-6.112772	2.012678
H	-2.628579	-4.332265	1.799541
C	-4.498247	3.618918	-0.943514
C	-5.458431	4.615095	-0.824323
C	-5.417958	5.500091	0.245279

C	-4.409532	5.387304	1.194679
C	-3.446921	4.396726	1.072405
H	-4.522371	2.934033	-1.782813
H	-6.236018	4.703971	-1.572677
H	-6.168440	6.274827	0.338974
H	-4.374962	6.069592	2.034669
H	-2.660723	4.303281	1.811994
C	4.465347	3.653604	-0.957886
C	5.417958	4.657609	-0.843984
C	5.372863	5.545685	0.222869
C	4.367398	5.428037	1.174834
C	3.412345	4.429539	1.057866
H	4.493114	2.966165	-1.794985
H	6.193216	4.750148	-1.594309
H	6.117432	6.326579	0.312425
H	4.329261	6.112772	2.012678
H	2.628579	4.332265	1.799541
C	4.498247	-3.618918	-0.943514
C	5.458431	-4.615095	-0.824323
C	5.417958	-5.500091	0.245279
C	4.409532	-5.387304	1.194679
C	3.446921	-4.396726	1.072405
H	4.522371	-2.934033	-1.782813
H	6.236018	-4.703971	-1.572677
H	6.168440	-6.274827	0.338974
H	4.374962	-6.069592	2.034669
H	2.660723	-4.303281	1.811994

M06-2X/TZVP geometries – Group II

tetrafluorobenzene S_0

C	-1.188886	0.692623	0.000000
C	-1.188886	-0.692623	0.000000
C	0.000000	-1.395870	0.000000
C	1.188886	-0.692623	0.000000
C	1.188886	0.692623	0.000000
C	0.000000	1.395870	0.000000
F	-2.350202	-1.346075	0.000000
H	0.000000	-2.476914	0.000000
F	2.350202	-1.346075	0.000000
F	2.350202	1.346075	0.000000
H	0.000000	2.476914	0.000000
F	-2.350202	1.346075	0.000000

tetrafluorobenzene S_1

C	1.158490	-0.708283	0.107844
C	1.158490	0.708283	0.107844
C	0.000000	1.464190	0.338466
C	-1.158490	0.708283	0.107844
C	-1.158490	-0.708283	0.107844
C	0.000000	-1.464190	0.338466
F	2.293934	1.310715	-0.229603
H	0.000000	2.510884	0.603175
F	-2.293934	1.310715	-0.229603
F	-2.293934	-1.310715	-0.229603
H	0.000000	-2.510884	0.603175
F	2.293934	-1.310715	-0.229603

benzonitrile S_0

C	0.000000	0.000000	-1.050902
C	-1.210762	0.000000	-0.358628
C	-1.204758	0.000000	1.027084
C	0.000000	0.000000	1.719255
C	1.204758	0.000000	1.027084
C	1.210762	0.000000	-0.358628
H	-2.141603	0.000000	-0.910132
H	-2.142119	0.000000	1.567739
H	0.000000	0.000000	2.801662
H	2.142119	0.000000	1.567739
H	2.141603	0.000000	-0.910132
C	0.000000	0.000000	-2.486946
N	0.000000	0.000000	-3.635185

benzonitrile S_1

C	0.000000	0.000000	-1.101751
C	-1.225520	0.000000	-0.372970
C	-1.215189	0.000000	1.045782
C	0.000000	0.000000	1.764551
C	1.215189	0.000000	1.045782
C	1.225520	0.000000	-0.372970
H	-2.163247	0.000000	-0.910909
H	-2.159027	0.000000	1.573635
H	0.000000	0.000000	2.844180
H	2.159027	0.000000	1.573635
H	2.163247	0.000000	-0.910909
C	0.000000	0.000000	-2.511353
N	0.000000	0.000000	-3.666702

o-fluorophenol, *cis* S_0

C	0.325793	1.451406	0.000000
C	-0.871368	0.773115	0.000000
C	-0.947025	-0.613599	0.000000
C	0.237366	-1.336051	0.000000
C	1.455452	-0.670447	0.000000
C	1.506366	0.717737	0.000000
F	-2.044486	1.448725	0.000000
O	-2.138453	-1.261468	0.000000
H	0.180175	-2.416423	0.000000
H	2.372551	-1.244615	0.000000
H	2.457509	1.232062	0.000000
H	0.318907	2.533139	0.000000
H	-2.852776	-0.613601	0.000000

o-fluorophenol, *cis* S_1

C	1.222559	-0.274561	-0.740053
C	0.001514	-0.012885	-0.095050
C	-0.020633	-0.024397	1.353203
C	1.161453	0.077335	2.090359
C	2.366984	0.133277	1.402190
C	2.385897	-0.043734	0.003662
F	-0.847798	0.961788	-0.651114
O	-1.175387	-0.210356	1.990338
H	1.118991	-0.046756	3.166168
H	3.298606	0.235352	1.940970
H	3.333072	0.027751	-0.521516
H	1.269712	-0.433671	-1.808941
H	-1.859591	-0.389144	1.319725

o-fluorophenol, *trans* S_0

C	0.289912	1.258725	0.000000
C	-0.944181	0.614538	0.000000
C	-0.961013	-0.773667	0.000000
C	0.227665	-1.494068	0.000000
C	1.446198	-0.833904	0.000000
C	1.474727	0.556663	0.000000
O	-2.057879	1.390018	0.000000
H	-1.914707	-1.290261	0.000000
H	0.193269	-2.575366	0.000000
H	2.372655	-1.391532	0.000000
H	2.404022	1.110790	0.000000

F	0.309835	2.597855	0.000000
H	-2.840514	0.830208	0.000000

o-fluorophenol, *trans* S_1

C	0.819948	1.031578	0.113171
C	-0.588297	0.970582	0.095057
C	-1.274893	-0.289159	0.141528
C	-0.474285	-1.415834	-0.077157
C	0.938065	-1.327824	-0.076923
C	1.618264	-0.127307	0.200538
O	-1.244750	2.109054	-0.136034
H	-2.295791	-0.355520	0.498896
H	-0.930437	-2.388885	-0.213064
H	1.508862	-2.228020	-0.276419
H	2.687296	-0.063966	0.327518
F	1.389750	2.200184	-0.195707
H	-2.153761	1.885118	-0.401406

m-fluorophenol, *cis* S_0

C	0.308886	1.405738	0.000000
C	-0.926973	0.786679	0.000000
C	-0.964700	-0.602908	0.000000
C	0.214999	-1.341040	0.000000
C	1.431810	-0.680203	0.000000
C	1.499178	0.709006	0.000000
O	-2.135166	-1.295236	0.000000
F	0.339047	2.749223	0.000000
H	0.155071	-2.420438	0.000000
H	2.348275	-1.255923	0.000000
H	2.437867	1.244089	0.000000
H	-1.828187	1.387500	0.000000
H	-2.880107	-0.686486	0.000000

m-fluorophenol, *cis* S_1

C	1.217941	-0.039379	-0.679726
C	-0.047806	0.106430	-0.101998
C	-0.023088	0.044973	1.321519
C	1.169554	0.024799	2.079241
C	2.426354	0.187334	1.439849
C	2.425500	-0.041964	0.041596
O	-1.167460	-0.069543	2.007522
F	1.293770	-0.188800	-2.007827
H	1.084069	-0.199019	3.135607

H	3.345405	0.237776	1.999502
H	3.339295	-0.240226	-0.506129
H	-0.913777	0.416946	-0.670629
H	-1.894397	-0.239327	1.391422

m-fluorophenol, *trans* S_0

C	0.268395	1.301996	0.000000
C	-0.946779	0.626886	0.000000
C	-0.982446	-0.764026	0.000000
C	0.207536	-1.478682	0.000000
C	1.433201	-0.829550	0.000000
C	1.426201	0.553698	0.000000
O	-2.072851	1.389211	0.000000
H	-1.933886	-1.282969	0.000000
H	0.177115	-2.560413	0.000000
H	2.371508	-1.365313	0.000000
F	2.601301	1.203926	0.000000
H	0.301573	2.382114	0.000000
H	-2.850867	0.823130	0.000000

m-fluorophenol, *trans* S_1

C	1.086258	-0.016819	0.000000
C	0.328819	1.180418	0.000000
C	-1.091223	1.209931	0.000000
C	-1.824376	-0.005771	0.000000
C	-1.085596	-1.216876	0.000000
C	0.319920	-1.194190	0.000000
O	1.035015	2.319614	0.000000
H	-1.597994	2.167904	0.000000
H	-2.901980	-0.012320	0.000000
H	-1.580394	-2.179086	0.000000
F	0.964773	-2.367183	0.000000
H	2.163705	-0.012170	0.000000
H	0.441924	3.080694	0.000000

p-fluorophenol S_0

C	0.271685	1.314121	0.000000
C	-0.947258	0.644972	0.000000
C	-0.979382	-0.744058	0.000000
C	0.206274	-1.468494	0.000000
C	1.403763	-0.785117	0.000000
C	1.456515	0.596206	0.000000
O	-2.078001	1.408743	0.000000

H	-1.929645	-1.266079	0.000000
H	0.206045	-2.550018	0.000000
F	2.555569	-1.483368	0.000000
H	2.416891	1.093799	0.000000
H	0.273638	2.395681	0.000000
H	-2.856114	0.843600	0.000000

p-fluorophenol S_1

C	1.266286	0.678345	0.000000
C	0.026471	1.358842	0.000000
C	-1.238185	0.708541	0.000000
C	-1.250999	-0.703544	0.000000
C	-0.006217	-1.361186	0.000000
C	1.252333	-0.735156	0.000000
O	0.093103	2.694367	0.000000
H	-2.151810	1.288626	0.000000
H	-2.159753	-1.285212	0.000000
F	-0.026790	-2.690557	0.000000
H	2.149102	-1.334428	0.000000
H	2.178594	1.255028	0.000000
H	-0.795437	3.071929	0.000000

phenylacetylene S_0

C	1.206522	0.000000	-0.013560
C	0.000000	0.000000	-0.718213
C	-1.206522	0.000000	-0.013560
C	-1.202631	0.000000	1.372388
C	0.000000	0.000000	2.068166
C	1.202631	0.000000	1.372388
C	0.000000	0.000000	-2.150544
C	0.000000	0.000000	-3.350600
H	-2.138813	0.000000	-0.563034
H	-2.141391	0.000000	1.911408
H	0.000000	0.000000	3.150604
H	2.141391	0.000000	1.911408
H	2.138813	0.000000	-0.563034
H	0.000000	0.000000	-4.413835

phenylacetylene S_1

C	1.231734	0.000000	-0.029424
C	0.000000	0.000000	-0.751325
C	-1.231734	0.000000	-0.029424
C	-1.222606	0.000000	1.389903

C	0.000000	0.000000	2.094189
C	1.222606	0.000000	1.389903
C	0.000000	0.000000	-2.153939
C	0.000000	0.000000	-3.362725
H	-2.163128	0.000000	-0.577163
H	-2.159594	0.000000	1.928889
H	0.000000	0.000000	3.175333
H	2.159594	0.000000	1.928889
H	2.163128	0.000000	-0.577163
H	0.000000	0.000000	-4.425943

aniline S_0

C	0.917225	0.029270	0.000000
C	0.205722	0.037335	1.201817
C	-1.180271	0.042490	1.196547
C	-1.886026	0.046138	0.000000
C	-1.180271	0.042490	-1.196547
C	0.205722	0.037335	-1.201817
H	0.747724	0.040129	2.140657
H	-2.967613	0.050034	0.000000
H	-1.713366	0.045896	2.139312
H	-1.713366	0.045896	-2.139312
H	0.747724	0.040129	-2.140657
N	2.310885	0.079876	0.000000
H	2.752961	-0.268503	-0.836186
H	2.752961	-0.268503	0.836186

aniline S_1

C	0.894975	-0.034134	0.000000
C	0.224229	-0.008473	1.248952
C	-1.192689	0.045615	1.237701
C	-1.864098	0.071182	0.000000
C	-1.192689	0.045615	-1.237701
C	0.224229	-0.008473	-1.248952
H	0.794101	-0.030281	2.167952
H	-2.947249	0.112419	0.000000
H	-1.752629	0.066976	2.160567
H	-1.752629	0.066976	-2.160567
H	0.794101	-0.030281	-2.167952
N	2.246717	-0.085949	0.000000
H	2.761809	-0.105606	-0.864696
H	2.761809	-0.105606	0.864696

catechol S_0

C	0.469923	1.276737	0.000000
C	-0.745083	0.617803	0.000000
C	-0.795256	-0.777346	0.000000
C	0.383385	-1.502156	0.000000
C	1.606569	-0.841482	0.000000
C	1.653120	0.544194	0.000000
O	-1.968689	1.240196	0.000000
O	-1.990975	-1.420388	0.000000
H	0.322363	-2.582445	0.000000
H	2.523216	-1.416143	0.000000
H	2.602618	1.062125	0.000000
H	0.491837	2.361149	0.000000
H	-1.860081	2.195381	0.000000
H	-2.692948	-0.757627	0.000000

catechol S_1

C	0.473891	1.349304	0.000000
C	-0.755447	0.625197	0.000000
C	-0.800532	-0.784571	0.000000
C	0.388091	-1.575170	0.000000
C	1.595596	-0.859218	0.000000
C	1.637594	0.557971	0.000000
O	-1.965725	1.239744	0.000000
O	-1.983386	-1.414853	0.000000
H	0.322394	-2.650461	0.000000
H	2.534896	-1.396273	0.000000
H	2.605928	1.041733	0.000000
H	0.494718	2.428761	0.000000
H	-1.853353	2.196131	0.000000
H	-2.694663	-0.758296	0.000000

resorcinol, isomer 1 S_0

C	0.075029	1.145527	0.000000
C	-1.135818	0.463947	0.000000
C	-1.167908	-0.924679	0.000000
C	0.032958	-1.624709	0.000000
C	1.249819	-0.966653	0.000000
C	1.260820	0.425491	0.000000
O	-2.266202	1.224640	0.000000
H	-2.115324	-1.450557	0.000000
H	0.014422	-2.707086	0.000000
H	2.188963	-1.501538	0.000000
O	2.476053	1.039477	0.000000

H	0.068233	2.228976	0.000000
H	-3.039946	0.652763	0.000000
H	2.358900	1.994391	0.000000

resorcinol, isomer 1 S_1

C	0.000585	1.046867	0.253653
C	-1.174005	0.310408	0.055097
C	-1.164309	-1.103931	-0.023298
C	-0.001622	-1.840911	0.355291
C	1.168966	-1.108586	-0.013132
C	1.176092	0.301499	0.049376
O	-2.319463	1.003229	-0.093773
H	-2.028717	-1.602768	-0.458047
H	-0.005048	-2.918573	0.358572
H	2.043956	-1.595700	-0.431765
O	2.365379	0.905243	-0.135948
H	-0.014920	2.105990	0.463682
H	-3.067277	0.396193	-0.140527
H	2.231376	1.857160	-0.219530

resorcinol, isomer 2 S_0

C	1.196044	0.000000	-0.544789
C	0.000000	0.000000	-1.246160
C	-1.196044	0.000000	-0.544789
C	-1.207489	0.000000	0.847904
C	0.000000	0.000000	1.529222
C	1.207489	0.000000	0.847904
O	-2.341561	0.000000	-1.281084
O	2.341561	0.000000	-1.281084
H	-2.146871	0.000000	1.387995
H	0.000000	0.000000	2.611674
H	2.146871	0.000000	1.387995
H	0.000000	0.000000	-2.326959
H	-3.103773	0.000000	-0.694154
H	3.103773	0.000000	-0.694154

resorcinol, isomer 2 S_1

C	1.193673	0.000000	-0.330419
C	0.000000	0.000000	-1.082271
C	-1.193673	0.000000	-0.330419
C	-1.210541	0.000000	1.086801
C	0.000000	0.000000	1.826971
C	1.210541	0.000000	1.086801

O	-2.344905	0.000000	-1.034772
O	2.344905	0.000000	-1.034772
H	-2.166328	0.000000	1.599331
H	0.000000	0.000000	2.904498
H	2.166328	0.000000	1.599331
H	0.000000	0.000000	-2.159437
H	-3.099398	0.000000	-0.435363
H	3.099398	0.000000	-0.435363

resorcinol, isomer 3 S_0

C	1.201167	0.000000	-0.287104
C	0.000000	0.000000	-0.988394
C	-1.201167	0.000000	-0.287104
C	-1.210122	0.000000	1.101387
C	0.000000	0.000000	1.778471
C	1.210122	0.000000	1.101387
O	-2.406400	0.000000	-0.922747
O	2.406400	0.000000	-0.922747
H	-2.157250	0.000000	1.622053
H	0.000000	0.000000	2.861055
H	2.157250	0.000000	1.622053
H	0.000000	0.000000	-2.074397
H	2.276884	0.000000	-1.875717
H	-2.276884	0.000000	-1.875717

resorcinol, isomer 3 S_1

C	-0.024806	-0.304653	1.183381
C	-0.148249	-1.073242	0.000000
C	-0.024806	-0.304653	-1.183381
C	0.035974	1.106820	-1.193952
C	-0.110992	1.849466	0.000000
C	0.035974	1.106820	1.193952
O	0.075829	-0.914696	-2.380728
O	0.075829	-0.914696	2.380728
H	0.241601	1.586506	-2.143542
H	-0.120687	2.926725	0.000000
H	0.241601	1.586506	2.143542
H	-0.650475	-2.037488	0.000000
H	0.248060	-1.855227	2.236013
H	0.248060	-1.855227	-2.236013

hydroquinone, *cis* S_0

C	-0.695682	0.000000	1.090043

C	0.695682	0.000000	1.090043
C	1.391412	0.000000	-0.108597
C	0.691286	0.000000	-1.310594
C	-0.691286	0.000000	-1.310594
C	-1.391412	0.000000	-0.108597
O	2.757755	0.000000	-0.176175
O	-2.757755	0.000000	-0.176175
H	1.248242	0.000000	-2.238106
H	-1.248242	0.000000	-2.238106
H	-1.232727	0.000000	2.032196
H	1.232727	0.000000	2.032196
H	-3.127097	0.000000	0.711523
H	3.127097	0.000000	0.711523

hydroquinone, *cis* S_1

C	0.705035	0.000000	-1.133317
C	-0.705035	0.000000	-1.133317
C	-1.371356	0.000000	0.119358
C	-0.705480	0.000000	1.362272
C	0.705480	0.000000	1.362272
C	1.371356	0.000000	0.119358
O	-2.711530	0.000000	0.165798
O	2.711530	0.000000	0.165798
H	-1.290473	0.000000	2.268949
H	1.290473	0.000000	2.268949
H	1.274671	0.000000	-2.053330
H	-1.274671	0.000000	-2.053330
H	3.071717	0.000000	-0.728961
H	-3.071717	0.000000	-0.728961

hydroquinone, *trans* S_0

C	0.020931	1.387773	0.000000
C	-1.192935	0.716276	0.000000
C	-1.209547	-0.673224	0.000000
C	-0.020931	-1.387773	0.000000
C	1.192935	-0.716276	0.000000
C	1.209547	0.673224	0.000000
O	-2.333329	1.472042	0.000000
H	-2.155314	-1.204277	0.000000
H	-0.021455	-2.469538	0.000000
O	2.333329	-1.472042	0.000000
H	2.155314	1.204277	0.000000
H	0.021455	2.469538	0.000000
H	-3.103720	0.896752	0.000000

H	3.103720	-0.896752	0.000000

hydroquinone, *trans* S_1

C	1.262363	0.674889	0.000000
C	0.034305	1.370854	0.000000
C	-1.232585	0.735546	0.000000
C	-1.262363	-0.674889	0.000000
C	-0.034305	-1.370854	0.000000
C	1.232585	-0.735546	0.000000
O	0.118824	2.709442	0.000000
H	-2.140060	1.324951	0.000000
H	-2.181588	-1.240524	0.000000
O	-0.118824	-2.709442	0.000000
H	2.140060	-1.324951	0.000000
H	2.181588	1.240524	0.000000
H	-0.766867	3.092717	0.000000
H	0.766867	-3.092717	0.000000

salicylic acid S_0

C	1.099566	1.595767	0.000000
C	1.132728	0.198811	0.000000
C	-0.080507	-0.514006	0.000000
C	-1.295650	0.182790	0.000000
C	-1.317386	1.560044	0.000000
C	-0.108239	2.260764	0.000000
O	2.334279	-0.391055	0.000000
C	-0.045483	-1.980241	0.000000
O	-1.250638	-2.564096	0.000000
O	0.972996	-2.645561	0.000000
H	-2.216144	-0.385157	0.000000
H	2.042336	2.126002	0.000000
H	-2.258473	2.092255	0.000000
H	-0.115581	3.343754	0.000000
H	2.209088	-1.359339	0.000000
H	-1.102895	-3.520732	0.000000

salicylic acid S_1

C	1.003868	1.913647	0.000000
C	0.968847	0.510301	0.000000
C	-0.300341	-0.222569	0.000000
C	-1.460435	0.537211	0.000000
C	-1.400979	1.959069	0.000000
C	-0.191979	2.652348	0.000000

O	2.068611	-0.182352	0.000000
C	-0.234107	-1.646038	0.000000
O	-1.409769	-2.304113	0.000000
O	0.851830	-2.293226	0.000000
H	-2.420954	0.039983	0.000000
H	1.975900	2.388818	0.000000
H	-2.333104	2.509963	0.000000
H	-0.173563	3.731944	0.000000
H	1.767297	-1.210267	0.000000
H	-1.200542	-3.247773	0.000000

o-cresol, *cis* S_0

C	1.961540	0.512445	0.000000
C	0.729564	1.150265	0.000000
C	-0.463130	0.433302	0.000000
C	-0.388533	-0.961838	0.000000
C	0.837343	-1.613782	0.000000
C	2.010077	-0.875722	0.000000
C	-1.800173	1.122679	0.000000
O	-1.506955	-1.745269	0.000000
H	0.847324	-2.695733	0.000000
H	2.963409	-1.388626	0.000000
H	2.874048	1.093665	0.000000
H	0.684104	2.233433	0.000000
H	-2.296420	-1.195682	0.000000
H	-2.389531	0.863583	0.884903
H	-1.673136	2.203706	0.000000
H	-2.389531	0.863583	-0.884903

o-cresol, *cis* S_1

C	1.853709	-0.057531	-0.780753
C	0.625805	0.102051	-1.458478
C	-0.587821	0.052731	-0.716501
C	-0.471880	0.090273	0.706676
C	0.766482	0.028374	1.397278
C	1.938155	-0.102180	0.628420
C	-1.891923	-0.096011	-1.426252
O	-1.558643	0.155157	1.485625
H	0.769787	0.146029	2.470440
H	2.902484	-0.201073	1.106040
H	2.764374	-0.150253	-1.360689
H	0.596297	0.136475	-2.538312
H	-2.345408	0.308581	0.944484
H	-2.705028	-0.450401	-0.786698

H	-2.218227	0.843144	-1.890918
H	-1.788745	-0.824856	-2.237952

o-cresol, *trans* S_0

C	2.421293	0.000019	0.031229
C	1.249430	-0.000042	-0.714024
C	0.036519	-0.000020	-0.020748
C	0.001391	0.000060	1.366631
C	1.188602	0.000110	2.088394
C	2.403617	0.000093	1.422034
C	1.243446	-0.000109	-2.214900
O	-1.099292	-0.000074	-0.780266
H	-0.953638	0.000089	1.881705
H	1.156711	0.000178	3.170413
H	3.332184	0.000143	1.977479
H	3.369250	-0.000003	-0.494785
H	-1.871971	-0.000070	-0.207208
H	2.261025	-0.000087	-2.603019
H	0.720102	-0.876490	-2.601448
H	0.720037	0.876201	-2.601517

o-cresol, *trans* S_1

C	2.423038	0.283546	-0.007775
C	1.215588	0.119067	-0.748377
C	0.007583	0.002921	-0.015880
C	-0.053057	-0.069310	1.411602
C	1.174426	-0.076940	2.095173
C	2.387052	0.078554	1.384354
C	1.252454	-0.029093	-2.228630
O	-1.127506	-0.100473	-0.720359
H	-0.998080	0.067844	1.921739
H	1.199194	-0.161843	3.173047
H	3.317315	0.049427	1.939395
H	3.359808	0.423457	-0.527298
H	-1.835050	-0.397209	-0.128561
H	1.893739	-0.873126	-2.511045
H	0.263136	-0.179357	-2.653470
H	1.699050	0.862537	-2.683935

m-cresol, *cis* S_0

C	1.157957	-0.012057	2.081904
C	2.368191	-0.008994	1.409897
C	2.412985	0.006830	0.020198

C	1.234834	0.017321	-0.718466
C	0.016637	0.016991	-0.041655
C	-0.022083	0.001542	1.346365
C	1.261414	0.001451	-2.223327
O	-1.193946	0.002231	2.043629
H	1.103670	-0.021413	3.162160
H	3.290588	-0.015915	1.977185
H	3.367085	0.011938	-0.492535
H	-0.911959	0.030284	-0.605445
H	-1.935864	0.013898	1.431366
H	2.221888	0.350509	-2.601065
H	1.102485	-1.011431	-2.600546
H	0.478418	0.636186	-2.639716

m-cresol, *cis* S_1

C	1.165367	0.002444	2.118496
C	2.407852	0.089500	1.447759
C	2.406903	0.029874	0.035084
C	1.218366	0.005609	-0.740617
C	-0.030746	0.029622	-0.073974
C	-0.018681	0.008731	1.348563
C	1.264610	-0.029821	-2.230332
O	-1.172391	-0.035969	2.028337
H	1.083753	-0.119107	3.189489
H	3.336940	0.114759	1.995825
H	3.355219	0.011017	-0.490846
H	-0.954246	0.212388	-0.611226
H	-1.902462	-0.176979	1.410577
H	2.279730	0.098019	-2.604703
H	0.875682	-0.980558	-2.614421
H	0.636383	0.759840	-2.658072

m-cresol, *trans* S_0

C	-1.191806	-1.097691	0.000000
C	0.197022	-1.209012	0.000000
C	0.967729	-0.051290	0.000000
C	0.363387	1.197954	0.000000
C	-1.023429	1.307623	0.000000
C	-1.792413	0.153433	0.000000
C	0.872062	-2.554823	0.000000
O	1.183144	2.287851	0.000000
H	-1.493884	2.284805	0.000000
H	-2.872202	0.234058	0.000000
H	-1.802424	-1.992099	0.000000

H	2.050035	-0.102640	0.000000
H	0.653648	3.091032	0.000000
H	0.140531	-3.361865	0.000000
H	1.506842	-2.669405	-0.880424
H	1.506842	-2.669405	0.880424

m-cresol, *trans* S_1

C	-1.203515	-1.057536	0.000000
C	0.203502	-1.232575	0.000000
C	1.024943	-0.075641	0.000000
C	0.397843	1.191829	0.000000
C	-1.011274	1.369653	0.000000
C	-1.826302	0.214916	0.000000
C	0.826918	-2.586769	0.000000
O	1.214583	2.255223	0.000000
H	-1.431119	2.367771	0.000000
H	-2.902702	0.294523	0.000000
H	-1.829597	-1.942754	0.000000
H	2.104024	-0.129028	0.000000
H	0.696847	3.069699	0.000000
H	0.075165	-3.375895	0.000000
H	1.468582	-2.724200	-0.877885
H	1.468582	-2.724200	0.877885

p-cresol S_0

C	0.712141	0.009766	-1.187480
C	-0.671861	0.011732	-1.196696
C	-1.368025	0.000169	0.007031
C	-0.670242	-0.015183	1.206492
C	0.719686	-0.016702	1.196574
C	1.435679	-0.002602	0.005697
O	-2.731559	0.000427	-0.055073
C	2.941092	0.021653	-0.004577
H	-1.208930	-0.028749	2.148146
H	1.253470	-0.031295	2.140019
H	1.246212	0.016285	-2.131247
H	-1.231357	0.019093	-2.122889
H	-3.096328	-0.010547	0.834804
H	3.340672	-0.653968	-0.762153
H	3.315953	1.023654	-0.225675
H	3.344956	-0.278356	0.962327

p-cresol S_1

C	0.731528	-0.078951	-1.236715
C	-0.680169	-0.022970	-1.244396
C	-1.349779	-0.002752	-0.000929
C	-0.679126	0.003934	1.251131
C	0.731348	-0.037282	1.238290
C	1.427211	-0.043820	-0.000186
O	-2.687684	0.027515	-0.048660
C	2.912912	0.039925	-0.000882
H	-1.247140	0.006919	2.172639
H	1.294368	-0.037090	2.161295
H	1.291036	-0.100705	-2.161239
H	-1.265149	0.006017	-2.151521
H	-3.046613	0.068310	0.846360
H	3.335209	-0.462806	-0.872752
H	3.228012	1.090195	-0.045116
H	3.335586	-0.391059	0.907970

o-methoxyphenol S_0

C	2.021551	-0.083663	0.000000
C	0.866580	0.698786	0.000000
C	-0.373359	0.084229	0.000000
C	-0.468858	-1.314408	0.000000
C	0.679610	-2.081761	0.000000
C	1.927282	-1.464285	0.000000
O	-1.583953	0.720701	0.000000
O	-1.687678	-1.910545	0.000000
H	0.578686	-3.159107	0.000000
H	2.823220	-2.071068	0.000000
H	2.989453	0.399435	0.000000
H	0.946647	1.777098	0.000000
C	-1.578491	2.133274	0.000000
H	-2.358242	-1.215636	0.000000
H	-2.619917	2.443501	0.000000
H	-1.081265	2.521725	0.892835
H	-1.081265	2.521725	-0.892835

o-methoxyphenol S_1

C	2.465364	0.089281	0.053523
C	1.378435	-0.290631	-0.750655
C	0.108819	-0.236517	-0.095308
C	0.018697	-0.165820	1.317550
C	1.182335	-0.121809	2.136398
C	2.374714	0.157018	1.464090
O	-1.067459	0.042246	-0.719221

O	-1.171806	0.049556	1.891461
H	1.103699	-0.237402	3.206374
H	3.264197	0.421001	2.024477
H	3.417052	0.326766	-0.411256
H	1.496813	-0.586925	-1.781981
C	-1.076119	0.109968	-2.138397
H	-1.852671	0.062428	1.198686
H	-2.099957	0.338469	-2.420567
H	-0.403970	0.892926	-2.492037
H	-0.779584	-0.850565	-2.565057

m-methoxyphenol, isomer 1 S_0

C	0.927167	1.446899	0.000000
C	-0.261760	0.719460	0.000000
C	-0.234294	-0.672492	0.000000
C	0.996503	-1.327782	0.000000
C	2.185918	-0.617016	0.000000
C	2.133979	0.771264	0.000000
H	-1.146558	-1.255148	0.000000
O	1.077612	-2.688837	0.000000
H	3.122786	-1.155987	0.000000
H	3.057640	1.336170	0.000000
H	0.875040	2.526624	0.000000
O	-1.406452	1.449858	0.000000
H	0.195107	-3.070817	0.000000
C	-2.634635	0.756000	0.000000
H	-3.411519	1.515949	0.000000
H	-2.738266	0.132928	-0.893238
H	-2.738266	0.132928	0.893238

m-methoxyphenol, isomer 1 S_1

C	1.173552	-0.010020	-0.618239
C	-0.029376	-0.052058	0.122739
C	-0.049756	-0.173889	1.534695
C	1.224293	-0.021655	2.134973
C	2.431349	0.018251	1.405457
C	2.433336	-0.198716	0.006651
H	-0.894064	-0.558062	2.091232
O	1.326481	0.143657	3.469531
H	3.331462	0.280606	1.949434
H	3.347862	-0.224437	-0.562192
H	1.089751	0.211762	-1.675927
O	-1.147324	0.070968	-0.616465
H	0.447155	0.325231	3.828046

C	-2.400349	0.050421	0.044524
H	-3.146065	0.250498	-0.719647
H	-2.588261	-0.930310	0.487685
H	-2.441736	0.817754	0.820242

m-methoxyphenol, isomer 2 S_0

C	0.344833	2.156580	0.000000
C	-0.838125	1.446054	0.000000
C	-0.796750	0.049057	0.000000
C	0.420066	-0.619637	0.000000
C	1.600057	0.121339	0.000000
C	1.576544	1.507202	0.000000
O	-1.999889	-0.577500	0.000000
C	-2.006955	-1.989624	0.000000
O	2.761340	-0.593406	0.000000
H	0.495814	-1.696883	0.000000
H	2.501298	2.072138	0.000000
H	0.316205	3.238821	0.000000
H	-1.800794	1.937803	0.000000
H	-3.052463	-2.286017	0.000000
H	-1.515939	-2.387881	-0.892319
H	-1.515939	-2.387881	0.892319
H	3.510688	0.009845	0.000000

m-methoxyphenol, isomer 2 S_1

C	1.249912	-0.380815	-0.696613
C	0.096209	-0.025850	0.072360
C	0.118667	-0.102292	1.484091
C	1.322983	-0.285732	2.191242
C	2.466387	-0.043787	1.418627
C	2.415753	0.048495	0.006972
O	-1.073466	0.051745	2.081086
C	-1.117988	0.072212	3.498264
O	3.625606	0.141715	2.081037
H	1.399666	-0.469716	3.249435
H	3.244447	0.530056	-0.510055
H	1.220760	-0.372657	-1.774164
H	-0.797228	0.383374	-0.389104
H	-2.156087	0.253583	3.761691
H	-0.797175	-0.886541	3.910772
H	-0.487032	0.871359	3.893111
H	4.353716	0.214850	1.453147

p-methoxyphenol, *cis* S_0

C	-0.318630	0.733390	0.000000
C	-1.548592	0.073384	0.000000
C	-1.606193	-1.304612	0.000000
C	-0.430169	-2.052215	0.000000
C	0.791156	-1.402999	0.000000
C	0.853625	-0.009531	0.000000
O	-0.552187	-3.414556	0.000000
O	-0.373078	2.095851	0.000000
C	0.852165	2.792356	0.000000
H	1.822289	0.469354	0.000000
H	-2.451992	0.669159	0.000000
H	-2.555171	-1.824352	0.000000
H	1.711514	-1.977044	0.000000
H	0.601460	3.849868	0.000000
H	1.441553	2.559871	0.892219
H	1.441553	2.559871	-0.892219
H	0.320698	-3.817775	0.000000

p-methoxyphenol, *cis* S_1

C	1.322692	-0.017717	-0.619795
C	0.048241	-0.046871	0.002123
C	-0.018254	0.023127	1.409178
C	1.189396	0.000128	2.131217
C	2.468005	-0.051697	1.516532
C	2.539780	0.013432	0.108859
O	1.090059	0.025402	3.469194
O	1.282973	-0.019785	-1.955281
C	2.491505	0.015529	-2.697456
H	3.494564	0.041316	-0.391212
H	-0.830178	-0.077386	-0.623916
H	-0.950816	0.090579	1.948421
H	3.360856	-0.119485	2.124658
H	2.197702	0.009713	-3.742855
H	3.053040	0.924484	-2.474515
H	3.102377	-0.862120	-2.478676
H	1.971587	0.051332	3.860523

p-methoxyphenol, *trans* S_0

C	-0.655664	1.304635	0.000000
C	-1.885173	0.671141	0.000000
C	-1.955945	-0.719105	0.000000
C	-0.787393	-1.461639	0.000000
C	0.450647	-0.828654	0.000000

C	0.521378	0.560846	0.000000
O	-3.143124	-1.399013	0.000000
H	1.345983	-1.434181	0.000000
O	1.681441	1.277674	0.000000
H	-0.584844	2.384308	0.000000
H	-2.795178	1.261736	0.000000
H	-3.873788	-0.774092	0.000000
H	-0.854583	-2.541486	0.000000
C	2.890923	0.553248	0.000000
H	3.687889	1.292369	0.000000
H	2.978711	-0.073904	0.892347
H	2.978711	-0.073904	-0.892347

p-methoxyphenol, *trans* S_1

C	0.122765	-0.028834	-1.394510
C	-1.276746	-0.025958	-1.220436
C	-1.776623	0.019368	0.102227
C	-0.951804	0.065594	1.247129
C	0.449018	0.017729	1.078816
C	0.955258	-0.005615	-0.244749
O	-3.099014	0.032425	0.329981
H	1.104444	0.039616	1.934278
O	2.262540	-0.019144	-0.520525
H	0.590916	-0.057694	-2.366486
H	-1.956196	-0.111564	-2.058246
H	-3.571840	0.052349	-0.510790
H	-1.415347	0.137320	2.219479
C	3.205957	-0.017719	0.538959
H	4.182550	-0.058390	0.065612
H	3.118115	0.895333	1.130656
H	3.066797	-0.890507	1.179303

1-naphthol, *cis* S_0

C	0.828598	1.513983	0.007829
C	0.525184	0.121669	-0.007793
C	-0.841812	-0.267183	-0.000307
C	-1.854754	0.721569	-0.013765
C	-1.519421	2.046271	-0.030117
C	-0.170162	2.449090	-0.015091
C	1.522697	-0.884767	-0.038309
C	1.185523	-2.209789	-0.030908
C	-0.171055	-2.598041	-0.000404
C	-1.154532	-1.649692	0.009386
O	2.115333	1.962751	0.015853

H	-2.198589	-1.940718	0.021113
H	-0.427332	-3.649889	0.006312
H	1.959876	-2.965569	-0.059827
H	2.573131	-0.621843	-0.093208
H	-2.891792	0.409319	-0.013016
H	-2.292617	2.803945	-0.045348
H	0.100867	3.496488	-0.008345
H	2.710868	1.262416	0.295942

1-naphthol, *cis* S_1

C	0.867958	1.463911	0.019731
C	0.537260	0.087854	-0.062570
C	-0.849255	-0.247147	0.016903
C	-1.791845	0.799903	-0.016643
C	-1.423553	2.170717	-0.034494
C	-0.102906	2.510400	-0.038978
C	1.503655	-0.928575	-0.141151
C	1.095444	-2.294056	-0.060281
C	-0.231199	-2.616525	0.044961
C	-1.224796	-1.602420	0.064987
O	2.134000	1.856753	0.164043
H	-2.272499	-1.860308	0.141472
H	-0.533335	-3.654085	0.106220
H	1.846451	-3.072450	-0.091016
H	2.544214	-0.707947	-0.347365
H	-2.844215	0.540850	-0.025380
H	-2.190601	2.932005	-0.070398
H	0.246835	3.533361	-0.033782
H	2.688387	1.087749	0.363724

1-naphthol, *trans* S_0

C	-0.714991	-0.539554	0.000000
C	-0.672681	-1.955648	0.000000
C	0.520971	-2.622728	0.000000
C	1.738111	-1.907395	0.000000
C	1.735386	-0.539303	0.000000
C	0.511860	0.170536	0.000000
H	-1.608673	-2.501989	0.000000
H	0.537330	-3.705362	0.000000
H	2.676565	-2.446990	0.000000
H	2.660735	0.020746	0.000000
C	-1.939993	0.175416	0.000000
C	-1.936661	1.540427	0.000000
C	-0.722689	2.261327	0.000000

C	0.471605	1.592805	0.000000
H	-2.870996	-0.377760	0.000000
H	-2.870654	2.087825	0.000000
H	-0.737140	3.345683	0.000000
O	1.678041	2.224641	0.000000
H	1.543885	3.177313	0.000000

1-naphthol, *trans* S_1

C	-0.943309	-0.393425	0.000000
C	-1.306500	-1.748989	0.000000
C	-0.311801	-2.767195	0.000000
C	1.014487	-2.426976	0.000000
C	1.417365	-1.059560	0.000000
C	0.448994	-0.047081	0.000000
H	-2.356273	-2.012534	0.000000
H	-0.611802	-3.806529	0.000000
H	1.775998	-3.196254	0.000000
H	2.465568	-0.798268	0.000000
C	-1.892297	0.645738	0.000000
C	-1.522333	2.018813	0.000000
C	-0.203600	2.366648	0.000000
C	0.780013	1.326086	0.000000
H	-2.944344	0.386770	0.000000
H	-2.292427	2.778252	0.000000
H	0.115400	3.402443	0.000000
O	2.086473	1.637251	0.000000
H	2.204710	2.593882	0.000000

2-naphthol, *cis* S_0

C	0.596714	2.007293	0.000000
C	0.618399	0.592625	0.000000
C	-0.608687	-0.119413	0.000000
C	-1.820724	0.614040	0.000000
C	-1.810608	1.981736	0.000000
C	-0.588577	2.689912	0.000000
C	1.830941	-0.143960	0.000000
C	1.829565	-1.506766	0.000000
C	0.601522	-2.210104	0.000000
C	-0.588609	-1.535848	0.000000
H	-1.529099	-2.077990	0.000000
H	1.540161	2.541378	0.000000
H	-0.595820	3.772239	0.000000
H	-2.744832	2.529187	0.000000
H	-2.759488	0.072062	0.000000

H	2.769982	0.397347	0.000000
H	2.747535	-2.079542	0.000000
O	0.696342	-3.568721	0.000000
H	-0.184726	-3.955465	0.000000

2-naphthol, *cis* S_1

C	0.601906	1.985924	0.000000
C	0.645183	0.584053	0.000000
C	-0.629423	-0.117208	0.000000
C	-1.833042	0.607290	0.000000
C	-1.841918	2.016472	0.000000
C	-0.625883	2.682736	0.000000
C	1.848890	-0.150934	0.000000
C	1.881205	-1.553156	0.000000
C	0.656720	-2.213284	0.000000
C	-0.584741	-1.517290	0.000000
H	-1.507660	-2.089621	0.000000
H	1.530366	2.543797	0.000000
H	-0.605032	3.765984	0.000000
H	-2.774137	2.561987	0.000000
H	-2.767522	0.058261	0.000000
H	2.780877	0.401686	0.000000
H	2.799327	-2.119432	0.000000
O	0.663821	-3.554173	0.000000
H	-0.238927	-3.893082	0.000000

2-naphthol, *trans* S_0

C	0.509622	2.009159	0.000000
C	0.537171	0.593464	0.000000
C	-0.687950	-0.125981	0.000000
C	-1.903402	0.604612	0.000000
C	-1.898034	1.971153	0.000000
C	-0.677999	2.685314	0.000000
C	1.749068	-0.136290	0.000000
C	1.748906	-1.502230	0.000000
C	0.525078	-2.210618	0.000000
C	-0.666198	-1.538446	0.000000
H	-1.592011	-2.099939	0.000000
H	1.450361	2.548045	0.000000
H	-0.689938	3.767599	0.000000
H	-2.834310	2.515060	0.000000
H	-2.839358	0.058277	0.000000
H	2.687825	0.405392	0.000000
H	2.684289	-2.051995	0.000000

O	0.499472	-3.574109	0.000000
H	1.397419	-3.918466	0.000000

2-naphthol, *trans* S_1

C	0.513447	1.990079	0.000000
C	0.559180	0.588591	0.000000
C	-0.710387	-0.117318	0.000000
C	-1.914826	0.603320	0.000000
C	-1.927905	2.014395	0.000000
C	-0.717083	2.684511	0.000000
C	1.765527	-0.141249	0.000000
C	1.800079	-1.545647	0.000000
C	0.573644	-2.207843	0.000000
C	-0.666296	-1.518167	0.000000
H	-1.572971	-2.109781	0.000000
H	1.440570	2.550349	0.000000
H	-0.699327	3.767781	0.000000
H	-2.862655	2.555817	0.000000
H	-2.847239	0.051172	0.000000
H	2.696342	0.413392	0.000000
H	2.731875	-2.094621	0.000000
O	0.478570	-3.546100	0.000000
H	1.359456	-3.938672	0.000000

5-methoxysalicylic acid S_0

C	2.275687	-0.167461	0.000000
C	1.565620	-1.341591	0.000000
C	0.162329	-1.335984	0.000000
C	-0.507991	-0.132687	0.000000
C	0.213900	1.075749	0.000000
C	1.612973	1.066807	0.000000
O	-0.432202	-2.559967	0.000000
C	-1.842491	-2.590019	0.000000
C	-0.487518	2.363211	0.000000
O	-1.824786	2.267287	0.000000
O	2.371346	2.174202	0.000000
O	0.060888	3.448705	0.000000
H	-2.124241	-3.639473	0.000000
H	-2.248906	-2.104406	-0.892356
H	-2.248906	-2.104406	0.892356
H	-1.586397	-0.080822	0.000000
H	3.357332	-0.164390	0.000000
H	2.072193	-2.298307	0.000000
H	1.784970	2.953568	0.000000

H	-2.173780	3.169984	0.000000

5-methoxysalicylic acid S_1

C	2.176735	-0.136544	0.000000
C	1.729844	-1.455393	0.000000
C	0.338247	-1.684782	0.000000
C	-0.604226	-0.623280	0.000000
C	-0.167544	0.698222	0.000000
C	1.270112	0.929518	0.000000
O	-0.027210	-2.967146	0.000000
C	-1.405420	-3.313625	0.000000
C	-1.035349	1.831961	0.000000
O	-2.361017	1.556523	0.000000
O	1.706091	2.166065	0.000000
O	-0.640658	3.022083	0.000000
H	-1.434681	-4.398852	0.000000
H	-1.899884	-2.929888	-0.894014
H	-1.899884	-2.929888	0.894014
H	-1.666116	-0.820153	0.000000
H	3.231084	0.104866	0.000000
H	2.401774	-2.299795	0.000000
H	0.875828	2.771409	0.000000
H	-2.815677	2.409475	0.000000

m-dimethoxybenzene, *trans* S_0

C	0.000000	-0.705904	-0.178327
C	0.000000	0.705904	-0.178327
C	0.000000	1.388475	1.025937
C	0.000000	0.689114	2.234937
C	0.000000	-0.689114	2.234937
C	0.000000	-1.388475	1.025937
O	0.000000	1.288726	-1.401205
H	0.000000	2.469030	1.037566
H	0.000000	1.239215	3.166559
H	0.000000	-1.239215	3.166559
H	0.000000	-2.469030	1.037566
O	0.000000	-1.288726	-1.401205
C	0.000000	-2.697936	-1.447573
H	0.000000	-2.964203	-2.501188
H	0.892269	-3.111800	-0.968343
H	-0.892269	-3.111800	-0.968343
C	0.000000	2.697936	-1.447573
H	0.000000	2.964203	-2.501188
H	-0.892269	3.111800	-0.968343

H	0.892269	3.111800	-0.968343

m-dimethoxybenzene, *trans* S_1

C	-0.157917	-1.063951	-1.443138
C	-0.264073	0.163396	-0.708687
C	-0.264073	0.163396	0.708687
C	-0.157917	-1.063951	1.443138
C	0.288905	-2.167027	0.705994
C	0.288905	-2.167027	-0.705994
O	-0.173493	1.374560	-1.282961
C	-0.009584	1.445422	-2.690574
O	-0.173493	1.374560	1.282961
C	-0.009584	1.445422	2.690574
H	-0.392023	-1.132513	2.494468
H	0.612819	-3.064758	1.221911
H	0.612819	-3.064758	-1.221911
H	-0.392023	-1.132513	-2.494468
H	0.071358	2.503370	-2.923629
H	0.893776	0.921218	-3.006487
H	-0.876678	1.022723	-3.202775
H	0.071358	2.503370	2.923629
H	-0.876678	1.022723	3.202775
H	0.893776	0.921218	3.006487

3P-propionic acid, *gauche* S_0

C	-0.997840	0.880304	-1.161539
C	-0.372401	0.679093	0.068110
C	-1.036328	-0.062196	1.042806
C	-2.297300	-0.589291	0.792376
C	-2.911169	-0.382692	-0.435560
C	-2.256921	0.354597	-1.414751
C	1.010750	1.230581	0.312825
C	2.100357	0.310350	-0.238048
C	2.253317	-0.944310	0.582379
O	1.918934	-1.076680	1.727737
O	2.857624	-1.928485	-0.108638
H	1.902360	0.029054	-1.273352
H	3.075251	0.807218	-0.223610
H	1.173703	1.370834	1.382050
H	1.104091	2.205318	-0.169354
H	-0.552916	-0.231732	1.997377
H	-2.801675	-1.161241	1.561313
H	-3.895010	-0.791112	-0.628948
H	-2.729608	0.524252	-2.374250

H	-0.493906	1.461926	-1.926763
H	2.948698	-2.685809	0.487849

3P-propionic acid, *gauche* S_1

C	-0.998415	0.967587	-1.181219
C	-0.356855	0.712466	0.064880
C	-1.026656	-0.067735	1.050792
C	-2.309219	-0.611581	0.785300
C	-2.931833	-0.362278	-0.462276
C	-2.274534	0.412371	-1.451342
C	1.028058	1.219093	0.299448
C	2.097168	0.257788	-0.242023
C	2.255884	-0.962443	0.627865
O	1.950101	-1.042845	1.786032
O	2.836449	-1.979157	-0.035241
H	1.869596	-0.058912	-1.260462
H	3.076009	0.746989	-0.268837
H	1.202331	1.365349	1.367175
H	1.150772	2.181490	-0.204332
H	-0.531912	-0.255225	1.994367
H	-2.807911	-1.213766	1.531287
H	-3.914002	-0.767304	-0.665404
H	-2.750704	0.584236	-2.406622
H	-0.503067	1.584733	-1.920069
H	2.938749	-2.710865	0.590682

3P-propionic acid, *anti* S_0

C	1.439005	-0.447292	0.000000
C	0.544662	0.789787	0.000000
C	2.901904	-0.095854	0.000000
H	1.242752	-1.076223	0.872427
H	1.242752	-1.076223	-0.872427
C	-0.911487	0.402304	0.000000
H	0.776342	1.399114	0.874999
H	0.776342	1.399114	-0.874999
C	-1.592227	0.196944	1.197729
C	-2.921575	-0.204102	1.200509
C	-3.589915	-0.406432	0.000000
C	-2.921575	-0.204102	-1.200509
C	-1.592227	0.196944	-1.197729
H	-1.075272	0.360699	2.137257
H	-3.437886	-0.354377	2.140427
H	-4.627311	-0.715572	0.000000
H	-3.437886	-0.354377	-2.140427

H	-1.075272	0.360699	-2.137257
O	3.681116	-1.195992	0.000000
O	3.358570	1.013512	0.000000
H	4.602026	-0.897249	0.000000

3P-propionic acid, *anti* S_1

C	1.436562	-0.431580	0.000000
C	0.560925	0.828388	0.000000
C	2.903748	-0.098190	0.000000
H	1.227411	-1.053490	0.873892
H	1.227411	-1.053490	-0.873892
C	-0.886379	0.470885	0.000000
H	0.806767	1.427179	0.879838
H	0.806767	1.427179	-0.879838
C	-1.568776	0.254141	1.230763
C	-2.901112	-0.229439	1.231819
C	-3.564597	-0.454085	0.000000
C	-2.901112	-0.229439	-1.231819
C	-1.568776	0.254141	-1.230763
H	-1.057168	0.457034	2.162935
H	-3.412696	-0.419684	2.164550
H	-4.589893	-0.799153	0.000000
H	-3.412696	-0.419684	-2.164550
H	-1.057168	0.457034	-2.162935
O	3.667277	-1.208829	0.000000
O	3.373606	1.005634	0.000000
H	4.592525	-0.923395	0.000000

fluorine S_0

C	0.000000	0.000000	-1.791376
C	0.000000	1.179027	-0.847741
C	0.000000	0.734265	0.481192
C	0.000000	-0.734265	0.481192
C	0.000000	1.643662	1.530235
C	0.000000	3.002242	1.237652
C	0.000000	3.444036	-0.082504
C	0.000000	2.532527	-1.134573
H	0.000000	2.881817	-2.160559
H	0.000000	4.506301	-0.291752
H	0.000000	3.725001	2.043818
H	0.000000	1.304100	2.559144
C	0.000000	-1.643662	1.530235
C	0.000000	-3.002242	1.237652
C	0.000000	-3.444036	-0.082504

C	0.000000	-2.532527	-1.134573
C	0.000000	-1.179027	-0.847741
H	0.000000	-1.304100	2.559144
H	0.000000	-3.725001	2.043818
H	0.000000	-4.506301	-0.291752
H	0.000000	-2.881817	-2.160559
H	-0.880767	0.000000	-2.439214
H	0.880767	0.000000	-2.439214

fluorine S_1

C	0.000000	0.000000	-1.868667
C	0.000000	1.178727	-0.918744
C	0.000000	0.695379	0.449810
C	0.000000	-0.695379	0.449810
C	0.000000	1.635475	1.536005
C	0.000000	2.973334	1.229564
C	0.000000	3.429703	-0.106011
C	0.000000	2.519286	-1.185822
H	0.000000	2.886008	-2.205166
H	0.000000	4.493837	-0.302822
H	0.000000	3.706012	2.027474
H	0.000000	1.289421	2.561205
C	0.000000	-1.635475	1.536005
C	0.000000	-2.973334	1.229564
C	0.000000	-3.429703	-0.106011
C	0.000000	-2.519286	-1.185822
C	0.000000	-1.178727	-0.918744
H	0.000000	-1.289421	2.561205
H	0.000000	-3.706012	2.027474
H	0.000000	-4.493837	-0.302822
H	0.000000	-2.886008	-2.205166
H	-0.880085	0.000000	-2.518997
H	0.880085	0.000000	-2.518997

phenanthrene S_0

C	0.727724	0.000000	-0.349062
C	-0.727724	0.000000	-0.349062
C	-1.414694	0.000000	0.885521
C	-0.674288	0.000000	2.114809
C	0.674288	0.000000	2.114809
C	1.414694	0.000000	0.885521
C	-1.491776	0.000000	-1.532936
C	-2.823028	0.000000	0.901048
H	-1.228489	0.000000	3.046186

H	1.228489	0.000000	3.046186
C	1.491776	0.000000	-1.532936
C	2.866019	0.000000	-1.495818
C	3.542326	0.000000	-0.267772
C	2.823028	0.000000	0.901048
H	0.999092	0.000000	-2.495161
H	3.428517	0.000000	-2.420841
H	4.624491	0.000000	-0.244339
H	3.331325	0.000000	1.858456
C	-3.542326	0.000000	-0.267772
C	-2.866019	0.000000	-1.495818
H	-0.999092	0.000000	-2.495161
H	-3.428517	0.000000	-2.420841
H	-4.624491	0.000000	-0.244339
H	-3.331325	0.000000	1.858456

phenanthrene S_1

C	0.710344	0.000000	-0.388347
C	-0.710344	0.000000	-0.388347
C	-1.431911	0.000000	0.883092
C	-0.694399	0.000000	2.079910
C	0.694399	0.000000	2.079910
C	1.431911	0.000000	0.883092
C	-1.490768	0.000000	-1.570032
C	-2.836045	0.000000	0.885631
H	-1.232050	0.000000	3.020840
H	1.232050	0.000000	3.020840
C	1.490768	0.000000	-1.570032
C	2.877666	0.000000	-1.525457
C	3.563064	0.000000	-0.299379
C	2.836045	0.000000	0.885631
H	1.006799	0.000000	-2.536223
H	3.437171	0.000000	-2.452172
H	4.644126	0.000000	-0.278738
H	3.349864	0.000000	1.839914
C	-3.563064	0.000000	-0.299379
C	-2.877666	0.000000	-1.525457
H	-1.006799	0.000000	-2.536223
H	-3.437171	0.000000	-2.452172
H	-4.644126	0.000000	-0.278738
H	-3.349864	0.000000	1.839914

2,4,6,8-decatetraene S_0

C	-2.584955	-5.002335	0.000000

C	-2.464127	-3.512769	0.000000
C	-1.310516	-2.841749	0.000000
C	-1.210360	-1.394935	0.000000
C	-0.050151	-0.721087	0.000000
C	0.050151	0.721087	0.000000
C	1.210360	1.394935	0.000000
C	1.310516	2.841749	0.000000
C	2.464127	3.512769	0.000000
C	2.584955	5.002335	0.000000
H	-0.373916	-3.395720	0.000000
H	-2.144922	-0.838091	0.000000
H	0.883975	-1.278617	0.000000
H	-0.883975	1.278617	0.000000
H	2.144922	0.838091	0.000000
H	0.373916	3.395720	0.000000
H	3.393361	2.947039	0.000000
H	-3.393361	-2.947039	0.000000
H	1.603539	5.477098	0.000000
H	3.134790	5.350760	0.877959
H	3.134790	5.350760	-0.877959
H	-1.603539	-5.477098	0.000000
H	-3.134790	-5.350760	0.877959
H	-3.134790	-5.350760	-0.877959

2,4,6,8-decatetraene S_1

C	-2.572276	-5.011606	0.000000
C	-2.513884	-3.527221	0.000000
C	-1.352296	-2.804705	0.000000
C	-1.267317	-1.400403	0.000000
C	-0.052825	-0.692749	0.000000
C	0.052825	0.692749	0.000000
C	1.267317	1.400403	0.000000
C	1.352296	2.804705	0.000000
C	2.513884	3.527221	0.000000
C	2.572276	5.011606	0.000000
H	-0.412250	-3.354990	0.000000
H	-2.192357	-0.828848	0.000000
H	0.866965	-1.273841	0.000000
H	-0.866965	1.273841	0.000000
H	2.192357	0.828848	0.000000
H	0.412250	3.354990	0.000000
H	3.458773	2.989014	0.000000
H	-3.458773	-2.989014	0.000000
H	1.572654	5.447873	0.000000
H	3.111192	5.393845	0.875505

H	3.111192	5.393845	-0.875505
H	-1.572654	-5.447873	0.000000
H	-3.111192	-5.393845	0.875505
H	-3.111192	-5.393845	-0.875505

tetracene S_0

C	3.694634	1.404410	0.000000
C	2.433944	0.720705	0.000000
C	2.433944	-0.720705	0.000000
C	3.694634	-1.404410	0.000000
C	4.861350	-0.715780	0.000000
C	4.861350	0.715780	0.000000
C	1.229932	1.400020	0.000000
C	0.000000	0.719880	0.000000
C	0.000000	-0.719880	0.000000
C	1.229932	-1.400020	0.000000
C	-1.229932	1.400020	0.000000
C	-2.433944	0.720705	0.000000
C	-2.433944	-0.720705	0.000000
C	-1.229932	-1.400020	0.000000
C	-3.694634	1.404410	0.000000
C	-4.861350	0.715780	0.000000
C	-4.861350	-0.715780	0.000000
C	-3.694634	-1.404410	0.000000
H	-3.690599	-2.488189	0.000000
H	-5.806109	-1.244361	0.000000
H	-5.806109	1.244361	0.000000
H	-3.690599	2.488189	0.000000
H	-1.230040	-2.484929	0.000000
H	-1.230040	2.484929	0.000000
H	1.230040	-2.484929	0.000000
H	1.230040	2.484929	0.000000
H	3.690599	-2.488189	0.000000
H	5.806109	-1.244361	0.000000
H	5.806109	1.244361	0.000000
H	3.690599	2.488189	0.000000

tetracene S_1

C	3.693373	1.393406	0.000000
C	2.464776	0.717157	0.000000
C	2.464776	-0.717157	0.000000
C	3.693373	-1.393406	0.000000
C	4.894888	-0.696899	0.000000
C	4.894888	0.696899	0.000000

C	1.225179	1.396347	0.000000
C	0.000000	0.725031	0.000000
C	0.000000	-0.725031	0.000000
C	1.225179	-1.396347	0.000000
C	-1.225179	1.396347	0.000000
C	-2.464776	0.717157	0.000000
C	-2.464776	-0.717157	0.000000
C	-1.225179	-1.396347	0.000000
C	-3.693373	1.393406	0.000000
C	-4.894888	0.696899	0.000000
C	-4.894888	-0.696899	0.000000
C	-3.693373	-1.393406	0.000000
H	-3.693528	-2.477165	0.000000
H	-5.831498	-1.239099	0.000000
H	-5.831498	1.239099	0.000000
H	-3.693528	2.477165	0.000000
H	-1.227389	-2.481379	0.000000
H	-1.227389	2.481379	0.000000
H	1.227389	-2.481379	0.000000
H	1.227389	2.481379	0.000000
H	3.693528	-2.477165	0.000000
H	5.831498	-1.239099	0.000000
H	5.831498	1.239099	0.000000
H	3.693528	2.477165	0.000000

perylene S_0

C	0.115457	1.467257	-2.412133
C	0.038179	0.737575	-1.244392
C	0.010959	1.435762	-0.000150
C	0.034642	2.857817	-0.000149
C	0.098305	3.556880	-1.227557
C	0.146570	2.871319	-2.407612
C	-0.010561	3.558624	1.227010
C	-0.069069	2.874620	2.407548
C	-0.070016	1.470252	2.412429
C	-0.013213	0.738519	1.244688
C	-0.038179	-0.737575	-1.244392
C	-0.010959	-1.435762	-0.000150
C	0.013213	-0.738519	1.244688
C	-0.034642	-2.857817	-0.000149
C	0.010561	-3.558624	1.227010
C	0.069069	-2.874620	2.407548
C	0.070016	-1.470252	2.412429
C	-0.115457	-1.467257	-2.412133
C	-0.146570	-2.871319	-2.407612

C	-0.098305	-3.556880	-1.227557
H	0.000777	4.641838	1.210124
H	-0.112105	3.408032	3.348643
H	-0.116885	0.969642	3.368783
H	-0.000777	-4.641838	1.210124
H	0.112105	-3.408032	3.348643
H	0.116885	-0.969642	3.368783
H	-0.114420	-4.640038	-1.210905
H	-0.206340	-3.403302	-3.348607
H	-0.159528	-0.964853	-3.367718
H	0.114420	4.640038	-1.210905
H	0.206340	3.403302	-3.348607
H	0.159528	0.964853	-3.367718

perylene S_1

C	-0.006287	1.465712	-2.444722
C	-0.006683	0.718028	-1.237487
C	0.013028	1.416432	0.000001
C	0.007203	2.846547	-0.000001
C	0.009291	3.538081	-1.226442
C	-0.001093	2.846623	-2.428991
C	0.009504	3.538086	1.226433
C	-0.000649	2.846630	2.428988
C	-0.005898	1.465721	2.444725
C	-0.006587	0.718029	1.237492
C	0.006683	-0.718028	-1.237487
C	-0.013028	-1.416432	0.000001
C	0.006587	-0.718029	1.237492
C	-0.007203	-2.846547	-0.000001
C	-0.009504	-3.538086	1.226433
C	0.000649	-2.846630	2.428988
C	0.005898	-1.465721	2.444725
C	0.006287	-1.465712	-2.444722
C	0.001093	-2.846623	-2.428991
C	-0.009291	-3.538081	-1.226442
H	0.013013	4.621365	1.215871
H	-0.004062	3.392670	3.363849
H	-0.028469	0.958906	3.397291
H	-0.013013	-4.621365	1.215871
H	0.004062	-3.392670	3.363849
H	0.028469	-0.958906	3.397291
H	-0.012785	-4.621361	-1.215882
H	0.004743	-3.392658	-3.363854
H	0.029140	-0.958888	-3.397278
H	0.012785	4.621361	-1.215882

H	-0.004743	3.392658	-3.363854
H	-0.029140	0.958888	-3.397278

M06-HF/TZVP geometries – Group I

pyrazine S_0

C	1.127486	-0.695198	0.000000
C	1.127486	0.695198	0.000000
N	0.000000	1.392107	0.000000
C	-1.127486	0.695198	0.000000
C	-1.127486	-0.695198	0.000000
N	0.000000	-1.392107	0.000000
H	-2.053929	-1.250428	0.000000
H	2.053929	-1.250428	0.000000
H	2.053929	1.250428	0.000000
H	-2.053929	1.250428	0.000000

pyrazine S_1

C	-1.185347	0.656584	0.000000
C	-1.138475	-0.735169	0.000000
N	0.045667	-1.355194	0.000000
C	1.185347	-0.656584	0.000000
C	1.138475	0.735169	0.000000
N	-0.045667	1.355194	0.000000
H	2.058022	1.298798	0.000000
H	-2.140579	1.157580	0.000000
H	-2.058022	-1.298798	0.000000
H	2.140579	-1.157580	0.000000

2,6-difluoropyridine S_0

C	1.110202	0.000000	-0.871840
N	0.000000	0.000000	-1.558535
C	-1.110202	0.000000	-0.871840
C	-1.201421	0.000000	0.507674
C	0.000000	0.000000	1.200869
C	1.201421	0.000000	0.507674
F	-2.237282	0.000000	-1.588490
H	-2.163829	0.000000	0.991274
H	0.000000	0.000000	2.280850
H	2.163829	0.000000	0.991274
F	2.237282	0.000000	-1.588490

2,6-difluoropyridine S_1

C	-1.091712	0.000000	-0.337381
N	0.000000	0.000000	-1.101717
C	1.091712	0.000000	-0.337381
C	1.184885	0.000000	1.073822
C	0.000000	0.000000	1.851200
C	-1.184885	0.000000	1.073822
F	2.234066	0.000000	-1.002373
H	2.174930	0.000000	1.503288
H	0.000000	0.000000	2.925098
H	-2.174930	0.000000	1.503288
F	-2.234066	0.000000	-1.002373

2-fluoropyridine S_0

C	-1.309857	0.499947	0.000000
N	-1.359221	-0.796992	0.000000
C	-0.196411	-1.450472	0.000000
C	1.029466	-0.808421	0.000000
C	1.043389	0.583705	0.000000
C	-0.155427	1.271064	0.000000
H	-0.262311	-2.528526	0.000000
H	1.943590	-1.381243	0.000000
H	1.978039	1.125820	0.000000
H	-0.221607	2.347074	0.000000
F	-2.489660	1.138033	0.000000

2-fluoropyridine S_1

C	-1.317280	0.482677	0.000000
N	-1.435122	-0.842825	0.000000
C	-0.230846	-1.458279	0.000000
C	1.028282	-0.786393	0.000000
C	1.112842	0.622232	0.000000
C	-0.146483	1.274544	0.000000
H	-0.248036	-2.537835	0.000000
H	1.918018	-1.399425	0.000000
H	2.046093	1.156239	0.000000
H	-0.263196	2.346959	0.000000
F	-2.464281	1.142098	0.000000

2-hydroxypyridine S_0

C	-0.975687	0.751186	0.000000
C	-0.962731	-0.645014	0.000000

N	0.133336	-1.368099	0.000000
C	1.306040	-0.733350	0.000000
C	1.418797	0.643756	0.000000
C	0.243393	1.394560	0.000000
O	-2.141531	-1.298283	0.000000
H	2.182675	-1.364877	0.000000
H	2.389629	1.113479	0.000000
H	0.283319	2.474409	0.000000
H	-1.917619	1.275657	0.000000
H	-1.959620	-2.243423	0.000000

2-hydroxypyridine S_1

C	-0.986545	0.767540	0.000000
C	-0.961413	-0.643178	0.000000
N	0.129621	-1.456799	0.000000
C	1.287553	-0.775853	0.000000
C	1.388126	0.644978	0.000000
C	0.245890	1.469600	0.000000
O	-2.111290	-1.281237	0.000000
H	2.192841	-1.364536	0.000000
H	2.381227	1.071718	0.000000
H	0.300947	2.543450	0.000000
H	-1.949793	1.253454	0.000000
H	-1.917165	-2.229138	0.000000

2-pyridone S_0

C	-1.243772	0.701331	0.000000
N	-1.135171	-0.682465	0.000000
C	0.034616	-1.379434	0.000000
C	1.220460	-0.737487	0.000000
C	1.202047	0.696536	0.000000
C	0.043326	1.388730	0.000000
H	-2.018475	-1.171035	0.000000
H	-0.060459	-2.454280	0.000000
H	2.144516	-1.289624	0.000000
H	2.141903	1.230669	0.000000
H	0.005239	2.466566	0.000000
O	-2.334229	1.230503	0.000000

2-pyridone S_1

C	-1.402447	0.118803	0.000000
N	-0.725714	-1.164466	0.000000
C	0.610936	-1.252247	0.000000

C	1.403785	-0.077776	0.000000
C	0.826328	1.185387	0.000000
C	-0.597927	1.275682	0.000000
H	-1.333874	-1.969733	0.000000
H	1.048706	-2.237623	0.000000
H	2.475659	-0.205085	0.000000
H	1.434449	2.073579	0.000000
H	-1.119901	2.218540	0.000000
O	-2.620001	0.034928	0.000000

2-methylpyrimidine S_0

C	0.000076	1.961887	0.000000
C	-1.172683	1.221294	0.000000
N	-1.169707	-0.102282	0.000000
C	0.012093	-0.716181	0.000000
N	1.185937	-0.094102	0.000000
C	1.176496	1.233167	0.000000
H	-2.141944	1.701118	0.000000
H	2.142078	1.720047	0.000000
H	-0.005128	3.039897	0.000000
C	0.003620	-2.222499	0.000000
H	1.024215	-2.589927	0.000000
H	-0.527531	-2.576210	0.882195
H	-0.527531	-2.576210	-0.882195

2-methylpyrimidine S_1

C	-0.001258	2.007760	0.000000
C	-1.193958	1.296092	0.000000
N	-1.090295	-0.068343	0.000000
C	0.017740	-0.792386	0.000000
N	1.112808	-0.075679	0.000000
C	1.186870	1.293055	0.000000
H	-2.175044	1.734641	0.000000
H	2.164547	1.739551	0.000000
H	-0.003299	3.087770	0.000000
C	0.001610	-2.289765	0.000000
H	1.026074	-2.648818	0.000000
H	-0.522897	-2.641944	0.886322
H	-0.522897	-2.641944	-0.886322

5-methylpyrimidine S_0

C	0.873794	0.851131	0.000000
C	-0.357762	0.212317	0.000000

C	-0.299766	-1.176935	0.000000
N	0.842120	-1.847683	0.000000
C	1.957389	-1.129814	0.000000
N	2.025671	0.191499	0.000000
H	2.891394	-1.672383	0.000000
H	-1.207972	-1.767531	0.000000
H	0.936974	1.931936	0.000000
C	-1.669339	0.961179	0.000000
H	-1.490479	2.034249	0.000000
H	-2.251012	0.706008	-0.884518
H	-2.251012	0.706008	0.884518

5-methylpyrimidine S_1

C	0.839266	0.882943	0.000000
C	-0.375734	0.228881	0.000000
C	-0.348022	-1.175105	0.000000
N	0.872831	-1.772564	0.000000
C	2.045437	-1.178573	0.000000
N	1.993157	0.134124	0.000000
H	2.972794	-1.725304	0.000000
H	-1.226393	-1.795986	0.000000
H	0.944279	1.953595	0.000000
C	-1.686245	0.976324	0.000000
H	-1.508508	2.048938	0.000000
H	-2.261436	0.711369	-0.885928
H	-2.261436	0.711369	0.885928

7-azaindole S_0

N	-0.631108	1.836233	0.000000
C	-0.666354	0.470818	0.000000
C	0.665438	0.005274	0.000000
C	1.509771	1.170079	0.000000
C	0.679681	2.248188	0.000000
C	0.842241	-1.379115	0.000000
C	-0.289734	-2.169150	0.000000
C	-1.563004	-1.571794	0.000000
N	-1.766189	-0.268000	0.000000
H	-2.449438	-2.191270	0.000000
H	1.830666	-1.817642	0.000000
H	-0.215333	-3.245378	0.000000
H	-1.449895	2.419323	0.000000
H	2.584189	1.195969	0.000000
H	0.919089	3.296466	0.000000

7-azaindole S_1

N	-0.610148	1.872917	0.000000
C	-0.666077	0.456778	0.000000
C	0.675287	0.000458	0.000000
C	1.492413	1.130545	0.000000
C	0.640304	2.303436	0.000000
C	0.885789	-1.410970	0.000000
C	-0.302458	-2.180343	0.000000
C	-1.545215	-1.599439	0.000000
N	-1.773472	-0.213526	0.000000
H	-2.440072	-2.200655	0.000000
H	1.867877	-1.851325	0.000000
H	-0.242894	-3.258289	0.000000
H	-1.447276	2.438517	0.000000
H	2.567906	1.165395	0.000000
H	0.898045	3.346520	0.000000

7-hydroxyquinoline, *cis* S_0

N	0.455372	1.963394	0.000000
C	0.425691	0.604797	0.000000
C	-0.781707	-0.121744	0.000000
C	-1.992416	0.608963	0.000000
C	-1.946648	1.971155	0.000000
C	-0.677734	2.604210	0.000000
C	1.662807	-0.088129	0.000000
C	1.674356	-1.450928	0.000000
C	0.462263	-2.193124	0.000000
C	-0.730764	-1.542284	0.000000
H	-0.619901	3.685065	0.000000
H	-1.657322	-2.100517	0.000000
H	0.528161	-3.270474	0.000000
O	2.815101	-2.191338	0.000000
H	2.569311	0.501936	0.000000
H	-2.934861	0.077423	0.000000
H	-2.843927	2.570741	0.000000
H	3.592219	-1.629136	0.000000

7-hydroxyquinoline, *cis* S_1

N	0.482534	1.979333	0.000000
C	0.450747	0.637665	0.000000
C	-0.794141	-0.148869	0.000000
C	-1.991154	0.587208	0.000000
C	-1.919714	1.984148	0.000000

C	-0.676040	2.639802	0.000000
C	1.644581	-0.071194	0.000000
C	1.647608	-1.497579	0.000000
C	0.473773	-2.256769	0.000000
C	-0.733677	-1.561987	0.000000
H	-0.623005	3.717485	0.000000
H	-1.666192	-2.109564	0.000000
H	0.535397	-3.331671	0.000000
O	2.807498	-2.151880	0.000000
H	2.574294	0.482147	0.000000
H	-2.944969	0.080529	0.000000
H	-2.825456	2.573003	0.000000
H	3.557917	-1.551797	0.000000

7-hydroxyquinoline, *trans* S_0

N	0.506139	2.036308	0.000000
C	0.474210	0.674731	0.000000
C	-0.738353	-0.045423	0.000000
C	-1.949108	0.690145	0.000000
C	-1.897562	2.050192	0.000000
C	-0.623609	2.679077	0.000000
C	1.705895	-0.019631	0.000000
C	1.714017	-1.383088	0.000000
C	0.498944	-2.117889	0.000000
C	-0.695222	-1.461962	0.000000
H	-0.561947	3.759959	0.000000
H	-1.622917	-2.017471	0.000000
H	0.528698	-3.199760	0.000000
O	2.914741	-2.025022	0.000000
H	2.627783	0.540825	0.000000
H	-2.893094	0.161956	0.000000
H	-2.792570	2.653813	0.000000
H	2.803934	-2.976739	0.000000

7-hydroxyquinoline, *trans* S_1

N	0.526124	2.053529	0.000000
C	0.491233	0.715078	0.000000
C	-0.751712	-0.066585	0.000000
C	-1.947063	0.670137	0.000000
C	-1.873171	2.068916	0.000000
C	-0.631959	2.720373	0.000000
C	1.684793	0.000919	0.000000
C	1.683423	-1.422085	0.000000
C	0.508031	-2.183190	0.000000

C	-0.697061	-1.479858	0.000000
H	-0.573518	3.797558	0.000000
H	-1.632012	-2.023473	0.000000
H	0.539040	-3.261518	0.000000
O	2.888994	-1.988573	0.000000
H	2.629303	0.522587	0.000000
H	-2.902173	0.165827	0.000000
H	-2.778813	2.658082	0.000000
H	2.836521	-2.947702	0.000000

2-hydroxyquinoline, enol S_0

C	0.431293	1.904228	0.000000
C	0.480020	0.488863	0.000000
C	-0.715923	-0.252862	0.000000
C	-1.952966	0.436632	0.000000
C	-1.976905	1.801900	0.000000
C	-0.772273	2.548552	0.000000
C	1.697943	-0.243570	0.000000
C	1.665472	-1.598886	0.000000
C	0.387327	-2.243992	0.000000
N	-0.734057	-1.615002	0.000000
O	0.318799	-3.594212	0.000000
H	1.359217	2.460284	0.000000
H	-0.813532	3.627946	0.000000
H	-2.922389	2.324239	0.000000
H	-2.856411	-0.155397	0.000000
H	2.640629	0.286885	0.000000
H	2.573014	-2.185320	0.000000
H	1.190741	-3.990287	0.000000

2-hydroxyquinoline, enol S_1

C	0.445717	1.885478	0.000000
C	0.533764	0.492319	0.000000
C	-0.741595	-0.265830	0.000000
C	-1.971781	0.433681	0.000000
C	-2.012396	1.827034	0.000000
C	-0.802471	2.535286	0.000000
C	1.732993	-0.234797	0.000000
C	1.694324	-1.630590	0.000000
C	0.423697	-2.236572	0.000000
N	-0.750995	-1.598646	0.000000
O	0.305528	-3.561545	0.000000
H	1.352630	2.474070	0.000000
H	-0.819594	3.616431	0.000000

H	-2.952879	2.353335	0.000000
H	-2.870464	-0.165476	0.000000
H	2.675797	0.292036	0.000000
H	2.592699	-2.227845	0.000000
H	1.165016	-3.988349	0.000000

2-hydroxyquinoline, keto S_0

N	0.560440	1.704684	0.000000
C	0.598640	0.325399	0.000000
C	-0.606948	-0.382287	0.000000
C	-1.842355	0.379892	0.000000
C	-1.840092	1.717458	0.000000
C	-0.577941	2.478447	0.000000
C	1.817679	-0.361213	0.000000
C	1.820475	-1.739556	0.000000
C	0.620535	-2.460626	0.000000
C	-0.578282	-1.781416	0.000000
H	-1.515624	-2.321245	0.000000
H	0.637934	-3.539932	0.000000
H	2.763065	-2.266909	0.000000
H	2.746356	0.192863	0.000000
H	-2.776549	-0.166889	0.000000
H	-2.741079	2.310193	0.000000
O	-0.512284	3.686198	0.000000
H	1.426051	2.224958	0.000000

2-hydroxyquinoline, keto S_1

N	0.571365	1.669699	0.000000
C	0.618791	0.336570	0.000000
C	-0.668014	-0.379307	0.000000
C	-1.856233	0.361545	0.000000
C	-1.857857	1.759836	0.000000
C	-0.635514	2.472131	0.000000
C	1.845019	-0.358476	0.000000
C	1.853022	-1.738942	0.000000
C	0.623190	-2.443841	0.000000
C	-0.593786	-1.789635	0.000000
H	-1.515339	-2.353710	0.000000
H	0.641265	-3.524547	0.000000
H	2.785615	-2.280129	0.000000
H	2.766561	0.207556	0.000000
H	-2.794030	-0.174409	0.000000
H	-2.763304	2.341652	0.000000
O	-0.440564	3.671644	0.000000

H	1.419814	2.222374	0.000000

dibenzofuran S_0

C	1.721547	0.000000	-1.359186
C	0.725033	0.000000	-0.382029
C	1.099430	0.000000	0.971129
C	2.416241	0.000000	1.395372
C	3.393078	0.000000	0.403744
C	3.051117	0.000000	-0.954809
C	-0.725033	0.000000	-0.382029
C	-1.099430	0.000000	0.971129
O	0.000000	0.000000	1.799285
C	-1.721547	0.000000	-1.359186
C	-3.051117	0.000000	-0.954809
C	-3.393078	0.000000	0.403744
C	-2.416241	0.000000	1.395372
H	-2.666677	0.000000	2.448186
H	-4.437585	0.000000	0.689760
H	-3.837606	0.000000	-1.699501
H	-1.466221	0.000000	-2.412142
H	1.466221	0.000000	-2.412142
H	3.837606	0.000000	-1.699501
H	4.437585	0.000000	0.689760
H	2.666677	0.000000	2.448186

dibenzofuran S_1

C	0.000000	1.728507	-1.533998
C	0.000000	0.712933	-0.574828
C	0.000000	1.099268	0.802872
C	0.000000	2.405417	1.257844
C	0.000000	3.409831	0.271387
C	0.000000	3.066749	-1.086696
C	0.000000	-0.712933	-0.574828
C	0.000000	-1.099268	0.802872
O	0.000000	0.000000	1.585538
C	0.000000	-1.728507	-1.533998
C	0.000000	-3.066749	-1.086696
C	0.000000	-3.409831	0.271387
C	0.000000	-2.405417	1.257844
H	0.000000	-2.625072	2.314161
H	0.000000	-4.448327	0.563263
H	0.000000	-3.857232	-1.823341
H	0.000000	-1.504175	-2.589722
H	0.000000	1.504175	-2.589722

H	0.000000	3.857232	-1.823341
H	0.000000	4.448327	0.563263
H	0.000000	2.625072	2.314161

pyrrolo[3,2-*h*]quinoline S_0

C	0.140370	-0.681141	0.000000
N	0.063150	-2.026925	0.000000
C	1.183087	-2.703236	0.000000
C	2.456493	-2.096564	0.000000
C	2.536034	-0.729287	0.000000
C	1.352513	0.035976	0.000000
H	1.096759	-3.781451	0.000000
H	3.342201	-2.713911	0.000000
H	3.494072	-0.226854	0.000000
C	-1.053286	0.090159	0.000000
C	-1.056648	1.480845	0.000000
C	0.188912	2.178305	0.000000
C	1.349875	1.474660	0.000000
H	0.200858	3.258907	0.000000
H	2.302296	1.985564	0.000000
C	-2.430679	1.885091	0.000000
C	-3.175483	0.737755	0.000000
N	-2.338749	-0.345491	0.000000
H	-2.596119	-1.318351	0.000000
H	-2.812898	2.890023	0.000000
H	-4.242747	0.605925	0.000000

pyrrolo[3,2-*h*]quinoline S_1

C	0.152329	-0.709155	0.000000
N	0.031080	-2.009002	0.000000
C	1.204998	-2.737535	0.000000
C	2.435356	-2.138672	0.000000
C	2.556142	-0.730474	0.000000
C	1.371224	0.037178	0.000000
H	1.090895	-3.808762	0.000000
H	3.324141	-2.752992	0.000000
H	3.523763	-0.253412	0.000000
C	-1.029196	0.107188	0.000000
C	-1.058974	1.553395	0.000000
C	0.132538	2.233230	0.000000
C	1.330817	1.448060	0.000000
H	0.183919	3.309919	0.000000
H	2.277358	1.971155	0.000000
C	-2.467742	1.907296	0.000000

C	-3.165479	0.748577	0.000000
N	-2.282123	-0.334057	0.000000
H	-2.502779	-1.320086	0.000000
H	-2.881031	2.899633	0.000000
H	-4.227245	0.578515	0.000000

carbazole S_0

C	1.125490	0.000000	-0.893408
N	0.000000	0.000000	-1.690493
C	-1.125490	0.000000	-0.893408
C	-0.727123	0.000000	0.455179
C	0.727123	0.000000	0.455179
C	-1.692698	0.000000	1.460054
C	-3.028374	0.000000	1.104585
C	-3.408434	0.000000	-0.246079
C	-2.470603	0.000000	-1.260637
C	2.470603	0.000000	-1.260637
C	3.408434	0.000000	-0.246079
C	3.028374	0.000000	1.104585
C	1.692698	0.000000	1.460054
H	-2.769098	0.000000	-2.299559
H	-4.459225	0.000000	-0.499218
H	-3.789546	0.000000	1.870152
H	-1.399284	0.000000	2.500825
H	1.399284	0.000000	2.500825
H	3.789546	0.000000	1.870152
H	4.459225	0.000000	-0.499218
H	2.769098	0.000000	-2.299559
H	0.000000	0.000000	-2.694254

carbazole S_1

C	1.137857	0.000000	-0.836071
N	0.000000	0.000000	-1.598979
C	-1.137857	0.000000	-0.836071
C	-0.715014	0.000000	0.538980
C	0.715014	0.000000	0.538980
C	-1.702782	0.000000	1.523142
C	-3.054106	0.000000	1.116040
C	-3.440936	0.000000	-0.224423
C	-2.461764	0.000000	-1.240456
C	2.461764	0.000000	-1.240456
C	3.440936	0.000000	-0.224423
C	3.054106	0.000000	1.116040
C	1.702782	0.000000	1.523142

H	-2.731791	0.000000	-2.286859
H	-4.487641	0.000000	-0.484422
H	-3.820346	0.000000	1.878620
H	-1.449143	0.000000	2.572489
H	1.449143	0.000000	2.572489
H	3.820346	0.000000	1.878620
H	4.487641	0.000000	-0.484422
H	2.731791	0.000000	-2.286859
H	0.000000	0.000000	-2.607728

tryptamine, A-ph S_0

C	-2.133535	0.146251	0.893353
N	-1.252649	0.119945	1.951318
C	0.026431	0.038109	1.465606
C	-0.057798	0.007899	0.061297
C	-1.457620	0.078822	-0.285412
C	1.250646	-0.007419	2.140328
C	2.392315	-0.082122	1.373946
C	2.331588	-0.107438	-0.033924
C	1.122776	-0.062218	-0.692831
C	-2.030481	0.029724	-1.672921
C	-1.990869	-1.394526	-2.246282
N	-2.441768	-1.381203	-3.637778
H	1.298840	0.015492	3.219709
H	3.356495	-0.118933	1.860355
H	3.250509	-0.159624	-0.598737
H	1.081068	-0.076106	-1.773108
H	-1.505148	0.176092	2.920741
H	-3.193777	0.216510	1.068075
H	-1.465605	0.681565	-2.338349
H	-3.063474	0.380858	-1.654136
H	-2.584980	-2.044766	-1.598254
H	-0.962071	-1.748729	-2.227832
H	-3.411354	-1.105635	-3.714219
H	-2.326947	-2.280168	-4.083575

tryptamine, A-ph S_1

C	-2.182740	0.167636	0.886616
N	-1.307516	0.104164	1.891887
C	0.015063	0.056578	1.427581
C	-0.059449	0.129327	0.014945
C	-1.416004	0.183192	-0.336543
C	1.178571	-0.112452	2.133484
C	2.397029	-0.156513	1.332186

C	2.357152	-0.086181	-0.033370
C	1.136814	0.056931	-0.751445
C	-1.988381	0.091822	-1.707037
C	-1.952427	-1.377983	-2.181802
N	-2.497867	-1.464910	-3.533357
H	1.205953	-0.213568	3.206465
H	3.343597	-0.252826	1.841369
H	3.282611	-0.125328	-0.589138
H	1.124153	0.163487	-1.824352
H	-1.554394	0.110911	2.869383
H	-3.241999	0.267115	1.043945
H	-1.400311	0.683720	-2.406219
H	-3.018259	0.451213	-1.714780
H	-2.482479	-1.995812	-1.451365
H	-0.910355	-1.691586	-2.205488
H	-3.496758	-1.311510	-3.548602
H	-2.299432	-2.355049	-3.967036

tryptamine, A-py S_0

C	-2.125886	0.121553	0.864618
N	-1.257370	0.109687	1.932450
C	0.027908	0.039305	1.462291
C	-0.039354	0.000889	0.056777
C	-1.436101	0.054420	-0.306266
C	1.243929	0.009575	2.152476
C	2.396223	-0.057204	1.401466
C	2.353329	-0.090849	-0.006736
C	1.152143	-0.062043	-0.680543
C	-2.006698	0.000691	-1.695008
C	-1.939007	-1.418098	-2.277995
N	-2.483721	-1.417892	-3.636331
H	1.277937	0.038009	3.232301
H	3.354349	-0.081833	1.900457
H	3.279626	-0.137919	-0.559868
H	1.126223	-0.085138	-1.761048
H	-1.521786	0.167073	2.898635
H	-3.188955	0.181859	1.025209
H	-1.450900	0.682449	-2.341995
H	-3.047694	0.318835	-1.688860
H	-2.559989	-2.066064	-1.662456
H	-0.909233	-1.779758	-2.220599
H	-1.924012	-0.854655	-4.262048
H	-2.551050	-2.350503	-4.017818

tryptamine, A-py S_1

C	-2.179028	0.135296	0.867832
N	-1.311641	0.081855	1.879283
C	0.015480	0.054397	1.424919
C	-0.048988	0.129965	0.012515
C	-1.403301	0.164483	-0.349136
C	1.175854	-0.102948	2.139967
C	2.399721	-0.131468	1.347152
C	2.370279	-0.057653	-0.018746
C	1.154055	0.073800	-0.745805
C	-1.967763	0.066464	-1.721976
C	-1.897003	-1.401761	-2.199346
N	-2.478387	-1.505745	-3.534695
H	1.196582	-0.206476	3.212725
H	3.343611	-0.218773	1.863056
H	3.300905	-0.085559	-0.566520
H	1.149050	0.184706	-1.818156
H	-1.566349	0.082268	2.854877
H	-3.241320	0.215706	1.015365
H	-1.382722	0.687139	-2.402188
H	-3.006762	0.389403	-1.748036
H	-2.492372	-2.009153	-1.519069
H	-0.856062	-1.728820	-2.137348
H	-1.915475	-1.027162	-4.225059
H	-2.588455	-2.467586	-3.822510

tryptamine, A-up S_0

C	-2.124916	0.139114	0.880848
N	-1.253182	0.100251	1.945235
C	0.030079	0.030390	1.469490
C	-0.041641	0.020808	0.063956
C	-1.438893	0.093167	-0.293492
C	1.247854	-0.021463	2.155179
C	2.397129	-0.081776	1.399233
C	2.349691	-0.087605	-0.009266
C	1.146986	-0.036210	-0.678607
C	-2.007970	0.060499	-1.683214
C	-1.949871	-1.357573	-2.289856
N	-2.433696	-1.456780	-3.662622
H	1.285211	-0.014781	3.235201
H	3.356644	-0.123594	1.894268
H	3.273852	-0.131617	-0.566118
H	1.117975	-0.038997	-1.759237
H	-1.514354	0.136903	2.913345
H	-3.186889	0.202359	1.047531

H	-1.450537	0.745882	-2.324380
H	-3.046235	0.394492	-1.661588
H	-2.542287	-2.026188	-1.667545
H	-0.923482	-1.718766	-2.262197
H	-1.886275	-0.894423	-4.299148
H	-3.403954	-1.186179	-3.743773

tryptamine, A-up S_1

C	-2.175807	0.151358	0.877718
N	-1.306217	0.067038	1.886118
C	0.019926	0.042585	1.430515
C	-0.045084	0.152210	0.020140
C	-1.400561	0.207926	-0.339198
C	1.180322	-0.132515	2.140683
C	2.403637	-0.149598	1.347253
C	2.373102	-0.044590	-0.015971
C	1.155966	0.109219	-0.738703
C	-1.961164	0.131724	-1.712257
C	-1.935012	-1.351091	-2.193090
N	-2.441751	-1.561251	-3.537615
H	1.201201	-0.259814	3.210999
H	3.347096	-0.255260	1.860295
H	3.302437	-0.065834	-0.566205
H	1.151303	0.238884	-1.809015
H	-1.559775	0.043514	2.861720
H	-3.236910	0.235951	1.030981
H	-1.354901	0.728187	-2.393979
H	-2.987987	0.497833	-1.733166
H	-2.524327	-1.950278	-1.501106
H	-0.905701	-1.701779	-2.143502
H	-1.888306	-1.092745	-4.240628
H	-3.410266	-1.293755	-3.638768

tryptamine, Ph-out S_0

C	-0.005760	0.003631	0.066715
C	0.037600	0.053621	1.472724
C	1.242495	0.054855	2.183771
C	2.407210	0.007073	1.451312
C	2.387099	-0.043653	0.042198
C	1.198942	-0.046633	-0.654057
N	-1.256346	0.099995	1.922296
H	1.257560	0.091755	3.263808
H	3.357735	0.006934	1.964749
H	3.322902	-0.082492	-0.495543

H	1.180458	-0.108181	-1.732879
C	-1.398496	0.026483	-0.319345
C	-2.107816	0.087418	0.841385
H	-1.537618	0.150732	2.883971
H	-3.174255	0.136854	0.986088
C	-1.959083	-0.018281	-1.715529
H	-1.311733	0.547811	-2.384067
C	-2.076074	-1.452732	-2.252224
H	-2.946920	0.442820	-1.717020
H	-2.478866	-1.413573	-3.263432
N	-0.752566	-2.068068	-2.319818
H	-2.774931	-2.004633	-1.616810
H	-0.349635	-2.176723	-1.397296
H	-0.776931	-2.970902	-2.771789

tryptamine, Ph-out S_1

C	-0.001605	0.026423	0.033260
C	0.037110	0.046965	1.451390
C	1.187803	0.019418	2.195502
C	2.431591	0.002123	1.431985
C	2.427125	-0.025882	0.064972
C	1.222823	-0.029931	-0.692985
N	-1.296885	0.079933	1.878896
H	1.190052	0.029234	3.273861
H	3.366148	0.006330	1.971356
H	3.368769	-0.045326	-0.464280
H	1.231296	-0.065466	-1.770321
C	-1.349621	0.062973	-0.355485
C	-2.147141	0.082366	0.849959
H	-1.569866	0.104346	2.848769
H	-3.214296	0.127535	0.974947
C	-1.923036	-0.000090	-1.729784
H	-1.251816	0.488815	-2.433376
C	-2.101563	-1.468659	-2.179461
H	-2.892814	0.499150	-1.739852
H	-2.614613	-1.465037	-3.139666
N	-0.792916	-2.078734	-2.363935
H	-2.731575	-1.981914	-1.446312
H	-0.235492	-2.062771	-1.517165
H	-0.854487	-3.027680	-2.703063

tryptamine, Ph-up S_0

C	-2.084656	0.031084	0.805550
N	-1.247434	0.009062	1.896836

C	0.052259	0.024052	1.463896
C	0.026553	0.054470	0.056331
C	-1.359678	0.056198	-0.347360
C	1.247750	0.015720	2.190503
C	2.423078	0.041364	1.474652
C	2.422515	0.077769	0.064808
C	1.242651	0.084833	-0.644413
C	-1.900505	0.035969	-1.751016
C	-2.101352	-1.405814	-2.269498
N	-0.902287	-2.232299	-2.280908
H	1.247605	-0.010968	3.271204
H	3.366240	0.034229	2.001129
H	3.365852	0.101960	-0.460312
H	1.250613	0.115830	-1.724930
H	-1.541380	-0.002786	2.856040
H	-3.153807	0.033591	0.937559
H	-1.211352	0.564603	-2.410883
H	-2.856187	0.561235	-1.779301
H	-2.499127	-1.370281	-3.283201
H	-2.840713	-1.898317	-1.639077
H	-0.486897	-2.292684	-1.359812
H	-0.206093	-1.879188	-2.922739

tryptamine, Ph-up S_1

C	-2.150559	0.108316	0.841430
N	-1.303325	0.068292	1.870514
C	0.032051	0.050934	1.443746
C	-0.004438	0.097913	0.027400
C	-1.352137	0.129307	-0.361875
C	1.181137	-0.036981	2.187694
C	2.423617	-0.033754	1.424641
C	2.423698	0.015266	0.058098
C	1.220714	0.078120	-0.700406
C	-1.911168	0.041551	-1.734421
C	-2.040854	-1.456923	-2.164099
N	-0.787806	-2.168927	-2.292323
H	1.181212	-0.095788	3.264505
H	3.357492	-0.074451	1.963997
H	3.367379	0.015863	-0.467757
H	1.238116	0.160793	-1.775047
H	-1.577608	0.065455	2.840323
H	-3.217825	0.154475	0.966202
H	-1.254372	0.552195	-2.437744
H	-2.899042	0.504415	-1.764909
H	-2.557416	-1.488858	-3.122197

H	-2.660207	-1.970481	-1.430629
H	-0.235922	-2.150569	-1.442722
H	-0.219076	-1.816554	-3.049329

tryptamine, Py-out S_0

C	0.512748	0.465069	0.205299
C	0.578994	0.510782	1.610798
C	1.791835	0.451948	2.303932
C	2.943776	0.348503	1.555890
C	2.901903	0.306073	0.147789
C	1.703717	0.364696	-0.529296
N	-0.704871	0.618277	2.079285
H	1.823386	0.488060	3.383692
H	3.899980	0.301221	2.056697
H	3.827181	0.229315	-0.403523
H	1.679815	0.335694	-1.609714
C	-0.881723	0.556564	-0.159737
C	-1.571866	0.644508	1.010186
H	-0.968489	0.675480	3.045530
H	-2.635224	0.721491	1.163238
C	-1.455693	0.497529	-1.547102
H	-0.890757	1.157880	-2.205839
C	-1.423724	-0.934512	-2.105857
H	-2.492492	0.829168	-1.523966
H	-0.383741	-1.265119	-2.179210
N	-2.239388	-1.799457	-1.256893
H	-1.859144	-0.928918	-3.103833
H	-2.295249	-2.741062	-1.618523
H	-1.860956	-1.833191	-0.318823

tryptamine, Py-out S_1

C	0.503946	0.494692	0.173945
C	0.574734	0.502680	1.587905
C	1.739762	0.406730	2.307622
C	2.959926	0.326366	1.510536
C	2.924435	0.324695	0.143507
C	1.704119	0.405122	-0.585727
N	-0.748148	0.594584	2.046429
H	1.767923	0.402251	3.385402
H	3.906333	0.268540	2.025763
H	3.852660	0.265821	-0.405574
H	1.692885	0.424648	-1.663489
C	-0.850271	0.587521	-0.183359
C	-1.618544	0.640443	1.037784

H	-0.997027	0.622414	3.022678
H	-2.682803	0.702192	1.179320
C	-1.426423	0.520477	-1.555080
H	-0.827856	1.138335	-2.225152
C	-1.406309	-0.939174	-2.059675
H	-2.457190	0.870534	-1.549097
H	-0.366019	-1.268315	-2.115955
N	-2.228472	-1.768823	-1.182188
H	-1.842589	-0.961877	-3.056098
H	-2.376576	-2.690364	-1.568471
H	-1.798506	-1.869502	-0.271035

tryptamine, Py-up S_0

C	-2.130818	0.259734	0.874176
N	-1.260024	0.218324	1.939830
C	0.019151	0.084282	1.465581
C	-0.054217	0.037834	0.060985
C	-1.448248	0.154621	-0.298822
C	1.233904	0.003606	2.153527
C	2.379846	-0.122529	1.400179
C	2.330858	-0.166207	-0.007697
C	1.131174	-0.086334	-0.679291
C	-2.019838	0.104012	-1.685837
C	-1.981695	-1.330206	-2.263362
N	-2.734959	-2.311904	-1.495575
H	1.271171	0.040107	3.232981
H	3.337336	-0.187692	1.896632
H	3.251997	-0.261766	-0.562955
H	1.102105	-0.116959	-1.759469
H	-1.517624	0.283653	2.907146
H	-3.190057	0.369051	1.035883
H	-1.457935	0.773487	-2.339504
H	-3.055083	0.447754	-1.662845
H	-0.948334	-1.669898	-2.311244
H	-2.374414	-1.316681	-3.279221
H	-3.717664	-2.077220	-1.450929
H	-2.378110	-2.379448	-0.551280

tryptamine, Py-up S_1

C	-2.188574	0.278984	0.896853
N	-1.312448	0.215310	1.902073
C	0.004209	0.089769	1.437209
C	-0.074049	0.091397	0.022639
C	-1.428482	0.205873	-0.328154

C	1.166918	-0.056675	2.149311
C	2.382266	-0.174173	1.348572
C	2.339628	-0.166297	-0.017754
C	1.119860	-0.034457	-0.740022
C	-2.006418	0.127177	-1.696187
C	-1.949061	-1.339389	-2.214474
N	-2.685080	-2.302207	-1.412996
H	1.197732	-0.080437	3.226682
H	3.327372	-0.270266	1.860239
H	3.261819	-0.254655	-0.573100
H	1.107646	0.002758	-1.817323
H	-1.554012	0.262095	2.879403
H	-3.245146	0.408702	1.049896
H	-1.427916	0.761046	-2.370629
H	-3.042304	0.468259	-1.689446
H	-0.906497	-1.651192	-2.241206
H	-2.340086	-1.362384	-3.230050
H	-3.666288	-2.072940	-1.336814
H	-2.292570	-2.396668	-0.485808

porphycene S_0

C	-3.413519	1.867761	0.000047
C	-2.356483	0.883850	0.000012
N	-1.183131	1.541563	-0.000043
C	-1.391332	2.881472	-0.000010
C	-2.822048	3.090255	0.000026
C	-0.408330	3.864715	-0.000014
C	0.978451	3.727715	-0.000026
C	1.776054	2.584130	-0.000013
H	-0.151880	1.164188	-0.000114
N	1.359084	1.293574	0.000011
C	3.234349	2.610694	-0.000018
C	3.648464	1.324554	0.000004
C	2.440209	0.514834	0.000008
C	2.360707	-0.889714	0.000019
C	3.409025	-1.862630	0.000075
C	2.813191	-3.093811	0.000062
C	1.395780	-2.883277	-0.000011
N	1.185220	-1.548072	-0.000046
C	0.395147	-3.871706	-0.000046
C	-0.975765	-3.735694	-0.000050
C	-1.781657	-2.576208	-0.000021
C	-3.236654	-2.605965	0.000010
C	-3.652945	-1.317120	0.000039
C	-2.449421	-0.510643	0.000012

N	-1.361904	-1.300700	-0.000009
H	0.158748	-1.171501	-0.000132
H	3.291886	-4.057591	0.000098
H	4.462329	-1.643152	0.000124
H	0.775748	-4.884086	-0.000062
H	-1.537458	-4.660336	-0.000073
H	-3.837318	-3.500418	0.000011
H	-4.662198	-0.943787	0.000064
H	-4.466025	1.644226	0.000076
H	-3.298393	4.055446	0.000039
H	-0.787068	4.877432	0.000012
H	1.534789	4.655642	-0.000039
H	3.834926	3.505376	-0.000032
H	4.656326	0.947890	0.000009

porphycene S_1

C	-3.429958	1.868229	0.000045
C	-2.392145	0.886792	0.000008
N	-1.196877	1.554197	-0.000050
C	-1.408758	2.876652	-0.000013
C	-2.824377	3.096991	0.000025
C	-0.391677	3.884782	-0.000012
C	0.961782	3.744376	-0.000025
C	1.789474	2.566892	-0.000012
H	-0.181363	1.170847	-0.000120
N	1.370440	1.301903	0.000010
C	3.237214	2.609599	-0.000017
C	3.666754	1.318916	0.000008
C	2.478033	0.506643	0.000008
C	2.388737	-0.887833	0.000015
C	3.426570	-1.869300	0.000072
C	2.821026	-3.097979	0.000057
C	1.405387	-2.877620	-0.000013
N	1.193415	-1.555295	-0.000050
C	0.388385	-3.886109	-0.000044
C	-0.964987	-3.745633	-0.000049
C	-1.792705	-2.568033	-0.000023
C	-3.240345	-2.610670	0.000011
C	-3.669909	-1.319957	0.000040
C	-2.481282	-0.507722	0.000009
N	-1.373655	-1.302990	-0.000012
H	0.177141	-1.172136	-0.000133
H	3.291049	-4.066016	0.000094
H	4.480920	-1.655726	0.000121
H	0.774651	-4.895554	-0.000053

H	-1.533632	-4.666601	-0.000066
H	-3.834697	-3.509405	0.000015
H	-4.681988	-0.955051	0.000068
H	-4.484306	1.654645	0.000075
H	-3.294314	4.065063	0.000040
H	-0.777868	4.894288	0.000019
H	1.530389	4.665367	-0.000038
H	3.831553	3.508343	-0.000030
H	4.678829	0.954008	0.000015

porphine S_0

N	-0.000191	2.016498	-0.025205
N	-0.000086	-0.000001	2.087514
C	-0.000144	2.837133	1.078293
C	-0.000180	4.241636	0.662319
C	0.000011	2.439249	2.383744
C	0.000066	1.112174	2.862532
C	0.000283	0.689289	4.211807
H	-0.000135	5.084155	1.333913
H	0.000108	3.210728	3.141600
H	0.000439	1.350206	5.061409
H	-0.000256	-0.000001	1.072695
N	-0.000017	-2.016503	-0.025206
N	0.000127	-0.000001	-2.099811
C	-0.000111	-2.837132	1.078296
C	-0.000067	-2.818254	-1.076544
C	-0.000226	2.818251	-1.076541
C	-0.000218	-4.241635	0.662320
C	-0.000208	-4.233291	-0.679558
C	-0.000246	4.233289	-0.679558
C	-0.000085	-2.439248	2.383747
C	0.000060	-2.415655	-2.436185
C	-0.000080	2.415654	-2.436180
C	0.000023	-1.112174	2.862533
C	0.000139	-1.123989	-2.871768
C	0.000074	1.123989	-2.871766
C	0.000258	-0.689288	4.211808
C	0.000271	-0.672087	-4.260059
C	0.000232	0.672090	-4.260058
H	-0.000293	-5.084153	1.333914
H	-0.000266	-5.066548	-1.361994
H	-0.000265	5.066546	-1.361996
H	-0.000157	-3.210727	3.141604
H	0.000093	-3.191936	-3.186405
H	-0.000094	3.191937	-3.186399

H	0.000387	-1.350204	5.061411
H	0.000376	-1.339747	-5.104912
H	0.000297	1.339751	-5.104910
H	0.000083	-0.000002	-1.086400

porphine S_1

N	0.000000	-2.035396	0.000000
N	2.092271	0.000000	0.000000
C	1.080167	-2.846937	0.000000
C	0.671393	-4.256214	0.000000
C	2.413511	-2.436162	0.000000
C	2.869708	-1.121438	0.000000
C	4.236096	-0.682398	0.000000
H	1.347115	-5.094993	0.000000
H	3.171019	-3.206456	0.000000
H	5.084544	-1.345019	0.000000
H	1.079961	0.000000	0.000000
N	0.000000	2.035396	0.000000
N	-2.092271	0.000000	0.000000
C	1.080167	2.846937	0.000000
C	-1.080167	2.846937	0.000000
C	-1.080167	-2.846937	0.000000
C	0.671393	4.256214	0.000000
C	-0.671393	4.256214	0.000000
C	-0.671393	-4.256214	0.000000
C	2.413511	2.436162	0.000000
C	-2.413511	2.436162	0.000000
C	-2.413511	-2.436162	0.000000
C	2.869708	1.121438	0.000000
C	-2.869708	1.121438	0.000000
C	-2.869708	-1.121438	0.000000
C	4.236096	0.682398	0.000000
C	-4.236096	0.682398	0.000000
C	-4.236096	-0.682398	0.000000
H	1.347115	5.094993	0.000000
H	-1.347115	5.094993	0.000000
H	-1.347115	-5.094993	0.000000
H	3.171019	3.206456	0.000000
H	-3.171019	3.206456	0.000000
H	-3.171019	-3.206456	0.000000
H	5.084544	1.345019	0.000000
H	-5.084544	1.345019	0.000000
H	-5.084544	-1.345019	0.000000
H	-1.079961	0.000000	0.000000

chlorin S_0

C	0.000000	4.205509	0.763144
C	0.000000	2.863143	1.185260
N	0.000000	2.087387	0.057805
C	0.000000	2.862090	-1.042643
C	0.000000	4.207214	-0.620493
C	0.000000	2.385067	2.504382
C	0.000000	1.081154	2.920852
N	0.000000	-0.028836	2.103702
C	0.000000	-1.072410	2.910563
C	0.000000	-0.675231	4.314104
C	0.000000	0.673537	4.316559
C	0.000000	-2.442984	2.493667
C	0.000000	-2.868006	1.211460
N	0.000000	-2.082664	0.079541
C	0.000000	-2.841122	-1.042473
C	0.000000	-4.239179	-0.599265
C	0.000000	-4.252594	0.741622
C	0.000000	-2.421220	-2.342810
C	0.000000	-1.075733	-2.785932
C	0.000000	-0.781007	-4.283443
C	0.000000	0.755819	-4.316351
C	0.000000	1.119603	-2.831362
N	0.000000	-0.012166	-2.032111
C	0.000000	2.394776	-2.396968
H	0.884300	-1.215895	-4.744004
H	0.000000	-3.189192	-3.101436
H	0.000000	-5.076606	-1.275732
H	0.000000	-1.351354	5.152192
H	0.000000	1.344791	5.159839
H	0.884820	1.156988	-4.802775
H	0.000000	-3.196395	3.267551
H	0.000000	3.147154	3.272826
H	0.000000	3.176242	-3.144336
H	0.000000	-5.106034	1.398826
H	0.000000	5.055794	1.423240
H	0.000000	5.057457	-1.279815
H	-0.884820	1.156988	-4.802775
H	-0.884300	-1.215895	-4.744004
H	0.000000	1.075276	0.057360
H	0.000000	-1.071469	0.104362

chlorin S_1

C	0.000000	-4.230498	0.920483

C	0.000000	-2.868441	1.362366
N	0.000000	-2.087654	0.240946
C	0.000000	-2.860523	-0.881622
C	0.000000	-4.225675	-0.446711
C	0.000000	-2.411882	2.679153
C	0.000000	-1.080249	3.080030
N	0.000000	0.000000	2.268704
C	0.000000	1.080249	3.080030
C	0.000000	0.669517	4.494715
C	0.000000	-0.669517	4.494715
C	0.000000	2.411882	2.679153
C	0.000000	2.868441	1.362366
N	0.000000	2.087654	0.240946
C	0.000000	2.860523	-0.881622
C	0.000000	4.225675	-0.446711
C	0.000000	4.230498	0.920483
C	0.000000	2.412025	-2.205502
C	0.000000	1.097174	-2.643266
C	0.000000	0.768098	-4.132633
C	0.000000	-0.768098	-4.132633
C	0.000000	-1.097174	-2.643266
N	0.000000	0.000000	-1.865410
C	0.000000	-2.412025	-2.205502
H	-0.884550	1.186924	-4.607050
H	0.000000	3.183174	-2.962283
H	0.000000	5.071868	-1.112073
H	0.000000	1.346343	5.332701
H	0.000000	-1.346343	5.332701
H	-0.884550	-1.186924	-4.607050
H	0.000000	3.167360	3.450840
H	0.000000	-3.167360	3.450840
H	0.000000	-3.183174	-2.962283
H	0.000000	5.081115	1.580446
H	0.000000	-5.081115	1.580446
H	0.000000	-5.071868	-1.112073
H	0.884550	-1.186924	-4.607050
H	0.884550	1.186924	-4.607050
H	0.000000	-1.076341	0.254873
H	0.000000	1.076341	0.254873

Zn-tetraphenylporphine S_0

C	-3.856795	4.103898	1.189685
C	-3.485260	3.485269	-0.000026
C	-4.103602	3.856555	-1.189964
C	-5.085799	4.838828	-1.190292

C	-5.454334	5.454424	-0.000483
C	-4.839030	5.086135	1.189555
C	-2.425282	2.425282	0.000201
C	-1.095438	2.850630	0.004806
N	0.000000	2.049910	0.017752
C	1.095438	2.850630	0.004806
C	0.675787	4.241322	-0.020094
C	-0.675787	4.241322	-0.020094
C	2.425282	2.425282	0.000201
C	3.485260	3.485269	-0.000026
C	4.103602	3.856555	-1.189964
C	5.085799	4.838828	-1.190292
C	5.454334	5.454424	-0.000483
C	4.839030	5.086135	1.189555
C	3.856795	4.103898	1.189685
C	-2.850632	1.095439	-0.004348
N	-2.049910	0.000000	-0.017165
C	-2.850632	-1.095439	-0.004348
C	-4.241327	-0.675787	0.020391
C	-4.241327	0.675787	0.020391
C	-2.425282	-2.425282	0.000201
C	-3.485260	-3.485269	-0.000026
C	-4.103602	-3.856555	-1.189964
C	-5.085799	-4.838828	-1.190292
C	-5.454334	-5.454424	-0.000483
C	-4.839030	-5.086135	1.189555
C	-3.856795	-4.103898	1.189685
C	2.850632	1.095439	-0.004348
N	2.049910	0.000000	-0.017165
C	2.850632	-1.095439	-0.004348
C	4.241327	-0.675787	0.020391
C	4.241327	0.675787	0.020391
C	2.425282	-2.425282	0.000201
C	3.485260	-3.485269	-0.000026
C	4.103602	-3.856555	-1.189964
C	5.085799	-4.838828	-1.190292
C	5.454334	-5.454424	-0.000483
C	4.839030	-5.086135	1.189555
C	3.856795	-4.103898	1.189685
C	1.095438	-2.850630	0.004806
N	0.000000	-2.049910	0.017752
C	-1.095438	-2.850630	0.004806
C	-0.675787	-4.241322	-0.020094
C	0.675787	-4.241322	-0.020094
H	1.346670	-5.083013	-0.042989
H	5.083022	-1.346670	0.043150

H	1.346670	5.083013	-0.042989
H	-1.346670	5.083013	-0.042989
H	-1.346670	-5.083013	-0.042989
H	5.083022	1.346670	0.043150
H	-5.083022	1.346670	0.043150
H	-5.083022	-1.346670	0.043150
H	3.807976	3.371280	-2.109758
H	5.560956	5.123909	-2.117661
H	6.218412	6.218538	-0.000658
H	5.124300	5.561527	2.116745
H	3.371737	3.808476	2.109660
H	3.807976	-3.371280	-2.109758
H	5.560956	-5.123909	-2.117661
H	6.218412	-6.218538	-0.000658
H	5.124300	-5.561527	2.116745
H	3.371737	-3.808476	2.109660
H	-3.807976	-3.371280	-2.109758
H	-5.560956	-5.123909	-2.117661
H	-6.218412	-6.218538	-0.000658
H	-5.124300	-5.561527	2.116745
H	-3.371737	-3.808476	2.109660
H	-3.807976	3.371280	-2.109758
H	-5.560956	5.123909	-2.117661
H	-6.218412	6.218538	-0.000658
H	-5.124300	5.561527	2.116745
H	-3.371737	3.808476	2.109660
Zn	0.000000	0.000000	0.000382

Zn-tetraphenylporphine S_1

C	-3.691586	4.268525	1.137066
C	-3.491377	3.489164	0.000549
C	-4.281309	3.705387	-1.125556
C	-5.260389	4.690422	-1.115316
C	-5.457153	5.464499	0.021388
C	-4.671615	5.252286	1.147576
C	-2.438728	2.429103	-0.008318
C	-1.098803	2.850930	-0.003421
N	0.000000	2.044536	0.036589
C	1.098803	2.850930	-0.003421
C	0.678328	4.234460	-0.076657
C	-0.678328	4.234460	-0.076657
C	2.438728	2.429103	-0.008318
C	3.491377	3.489164	0.000549
C	4.281309	3.705387	-1.125556
C	5.260389	4.690422	-1.115316

C	5.457153	5.464499	0.021388
C	4.671615	5.252286	1.147576
C	3.691586	4.268525	1.137066
C	-2.870696	1.096768	-0.017900
N	-2.069685	0.000000	-0.062005
C	-2.870696	-1.096768	-0.017900
C	-4.262716	-0.675163	0.060424
C	-4.262716	0.675163	0.060424
C	-2.438728	-2.429103	-0.008318
C	-3.491377	-3.489164	0.000549
C	-4.281309	-3.705387	-1.125556
C	-5.260389	-4.690422	-1.115316
C	-5.457153	-5.464499	0.021388
C	-4.671615	-5.252286	1.147576
C	-3.691586	-4.268525	1.137066
C	2.870696	1.096768	-0.017900
N	2.069685	0.000000	-0.062005
C	2.870696	-1.096768	-0.017900
C	4.262716	-0.675163	0.060424
C	4.262716	0.675163	0.060424
C	2.438728	-2.429103	-0.008318
C	3.491377	-3.489164	0.000549
C	4.281309	-3.705387	-1.125556
C	5.260389	-4.690422	-1.115316
C	5.457153	-5.464499	0.021388
C	4.671615	-5.252286	1.147576
C	3.691586	-4.268525	1.137066
C	1.098803	-2.850930	-0.003421
N	0.000000	-2.044536	0.036589
C	-1.098803	-2.850930	-0.003421
C	-0.678328	-4.234460	-0.076657
C	0.678328	-4.234460	-0.076657
H	1.345920	-5.076095	-0.141518
H	5.101707	-1.345659	0.128676
H	1.345920	5.076095	-0.141518
H	-1.345920	5.076095	-0.141518
H	-1.345920	-5.076095	-0.141518
H	5.101707	1.345659	0.128676
H	-5.101707	1.345659	0.128676
H	-5.101707	-1.345659	0.128676
H	4.115834	3.102260	-2.007935
H	5.863945	4.857256	-1.995971
H	6.219224	6.230531	0.029626
H	4.825315	5.847498	2.036212
H	3.077621	4.091954	2.009708
H	4.115834	-3.102260	-2.007935

H	5.863945	-4.857256	-1.995971
H	6.219224	-6.230531	0.029626
H	4.825315	-5.847498	2.036212
H	3.077621	-4.091954	2.009708
H	-4.115834	-3.102260	-2.007935
H	-5.863945	-4.857256	-1.995971
H	-6.219224	-6.230531	0.029626
H	-4.825315	-5.847498	2.036212
H	-3.077621	-4.091954	2.009708
H	-4.115834	3.102260	-2.007935
H	-5.863945	4.857256	-1.995971
H	-6.219224	6.230531	0.029626
H	-4.825315	5.847498	2.036212
H	-3.077621	4.091954	2.009708
Zn	0.000000	0.000000	-0.011848

tetraphenylporphine S_0

C	4.229068	0.679556	0.023542
C	2.859074	1.116974	-0.000250
N	2.083481	0.000005	-0.012110
C	2.859070	-1.116968	-0.000296
C	4.229063	-0.679556	0.023515
C	2.415167	-2.434199	-0.001191
C	1.076577	-2.829993	-0.002907
N	0.000002	-2.016999	0.011808
C	-1.076574	-2.829991	-0.002847
C	-0.671456	-4.238595	-0.034589
C	0.671458	-4.238600	-0.034599
C	-2.415167	-2.434203	-0.001096
C	-2.859074	-1.116974	-0.000250
N	-2.083481	-0.000005	-0.012110
C	-2.859070	1.116968	-0.000296
C	-4.229063	0.679556	0.023515
C	-4.229068	-0.679556	0.023542
C	-2.415167	2.434199	-0.001191
C	-1.076577	2.829993	-0.002907
N	-0.000002	2.016999	0.011808
C	1.076574	2.829991	-0.002847
C	0.671456	4.238595	-0.034589
C	-0.671458	4.238600	-0.034599
C	2.415167	2.434203	-0.001096
H	-1.348221	5.075470	-0.061534
C	-3.471124	3.497866	0.000598
H	-5.072958	1.347225	0.043902
H	-1.069131	-0.000003	-0.014688

H	-1.348226	-5.075462	-0.061501
H	1.348221	-5.075470	-0.061534
H	1.348226	5.075462	-0.061501
C	-3.471123	-3.497870	0.000713
C	3.471124	-3.497866	0.000598
C	3.471123	3.497870	0.000713
H	-5.072968	-1.347216	0.043960
H	5.072958	-1.347225	0.043902
H	5.072968	1.347216	0.043960
H	1.069131	0.000003	-0.014688
C	-4.086319	-3.875423	-1.188813
C	-5.064402	-4.861868	-1.186719
C	-5.431696	-5.474506	0.004978
C	-4.819677	-5.099282	1.194599
C	-3.841758	-4.112803	1.192601
H	-3.789754	-3.393739	-2.110238
H	-5.536583	-5.153047	-2.113723
H	-6.191920	-6.242466	0.006575
H	-5.103583	-5.573159	2.122958
H	-3.357673	-3.812789	2.111617
C	-4.086297	3.875395	-1.188951
C	-5.064400	4.861822	-1.186893
C	-5.431735	5.474465	0.004787
C	-4.819733	5.099268	1.194427
C	-3.841797	4.112808	1.192465
H	-3.789702	3.393699	-2.110361
H	-5.536563	5.152980	-2.113913
H	-6.191977	6.242406	0.006355
H	-5.103669	5.573155	2.122772
H	-3.357731	3.812815	2.111498
C	4.086319	3.875423	-1.188813
C	5.064402	4.861868	-1.186719
C	5.431696	5.474506	0.004978
C	4.819677	5.099282	1.194599
C	3.841758	4.112803	1.192601
H	3.789754	3.393739	-2.110238
H	5.536583	5.153047	-2.113723
H	6.191920	6.242466	0.006575
H	5.103583	5.573159	2.122958
H	3.357673	3.812789	2.111617
C	4.086297	-3.875395	-1.188951
C	5.064400	-4.861822	-1.186893
C	5.431735	-5.474465	0.004787
C	4.819733	-5.099268	1.194427
C	3.841797	-4.112808	1.192465
H	3.789702	-3.393699	-2.110361

H	5.536563	-5.152980	-2.113913
H	6.191977	-6.242406	0.006355
H	5.103669	-5.573155	2.122772
H	3.357731	-3.812815	2.111498

tetraphenylporphine S_1

C	-0.922479	-4.192012	0.162133
C	-0.011996	-3.082845	0.064026
N	-0.767150	-1.951787	-0.017893
C	-2.092570	-2.263536	0.004044
C	-2.188384	-3.693600	0.122114
C	-3.159861	-1.362211	-0.049968
C	-3.036593	0.033757	-0.059297
N	-1.882314	0.738080	0.032464
C	-2.244395	2.041886	0.000912
C	-3.693719	2.180156	-0.140218
C	-4.187067	0.928204	-0.181888
C	-1.382989	3.149027	0.057283
C	0.011996	3.082846	0.064023
N	0.767150	1.951788	-0.017893
C	2.092570	2.263537	0.004045
C	2.188384	3.693601	0.122113
C	0.922479	4.192013	0.162130
C	3.159861	1.362212	-0.049968
C	3.036593	-0.033756	-0.059297
N	1.882314	-0.738080	0.032468
C	2.244395	-2.041885	0.000911
C	3.693718	-2.180155	-0.140227
C	4.187066	-0.928203	-0.181896
C	1.382989	-3.149026	0.057284
H	5.207769	-0.611177	-0.305006
C	4.527980	1.956965	-0.098946
H	3.118034	4.230446	0.187552
H	0.394603	1.008299	-0.048604
H	-4.221286	3.114426	-0.222191
H	-5.207771	0.611179	-0.304993
H	4.221285	-3.114425	-0.222204
C	-1.989409	4.511617	0.110124
C	-4.527980	-1.956965	-0.098946
C	1.989409	-4.511616	0.110124
H	0.613388	5.216546	0.267544
H	-3.118034	-4.230445	0.187554
H	-0.613388	-5.216545	0.267549
H	-0.394603	-1.008298	-0.048605
C	-1.845515	5.394214	-0.957880

C	-2.414500	6.660012	-0.901447
C	-3.128766	7.053014	0.223845
C	-3.275172	6.175801	1.291721
C	-2.708093	4.909819	1.235488
H	-1.295360	5.077069	-1.833460
H	-2.304709	7.336330	-1.736820
H	-3.571034	8.037675	0.268633
H	-3.826885	6.478031	2.170430
H	-2.814542	4.219660	2.060942
C	4.938787	2.670556	-1.222871
C	6.210978	3.224454	-1.274550
C	7.081079	3.070619	-0.202096
C	6.675095	2.361752	0.922072
C	5.403373	1.805852	0.973836
H	4.256559	2.778200	-2.054935
H	6.523818	3.769331	-2.153751
H	8.071124	3.501043	-0.243082
H	7.347285	2.243767	1.759651
H	5.077940	1.254324	1.845309
C	1.845520	-5.394212	-0.957881
C	2.414504	-6.660010	-0.901448
C	3.128765	-7.053014	0.223847
C	3.275167	-6.175802	1.291725
C	2.708089	-4.909819	1.235491
H	1.295368	-5.077066	-1.833463
H	2.304717	-7.336326	-1.736823
H	3.571032	-8.037675	0.268636
H	3.826876	-6.478034	2.170436
H	2.814534	-4.219662	2.060946
C	-4.938786	-2.670556	-1.222871
C	-6.210976	-3.224455	-1.274552
C	-7.081077	-3.070622	-0.202096
C	-6.675094	-2.361757	0.922072
C	-5.403373	-1.805854	0.973836
H	-4.256559	-2.778198	-2.054936
H	-6.523816	-3.769332	-2.153753
H	-8.071121	-3.501049	-0.243083
H	-7.347284	-2.243773	1.759651
H	-5.077940	-1.254327	1.845310

M06-HF/TZVP geometries – Group II

tetrafluorobenzene S_0

C	-1.186994	0.691194	0.000000

C	-1.186994	-0.691194	0.000000
C	0.000000	-1.394354	0.000000
C	1.186994	-0.691194	0.000000
C	1.186994	0.691194	0.000000
C	0.000000	1.394354	0.000000
F	-2.350057	-1.351609	0.000000
H	0.000000	-2.474113	0.000000
F	2.350057	-1.351609	0.000000
F	2.350057	1.351609	0.000000
H	0.000000	2.474113	0.000000
F	-2.350057	1.351609	0.000000

tetrafluorobenzene S_1

C	1.144987	-0.708154	0.105255
C	1.144987	0.708154	0.105255
C	0.000000	1.458485	0.400006
C	-1.144987	0.708154	0.105255
C	-1.144987	-0.708154	0.105255
C	0.000000	-1.458485	0.400006
F	2.267585	1.316119	-0.281158
H	0.000000	2.505655	0.649924
F	-2.267585	1.316119	-0.281158
F	-2.267585	-1.316119	-0.281158
H	0.000000	-2.505655	0.649924
F	2.267585	-1.316119	-0.281158

benzonitrile S_0

C	0.000000	0.000000	-1.043494
C	-1.211848	0.000000	-0.359468
C	-1.205815	0.000000	1.027150
C	0.000000	0.000000	1.717963
C	1.205815	0.000000	1.027150
C	1.211848	0.000000	-0.359468
H	-2.138965	0.000000	-0.912885
H	-2.140837	0.000000	1.567084
H	0.000000	0.000000	2.798337
H	2.140837	0.000000	1.567084
H	2.138965	0.000000	-0.912885
C	0.000000	0.000000	-2.489284
N	0.000000	0.000000	-3.627277

benzonitrile S_1

C	0.000000	0.000000	-1.089630

C	-1.219457	0.000000	-0.371095
C	-1.211706	0.000000	1.039983
C	0.000000	0.000000	1.753539
C	1.211706	0.000000	1.039983
C	1.219457	0.000000	-0.371095
H	-2.150596	0.000000	-0.901941
H	-2.146503	0.000000	1.565245
H	0.000000	0.000000	2.824748
H	2.146503	0.000000	1.565245
H	2.150596	0.000000	-0.901941
C	0.000000	0.000000	-2.510024
N	0.000000	0.000000	-3.643018

o-fluorophenol, *cis* S_0

C	0.328414	1.451261	0.000000
C	-0.868137	0.773341	0.000000
C	-0.945459	-0.610922	0.000000
C	0.237501	-1.333579	0.000000
C	1.456943	-0.670301	0.000000
C	1.508860	0.718085	0.000000
F	-2.040613	1.459556	0.000000
O	-2.136516	-1.259917	0.000000
H	0.175619	-2.411715	0.000000
H	2.371626	-1.244208	0.000000
H	2.457839	1.231069	0.000000
H	0.318931	2.531081	0.000000
H	-2.864996	-0.633770	0.000000

o-fluorophenol, *cis* S_1

C	0.321191	1.519085	0.000000
C	-0.881973	0.792425	0.000000
C	-0.941019	-0.617874	0.000000
C	0.244042	-1.408490	0.000000
C	1.458110	-0.696406	0.000000
C	1.491026	0.722884	0.000000
F	-2.067372	1.442081	0.000000
O	-2.116838	-1.237349	0.000000
H	0.166931	-2.481137	0.000000
H	2.395431	-1.230285	0.000000
H	2.453913	1.212536	0.000000
H	0.326117	2.594508	0.000000
H	-2.849546	-0.611997	0.000000

o-fluorophenol, *trans* S_0

C	0.289187	1.254050	0.000000
C	-0.943095	0.612056	0.000000
C	-0.960426	-0.775081	0.000000
C	0.229413	-1.494591	0.000000
C	1.447833	-0.834647	0.000000
C	1.474938	0.556044	0.000000
O	-2.058841	1.384697	0.000000
H	-1.910176	-1.292994	0.000000
H	0.194796	-2.573799	0.000000
H	2.372852	-1.390189	0.000000
H	2.400875	1.111768	0.000000
F	0.313649	2.598230	0.000000
H	-2.851015	0.844457	0.000000

o-fluorophenol, *trans* S_1

C	0.823196	0.999390	0.095773
C	-0.586331	0.956505	0.096890
C	-1.264115	-0.294918	0.231727
C	-0.474163	-1.401079	-0.056051
C	0.939571	-1.293512	-0.094369
C	1.610756	-0.138204	0.379289
O	-1.238269	2.083983	-0.167946
H	-2.305127	-0.353918	0.508559
H	-0.923508	-2.369480	-0.232900
H	1.511202	-2.122303	-0.494477
H	2.675348	-0.074045	0.514830
F	1.393764	2.111205	-0.409658
H	-2.162354	1.896375	-0.371668

m-fluorophenol, *cis* S_0

C	0.310641	1.401969	0.000000
C	-0.925878	0.787309	0.000000
C	-0.962567	-0.600799	0.000000
C	0.215386	-1.339587	0.000000
C	1.433367	-0.680646	0.000000
C	1.500984	0.709024	0.000000
O	-2.134841	-1.291399	0.000000
F	0.340570	2.751765	0.000000
H	0.151072	-2.416764	0.000000
H	2.347812	-1.255511	0.000000
H	2.436702	1.245021	0.000000
H	-1.822521	1.391473	0.000000
H	-2.890728	-0.701854	0.000000

m-fluorophenol, *cis* S_1

C	0.286167	1.411127	0.000000
C	-0.986880	0.832625	0.000000
C	-0.961342	-0.592470	0.000000
C	0.227839	-1.360436	0.000000
C	1.493116	-0.723018	0.000000
C	1.495918	0.693189	0.000000
O	-2.104376	-1.279289	0.000000
F	0.364145	2.752669	0.000000
H	0.119072	-2.434089	0.000000
H	2.410421	-1.284013	0.000000
H	2.414671	1.261581	0.000000
H	-1.889392	1.419968	0.000000
H	-2.869360	-0.697845	0.000000

m-fluorophenol, *trans* S_0

C	0.267838	1.298988	0.000000
C	-0.945438	0.623559	0.000000
C	-0.982042	-0.766068	0.000000
C	0.209232	-1.479875	0.000000
C	1.435016	-0.830786	0.000000
C	1.423881	0.550955	0.000000
O	-2.072285	1.386018	0.000000
H	-1.929788	-1.286346	0.000000
H	0.179231	-2.559515	0.000000
H	2.372835	-1.362877	0.000000
F	2.602909	1.207170	0.000000
H	0.299974	2.377353	0.000000
H	-2.861365	0.841432	0.000000

m-fluorophenol, *trans* S_1

C	1.087635	-0.017492	0.000000
C	0.327143	1.177857	0.000000
C	-1.095296	1.207732	0.000000
C	-1.826986	-0.004616	0.000000
C	-1.085872	-1.214713	0.000000
C	0.319356	-1.188595	0.000000
O	1.025980	2.313252	0.000000
H	-1.600245	2.163331	0.000000
H	-2.902609	-0.012925	0.000000
H	-1.574753	-2.177733	0.000000
F	0.964832	-2.368030	0.000000
H	2.162656	-0.011379	0.000000

H	0.457010	3.087458	0.000000

p-fluorophenol S_0

C	0.271360	1.312866	0.000000
C	-0.945283	0.642114	0.000000
C	-0.979116	-0.745627	0.000000
C	0.207562	-1.469232	0.000000
C	1.401748	-0.783529	0.000000
C	1.457163	0.596440	0.000000
O	-2.077476	1.404838	0.000000
H	-1.925637	-1.268774	0.000000
H	0.209958	-2.548798	0.000000
F	2.558813	-1.484491	0.000000
H	2.416371	1.091888	0.000000
H	0.269956	2.392227	0.000000
H	-2.865439	0.860068	0.000000

p-fluorophenol S_1

C	1.266010	0.676195	0.000000
C	0.025115	1.356622	0.000000
C	-1.243113	0.707167	0.000000
C	-1.251328	-0.701576	0.000000
C	-0.005271	-1.355944	0.000000
C	1.254515	-0.734052	0.000000
O	0.089784	2.685143	0.000000
H	-2.156196	1.282793	0.000000
H	-2.155974	-1.286255	0.000000
F	-0.026231	-2.690650	0.000000
H	2.148632	-1.334058	0.000000
H	2.174118	1.255407	0.000000
H	-0.783363	3.084801	0.000000

phenylacetylene S_0

C	1.207062	0.000000	-0.013745
C	0.000000	0.000000	-0.711790
C	-1.207062	0.000000	-0.013745
C	-1.203603	0.000000	1.373043
C	0.000000	0.000000	2.067734
C	1.203603	0.000000	1.373043
C	0.000000	0.000000	-2.153422
C	0.000000	0.000000	-3.349020
H	-2.135639	0.000000	-0.564706
H	-2.140126	0.000000	1.910803
H	0.000000	0.000000	3.147979

H	2.140126	0.000000	1.910803
H	2.135639	0.000000	-0.564706
H	0.000000	0.000000	-4.412289

phenylacetylene S_1

C	1.229743	0.000000	-0.028561
C	0.000000	0.000000	-0.746307
C	-1.229743	0.000000	-0.028561
C	-1.222464	0.000000	1.389718
C	0.000000	0.000000	2.098721
C	1.222464	0.000000	1.389718
C	0.000000	0.000000	-2.161832
C	0.000000	0.000000	-3.363354
H	-2.159071	0.000000	-0.575652
H	-2.158897	0.000000	1.925428
H	0.000000	0.000000	3.177426
H	2.158897	0.000000	1.925428
H	2.159071	0.000000	-0.575652
H	0.000000	0.000000	-4.426538

aniline S_0

C	0.914561	0.024085	0.000000
C	0.204724	0.036391	1.201852
C	-1.181755	0.042339	1.196407
C	-1.887729	0.046214	0.000000
C	-1.181755	0.042339	-1.196407
C	0.204724	0.036391	-1.201852
H	0.744363	0.040891	2.138832
H	-2.967095	0.051272	0.000000
H	-1.713162	0.048235	2.137243
H	-1.713162	0.048235	-2.137243
H	0.744363	0.040891	-2.138832
N	2.308290	0.056299	0.000000
H	2.761823	-0.256785	-0.840786
H	2.761823	-0.256785	0.840786

aniline S_1

C	0.898598	-0.034293	0.000000
C	0.223586	-0.008487	1.253735
C	-1.187372	0.045392	1.239641
C	-1.860262	0.071067	0.000000
C	-1.187372	0.045392	-1.239641
C	0.223586	-0.008487	-1.253735
H	0.791923	-0.030235	2.170790

H	-2.941239	0.112270	0.000000
H	-1.748011	0.066789	2.159721
H	-1.748011	0.066789	-2.159721
H	0.791923	-0.030235	-2.170790
N	2.238521	-0.085617	0.000000
H	2.752060	-0.105183	-0.864005
H	2.752060	-0.105183	0.864005

catechol S_0

C	0.472184	1.276257	0.000000
C	-0.741905	0.617133	0.000000
C	-0.791893	-0.775701	0.000000
C	0.384563	-1.501694	0.000000
C	1.608655	-0.842343	0.000000
C	1.655275	0.543352	0.000000
O	-1.963724	1.242783	0.000000
O	-1.989187	-1.414551	0.000000
H	0.319155	-2.579710	0.000000
H	2.523341	-1.415999	0.000000
H	2.602522	1.060096	0.000000
H	0.496056	2.358212	0.000000
H	-1.876160	2.197088	0.000000
H	-2.698881	-0.764922	0.000000

catechol S_1

C	0.475165	1.354839	0.000000
C	-0.748634	0.626173	0.000000
C	-0.794191	-0.784382	0.000000
C	0.389943	-1.581155	0.000000
C	1.592787	-0.862209	0.000000
C	1.634741	0.557762	0.000000
O	-1.956992	1.234610	0.000000
O	-1.976616	-1.400053	0.000000
H	0.318460	-2.653696	0.000000
H	2.532986	-1.393254	0.000000
H	2.603470	1.035687	0.000000
H	0.497873	2.431582	0.000000
H	-1.873985	2.190750	0.000000
H	-2.695009	-0.756653	0.000000

resorcinol, isomer 1 S_0

C	0.073420	1.142692	0.000000
C	-1.135296	0.459483	0.000000

C	-1.168351	-0.927598	0.000000
C	0.034294	-1.626015	0.000000
C	1.250241	-0.966486	0.000000
C	1.258611	0.424448	0.000000
O	-2.266248	1.220661	0.000000
H	-2.111578	-1.455266	0.000000
H	0.016799	-2.706284	0.000000
H	2.189431	-1.496461	0.000000
O	2.472941	1.041455	0.000000
H	0.059804	2.223699	0.000000
H	-3.051344	0.670436	0.000000
H	2.377276	1.995225	0.000000

resorcinol, isomer 1 S_1

C	0.074135	1.222807	0.000000
C	-1.124495	0.483224	0.000000
C	-1.165639	-0.935594	0.000000
C	0.026482	-1.699169	0.000000
C	1.245439	-0.974437	0.000000
C	1.252072	0.438870	0.000000
O	-2.262643	1.198344	0.000000
H	-2.130983	-1.424582	0.000000
H	0.008714	-2.774300	0.000000
H	2.203790	-1.471429	0.000000
O	2.462696	1.023744	0.000000
H	0.064314	2.299195	0.000000
H	-3.038483	0.632868	0.000000
H	2.384599	1.980448	0.000000

resorcinol, isomer 2 S_0

C	1.195051	0.000000	-0.541042
C	0.000000	0.000000	-1.241395
C	-1.195051	0.000000	-0.541042
C	-1.208412	0.000000	0.850427
C	0.000000	0.000000	1.530774
C	1.208412	0.000000	0.850427
O	-2.340571	0.000000	-1.278260
O	2.340571	0.000000	-1.278260
H	-2.144061	0.000000	1.391553
H	0.000000	0.000000	2.611121
H	2.144061	0.000000	1.391553
H	0.000000	0.000000	-2.320189
H	-3.114748	0.000000	-0.713072
H	3.114748	0.000000	-0.713072

resorcinol, isomer 2 S_1

C	1.190010	0.000000	-0.329410
C	0.000000	0.000000	-1.082744
C	-1.190010	0.000000	-0.329410
C	-1.208955	0.000000	1.089763
C	0.000000	0.000000	1.829997
C	1.208955	0.000000	1.089763
O	-2.339786	0.000000	-1.027722
O	2.339786	0.000000	-1.027722
H	-2.162232	0.000000	1.601075
H	0.000000	0.000000	2.905537
H	2.162232	0.000000	1.601075
H	0.000000	0.000000	-2.157442
H	-3.106631	0.000000	-0.450922
H	3.106631	0.000000	-0.450922

resorcinol, isomer 3 S_0

C	1.199400	0.000000	-0.285380
C	0.000000	0.000000	-0.987531
C	-1.199400	0.000000	-0.285380
C	-1.209989	0.000000	1.101546
C	0.000000	0.000000	1.779426
C	1.209989	0.000000	1.101546
O	-2.404353	0.000000	-0.923136
O	2.404353	0.000000	-0.923136
H	-2.156599	0.000000	1.618091
H	0.000000	0.000000	2.859851
H	2.156599	0.000000	1.618091
H	0.000000	0.000000	-2.070779
H	2.297444	0.000000	-1.875365
H	-2.297444	0.000000	-1.875365

resorcinol, isomer 3 S_1

C	-0.034229	-0.310281	1.161268
C	-0.320141	-1.039916	0.000000
C	-0.034229	-0.310281	-1.161268
C	0.139227	1.091108	-1.113842
C	-0.361725	1.842099	0.000000
C	0.139227	1.091108	1.113842
O	0.129883	-0.902445	-2.355812
O	0.129883	-0.902445	2.355812
H	0.697982	1.560715	-1.913780

H	-0.331707	2.917381	0.000000
H	0.697982	1.560715	1.913780
H	-0.650956	-2.067307	0.000000
H	0.169897	-1.857698	2.263527
H	0.169897	-1.857698	-2.263527

hydroquinone, *cis* S_0

C	-0.696067	0.000000	1.090964
C	0.696067	0.000000	1.090964
C	1.389431	0.000000	-0.107292
C	0.691231	0.000000	-1.309307
C	-0.691231	0.000000	-1.309307
C	-1.389431	0.000000	-0.107292
O	2.756362	0.000000	-0.173859
O	-2.756362	0.000000	-0.173859
H	1.249356	0.000000	-2.233467
H	-1.249356	0.000000	-2.233467
H	-1.229821	0.000000	2.031861
H	1.229821	0.000000	2.031861
H	-3.145082	0.000000	0.701390
H	3.145082	0.000000	0.701390

hydroquinone, *cis* S_1

C	0.703387	0.000000	-1.136950
C	-0.703387	0.000000	-1.136950
C	-1.369521	0.000000	0.118964
C	-0.703904	0.000000	1.362472
C	0.703904	0.000000	1.362472
C	1.369521	0.000000	0.118964
O	-2.703961	0.000000	0.163166
O	2.703961	0.000000	0.163166
H	-1.290452	0.000000	2.265670
H	1.290452	0.000000	2.265670
H	1.269924	0.000000	-2.055619
H	-1.269924	0.000000	-2.055619
H	3.086484	0.000000	-0.716932
H	-3.086484	0.000000	-0.716932

hydroquinone, *trans* S_0

C	0.019271	1.386852	0.000000
C	-1.192066	0.713835	0.000000
C	-1.209658	-0.674625	0.000000
C	-0.019271	-1.386852	0.000000

C	1.192066	-0.713835	0.000000
C	1.209658	0.674625	0.000000
O	-2.334010	1.468244	0.000000
H	-2.151341	-1.207332	0.000000
H	-0.015943	-2.466365	0.000000
O	2.334010	-1.468244	0.000000
H	2.151341	1.207332	0.000000
H	0.015943	2.466365	0.000000
H	-3.114364	0.913001	0.000000
H	3.114364	-0.913001	0.000000

hydroquinone, *trans* S_1

C	1.261307	0.672896	0.000000
C	0.031988	1.368576	0.000000
C	-1.237695	0.734064	0.000000
C	-1.261307	-0.672896	0.000000
C	-0.031988	-1.368576	0.000000
C	1.237695	-0.734064	0.000000
O	0.115093	2.701013	0.000000
H	-2.145092	1.318682	0.000000
H	-2.175573	-1.242350	0.000000
O	-0.115093	-2.701013	0.000000
H	2.145092	-1.318682	0.000000
H	2.175573	1.242350	0.000000
H	-0.754990	3.106706	0.000000
H	0.754990	-3.106706	0.000000

salicylic acid S_0

C	1.100808	1.596628	0.000000
C	1.129177	0.199573	0.000000
C	-0.082945	-0.503363	0.000000
C	-1.300259	0.185631	0.000000
C	-1.318819	1.562782	0.000000
C	-0.106953	2.261105	0.000000
O	2.322460	-0.404743	0.000000
C	-0.043117	-1.975601	0.000000
O	-1.231811	-2.573351	0.000000
O	0.977760	-2.625692	0.000000
H	-2.218682	-0.382390	0.000000
H	2.043747	2.121724	0.000000
H	-2.256284	2.096349	0.000000
H	-0.114136	3.342098	0.000000
H	2.195372	-1.372126	0.000000
H	-1.096318	-3.528625	0.000000

salicylic acid S_1

C	1.013546	1.921051	0.000000
C	0.978798	0.516927	0.000000
C	-0.313935	-0.224543	0.000000
C	-1.476289	0.540282	0.000000
C	-1.402176	1.948848	0.000000
C	-0.179336	2.647041	0.000000
O	2.053489	-0.185720	0.000000
C	-0.239731	-1.634989	0.000000
O	-1.390687	-2.317851	0.000000
O	0.852170	-2.269869	0.000000
H	-2.437291	0.049144	0.000000
H	1.983914	2.394475	0.000000
H	-2.326201	2.509044	0.000000
H	-0.168271	3.725169	0.000000
H	1.744497	-1.223679	0.000000
H	-1.181919	-3.258385	0.000000

o-cresol, *cis* S_0

C	1.962167	0.513364	0.000000
C	0.729919	1.150781	0.000000
C	-0.461612	0.432774	0.000000
C	-0.386812	-0.959491	0.000000
C	0.837226	-1.612360	0.000000
C	2.010639	-0.875197	0.000000
C	-1.807483	1.126567	0.000000
O	-1.506506	-1.740882	0.000000
H	0.843980	-2.692077	0.000000
H	2.961433	-1.387149	0.000000
H	2.872912	1.093308	0.000000
H	0.684990	2.231619	0.000000
H	-2.304452	-1.210173	0.000000
H	-2.384419	0.862287	0.888635
H	-1.667560	2.204351	0.000000
H	-2.384419	0.862287	-0.888635

o-cresol, *cis* S_1

C	1.957979	0.504525	0.000000
C	0.722711	1.193722	0.000000
C	-0.487945	0.456384	0.000000
C	-0.377863	-0.965361	0.000000
C	0.854973	-1.670611	0.000000

C	2.041502	-0.908899	0.000000
C	-1.835904	1.129496	0.000000
O	-1.478533	-1.721399	0.000000
H	0.835799	-2.747135	0.000000
H	3.006746	-1.389081	0.000000
H	2.873611	1.079125	0.000000
H	0.703470	2.272182	0.000000
H	-2.278957	-1.189524	0.000000
H	-2.420826	0.874610	0.889771
H	-1.695935	2.207365	0.000000
H	-2.420826	0.874610	-0.889771

o-cresol, *trans* S_0

C	2.421866	0.000038	0.030735
C	1.248909	-0.000036	-0.711654
C	0.038599	-0.000023	-0.019217
C	0.002108	0.000038	1.366930
C	1.190380	0.000103	2.087935
C	2.405269	0.000088	1.421525
C	1.242207	-0.000117	-2.222465
O	-1.100314	-0.000036	-0.775268
H	-0.948868	0.000067	1.884088
H	1.158279	0.000151	3.167241
H	3.332176	0.000151	1.975820
H	3.367385	0.000029	-0.494649
H	-1.882737	-0.000024	-0.222024
H	2.262875	-0.000095	-2.598104
H	0.720329	-0.880227	-2.595403
H	0.720244	0.879890	-2.595519

o-cresol, *trans* S_1

C	2.468043	-0.000105	0.003878
C	1.258198	-0.000095	-0.741876
C	0.039891	-0.000113	-0.019562
C	-0.049725	0.000268	1.408010
C	1.166805	0.000069	2.115198
C	2.398331	0.000144	1.413080
C	1.239917	-0.000088	-2.244606
O	-1.079401	-0.000289	-0.751231
H	-1.009002	0.000095	1.901616
H	1.171887	0.000070	3.193865
H	3.315201	0.000278	1.986155
H	3.419190	-0.000094	-0.502653
H	-1.860369	0.000122	-0.191939

H	2.260368	0.000027	-2.619911
H	0.719786	-0.880927	-2.625027
H	0.719586	0.880634	-2.625026

m-cresol, *cis* S_0

C	1.158209	-0.009297	2.080129
C	2.369359	-0.003194	1.409697
C	2.414843	0.010608	0.019479
C	1.237388	0.016256	-0.717245
C	0.018306	0.012247	-0.043192
C	-0.019539	-0.001453	1.343167
C	1.262063	0.000991	-2.232014
O	-1.193550	-0.004759	2.039241
H	1.100080	-0.017706	3.157487
H	3.289250	-0.006696	1.976930
H	3.367318	0.017404	-0.491503
H	-0.906322	0.020548	-0.608819
H	-1.947005	0.003973	1.447261
H	2.235797	0.316792	-2.599435
H	1.063178	-1.006499	-2.597712
H	0.502926	0.670155	-2.633521

m-cresol, *cis* S_1

C	1.167115	0.009593	2.128469
C	2.412882	0.063543	1.452907
C	2.411888	0.040750	0.034009
C	1.219368	0.003465	-0.743906
C	-0.030678	0.001888	-0.072560
C	-0.022230	-0.013493	1.354465
C	1.263999	-0.009653	-2.247788
O	-1.168203	-0.059801	2.024981
H	1.077197	-0.035438	3.209374
H	3.348078	0.095857	2.002382
H	3.364786	0.052827	-0.494897
H	-0.971877	0.035885	-0.618335
H	-1.913563	-0.127242	1.418555
H	2.297929	0.012549	-2.610179
H	0.769992	-0.914405	-2.636351
H	0.725619	0.863047	-2.651176

m-cresol, *trans* S_0

C	-1.193136	-1.100141	0.000000
C	0.194601	-1.208803	0.000000

C	0.964801	-0.052196	0.000000
C	0.360369	1.195763	0.000000
C	-1.025212	1.306714	0.000000
C	-1.793532	0.151353	0.000000
C	0.877388	-2.562070	0.000000
O	1.180652	2.286560	0.000000
H	-1.497288	2.279947	0.000000
H	-2.871207	0.232153	0.000000
H	-1.802758	-1.992347	0.000000
H	2.045150	-0.100697	0.000000
H	0.673311	3.099921	0.000000
H	0.140616	-3.361990	0.000000
H	1.505665	-2.662822	-0.884348
H	1.505665	-2.662822	0.884348

m-cresol, *trans* S_1

C	-1.203000	-1.057300	0.000000
C	0.203986	-1.230391	0.000000
C	1.024177	-0.078296	0.000000
C	0.395340	1.188623	0.000000
C	-1.015579	1.370013	0.000000
C	-1.827647	0.216337	0.000000
C	0.832885	-2.594744	0.000000
O	1.207184	2.248268	0.000000
H	-1.435098	2.364915	0.000000
H	-2.902157	0.293556	0.000000
H	-1.827636	-1.940816	0.000000
H	2.101263	-0.127425	0.000000
H	0.714041	3.072663	0.000000
H	0.075640	-3.376033	0.000000
H	1.466541	-2.717178	-0.882277
H	1.466541	-2.717178	0.882277

p-cresol S_0

C	0.713916	0.025152	-1.185945
C	-0.669967	0.025560	-1.194536
C	-1.364018	0.000021	0.009464
C	-0.669599	-0.026592	1.208428
C	0.721931	-0.026348	1.198116
C	1.434937	0.000568	0.008051
O	-2.728523	-0.000194	-0.052371
C	2.950754	0.020132	-0.007309
H	-1.204959	-0.049234	2.148653
H	1.253310	-0.048736	2.139622

H	1.247498	0.043479	-2.127146
H	-1.231318	0.043186	-2.116699
H	-3.112911	-0.020020	0.824835
H	3.332656	-0.723116	-0.705748
H	3.312917	1.000930	-0.314832
H	3.344938	-0.199413	0.982716

p-cresol S_1

C	0.723583	-0.563234	-1.211302
C	-0.554310	0.054567	-1.171513
C	-1.305432	0.008375	0.022400
C	-0.698846	-0.308758	1.265444
C	0.689439	-0.238398	1.244319
C	1.390821	-0.207963	0.020501
O	-2.598335	0.338061	-0.056104
C	2.829289	0.235370	-0.052814
H	-1.273785	-0.474904	2.162611
H	1.254673	-0.212840	2.167073
H	1.283153	-0.602421	-2.131572
H	-0.974900	0.582267	-2.016888
H	-2.987559	0.415017	0.820052
H	3.395542	-0.477739	-0.654915
H	2.892764	1.213126	-0.533718
H	3.265453	0.304854	0.941718

o-methoxyphenol S_0

C	2.021841	-0.083708	0.000000
C	0.866027	0.698937	0.000000
C	-0.372173	0.083852	0.000000
C	-0.465920	-1.313008	0.000000
C	0.679854	-2.081063	0.000000
C	1.928292	-1.463840	0.000000
O	-1.578582	0.723037	0.000000
O	-1.687103	-1.902922	0.000000
H	0.575028	-3.155982	0.000000
H	2.823106	-2.068834	0.000000
H	2.986991	0.399095	0.000000
H	0.947450	1.775233	0.000000
C	-1.577323	2.139230	0.000000
H	-2.364138	-1.218731	0.000000
H	-2.620402	2.437968	0.000000
H	-1.081474	2.515369	0.895437
H	-1.081474	2.515369	-0.895437

o-methoxyphenol S_1

C	2.438007	0.136992	0.051997
C	1.410532	-0.408798	-0.741295
C	0.137410	-0.187501	-0.106392
C	0.027545	-0.187563	1.308387
C	1.181136	-0.194998	2.129105
C	2.357659	0.143296	1.469000
O	-0.968381	0.301525	-0.723743
O	-1.170072	-0.013302	1.866603
H	1.093467	-0.318021	3.194996
H	3.238607	0.422570	2.032309
H	3.324287	0.552247	-0.412741
H	1.523133	-0.628359	-1.787451
C	-1.070183	0.111647	-2.129694
H	-1.840541	0.059225	1.174208
H	-2.062793	0.451574	-2.403879
H	-0.313177	0.705180	-2.638767
H	-0.948076	-0.945726	-2.364563

m-methoxyphenol, isomer 1 S_0

C	0.928341	1.449182	0.000000
C	-0.260395	0.723156	0.000000
C	-0.236281	-0.667501	0.000000
C	0.993486	-1.322675	0.000000
C	2.183144	-0.616442	0.000000
C	2.134515	0.772797	0.000000
H	-1.148400	-1.246224	0.000000
O	1.070381	-2.684852	0.000000
H	3.115569	-1.158368	0.000000
H	3.057499	1.334462	0.000000
H	0.874252	2.526753	0.000000
O	-1.407861	1.446560	0.000000
H	0.199791	-3.083812	0.000000
C	-2.637737	0.749610	0.000000
H	-3.409511	1.512104	0.000000
H	-2.728396	0.132625	-0.895862
H	-2.728396	0.132625	0.895862

m-methoxyphenol, isomer 1 S_1

C	1.209360	0.030074	-0.542021
C	-0.025979	-0.101586	0.140111
C	-0.043058	-0.325841	1.524334
C	1.194838	-0.038528	2.111887

C	2.361894	0.086244	1.325517
C	2.415369	-0.510187	0.021904
H	-0.917744	-0.584442	2.097413
O	1.326784	0.181004	3.431832
H	3.184198	0.667802	1.723030
H	3.332045	-0.515993	-0.541613
H	1.214242	0.569672	-1.480323
O	-1.124680	0.050825	-0.603886
H	0.468307	0.242017	3.857341
C	-2.384766	0.059052	0.050618
H	-3.117115	0.253812	-0.724885
H	-2.576607	-0.911188	0.507940
H	-2.408779	0.847263	0.803540

m-methoxyphenol, isomer 2 S_0

C	0.342612	2.157583	0.000000
C	-0.840631	1.448411	0.000000
C	-0.799877	0.051960	0.000000
C	0.415259	-0.616306	0.000000
C	1.595032	0.123811	0.000000
C	1.575191	1.507656	0.000000
O	-1.997546	-0.581075	0.000000
C	-2.002198	-1.996145	0.000000
O	2.755764	-0.593165	0.000000
H	0.496191	-1.691340	0.000000
H	2.496994	2.072476	0.000000
H	0.315173	3.237763	0.000000
H	-1.801807	1.937452	0.000000
H	-3.047532	-2.286990	0.000000
H	-1.510201	-2.380196	-0.894629
H	-1.510201	-2.380196	0.894629
H	3.517766	-0.011689	0.000000

m-methoxyphenol, isomer 2 S_1

C	0.348951	2.227701	0.000000
C	-0.832789	1.441545	0.000000
C	-0.781155	0.026904	0.000001
C	0.439800	-0.698230	0.000001
C	1.598089	0.104824	0.000000
C	1.574811	1.522818	0.000000
O	-1.974479	-0.577839	0.000001
C	-2.027724	-1.996512	0.000000
O	2.771196	-0.554886	0.000000
H	0.527739	-1.768354	0.000001

H	2.516818	2.055641	0.000000
H	0.313150	3.302433	-0.000001
H	-1.814288	1.890977	0.000000
H	-3.082897	-2.247072	0.000000
H	-1.547095	-2.389477	-0.895144
H	-1.547094	-2.389479	0.895142
H	3.516956	0.049016	0.000000

p-methoxyphenol, *cis* S_0

C	-0.321411	0.734926	0.000000
C	-1.550299	0.074065	0.000000
C	-1.605427	-1.303686	0.000000
C	-0.427843	-2.047878	0.000000
C	0.791371	-1.399333	0.000000
C	0.850826	-0.004617	0.000000
O	-0.547061	-3.411218	0.000000
O	-0.369153	2.096085	0.000000
C	0.859731	2.792963	0.000000
H	1.817285	0.473157	0.000000
H	-2.451733	0.669145	0.000000
H	-2.549694	-1.826914	0.000000
H	1.712133	-1.967898	0.000000
H	0.603901	3.847490	0.000000
H	1.436893	2.552509	0.894574
H	1.436893	2.552509	-0.894574
H	0.313589	-3.831284	0.000000

p-methoxyphenol, *cis* S_1

C	1.319260	-0.052423	-0.618871
C	0.050133	-0.154133	0.013164
C	-0.009998	0.078640	1.395981
C	1.189371	0.001503	2.124588
C	2.461247	-0.179053	1.503260
C	2.532651	0.041699	0.116720
O	1.103860	0.106879	3.454624
O	1.288368	-0.050879	-1.946308
C	2.496912	0.052257	-2.688327
H	3.483085	0.151486	-0.377364
H	-0.824665	-0.255090	-0.606705
H	-0.929771	0.277913	1.921363
H	3.336597	-0.403035	2.094856
H	2.198120	0.025071	-3.730234
H	2.993538	0.994147	-2.462024
H	3.146884	-0.791325	-2.459919

H	1.977939	0.156327	3.852196

p-methoxyphenol, *trans* S_0

C	-0.655224	1.306281	0.000000
C	-1.884792	0.673225	0.000000
C	-1.952272	-0.716555	0.000000
C	-0.785141	-1.457564	0.000000
C	0.453196	-0.824392	0.000000
C	0.521708	0.563864	0.000000
O	-3.139967	-1.397071	0.000000
H	1.346792	-1.429362	0.000000
O	1.683957	1.274224	0.000000
H	-0.581897	2.383781	0.000000
H	-2.792291	1.263348	0.000000
H	-3.882715	-0.792005	0.000000
H	-0.854824	-2.535253	0.000000
C	2.895576	0.546618	0.000000
H	3.687316	1.288546	0.000000
H	2.970283	-0.073851	0.894969
H	2.970283	-0.073851	-0.894969

p-methoxyphenol, *trans* S_1

C	0.106818	0.053738	-1.385488
C	-1.266538	-0.185978	-1.209914
C	-1.770269	0.013454	0.102067
C	-0.934503	0.145099	1.231760
C	0.445466	-0.074454	1.080399
C	0.953560	0.009843	-0.246655
O	-3.086824	0.095818	0.321317
H	1.094333	-0.141578	1.936001
O	2.253512	0.065097	-0.513510
H	0.569521	0.146129	-2.354794
H	-1.925446	-0.424076	-2.030737
H	-3.570676	0.117267	-0.509307
H	-1.388745	0.370276	2.183466
C	3.200375	-0.021567	0.544152
H	4.171499	0.026301	0.065022
H	3.075661	0.816867	1.227736
H	3.083045	-0.967927	1.069183

1-naphthol, *cis* S_0

C	0.829069	1.507680	-0.008087
C	0.520578	0.114493	-0.021455

C	-0.838013	-0.269189	0.004086
C	-1.853672	0.722766	-0.010675
C	-1.517723	2.042833	-0.042709
C	-0.160594	2.443224	-0.033763
C	1.524041	-0.889651	-0.073947
C	1.184818	-2.210759	-0.053687
C	-0.175565	-2.599732	0.008569
C	-1.157289	-1.653683	0.028390
O	2.127665	1.935659	-0.007230
H	-2.199402	-1.942484	0.058875
H	-0.429811	-3.650023	0.027194
H	1.954190	-2.967716	-0.100642
H	2.565679	-0.615780	-0.164979
H	-2.889171	0.411853	-0.000049
H	-2.286515	2.801558	-0.061954
H	0.114549	3.487694	-0.030976
H	2.687177	1.331267	0.483036

1-naphthol, *cis* S_1

C	0.872081	1.459243	0.023968
C	0.540929	0.087808	-0.069471
C	-0.854694	-0.247439	0.029434
C	-1.793236	0.792888	-0.015889
C	-1.417034	2.172199	-0.049647
C	-0.102789	2.510531	-0.058516
C	1.492736	-0.926508	-0.176476
C	1.091476	-2.298735	-0.087208
C	-0.229006	-2.620405	0.046315
C	-1.218654	-1.598945	0.088442
O	2.133377	1.849459	0.202428
H	-2.260622	-1.860552	0.194570
H	-0.535653	-3.653298	0.116753
H	1.844974	-3.070397	-0.133558
H	2.527184	-0.704639	-0.399701
H	-2.844324	0.540144	-0.024440
H	-2.183745	2.930409	-0.096436
H	0.251199	3.529570	-0.070342
H	2.685801	1.108657	0.479754

1-naphthol, *trans* S_0

C	-0.713324	-0.538763	0.000000
C	-0.673600	-1.957912	0.000000
C	0.518808	-2.621590	0.000000
C	1.738982	-1.901758	0.000000

C	1.734998	-0.536864	0.000000
C	0.505080	0.168101	0.000000
H	-1.607047	-2.503994	0.000000
H	0.537612	-3.701818	0.000000
H	2.675318	-2.440158	0.000000
H	2.655106	0.027110	0.000000
C	-1.943395	0.175050	0.000000
C	-1.939606	1.536306	0.000000
C	-0.721233	2.261074	0.000000
C	0.467665	1.592475	0.000000
H	-2.871628	-0.378198	0.000000
H	-2.870754	2.083873	0.000000
H	-0.739275	3.342679	0.000000
O	1.676431	2.220855	0.000000
H	1.569873	3.173520	0.000000

1-naphthol, *trans* S_1

C	-0.951482	-0.397287	0.000000
C	-1.304179	-1.749013	0.000000
C	-0.311121	-2.773351	0.000000
C	1.010835	-2.424761	0.000000
C	1.408137	-1.052726	0.000000
C	0.446852	-0.040985	0.000000
H	-2.350801	-2.016951	0.000000
H	-0.611591	-3.809612	0.000000
H	1.778240	-3.184941	0.000000
H	2.454886	-0.793221	0.000000
C	-1.897085	0.639121	0.000000
C	-1.516309	2.015521	0.000000
C	-0.204454	2.372269	0.000000
C	0.783451	1.324376	0.000000
H	-2.948512	0.389282	0.000000
H	-2.287396	2.771564	0.000000
H	0.108563	3.406921	0.000000
O	2.087965	1.636576	0.000000
H	2.228323	2.586291	0.000000

2-naphthol, *cis* S_0

C	0.597143	2.010257	0.000000
C	0.614914	0.591980	0.000000
C	-0.604574	-0.115649	0.000000
C	-1.821526	0.615380	0.000000
C	-1.811837	1.980030	0.000000
C	-0.585738	2.690893	0.000000

C	1.832483	-0.143794	0.000000
C	1.829486	-1.503249	0.000000
C	0.596843	-2.206914	0.000000
C	-0.589746	-1.536461	0.000000
H	-1.530513	-2.073258	0.000000
H	1.539517	2.541958	0.000000
H	-0.595416	3.771094	0.000000
H	-2.743262	2.527068	0.000000
H	-2.757982	0.073594	0.000000
H	2.769910	0.396345	0.000000
H	2.742125	-2.079748	0.000000
O	0.693018	-3.566235	0.000000
H	-0.174856	-3.973281	0.000000

2-naphthol, *cis* S_1

C	0.606443	1.985131	0.000000
C	0.652771	0.584512	0.000000
C	-0.638830	-0.118931	0.000000
C	-1.840265	0.608633	0.000000
C	-1.846268	2.011369	0.000000
C	-0.618753	2.675653	0.000000
C	1.854219	-0.148011	0.000000
C	1.880712	-1.547347	0.000000
C	0.650508	-2.204377	0.000000
C	-0.593291	-1.515179	0.000000
H	-1.512661	-2.088115	0.000000
H	1.531024	2.545711	0.000000
H	-0.598723	3.757042	0.000000
H	-2.772274	2.561888	0.000000
H	-2.773815	0.061895	0.000000
H	2.785517	0.401879	0.000000
H	2.791745	-2.120356	0.000000
O	0.664588	-3.542672	0.000000
H	-0.222637	-3.908715	0.000000

2-naphthol, *trans* S_0

C	0.509827	2.012916	0.000000
C	0.533768	0.592678	0.000000
C	-0.683182	-0.122464	0.000000
C	-1.904782	0.605238	0.000000
C	-1.900152	1.968416	0.000000
C	-0.675514	2.686227	0.000000
C	1.750736	-0.135642	0.000000
C	1.751568	-1.498544	0.000000

C	0.522917	-2.207810	0.000000
C	-0.664585	-1.538909	0.000000
H	-1.588117	-2.100383	0.000000
H	1.449567	2.549293	0.000000
H	-0.691136	3.766399	0.000000
H	-2.833490	2.512235	0.000000
H	-2.837729	0.057806	0.000000
H	2.687409	0.405763	0.000000
H	2.685011	-2.045866	0.000000
O	0.500920	-3.571690	0.000000
H	1.386974	-3.935664	0.000000

2-naphthol, *trans* S_1

C	0.517162	1.987632	0.000000
C	0.566444	0.587973	0.000000
C	-0.719368	-0.117968	0.000000
C	-1.921599	0.604164	0.000000
C	-1.933632	2.009854	0.000000
C	-0.711942	2.676039	0.000000
C	1.770558	-0.139327	0.000000
C	1.803586	-1.541589	0.000000
C	0.570878	-2.199004	0.000000
C	-0.670898	-1.514958	0.000000
H	-1.569951	-2.113933	0.000000
H	1.439614	2.551804	0.000000
H	-0.693472	3.757488	0.000000
H	-2.862380	2.555724	0.000000
H	-2.852456	0.053138	0.000000
H	2.700001	0.413731	0.000000
H	2.732085	-2.090313	0.000000
O	0.483765	-3.535062	0.000000
H	1.351603	-3.945382	0.000000

5-methoxysalicylic acid S_0

C	2.275916	-0.168122	0.000000
C	1.565547	-1.340714	0.000000
C	0.161085	-1.336962	0.000000
C	-0.510430	-0.137087	0.000000
C	0.217479	1.066406	0.000000
C	1.609630	1.065280	0.000000
O	-0.435323	-2.558067	0.000000
C	-1.848943	-2.592370	0.000000
C	-0.483603	2.361705	0.000000
O	-1.813402	2.284583	0.000000

O	2.356770	2.179522	0.000000
O	0.074507	3.434659	0.000000
H	-2.119590	-3.642750	0.000000
H	-2.242631	-2.107708	-0.894885
H	-2.242631	-2.107708	0.894885
H	-1.587329	-0.081843	0.000000
H	3.355611	-0.160765	0.000000
H	2.067620	-2.297241	0.000000
H	1.773732	2.960027	0.000000
H	-2.173996	3.179156	0.000000

5-methoxysalicylic acid S_1

C	2.184466	-0.136226	0.000000
C	1.728019	-1.447974	0.000000
C	0.329504	-1.683285	0.000000
C	-0.617851	-0.635354	0.000000
C	-0.179908	0.686687	0.000000
C	1.278150	0.930915	0.000000
O	-0.025088	-2.964286	0.000000
C	-1.402067	-3.321580	0.000000
C	-1.024200	1.821500	0.000000
O	-2.347980	1.601670	0.000000
O	1.675715	2.160609	0.000000
O	-0.597690	3.003858	0.000000
H	-1.416883	-4.405607	0.000000
H	-1.888020	-2.938112	-0.896288
H	-1.888020	-2.938112	0.896288
H	-1.677890	-0.832551	0.000000
H	3.237389	0.102788	0.000000
H	2.391192	-2.296441	0.000000
H	0.803477	2.764345	0.000000
H	-2.790264	2.457933	0.000000

m-dimethoxybenzene, *trans* S_0

C	0.000000	-0.705259	-0.183780
C	0.000000	0.705259	-0.183780
C	0.000000	1.386952	1.019089
C	0.000000	0.688579	2.230013
C	0.000000	-0.688579	2.230013
C	0.000000	-1.386952	1.019089
O	0.000000	1.297150	-1.399232
H	0.000000	2.465612	1.031517
H	0.000000	1.238064	3.159249
H	0.000000	-1.238064	3.159249

H	0.000000	-2.465612	1.031517
O	0.000000	-1.297150	-1.399232
C	0.000000	-2.709376	-1.441333
H	0.000000	-2.970873	-2.494316
H	0.894662	-3.108602	-0.960593
H	-0.894662	-3.108602	-0.960593
C	0.000000	2.709376	-1.441333
H	0.000000	2.970873	-2.494316
H	-0.894662	3.108602	-0.960593
H	0.894662	3.108602	-0.960593

m-dimethoxybenzene, *trans* S_1

C	-0.262004	-1.068355	-1.433878
C	-0.288000	0.170774	-0.709791
C	-0.288000	0.170774	0.709791
C	-0.262004	-1.068355	1.433878
C	0.307157	-2.119290	0.708265
C	0.307157	-2.119290	-0.708265
O	-0.127385	1.361990	-1.289470
C	0.002253	1.417983	-2.703219
O	-0.127385	1.361990	1.289470
C	0.002253	1.417983	2.703219
H	-0.463115	-1.133451	2.488220
H	0.722329	-2.976926	1.222872
H	0.722329	-2.976926	-1.222872
H	-0.463115	-1.133451	-2.488220
H	0.124936	2.469463	-2.938060
H	0.875026	0.850558	-3.023201
H	-0.898107	1.029693	-3.178366
H	0.124936	2.469463	2.938060
H	-0.898107	1.029693	3.178366
H	0.875026	0.850558	3.023201

3P-propionic acid, *gauche* S_0

C	-0.997823	0.897258	-1.157947
C	-0.364573	0.686669	0.064999
C	-1.009995	-0.075788	1.034632
C	-2.263794	-0.620239	0.782036
C	-2.886714	-0.406880	-0.440202
C	-2.249973	0.355204	-1.412538
C	1.018369	1.256476	0.310277
C	2.108271	0.326633	-0.246166
C	2.237446	-0.926500	0.591691
O	1.973225	-1.010491	1.754610

O	2.728589	-1.965653	-0.096003
H	1.898057	0.034211	-1.271828
H	3.085282	0.812424	-0.216717
H	1.182855	1.394309	1.376168
H	1.102536	2.222489	-0.184534
H	-0.521319	-0.249195	1.983345
H	-2.754661	-1.209572	1.543425
H	-3.861977	-0.828374	-0.634765
H	-2.729511	0.530977	-2.364911
H	-0.507065	1.495285	-1.915767
H	2.812785	-2.719262	0.500203

3P-propionic acid, *gauche* S_1

C	-0.955350	0.980372	-1.139363
C	-0.301491	0.809316	0.111672
C	-0.903080	0.019239	1.128055
C	-2.038058	-0.775318	0.831533
C	-2.664141	-0.625646	-0.429906
C	-2.076497	0.168348	-1.443823
C	1.073072	1.375981	0.319311
C	2.154645	0.412547	-0.238133
C	2.066970	-0.892927	0.519663
O	2.257490	-1.004064	1.696018
O	1.736147	-1.936255	-0.247653
H	1.997946	0.230406	-1.296180
H	3.143326	0.830813	-0.061015
H	1.260055	1.521656	1.381871
H	1.160968	2.330199	-0.199514
H	-0.462643	0.001134	2.114448
H	-2.446813	-1.444262	1.571600
H	-3.607414	-1.116737	-0.620667
H	-2.494139	0.168273	-2.438700
H	-0.553113	1.664921	-1.870979
H	1.652130	-2.718014	0.311772

3P-propionic acid, *anti* S_0

C	1.427400	-0.447595	0.000000
C	0.547345	0.808213	0.000000
C	2.898660	-0.104058	0.000000
H	1.230775	-1.063312	0.877581
H	1.230775	-1.063312	-0.877581
C	-0.913989	0.410653	0.000000
H	0.775664	1.407406	0.878482
H	0.775664	1.407406	-0.878482

C	-1.590532	0.202752	1.198504
C	-2.917401	-0.208325	1.201178
C	-3.583554	-0.415566	0.000000
C	-2.917401	-0.208325	-1.201178
C	-1.590532	0.202752	-1.198504
H	-1.075803	0.369230	2.135918
H	-3.431508	-0.362440	2.138838
H	-4.616314	-0.732600	0.000000
H	-3.431508	-0.362440	-2.138838
H	-1.075803	0.369230	-2.135918
O	3.678562	-1.197145	0.000000
O	3.360218	0.997600	0.000000
H	4.602121	-0.918801	0.000000

3P-propionic acid, *anti* S_1

C	1.394962	-0.454671	0.000000
C	0.554561	0.835810	0.000000
C	2.874231	-0.145470	0.000000
H	1.179531	-1.060469	0.879161
H	1.179531	-1.060469	-0.879161
C	-0.909456	0.503850	0.000000
H	0.804164	1.422432	0.882410
H	0.804164	1.422432	-0.882410
C	-1.592290	0.310756	1.230790
C	-2.883435	-0.273204	1.232141
C	-3.551304	-0.472724	0.000000
C	-2.883435	-0.273204	-1.232141
C	-1.592290	0.310756	-1.230790
H	-1.107326	0.575993	2.158810
H	-3.369894	-0.524063	2.161465
H	-4.589765	-0.770749	0.000000
H	-3.369894	-0.524063	-2.161465
H	-1.107326	0.575993	-2.158810
O	3.629561	-1.255057	0.000000
O	3.358851	0.946869	0.000000
H	4.559700	-0.999425	0.000000

fluorine S_0

C	0.000000	0.000000	-1.801700
C	0.000000	1.182082	-0.848048
C	0.000000	0.738954	0.477236
C	0.000000	-0.738954	0.477236
C	0.000000	1.642540	1.529072
C	0.000000	3.001949	1.239173

C	0.000000	3.445774	-0.080527
C	0.000000	2.535731	-1.134216
H	0.000000	2.884672	-2.157931
H	0.000000	4.505948	-0.287928
H	0.000000	3.721175	2.045062
H	0.000000	1.299832	2.554260
C	0.000000	-1.642540	1.529072
C	0.000000	-3.001949	1.239173
C	0.000000	-3.445774	-0.080527
C	0.000000	-2.535731	-1.134216
C	0.000000	-1.182082	-0.848048
H	0.000000	-1.299832	2.554260
H	0.000000	-3.721175	2.045062
H	0.000000	-4.505948	-0.287928
H	0.000000	-2.884672	-2.157931
H	-0.887121	0.000000	-2.435292
H	0.887121	0.000000	-2.435292

fluorine S_1

C	0.000000	0.000000	-1.886431
C	0.000000	1.180690	-0.924825
C	0.000000	0.692471	0.445134
C	0.000000	-0.692471	0.445134
C	0.000000	1.629897	1.537542
C	0.000000	2.966263	1.234023
C	0.000000	3.425237	-0.101844
C	0.000000	2.519546	-1.186524
H	0.000000	2.889933	-2.202076
H	0.000000	4.487462	-0.294838
H	0.000000	3.696005	2.031199
H	0.000000	1.280675	2.558733
C	0.000000	-1.629897	1.537542
C	0.000000	-2.966263	1.234023
C	0.000000	-3.425237	-0.101844
C	0.000000	-2.519546	-1.186524
C	0.000000	-1.180690	-0.924825
H	0.000000	-1.280675	2.558733
H	0.000000	-3.696005	2.031199
H	0.000000	-4.487462	-0.294838
H	0.000000	-2.889933	-2.202076
H	-0.886515	0.000000	-2.521147
H	0.886515	0.000000	-2.521147

phenanthrene S_0

C	0.731077	0.000000	-0.345993
C	-0.731077	0.000000	-0.345993
C	-1.413983	0.000000	0.881101
C	-0.671880	0.000000	2.119102
C	0.671880	0.000000	2.119102
C	1.413983	0.000000	0.881101
C	-1.490633	0.000000	-1.533828
C	-2.822943	0.000000	0.900767
H	-1.226254	0.000000	3.047567
H	1.226254	0.000000	3.047567
C	1.490633	0.000000	-1.533828
C	2.863662	0.000000	-1.497324
C	3.540887	0.000000	-0.267649
C	2.822943	0.000000	0.900767
H	0.998730	0.000000	-2.493302
H	3.424740	0.000000	-2.420567
H	4.620967	0.000000	-0.245239
H	3.330614	0.000000	1.855455
C	-3.540887	0.000000	-0.267649
C	-2.863662	0.000000	-1.497324
H	-0.998730	0.000000	-2.493302
H	-3.424740	0.000000	-2.420567
H	-4.620967	0.000000	-0.245239
H	-3.330614	0.000000	1.855455

phenanthrene S_1

C	0.707510	0.000000	-0.391527
C	-0.707510	0.000000	-0.391527
C	-1.431089	0.000000	0.884951
C	-0.694849	0.000000	2.080288
C	0.694849	0.000000	2.080288
C	1.431089	0.000000	0.884951
C	-1.487991	0.000000	-1.572882
C	-2.837750	0.000000	0.887238
H	-1.229243	0.000000	3.020269
H	1.229243	0.000000	3.020269
C	1.487991	0.000000	-1.572882
C	2.872738	0.000000	-1.525954
C	3.560063	0.000000	-0.295804
C	2.837750	0.000000	0.887238
H	1.007679	0.000000	-2.538039
H	3.432230	0.000000	-2.450067
H	4.639135	0.000000	-0.277728
H	3.352257	0.000000	1.838294
C	-3.560063	0.000000	-0.295804

C	-2.872738	0.000000	-1.525954
H	-1.007679	0.000000	-2.538039
H	-3.432230	0.000000	-2.450067
H	-4.639135	0.000000	-0.277728
H	-3.352257	0.000000	1.838294

2,4,6,8-decatetraene S_0

C	-2.587806	-5.012726	0.000000
C	-2.462107	-3.510306	0.000000
C	-1.306449	-2.852543	0.000000
C	-1.208545	-1.390019	0.000000
C	-0.048531	-0.729380	0.000000
C	0.048531	0.729380	0.000000
C	1.208545	1.390019	0.000000
C	1.306449	2.852543	0.000000
C	2.462107	3.510306	0.000000
C	2.587806	5.012726	0.000000
H	-0.372313	-3.403653	0.000000
H	-2.141011	-0.836391	0.000000
H	0.883801	-1.283077	0.000000
H	-0.883801	1.283077	0.000000
H	2.141011	0.836391	0.000000
H	0.372313	3.403653	0.000000
H	3.387371	2.943934	0.000000
H	-3.387371	-2.943934	0.000000
H	1.604559	5.478821	0.000000
H	3.136249	5.345955	0.881652
H	3.136249	5.345955	-0.881652
H	-1.604559	-5.478821	0.000000
H	-3.136249	-5.345955	0.881652
H	-3.136249	-5.345955	-0.881652

2,4,6,8-decatetraene S_1

C	-2.570626	-5.018272	0.000000
C	-2.511594	-3.519349	0.000000
C	-1.350112	-2.804847	0.000000
C	-1.271988	-1.395450	0.000000
C	-0.050311	-0.692018	0.000000
C	0.050311	0.692018	0.000000
C	1.271988	1.395450	0.000000
C	1.350112	2.804847	0.000000
C	2.511594	3.519349	0.000000
C	2.570626	5.018272	0.000000
H	-0.412129	-3.351398	0.000000

H	-2.193689	-0.826009	0.000000
H	0.864595	-1.273647	0.000000
H	-0.864595	1.273647	0.000000
H	2.193689	0.826009	0.000000
H	0.412129	3.351398	0.000000
H	3.454033	2.983297	0.000000
H	-3.454033	-2.983297	0.000000
H	1.568073	5.442552	0.000000
H	3.106382	5.384106	0.880246
H	3.106382	5.384106	-0.880246
H	-1.568073	-5.442552	0.000000
H	-3.106382	-5.384106	0.880246
H	-3.106382	-5.384106	-0.880246

tetracene S_0

C	3.696673	1.408690	0.000000
C	2.428322	0.718624	0.000000
C	2.428322	-0.718624	0.000000
C	3.696673	-1.408690	0.000000
C	4.856710	-0.721340	0.000000
C	4.856710	0.721340	0.000000
C	1.230646	1.399958	0.000000
C	0.000000	0.715341	0.000000
C	0.000000	-0.715341	0.000000
C	1.230646	-1.399958	0.000000
C	-1.230646	1.399958	0.000000
C	-2.428322	0.718624	0.000000
C	-2.428322	-0.718624	0.000000
C	-1.230646	-1.399958	0.000000
C	-3.696673	1.408690	0.000000
C	-4.856710	0.721340	0.000000
C	-4.856710	-0.721340	0.000000
C	-3.696673	-1.408690	0.000000
H	-3.691184	-2.490138	0.000000
H	-5.801240	-1.245180	0.000000
H	-5.801240	1.245180	0.000000
H	-3.691184	2.490138	0.000000
H	-1.229837	-2.482490	0.000000
H	-1.229837	2.482490	0.000000
H	1.229837	-2.482490	0.000000
H	1.229837	2.482490	0.000000
H	3.691184	-2.490138	0.000000
H	5.801240	-1.245180	0.000000
H	5.801240	1.245180	0.000000
H	3.691184	2.490138	0.000000

tetracene S_1

C	3.690492	1.393072	0.000000
C	2.464734	0.713807	0.000000
C	2.464734	-0.713807	0.000000
C	3.690492	-1.393072	0.000000
C	4.890824	-0.697692	0.000000
C	4.890824	0.697692	0.000000
C	1.222238	1.398478	0.000000
C	0.000000	0.727748	0.000000
C	0.000000	-0.727748	0.000000
C	1.222238	-1.398478	0.000000
C	-1.222238	1.398478	0.000000
C	-2.464734	0.713807	0.000000
C	-2.464734	-0.713807	0.000000
C	-1.222238	-1.398478	0.000000
C	-3.690492	1.393072	0.000000
C	-4.890824	0.697692	0.000000
C	-4.890824	-0.697692	0.000000
C	-3.690492	-1.393072	0.000000
H	-3.690633	-2.474552	0.000000
H	-5.825522	-1.238317	0.000000
H	-5.825522	1.238317	0.000000
H	-3.690633	2.474552	0.000000
H	-1.227258	-2.480857	0.000000
H	-1.227258	2.480857	0.000000
H	1.227258	-2.480857	0.000000
H	1.227258	2.480857	0.000000
H	3.690633	-2.474552	0.000000
H	5.825522	-1.238317	0.000000
H	5.825522	1.238317	0.000000
H	3.690633	2.474552	0.000000

perylene S_0

C	0.213259	1.457242	-2.403586
C	0.064538	0.739762	-1.243101
C	0.011320	1.440309	-0.000353
C	0.036177	2.853112	-0.000162
C	0.159206	3.553891	-1.226624
C	0.262406	2.867309	-2.398984
C	-0.068890	3.557396	1.225779
C	-0.183977	2.873930	2.398924
C	-0.168419	1.463201	2.403987
C	-0.039278	0.741651	1.243466

C	-0.064538	-0.739762	-1.243101
C	-0.011320	-1.440309	-0.000353
C	0.039278	-0.741651	1.243466
C	-0.036177	-2.853112	-0.000162
C	0.068890	-3.557396	1.225779
C	0.183977	-2.873930	2.398924
C	0.168419	-1.463201	2.403987
C	-0.213259	-1.457242	-2.403586
C	-0.262406	-2.867309	-2.398984
C	-0.159206	-3.553891	-1.226624
H	-0.061556	4.638491	1.209538
H	-0.281777	3.403542	3.335280
H	-0.261466	0.960926	3.353979
H	0.061556	-4.638491	1.209538
H	0.281777	-3.403542	3.335280
H	0.261466	-0.960926	3.353979
H	-0.179956	-4.634816	-1.210737
H	-0.376175	-3.394060	-3.335149
H	-0.301818	-0.951569	-3.352255
H	0.179956	4.634816	-1.210737
H	0.376175	3.394060	-3.335149
H	0.301818	0.951569	-3.352255

perylene S_1

C	-0.006561	1.462266	-2.444351
C	-0.006760	0.717610	-1.234732
C	0.015806	1.413868	0.000001
C	0.006650	2.842635	-0.000001
C	0.009580	3.534744	-1.225428
C	-0.001105	2.843493	-2.428620
C	0.009775	3.534749	1.225419
C	-0.000693	2.843500	2.428618
C	-0.006189	1.462276	2.444354
C	-0.006669	0.717611	1.234738
C	0.006760	-0.717610	-1.234732
C	-0.015806	-1.413868	0.000001
C	0.006669	-0.717611	1.234738
C	-0.006650	-2.842635	-0.000001
C	-0.009775	-3.534749	1.225419
C	0.000693	-2.843500	2.428618
C	0.006189	-1.462276	2.444354
C	0.006561	-1.462266	-2.444351
C	0.001105	-2.843493	-2.428620
C	-0.009580	-3.534744	-1.225428
H	0.013113	4.615767	1.216165

H	-0.004160	3.388256	3.361405
H	-0.030497	0.957213	3.394822
H	-0.013113	-4.615767	1.216165
H	0.004160	-3.388256	3.361405
H	0.030497	-0.957213	3.394822
H	-0.012907	-4.615762	-1.216177
H	0.004791	-3.388244	-3.361410
H	0.031154	-0.957194	-3.394808
H	0.012907	4.615762	-1.216177
H	-0.004791	3.388244	-3.361410
H	-0.031154	0.957194	-3.394808

CAM-B3LYP/TZVP geometries – Group I

pyrazine S_0

C	1.126638	-0.693086	0.000000
C	1.126638	0.693086	0.000000
N	0.000000	1.393917	0.000000
C	-1.126638	0.693086	0.000000
C	-1.126638	-0.693086	0.000000
N	0.000000	-1.393917	0.000000
H	-2.056557	-1.249635	0.000000
H	2.056557	-1.249635	0.000000
H	2.056557	1.249635	0.000000
H	-2.056557	1.249635	0.000000

pyrazine S_1

C	-1.200798	0.664784	0.000000
C	-1.116245	-0.735393	0.000000
N	0.024738	-1.348730	0.000000
C	1.200798	-0.664784	0.000000
C	1.116245	0.735393	0.000000
N	-0.024738	1.348730	0.000000
H	2.043089	1.301406	0.000000
H	-2.152341	1.170187	0.000000
H	-2.043089	-1.301406	0.000000
H	2.152341	-1.170187	0.000000

2,6-difluoropyridine S_0

C	1.111700	0.000000	-0.872572
N	0.000000	0.000000	-1.560292
C	-1.111700	0.000000	-0.872572

C	-1.198699	0.000000	0.505117
C	0.000000	0.000000	1.197729
C	1.198699	0.000000	0.505117
F	-2.237911	0.000000	-1.586722
H	-2.159967	0.000000	0.995903
H	0.000000	0.000000	2.279529
H	2.159967	0.000000	0.995903
F	2.237911	0.000000	-1.586722

2,6-difluoropyridine S_1

C	-1.098440	0.000000	-0.334304
N	0.000000	0.000000	-1.095748
C	1.098440	0.000000	-0.334304
C	1.189266	0.000000	1.070349
C	0.000000	0.000000	1.841500
C	-1.189266	0.000000	1.070349
F	2.236219	0.000000	-1.008796
H	2.173883	0.000000	1.515958
H	0.000000	0.000000	2.917130
H	-2.173883	0.000000	1.515958
F	-2.236219	0.000000	-1.008796

2-fluoropyridine S_0

C	-1.310995	0.501789	0.000000
N	-1.360589	-0.797986	0.000000
C	-0.195811	-1.448482	0.000000
C	1.026468	-0.806791	0.000000
C	1.040100	0.582038	0.000000
C	-0.157202	1.267851	0.000000
H	-0.257899	-2.530087	0.000000
H	1.943741	-1.378362	0.000000
H	1.976444	1.124599	0.000000
H	-0.215350	2.346400	0.000000
F	-2.488918	1.139020	0.000000

2-fluoropyridine S_1

C	-1.317414	0.490002	0.000000
N	-1.430927	-0.839560	0.000000
C	-0.224103	-1.461784	0.000000
C	1.027188	-0.790600	0.000000
C	1.103480	0.616504	0.000000
C	-0.151773	1.279234	0.000000
H	-0.248252	-2.543375	0.000000

H	1.924979	-1.394126	0.000000
H	2.039234	1.149238	0.000000
H	-0.252822	2.354472	0.000000
F	-2.469600	1.139983	0.000000

2-hydroxypyridine S_0

C	-0.975419	0.749724	0.000000
C	-0.967066	-0.643193	0.000000
N	0.130848	-1.370917	0.000000
C	1.302196	-0.733083	0.000000
C	1.414472	0.640806	0.000000
C	0.242471	1.390767	0.000000
O	-2.146016	-1.296833	0.000000
H	2.183298	-1.364118	0.000000
H	2.386783	1.112285	0.000000
H	0.283943	2.472494	0.000000
H	-1.914486	1.283609	0.000000
H	-1.941025	-2.241539	0.000000

2-hydroxypyridine S_1

C	-0.994649	0.765596	0.000000
C	-0.966536	-0.636072	0.000000
N	0.119780	-1.447653	0.000000
C	1.291327	-0.772203	0.000000
C	1.388416	0.641945	0.000000
C	0.248794	1.458865	0.000000
O	-2.123267	-1.287401	0.000000
H	2.191987	-1.371478	0.000000
H	2.378554	1.078908	0.000000
H	0.307784	2.534343	0.000000
H	-1.950822	1.267662	0.000000
H	-1.891367	-2.232514	0.000000

2-pyridone S_0

C	-1.243081	0.709583	0.000000
N	-1.133918	-0.684603	0.000000
C	0.034263	-1.379744	0.000000
C	1.218260	-0.732192	0.000000
C	1.200380	0.691020	0.000000
C	0.038857	1.382517	0.000000
H	-2.018084	-1.172703	0.000000
H	-0.053947	-2.457214	0.000000
H	2.144931	-1.284642	0.000000

H	2.141153	1.228025	0.000000
H	0.011164	2.462536	0.000000
O	-2.339978	1.237429	0.000000

2-pyridone S_1

C	-1.384599	0.106118	0.000000
N	-0.728719	-1.137655	0.000000
C	0.622217	-1.250713	0.000000
C	1.408882	-0.075470	0.000000
C	0.828280	1.169318	0.000000
C	-0.607467	1.263564	0.000000
H	-1.340875	-1.941085	0.000000
H	1.042674	-2.243798	0.000000
H	2.483619	-0.192264	0.000000
H	1.433584	2.062871	0.000000
H	-1.125532	2.209565	0.000000
O	-2.632064	0.029538	0.000000

2-methylpyrimidine S_0

C	0.000149	1.958213	0.000000
C	-1.170494	1.221631	0.000000
N	-1.174808	-0.103013	0.000000
C	0.010659	-0.715555	0.000000
N	1.189218	-0.095813	0.000000
C	1.174075	1.232225	0.000000
H	-2.140604	1.707485	0.000000
H	2.140930	1.724141	0.000000
H	-0.004492	3.038679	0.000000
C	0.004735	-2.210752	0.000000
H	1.022039	-2.592045	0.000000
H	-0.525709	-2.582597	0.877206
H	-0.525709	-2.582597	-0.877206

2-methylpyrimidine S_1

C	-0.014082	2.006782	0.000000
C	-1.164577	1.276476	0.000000
N	-1.144871	-0.093712	0.000000
C	0.010975	-0.782542	0.000000
N	1.081798	-0.065577	0.000000
C	1.202046	1.288173	0.000000
H	-2.142634	1.738165	0.000000
H	2.187282	1.722059	0.000000
H	-0.025632	3.088036	0.000000

C	0.012849	-2.266032	0.000000
H	1.030629	-2.648559	0.000000
H	-0.516891	-2.631640	0.880246
H	-0.516891	-2.631640	-0.880246

5-methylpyrimidine S_0

C	0.871515	0.848194	0.000000
C	-0.358437	0.209931	0.000000
C	-0.298403	-1.177335	0.000000
N	0.843012	-1.851747	0.000000
C	1.955566	-1.128097	0.000000
N	2.027672	0.194169	0.000000
H	2.893288	-1.671550	0.000000
H	-1.208900	-1.769857	0.000000
H	0.930122	1.932581	0.000000
C	-1.657719	0.956735	0.000000
H	-1.488895	2.032976	0.000000
H	-2.254410	0.711990	-0.879967
H	-2.254410	0.711990	0.879967

5-methylpyrimidine S_1

C	0.841549	0.854907	0.000000
C	-0.375000	0.242265	0.000000
C	-0.346163	-1.188052	0.000000
N	0.878507	-1.750817	0.000000
C	2.030309	-1.177049	0.000000
N	2.025904	0.165507	0.000000
H	2.954871	-1.734694	0.000000
H	-1.217100	-1.822350	0.000000
H	0.928063	1.934185	0.000000
C	-1.673971	0.977883	0.000000
H	-1.513704	2.055182	0.000000
H	-2.266637	0.721523	-0.880670
H	-2.266637	0.721523	0.880670

7-azaindole S_0

N	-0.632597	1.839006	0.000000
C	-0.672026	0.470824	0.000000
C	0.661916	0.006420	0.000000
C	1.503764	1.164723	0.000000
C	0.681332	2.246926	0.000000
C	0.840004	-1.373183	0.000000
C	-0.290722	-2.165804	0.000000

C	-1.558909	-1.576474	0.000000
N	-1.769072	-0.268149	0.000000
H	-2.445134	-2.200768	0.000000
H	1.829444	-1.813411	0.000000
H	-0.210263	-3.244224	0.000000
H	-1.446213	2.428989	0.000000
H	2.580595	1.189421	0.000000
H	0.927900	3.295703	0.000000

7-azaindole S_1

N	-0.606518	1.870308	0.000000
C	-0.660848	0.451139	0.000000
C	0.656903	-0.003559	0.000000
C	1.485706	1.139277	0.000000
C	0.648560	2.299935	0.000000
C	0.884110	-1.404387	0.000000
C	-0.302975	-2.177185	0.000000
C	-1.545096	-1.595597	0.000000
N	-1.789401	-0.223242	0.000000
H	-2.434776	-2.211649	0.000000
H	1.870336	-1.840792	0.000000
H	-0.243384	-3.257579	0.000000
H	-1.439407	2.441367	0.000000
H	2.563526	1.168979	0.000000
H	0.913272	3.343006	0.000000

7-hydroxyquinoline, *cis* S_0

N	0.458493	1.964297	0.000000
C	0.431489	0.606591	0.000000
C	-0.782474	-0.123022	0.000000
C	-1.985892	0.607493	0.000000
C	-1.941347	1.970511	0.000000
C	-0.681895	2.601298	0.000000
C	1.658933	-0.090535	0.000000
C	1.671652	-1.455721	0.000000
C	0.464640	-2.190860	0.000000
C	-0.727487	-1.537438	0.000000
H	-0.625945	3.685536	0.000000
H	-1.654225	-2.098454	0.000000
H	0.521088	-3.270887	0.000000
O	2.813801	-2.193483	0.000000
H	2.572317	0.491901	0.000000
H	-2.931392	0.077776	0.000000
H	-2.843039	2.567458	0.000000

H	3.581283	-1.612451	0.000000

7-hydroxyquinoline, *cis* S_1

N	0.485682	1.967441	0.000000
C	0.434426	0.629561	0.000000
C	-0.789075	-0.139878	0.000000
C	-1.990217	0.592843	0.000000
C	-1.915898	1.992017	0.000000
C	-0.686639	2.635838	0.000000
C	1.632799	-0.087088	0.000000
C	1.649932	-1.512095	0.000000
C	0.481586	-2.258462	0.000000
C	-0.720212	-1.552601	0.000000
H	-0.623761	3.715622	0.000000
H	-1.653139	-2.103518	0.000000
H	0.524144	-3.336392	0.000000
O	2.822098	-2.153817	0.000000
H	2.563358	0.469450	0.000000
H	-2.945301	0.085769	0.000000
H	-2.824590	2.580508	0.000000
H	3.554804	-1.525190	0.000000

7-hydroxyquinoline, *trans* S_0

N	0.508595	2.037070	0.000000
C	0.479524	0.677018	0.000000
C	-0.739720	-0.046939	0.000000
C	-1.942326	0.688323	0.000000
C	-1.892499	2.049519	0.000000
C	-0.628479	2.676162	0.000000
C	1.703301	-0.019970	0.000000
C	1.712853	-1.385380	0.000000
C	0.502179	-2.114025	0.000000
C	-0.691669	-1.457844	0.000000
H	-0.569863	3.760408	0.000000
H	-1.619250	-2.017379	0.000000
H	0.530913	-3.198147	0.000000
O	2.914761	-2.024262	0.000000
H	2.627199	0.540425	0.000000
H	-2.889600	0.161721	0.000000
H	-2.791499	2.650565	0.000000
H	2.785562	-2.977246	0.000000

7-hydroxyquinoline, *trans* S_1

N	0.528782	2.042898	0.000000
C	0.476496	0.706896	0.000000
C	-0.748336	-0.057311	0.000000
C	-1.948817	0.676486	0.000000
C	-1.872661	2.076280	0.000000
C	-0.643802	2.714842	0.000000
C	1.676785	-0.012078	0.000000
C	1.686984	-1.433712	0.000000
C	0.515530	-2.179517	0.000000
C	-0.685750	-1.468864	0.000000
H	-0.577352	3.794540	0.000000
H	-1.620338	-2.017161	0.000000
H	0.536428	-3.260720	0.000000
O	2.903964	-1.987389	0.000000
H	2.618575	0.518487	0.000000
H	-2.904415	0.170212	0.000000
H	-2.780097	2.666637	0.000000
H	2.838007	-2.950506	0.000000

2-hydroxyquinoline, enol S_0

C	0.429143	1.898097	0.000000
C	0.482386	0.488197	0.000000
C	-0.720152	-0.255952	0.000000
C	-1.949176	0.437409	0.000000
C	-1.971621	1.802873	0.000000
C	-0.773482	2.544117	0.000000
C	1.692263	-0.244167	0.000000
C	1.660355	-1.600606	0.000000
C	0.392495	-2.243849	0.000000
N	-0.735863	-1.615302	0.000000
O	0.316386	-3.595966	0.000000
H	1.356619	2.458494	0.000000
H	-0.811641	3.625552	0.000000
H	-2.919726	2.325467	0.000000
H	-2.858171	-0.148607	0.000000
H	2.637574	0.285258	0.000000
H	2.572898	-2.184131	0.000000
H	1.199712	-3.976884	0.000000

2-hydroxyquinoline, enol S_1

C	0.435605	1.876917	0.000000
C	0.526310	0.488600	0.000000
C	-0.724817	-0.259788	0.000000
C	-1.955818	0.438790	0.000000

C	-2.007409	1.834403	0.000000
C	-0.813681	2.539039	0.000000
C	1.729299	-0.234739	0.000000
C	1.691423	-1.635562	0.000000
C	0.431835	-2.237399	0.000000
N	-0.746555	-1.598965	0.000000
O	0.295120	-3.568761	0.000000
H	1.343194	2.467761	0.000000
H	-0.824001	3.621664	0.000000
H	-2.955562	2.351690	0.000000
H	-2.856458	-0.160332	0.000000
H	2.672900	0.293793	0.000000
H	2.593890	-2.230748	0.000000
H	1.164716	-3.986343	0.000000

2-hydroxyquinoline, keto S_0

N	0.558396	1.702496	0.000000
C	0.599782	0.325580	0.000000
C	-0.610436	-0.381849	0.000000
C	-1.832616	0.378040	0.000000
C	-1.830552	1.718607	0.000000
C	-0.586253	2.482013	0.000000
C	1.813554	-0.363395	0.000000
C	1.817077	-1.740039	0.000000
C	0.620399	-2.457260	0.000000
C	-0.576705	-1.779259	0.000000
H	-1.513687	-2.322908	0.000000
H	0.636053	-3.538584	0.000000
H	2.761368	-2.268851	0.000000
H	2.744886	0.189704	0.000000
H	-2.770637	-0.165295	0.000000
H	-2.740712	2.300766	0.000000
O	-0.513116	3.695883	0.000000
H	1.423220	2.224372	0.000000

2-hydroxyquinoline, keto S_1

N	0.561891	1.673208	0.000000
C	0.611327	0.326586	0.000000
C	-0.664707	-0.380517	0.000000
C	-1.851858	0.363784	0.000000
C	-1.850780	1.761603	0.000000
C	-0.628350	2.467717	0.000000
C	1.832505	-0.360353	0.000000
C	1.851321	-1.744184	0.000000

C	0.629776	-2.442330	0.000000
C	-0.589819	-1.785574	0.000000
H	-1.509481	-2.355350	0.000000
H	0.642519	-3.524790	0.000000
H	2.788489	-2.281049	0.000000
H	2.754335	0.208635	0.000000
H	-2.791566	-0.172300	0.000000
H	-2.758959	2.342567	0.000000
O	-0.438912	3.679936	0.000000
H	1.412268	2.222418	0.000000

dibenzofuran S_0

C	1.715739	0.000000	-1.352856
C	0.724613	0.000000	-0.379243
C	1.094766	0.000000	0.966047
C	2.406849	0.000000	1.389215
C	3.379107	0.000000	0.402622
C	3.039417	0.000000	-0.950764
C	-0.724613	0.000000	-0.379243
C	-1.094766	0.000000	0.966047
O	0.000000	0.000000	1.789497
C	-1.715739	0.000000	-1.352856
C	-3.039417	0.000000	-0.950764
C	-3.379107	0.000000	0.402622
C	-2.406849	0.000000	1.389215
H	-2.655757	0.000000	2.441222
H	-4.422836	0.000000	0.688430
H	-3.825107	0.000000	-1.694645
H	-1.459965	0.000000	-2.404609
H	1.459965	0.000000	-2.404609
H	3.825107	0.000000	-1.694645
H	4.422836	0.000000	0.688430
H	2.655757	0.000000	2.441222

dibenzofuran S_1

C	0.000000	1.724796	-1.527066
C	0.000000	0.710328	-0.565997
C	0.000000	1.102348	0.803136
C	0.000000	2.404037	1.252324
C	0.000000	3.409429	0.264317
C	0.000000	3.062612	-1.085893
C	0.000000	-0.710328	-0.565997
C	0.000000	-1.102348	0.803136
O	0.000000	0.000000	1.600711

C	0.000000	-1.724796	-1.527066
C	0.000000	-3.062612	-1.085893
C	0.000000	-3.409429	0.264317
C	0.000000	-2.404037	1.252324
H	0.000000	-2.631930	2.308544
H	0.000000	-4.449428	0.555870
H	0.000000	-3.850921	-1.827623
H	0.000000	-1.499749	-2.584257
H	0.000000	1.499749	-2.584257
H	0.000000	3.850921	-1.827623
H	0.000000	4.449428	0.555870
H	0.000000	2.631930	2.308544

pyrrolo[3,2-*h*]quinoline S_0

C	0.135014	-0.682836	0.000000
N	0.064113	-2.030548	0.000000
C	1.191460	-2.701010	0.000000
C	2.455897	-2.093768	0.000000
C	2.532180	-0.726880	0.000000
C	1.354218	0.037613	0.000000
H	1.109760	-3.783011	0.000000
H	3.346807	-2.706853	0.000000
H	3.492866	-0.225349	0.000000
C	-1.050752	0.084265	0.000000
C	-1.055012	1.478388	0.000000
C	0.182587	2.170287	0.000000
C	1.345257	1.466063	0.000000
H	0.198576	3.252875	0.000000
H	2.296948	1.983055	0.000000
C	-2.423190	1.883231	0.000000
C	-3.174622	0.743992	0.000000
N	-2.343148	-0.345743	0.000000
H	-2.610516	-1.315212	0.000000
H	-2.803814	2.891062	0.000000
H	-4.244619	0.620378	0.000000

pyrrolo[3,2-*h*]quinoline S_1

C	0.149985	-0.697502	0.000000
N	0.020136	-2.020323	0.000000
C	1.201461	-2.725524	0.000000
C	2.433170	-2.130836	0.000000
C	2.557059	-0.724374	0.000000
C	1.362324	0.029270	0.000000
H	1.102332	-3.802959	0.000000

H	3.319831	-2.751684	0.000000
H	3.523191	-0.240911	0.000000
C	-1.025428	0.101004	0.000000
C	-1.059031	1.545086	0.000000
C	0.138689	2.220427	0.000000
C	1.319961	1.449328	0.000000
H	0.189459	3.299867	0.000000
H	2.269080	1.972495	0.000000
C	-2.453604	1.902255	0.000000
C	-3.161213	0.749769	0.000000
N	-2.285648	-0.339460	0.000000
H	-2.511291	-1.323314	0.000000
H	-2.864182	2.897528	0.000000
H	-4.226292	0.589857	0.000000

carbazole S_0

C	1.127104	0.000000	-0.894816
N	0.000000	0.000000	-1.692349
C	-1.127104	0.000000	-0.894816
C	-0.723412	0.000000	0.453714
C	0.723412	0.000000	0.453714
C	-1.688604	0.000000	1.454391
C	-3.024463	0.000000	1.101394
C	-3.406196	0.000000	-0.242165
C	-2.467272	0.000000	-1.256281
C	2.467272	0.000000	-1.256281
C	3.406196	0.000000	-0.242165
C	3.024463	0.000000	1.101394
C	1.688604	0.000000	1.454391
H	-2.770316	0.000000	-2.295702
H	-4.458599	0.000000	-0.495409
H	-3.784948	0.000000	1.870996
H	-1.398452	0.000000	2.497649
H	1.398452	0.000000	2.497649
H	3.784948	0.000000	1.870996
H	4.458599	0.000000	-0.495409
H	2.770316	0.000000	-2.295702
H	0.000000	0.000000	-2.696154

carbazole S_1

C	1.139156	0.000000	-0.836014
N	0.000000	0.000000	-1.607657
C	-1.139156	0.000000	-0.836014
C	-0.713749	0.000000	0.528843

C	0.713749	0.000000	0.528843
C	-1.700122	0.000000	1.516629
C	-3.049788	0.000000	1.116601
C	-3.438853	0.000000	-0.217253
C	-2.459446	0.000000	-1.234615
C	2.459446	0.000000	-1.234615
C	3.438853	0.000000	-0.217253
C	3.049788	0.000000	1.116601
C	1.700122	0.000000	1.516629
H	-2.735254	0.000000	-2.280992
H	-4.487201	0.000000	-0.477487
H	-3.814522	0.000000	1.883299
H	-1.443590	0.000000	2.566641
H	1.443590	0.000000	2.566641
H	3.814522	0.000000	1.883299
H	4.487201	0.000000	-0.477487
H	2.735254	0.000000	-2.280992
H	0.000000	0.000000	-2.616273

tryptamine, A-ph S_0

C	-2.127166	0.137939	0.887979
N	-1.251262	0.129636	1.952323
C	0.031976	0.045046	1.472796
C	-0.049982	-0.005671	0.067059
C	-1.444496	0.055496	-0.284920
C	1.249336	0.014004	2.146159
C	2.396375	-0.067106	1.386596
C	2.339055	-0.113869	-0.013678
C	1.131371	-0.083780	-0.675833
C	-2.017520	0.006219	-1.663713
C	-1.985835	-1.389839	-2.281624
N	-2.484456	-1.351334	-3.651820
H	1.296935	0.053530	3.227401
H	3.359863	-0.092966	1.879167
H	3.260395	-0.173297	-0.578447
H	1.099110	-0.116398	-1.757892
H	-1.510808	0.199143	2.919223
H	-3.190066	0.208496	1.055640
H	-1.474193	0.682918	-2.327380
H	-3.052329	0.360410	-1.641272
H	-2.540473	-2.076168	-1.627483
H	-0.954774	-1.746352	-2.308394
H	-3.466453	-1.105914	-3.676117
H	-2.382015	-2.247763	-4.108400

tryptamine, A-ph S_1

C	-2.175983	0.157086	0.908481
N	-1.290780	0.127032	1.914400
C	0.025906	0.052035	1.439577
C	-0.053830	0.045692	0.041016
C	-1.427218	0.108274	-0.306877
C	1.207514	-0.031697	2.154771
C	2.404842	-0.112721	1.350328
C	2.357637	-0.116866	-0.017544
C	1.130513	-0.038964	-0.732595
C	-2.006247	0.045586	-1.666071
C	-1.965545	-1.377332	-2.243413
N	-2.501728	-1.383019	-3.596327
H	1.245773	-0.039297	3.233939
H	3.361318	-0.172066	1.852958
H	3.283468	-0.177411	-0.575411
H	1.108036	-0.008415	-1.812071
H	-1.532511	0.169680	2.892120
H	-3.236448	0.248672	1.067753
H	-1.445865	0.692020	-2.344351
H	-3.041107	0.398739	-1.653732
H	-2.488285	-2.054818	-1.555267
H	-0.924782	-1.701481	-2.282326
H	-3.505883	-1.257242	-3.600283
H	-2.296225	-2.251107	-4.071745

tryptamine, A-py S_0

C	-2.119976	0.112485	0.865240
N	-1.254226	0.119316	1.937452
C	0.034188	0.046167	1.470674
C	-0.033930	-0.013703	0.064254
C	-1.425728	0.029988	-0.300938
C	1.245041	0.032238	2.156165
C	2.400663	-0.040477	1.408971
C	2.357722	-0.096350	0.008578
C	1.156219	-0.083871	-0.665236
C	-1.996495	-0.025519	-1.680707
C	-1.946290	-1.418038	-2.304355
N	-2.519516	-1.391672	-3.645946
H	1.281110	0.078135	3.237593
H	3.359324	-0.053082	1.911320
H	3.285198	-0.150031	-0.546670
H	1.136242	-0.126662	-1.747254
H	-1.523879	0.189972	2.901539

H	-3.185182	0.172918	1.021418
H	-1.454431	0.670151	-2.330387
H	-3.035460	0.308134	-1.673360
H	-2.543589	-2.097059	-1.693034
H	-0.914117	-1.791013	-2.274275
H	-1.955697	-0.828801	-4.270916
H	-2.577279	-2.320837	-4.041017

tryptamine, A-py S_1

C	-2.169197	0.117784	0.884078
N	-1.295521	0.101664	1.899236
C	0.027873	0.047055	1.438466
C	-0.036524	0.036877	0.039785
C	-1.406721	0.079696	-0.322890
C	1.203562	-0.013517	2.167010
C	2.409446	-0.076637	1.374983
C	2.377775	-0.084776	0.006469
C	1.157195	-0.028904	-0.721877
C	-1.976563	0.014818	-1.684883
C	-1.911188	-1.405443	-2.270064
N	-2.512867	-1.423499	-3.594317
H	1.230836	-0.015670	3.246455
H	3.361580	-0.118907	1.887622
H	3.310869	-0.131924	-0.540495
H	1.145739	-0.005915	-1.801685
H	-1.548821	0.139999	2.874180
H	-3.233252	0.187645	1.030070
H	-1.416186	0.683824	-2.344759
H	-3.017686	0.340819	-1.690899
H	-2.483113	-2.076850	-1.626888
H	-0.868058	-1.743271	-2.244569
H	-1.937033	-0.933650	-4.267449
H	-2.642236	-2.368839	-3.928478

tryptamine, A-up S_0

C	-2.119182	0.127812	0.877004
N	-1.251303	0.106990	1.947162
C	0.035811	0.036365	1.476224
C	-0.035117	0.007042	0.069180
C	-1.427273	0.068485	-0.292219
C	1.247838	0.000246	2.158819
C	2.401329	-0.064284	1.407707
C	2.355435	-0.090713	0.006540
C	1.152905	-0.055714	-0.664469

C	-1.994553	0.032151	-1.673879
C	-1.956635	-1.362056	-2.315728
N	-2.465541	-1.439128	-3.676486
H	1.286355	0.022731	3.240878
H	3.360873	-0.094148	1.907600
H	3.281401	-0.139779	-0.551561
H	1.130938	-0.076618	-1.747085
H	-1.518687	0.155219	2.913279
H	-3.183643	0.189971	1.037806
H	-1.447950	0.728397	-2.318350
H	-3.030813	0.381272	-1.654571
H	-2.530093	-2.054066	-1.695645
H	-0.931486	-1.736776	-2.314887
H	-1.928534	-0.856293	-4.305934
H	-3.430836	-1.139197	-3.728145

tryptamine, A-up S_1

C	-2.166086	0.121045	0.890316
N	-1.289862	0.078877	1.903754
C	0.032515	0.034711	1.441710
C	-0.032477	0.059532	0.042952
C	-1.403595	0.118992	-0.317650
C	1.208689	-0.043725	2.167501
C	2.414015	-0.090965	1.374405
C	2.381135	-0.067269	0.006390
C	1.159844	0.008723	-0.719676
C	-1.965439	0.078246	-1.680162
C	-1.958145	-1.361313	-2.263727
N	-2.469552	-1.479958	-3.611088
H	1.236275	-0.070510	3.246660
H	3.366214	-0.148480	1.885338
H	3.313370	-0.105370	-0.542728
H	1.148476	0.049226	-1.799049
H	-1.541930	0.093711	2.879715
H	-3.229298	0.191839	1.041603
H	-1.372412	0.713243	-2.343265
H	-2.991514	0.455049	-1.686450
H	-2.544634	-2.009960	-1.611155
H	-0.934186	-1.736567	-2.240924
H	-1.923933	-0.948745	-4.276403
H	-3.436250	-1.192412	-3.684847

tryptamine, Ph-out S_0

C	0.006284	-0.000803	0.083307

C	0.046411	0.065233	1.490896
C	1.243668	0.079899	2.200474
C	2.414299	0.031937	1.475506
C	2.398851	-0.031299	0.074459
C	1.212111	-0.047710	-0.624845
N	-1.251363	0.111085	1.934179
H	1.257385	0.129452	3.282285
H	3.363355	0.042770	1.995978
H	3.337862	-0.067562	-0.462602
H	1.207060	-0.112952	-1.705095
C	-1.380831	0.012387	-0.307655
C	-2.097058	0.085861	0.847111
H	-1.538953	0.188795	2.892583
H	-3.165558	0.133194	0.985176
C	-1.938206	-0.044062	-1.696444
H	-1.303240	0.532718	-2.372781
C	-2.083072	-1.456305	-2.261302
H	-2.923056	0.429169	-1.704597
H	-2.545262	-1.387228	-3.248735
N	-0.785489	-2.100347	-2.421802
H	-2.774041	-2.020649	-1.618857
H	-0.339991	-2.248807	-1.524749
H	-0.876192	-3.000668	-2.873279

tryptamine, Ph-out S_1

C	0.000726	0.022294	0.065705
C	0.036031	0.081590	1.466585
C	1.195086	0.058066	2.221574
C	2.421315	-0.009204	1.461104
C	2.419272	-0.067823	0.094005
C	1.215236	-0.063971	-0.663530
N	-1.294627	0.140112	1.898965
H	1.196899	0.101869	3.300613
H	3.361652	-0.015026	1.996558
H	3.364169	-0.117978	-0.431985
H	1.226684	-0.086697	-1.742890
C	-1.362706	0.047600	-0.325950
C	-2.148484	0.116608	0.867081
H	-1.566719	0.208812	2.867197
H	-3.215397	0.185332	0.991318
C	-1.934841	-0.042539	-1.689502
H	-1.301449	0.494349	-2.397976
C	-2.077226	-1.490716	-2.189837
H	-2.923889	0.422097	-1.696401
H	-2.677788	-1.468510	-3.101576

N	-0.781994	-2.057546	-2.516446
H	-2.644683	-2.062902	-1.442078
H	-0.156225	-2.072452	-1.719027
H	-0.866050	-2.999245	-2.874299

tryptamine, Ph-up S_0

C	-2.072974	0.022076	0.815215
N	-1.240309	0.016932	1.912272
C	0.062724	0.034519	1.484301
C	0.038984	0.044721	0.074761
C	-1.341763	0.034322	-0.332888
C	1.251412	0.047334	2.208087
C	2.430961	0.075091	1.496998
C	2.432938	0.091286	0.094516
C	1.253978	0.076404	-0.617176
C	-1.874583	0.010333	-1.731197
C	-2.118527	-1.403089	-2.283133
N	-0.957187	-2.270843	-2.380916
H	1.251865	0.037895	3.291013
H	3.373445	0.086217	2.028984
H	3.378227	0.117388	-0.431871
H	1.269338	0.091511	-1.699743
H	-1.541238	0.025026	2.869794
H	-3.143751	0.023061	0.943229
H	-1.182550	0.536466	-2.395187
H	-2.817527	0.562833	-1.773353
H	-2.563933	-1.321954	-3.277683
H	-2.858059	-1.903461	-1.653535
H	-0.511483	-2.390066	-1.480027
H	-0.266338	-1.894372	-3.017403

tryptamine, Ph-up S_1

C	-2.151453	0.127600	0.860527
N	-1.299993	0.118961	1.894852
C	0.032092	0.077191	1.463315
C	-0.000570	0.072152	0.062512
C	-1.363822	0.100662	-0.330442
C	1.190704	0.016739	2.219228
C	2.415539	-0.028657	1.458612
C	2.417714	-0.030587	0.090057
C	1.214830	0.013470	-0.668947
C	-1.917377	0.004665	-1.691594
C	-2.019741	-1.472018	-2.191342
N	-0.775866	-2.149664	-2.445028

H	1.190649	0.011576	3.299023
H	3.355247	-0.062841	1.994244
H	3.364475	-0.061887	-0.434095
H	1.233936	0.082815	-1.746316
H	-1.574154	0.159983	2.863924
H	-3.218865	0.189840	0.985004
H	-1.294159	0.559042	-2.396517
H	-2.921527	0.436685	-1.718152
H	-2.605083	-1.464153	-3.112870
H	-2.591233	-2.044651	-1.459078
H	-0.163123	-2.170273	-1.638519
H	-0.264561	-1.737039	-3.213309

tryptamine, Py-out S_0

C	0.519294	0.453394	0.223581
C	0.594960	0.528072	1.629079
C	1.807683	0.489349	2.310137
C	2.957747	0.375704	1.559311
C	2.907449	0.304146	0.159995
C	1.704065	0.342137	-0.509820
N	-0.689226	0.640653	2.100500
H	1.849549	0.548118	3.390729
H	3.917799	0.343008	2.058085
H	3.830831	0.218916	-0.398105
H	1.678409	0.288264	-1.591065
C	-0.873045	0.531603	-0.136288
C	-1.560135	0.643323	1.032312
H	-0.952460	0.729393	3.064929
H	-2.623282	0.728323	1.189975
C	-1.450377	0.470433	-1.514366
H	-0.892091	1.136874	-2.177607
C	-1.445305	-0.934917	-2.114609
H	-2.481389	0.828187	-1.492954
H	-0.407293	-1.283702	-2.204036
N	-2.288262	-1.827603	-1.329387
H	-1.855234	-0.883511	-3.125492
H	-2.324166	-2.752612	-1.736600
H	-1.925502	-1.917551	-0.388287

tryptamine, Py-out S_1

C	0.523012	0.481543	0.206252
C	0.599395	0.532166	1.603340
C	1.780104	0.473300	2.324959
C	2.978108	0.367374	1.525475

C	2.934860	0.319934	0.158351
C	1.708721	0.372555	-0.562284
N	-0.718555	0.628363	2.073132
H	1.816687	0.512095	3.403417
H	3.933804	0.325164	2.031488
H	3.862402	0.241820	-0.394444
H	1.688790	0.357937	-1.641978
C	-0.850339	0.549832	-0.146678
C	-1.600951	0.634699	1.065685
H	-0.962856	0.688636	3.049348
H	-2.664082	0.706034	1.216251
C	-1.429545	0.484524	-1.506189
H	-0.839579	1.115913	-2.175763
C	-1.431967	-0.943341	-2.074812
H	-2.456248	0.854367	-1.499736
H	-0.394460	-1.294619	-2.132074
N	-2.302551	-1.809256	-1.292388
H	-1.822948	-0.900623	-3.092339
H	-2.449765	-2.695468	-1.756541
H	-1.902048	-2.002960	-0.382484

tryptamine, Py-up S_0

C	-2.116581	0.250027	0.894500
N	-1.242144	0.230250	1.959779
C	0.038046	0.097347	1.482852
C	-0.044017	0.027829	0.077872
C	-1.436160	0.129321	-0.277183
C	1.252578	0.036842	2.159224
C	2.397362	-0.093918	1.403478
C	2.340581	-0.161350	0.004138
C	1.135614	-0.101884	-0.660776
C	-2.012058	0.076228	-1.654301
C	-2.003153	-1.331574	-2.272589
N	-2.788120	-2.335784	-1.575259
H	1.299568	0.091553	3.239781
H	3.358667	-0.144308	1.898286
H	3.260143	-0.261478	-0.557656
H	1.105249	-0.153387	-1.742010
H	-1.499644	0.322341	2.925418
H	-3.176406	0.361143	1.059227
H	-1.457069	0.751062	-2.313713
H	-3.042093	0.443599	-1.632534
H	-0.975121	-1.694334	-2.333376
H	-2.368721	-1.268334	-3.299925
H	-3.767579	-2.080896	-1.546555

H	-2.470421	-2.440675	-0.619788

tryptamine, Py-up S_1

C	-2.162122	0.253744	0.932010
N	-1.271406	0.234403	1.934691
C	0.039853	0.110826	1.457586
C	-0.046592	0.061249	0.059969
C	-1.420851	0.152804	-0.284882
C	1.222056	0.023785	2.171138
C	2.414355	-0.112280	1.366960
C	2.361162	-0.159305	0.000701
C	1.132477	-0.076081	-0.712574
C	-2.003268	0.087338	-1.639307
C	-1.983978	-1.343905	-2.237443
N	-2.798782	-2.332802	-1.566706
H	1.264366	0.057323	3.249690
H	3.370861	-0.179532	1.868353
H	3.282446	-0.261554	-0.558529
H	1.108222	-0.090367	-1.792285
H	-1.506946	0.309839	2.912053
H	-3.218646	0.380002	1.093239
H	-1.426512	0.732543	-2.308896
H	-3.032961	0.454721	-1.630847
H	-0.952789	-1.699551	-2.250371
H	-2.310905	-1.276047	-3.276544
H	-3.777755	-2.079288	-1.552309
H	-2.493765	-2.498237	-0.616782

porphycene S_0

C	-3.425118	1.914094	0.000000
C	-2.416675	0.907691	0.000000
N	-1.221180	1.542741	0.000000
C	-1.387482	2.890295	0.000000
C	-2.796146	3.126731	0.000000
C	-0.362915	3.840292	0.000000
C	1.012696	3.690492	0.000000
C	1.828253	2.550165	0.000000
H	-0.263033	1.127622	0.000000
N	1.414174	1.263874	0.000000
C	3.277141	2.589097	0.000000
C	3.703790	1.304686	0.000000
C	2.511847	0.490895	0.000000
C	2.416675	-0.907691	0.000000
C	3.425118	-1.914094	0.000000

C	2.796146	-3.126731	0.000000
C	1.387482	-2.890295	0.000000
N	1.221180	-1.542741	0.000000
C	0.362915	-3.840292	0.000000
C	-1.012696	-3.690492	0.000000
C	-1.828253	-2.550165	0.000000
C	-3.277141	-2.589097	0.000000
C	-3.703790	-1.304686	0.000000
C	-2.511847	-0.490895	0.000000
N	-1.414174	-1.263874	0.000000
H	0.263033	-1.127622	0.000000
H	3.255876	-4.102042	0.000000
H	4.486886	-1.729918	0.000000
H	0.719633	-4.863482	0.000000
H	-1.568292	-4.621445	0.000000
H	-3.878519	-3.485064	0.000000
H	-4.720547	-0.945506	0.000000
H	-4.486886	1.729918	0.000000
H	-3.255876	4.102042	0.000000
H	-0.719633	4.863482	0.000000
H	1.568292	4.621445	0.000000
H	3.878519	3.485064	0.000000
H	4.720547	0.945506	0.000000

porphycene S_1

C	-3.419140	1.952876	0.000000
C	-2.429520	0.933620	0.000000
N	-1.212514	1.559943	0.000000
C	-1.366396	2.901674	0.000000
C	-2.769771	3.159345	0.000000
C	-0.318564	3.853811	0.000000
C	1.041962	3.688460	0.000000
C	1.868750	2.528200	0.000000
H	-0.263333	1.131274	0.000000
N	1.439230	1.254773	0.000000
C	3.309418	2.558183	0.000000
C	3.732268	1.264329	0.000000
C	2.547690	0.461757	0.000000
C	2.429520	-0.933620	0.000000
C	3.419140	-1.952876	0.000000
C	2.769771	-3.159345	0.000000
C	1.366396	-2.901674	0.000000
N	1.212514	-1.559943	0.000000
C	0.318564	-3.853811	0.000000
C	-1.041962	-3.688460	0.000000

C	-1.868750	-2.528200	0.000000
C	-3.309418	-2.558183	0.000000
C	-3.732268	-1.264329	0.000000
C	-2.547690	-0.461757	0.000000
N	-1.439230	-1.254773	0.000000
H	0.263333	-1.131274	0.000000
H	3.213998	-4.141802	0.000000
H	4.483406	-1.784436	0.000000
H	0.667768	-4.879172	0.000000
H	-1.609734	-4.612530	0.000000
H	-3.917775	-3.449502	0.000000
H	-4.747746	-0.902395	0.000000
H	-4.483406	1.784436	0.000000
H	-3.213998	4.141802	0.000000
H	-0.667768	4.879172	0.000000
H	1.609734	4.612530	0.000000
H	3.917775	3.449502	0.000000
H	4.747746	0.902395	0.000000

porphine S_0

N	0.000000	-2.019344	0.000000
N	2.098453	0.000000	0.000000
C	1.079234	-2.835028	0.000000
C	0.672351	-4.230773	0.000000
C	2.406382	-2.424451	0.000000
C	2.872650	-1.122013	0.000000
C	4.230767	-0.680300	0.000000
H	1.342627	-5.076502	0.000000
H	3.161591	-3.199760	0.000000
H	5.084732	-1.338377	0.000000
H	1.086278	0.000000	0.000000
N	0.000000	2.019344	0.000000
N	-2.098453	0.000000	0.000000
C	1.079234	2.835028	0.000000
C	-1.079234	2.835028	0.000000
C	-1.079234	-2.835028	0.000000
C	0.672351	4.230773	0.000000
C	-0.672351	4.230773	0.000000
C	-0.672351	-4.230773	0.000000
C	2.406382	2.424451	0.000000
C	-2.406382	2.424451	0.000000
C	-2.406382	-2.424451	0.000000
C	2.872650	1.122013	0.000000
C	-2.872650	1.122013	0.000000
C	-2.872650	-1.122013	0.000000

C	4.230767	0.680300	0.000000
C	-4.230767	0.680300	0.000000
C	-4.230767	-0.680300	0.000000
H	1.342627	5.076502	0.000000
H	-1.342627	5.076502	0.000000
H	-1.342627	-5.076502	0.000000
H	3.161591	3.199760	0.000000
H	-3.161591	3.199760	0.000000
H	-3.161591	-3.199760	0.000000
H	5.084732	1.338377	0.000000
H	-5.084732	1.338377	0.000000
H	-5.084732	-1.338377	0.000000
H	-1.086278	0.000000	0.000000

porphine S_1

N	0.000000	-2.038321	0.000000
N	2.096582	0.000000	0.000000
C	1.082390	-2.857640	0.000000
C	0.673776	-4.249774	0.000000
C	2.411675	-2.433131	0.000000
C	2.874776	-1.124934	0.000000
C	4.232112	-0.681987	0.000000
H	1.342303	-5.096634	0.000000
H	3.171371	-3.203976	0.000000
H	5.086822	-1.338950	0.000000
H	1.086034	0.000000	0.000000
N	0.000000	2.038321	0.000000
N	-2.096582	0.000000	0.000000
C	1.082390	2.857640	0.000000
C	-1.082390	2.857640	0.000000
C	-1.082390	-2.857640	0.000000
C	0.673776	4.249774	0.000000
C	-0.673776	4.249774	0.000000
C	-0.673776	-4.249774	0.000000
C	2.411675	2.433131	0.000000
C	-2.411675	2.433131	0.000000
C	-2.411675	-2.433131	0.000000
C	2.874776	1.124934	0.000000
C	-2.874776	1.124934	0.000000
C	-2.874776	-1.124934	0.000000
C	4.232112	0.681987	0.000000
C	-4.232112	0.681987	0.000000
C	-4.232112	-0.681987	0.000000
H	1.342303	5.096634	0.000000
H	-1.342303	5.096634	0.000000

H	-1.342303	-5.096634	0.000000
H	3.171371	3.203976	0.000000
H	-3.171371	3.203976	0.000000
H	-3.171371	-3.203976	0.000000
H	5.086822	1.338950	0.000000
H	-5.086822	1.338950	0.000000
H	-5.086822	-1.338950	0.000000
H	-1.086034	0.000000	0.000000

chlorin S_0

C	0.000000	-4.224022	0.919736
C	0.000000	-2.872242	1.371718
N	0.000000	-2.088595	0.240423
C	0.000000	-2.853798	-0.876366
C	0.000000	-4.215322	-0.441359
C	0.000000	-2.410082	2.665576
C	0.000000	-1.078578	3.089395
N	0.000000	0.000000	2.272230
C	0.000000	1.078578	3.089395
C	0.000000	0.676100	4.475087
C	0.000000	-0.676100	4.475087
C	0.000000	2.410082	2.665576
C	0.000000	2.872242	1.371718
N	0.000000	2.088595	0.240423
C	0.000000	2.853798	-0.876366
C	0.000000	4.215322	-0.441359
C	0.000000	4.224022	0.919736
C	0.000000	2.400686	-2.195162
C	0.000000	1.097881	-2.641672
C	0.000000	0.763950	-4.122143
C	0.000000	-0.763950	-4.122143
C	0.000000	-1.097881	-2.641672
N	0.000000	0.000000	-1.868151
C	0.000000	-2.400686	-2.195162
H	-0.877728	1.186590	-4.612119
H	0.000000	3.176407	-2.950166
H	0.000000	5.064362	-1.105512
H	0.000000	1.344712	5.322220
H	0.000000	-1.344712	5.322220
H	-0.877728	-1.186590	-4.612119
H	0.000000	3.167771	3.439245
H	0.000000	-3.167771	3.439245
H	0.000000	-3.176407	-2.950166
H	0.000000	5.083292	1.571215
H	0.000000	-5.083292	1.571215

H	0.000000	-5.064362	-1.105512
H	0.877728	-1.186590	-4.612119
H	0.877728	1.186590	-4.612119
H	0.000000	-1.078484	0.259958
H	0.000000	1.078484	0.259958

chlorin S_1

C	0.000000	-4.231223	0.920279
C	0.000000	-2.878436	1.368042
N	0.000000	-2.095421	0.241319
C	0.000000	-2.868065	-0.883550
C	0.000000	-4.224746	-0.446445
C	0.000000	-2.412720	2.675777
C	0.000000	-1.082452	3.088975
N	0.000000	0.000000	2.270397
C	0.000000	1.082452	3.088975
C	0.000000	0.672116	4.485783
C	0.000000	-0.672116	4.485783
C	0.000000	2.412720	2.675777
C	0.000000	2.878436	1.368042
N	0.000000	2.095421	0.241319
C	0.000000	2.868065	-0.883550
C	0.000000	4.224746	-0.446445
C	0.000000	4.231223	0.920279
C	0.000000	2.409967	-2.202678
C	0.000000	1.099257	-2.645850
C	0.000000	0.763209	-4.121688
C	0.000000	-0.763209	-4.121688
C	0.000000	-1.099257	-2.645850
N	0.000000	0.000000	-1.864889
C	0.000000	-2.409967	-2.202678
H	-0.877316	1.186532	-4.613369
H	0.000000	3.181430	-2.961770
H	0.000000	5.076126	-1.107753
H	0.000000	1.342288	5.331470
H	0.000000	-1.342288	5.331470
H	-0.877316	-1.186532	-4.613369
H	0.000000	3.168635	3.449984
H	0.000000	-3.168635	3.449984
H	0.000000	-3.181430	-2.961770
H	0.000000	5.088813	1.573617
H	0.000000	-5.088813	1.573617
H	0.000000	-5.076126	-1.107753
H	0.877316	-1.186532	-4.613369
H	0.877316	1.186532	-4.613369

H	0.000000	-1.085675	0.258483
H	0.000000	1.085675	0.258483

Zn-tetraphenylporphine S_0

C	-3.781829	4.191866	1.161199
C	-3.485735	3.485722	0.000021
C	-4.191893	3.781803	-1.161152
C	-5.171242	4.762205	-1.162367
C	-5.459463	5.459414	0.000028
C	-4.762247	5.171199	1.162419
C	-2.428862	2.428860	0.000018
C	-1.098186	2.849287	-0.005399
N	0.000000	2.038877	0.019262
C	1.098186	2.849287	-0.005399
C	0.674913	4.224611	-0.056007
C	-0.674913	4.224611	-0.056007
C	2.428862	2.428860	0.000018
C	3.485735	3.485722	0.000021
C	4.191893	3.781803	-1.161152
C	5.171242	4.762205	-1.162367
C	5.459463	5.459414	0.000028
C	4.762247	5.171199	1.162419
C	3.781829	4.191866	1.161199
C	-2.849286	1.098184	0.005405
N	-2.038877	0.000000	-0.019341
C	-2.849286	-1.098184	0.005405
C	-4.224612	-0.674913	0.055969
C	-4.224612	0.674913	0.055969
C	-2.428862	-2.428860	0.000018
C	-3.485735	-3.485722	0.000021
C	-4.191893	-3.781803	-1.161152
C	-5.171242	-4.762205	-1.162367
C	-5.459463	-5.459414	0.000028
C	-4.762247	-5.171199	1.162419
C	-3.781829	-4.191866	1.161199
C	2.849286	1.098184	0.005405
N	2.038877	0.000000	-0.019341
C	2.849286	-1.098184	0.005405
C	4.224612	-0.674913	0.055969
C	4.224612	0.674913	0.055969
C	2.428862	-2.428860	0.000018
C	3.485735	-3.485722	0.000021
C	4.191893	-3.781803	-1.161152
C	5.171242	-4.762205	-1.162367
C	5.459463	-5.459414	0.000028

C	4.762247	-5.171199	1.162419
C	3.781829	-4.191866	1.161199
C	1.098186	-2.849287	-0.005399
N	0.000000	-2.038877	0.019262
C	-1.098186	-2.849287	-0.005399
C	-0.674913	-4.224611	-0.056007
C	0.674913	-4.224611	-0.056007
H	1.333648	-5.075397	-0.097286
H	5.075398	-1.333649	0.097240
H	1.333648	5.075397	-0.097286
H	-1.333648	5.075397	-0.097286
H	-1.333648	-5.075397	-0.097286
H	5.075398	1.333649	0.097240
H	-5.075398	1.333649	0.097240
H	-5.075398	-1.333649	0.097240
H	3.966672	3.239101	-2.070609
H	5.709145	4.983043	-2.075622
H	6.224902	6.224840	0.000030
H	4.983093	5.709093	2.075678
H	3.239123	3.966650	2.070654
H	3.966672	-3.239101	-2.070609
H	5.709145	-4.983043	-2.075622
H	6.224902	-6.224840	0.000030
H	4.983093	-5.709093	2.075678
H	3.239123	-3.966650	2.070654
H	-3.966672	-3.239101	-2.070609
H	-5.709145	-4.983043	-2.075622
H	-6.224902	-6.224840	0.000030
H	-4.983093	-5.709093	2.075678
H	-3.239123	-3.966650	2.070654
H	-3.966672	3.239101	-2.070609
H	-5.709145	4.983043	-2.075622
H	-6.224902	6.224840	0.000030
H	-4.983093	5.709093	2.075678
H	-3.239123	3.966650	2.070654
Zn	0.000000	0.000000	-0.000080

Zn-tetraphenylporphine S_1

C	-3.660136	4.324011	1.102030
C	-3.488384	3.490809	-0.000070
C	-4.320261	3.664632	-1.102996
C	-5.295231	4.648601	-1.106131
C	-5.458659	5.470793	-0.002423
C	-4.639010	5.304331	1.102514
C	-2.438491	2.434906	0.000547

C	-1.101094	2.849967	-0.011951
N	0.000000	2.036096	0.051257
C	1.101094	2.849967	-0.011951
C	0.676238	4.218954	-0.127356
C	-0.676238	4.218954	-0.127356
C	2.438491	2.434906	0.000547
C	3.488384	3.490809	-0.000070
C	4.320261	3.664632	-1.102996
C	5.295231	4.648601	-1.106131
C	5.458659	5.470793	-0.002423
C	4.639010	5.304331	1.102514
C	3.660136	4.324011	1.102030
C	-2.868834	1.098492	0.014618
N	-2.057658	0.000000	-0.049373
C	-2.868834	-1.098492	0.014618
C	-4.237785	-0.676872	0.129700
C	-4.237785	0.676872	0.129700
C	-2.438491	-2.434906	0.000547
C	-3.488384	-3.490809	-0.000070
C	-4.320261	-3.664632	-1.102996
C	-5.295231	-4.648601	-1.106131
C	-5.458659	-5.470793	-0.002423
C	-4.639010	-5.304331	1.102514
C	-3.660136	-4.324011	1.102030
C	2.868834	1.098492	0.014618
N	2.057658	0.000000	-0.049373
C	2.868834	-1.098492	0.014618
C	4.237785	-0.676872	0.129700
C	4.237785	0.676872	0.129700
C	2.438491	-2.434906	0.000547
C	3.488384	-3.490809	-0.000070
C	4.320261	-3.664632	-1.102996
C	5.295231	-4.648601	-1.106131
C	5.458659	-5.470793	-0.002423
C	4.639010	-5.304331	1.102514
C	3.660136	-4.324011	1.102030
C	1.101094	-2.849967	-0.011951
N	0.000000	-2.036096	0.051257
C	-1.101094	-2.849967	-0.011951
C	-0.676238	-4.218954	-0.127356
C	0.676238	-4.218954	-0.127356
H	1.332297	-5.067337	-0.219545
H	5.085239	-1.334140	0.220808
H	1.332297	5.067337	-0.219545
H	-1.332297	5.067337	-0.219545
H	-1.332297	-5.067337	-0.219545

H	5.085239	1.334140	0.220808
H	-5.085239	1.334140	0.220808
H	-5.085239	-1.334140	0.220808
H	4.192725	3.025630	-1.967566
H	5.927750	4.774807	-1.975676
H	6.222005	6.238268	-0.003450
H	4.762953	5.938681	1.971051
H	3.022871	4.194048	1.967475
H	4.192725	-3.025630	-1.967566
H	5.927750	-4.774807	-1.975676
H	6.222005	-6.238268	-0.003450
H	4.762953	-5.938681	1.971051
H	3.022871	-4.194048	1.967475
H	-4.192725	-3.025630	-1.967566
H	-5.927750	-4.774807	-1.975676
H	-6.222005	-6.238268	-0.003450
H	-4.762953	-5.938681	1.971051
H	-3.022871	-4.194048	1.967475
H	-4.192725	3.025630	-1.967566
H	-5.927750	4.774807	-1.975676
H	-6.222005	6.238268	-0.003450
H	-4.762953	5.938681	1.971051
H	-3.022871	4.194048	1.967475
Zn	0.000000	0.000000	0.001256

tetraphenylporphine S_0

C	-0.679158	4.221493	0.063330
C	-1.123724	2.865922	0.006731
N	0.000001	2.088925	-0.022180
C	1.123724	2.865924	0.006761
C	0.679155	4.221494	0.063351
C	2.442638	2.421401	-0.006017
C	2.842506	1.081499	-0.022606
N	2.025494	0.000001	0.007579
C	2.842506	-1.081497	-0.022634
C	4.235793	-0.671254	-0.089221
C	4.235793	0.671257	-0.089202
C	2.442638	-2.421399	-0.006067
C	1.123724	-2.865922	0.006731
N	-0.000001	-2.088925	-0.022180
C	-1.123724	-2.865924	0.006761
C	-0.679155	-4.221494	0.063351
C	0.679158	-4.221493	0.063330
C	-2.442638	-2.421401	-0.006017
C	-2.842506	-1.081499	-0.022606

N	-2.025494	-0.000001	0.007579
C	-2.842506	1.081497	-0.022634
C	-4.235793	0.671254	-0.089221
C	-4.235793	-0.671257	-0.089202
C	-2.442638	2.421399	-0.006067
H	-5.083260	-1.333740	-0.141064
C	-3.503002	-3.474741	0.001163
H	-1.332960	-5.075367	0.106923
H	-0.000002	-1.077376	-0.033019
H	5.083260	-1.333735	-0.141103
H	5.083260	1.333740	-0.141064
H	-5.083260	1.333735	-0.141103
C	3.503001	-3.474741	0.001068
C	3.503002	3.474741	0.001163
C	-3.503001	3.474741	0.001068
H	1.332966	-5.075365	0.106882
H	1.332960	5.075367	0.106923
H	-1.332966	5.075365	0.106882
H	0.000002	1.077376	-0.033019
C	3.791463	-4.198853	-1.150977
C	4.775072	-5.175038	-1.144340
C	5.482351	-5.442248	0.016949
C	5.201179	-4.727379	1.170377
C	4.218739	-3.750226	1.161532
H	3.242348	-3.988436	-2.060165
H	4.991010	-5.726219	-2.050812
H	6.250593	-6.204832	0.022965
H	5.747434	-4.931498	2.082539
H	3.999590	-3.192723	2.063434
C	-3.791486	-4.198885	-1.150857
C	-4.775098	-5.175067	-1.144175
C	-5.482358	-5.442242	0.017133
C	-5.201164	-4.727341	1.170536
C	-4.218722	-3.750191	1.161647
H	-3.242387	-3.988495	-2.060061
H	-4.991053	-5.726274	-2.050628
H	-6.250602	-6.204824	0.023184
H	-5.747404	-4.931433	2.082713
H	-3.999556	-3.192663	2.063528
C	-3.791463	4.198853	-1.150977
C	-4.775072	5.175038	-1.144340
C	-5.482351	5.442248	0.016949
C	-5.201179	4.727379	1.170377
C	-4.218739	3.750226	1.161532
H	-3.242348	3.988436	-2.060165
H	-4.991010	5.726219	-2.050812

H	-6.250593	6.204832	0.022965
H	-5.747434	4.931498	2.082539
H	-3.999590	3.192723	2.063434
C	3.791486	4.198885	-1.150857
C	4.775098	5.175067	-1.144175
C	5.482358	5.442242	0.017133
C	5.201164	4.727341	1.170536
C	4.218722	3.750191	1.161647
H	3.242387	3.988495	-2.060061
H	4.991053	5.726274	-2.050628
H	6.250602	6.204824	0.023184
H	5.747404	4.931433	2.082713
H	3.999556	3.192663	2.063528

tetraphenylporphine S_1

C	4.211672	0.744179	0.127178
C	2.853628	1.170941	0.016072
N	2.091756	0.032144	-0.045475
C	2.887556	-1.083381	0.011999
C	4.232155	-0.616373	0.124435
C	2.466323	-2.413868	-0.017505
C	1.127698	-2.848806	-0.055584
N	0.030977	-2.046743	0.005809
C	-1.040912	-2.881916	-0.051669
C	-0.609508	-4.258300	-0.176654
C	0.738025	-4.237719	-0.179320
C	-2.392168	-2.488040	-0.010232
C	-2.853628	-1.170941	0.016072
N	-2.091756	-0.032144	-0.045475
C	-2.887556	1.083381	0.011999
C	-4.232155	0.616373	0.124435
C	-4.211672	-0.744179	0.127178
C	-2.466323	2.413868	-0.017505
C	-1.127698	2.848806	-0.055584
N	-0.030977	2.046743	0.005809
C	1.040912	2.881916	-0.051669
C	0.609508	4.258300	-0.176654
C	-0.738025	4.237719	-0.179320
C	2.392168	2.488040	-0.010232
H	-1.410364	5.073285	-0.273086
C	-3.534126	3.452797	-0.005160
H	-5.094488	1.254564	0.207512
H	-1.082026	-0.017198	-0.069035
H	-1.256477	-5.113936	-0.267921
H	1.410364	-5.073285	-0.273086

H	1.256477	5.113936	-0.267921
C	-3.427199	-3.559443	0.009541
C	3.534126	-3.452797	-0.005160
C	3.427199	3.559443	0.009541
H	-5.054536	-1.407534	0.212772
H	5.094488	-1.254564	0.207512
H	5.054536	1.407534	0.212772
H	1.082026	0.017198	-0.069035
C	-4.266741	-3.760097	-1.082356
C	-5.226721	-4.759097	-1.062021
C	-5.365065	-5.569061	0.053649
C	-4.535499	-5.376426	1.147272
C	-3.572132	-4.381589	1.123637
H	-4.157029	-3.131723	-1.957142
H	-5.866391	-4.906462	-1.922944
H	-6.116088	-6.348413	0.070753
H	-4.639328	-6.002337	2.024491
H	-2.925319	-4.232310	1.978799
C	-4.374005	3.624058	-1.101773
C	-5.365065	4.592331	-1.089092
C	-5.534597	5.400377	0.023672
C	-4.704989	5.236786	1.121975
C	-3.710606	4.272748	1.105986
H	-4.240257	2.996927	-1.974099
H	-6.004716	4.717126	-1.953588
H	-6.309972	6.155613	0.034949
H	-4.833071	5.861299	1.996981
H	-3.063980	4.146001	1.964924
C	4.266741	3.760097	-1.082356
C	5.226721	4.759097	-1.062021
C	5.365065	5.569061	0.053649
C	4.535499	5.376426	1.147272
C	3.572132	4.381589	1.123637
H	4.157029	3.131723	-1.957142
H	5.866391	4.906462	-1.922944
H	6.116088	6.348413	0.070753
H	4.639328	6.002337	2.024491
H	2.925319	4.232310	1.978799
C	4.374005	-3.624058	-1.101773
C	5.365065	-4.592331	-1.089092
C	5.534597	-5.400377	0.023672
C	4.704989	-5.236786	1.121975
C	3.710606	-4.272748	1.105986
H	4.240257	-2.996927	-1.974099
H	6.004716	-4.717126	-1.953588
H	6.309972	-6.155613	0.034949

H	4.833071	-5.861299	1.996981
H	3.063980	-4.146001	1.964924

CAM-B3LYP/TZVP geometries – Group II

tetrafluorobenzene S_0

C	-1.186683	0.691323	0.000000
C	-1.186683	-0.691323	0.000000
C	0.000000	-1.393072	0.000000
C	1.186683	-0.691323	0.000000
C	1.186683	0.691323	0.000000
C	0.000000	1.393072	0.000000
F	-2.350141	-1.347609	0.000000
H	0.000000	-2.473768	0.000000
F	2.350141	-1.347609	0.000000
F	2.350141	1.347609	0.000000
H	0.000000	2.473768	0.000000
F	-2.350141	1.347609	0.000000

tetrafluorobenzene S_1

C	1.161874	-0.705860	0.107230
C	1.161874	0.705860	0.107230
C	0.000000	1.461433	0.305642
C	-1.161874	0.705860	0.107230
C	-1.161874	-0.705860	0.107230
C	0.000000	-1.461433	0.305642
F	2.305639	1.315120	-0.201809
H	0.000000	2.505500	0.581639
F	-2.305639	1.315120	-0.201809
F	-2.305639	-1.315120	-0.201809
H	0.000000	-2.505500	0.581639
F	2.305639	-1.315120	-0.201809

benzonitrile S_0

C	0.000000	0.000000	-1.052066
C	-1.207438	0.000000	-0.357767
C	-1.201751	0.000000	1.024940
C	0.000000	0.000000	1.716328
C	1.201751	0.000000	1.024940
C	1.207438	0.000000	-0.357767
H	-2.139765	0.000000	-0.905875
H	-2.139223	0.000000	1.565028

H	0.000000	0.000000	2.798559
H	2.139223	0.000000	1.565028
H	2.139765	0.000000	-0.905875
C	0.000000	0.000000	-2.484211
N	0.000000	0.000000	-3.631253

benzonitrile S_1

C	0.000000	0.000000	-1.102010
C	-1.222482	0.000000	-0.372116
C	-1.212237	0.000000	1.043259
C	0.000000	0.000000	1.760446
C	1.212237	0.000000	1.043259
C	1.222482	0.000000	-0.372116
H	-2.160935	0.000000	-0.907206
H	-2.155430	0.000000	1.571136
H	0.000000	0.000000	2.839835
H	2.155430	0.000000	1.571136
H	2.160935	0.000000	-0.907206
C	0.000000	0.000000	-2.507017
N	0.000000	0.000000	-3.661400

o-fluorophenol, *cis* S_0

C	0.325657	1.448449	0.000000
C	-0.869174	0.771496	0.000000
C	-0.945298	-0.612362	0.000000
C	0.237143	-1.333229	0.000000
C	1.452925	-0.669010	0.000000
C	1.503981	0.716555	0.000000
F	-2.045263	1.450873	0.000000
O	-2.136514	-1.261125	0.000000
H	0.182453	-2.413452	0.000000
H	2.370002	-1.242943	0.000000
H	2.455436	1.230132	0.000000
H	0.321513	2.529968	0.000000
H	-2.852852	-0.615372	0.000000

o-fluorophenol, *cis* S_1

C	1.236481	-0.232152	-0.738760
C	0.008256	-0.082187	-0.089730
C	-0.005818	-0.031112	1.347279
C	1.174634	0.029406	2.090682
C	2.388866	0.103481	1.411219
C	2.403585	-0.012111	0.013324

F	-0.978965	0.738551	-0.685362
O	-1.172339	-0.097660	1.984180
H	1.124950	-0.115848	3.162694
H	3.316569	0.203679	1.955552
H	3.346873	0.090754	-0.511835
H	1.286452	-0.366883	-1.810260
H	-1.874165	-0.227918	1.320956

o-fluorophenol, *trans* S_0

C	0.289912	1.257003	0.000000
C	-0.942206	0.614352	0.000000
C	-0.958505	-0.771617	0.000000
C	0.227356	-1.491188	0.000000
C	1.443690	-0.832382	0.000000
C	1.471877	0.555294	0.000000
O	-2.058713	1.386554	0.000000
H	-1.911198	-1.289514	0.000000
H	0.192912	-2.572410	0.000000
H	2.370210	-1.389768	0.000000
H	2.402614	1.106400	0.000000
F	0.313786	2.599728	0.000000
H	-2.841745	0.827548	0.000000

o-fluorophenol, *trans* S_1

C	0.817781	1.031378	0.102194
C	-0.585987	0.970015	0.084215
C	-1.270300	-0.287388	0.099697
C	-0.469443	-1.422165	-0.074348
C	0.938629	-1.334720	-0.065852
C	1.616324	-0.126383	0.164828
O	-1.250980	2.113356	-0.101746
H	-2.296888	-0.352565	0.440903
H	-0.928150	-2.396054	-0.185546
H	1.511945	-2.241286	-0.218410
H	2.685429	-0.061767	0.289269
F	1.394509	2.208957	-0.172578
H	-2.162897	1.898622	-0.362625

m-fluorophenol, *cis* S_0

C	0.308844	1.403467	0.000000
C	-0.924405	0.785082	0.000000
C	-0.962838	-0.602140	0.000000
C	0.214703	-1.338456	0.000000

C	1.429125	-0.678568	0.000000
C	1.496432	0.707980	0.000000
O	-2.134176	-1.293843	0.000000
F	0.339697	2.750416	0.000000
H	0.157419	-2.417776	0.000000
H	2.345546	-1.253959	0.000000
H	2.436526	1.240258	0.000000
H	-1.825613	1.385161	0.000000
H	-2.881260	-0.687622	0.000000

m-fluorophenol, *cis* S_1

C	1.225767	-0.039253	-0.684813
C	-0.044543	0.024216	-0.099103
C	-0.021003	0.030141	1.323643
C	1.164470	0.019534	2.083588
C	2.424304	0.100658	1.440104
C	2.429754	-0.032525	0.034013
O	-1.172818	-0.015334	2.009285
F	1.300013	-0.118905	-2.023244
H	1.075616	-0.097726	3.154793
H	3.343116	0.131291	2.001472
H	3.353417	-0.120815	-0.522486
H	-0.918170	0.310569	-0.668792
H	-1.904563	-0.191851	1.401490

m-fluorophenol, *trans* S_0

C	0.268354	1.299035	0.000000
C	-0.944971	0.625945	0.000000
C	-0.980164	-0.762444	0.000000
C	0.207577	-1.475988	0.000000
C	1.430847	-0.827883	0.000000
C	1.423860	0.552399	0.000000
O	-2.072182	1.387400	0.000000
H	-1.930792	-1.282565	0.000000
H	0.177303	-2.557604	0.000000
H	2.368128	-1.365070	0.000000
F	2.602102	1.204227	0.000000
H	0.301876	2.378849	0.000000
H	-2.851939	0.823709	0.000000

m-fluorophenol, *trans* S_1

C	1.079930	-0.016077	0.000000
C	0.327142	1.179962	0.000000

C	-1.088421	1.208884	0.000000
C	-1.819495	-0.006210	0.000000
C	-1.083634	-1.215802	0.000000
C	0.317644	-1.194042	0.000000
O	1.034791	2.319871	0.000000
H	-1.597459	2.164740	0.000000
H	-2.896919	-0.012931	0.000000
H	-1.581485	-2.175620	0.000000
F	0.966927	-2.369159	0.000000
H	2.156831	-0.011598	0.000000
H	0.443002	3.082130	0.000000

p-fluorophenol S_0

C	0.271326	1.311308	0.000000
C	-0.945792	0.644374	0.000000
C	-0.976933	-0.742146	0.000000
C	0.206609	-1.465258	0.000000
C	1.401973	-0.784040	0.000000
C	1.453829	0.594404	0.000000
O	-2.077680	1.407246	0.000000
H	-1.925895	-1.266010	0.000000
H	0.203595	-2.546481	0.000000
F	2.557162	-1.484183	0.000000
H	2.412666	1.094295	0.000000
H	0.276365	2.392549	0.000000
H	-2.857246	0.843932	0.000000

p-fluorophenol S_1

C	1.262725	0.678029	0.000000
C	0.027237	1.357636	0.000000
C	-1.232970	0.707949	0.000000
C	-1.247438	-0.702885	0.000000
C	-0.006482	-1.359880	0.000000
C	1.248108	-0.734186	0.000000
O	0.091625	2.694728	0.000000
H	-2.147003	1.285952	0.000000
H	-2.157966	-1.280929	0.000000
F	-0.026673	-2.692359	0.000000
H	2.146406	-1.330571	0.000000
H	2.176747	1.250999	0.000000
H	-0.797621	3.071110	0.000000

phenylacetylene S_0

C	1.203167	0.000000	-0.013243
C	0.000000	0.000000	-0.719475
C	-1.203167	0.000000	-0.013243
C	-1.199541	0.000000	1.369818
C	0.000000	0.000000	2.064871
C	1.199541	0.000000	1.369818
C	0.000000	0.000000	-2.148902
C	0.000000	0.000000	-3.346027
H	-2.136964	0.000000	-0.559262
H	-2.138522	0.000000	1.908147
H	0.000000	0.000000	3.147186
H	2.138522	0.000000	1.908147
H	2.136964	0.000000	-0.559262
H	0.000000	0.000000	-4.408593

phenylacetylene S_1

C	1.228227	0.000000	-0.029104
C	0.000000	0.000000	-0.752371
C	-1.228227	0.000000	-0.029104
C	-1.219473	0.000000	1.387051
C	0.000000	0.000000	2.090545
C	1.219473	0.000000	1.387051
C	0.000000	0.000000	-2.151889
C	0.000000	0.000000	-3.357382
H	-2.160799	0.000000	-0.573398
H	-2.156416	0.000000	1.925257
H	0.000000	0.000000	3.171344
H	2.156416	0.000000	1.925257
H	2.160799	0.000000	-0.573398
H	0.000000	0.000000	-4.419858

aniline S_0

C	0.916126	0.026431	0.000000
C	0.204032	0.034474	1.198934
C	-1.179193	0.042897	1.193596
C	-1.884273	0.047695	0.000000
C	-1.179193	0.042897	-1.193596
C	0.204032	0.034474	-1.198934
H	0.742897	0.036277	2.139356
H	-2.965853	0.054105	0.000000
H	-1.711666	0.047051	2.136536
H	-1.711666	0.047051	-2.136536
H	0.742897	0.036277	-2.139356
N	2.306144	0.066950	0.000000

H	2.757863	-0.258285	-0.838507
H	2.757863	-0.258285	0.838507

aniline S_1

C	0.894691	-0.034154	0.000000
C	0.223350	-0.008481	1.243689
C	-1.192413	0.045594	1.234105
C	-1.863008	0.071162	0.000000
C	-1.192413	0.045594	-1.234105
C	0.223350	-0.008481	-1.243689
H	0.789843	-0.030162	2.164494
H	-2.945622	0.112424	0.000000
H	-1.750587	0.066903	2.157758
H	-1.750587	0.066903	-2.157758
H	0.789843	-0.030162	-2.164494
N	2.247736	-0.085962	0.000000
H	2.762903	-0.105599	-0.863656
H	2.762903	-0.105599	0.863656

catechol S_0

C	0.469742	1.273766	0.000000
C	-0.743385	0.616338	0.000000
C	-0.793566	-0.776151	0.000000
C	0.383164	-1.499226	0.000000
C	1.604138	-0.840033	0.000000
C	1.650669	0.542907	0.000000
O	-1.966575	1.241307	0.000000
O	-1.989362	-1.420296	0.000000
H	0.324672	-2.579391	0.000000
H	2.520756	-1.414535	0.000000
H	2.600523	1.060078	0.000000
H	0.494094	2.357942	0.000000
H	-1.861668	2.196739	0.000000
H	-2.693200	-0.759446	0.000000

catechol S_1

C	0.473156	1.342957	0.000000
C	-0.755741	0.623035	0.000000
C	-0.800023	-0.782568	0.000000
C	0.387459	-1.568612	0.000000
C	1.595670	-0.856688	0.000000
C	1.637107	0.555859	0.000000
O	-1.964324	1.243592	0.000000

O	-1.982436	-1.417538	0.000000
H	0.324017	-2.643920	0.000000
H	2.532991	-1.396210	0.000000
H	2.603729	1.041775	0.000000
H	0.496029	2.422275	0.000000
H	-1.851169	2.199748	0.000000
H	-2.696464	-0.763704	0.000000

resorcinol, isomer 1 S_0

C	0.075040	1.142820	0.000000
C	-1.133930	0.463028	0.000000
C	-1.165581	-0.923019	0.000000
C	0.032970	-1.621802	0.000000
C	1.247574	-0.964970	0.000000
C	1.258959	0.424447	0.000000
O	-2.265631	1.222432	0.000000
H	-2.112239	-1.450053	0.000000
H	0.014476	-2.704058	0.000000
H	2.185545	-1.501559	0.000000
O	2.474016	1.039297	0.000000
H	0.069183	2.226010	0.000000
H	-3.040860	0.652732	0.000000
H	2.360478	1.994686	0.000000

resorcinol, isomer 1 S_1

C	-0.001616	1.057442	0.052315
C	-1.189976	0.304495	-0.000880
C	-1.200368	-1.106964	-0.034018
C	-0.000087	-1.846211	0.093131
C	1.205940	-1.107828	0.005193
C	1.190976	0.299580	0.028607
O	-2.343328	1.006256	-0.037351
H	-2.147427	-1.617529	-0.171640
H	-0.001409	-2.923333	0.091992
H	2.163028	-1.599239	-0.106829
O	2.392403	0.914873	-0.014556
H	-0.022942	2.110012	0.295595
H	-3.097882	0.407091	-0.003706
H	2.263681	1.857476	-0.178202

resorcinol, isomer 2 S_0

C	1.194078	0.000000	-0.543984
C	0.000000	0.000000	-1.243606

C	-1.194078	0.000000	-0.543984
C	-1.205154	0.000000	0.846152
C	0.000000	0.000000	1.526314
C	1.205154	0.000000	0.846152
O	-2.340820	0.000000	-1.279033
O	2.340820	0.000000	-1.279033
H	-2.143875	0.000000	1.387192
H	0.000000	0.000000	2.608675
H	2.143875	0.000000	1.387192
H	0.000000	0.000000	-2.324124
H	-3.104600	0.000000	-0.694197
H	3.104600	0.000000	-0.694197

resorcinol, isomer 2 S_1

C	1.193235	0.000000	-0.328062
C	0.000000	0.000000	-1.075730
C	-1.193235	0.000000	-0.328062
C	-1.209683	0.000000	1.084361
C	0.000000	0.000000	1.822068
C	1.209683	0.000000	1.084361
O	-2.345722	0.000000	-1.034603
O	2.345722	0.000000	-1.034603
H	-2.163289	0.000000	1.599425
H	0.000000	0.000000	2.899433
H	2.163289	0.000000	1.599425
H	0.000000	0.000000	-2.152619
H	-3.101891	0.000000	-0.437241
H	3.101891	0.000000	-0.437241

resorcinol, isomer 3 S_0

C	1.199404	0.000000	-0.285915
C	0.000000	0.000000	-0.985474
C	-1.199404	0.000000	-0.285915
C	-1.207924	0.000000	1.099811
C	0.000000	0.000000	1.775560
C	1.207924	0.000000	1.099811
O	-2.404405	0.000000	-0.922515
O	2.404405	0.000000	-0.922515
H	-2.153779	0.000000	1.622423
H	0.000000	0.000000	2.858013
H	2.153779	0.000000	1.622423
H	0.000000	0.000000	-2.071269
H	2.278122	0.000000	-1.875979
H	-2.278122	0.000000	-1.875979

resorcinol, isomer 3 S_1

C	-0.019486	-0.302054	1.185559
C	-0.099985	-1.070347	0.000000
C	-0.019486	-0.302054	-1.185559
C	0.026138	1.105174	-1.197281
C	-0.081257	1.844475	0.000000
C	0.026138	1.105174	1.197281
O	0.053602	-0.914514	-2.385967
O	0.053602	-0.914514	2.385967
H	0.174133	1.591892	-2.152597
H	-0.085686	2.921725	0.000000
H	0.174133	1.591892	2.152597
H	-0.578892	-2.046753	0.000000
H	0.233155	-1.854372	2.248621
H	0.233155	-1.854372	-2.248621

hydroquinone, *cis* S_0

C	-0.694479	0.000000	1.087016
C	0.694479	0.000000	1.087016
C	1.389775	0.000000	-0.108784
C	0.690038	0.000000	-1.307801
C	-0.690038	0.000000	-1.307801
C	-1.389775	0.000000	-0.108784
O	2.756833	0.000000	-0.175184
O	-2.756833	0.000000	-0.175184
H	1.244299	0.000000	-2.236574
H	-1.244299	0.000000	-2.236574
H	-1.229478	0.000000	2.030069
H	1.229478	0.000000	2.030069
H	-3.128678	0.000000	0.711548
H	3.128678	0.000000	0.711548

hydroquinone, *cis* S_1

C	0.704564	0.000000	-1.128276
C	-0.704564	0.000000	-1.128276
C	-1.369667	0.000000	0.120154
C	-0.705057	0.000000	1.358680
C	0.705057	0.000000	1.358680
C	1.369667	0.000000	0.120154
O	-2.711859	0.000000	0.164058
O	2.711859	0.000000	0.164058
H	-1.286432	0.000000	2.267263

H	1.286432	0.000000	2.267263
H	1.271744	0.000000	-2.049389
H	-1.271744	0.000000	-2.049389
H	3.070453	0.000000	-0.731720
H	-3.070453	0.000000	-0.731720

hydroquinone, *trans* S_0

C	0.020605	1.384747	0.000000
C	-1.191399	0.715628	0.000000
C	-1.206971	-0.671228	0.000000
C	-0.020605	-1.384747	0.000000
C	1.191399	-0.715628	0.000000
C	1.206971	0.671228	0.000000
O	-2.333135	1.470542	0.000000
H	-2.151452	-1.204045	0.000000
H	-0.024114	-2.466229	0.000000
O	2.333135	-1.470542	0.000000
H	2.151452	1.204045	0.000000
H	0.024114	2.466229	0.000000
H	-3.105019	0.897163	0.000000
H	3.105019	-0.897163	0.000000

hydroquinone, *trans* S_1

C	1.258672	0.674511	0.000000
C	0.035123	1.369117	0.000000
C	-1.227719	0.734873	0.000000
C	-1.258672	-0.674511	0.000000
C	-0.035123	-1.369117	0.000000
C	1.227719	-0.734873	0.000000
O	0.117417	2.709501	0.000000
H	-2.135915	1.322417	0.000000
H	-2.179979	-1.236075	0.000000
O	-0.117417	-2.709501	0.000000
H	2.135915	-1.322417	0.000000
H	2.179979	1.236075	0.000000
H	-0.768647	3.092264	0.000000
H	0.768647	-3.092264	0.000000

salicylic acid S_0

C	1.097780	1.593760	0.000000
C	1.128712	0.199448	0.000000
C	-0.083564	-0.513452	0.000000
C	-1.295025	0.187039	0.000000

C	-1.314298	1.560960	0.000000
C	-0.106342	2.258862	0.000000
O	2.324727	-0.398227	0.000000
C	-0.043942	-1.973699	0.000000
O	-1.242627	-2.570814	0.000000
O	0.981116	-2.633574	0.000000
H	-2.217359	-0.376509	0.000000
H	2.039808	2.124648	0.000000
H	-2.254499	2.094663	0.000000
H	-0.112346	3.341638	0.000000
H	2.183394	-1.368552	0.000000
H	-1.085534	-3.526191	0.000000

salicylic acid S_1

C	0.998895	1.907910	0.000000
C	0.963048	0.510481	0.000000
C	-0.295912	-0.224507	0.000000
C	-1.454356	0.536532	0.000000
C	-1.397816	1.957010	0.000000
C	-0.195398	2.649683	0.000000
O	2.075174	-0.175535	0.000000
C	-0.235228	-1.648195	0.000000
O	-1.417518	-2.298520	0.000000
O	0.842191	-2.303335	0.000000
H	-2.415087	0.042100	0.000000
H	1.969660	2.384447	0.000000
H	-2.331811	2.503754	0.000000
H	-0.174288	3.728857	0.000000
H	1.794048	-1.189994	0.000000
H	-1.215023	-3.243742	0.000000

o-cresol, *cis* S_0

C	1.958136	0.510775	0.000000
C	0.728232	1.146657	0.000000
C	-0.462755	0.431383	0.000000
C	-0.386917	-0.961464	0.000000
C	0.837367	-1.610945	0.000000
C	2.007484	-0.874364	0.000000
C	-1.796966	1.123001	0.000000
O	-1.504723	-1.747103	0.000000
H	0.850150	-2.692629	0.000000
H	2.961170	-1.386270	0.000000
H	2.870241	1.092435	0.000000
H	0.684300	2.229438	0.000000

H	-2.296493	-1.201650	0.000000
H	-2.389536	0.868425	0.883926
H	-1.670155	2.203897	0.000000
H	-2.389536	0.868425	-0.883926

o-cresol, *cis* S_1

C	1.859914	-0.063995	-0.778855
C	0.626147	-0.021409	-1.456760
C	-0.586310	-0.015500	-0.714103
C	-0.467590	0.059042	0.703229
C	0.769595	0.052681	1.390802
C	1.948777	-0.035445	0.626843
C	-1.895303	-0.035114	-1.422930
O	-1.555332	0.121898	1.484584
H	0.767677	0.132121	2.466770
H	2.915333	-0.063116	1.107667
H	2.772603	-0.117448	-1.358717
H	0.595609	-0.051539	-2.536155
H	-2.353513	0.159545	0.942045
H	-2.738568	-0.350191	-0.801350
H	-2.152757	0.944564	-1.847780
H	-1.856862	-0.735586	-2.262879

o-cresol, *trans* S_0

C	2.414497	0.000025	0.030414
C	1.244693	-0.000020	-0.713872
C	0.035249	0.000002	-0.019103
C	0.003746	0.000058	1.365828
C	1.188594	0.000117	2.085232
C	2.399802	0.000077	1.418169
C	1.248163	-0.000109	-2.213143
O	-1.106437	-0.000040	-0.771706
H	-0.949855	0.000079	1.883048
H	1.157826	0.000152	3.167081
H	3.329683	0.000126	1.971053
H	3.362535	0.000010	-0.494414
H	-1.877165	-0.000047	-0.196205
H	2.267667	-0.000064	-2.596187
H	0.729925	-0.875437	-2.608041
H	0.729785	0.875069	-2.608184

o-cresol, *trans* S_1

C	2.426456	0.221340	-0.007304

C	1.218014	0.083617	-0.750224
C	0.015001	-0.029249	-0.015154
C	-0.043753	-0.092309	1.407221
C	1.176311	-0.044379	2.102135
C	2.386342	0.096417	1.390682
C	1.250504	-0.008929	-2.232239
O	-1.125349	-0.126239	-0.716947
H	-0.996779	-0.009352	1.913152
H	1.194028	-0.092923	3.181543
H	3.313541	0.121732	1.949346
H	3.366256	0.340756	-0.525542
H	-1.846425	-0.367482	-0.119307
H	1.855763	-0.866260	-2.552930
H	0.258119	-0.105413	-2.664356
H	1.730661	0.878671	-2.660097

m-cresol, *cis* S_0

C	1.158281	-0.002895	2.079475
C	2.365371	0.013171	1.409132
C	2.410589	0.021785	0.021521
C	1.235926	0.012824	-0.717009
C	0.019952	-0.001444	-0.040149
C	-0.019436	-0.009887	1.344795
C	1.261250	0.002214	-2.220184
O	-1.192404	-0.023001	2.040816
H	1.106198	-0.007807	3.159574
H	3.287805	0.021140	1.975952
H	3.365418	0.036504	-0.488554
H	-0.908477	-0.004969	-0.603525
H	-1.936040	-0.026722	1.430601
H	2.262011	0.206806	-2.598281
H	0.951100	-0.969703	-2.610029
H	0.584754	0.751355	-2.634184

m-cresol, *cis* S_1

C	1.164303	0.009301	2.118137
C	2.405285	0.063389	1.444389
C	2.405313	0.031711	0.034035
C	1.220631	0.002706	-0.741684
C	-0.024773	-0.016972	-0.068726
C	-0.015208	-0.007285	1.348906
C	1.265520	-0.010437	-2.229292
O	-1.171679	-0.035063	2.029415
H	1.084868	-0.043853	3.193828

H	3.334478	0.085541	1.992027
H	3.354236	0.039211	-0.488635
H	-0.958852	0.076452	-0.608725
H	-1.909973	-0.131620	1.414454
H	2.286252	0.061127	-2.603050
H	0.820988	-0.927622	-2.634171
H	0.690891	0.822785	-2.650970

m-cresol, *trans* S_0

C	-1.187329	-1.095452	0.000000
C	0.199101	-1.206717	0.000000
C	0.966239	-0.049359	0.000000
C	0.362083	1.197037	0.000000
C	-1.022007	1.305269	0.000000
C	-1.788010	0.152634	0.000000
C	0.869519	-2.552541	0.000000
O	1.180034	2.288993	0.000000
H	-1.494480	2.281252	0.000000
H	-2.867776	0.231447	0.000000
H	-1.798140	-1.989253	0.000000
H	2.048053	-0.099295	0.000000
H	0.652438	3.093287	0.000000
H	0.136924	-3.358521	0.000000
H	1.504219	-2.675128	-0.879417
H	1.504219	-2.675128	0.879417

m-cresol, *trans* S_1

C	-1.198992	-1.055988	0.000000
C	0.204237	-1.230976	0.000000
C	1.021763	-0.072493	0.000000
C	0.396294	1.191041	0.000000
C	-1.008234	1.367234	0.000000
C	-1.821016	0.213064	0.000000
C	0.825075	-2.584279	0.000000
O	1.212828	2.257128	0.000000
H	-1.430987	2.363681	0.000000
H	-2.897234	0.292102	0.000000
H	-1.825540	-1.939727	0.000000
H	2.100297	-0.125001	0.000000
H	0.694568	3.071367	0.000000
H	0.072185	-3.372416	0.000000
H	1.465619	-2.729860	-0.877324
H	1.465619	-2.729860	0.877324

p-cresol S_0

C	0.710131	0.020948	-1.184474
C	-0.671032	0.021673	-1.192956
C	-1.366619	0.000222	0.007625
C	-0.668648	-0.023426	1.203270
C	0.718908	-0.023747	1.192856
C	1.434657	-0.000081	0.005327
O	-2.730646	0.000040	-0.052928
C	2.938360	0.020428	-0.005266
H	-1.204082	-0.044010	2.146359
H	1.250700	-0.044495	2.136729
H	1.240780	0.035617	-2.129569
H	-1.227414	0.036259	-2.120595
H	-3.097784	-0.017252	0.835892
H	3.341309	-0.703043	-0.715613
H	3.320039	1.003685	-0.289638
H	3.342901	-0.217441	0.978281

p-cresol S_1

C	0.730193	-0.064961	-1.233023
C	-0.680660	-0.026247	-1.240486
C	-1.349209	-0.003169	-0.001500
C	-0.678526	0.007825	1.245349
C	0.730968	-0.025956	1.233753
C	1.427285	-0.035723	-0.001011
O	-2.689070	0.021327	-0.046936
C	2.911624	0.034202	-0.000979
H	-1.243236	0.018417	2.168470
H	1.289980	-0.023203	2.158430
H	1.285752	-0.086030	-2.159255
H	-1.261612	-0.011539	-2.150032
H	-3.048063	0.054447	0.848590
H	3.332520	-0.457401	-0.879317
H	3.241105	1.080060	-0.025649
H	3.332497	-0.416669	0.898887

o-methoxyphenol S_0

C	2.025133	-0.090351	0.000000
C	0.874244	0.692766	0.000000
C	-0.365119	0.083411	0.000000
C	-0.464328	-1.312309	0.000000
C	0.680132	-2.080865	0.000000
C	1.927255	-1.468088	0.000000

O	-1.574471	0.723219	0.000000
O	-1.685552	-1.904388	0.000000
H	0.579425	-3.157957	0.000000
H	2.821334	-2.077287	0.000000
H	2.994465	0.389727	0.000000
H	0.957300	1.770203	0.000000
C	-1.587110	2.136222	0.000000
H	-2.353589	-1.206579	0.000000
H	-2.632693	2.431741	0.000000
H	-1.098212	2.535268	0.892149
H	-1.098212	2.535268	-0.892149

o-methoxyphenol S_1

C	2.483882	0.073422	0.066521
C	1.383723	-0.226578	-0.750391
C	0.117036	-0.217904	-0.095517
C	0.023633	-0.142124	1.311910
C	1.179894	-0.082892	2.136331
C	2.387447	0.143919	1.471867
O	-1.071068	-0.018773	-0.726187
O	-1.174145	0.046759	1.884264
H	1.093968	-0.189976	3.206346
H	3.282332	0.367554	2.039430
H	3.451011	0.248185	-0.391322
H	1.504168	-0.520889	-1.782126
C	-1.094517	0.096486	-2.144047
H	-1.851849	0.048676	1.187757
H	-2.128285	0.297846	-2.409436
H	-0.455769	0.913563	-2.479138
H	-0.772900	-0.837284	-2.608183

m-methoxyphenol, isomer 1 S_0

C	0.926760	1.441862	0.000000
C	-0.258604	0.713753	0.000000
C	-0.227099	-0.675230	0.000000
C	1.002036	-1.328438	0.000000
C	2.187295	-0.616258	0.000000
C	2.132308	0.769267	0.000000
H	-1.139065	-1.256923	0.000000
O	1.084342	-2.689646	0.000000
H	3.126852	-1.150215	0.000000
H	3.054899	1.335575	0.000000
H	0.875590	2.521421	0.000000
O	-1.405071	1.441372	0.000000

H	0.203413	-3.075339	0.000000
C	-2.641290	0.760439	0.000000
H	-3.408666	1.529736	0.000000
H	-2.756851	0.139312	-0.892528
H	-2.756851	0.139312	0.892528

m-methoxyphenol, isomer 1 S_1

C	1.166747	-0.008986	-0.619083
C	-0.028855	-0.034679	0.126326
C	-0.046066	-0.081657	1.542699
C	1.236074	-0.010859	2.141124
C	2.438732	0.013528	1.412696
C	2.430621	-0.113524	0.007499
H	-0.890037	-0.467380	2.100169
O	1.344642	0.091978	3.483633
H	3.356511	0.164485	1.966008
H	3.343339	-0.128811	-0.564406
H	1.076527	0.105786	-1.691357
O	-1.152017	0.030215	-0.615752
H	0.476434	0.303360	3.852855
C	-2.414139	0.032791	0.030398
H	-3.146204	0.241779	-0.744519
H	-2.626972	-0.942212	0.473995
H	-2.457027	0.804186	0.800453

m-methoxyphenol, isomer 2 S_0

C	0.345716	2.154374	0.000000
C	-0.833655	1.442986	0.000000
C	-0.789989	0.048735	0.000000
C	0.426447	-0.615033	0.000000
C	1.603245	0.125469	0.000000
C	1.576581	1.508702	0.000000
O	-1.991613	-0.580618	0.000000
C	-2.014374	-1.993376	0.000000
O	2.766899	-0.585911	0.000000
H	0.501159	-1.691557	0.000000
H	2.499202	2.076901	0.000000
H	0.314768	3.236424	0.000000
H	-1.796025	1.934799	0.000000
H	-3.063409	-2.276620	0.000000
H	-1.530933	-2.400845	-0.891660
H	-1.530933	-2.400845	0.891660
H	3.516902	0.016424	0.000000

m-methoxyphenol, isomer 2 S_1

C	1.240065	-0.081338	-0.704666
C	0.057655	-0.013241	0.077199
C	0.111257	-0.033897	1.485376
C	1.335190	-0.049364	2.197536
C	2.497182	-0.000720	1.401753
C	2.466549	0.028512	-0.007821
O	-1.090278	-0.012290	2.094867
C	-1.151384	0.024824	3.510328
O	3.672151	0.040657	2.070036
H	1.416483	-0.163442	3.264172
H	3.400274	0.135096	-0.548914
H	1.202386	-0.064945	-1.781093
H	-0.918423	0.056955	-0.382685
H	-2.206918	0.078112	3.761271
H	-0.719438	-0.878479	3.945370
H	-0.634992	0.902900	3.902227
H	4.407370	0.030661	1.446943

p-methoxyphenol, *cis* S_0

C	-0.314502	0.727474	0.000000
C	-1.542998	0.070422	0.000000
C	-1.603213	-1.304986	0.000000
C	-0.431990	-2.054523	0.000000
C	0.788055	-1.408390	0.000000
C	0.852599	-0.017438	0.000000
O	-0.556347	-3.417174	0.000000
O	-0.365742	2.090249	0.000000
C	0.851898	2.800953	0.000000
H	1.821375	0.459807	0.000000
H	-2.446408	0.665419	0.000000
H	-2.554525	-1.819790	0.000000
H	1.708194	-1.982310	0.000000
H	0.587473	3.855091	0.000000
H	1.446046	2.580510	0.891758
H	1.446046	2.580510	-0.891758
H	0.314038	-3.825802	0.000000

p-methoxyphenol, *cis* S_1

C	1.326247	-0.003279	-0.614298
C	0.053660	-0.006999	0.003085
C	-0.015347	0.000171	1.411404
C	1.187018	-0.001108	2.133462

C	2.464213	0.001625	1.522817
C	2.537179	-0.003951	0.114710
O	1.086863	-0.000193	3.473175
O	1.289539	-0.003888	-1.951492
C	2.492547	0.003665	-2.706507
H	3.492575	-0.006320	-0.383369
H	-0.825485	-0.004430	-0.621780
H	-0.951871	0.008271	1.947006
H	3.358449	-0.016326	2.131669
H	2.186413	0.002403	-3.748293
H	3.076947	0.899918	-2.495293
H	3.087268	-0.886112	-2.496590
H	1.967317	0.016536	3.867295

p-methoxyphenol, *trans* S_0

C	-0.655589	1.299015	0.000000
C	-1.884127	0.668631	0.000000
C	-1.958538	-0.718713	0.000000
C	-0.793604	-1.461408	0.000000
C	0.443087	-0.831084	0.000000
C	0.517870	0.555059	0.000000
O	-3.148124	-1.395468	0.000000
H	1.337016	-1.437268	0.000000
O	1.680305	1.268758	0.000000
H	-0.585483	2.378393	0.000000
H	-2.791709	1.262373	0.000000
H	-3.879806	-0.771762	0.000000
H	-0.860121	-2.541017	0.000000
C	2.897730	0.556842	0.000000
H	3.685759	1.305281	0.000000
H	2.997663	-0.068827	0.891660
H	2.997663	-0.068827	-0.891660

p-methoxyphenol, *trans* S_1

C	0.121884	-0.053727	-1.388400
C	-1.276846	-0.017639	-1.215589
C	-1.778540	0.027565	0.101167
C	-0.957767	0.057985	1.244663
C	0.442479	0.033762	1.075221
C	0.950507	-0.018135	-0.241016
O	-3.102922	0.050375	0.325503
H	1.096606	0.059235	1.930755
O	2.260010	-0.043332	-0.513247
H	0.587111	-0.093626	-2.360860

H	-1.953590	-0.047425	-2.059015
H	-3.576789	0.033731	-0.514801
H	-1.419409	0.098078	2.219131
C	3.213944	-0.015400	0.539045
H	4.186092	-0.043815	0.056188
H	3.118870	0.900494	1.123302
H	3.099150	-0.883817	1.188655

1-naphthol, *cis* S_0

C	0.825817	1.513809	0.012161
C	0.524045	0.123155	-0.002309
C	-0.841040	-0.266313	-0.005030
C	-1.852049	0.720826	-0.015333
C	-1.517745	2.042902	-0.020849
C	-0.172332	2.445878	-0.004073
C	1.518222	-0.883582	-0.019790
C	1.182981	-2.205926	-0.018801
C	-0.170567	-2.593293	-0.006221
C	-1.151483	-1.646873	-0.002690
O	2.110317	1.967521	0.025287
H	-2.194352	-1.939881	-0.000243
H	-0.427126	-3.644735	-0.004765
H	1.958089	-2.960901	-0.034296
H	2.570120	-0.623204	-0.050246
H	-2.888974	0.410313	-0.020405
H	-2.291544	2.799648	-0.031477
H	0.094999	3.493751	0.004367
H	2.722631	1.246916	0.194710

1-naphthol, *cis* S_1

C	0.866857	1.462420	0.015677
C	0.536204	0.090161	-0.053035
C	-0.850381	-0.246657	0.013282
C	-1.791067	0.797582	-0.013948
C	-1.421148	2.164323	-0.026919
C	-0.103319	2.503748	-0.033632
C	1.498180	-0.928875	-0.121149
C	1.090849	-2.291432	-0.051283
C	-0.233445	-2.614346	0.038308
C	-1.223445	-1.599637	0.054496
O	2.137203	1.861711	0.134025
H	-2.271302	-1.859924	0.116826
H	-0.537068	-3.651629	0.090713
H	1.843114	-3.068579	-0.077384

H	2.544698	-0.710522	-0.296205
H	-2.843233	0.541203	-0.018529
H	-2.188063	2.925760	-0.055116
H	0.242052	3.527693	-0.027122
H	2.703315	1.096990	0.310974

1-naphthol, *trans* S_0

C	-0.712753	-0.538719	0.000000
C	-0.670250	-1.952335	0.000000
C	0.519841	-2.619299	0.000000
C	1.734530	-1.906443	0.000000
C	1.732185	-0.541578	0.000000
C	0.512663	0.171079	0.000000
H	-1.605412	-2.499110	0.000000
H	0.534700	-3.701804	0.000000
H	2.672567	-2.446426	0.000000
H	2.659004	0.014388	0.000000
C	-1.935421	0.175664	0.000000
C	-1.932970	1.537565	0.000000
C	-0.721842	2.256931	0.000000
C	0.470713	1.591043	0.000000
H	-2.866910	-0.375912	0.000000
H	-2.867076	2.084365	0.000000
H	-0.738040	3.341135	0.000000
O	1.674970	2.228541	0.000000
H	1.539511	3.180904	0.000000

1-naphthol, *trans* S_1

C	-0.941877	-0.392248	0.000000
C	-1.303061	-1.745262	0.000000
C	-0.312576	-2.763182	0.000000
C	1.011187	-2.423905	0.000000
C	1.413322	-1.060588	0.000000
C	0.450162	-0.044876	0.000000
H	-2.352320	-2.010083	0.000000
H	-0.614079	-3.801914	0.000000
H	1.772408	-3.193303	0.000000
H	2.462002	-0.803688	0.000000
C	-1.889808	0.644091	0.000000
C	-1.519399	2.012600	0.000000
C	-0.203086	2.359926	0.000000
C	0.779902	1.324231	0.000000
H	-2.941534	0.386646	0.000000
H	-2.288901	2.772469	0.000000

H	0.112739	3.396359	0.000000
O	2.087939	1.642357	0.000000
H	2.201301	2.599445	0.000000

2-naphthol, *cis* S_0

C	0.594244	2.004333	0.000000
C	0.617687	0.592309	0.000000
C	-0.608081	-0.119094	0.000000
C	-1.816781	0.614688	0.000000
C	-1.806826	1.979556	0.000000
C	-0.588371	2.685648	0.000000
C	1.826552	-0.144668	0.000000
C	1.825741	-1.504830	0.000000
C	0.601849	-2.206518	0.000000
C	-0.585602	-1.533254	0.000000
H	-1.525006	-2.076144	0.000000
H	1.535721	2.540714	0.000000
H	-0.594577	3.767819	0.000000
H	-2.741190	2.526316	0.000000
H	-2.756475	0.075405	0.000000
H	2.766411	0.394055	0.000000
H	2.745609	-2.073674	0.000000
O	0.694438	-3.566383	0.000000
H	-0.185352	-3.956266	0.000000

2-naphthol, *cis* S_1

C	0.599708	1.984720	0.000000
C	0.644140	0.585418	0.000000
C	-0.625850	-0.117665	0.000000
C	-1.826833	0.606229	0.000000
C	-1.836265	2.013455	0.000000
C	-0.626091	2.680267	0.000000
C	1.844628	-0.149834	0.000000
C	1.874854	-1.551181	0.000000
C	0.656914	-2.211285	0.000000
C	-0.581128	-1.515810	0.000000
H	-1.503973	-2.086903	0.000000
H	1.526709	2.543941	0.000000
H	-0.606628	3.763077	0.000000
H	-2.769867	2.556717	0.000000
H	-2.762354	0.059909	0.000000
H	2.778167	0.398997	0.000000
H	2.795698	-2.113056	0.000000
O	0.660621	-3.554346	0.000000

H	-0.242442	-3.892639	0.000000

2-naphthol, *trans* S_0

C	0.507207	2.006428	0.000000
C	0.536291	0.592943	0.000000
C	-0.687118	-0.125515	0.000000
C	-1.899781	0.605351	0.000000
C	-1.894555	1.968972	0.000000
C	-0.677685	2.681260	0.000000
C	1.745285	-0.137230	0.000000
C	1.745306	-1.500264	0.000000
C	0.524740	-2.207408	0.000000
C	-0.663617	-1.536156	0.000000
H	-1.589005	-2.097200	0.000000
H	1.446297	2.547069	0.000000
H	-0.689256	3.763414	0.000000
H	-2.830803	2.512531	0.000000
H	-2.836411	0.061246	0.000000
H	2.684513	0.402487	0.000000
H	2.681545	-2.047890	0.000000
O	0.500049	-3.571640	0.000000
H	1.397008	-3.918398	0.000000

2-naphthol, *trans* S_1

C	0.511268	1.989097	0.000000
C	0.558321	0.590120	0.000000
C	-0.707049	-0.117636	0.000000
C	-1.908808	0.602430	0.000000
C	-1.922353	2.011311	0.000000
C	-0.717057	2.682088	0.000000
C	1.761381	-0.140051	0.000000
C	1.793429	-1.543487	0.000000
C	0.573060	-2.205666	0.000000
C	-0.663154	-1.516622	0.000000
H	-1.570366	-2.106089	0.000000
H	1.436923	2.550735	0.000000
H	-0.700847	3.764946	0.000000
H	-2.858409	2.550587	0.000000
H	-2.842256	0.053016	0.000000
H	2.693762	0.410799	0.000000
H	2.727056	-2.089399	0.000000
O	0.477497	-3.545821	0.000000
H	1.357605	-3.940351	0.000000

5-methoxysalicylic acid S_0

C	2.271540	-0.165280	0.000000
C	1.561506	-1.335905	0.000000
C	0.160623	-1.329833	0.000000
C	-0.506443	-0.129256	0.000000
C	0.212994	1.079716	0.000000
C	1.611308	1.067292	0.000000
O	-0.433487	-2.554681	0.000000
C	-1.843735	-2.605192	0.000000
C	-0.478430	2.365512	0.000000
O	-1.817090	2.287719	0.000000
O	2.363344	2.177246	0.000000
O	0.081051	3.448468	0.000000
H	-2.108944	-3.658908	0.000000
H	-2.261136	-2.128638	-0.891691
H	-2.261136	-2.128638	0.891691
H	-1.583765	-0.079573	0.000000
H	3.352847	-0.165756	0.000000
H	2.068713	-2.291768	0.000000
H	1.764229	2.952123	0.000000
H	-2.153967	3.195354	0.000000

5-methoxysalicylic acid S_1

C	2.171237	-0.134137	0.000000
C	1.725428	-1.452908	0.000000
C	0.338802	-1.679005	0.000000
C	-0.598140	-0.616736	0.000000
C	-0.163555	0.704034	0.000000
C	1.269569	0.929075	0.000000
O	-0.032804	-2.960491	0.000000
C	-1.409883	-3.320591	0.000000
C	-1.034489	1.834032	0.000000
O	-2.361149	1.554206	0.000000
O	1.714831	2.167636	0.000000
O	-0.647862	3.025337	0.000000
H	-1.426676	-4.405896	0.000000
H	-1.909553	-2.945068	-0.893410
H	-1.909553	-2.945068	0.893410
H	-1.658309	-0.814457	0.000000
H	3.225999	0.103759	0.000000
H	2.400305	-2.294438	0.000000
H	0.895794	2.775492	0.000000
H	-2.817938	2.406000	0.000000

m-dimethoxybenzene, *trans* S_0

C	0.000000	-0.130248	0.704691
C	0.000000	-0.130248	-0.704691
C	0.000000	1.072673	-1.384407
C	0.000000	2.279784	-0.687682
C	0.000000	2.279784	0.687682
C	0.000000	1.072673	1.384407
O	0.000000	-1.351252	-1.292315
H	0.000000	1.084409	-2.464339
H	0.000000	3.211405	-1.237717
H	0.000000	3.211405	1.237717
H	0.000000	1.084409	2.464339
O	0.000000	-1.351252	1.292315
C	0.000000	-1.411814	2.701415
H	0.000000	-2.468304	2.955848
H	0.891574	-0.939933	3.124002
H	-0.891573	-0.939933	3.124002
C	0.000000	-1.411814	-2.701415
H	0.000000	-2.468304	-2.955848
H	-0.891573	-0.939933	-3.124002
H	0.891574	-0.939933	-3.124002

m-dimethoxybenzene, *trans* S_1

C	-0.105744	-1.065382	-1.442139
C	-0.236637	0.155905	-0.706583
C	-0.236637	0.155905	0.706583
C	-0.105744	-1.065382	1.442139
C	0.271177	-2.191474	0.703569
C	0.271177	-2.191474	-0.703569
O	-0.195077	1.367415	-1.287685
C	-0.017584	1.459201	-2.693605
O	-0.195077	1.367415	1.287685
C	-0.017584	1.459201	2.693605
H	-0.337620	-1.129070	2.494005
H	0.541425	-3.104908	1.220805
H	0.541425	-3.104908	-1.220805
H	-0.337620	-1.129070	-2.494005
H	0.031663	2.521898	-2.913155
H	0.905274	0.970640	-3.007980
H	-0.863787	1.018214	-3.223481
H	0.031663	2.521898	2.913155
H	-0.863787	1.018214	3.223481
H	0.905274	0.970640	3.007980

3P-propionic acid, *gauche* S_0

C	-1.031237	0.900857	-1.163368
C	-0.387874	0.662816	0.047287
C	-1.048459	-0.089094	1.012899
C	-2.317795	-0.591587	0.772144
C	-2.947077	-0.349887	-0.438167
C	-2.299136	0.399473	-1.407538
C	1.001175	1.198460	0.289916
C	2.104942	0.278745	-0.231319
C	2.309852	-0.947603	0.615281
O	1.997096	-1.068042	1.768414
O	2.941060	-1.925872	-0.062189
H	1.917001	-0.031957	-1.259125
H	3.064494	0.804459	-0.237530
H	1.155314	1.363572	1.356130
H	1.103821	2.165597	-0.204777
H	-0.556343	-0.286726	1.956567
H	-2.817845	-1.173309	1.536272
H	-3.939470	-0.740093	-0.624439
H	-2.784936	0.599498	-2.354285
H	-0.535635	1.494908	-1.923327
H	3.071061	-2.664234	0.551163

3P-propionic acid, *gauche* S_1

C	-1.064518	0.994597	-1.171777
C	-0.360253	0.695808	0.027104
C	-0.996935	-0.088640	1.027644
C	-2.306508	-0.585182	0.824392
C	-2.989797	-0.292679	-0.377891
C	-2.370341	0.491328	-1.378705
C	1.041661	1.174468	0.206128
C	2.098199	0.180954	-0.298957
C	2.328465	-0.972440	0.638669
O	2.096421	-0.981074	1.817085
O	2.887192	-2.024117	0.009989
H	1.842992	-0.206638	-1.284854
H	3.064497	0.684224	-0.402085
H	1.237706	1.375863	1.260773
H	1.172601	2.110185	-0.341847
H	-0.462910	-0.309338	1.940795
H	-2.780165	-1.189111	1.584657
H	-3.990353	-0.670785	-0.535105
H	-2.896090	0.708499	-2.297446
H	-0.595871	1.613321	-1.925146

H	3.044018	-2.709255	0.676579

3P-propionic acid, *anti* S_0

C	1.453981	-0.447375	0.000000
C	0.541157	0.774888	0.000000
C	2.912935	-0.089913	0.000000
H	1.264058	-1.080334	0.869883
H	1.264058	-1.080334	-0.869883
C	-0.914488	0.387330	0.000000
H	0.766447	1.389373	0.872198
H	0.766447	1.389373	-0.872198
C	-1.598828	0.189804	1.194256
C	-2.928831	-0.198901	1.197186
C	-3.598243	-0.396049	0.000000
C	-2.928831	-0.198901	-1.197186
C	-1.598828	0.189804	-1.194256
H	-1.085111	0.350415	2.135347
H	-3.445512	-0.343375	2.137618
H	-4.638156	-0.696227	0.000000
H	-3.445512	-0.343375	-2.137618
H	-1.085111	0.350415	-2.135347
O	3.695742	-1.188598	0.000000
O	3.369502	1.020105	0.000000
H	4.615964	-0.886803	0.000000

3P-propionic acid, *anti* S_1

C	1.461858	-0.434996	0.000000
C	0.557058	0.802192	0.000000
C	2.922388	-0.083999	0.000000
H	1.265122	-1.063378	0.871124
H	1.265122	-1.063378	-0.871124
C	-0.887568	0.436574	0.000000
H	0.792508	1.408755	0.876489
H	0.792508	1.408755	-0.876489
C	-1.575885	0.230082	1.226310
C	-2.919184	-0.213877	1.227736
C	-3.586022	-0.431083	0.000000
C	-2.919184	-0.213877	-1.227736
C	-1.575885	0.230082	-1.226310
H	-1.063924	0.417465	2.160534
H	-3.435198	-0.383785	2.161536
H	-4.614749	-0.763779	0.000000
H	-3.435198	-0.383785	-2.161536
H	-1.063924	0.417465	-2.160534

O	3.698460	-1.187054	0.000000
O	3.383607	1.024017	0.000000
H	4.620715	-0.891237	0.000000

fluorine S_0

C	0.000000	0.000000	-1.787580
C	0.000000	1.178043	-0.845990
C	0.000000	0.733455	0.480116
C	0.000000	-0.733455	0.480116
C	0.000000	1.642463	1.526259
C	0.000000	2.998209	1.235301
C	0.000000	3.439266	-0.081898
C	0.000000	2.529108	-1.131295
H	0.000000	2.879716	-2.156537
H	0.000000	4.501283	-0.291474
H	0.000000	3.720603	2.041570
H	0.000000	1.305275	2.555417
C	0.000000	-1.642463	1.526259
C	0.000000	-2.998209	1.235301
C	0.000000	-3.439266	-0.081898
C	0.000000	-2.529108	-1.131295
C	0.000000	-1.178043	-0.845990
H	0.000000	-1.305275	2.555417
H	0.000000	-3.720603	2.041570
H	0.000000	-4.501283	-0.291474
H	0.000000	-2.879716	-2.156537
H	-0.878852	0.000000	-2.437670
H	0.878852	0.000000	-2.437670

fluorine S_1

C	0.000000	0.000000	-1.865103
C	0.000000	1.177176	-0.917084
C	0.000000	0.693799	0.450512
C	0.000000	-0.693799	0.450512
C	0.000000	1.636378	1.531691
C	0.000000	2.970821	1.227402
C	0.000000	3.425738	-0.106303
C	0.000000	2.515629	-1.180924
H	0.000000	2.883794	-2.199754
H	0.000000	4.489407	-0.304757
H	0.000000	3.702949	2.025402
H	0.000000	1.293306	2.557615
C	0.000000	-1.636378	1.531691
C	0.000000	-2.970821	1.227402

C	0.000000	-3.425738	-0.106303
C	0.000000	-2.515629	-1.180924
C	0.000000	-1.177176	-0.917084
H	0.000000	-1.293306	2.557615
H	0.000000	-3.702949	2.025402
H	0.000000	-4.489407	-0.304757
H	0.000000	-2.883794	-2.199754
H	-0.877899	0.000000	-2.519086
H	0.877899	0.000000	-2.519086

phenanthrene S_0

C	0.726726	0.000000	-0.347651
C	-0.726726	0.000000	-0.347651
C	-1.413368	0.000000	0.884912
C	-0.672691	0.000000	2.110532
C	0.672691	0.000000	2.110532
C	1.413368	0.000000	0.884912
C	-1.490475	0.000000	-1.528679
C	-2.819359	0.000000	0.898237
H	-1.223862	0.000000	3.043133
H	1.223862	0.000000	3.043133
C	1.490475	0.000000	-1.528679
C	2.861570	0.000000	-1.493127
C	3.536901	0.000000	-0.268036
C	2.819359	0.000000	0.898237
H	0.997549	0.000000	-2.490163
H	3.422963	0.000000	-2.418624
H	4.618963	0.000000	-0.244586
H	3.329371	0.000000	1.854143
C	-3.536901	0.000000	-0.268036
C	-2.861570	0.000000	-1.493127
H	-0.997549	0.000000	-2.490163
H	-3.422963	0.000000	-2.418624
H	-4.618963	0.000000	-0.244586
H	-3.329371	0.000000	1.854143

phenanthrene S_1

C	0.709519	0.000000	-0.387242
C	-0.709519	0.000000	-0.387242
C	-1.429730	0.000000	0.882422
C	-0.692451	0.000000	2.076318
C	0.692451	0.000000	2.076318
C	1.429730	0.000000	0.882422
C	-1.489233	0.000000	-1.566172

C	-2.831483	0.000000	0.882826
H	-1.227732	0.000000	3.017858
H	1.227732	0.000000	3.017858
C	1.489233	0.000000	-1.566172
C	2.872888	0.000000	-1.523173
C	3.556527	0.000000	-0.299424
C	2.831483	0.000000	0.882826
H	1.005009	0.000000	-2.531474
H	3.431670	0.000000	-2.449948
H	4.637455	0.000000	-0.278352
H	3.347192	0.000000	1.835401
C	-3.556527	0.000000	-0.299424
C	-2.872888	0.000000	-1.523173
H	-1.005009	0.000000	-2.531474
H	-3.431670	0.000000	-2.449948
H	-4.637455	0.000000	-0.278352
H	-3.347192	0.000000	1.835401

2,4,6,8-decatetraene S_0

C	-2.584003	-4.998839	0.000000
C	-2.459872	-3.512210	0.000000
C	-1.310598	-2.839535	0.000000
C	-1.207364	-1.395444	0.000000
C	-0.051613	-0.719831	0.000000
C	0.051613	0.719831	0.000000
C	1.207364	1.395444	0.000000
C	1.310598	2.839535	0.000000
C	2.459872	3.512210	0.000000
C	2.584003	4.998839	0.000000
H	-0.374619	-3.393339	0.000000
H	-2.141615	-0.839436	0.000000
H	0.882237	-1.276547	0.000000
H	-0.882237	1.276547	0.000000
H	2.141615	0.839436	0.000000
H	0.374619	3.393339	0.000000
H	3.390332	2.949512	0.000000
H	-3.390332	-2.949512	0.000000
H	1.606111	5.481032	0.000000
H	3.135261	5.348146	0.876907
H	3.135261	5.348146	-0.876907
H	-1.606111	-5.481032	0.000000
H	-3.135261	-5.348146	0.876907
H	-3.135261	-5.348146	-0.876907

2,4,6,8-decatetraene S_1

C	-2.571448	-5.008247	0.000000
C	-2.509330	-3.526186	0.000000
C	-1.352108	-2.802873	0.000000
C	-1.264488	-1.400912	0.000000
C	-0.053807	-0.691272	0.000000
C	0.053807	0.691272	0.000000
C	1.264488	1.400912	0.000000
C	1.352108	2.802873	0.000000
C	2.509330	3.526186	0.000000
C	2.571448	5.008247	0.000000
H	-0.412680	-3.352765	0.000000
H	-2.189008	-0.829778	0.000000
H	0.865591	-1.271607	0.000000
H	-0.865591	1.271607	0.000000
H	2.189008	0.829778	0.000000
H	0.412680	3.352765	0.000000
H	3.454885	2.990065	0.000000
H	-3.454885	-2.990065	0.000000
H	1.574710	5.451261	0.000000
H	3.111568	5.390810	0.874652
H	3.111568	5.390810	-0.874652
H	-1.574710	-5.451261	0.000000
H	-3.111568	-5.390810	0.874652
H	-3.111568	-5.390810	-0.874652

tetracene S_0

C	3.690563	1.400776	0.000000
C	2.431230	0.719368	0.000000
C	2.431230	-0.719368	0.000000
C	3.690563	-1.400776	0.000000
C	4.854769	-0.713899	0.000000
C	4.854769	0.713899	0.000000
C	1.228704	1.395845	0.000000
C	0.000000	0.718241	0.000000
C	0.000000	-0.718241	0.000000
C	1.228704	-1.395845	0.000000
C	-1.228704	1.395845	0.000000
C	-2.431230	0.719368	0.000000
C	-2.431230	-0.719368	0.000000
C	-1.228704	-1.395845	0.000000
C	-3.690563	1.400776	0.000000
C	-4.854769	0.713899	0.000000
C	-4.854769	-0.713899	0.000000
C	-3.690563	-1.400776	0.000000

H	-3.688873	-2.484125	0.000000
H	-5.799320	-1.242510	0.000000
H	-5.799320	1.242510	0.000000
H	-3.688873	2.484125	0.000000
H	-1.228845	-2.480006	0.000000
H	-1.228845	2.480006	0.000000
H	1.228845	-2.480006	0.000000
H	1.228845	2.480006	0.000000
H	3.688873	-2.484125	0.000000
H	5.799320	-1.242510	0.000000
H	5.799320	1.242510	0.000000
H	3.688873	2.484125	0.000000

tetracene S_1

C	3.689198	1.390320	0.000000
C	2.462092	0.715666	0.000000
C	2.462092	-0.715666	0.000000
C	3.689198	-1.390320	0.000000
C	4.887624	-0.695571	0.000000
C	4.887624	0.695571	0.000000
C	1.223430	1.392767	0.000000
C	0.000000	0.724114	0.000000
C	0.000000	-0.724114	0.000000
C	1.223430	-1.392767	0.000000
C	-1.223430	1.392767	0.000000
C	-2.462092	0.715666	0.000000
C	-2.462092	-0.715666	0.000000
C	-1.223430	-1.392767	0.000000
C	-3.689198	1.390320	0.000000
C	-4.887624	0.695571	0.000000
C	-4.887624	-0.695571	0.000000
C	-3.689198	-1.390320	0.000000
H	-3.691320	-2.473665	0.000000
H	-5.824337	-1.237316	0.000000
H	-5.824337	1.237316	0.000000
H	-3.691320	2.473665	0.000000
H	-1.226337	-2.477029	0.000000
H	-1.226337	2.477029	0.000000
H	1.226337	-2.477029	0.000000
H	1.226337	2.477029	0.000000
H	3.691320	-2.473665	0.000000
H	5.824337	-1.237316	0.000000
H	5.824337	1.237316	0.000000
H	3.691320	2.473665	0.000000

perylene S_0

C	0.020469	1.468858	-2.409118
C	0.010705	0.737778	-1.243158
C	0.014976	1.434379	-0.000006
C	0.034825	2.854787	0.000001
C	0.043954	3.552723	-1.226699
C	0.037065	2.869712	-2.405256
C	0.044042	3.552710	1.226709
C	0.037244	2.869688	2.405261
C	0.020627	1.468834	2.409110
C	0.010750	0.737773	1.243142
C	-0.010705	-0.737778	-1.243158
C	-0.014976	-1.434379	-0.000006
C	-0.010750	-0.737773	1.243142
C	-0.034825	-2.854787	0.000001
C	-0.044042	-3.552710	1.226709
C	-0.037244	-2.869688	2.405261
C	-0.020627	-1.468834	2.409110
C	-0.020469	-1.468858	-2.409118
C	-0.037065	-2.869712	-2.405256
C	-0.043954	-3.552723	-1.226699
H	0.057471	4.635465	1.211851
H	0.044807	3.402370	3.347483
H	0.016543	0.968243	3.365893
H	-0.057471	-4.635465	1.211851
H	-0.044807	-3.402370	3.347483
H	-0.016543	-0.968243	3.365893
H	-0.057381	-4.635478	-1.211830
H	-0.044546	-3.402405	-3.347473
H	-0.016298	-0.968285	-3.365909
H	0.057381	4.635478	-1.211830
H	0.044546	3.402405	-3.347473
H	0.016298	0.968285	-3.365909

perylene S_1

C	-0.005708	1.463360	-2.439428
C	-0.005949	0.716897	-1.234963
C	0.010831	1.414748	0.000000
C	0.007285	2.843320	-0.000001
C	0.008726	3.531924	-1.225232
C	-0.000845	2.840990	-2.424417
C	0.008896	3.531925	1.225227
C	-0.000494	2.840990	2.424416
C	-0.005408	1.463362	2.439428

C	-0.005872	0.716897	1.234964
C	0.005949	-0.716897	-1.234963
C	-0.010831	-1.414748	0.000000
C	0.005872	-0.716897	1.234964
C	-0.007285	-2.843320	-0.000001
C	-0.008896	-3.531925	1.225227
C	0.000494	-2.840990	2.424416
C	0.005408	-1.463362	2.439428
C	0.005708	-1.463360	-2.439428
C	0.000845	-2.840990	-2.424417
C	-0.008726	-3.531924	-1.225232
H	0.012501	4.614770	1.217489
H	-0.003736	3.386210	3.359586
H	-0.025869	0.954872	3.390632
H	-0.012501	-4.614770	1.217489
H	0.003736	-3.386210	3.359586
H	0.025869	-0.954872	3.390632
H	-0.012318	-4.614769	-1.217494
H	0.004272	-3.386208	-3.359588
H	0.026384	-0.954866	-3.390625
H	0.012318	4.614769	-1.217494
H	-0.004272	3.386208	-3.359588
H	-0.026384	0.954866	-3.390625

ωB97X-D/TZVP geometries – Group I

pyrazine S_0

C	1.126592	-0.694160	0.000000
C	1.126592	0.694160	0.000000
N	0.000000	1.398578	0.000000
C	-1.126592	0.694160	0.000000
C	-1.126592	-0.694160	0.000000
N	0.000000	-1.398578	0.000000
H	-2.057654	-1.250015	0.000000
H	2.057654	-1.250015	0.000000
H	2.057654	1.250015	0.000000
H	-2.057654	1.250015	0.000000

pyrazine S_1

C	-1.201919	0.666965	0.000000
C	-1.115993	-0.736831	0.000000
N	0.024036	-1.351302	0.000000
C	1.201919	-0.666965	0.000000

C	1.115993	0.736831	0.000000
N	-0.024036	1.351302	0.000000
H	2.043272	1.303340	0.000000
H	-2.154094	1.172365	0.000000
H	-2.043272	-1.303340	0.000000
H	2.154094	-1.172365	0.000000

2,6-difluoropyridine S_0

C	1.113535	0.000000	-0.874793
N	0.000000	0.000000	-1.564382
C	-1.113535	0.000000	-0.874793
C	-1.200200	0.000000	0.506069
C	0.000000	0.000000	1.199018
C	1.200200	0.000000	0.506069
F	-2.235049	0.000000	-1.588266
H	-2.160909	0.000000	0.999139
H	0.000000	0.000000	2.281486
H	2.160909	0.000000	0.999139
F	2.235049	0.000000	-1.588266

2,6-difluoropyridine S_1

C	-1.100137	0.000000	-0.336695
N	0.000000	0.000000	-1.101220
C	1.100137	0.000000	-0.336695
C	1.190973	0.000000	1.071140
C	0.000000	0.000000	1.843319
C	-1.190973	0.000000	1.071140
F	2.234620	0.000000	-1.010234
H	2.175086	0.000000	1.519528
H	0.000000	0.000000	2.919716
H	-2.175086	0.000000	1.519528
F	-2.234620	0.000000	-1.010234

2-fluoropyridine S_0

C	-1.314175	0.502701	0.000000
N	-1.364244	-0.800234	0.000000
C	-0.197164	-1.448794	0.000000
C	1.027725	-0.807150	0.000000
C	1.041564	0.583054	0.000000
C	-0.157185	1.269639	0.000000
H	-0.258206	-2.531153	0.000000
H	1.944981	-1.379809	0.000000
H	1.978048	1.126681	0.000000

H	-0.212562	2.348985	0.000000
F	-2.488790	1.136072	0.000000

2-fluoropyridine S_1

C	-1.320113	0.490466	0.000000
N	-1.435972	-0.842879	0.000000
C	-0.225455	-1.462101	0.000000
C	1.028241	-0.790934	0.000000
C	1.105939	0.618223	0.000000
C	-0.151377	1.281085	0.000000
H	-0.248651	-2.544628	0.000000
H	1.926349	-1.395311	0.000000
H	2.042512	1.150884	0.000000
H	-0.251829	2.357157	0.000000
F	-2.469652	1.138029	0.000000

2-hydroxypyridine S_0

C	-0.977282	0.750290	0.000000
C	-0.968870	-0.645270	0.000000
N	0.130665	-1.375633	0.000000
C	1.301788	-0.734813	0.000000
C	1.415124	0.641237	0.000000
C	0.242162	1.392300	0.000000
O	-2.145356	-1.297677	0.000000
H	2.183951	-1.365466	0.000000
H	2.388323	1.112262	0.000000
H	0.282720	2.474694	0.000000
H	-1.915815	1.286413	0.000000
H	-1.937410	-2.238338	0.000000

2-hydroxypyridine S_1

C	-0.996238	0.765707	0.000000
C	-0.967553	-0.638541	0.000000
N	0.119988	-1.452990	0.000000
C	1.291613	-0.773581	0.000000
C	1.389703	0.642923	0.000000
C	0.248720	1.460931	0.000000
O	-2.123820	-1.288373	0.000000
H	2.193384	-1.372582	0.000000
H	2.380976	1.079063	0.000000
H	0.306040	2.537232	0.000000
H	-1.952243	1.269676	0.000000
H	-1.890571	-2.229465	0.000000

2-pyridone S_0

C	-1.245908	0.711039	0.000000
N	-1.134849	-0.685198	0.000000
C	0.033211	-1.380423	0.000000
C	1.219543	-0.732271	0.000000
C	1.201960	0.691440	0.000000
C	0.038325	1.384003	0.000000
H	-2.016501	-1.175246	0.000000
H	-0.055131	-2.458415	0.000000
H	2.146013	-1.286157	0.000000
H	2.143128	1.228927	0.000000
H	0.013277	2.464767	0.000000
O	-2.343068	1.237544	0.000000

2-pyridone S_1

C	-1.385877	0.105025	0.000000
N	-0.729806	-1.137644	0.000000
C	0.622464	-1.251891	0.000000
C	1.410373	-0.075580	0.000000
C	0.829292	1.171006	0.000000
C	-0.608728	1.264887	0.000000
H	-1.338648	-1.941928	0.000000
H	1.041103	-2.246412	0.000000
H	2.485697	-0.193346	0.000000
H	1.434898	2.065137	0.000000
H	-1.126779	2.211721	0.000000
O	-2.633988	0.029016	0.000000

2-methylpyrimidine S_0

C	0.000010	1.959836	0.000000
C	-1.171845	1.221707	0.000000
N	-1.177940	-0.104703	0.000000
C	0.011026	-0.714707	0.000000
N	1.192930	-0.097074	0.000000
C	1.175538	1.232599	0.000000
H	-2.142372	1.707974	0.000000
H	2.142537	1.725460	0.000000
H	-0.004752	3.040846	0.000000
C	0.004636	-2.211945	0.000000
H	1.022376	-2.594804	0.000000
H	-0.526077	-2.582594	0.878412
H	-0.526077	-2.582594	-0.878412

2-methylpyrimidine S_1

C	-0.015112	2.008449	0.000000
C	-1.164519	1.275446	0.000000
N	-1.151615	-0.095134	0.000000
C	0.010047	-0.782129	0.000000
N	1.081654	-0.064703	0.000000
C	1.205467	1.288168	0.000000
H	-2.142648	1.739126	0.000000
H	2.190982	1.722638	0.000000
H	-0.026396	3.090205	0.000000
C	0.013373	-2.267314	0.000000
H	1.031795	-2.650422	0.000000
H	-0.516514	-2.632170	0.881352
H	-0.516514	-2.632170	-0.881352

5-methylpyrimidine S_0

C	0.873486	0.849529	0.000000
C	-0.358465	0.210927	0.000000
C	-0.298845	-1.178206	0.000000
N	0.842862	-1.855702	0.000000
C	1.955122	-1.128249	0.000000
N	2.031736	0.195783	0.000000
H	2.893351	-1.672443	0.000000
H	-1.210831	-1.769625	0.000000
H	0.932052	1.934682	0.000000
C	-1.659313	0.957450	0.000000
H	-1.492107	2.034861	0.000000
H	-2.254524	0.710486	-0.881136
H	-2.254524	0.710486	0.881136

5-methylpyrimidine S_1

C	0.844197	0.855364	0.000000
C	-0.374431	0.243401	0.000000
C	-0.347427	-1.189463	0.000000
N	0.878286	-1.751904	0.000000
C	2.030627	-1.176904	0.000000
N	2.030804	0.168482	0.000000
H	2.954334	-1.736816	0.000000
H	-1.219791	-1.822797	0.000000
H	0.929792	1.935586	0.000000
C	-1.675746	0.978158	0.000000
H	-1.517087	2.056642	0.000000

H	-2.266783	0.720130	-0.882019
H	-2.266783	0.720130	0.882019

7-azaindole S_0

N	-0.632523	1.838772	0.000000
C	-0.671656	0.470508	0.000000
C	0.664109	0.006216	0.000000
C	1.505727	1.165037	0.000000
C	0.680323	2.247332	0.000000
C	0.841887	-1.374650	0.000000
C	-0.291322	-2.167012	0.000000
C	-1.559927	-1.576027	0.000000
N	-1.772548	-0.265991	0.000000
H	-2.446993	-2.200374	0.000000
H	1.831241	-1.816180	0.000000
H	-0.210960	-3.245925	0.000000
H	-1.444343	2.428629	0.000000
H	2.582848	1.192402	0.000000
H	0.924155	3.297263	0.000000

7-azaindole S_1

N	-0.606525	1.868952	0.000000
C	-0.659819	0.450117	0.000000
C	0.658981	-0.005005	0.000000
C	1.487366	1.140017	0.000000
C	0.648086	2.300750	0.000000
C	0.887321	-1.406213	0.000000
C	-0.303837	-2.177947	0.000000
C	-1.546151	-1.593446	0.000000
N	-1.793772	-0.220463	0.000000
H	-2.436620	-2.210100	0.000000
H	1.873628	-1.843907	0.000000
H	-0.245109	-3.259010	0.000000
H	-1.438135	2.439128	0.000000
H	2.565785	1.171808	0.000000
H	0.908810	3.345339	0.000000

7-hydroxyquinoline, *cis* S_0

N	0.462083	1.966702	0.000000
C	0.432078	0.607499	0.000000
C	-0.782681	-0.123445	0.000000
C	-1.987771	0.607015	0.000000
C	-1.942580	1.971820	0.000000

C	-0.681311	2.602251	0.000000
C	1.660860	-0.090127	0.000000
C	1.675189	-1.458078	0.000000
C	0.465756	-2.193586	0.000000
C	-0.727689	-1.539064	0.000000
H	-0.625715	3.687220	0.000000
H	-1.655021	-2.100528	0.000000
H	0.519950	-3.274295	0.000000
O	2.815156	-2.193761	0.000000
H	2.574521	0.493513	0.000000
H	-2.934306	0.077738	0.000000
H	-2.844787	2.568937	0.000000
H	3.576269	-1.609801	0.000000

7-hydroxyquinoline, *cis* S_1

N	0.489293	1.970500	0.000000
C	0.434861	0.630861	0.000000
C	-0.789810	-0.140222	0.000000
C	-1.992433	0.592158	0.000000
C	-1.917040	1.993079	0.000000
C	-0.685525	2.636655	0.000000
C	1.635036	-0.085523	0.000000
C	1.653426	-1.512826	0.000000
C	0.482370	-2.261077	0.000000
C	-0.720674	-1.555256	0.000000
H	-0.623355	3.717381	0.000000
H	-1.654376	-2.106305	0.000000
H	0.524863	-3.339574	0.000000
O	2.822547	-2.154979	0.000000
H	2.565805	0.472666	0.000000
H	-2.948686	0.085729	0.000000
H	-2.826179	2.582041	0.000000
H	3.549876	-1.525299	0.000000

7-hydroxyquinoline, *trans* S_0

N	0.512068	2.039031	0.000000
C	0.479618	0.677459	0.000000
C	-0.740548	-0.047663	0.000000
C	-1.944848	0.687850	0.000000
C	-1.893596	2.050826	0.000000
C	-0.628027	2.676827	0.000000
C	1.705019	-0.019571	0.000000
C	1.716128	-1.387577	0.000000
C	0.502991	-2.116510	0.000000

C	-0.692393	-1.459957	0.000000
H	-0.568484	3.761713	0.000000
H	-1.620559	-2.019879	0.000000
H	0.529709	-3.201472	0.000000
O	2.916141	-2.023651	0.000000
H	2.629319	0.541553	0.000000
H	-2.893093	0.161673	0.000000
H	-2.793005	2.652276	0.000000
H	2.783538	-2.972906	0.000000

7-hydroxyquinoline, *trans* S_1

N	0.532460	2.045610	0.000000
C	0.476743	0.707951	0.000000
C	-0.749280	-0.057700	0.000000
C	-1.951229	0.675746	0.000001
C	-1.873671	2.077192	0.000000
C	-0.642711	2.715411	-0.000001
C	1.678777	-0.010926	0.000000
C	1.690105	-1.434785	0.000000
C	0.515973	-2.182401	0.000000
C	-0.686412	-1.471611	0.000000
H	-0.575893	3.795937	-0.000001
H	-1.621700	-2.020146	0.000000
H	0.536190	-3.264352	-0.000001
O	2.904949	-1.987352	0.000000
H	2.620986	0.520645	0.000001
H	-2.907587	0.169388	0.000001
H	-2.781560	2.668066	0.000000
H	2.833838	-2.946651	0.000000

2-hydroxyquinoline, enol S_0

C	0.430279	1.899594	0.000000
C	0.483564	0.488133	0.000000
C	-0.719646	-0.257813	0.000000
C	-1.950364	0.436077	0.000000
C	-1.973122	1.803286	0.000000
C	-0.774080	2.545782	0.000000
C	1.694822	-0.244154	0.000000
C	1.662434	-1.602407	0.000000
C	0.392946	-2.246793	0.000000
N	-0.738865	-1.618172	0.000000
O	0.314642	-3.596006	0.000000
H	1.358567	2.460079	0.000000
H	-0.813104	3.627818	0.000000

H	-2.921903	2.325808	0.000000
H	-2.860802	-0.149060	0.000000
H	2.641284	0.284578	0.000000
H	2.577007	-2.184134	0.000000
H	1.196342	-3.972615	0.000000

2-hydroxyquinoline, enol S_1

C	0.437265	1.879017	0.000000
C	0.527176	0.488831	0.000000
C	-0.725495	-0.261810	0.000000
C	-1.957950	0.437161	0.000000
C	-2.009010	1.833977	0.000000
C	-0.812858	2.540148	0.000000
C	1.731979	-0.234920	0.000000
C	1.693498	-1.636541	0.000000
C	0.430939	-2.239969	0.000000
N	-0.750373	-1.602812	0.000000
O	0.293907	-3.568967	0.000000
H	1.345976	2.469533	0.000000
H	-0.824524	3.623555	0.000000
H	-2.957417	2.351972	0.000000
H	-2.860259	-0.160906	0.000000
H	2.676694	0.293125	0.000000
H	2.597932	-2.230235	0.000000
H	1.162510	-3.981140	0.000000

2-hydroxyquinoline, keto S_0

N	0.558774	1.703464	0.000000
C	0.599789	0.326721	0.000000
C	-0.611362	-0.381931	0.000000
C	-1.834765	0.377909	0.000000
C	-1.832319	1.720371	0.000000
C	-0.586135	2.485549	0.000000
C	1.815492	-0.362681	0.000000
C	1.818945	-1.740744	0.000000
C	0.620963	-2.459164	0.000000
C	-0.577545	-1.781007	0.000000
H	-1.515437	-2.324555	0.000000
H	0.637522	-3.541073	0.000000
H	2.763719	-2.269764	0.000000
H	2.748013	0.189598	0.000000
H	-2.773887	-0.164978	0.000000
H	-2.744131	2.301142	0.000000
O	-0.511635	3.698923	0.000000

H	1.424018	2.222240	0.000000

2-hydroxyquinoline, keto S_1

N	0.561762	1.674688	0.000000
C	0.611422	0.327088	0.000000
C	-0.664831	-0.380667	0.000000
C	-1.854114	0.364178	0.000000
C	-1.852717	1.763415	0.000000
C	-0.627738	2.470617	0.000000
C	1.834539	-0.359567	0.000000
C	1.853091	-1.745202	0.000000
C	0.630468	-2.444381	0.000000
C	-0.590668	-1.787326	0.000000
H	-1.511442	-2.356664	0.000000
H	0.644037	-3.527546	0.000000
H	2.790930	-2.282060	0.000000
H	2.757640	0.208551	0.000000
H	-2.794645	-0.171901	0.000000
H	-2.762017	2.343835	0.000000
O	-0.438526	3.682378	0.000000
H	1.412809	2.220575	0.000000

dibenzofuran S_0

C	1.715971	0.000000	-1.355127
C	0.724691	0.000000	-0.380542
C	1.092263	0.000000	0.966753
C	2.406232	0.000000	1.391364
C	3.379421	0.000000	0.403634
C	3.040967	0.000000	-0.951636
C	-0.724691	0.000000	-0.380542
C	-1.092263	0.000000	0.966753
O	0.000000	0.000000	1.788936
C	-1.715971	0.000000	-1.355127
C	-3.040967	0.000000	-0.951636
C	-3.379421	0.000000	0.403634
C	-2.406232	0.000000	1.391364
H	-2.655325	0.000000	2.443819
H	-4.423646	0.000000	0.690091
H	-3.827324	0.000000	-1.695508
H	-1.459073	0.000000	-2.407149
H	1.459073	0.000000	-2.407149
H	3.827324	0.000000	-1.695508
H	4.423646	0.000000	0.690091
H	2.655325	0.000000	2.443819

dibenzofuran S_1

C	0.000000	1.724658	-1.529927
C	0.000000	0.710466	-0.567015
C	0.000000	1.099937	0.804579
C	0.000000	2.403705	1.254868
C	0.000000	3.409314	0.265446
C	0.000000	3.063611	-1.087429
C	0.000000	-0.710466	-0.567015
C	0.000000	-1.099937	0.804579
O	0.000000	0.000000	1.601742
C	0.000000	-1.724658	-1.529927
C	0.000000	-3.063611	-1.087429
C	0.000000	-3.409314	0.265446
C	0.000000	-2.403705	1.254868
H	0.000000	-2.632291	2.311505
H	0.000000	-4.449990	0.557191
H	0.000000	-3.852849	-1.828994
H	0.000000	-1.498031	-2.587384
H	0.000000	1.498031	-2.587384
H	0.000000	3.852849	-1.828994
H	0.000000	4.449990	0.557191
H	0.000000	2.632291	2.311505

pyrrolo[3,2-*h*]quinoline S_0

C	0.135542	-0.683711	0.000000
N	0.060662	-2.032509	0.000000
C	1.190478	-2.702245	0.000000
C	2.456698	-2.095733	0.000000
C	2.534774	-0.727240	0.000000
C	1.355370	0.038130	0.000000
H	1.107378	-3.784785	0.000000
H	3.347870	-2.709471	0.000000
H	3.496494	-0.226185	0.000000
C	-1.051132	0.084963	0.000000
C	-1.055783	1.480251	0.000000
C	0.182571	2.173044	0.000000
C	1.346719	1.468149	0.000000
H	0.198437	3.256216	0.000000
H	2.299121	1.985345	0.000000
C	-2.424958	1.884705	0.000000
C	-3.175342	0.742661	0.000000
N	-2.342854	-0.345772	0.000000
H	-2.609106	-1.314081	0.000000

H	-2.807416	2.892297	0.000000
H	-4.245515	0.615971	0.000000

pyrrolo[3,2-*h*]quinoline S_1

C	0.150529	-0.698387	0.000000
N	0.016748	-2.022064	0.000000
C	1.200401	-2.726185	0.000000
C	2.434116	-2.132611	0.000000
C	2.560128	-0.724461	0.000000
C	1.364760	0.029635	0.000000
H	1.100041	-3.804296	0.000000
H	3.320646	-2.754763	0.000000
H	3.527049	-0.240693	0.000000
C	-1.025019	0.102131	0.000000
C	-1.059672	1.546717	0.000000
C	0.138378	2.222952	0.000000
C	1.322356	1.450181	0.000000
H	0.189713	3.302900	0.000000
H	2.271918	1.974321	0.000000
C	-2.455961	1.903752	0.000000
C	-3.161345	0.747839	0.000000
N	-2.286293	-0.339122	0.000000
H	-2.512650	-1.321295	0.000000
H	-2.869245	2.898246	0.000000
H	-4.226606	0.585204	0.000000

carbazole S_0

C	1.126464	0.000000	-0.895839
N	0.000000	0.000000	-1.693132
C	-1.126464	0.000000	-0.895839
C	-0.723491	0.000000	0.454005
C	0.723491	0.000000	0.454005
C	-1.688453	0.000000	1.456250
C	-3.025878	0.000000	1.102669
C	-3.407554	0.000000	-0.242696
C	-2.468178	0.000000	-1.258403
C	2.468178	0.000000	-1.258403
C	3.407554	0.000000	-0.242696
C	3.025878	0.000000	1.102669
C	1.688453	0.000000	1.456250
H	-2.770815	0.000000	-2.298438
H	-4.460661	0.000000	-0.495732
H	-3.786958	0.000000	1.872359
H	-1.396505	0.000000	2.499617

H	1.396505	0.000000	2.499617
H	3.786958	0.000000	1.872359
H	4.460661	0.000000	-0.495732
H	2.770815	0.000000	-2.298438
H	0.000000	0.000000	-2.695411

carbazole S_1

C	1.139196	0.000000	-0.837246
N	0.000000	0.000000	-1.609079
C	-1.139196	0.000000	-0.837246
C	-0.713809	0.000000	0.528859
C	0.713809	0.000000	0.528859
C	-1.699899	0.000000	1.518733
C	-3.050842	0.000000	1.118256
C	-3.440246	0.000000	-0.217911
C	-2.460676	0.000000	-1.236839
C	2.460676	0.000000	-1.236839
C	3.440246	0.000000	-0.217911
C	3.050842	0.000000	1.118256
C	1.699899	0.000000	1.518733
H	-2.736001	0.000000	-2.283937
H	-4.489382	0.000000	-0.477756
H	-3.816146	0.000000	1.885179
H	-1.441519	0.000000	2.568949
H	1.441519	0.000000	2.568949
H	3.816146	0.000000	1.885179
H	4.489382	0.000000	-0.477756
H	2.736001	0.000000	-2.283937
H	0.000000	0.000000	-2.616120

tryptamine, A-ph S_0

C	-2.136691	0.149661	0.896260
N	-1.256006	0.129814	1.956382
C	0.024747	0.042809	1.471355
C	-0.063601	0.003413	0.064965
C	-1.458196	0.074317	-0.281239
C	1.247355	-0.001075	2.138316
C	2.390062	-0.083318	1.369306
C	2.324891	-0.118843	-0.032768
C	1.112010	-0.076396	-0.688009
C	-2.025696	0.021300	-1.662068
C	-1.972558	-1.382388	-2.266093
N	-2.439471	-1.362933	-3.647784
H	1.301486	0.028550	3.220052

H	3.357048	-0.119448	1.855658
H	3.243063	-0.178036	-0.603712
H	1.069261	-0.099918	-1.770816
H	-1.510798	0.192826	2.923498
H	-3.199065	0.221802	1.070035
H	-1.478116	0.697359	-2.324303
H	-3.063882	0.367830	-1.648637
H	-2.537549	-2.063653	-1.613499
H	-0.936888	-1.730096	-2.262492
H	-3.420904	-1.118912	-3.689675
H	-2.337914	-2.272285	-4.077362

tryptamine, A-ph S_1

C	-2.187524	0.174583	0.915465
N	-1.296583	0.128982	1.916608
C	0.017460	0.053434	1.435168
C	-0.068276	0.066366	0.036792
C	-1.443215	0.137133	-0.303741
C	1.202946	-0.055596	2.144129
C	2.394819	-0.137225	1.328342
C	2.340486	-0.123519	-0.040873
C	1.107969	-0.023563	-0.748959
C	-2.017010	0.064494	-1.665029
C	-1.947160	-1.367948	-2.221193
N	-2.449806	-1.401528	-3.586456
H	1.246588	-0.084171	3.223341
H	3.354841	-0.211490	1.823773
H	3.262937	-0.184388	-0.605440
H	1.075552	0.024611	-1.828507
H	-1.532556	0.160895	2.894592
H	-3.246976	0.270593	1.082665
H	-1.454928	0.710013	-2.344031
H	-3.056835	0.404440	-1.662890
H	-2.478642	-2.039195	-1.531593
H	-0.899710	-1.677360	-2.227184
H	-3.454042	-1.281896	-3.609677
H	-2.237766	-2.285286	-4.027973

tryptamine, A-py S_0

C	-2.130746	0.127534	0.872237
N	-1.260246	0.121451	1.940453
C	0.025719	0.044174	1.468330
C	-0.048690	-0.004058	0.061052
C	-1.440739	0.050837	-0.298604

C	1.241977	0.015156	2.147727
C	2.393465	-0.060242	1.391330
C	2.342855	-0.104093	-0.011093
C	1.136023	-0.077256	-0.678296
C	-2.006326	-0.009335	-1.680269
C	-1.929469	-1.409210	-2.289663
N	-2.489867	-1.409272	-3.636865
H	1.284568	0.050722	3.229806
H	3.355611	-0.084758	1.887863
H	3.267282	-0.158514	-0.572382
H	1.105617	-0.110072	-1.761328
H	-1.524999	0.186331	2.904815
H	-3.195484	0.191026	1.034230
H	-1.463456	0.688187	-2.328551
H	-3.049763	0.312752	-1.680846
H	-2.521514	-2.088931	-1.672409
H	-0.889607	-1.762826	-2.242060
H	-1.924409	-0.842549	-4.256428
H	-2.507890	-2.344662	-4.019938

tryptamine, A-py S_1

C	-2.181706	0.136905	0.889905
N	-1.302310	0.106307	1.900617
C	0.018550	0.048987	1.433577
C	-0.051838	0.056020	0.034945
C	-1.423589	0.107900	-0.320745
C	1.198302	-0.036806	2.156452
C	2.399048	-0.102688	1.353480
C	2.360383	-0.094881	-0.016540
C	1.134211	-0.017201	-0.738481
C	-1.988006	0.032065	-1.684771
C	-1.890522	-1.396971	-2.249189
N	-2.478482	-1.446474	-3.578943
H	1.230957	-0.058377	3.236141
H	3.354847	-0.159839	1.859360
H	3.290378	-0.143670	-0.569797
H	1.112960	0.023293	-1.818625
H	-1.549894	0.135981	2.875775
H	-3.244929	0.212280	1.043318
H	-1.427786	0.701662	-2.345307
H	-3.034327	0.342791	-1.700900
H	-2.456480	-2.067524	-1.598286
H	-0.838927	-1.711277	-2.204667
H	-1.904022	-0.945766	-4.244749
H	-2.556907	-2.400337	-3.903471

tryptamine, A-up S_0

C	-2.130242	0.140397	0.887508
N	-1.256281	0.107867	1.952331
C	0.027934	0.035141	1.474468
C	-0.050984	0.017654	0.066991
C	-1.443770	0.088471	-0.287017
C	1.246264	-0.014590	2.148932
C	2.394570	-0.080424	1.386902
C	2.339180	-0.094971	-0.015913
C	1.130469	-0.046906	-0.678290
C	-2.005569	0.045753	-1.670523
C	-1.943315	-1.357685	-2.295719
N	-2.416039	-1.457685	-3.668084
H	1.292809	-0.002509	3.231331
H	3.358259	-0.121013	1.879334
H	3.261276	-0.143931	-0.581438
H	1.096666	-0.058015	-1.761638
H	-1.517698	0.149976	2.918873
H	-3.194091	0.203769	1.055532
H	-1.455415	0.740321	-2.315204
H	-3.045504	0.386327	-1.661982
H	-2.527147	-2.044669	-1.678193
H	-0.913750	-1.721845	-2.261255
H	-1.867712	-0.869047	-4.281924
H	-3.378671	-1.154479	-3.741785

tryptamine, A-up S_1

C	-2.180883	0.145780	0.901530
N	-1.297020	0.089569	1.908394
C	0.021904	0.040781	1.437432
C	-0.051817	0.082754	0.039285
C	-1.425262	0.150977	-0.311360
C	1.203095	-0.067273	2.154543
C	2.401422	-0.121524	1.347918
C	2.359028	-0.081384	-0.021015
C	1.131076	0.021415	-0.737734
C	-1.983727	0.093940	-1.674963
C	-1.925674	-1.354278	-2.239924
N	-2.405091	-1.505480	-3.595966
H	1.237937	-0.114878	3.233363
H	3.358030	-0.197848	1.849643
H	3.286795	-0.124571	-0.578451
H	1.108361	0.081972	-1.816945

H	-1.541312	0.096882	2.884858
H	-3.242646	0.225805	1.062367
H	-1.400475	0.738218	-2.339133
H	-3.020347	0.441899	-1.690096
H	-2.507917	-2.008393	-1.587534
H	-0.890159	-1.697500	-2.188194
H	-1.860175	-0.957754	-4.247916
H	-3.373922	-1.231188	-3.686882

tryptamine, Ph-out S_0

C	0.001685	0.007399	0.078860
C	0.041777	0.061712	1.487609
C	1.241394	0.069060	2.196924
C	2.411406	0.023194	1.467684
C	2.394727	-0.030428	0.064566
C	1.205749	-0.038049	-0.634013
N	-1.255762	0.102794	1.931077
H	1.256506	0.110673	3.279460
H	3.362160	0.027579	1.986475
H	3.333125	-0.067060	-0.474609
H	1.195439	-0.097244	-1.715542
C	-1.384495	0.023417	-0.312094
C	-2.101842	0.084845	0.844465
H	-1.542588	0.171048	2.888915
H	-3.171009	0.127811	0.983139
C	-1.935346	-0.034896	-1.703502
H	-1.292018	0.535630	-2.378581
C	-2.075156	-1.454963	-2.254870
H	-2.920012	0.439565	-1.720029
H	-2.536171	-1.397735	-3.244450
N	-0.774373	-2.095673	-2.403576
H	-2.766467	-2.012719	-1.604812
H	-0.334414	-2.221804	-1.500129
H	-0.869346	-3.010048	-2.823756

tryptamine, Ph-out S_1

C	-0.001035	0.038091	0.058060
C	0.030862	0.074441	1.460091
C	1.189910	0.039022	2.217908
C	2.417034	-0.018142	1.454153
C	2.417173	-0.055450	0.084646
C	1.212251	-0.036755	-0.675457
N	-1.300632	0.120616	1.890815
H	1.190390	0.064643	3.298066

H	3.358008	-0.033902	1.989849
H	3.362812	-0.100172	-0.441757
H	1.219838	-0.049605	-1.756012
C	-1.364073	0.062288	-0.335129
C	-2.153618	0.108802	0.857357
H	-1.573449	0.171696	2.858365
H	-3.221686	0.169542	0.981276
C	-1.927257	-0.028885	-1.702979
H	-1.281670	0.497420	-2.409349
C	-2.070322	-1.485736	-2.183179
H	-2.914372	0.440521	-1.721550
H	-2.658362	-1.476197	-3.104102
N	-0.772322	-2.062944	-2.480412
H	-2.651741	-2.040434	-1.431215
H	-0.162538	-2.057300	-1.670353
H	-0.860211	-3.017440	-2.799882

tryptamine, Ph-up S_0

C	-2.091455	0.054002	0.824724
N	-1.251591	0.042680	1.915948
C	0.048440	0.039019	1.479731
C	0.016071	0.044304	0.069653
C	-1.366732	0.052863	-0.329189
C	1.243939	0.033736	2.195910
C	2.418965	0.035722	1.473515
C	2.411510	0.045425	0.069391
C	1.225742	0.050131	-0.634180
C	-1.902812	0.013323	-1.725376
C	-2.076067	-1.414720	-2.273648
N	-0.871150	-2.223454	-2.359275
H	1.252498	0.029230	3.279219
H	3.366316	0.031293	1.998190
H	3.353316	0.049676	-0.464936
H	1.229225	0.058265	-1.717751
H	-1.545223	0.058193	2.874127
H	-3.161941	0.067901	0.958733
H	-1.234875	0.571581	-2.389717
H	-2.871218	0.521277	-1.762245
H	-2.519560	-1.358960	-3.271561
H	-2.792551	-1.947895	-1.642842
H	-0.435184	-2.311094	-1.449695
H	-0.192014	-1.792867	-2.973666

tryptamine, Ph-up S_1

C	-2.162406	0.144579	0.858379
N	-1.307159	0.124121	1.890110
C	0.023315	0.079730	1.454281
C	-0.012823	0.090157	0.053293
C	-1.377388	0.124398	-0.334909
C	1.184665	-0.003373	2.206896
C	2.406048	-0.058181	1.437569
C	2.404133	-0.045787	0.067499
C	1.197246	0.024414	-0.687814
C	-1.927387	0.011131	-1.696277
C	-1.993700	-1.479074	-2.171360
N	-0.733543	-2.134562	-2.402430
H	1.188337	-0.023252	3.287062
H	3.348387	-0.111049	1.968589
H	3.348636	-0.085740	-0.461381
H	1.208442	0.108693	-1.765224
H	-1.577108	0.157821	2.859077
H	-3.229767	0.209927	0.986937
H	-1.308241	0.566132	-2.405366
H	-2.940066	0.422665	-1.731611
H	-2.572877	-1.499826	-3.097436
H	-2.558611	-2.048339	-1.430167
H	-0.135066	-2.125423	-1.584429
H	-0.219409	-1.699555	-3.156198

tryptamine, Py-out S_0

C	0.507277	0.456685	0.219205
C	0.584157	0.520991	1.625928
C	1.799394	0.472366	2.305266
C	2.948017	0.358096	1.549150
C	2.895166	0.294562	0.147731
C	1.689299	0.342556	-0.519922
N	-0.698998	0.636546	2.098783
H	1.845009	0.524122	3.386521
H	3.909421	0.320409	2.046239
H	3.818269	0.209183	-0.411995
H	1.656089	0.295696	-1.602158
C	-0.883582	0.547422	-0.139479
C	-1.570541	0.652215	1.031548
H	-0.959981	0.722996	3.062545
H	-2.634174	0.737176	1.189495
C	-1.453065	0.482254	-1.520451
H	-0.890257	1.147009	-2.182387
C	-1.429816	-0.931195	-2.106053
H	-2.487380	0.833364	-1.507499

H	-0.384589	-1.265064	-2.185857
N	-2.263031	-1.822623	-1.309042
H	-1.837442	-0.896856	-3.119328
H	-2.260750	-2.757932	-1.692456
H	-1.898472	-1.879980	-0.365765

tryptamine, Py-out S_1

C	0.494969	0.487034	0.200014
C	0.578249	0.529592	1.597166
C	1.761974	0.439518	2.313791
C	2.953552	0.314875	1.503497
C	2.902553	0.274635	0.134778
C	1.671538	0.354775	-0.579951
N	-0.735196	0.652721	2.073271
H	1.805903	0.467137	3.392908
H	3.912009	0.255780	2.004109
H	3.826866	0.184233	-0.422807
H	1.640385	0.351327	-1.660418
C	-0.878459	0.585866	-0.145754
C	-1.622386	0.683521	1.069813
H	-0.972669	0.714283	3.049595
H	-2.684243	0.768135	1.225972
C	-1.456568	0.507801	-1.505573
H	-0.885763	1.159440	-2.173696
C	-1.394181	-0.924331	-2.064533
H	-2.497003	0.838619	-1.499526
H	-0.338592	-1.221716	-2.124845
N	-2.212182	-1.821690	-1.260531
H	-1.796673	-0.910986	-3.079110
H	-2.282733	-2.729860	-1.698671
H	-1.791359	-1.960718	-0.349512

tryptamine, Py-up S_0

C	-2.129404	0.260062	0.886313
N	-1.257130	0.225641	1.952640
C	0.023069	0.089946	1.477122
C	-0.056657	0.033310	0.070543
C	-1.446214	0.148489	-0.286366
C	1.238120	0.017001	2.154740
C	2.383239	-0.114622	1.396433
C	2.327445	-0.171730	-0.005188
C	1.121957	-0.099678	-0.670958
C	-2.013636	0.090486	-1.666424
C	-1.988141	-1.327980	-2.265998

N	-2.738876	-2.334695	-1.534393
H	1.286019	0.062683	3.236130
H	3.344429	-0.172140	1.891977
H	3.247967	-0.272438	-0.566497
H	1.087041	-0.142374	-1.753286
H	-1.514722	0.313427	2.917174
H	-3.190179	0.370865	1.048893
H	-1.455396	0.762778	-2.326416
H	-3.047353	0.450151	-1.652534
H	-0.952269	-1.669224	-2.336713
H	-2.373480	-1.287758	-3.287862
H	-3.716213	-2.076930	-1.474513
H	-2.391097	-2.405650	-0.585930

tryptamine, Py-up S_1

C	-2.181705	0.282688	0.919422
N	-1.292917	0.240523	1.923696
C	0.017757	0.105449	1.447916
C	-0.065787	0.074084	0.049144
C	-1.438004	0.185801	-0.296748
C	1.198009	-0.011215	2.163459
C	2.389796	-0.152763	1.355427
C	2.338467	-0.182692	-0.013067
C	1.110056	-0.073480	-0.727829
C	-2.013561	0.109096	-1.654110
C	-1.957879	-1.332783	-2.228863
N	-2.709689	-2.337451	-1.507915
H	1.239953	0.003106	3.243035
H	3.345623	-0.235574	1.857335
H	3.260565	-0.288238	-0.571591
H	1.082010	-0.070218	-1.808483
H	-1.528403	0.308442	2.900121
H	-3.238267	0.415046	1.079370
H	-1.442969	0.758739	-2.325567
H	-3.051160	0.455411	-1.651618
H	-0.912923	-1.647571	-2.265531
H	-2.320624	-1.297987	-3.258322
H	-3.689138	-2.094991	-1.439616
H	-2.350689	-2.463793	-0.570755

porphycene S_0

C	-3.426107	1.908650	0.000000
C	-2.414021	0.904517	0.000000
N	-1.219694	1.540251	0.000000

C	-1.388187	2.887551	0.000000
C	-2.798748	3.122976	0.000000
C	-0.365749	3.841322	0.000000
C	1.011357	3.693551	0.000000
C	1.827033	2.551962	0.000000
H	-0.262248	1.126277	0.000000
N	1.410506	1.265932	0.000000
C	3.277546	2.591727	0.000000
C	3.703838	1.305721	0.000000
C	2.509259	0.494150	0.000000
C	2.414021	-0.904517	0.000000
C	3.426107	-1.908650	0.000000
C	2.798748	-3.122976	0.000000
C	1.388187	-2.887551	0.000000
N	1.219694	-1.540251	0.000000
C	0.365749	-3.841322	0.000000
C	-1.011357	-3.693551	0.000000
C	-1.827033	-2.551962	0.000000
C	-3.277546	-2.591727	0.000000
C	-3.703838	-1.305721	0.000000
C	-2.509259	-0.494150	0.000000
N	-1.410506	-1.265932	0.000000
H	0.262248	-1.126277	0.000000
H	3.259870	-4.098221	0.000000
H	4.487759	-1.720331	0.000000
H	0.726422	-4.864024	0.000000
H	-1.566746	-4.625688	0.000000
H	-3.879094	-3.488401	0.000000
H	-4.719979	-0.942648	0.000000
H	-4.487759	1.720331	0.000000
H	-3.259870	4.098221	0.000000
H	-0.726422	4.864024	0.000000
H	1.566746	4.625688	0.000000
H	3.879094	3.488401	0.000000
H	4.719979	0.942648	0.000000

porphycene S_1

C	-3.449300	1.897580	0.000000
C	-2.440755	0.894518	0.000000
N	-1.234786	1.538552	0.000000
C	-1.409367	2.878775	0.000000
C	-2.819092	3.114784	0.000000
C	-0.378948	3.849272	0.000000
C	0.986943	3.705727	0.000000
C	1.831329	2.558286	0.000000

H	-0.281510	1.123822	0.000000
N	1.418460	1.277172	0.000000
C	3.272308	2.610748	0.000000
C	3.714631	1.321686	0.000000
C	2.539125	0.503498	0.000000
C	2.440755	-0.894518	0.000000
C	3.449300	-1.897580	0.000000
C	2.819092	-3.114784	0.000000
C	1.409367	-2.878775	0.000000
N	1.234786	-1.538552	0.000000
C	0.378948	-3.849272	0.000000
C	-0.986943	-3.705727	0.000000
C	-1.831329	-2.558286	0.000000
C	-3.272308	-2.610748	0.000000
C	-3.714631	-1.321686	0.000000
C	-2.539125	-0.503498	0.000000
N	-1.418460	-1.277172	0.000000
H	0.281510	-1.123822	0.000000
H	3.278487	-4.090822	0.000000
H	4.510719	-1.708828	0.000000
H	0.746900	-4.868862	0.000000
H	-1.540133	-4.639691	0.000000
H	-3.866773	-3.512173	0.000000
H	-4.734732	-0.970943	0.000000
H	-4.510719	1.708828	0.000000
H	-3.278487	4.090822	0.000000
H	-0.746900	4.868862	0.000000
H	1.540133	4.639691	0.000000
H	3.866773	3.512173	0.000000
H	4.734732	0.970943	0.000000

porphine S_0

N	0.000000	-2.015135	0.000000
N	2.098550	0.000000	0.000000
C	1.078102	-2.833716	0.000000
C	0.673100	-4.231206	0.000000
C	2.406649	-2.424730	0.000000
C	2.872955	-1.121263	0.000000
C	4.232738	-0.680867	0.000000
H	1.345451	-5.076108	0.000000
H	3.162566	-3.200337	0.000000
H	5.085796	-1.341008	0.000000
H	1.086460	0.000000	0.000000
N	0.000000	2.015135	0.000000
N	-2.098550	0.000000	0.000000

C	1.078102	2.833716	0.000000
C	-1.078102	2.833716	0.000000
C	-1.078102	-2.833716	0.000000
C	0.673100	4.231206	0.000000
C	-0.673100	4.231206	0.000000
C	-0.673100	-4.231206	0.000000
C	2.406649	2.424730	0.000000
C	-2.406649	2.424730	0.000000
C	-2.406649	-2.424730	0.000000
C	2.872955	1.121263	0.000000
C	-2.872955	1.121263	0.000000
C	-2.872955	-1.121263	0.000000
C	4.232738	0.680867	0.000000
C	-4.232738	0.680867	0.000000
C	-4.232738	-0.680867	0.000000
H	1.345451	5.076108	0.000000
H	-1.345451	5.076108	0.000000
H	-1.345451	-5.076108	0.000000
H	3.162566	3.200337	0.000000
H	-3.162566	3.200337	0.000000
H	-3.162566	-3.200337	0.000000
H	5.085796	1.341008	0.000000
H	-5.085796	1.341008	0.000000
H	-5.085796	-1.341008	0.000000
H	-1.086460	0.000000	0.000000

porphine S_1

N	0.000000	-2.035219	0.000000
N	2.096875	0.000000	0.000000
C	1.081451	-2.857396	0.000000
C	0.674602	-4.251194	0.000000
C	2.412312	-2.434047	0.000000
C	2.875258	-1.124396	0.000000
C	4.234376	-0.682555	0.000000
H	1.345192	-5.097220	0.000000
H	3.172749	-3.205137	0.000000
H	5.088254	-1.341509	0.000000
H	1.086533	0.000000	0.000000
N	0.000000	2.035219	0.000000
N	-2.096875	0.000000	0.000000
C	1.081451	2.857396	0.000000
C	-1.081451	2.857396	0.000000
C	-1.081451	-2.857396	0.000000
C	0.674602	4.251194	0.000000
C	-0.674602	4.251194	0.000000

C	-0.674602	-4.251194	0.000000
C	2.412312	2.434047	0.000000
C	-2.412312	2.434047	0.000000
C	-2.412312	-2.434047	0.000000
C	2.875258	1.124396	0.000000
C	-2.875258	1.124396	0.000000
C	-2.875258	-1.124396	0.000000
C	4.234376	0.682555	0.000000
C	-4.234376	0.682555	0.000000
C	-4.234376	-0.682555	0.000000
H	1.345192	5.097220	0.000000
H	-1.345192	5.097220	0.000000
H	-1.345192	-5.097220	0.000000
H	3.172749	3.205137	0.000000
H	-3.172749	3.205137	0.000000
H	-3.172749	-3.205137	0.000000
H	5.088254	1.341509	0.000000
H	-5.088254	1.341509	0.000000
H	-5.088254	-1.341509	0.000000
H	-1.086533	0.000000	0.000000

chlorin S_0

C	0.000000	-4.225967	0.920130
C	0.000000	-2.872187	1.370753
N	0.000000	-2.088534	0.239440
C	0.000000	-2.854042	-0.875869
C	0.000000	-4.217498	-0.441817
C	0.000000	-2.410575	2.664947
C	0.000000	-1.077250	3.088950
N	0.000000	0.000000	2.268892
C	0.000000	1.077250	3.088950
C	0.000000	0.677214	4.475402
C	0.000000	-0.677214	4.475402
C	0.000000	2.410575	2.664947
C	0.000000	2.872187	1.370753
N	0.000000	2.088534	0.239440
C	0.000000	2.854042	-0.875869
C	0.000000	4.217498	-0.441817
C	0.000000	4.225967	0.920130
C	0.000000	2.401203	-2.196148
C	0.000000	1.096846	-2.639855
C	0.000000	0.764066	-4.121717
C	0.000000	-0.764066	-4.121717
C	0.000000	-1.096846	-2.639855
N	0.000000	0.000000	-1.862602

C	0.000000	-2.401203	-2.196148
H	-0.879124	1.187848	-4.609335
H	0.000000	3.176398	-2.952507
H	0.000000	5.065571	-1.108085
H	0.000000	1.347846	5.321773
H	0.000000	-1.347846	5.321773
H	-0.879124	-1.187848	-4.609335
H	0.000000	3.169436	3.438555
H	0.000000	-3.169436	3.438555
H	0.000000	-3.176398	-2.952507
H	0.000000	5.084300	1.573779
H	0.000000	-5.084300	1.573779
H	0.000000	-5.065571	-1.108085
H	0.879124	-1.187848	-4.609335
H	0.879124	1.187848	-4.609335
H	0.000000	-1.078405	0.257788
H	0.000000	1.078405	0.257788

chlorin S_1

C	0.000000	-4.233148	0.920686
C	0.000000	-2.878519	1.367108
N	0.000000	-2.095396	0.241172
C	0.000000	-2.868421	-0.883310
C	0.000000	-4.226799	-0.447168
C	0.000000	-2.413086	2.676614
C	0.000000	-1.081469	3.088492
N	0.000000	0.000000	2.267117
C	0.000000	1.081469	3.088492
C	0.000000	0.672831	4.487312
C	0.000000	-0.672831	4.487312
C	0.000000	2.413086	2.676614
C	0.000000	2.878519	1.367108
N	0.000000	2.095396	0.241172
C	0.000000	2.868421	-0.883310
C	0.000000	4.226799	-0.447168
C	0.000000	4.233148	0.920686
C	0.000000	2.410569	-2.203467
C	0.000000	1.098156	-2.645554
C	0.000000	0.763491	-4.122884
C	0.000000	-0.763491	-4.122884
C	0.000000	-1.098156	-2.645554
N	0.000000	0.000000	-1.861418
C	0.000000	-2.410569	-2.203467
H	-0.878689	1.187729	-4.612451
H	0.000000	3.181945	-2.963565

H	0.000000	5.077342	-1.110461
H	0.000000	1.345124	5.332115
H	0.000000	-1.345124	5.332115
H	-0.878689	-1.187729	-4.612451
H	0.000000	3.169935	3.450849
H	0.000000	-3.169935	3.450849
H	0.000000	-3.181945	-2.963565
H	0.000000	5.089821	1.576125
H	0.000000	-5.089821	1.576125
H	0.000000	-5.077342	-1.110461
H	0.878689	-1.187729	-4.612451
H	0.878689	1.187729	-4.612451
H	0.000000	-1.085734	0.257999
H	0.000000	1.085734	0.257999

Zn-tetraphenylporphine S_0

C	-3.794409	4.173228	1.168451
C	-3.483601	3.483572	-0.000012
C	-4.172756	3.793817	-1.168925
C	-5.153363	4.774894	-1.170219
C	-5.457417	5.457241	-0.000901
C	-4.775567	5.153764	1.168854
C	-2.427570	2.427577	0.000380
C	-1.096971	2.850581	0.004692
N	0.000000	2.039337	0.023637
C	1.096971	2.850581	0.004692
C	0.675802	4.228310	-0.032225
C	-0.675802	4.228310	-0.032225
C	2.427570	2.427577	0.000380
C	3.483601	3.483572	-0.000012
C	4.172756	3.793817	-1.168925
C	5.153363	4.774894	-1.170219
C	5.457417	5.457241	-0.000901
C	4.775567	5.153764	1.168854
C	3.794409	4.173228	1.168451
C	-2.850560	1.096972	-0.003798
N	-2.039312	0.000000	-0.022547
C	-2.850560	-1.096972	-0.003798
C	-4.228296	-0.675801	0.032828
C	-4.228296	0.675801	0.032828
C	-2.427570	-2.427577	0.000380
C	-3.483601	-3.483572	-0.000012
C	-4.172756	-3.793817	-1.168925
C	-5.153363	-4.774894	-1.170219
C	-5.457417	-5.457241	-0.000901

C	-4.775567	-5.153764	1.168854
C	-3.794409	-4.173228	1.168451
C	2.850560	1.096972	-0.003798
N	2.039312	0.000000	-0.022547
C	2.850560	-1.096972	-0.003798
C	4.228296	-0.675801	0.032828
C	4.228296	0.675801	0.032828
C	2.427570	-2.427577	0.000380
C	3.483601	-3.483572	-0.000012
C	4.172756	-3.793817	-1.168925
C	5.153363	-4.774894	-1.170219
C	5.457417	-5.457241	-0.000901
C	4.775567	-5.153764	1.168854
C	3.794409	-4.173228	1.168451
C	1.096971	-2.850581	0.004692
N	0.000000	-2.039337	0.023637
C	-1.096971	-2.850581	0.004692
C	-0.675802	-4.228310	-0.032225
C	0.675802	-4.228310	-0.032225
H	1.338339	-5.078020	-0.064247
H	5.078013	-1.338339	0.064665
H	1.338339	5.078020	-0.064247
H	-1.338339	5.078020	-0.064247
H	-1.338339	-5.078020	-0.064247
H	5.078013	1.338339	0.064665
H	-5.078013	1.338339	0.064665
H	-5.078013	-1.338339	0.064665
H	3.933503	3.260681	-2.081343
H	5.679073	5.007759	-2.088201
H	6.223220	6.222982	-0.001237
H	5.008892	5.679864	2.086497
H	3.261666	3.934433	2.081218
H	3.933503	-3.260681	-2.081343
H	5.679073	-5.007759	-2.088201
H	6.223220	-6.222982	-0.001237
H	5.008892	-5.679864	2.086497
H	3.261666	-3.934433	2.081218
H	-3.933503	-3.260681	-2.081343
H	-5.679073	-5.007759	-2.088201
H	-6.223220	-6.222982	-0.001237
H	-5.008892	-5.679864	2.086497
H	-3.261666	-3.934433	2.081218
H	-3.933503	3.260681	-2.081343
H	-5.679073	5.007759	-2.088201
H	-6.223220	6.222982	-0.001237
H	-5.008892	5.679864	2.086497

H	-3.261666	3.934433	2.081218
Zn	0.000000	0.000000	0.000545

Zn-tetraphenylporphine S_1

C	-3.638403	4.433470	1.002576
C	-3.491458	3.481672	-0.004867
C	-4.355402	3.525226	-1.098682
C	-5.338988	4.497419	-1.185656
C	-5.476977	5.440430	-0.176786
C	-4.624730	5.404899	0.917651
C	-2.437175	2.435956	0.069830
C	-1.100244	2.853263	0.037415
N	0.000000	2.043099	0.146063
C	1.100244	2.853263	0.037415
C	0.676759	4.215399	-0.156451
C	-0.676759	4.215399	-0.156451
C	2.437175	2.435956	0.069830
C	3.491458	3.481672	-0.004867
C	4.355402	3.525226	-1.098682
C	5.338988	4.497419	-1.185656
C	5.476977	5.440430	-0.176786
C	4.624730	5.404899	0.917651
C	3.638403	4.433470	1.002576
C	-2.866272	1.097442	0.135001
N	-2.055160	0.000000	0.058115
C	-2.866272	-1.097442	0.135001
C	-4.231103	-0.678306	0.290902
C	-4.231103	0.678306	0.290902
C	-2.437175	-2.435956	0.069830
C	-3.491458	-3.481672	-0.004867
C	-4.355402	-3.525226	-1.098682
C	-5.338988	-4.497419	-1.185656
C	-5.476977	-5.440430	-0.176786
C	-4.624730	-5.404899	0.917651
C	-3.638403	-4.433470	1.002576
C	2.866272	1.097442	0.135001
N	2.055160	0.000000	0.058115
C	2.866272	-1.097442	0.135001
C	4.231103	-0.678306	0.290902
C	4.231103	0.678306	0.290902
C	2.437175	-2.435956	0.069830
C	3.491458	-3.481672	-0.004867
C	4.355402	-3.525226	-1.098682
C	5.338988	-4.497419	-1.185656
C	5.476977	-5.440430	-0.176786

C	4.624730	-5.404899	0.917651
C	3.638403	-4.433470	1.002576
C	1.100244	-2.853263	0.037415
N	0.000000	-2.043099	0.146063
C	-1.100244	-2.853263	0.037415
C	-0.676759	-4.215399	-0.156451
C	0.676759	-4.215399	-0.156451
H	1.334190	-5.056604	-0.301239
H	5.075211	-1.337733	0.406084
H	1.334190	5.056604	-0.301239
H	-1.334190	5.056604	-0.301239
H	-1.334190	-5.056604	-0.301239
H	5.075211	1.337733	0.406084
H	-5.075211	1.337733	0.406084
H	-5.075211	-1.337733	0.406084
H	4.245689	2.790051	-1.886769
H	5.997823	4.520647	-2.045143
H	6.245927	6.200186	-0.242721
H	4.728899	6.135145	1.710843
H	2.974441	4.403884	1.858174
H	4.245689	-2.790051	-1.886769
H	5.997823	-4.520647	-2.045143
H	6.245927	-6.200186	-0.242721
H	4.728899	-6.135145	1.710843
H	2.974441	-4.403884	1.858174
H	-4.245689	-2.790051	-1.886769
H	-5.997823	-4.520647	-2.045143
H	-6.245927	-6.200186	-0.242721
H	-4.728899	-6.135145	1.710843
H	-2.974441	-4.403884	1.858174
H	-4.245689	2.790051	-1.886769
H	-5.997823	4.520647	-2.045143
H	-6.245927	6.200186	-0.242721
H	-4.728899	6.135145	1.710843
H	-2.974441	4.403884	1.858174
Zn	0.000000	0.000000	0.106741

tetraphenylporphine S_0

C	0.679811	-4.224469	0.017654
C	1.121948	-2.866372	-0.028042
N	0.000004	-2.089072	-0.055013
C	-1.121948	-2.866364	-0.028174
C	-0.679826	-4.224464	0.017563
C	-2.440126	-2.419417	-0.026284
C	-2.839789	-1.079428	-0.034475

N	-2.019312	0.000004	-0.018840
C	-2.839789	1.079438	-0.034346
C	-4.236146	0.672102	-0.073308
C	-4.236146	-0.672088	-0.073396
C	-2.440127	2.419427	-0.026054
C	-1.121948	2.866372	-0.028042
N	-0.000004	2.089072	-0.055013
C	1.121948	2.866364	-0.028174
C	0.679826	4.224464	0.017563
C	-0.679811	4.224469	0.017654
C	2.440126	2.419417	-0.026284
C	2.839789	1.079428	-0.034475
N	2.019312	-0.000004	-0.018840
C	2.839789	-1.079438	-0.034346
C	4.236146	-0.672102	-0.073308
C	4.236146	0.672088	-0.073396
C	2.440127	-2.419427	-0.026054
H	5.082692	1.338903	-0.106413
C	3.500526	3.471079	-0.000648
H	1.337956	5.076770	0.053769
H	-0.000010	1.077508	-0.060184
H	-5.082692	1.338921	-0.106239
H	-5.082692	-1.338903	-0.106413
H	5.082692	-1.338921	-0.106239
C	-3.500530	3.471079	-0.000185
C	-3.500526	-3.471079	-0.000648
C	3.500530	-3.471079	-0.000185
H	-1.337931	5.076779	0.053945
H	-1.337956	-5.076770	0.053769
H	1.337931	-5.076779	0.053945
H	0.000010	-1.077508	-0.060184
C	-3.827509	4.178651	-1.153343
C	-4.813283	5.154456	-1.125572
C	-5.482345	5.435201	0.057077
C	-5.161164	4.735296	1.211471
C	-4.176166	3.759326	1.182286
H	-3.306236	3.956159	-2.076807
H	-5.060803	5.693909	-2.031677
H	-6.251902	6.196863	0.078886
H	-5.677320	4.949990	2.139210
H	-3.923961	3.211297	2.082266
C	3.827387	4.178484	-1.153942
C	4.813148	5.154307	-1.126411
C	5.482317	5.435239	0.056132
C	5.161257	4.735501	1.210661
C	4.176271	3.759511	1.181715

H	3.306028	3.955847	-2.077323
H	5.060571	5.693630	-2.032620
H	6.251864	6.196916	0.077756
H	5.677497	4.950341	2.138318
H	3.924161	3.211612	2.081802
C	3.827509	-4.178651	-1.153343
C	4.813283	-5.154456	-1.125572
C	5.482345	-5.435201	0.057077
C	5.161164	-4.735296	1.211471
C	4.176166	-3.759326	1.182286
H	3.306236	-3.956159	-2.076807
H	5.060803	-5.693909	-2.031677
H	6.251902	-6.196863	0.078886
H	5.677320	-4.949990	2.139210
H	3.923961	-3.211297	2.082266
C	-3.827387	-4.178484	-1.153942
C	-4.813148	-5.154307	-1.126411
C	-5.482317	-5.435239	0.056132
C	-5.161257	-4.735501	1.210661
C	-4.176271	-3.759511	1.181715
H	-3.306028	-3.955847	-2.077323
H	-5.060571	-5.693630	-2.032620
H	-6.251864	-6.196916	0.077756
H	-5.677497	-4.950341	2.138318
H	-3.924161	-3.211612	2.081802

tetraphenylporphine S_1

C	-0.680902	4.215562	0.167017
C	-1.126339	2.871822	-0.028628
N	0.000000	2.098296	-0.137062
C	1.126339	2.871822	-0.028628
C	0.680902	4.215562	0.167017
C	2.449764	2.428349	-0.083809
C	2.858950	1.082609	-0.180449
N	2.038913	0.000000	-0.102335
C	2.858950	-1.082609	-0.180449
C	4.237114	-0.674889	-0.357624
C	4.237114	0.674889	-0.357624
C	2.449764	-2.428349	-0.083808
C	1.126339	-2.871822	-0.028628
N	0.000000	-2.098296	-0.137062
C	-1.126339	-2.871822	-0.028628
C	-0.680902	-4.215562	0.167017
C	0.680902	-4.215562	0.167017
C	-2.449764	-2.428349	-0.083809

C	-2.858950	-1.082609	-0.180449
N	-2.038913	0.000000	-0.102335
C	-2.858950	1.082609	-0.180449
C	-4.237114	0.674889	-0.357624
C	-4.237114	-0.674889	-0.357624
C	-2.449764	2.428349	-0.083808
H	-5.077753	-1.337557	-0.482149
C	-3.509773	-3.468768	-0.000448
H	-1.333546	-5.060634	0.307375
H	0.000000	-1.090009	-0.196700
H	5.077753	-1.337557	-0.482148
H	5.077753	1.337557	-0.482149
H	-5.077753	1.337557	-0.482148
C	3.509773	-3.468768	-0.000446
C	3.509773	3.468768	-0.000448
C	-3.509773	3.468768	-0.000446
H	1.333546	-5.060634	0.307375
H	1.333546	5.060634	0.307375
H	-1.333546	5.060634	0.307375
H	0.000000	1.090009	-0.196700
C	3.657649	-4.430781	-0.997643
C	4.648530	-5.396996	-0.904620
C	5.503409	-5.416219	0.188019
C	5.364148	-4.462289	1.186534
C	4.376224	-3.495211	1.091618
H	2.992835	-4.412474	-1.852977
H	4.754444	-6.135031	-1.690307
H	6.276049	-6.171630	0.260418
H	6.026082	-4.472523	2.043848
H	4.266295	-2.750145	1.870243
C	-3.657650	-4.430781	-0.997645
C	-4.648530	-5.396996	-0.904622
C	-5.503408	-5.416220	0.188017
C	-5.364147	-4.462290	1.186533
C	-4.376223	-3.495212	1.091617
H	-2.992835	-4.412473	-1.852979
H	-4.754444	-6.135031	-1.690309
H	-6.276048	-6.171631	0.260417
H	-6.026081	-4.472524	2.043847
H	-4.266295	-2.750146	1.870242
C	-3.657649	4.430781	-0.997643
C	-4.648530	5.396996	-0.904620
C	-5.503409	5.416219	0.188019
C	-5.364148	4.462289	1.186534
C	-4.376224	3.495211	1.091618
H	-2.992835	4.412474	-1.852977

H	-4.754444	6.135031	-1.690307
H	-6.276049	6.171630	0.260418
H	-6.026082	4.472523	2.043848
H	-4.266295	2.750145	1.870243
C	3.657650	4.430781	-0.997645
C	4.648530	5.396996	-0.904622
C	5.503408	5.416220	0.188017
C	5.364147	4.462290	1.186533
C	4.376223	3.495212	1.091617
H	2.992835	4.412473	-1.852979
H	4.754444	6.135031	-1.690309
H	6.276048	6.171631	0.260417
H	6.026081	4.472524	2.043847
H	4.266295	2.750146	1.870242

ωB97X-D/TZVP geometries – Group II

tetrafluorobenzene S_0

C	-1.190075	0.692879	0.000000
C	-1.190075	-0.692879	0.000000
C	0.000000	-1.393186	0.000000
C	1.190075	-0.692879	0.000000
C	1.190075	0.692879	0.000000
C	0.000000	1.393186	0.000000
F	-2.348528	-1.350973	0.000000
H	0.000000	-2.474377	0.000000
F	2.348528	-1.350973	0.000000
F	2.348528	1.350973	0.000000
H	0.000000	2.474377	0.000000
F	-2.348528	1.350973	0.000000

tetrafluorobenzene S_1

C	1.165416	-0.707629	0.106010
C	1.165416	0.707629	0.106010
C	0.000000	1.460638	0.314596
C	-1.165416	0.707629	0.106010
C	-1.165416	-0.707629	0.106010
C	0.000000	-1.460638	0.314596
F	2.302175	1.320477	-0.207028
H	0.000000	2.506338	0.585564
F	-2.302175	1.320477	-0.207028
F	-2.302175	-1.320477	-0.207028
H	0.000000	-2.506338	0.585564

F	2.302175	-1.320477	-0.207028

benzonitrile S_0

C	0.000000	0.000000	-1.052359
C	-1.209394	0.000000	-0.358347
C	-1.203298	0.000000	1.026169
C	0.000000	0.000000	1.718045
C	1.203298	0.000000	1.026169
C	1.209394	0.000000	-0.358347
H	-2.142509	0.000000	-0.906441
H	-2.141450	0.000000	1.566169
H	0.000000	0.000000	2.800928
H	2.141450	0.000000	1.566169
H	2.142509	0.000000	-0.906441
C	0.000000	0.000000	-2.485997
N	0.000000	0.000000	-3.635708

benzonitrile S_1

C	0.000000	0.000000	-1.103118
C	-1.224594	0.000000	-0.372923
C	-1.213948	0.000000	1.044661
C	0.000000	0.000000	1.763218
C	1.213948	0.000000	1.044661
C	1.224594	0.000000	-0.372923
H	-2.164038	0.000000	-0.907904
H	-2.158061	0.000000	1.572303
H	0.000000	0.000000	2.843306
H	2.158061	0.000000	1.572303
H	2.164038	0.000000	-0.907904
C	0.000000	0.000000	-2.509341
N	0.000000	0.000000	-3.666337

o-fluorophenol, *cis* S_0

C	0.325631	1.450017	0.000000
C	-0.873382	0.775161	0.000000
C	-0.949819	-0.612738	0.000000
C	0.235499	-1.333541	0.000000
C	1.453131	-0.669889	0.000000
C	1.505071	0.717104	0.000000
F	-2.043338	1.456780	0.000000
O	-2.135864	-1.265100	0.000000
H	0.181564	-2.414490	0.000000
H	2.370532	-1.244470	0.000000

H	2.457038	1.230964	0.000000
H	0.323745	2.532215	0.000000
H	-2.849797	-0.622033	0.000000

o-fluorophenol, *cis* S_1

C	1.233191	-0.253729	-0.739098
C	0.003837	-0.064179	-0.094437
C	-0.011901	-0.031599	1.347849
C	1.169996	0.037327	2.090550
C	2.383969	0.113820	1.408852
C	2.400419	-0.017838	0.011254
F	-0.944145	0.808574	-0.681529
O	-1.174969	-0.126644	1.988732
H	1.124184	-0.111265	3.163104
H	3.312636	0.218883	1.952022
H	3.343758	0.088293	-0.514971
H	1.285252	-0.399859	-1.809659
H	-1.870848	-0.261783	1.327272

o-fluorophenol, *trans* S_0

C	0.289639	1.261312	0.000000
C	-0.945170	0.617245	0.000000
C	-0.960331	-0.771243	0.000000
C	0.226498	-1.491828	0.000000
C	1.443936	-0.832606	0.000000
C	1.472727	0.556576	0.000000
O	-2.061160	1.385949	0.000000
H	-1.913036	-1.290533	0.000000
H	0.191189	-2.573655	0.000000
H	2.371353	-1.389672	0.000000
H	2.405447	1.105408	0.000000
F	0.315689	2.600486	0.000000
H	-2.836790	0.822561	0.000000

o-fluorophenol, *trans* S_1

C	0.819142	1.036153	0.097799
C	-0.587655	0.972496	0.075299
C	-1.271577	-0.286637	0.092386
C	-0.468878	-1.425560	-0.072756
C	0.941234	-1.337804	-0.060523
C	1.618781	-0.126951	0.168682
O	-1.254034	2.116280	-0.102752
H	-2.302403	-0.350526	0.424425

H	-0.928885	-2.399220	-0.185774
H	1.514603	-2.245405	-0.211196
H	2.688735	-0.060731	0.289059
F	1.398291	2.208052	-0.180274
H	-2.167385	1.899852	-0.334376

m-fluorophenol, *cis* S_0

C	0.308305	1.407719	0.000000
C	-0.926308	0.786040	0.000000
C	-0.966425	-0.603834	0.000000
C	0.213936	-1.340421	0.000000
C	1.429086	-0.679114	0.000000
C	1.497368	0.708923	0.000000
O	-2.134772	-1.293948	0.000000
F	0.338561	2.750210	0.000000
H	0.158548	-2.420521	0.000000
H	2.346533	-1.254091	0.000000
H	2.439526	1.238762	0.000000
H	-1.828853	1.385571	0.000000
H	-2.875506	-0.685297	0.000000

m-fluorophenol, *cis* S_1

C	1.227323	-0.034197	-0.690424
C	-0.045016	0.021400	-0.099570
C	-0.023833	0.024410	1.325157
C	1.163991	0.015135	2.086492
C	2.425517	0.102010	1.441109
C	2.432611	-0.027908	0.032016
O	-1.174209	-0.019844	2.011117
F	1.299085	-0.112236	-2.025107
H	1.076903	-0.102568	3.158385
H	3.345500	0.128923	2.002121
H	3.359178	-0.116980	-0.520772
H	-0.926567	0.282252	-0.670564
H	-1.905124	-0.160396	1.399990

m-fluorophenol, *trans* S_0

C	0.267698	1.300851	0.000000
C	-0.948347	0.627963	0.000000
C	-0.982184	-0.763397	0.000000
C	0.207263	-1.476692	0.000000
C	1.432133	-0.828530	0.000000
C	1.426850	0.554799	0.000000

O	-2.072177	1.388489	0.000000
H	-1.932663	-1.285313	0.000000
H	0.177108	-2.559013	0.000000
H	2.368606	-1.368276	0.000000
F	2.600832	1.205081	0.000000
H	0.301039	2.381407	0.000000
H	-2.846159	0.822640	0.000000

m-fluorophenol, *trans* S_1

C	1.082637	-0.015607	0.000000
C	0.328680	1.182642	0.000000
C	-1.089600	1.211052	0.000000
C	-1.820895	-0.006146	0.000000
C	-1.084380	-1.217630	0.000000
C	0.319789	-1.196630	0.000000
O	1.036412	2.321194	0.000000
H	-1.601410	2.166778	0.000000
H	-2.899131	-0.013045	0.000000
H	-1.584983	-2.176685	0.000000
F	0.967775	-2.368742	0.000000
H	2.160743	-0.010935	0.000000
H	0.443214	3.077902	0.000000

p-fluorophenol S_0

C	0.270870	1.312827	0.000000
C	-0.948793	0.646172	0.000000
C	-0.978580	-0.742686	0.000000
C	0.206181	-1.466566	0.000000
C	1.404319	-0.785552	0.000000
C	1.454716	0.595214	0.000000
O	-2.078281	1.407654	0.000000
H	-1.926860	-1.269192	0.000000
H	0.200069	-2.548332	0.000000
F	2.556315	-1.483821	0.000000
H	2.412684	1.097972	0.000000
H	0.279071	2.394628	0.000000
H	-2.851729	0.841670	0.000000

p-fluorophenol S_1

C	1.263780	0.679252	0.000000
C	0.026867	1.360728	0.000000
C	-1.235073	0.709296	0.000000
C	-1.249069	-0.703769	0.000000

C	-0.006473	-1.363196	0.000000
C	1.249982	-0.735176	0.000000
O	0.092302	2.696686	0.000000
H	-2.152607	1.284464	0.000000
H	-2.162086	-1.279171	0.000000
F	-0.026798	-2.692661	0.000000
H	2.150996	-1.328615	0.000000
H	2.180344	1.249862	0.000000
H	-0.795468	3.067893	0.000000

phenylacetylene S_0

C	1.205124	0.000000	-0.013496
C	0.000000	0.000000	-0.719264
C	-1.205124	0.000000	-0.013496
C	-1.201144	0.000000	1.371385
C	0.000000	0.000000	2.066841
C	1.201144	0.000000	1.371385
C	0.000000	0.000000	-2.150087
C	0.000000	0.000000	-3.349816
H	-2.139644	0.000000	-0.559741
H	-2.140764	0.000000	1.909715
H	0.000000	0.000000	3.149824
H	2.140764	0.000000	1.909715
H	2.139644	0.000000	-0.559741
H	0.000000	0.000000	-4.413246

phenylacetylene S_1

C	1.230217	0.000000	-0.029426
C	0.000000	0.000000	-0.753141
C	-1.230217	0.000000	-0.029426
C	-1.221175	0.000000	1.388879
C	0.000000	0.000000	2.094101
C	1.221175	0.000000	1.388879
C	0.000000	0.000000	-2.154127
C	0.000000	0.000000	-3.361975
H	-2.163946	0.000000	-0.573573
H	-2.159253	0.000000	1.926565
H	0.000000	0.000000	3.175591
H	2.159253	0.000000	1.926565
H	2.163946	0.000000	-0.573573
H	0.000000	0.000000	-4.425339

aniline S_0

C	0.918650	0.028889	0.000000
C	0.205445	0.036481	1.200563
C	-1.179513	0.042784	1.194974
C	-1.885209	0.046565	0.000000
C	-1.179513	0.042784	-1.194974
C	0.205445	0.036481	-1.200563
H	0.743289	0.038524	2.142278
H	-2.967453	0.051522	0.000000
H	-1.711895	0.046141	2.138655
H	-1.711895	0.046141	-2.138655
H	0.743289	0.038524	-2.142278
N	2.309788	0.074438	0.000000
H	2.754790	-0.264633	-0.836091
H	2.754790	-0.264633	0.836091

aniline S_1

C	0.896410	-0.034209	0.000000
C	0.224365	-0.008501	1.245726
C	-1.193706	0.045652	1.235879
C	-1.865164	0.071237	0.000000
C	-1.193706	0.045652	-1.235879
C	0.224365	-0.008501	-1.245726
H	0.789306	-0.030128	2.168566
H	-2.948618	0.112502	0.000000
H	-1.751324	0.066931	2.160773
H	-1.751324	0.066931	-2.160773
H	0.789306	-0.030128	-2.168566
N	2.250438	-0.086079	0.000000
H	2.764821	-0.105691	-0.862830
H	2.764821	-0.105691	0.862830

catechol S_0

C	0.468888	1.275724	0.000000
C	-0.747269	0.618916	0.000000
C	-0.797917	-0.777169	0.000000
C	0.381619	-1.500170	0.000000
C	1.604090	-0.840566	0.000000
C	1.651206	0.543893	0.000000
O	-1.966803	1.243269	0.000000
O	-1.989815	-1.422401	0.000000
H	0.324440	-2.581087	0.000000
H	2.521361	-1.415228	0.000000
H	2.601556	1.061396	0.000000
H	0.494922	2.360616	0.000000

H	-1.856890	2.194592	0.000000
H	-2.689389	-0.761785	0.000000

catechol S_1

C	0.472756	1.345294	0.000000
C	-0.759700	0.625751	0.000000
C	-0.804322	-0.783195	0.000000
C	0.386040	-1.569796	0.000000
C	1.596291	-0.857396	0.000000
C	1.638341	0.556944	0.000000
O	-1.965487	1.246446	0.000000
O	-1.983725	-1.420438	0.000000
H	0.323604	-2.645996	0.000000
H	2.534144	-1.397444	0.000000
H	2.605272	1.043746	0.000000
H	0.497894	2.425512	0.000000
H	-1.846830	2.198425	0.000000
H	-2.694278	-0.767853	0.000000

resorcinol, isomer 1 S_0

C	0.074948	1.145263	0.000000
C	-1.136365	0.465368	0.000000
C	-1.167203	-0.923257	0.000000
C	0.032782	-1.622076	0.000000
C	1.248906	-0.965275	0.000000
C	1.261476	0.426455	0.000000
O	-2.265811	1.223301	0.000000
H	-2.113605	-1.452109	0.000000
H	0.014020	-2.704999	0.000000
H	2.186473	-1.503742	0.000000
O	2.474200	1.039819	0.000000
H	0.069081	2.229215	0.000000
H	-3.034742	0.650821	0.000000
H	2.355840	1.991205	0.000000

resorcinol, isomer 1 S_1

C	-0.002107	1.058724	0.041210
C	-1.194444	0.305432	0.001851
C	-1.204143	-1.109046	-0.029612
C	0.000128	-1.848313	0.084408
C	1.208723	-1.108937	0.000537
C	1.194158	0.301182	0.022183
O	-2.345051	1.008046	-0.027049

H	-2.152621	-1.622220	-0.152454
H	-0.000705	-2.926251	0.077732
H	2.166217	-1.602825	-0.101841
O	2.394703	0.914655	-0.014953
H	-0.023165	2.119116	0.251661
H	-3.094265	0.407386	0.001936
H	2.263566	1.859172	-0.135959

resorcinol, isomer 2 S_0

C	1.196539	0.000000	-0.545932
C	0.000000	0.000000	-1.245687
C	-1.196539	0.000000	-0.545932
C	-1.206662	0.000000	0.846715
C	0.000000	0.000000	1.526795
C	1.206662	0.000000	0.846715
O	-2.340785	0.000000	-1.279919
O	2.340785	0.000000	-1.279919
H	-2.145105	0.000000	1.389607
H	0.000000	0.000000	2.609812
H	2.145105	0.000000	1.389607
H	0.000000	0.000000	-2.326845
H	-3.098467	0.000000	-0.692748
H	3.098467	0.000000	-0.692748

resorcinol, isomer 2 S_1

C	1.196142	0.000000	-0.330092
C	0.000000	0.000000	-1.078252
C	-1.196142	0.000000	-0.330092
C	-1.211557	0.000000	1.085453
C	0.000000	0.000000	1.823752
C	1.211557	0.000000	1.085453
O	-2.346148	0.000000	-1.036232
O	2.346148	0.000000	-1.036232
H	-2.164904	0.000000	1.602996
H	0.000000	0.000000	2.901957
H	2.164904	0.000000	1.602996
H	0.000000	0.000000	-2.156188
H	-3.096611	0.000000	-0.437303
H	3.096611	0.000000	-0.437303

resorcinol, isomer 3 S_0

C	1.201972	0.000000	-0.288231
C	0.000000	0.000000	-0.988087

C	-1.201972	0.000000	-0.288231
C	-1.209412	0.000000	1.099885
C	0.000000	0.000000	1.775607
C	1.209412	0.000000	1.099885
O	-2.404757	0.000000	-0.923097
O	2.404757	0.000000	-0.923097
H	-2.154819	0.000000	1.624458
H	0.000000	0.000000	2.858754
H	2.154819	0.000000	1.624458
H	0.000000	0.000000	-2.074774
H	2.273951	0.000000	-1.872525
H	-2.273951	0.000000	-1.872525

resorcinol, isomer 3 S_1

C	-0.017378	-0.303289	1.189076
C	-0.088870	-1.073187	0.000000
C	-0.017378	-0.303289	-1.189076
C	0.025146	1.106322	-1.199998
C	-0.082445	1.846383	0.000000
C	0.025146	1.106322	1.199998
O	0.051338	-0.914410	-2.388472
O	0.051338	-0.914410	2.388472
H	0.172466	1.595653	-2.154842
H	-0.083125	2.924368	0.000000
H	0.172466	1.595653	2.154842
H	-0.564217	-2.053091	0.000000
H	0.207836	-1.853795	2.248000
H	0.207836	-1.853795	-2.248000

hydroquinone, *cis* S_0

C	-0.695194	0.000000	1.088471
C	0.695194	0.000000	1.088471
C	1.392736	0.000000	-0.108739
C	0.690831	0.000000	-1.308894
C	-0.690831	0.000000	-1.308894
C	-1.392736	0.000000	-0.108739
O	2.756967	0.000000	-0.175089
O	-2.756967	0.000000	-0.175089
H	1.242827	0.000000	-2.239692
H	-1.242827	0.000000	-2.239692
H	-1.228323	0.000000	2.033358
H	1.228323	0.000000	2.033358
H	-3.122025	0.000000	0.710874
H	3.122025	0.000000	0.710874

hydroquinone, *cis* S_1

C	0.705606	0.000000	-1.130607
C	-0.705606	0.000000	-1.130607
C	-1.373081	0.000000	0.119583
C	-0.706026	0.000000	1.359923
C	0.706026	0.000000	1.359923
C	1.373081	0.000000	0.119583
O	-2.713241	0.000000	0.164787
O	2.713241	0.000000	0.164787
H	-1.285005	0.000000	2.270945
H	1.285005	0.000000	2.270945
H	1.269867	0.000000	-2.054655
H	-1.269867	0.000000	-2.054655
H	3.066865	0.000000	-0.729206
H	-3.066865	0.000000	-0.729206

hydroquinone, *trans* S_0

C	0.020587	1.386237	0.000000
C	-1.193914	0.717202	0.000000
C	-1.208247	-0.671944	0.000000
C	-0.020587	-1.386237	0.000000
C	1.193914	-0.717202	0.000000
C	1.208247	0.671944	0.000000
O	-2.333138	1.470792	0.000000
H	-2.152114	-1.207242	0.000000
H	-0.027160	-2.468274	0.000000
O	2.333138	-1.470792	0.000000
H	2.152114	1.207242	0.000000
H	0.027160	2.468274	0.000000
H	-3.098905	0.894760	0.000000
H	3.098905	-0.894760	0.000000

hydroquinone, *trans* S_1

C	1.260421	0.675717	0.000000
C	0.035022	1.372550	0.000000
C	-1.229472	0.735648	0.000000
C	-1.260421	-0.675717	0.000000
C	-0.035022	-1.372550	0.000000
C	1.229472	-0.735648	0.000000
O	0.117990	2.710888	0.000000
H	-2.140771	1.320444	0.000000
H	-2.184141	-1.234845	0.000000

O	-0.117990	-2.710888	0.000000
H	2.140771	-1.320444	0.000000
H	2.184141	1.234845	0.000000
H	-0.766900	3.088239	0.000000
H	0.766900	-3.088239	0.000000

salicylic acid S_0

C	1.099223	1.594702	0.000000
C	1.131595	0.197905	0.000000
C	-0.082828	-0.516042	0.000000
C	-1.295258	0.185944	0.000000
C	-1.315032	1.561661	0.000000
C	-0.106424	2.260372	0.000000
O	2.327938	-0.394916	0.000000
C	-0.045247	-1.980176	0.000000
O	-1.244839	-2.572580	0.000000
O	0.978707	-2.641653	0.000000
H	-2.219633	-0.375764	0.000000
H	2.040492	2.128122	0.000000
H	-2.256493	2.094385	0.000000
H	-0.111247	3.343784	0.000000
H	2.187671	-1.361419	0.000000
H	-1.088624	-3.524326	0.000000

salicylic acid S_1

C	1.000549	1.907801	0.000000
C	0.964098	0.508366	0.000000
C	-0.294418	-0.229145	0.000000
C	-1.455182	0.533850	0.000000
C	-1.398996	1.954973	0.000000
C	-0.194973	2.650517	0.000000
O	2.082283	-0.170219	0.000000
C	-0.236377	-1.656984	0.000000
O	-1.424590	-2.295962	0.000000
O	0.834368	-2.315843	0.000000
H	-2.416701	0.039427	0.000000
H	1.971064	2.386267	0.000000
H	-2.334107	2.501246	0.000000
H	-0.173595	3.730231	0.000000
H	1.813725	-1.168995	0.000000
H	-1.226566	-3.238583	0.000000

o-cresol, *cis* S_0

C	1.958858	0.511414	0.000000
C	0.727259	1.147098	0.000000
C	-0.465069	0.430939	0.000000
C	-0.390196	-0.964936	0.000000
C	0.837403	-1.613456	0.000000
C	2.008525	-0.875420	0.000000
C	-1.799553	1.125999	0.000000
O	-1.503874	-1.750337	0.000000
H	0.853118	-2.695809	0.000000
H	2.962766	-1.387549	0.000000
H	2.871601	1.093213	0.000000
H	0.682797	2.230703	0.000000
H	-2.291265	-1.203656	0.000000
H	-2.391387	0.872195	0.885698
H	-1.669597	2.207417	0.000000
H	-2.391387	0.872195	-0.885698

o-cresol, *cis* S_1

C	1.865283	-0.089529	-0.778563
C	0.628549	-0.102988	-1.456899
C	-0.586533	-0.065984	-0.716224
C	-0.468980	0.056153	0.700510
C	0.769674	0.085107	1.389143
C	1.954734	-0.003994	0.627069
C	-1.901430	-0.010960	-1.418334
O	-1.559442	0.145174	1.473546
H	0.767326	0.165075	2.465948
H	2.921423	0.005459	1.109465
H	2.779219	-0.141239	-1.357886
H	0.599426	-0.178593	-2.535089
H	-2.350385	0.120836	0.925220
H	-2.726883	-0.460388	-0.854260
H	-2.198096	1.017640	-1.670896
H	-1.844464	-0.561260	-2.360341

o-cresol, *trans* S_0

C	2.414760	0.000016	0.029819
C	1.243521	-0.000035	-0.715508
C	0.031163	-0.000007	-0.020679
C	0.001347	0.000066	1.367138
C	1.187870	0.000111	2.087053
C	2.400416	0.000089	1.419118
C	1.248783	-0.000112	-2.216587
O	-1.107942	-0.000064	-0.770780

H	-0.951407	0.000089	1.887433
H	1.156189	0.000168	3.169466
H	3.331159	0.000133	1.971801
H	3.363318	-0.000006	-0.495751
H	-1.872661	-0.000050	-0.192906
H	2.269856	-0.000059	-2.598043
H	0.731230	-0.877120	-2.610757
H	0.731104	0.876780	-2.610847

o-cresol, *trans* S_1

C	2.426102	0.224799	-0.008524
C	1.215756	0.083545	-0.752722
C	0.012322	-0.044316	-0.015397
C	-0.042739	-0.109463	1.409017
C	1.177798	-0.035161	2.106960
C	2.387550	0.114734	1.393075
C	1.251599	-0.007140	-2.236777
O	-1.126123	-0.143948	-0.717595
H	-0.997581	-0.071355	1.918786
H	1.194886	-0.083570	3.186973
H	3.315693	0.157107	1.950452
H	3.365277	0.350709	-0.528274
H	-1.851584	-0.339247	-0.116099
H	1.786235	-0.912191	-2.555527
H	0.257577	-0.024908	-2.678255
H	1.805923	0.840407	-2.656112

m-cresol, *cis* S_0

C	1.157217	-0.002186	2.081693
C	2.366096	0.016352	1.410975
C	2.412714	0.024848	0.022064
C	1.236874	0.013736	-0.717628
C	0.018878	-0.003094	-0.041090
C	-0.022950	-0.011696	1.346251
C	1.260261	0.002830	-2.222415
O	-1.193526	-0.027678	2.040422
H	1.107676	-0.007600	3.162457
H	3.288120	0.025833	1.979663
H	3.368463	0.040762	-0.487932
H	-0.908119	-0.008938	-0.608443
H	-1.930974	-0.033623	1.427785
H	2.265432	0.187565	-2.601484
H	0.929075	-0.964120	-2.608875
H	0.597063	0.766379	-2.633493

m-cresol, *cis* S_1

C	1.163401	-0.000284	2.121890
C	2.406454	0.046905	1.446383
C	2.407585	0.033247	0.033659
C	1.221605	0.015054	-0.743503
C	-0.025840	-0.006178	-0.068934
C	-0.019021	-0.007831	1.351090
C	1.264648	-0.009254	-2.232926
O	-1.173591	-0.034301	2.031412
H	1.087132	-0.048745	3.198636
H	3.335788	0.062939	1.995550
H	3.357889	0.043374	-0.488497
H	-0.960092	0.065878	-0.613882
H	-1.909511	-0.086523	1.413992
H	2.280107	0.118510	-2.608985
H	0.875994	-0.957578	-2.625987
H	0.639730	0.784156	-2.659961

m-cresol, *trans* S_0

C	-1.190482	-1.095944	0.000000
C	0.197535	-1.207783	0.000000
C	0.966938	-0.050110	0.000000
C	0.364285	1.199433	0.000000
C	-1.022514	1.307597	0.000000
C	-1.790170	0.154060	0.000000
C	0.871933	-2.553668	0.000000
O	1.181725	2.288015	0.000000
H	-1.496463	2.283599	0.000000
H	-2.870476	0.234636	0.000000
H	-1.802250	-1.990074	0.000000
H	2.049335	-0.104097	0.000000
H	0.651584	3.086672	0.000000
H	0.140201	-3.361634	0.000000
H	1.506954	-2.671089	-0.880593
H	1.506954	-2.671089	0.880593

m-cresol, *trans* S_1

C	-1.201144	-1.056549	0.000000
C	0.203842	-1.232460	0.000000
C	1.023174	-0.072508	0.000000
C	0.398279	1.194269	0.000000
C	-1.009531	1.370609	0.000000

C	-1.823343	0.214542	0.000000
C	0.827063	-2.586648	0.000000
O	1.214570	2.258051	0.000000
H	-1.434818	2.366899	0.000000
H	-2.900328	0.294130	0.000000
H	-1.828742	-1.940768	0.000000
H	2.102576	-0.127759	0.000000
H	0.694904	3.067283	0.000000
H	0.074045	-3.375934	0.000000
H	1.467967	-2.729071	-0.878247
H	1.467967	-2.729071	0.878247

p-cresol S_0

C	0.710104	-0.004750	-1.185951
C	-0.673386	-0.002220	-1.195109
C	-1.370759	-0.000291	0.006643
C	-0.670070	-0.003025	1.204837
C	0.718340	-0.005499	1.194504
C	1.435075	-0.004665	0.004642
O	-2.731893	-0.000728	-0.052961
C	2.940206	0.022760	-0.004509
H	-1.203922	-0.006582	2.149853
H	1.249894	-0.010642	2.139669
H	1.240653	-0.009489	-2.131933
H	-1.227135	-0.005239	-2.125094
H	-3.092061	-0.002023	0.835411
H	3.341769	-0.587927	-0.814972
H	3.315363	1.040218	-0.143403
H	3.349382	-0.354521	0.933674

p-cresol S_1

C	0.729958	-0.065125	-1.234435
C	-0.683139	-0.026510	-1.242281
C	-1.353847	-0.001100	-0.001203
C	-0.680506	0.008956	1.247450
C	0.731232	-0.030652	1.235687
C	1.428311	-0.039455	-0.000934
O	-2.691885	0.025344	-0.047724
C	2.914629	0.033796	-0.001013
H	-1.242031	0.032416	2.173327
H	1.289333	-0.027484	2.161978
H	1.284478	-0.085182	-2.162403
H	-1.261700	-0.017765	-2.154284
H	-3.045856	0.048176	0.846577

H	3.336921	-0.449739	-0.884042
H	3.238172	1.082307	-0.017523
H	3.337480	-0.422602	0.896113

o-methoxyphenol S_0

C	2.025384	-0.088782	0.000000
C	0.873213	0.695179	0.000000
C	-0.368392	0.085891	0.000000
C	-0.468603	-1.312644	0.000000
C	0.678637	-2.081440	0.000000
C	1.926917	-1.467997	0.000000
O	-1.575668	0.723707	0.000000
O	-1.686395	-1.905720	0.000000
H	0.579118	-3.159256	0.000000
H	2.821447	-2.077646	0.000000
H	2.994906	0.392073	0.000000
H	0.958686	1.773404	0.000000
C	-1.585449	2.133580	0.000000
H	-2.350962	-1.208893	0.000000
H	-2.631419	2.431249	0.000000
H	-1.095710	2.533648	0.893038
H	-1.095710	2.533648	-0.893038

o-methoxyphenol S_1

C	2.483298	0.060915	0.061300
C	1.380039	-0.247316	-0.753112
C	0.111860	-0.231150	-0.095840
C	0.018333	-0.136815	1.312761
C	1.177984	-0.070492	2.137419
C	2.386994	0.149825	1.467563
O	-1.077084	-0.065164	-0.728880
O	-1.177700	0.053222	1.885558
H	1.092907	-0.163544	3.209334
H	3.283067	0.379523	2.031918
H	3.451387	0.223898	-0.399722
H	1.499362	-0.551319	-1.782815
C	-1.089012	0.106791	-2.138500
H	-1.851142	0.044682	1.190437
H	-2.128755	0.273314	-2.408385
H	-0.482358	0.965334	-2.432438
H	-0.720620	-0.791713	-2.638517

m-methoxyphenol, isomer 1 S_0

C	0.925547	1.443215	0.000000
C	-0.262003	0.714839	0.000000
C	-0.229601	-0.676474	0.000000
C	1.000897	-1.331906	0.000000
C	2.187703	-0.617497	0.000000
C	2.131951	0.769371	0.000000
H	-1.143017	-1.258056	0.000000
O	1.082672	-2.690177	0.000000
H	3.129126	-1.149268	0.000000
H	3.055458	1.335394	0.000000
H	0.876287	2.523500	0.000000
O	-1.405516	1.442774	0.000000
H	0.202438	-3.069448	0.000000
C	-2.637776	0.759975	0.000000
H	-3.407998	1.527554	0.000000
H	-2.753084	0.138102	-0.893779
H	-2.753084	0.138102	0.893779

m-methoxyphenol, isomer 1 S_1

C	1.166960	-0.012607	-0.623077
C	-0.031588	-0.041738	0.121802
C	-0.048594	-0.095588	1.540577
C	1.233127	-0.007775	2.143046
C	2.437705	0.017548	1.413688
C	2.431185	-0.124694	0.006494
H	-0.894046	-0.480631	2.098609
O	1.339566	0.104770	3.483230
H	3.356082	0.184383	1.962985
H	3.346045	-0.136333	-0.563417
H	1.080191	0.119408	-1.694481
O	-1.152967	0.029705	-0.619352
H	0.465459	0.274140	3.848884
C	-2.408179	0.039906	0.033775
H	-3.148197	0.225135	-0.740820
H	-2.612331	-0.925869	0.504086
H	-2.452110	0.830242	0.786712

m-methoxyphenol, isomer 2 S_0

C	0.345516	2.154283	0.000000
C	-0.835435	1.442532	0.000000
C	-0.791913	0.046177	0.000000
C	0.426787	-0.617891	0.000000
C	1.606017	0.122925	0.000000
C	1.577695	1.508886	0.000000

O	-1.992340	-0.580302	0.000000
C	-2.012785	-1.990374	0.000000
O	2.767045	-0.587050	0.000000
H	0.501551	-1.695551	0.000000
H	2.500070	2.078860	0.000000
H	0.314133	3.236982	0.000000
H	-1.797209	1.936686	0.000000
H	-3.062350	-2.275356	0.000000
H	-1.528997	-2.399029	-0.892621
H	-1.528997	-2.399029	0.892621
H	3.511199	0.017259	0.000000

m-methoxyphenol, isomer 2 S_1

C	1.239477	-0.080793	-0.705434
C	0.055342	-0.016781	0.077264
C	0.108829	-0.039134	1.488048
C	1.335425	-0.053973	2.200619
C	2.500331	-0.001915	1.404098
C	2.468056	0.030786	-0.008425
O	-1.092000	-0.017342	2.094941
C	-1.149723	0.027194	3.507532
O	3.672490	0.039489	2.072611
H	1.417939	-0.175305	3.267567
H	3.401222	0.141423	-0.551358
H	1.200903	-0.062696	-1.782625
H	-0.920064	0.056437	-0.385263
H	-2.205534	0.085964	3.760000
H	-0.720319	-0.876189	3.948488
H	-0.629616	0.906580	3.895602
H	4.402374	0.036257	1.448236

p-methoxyphenol, *cis* S_0

C	-0.314687	0.731128	0.000000
C	-1.544019	0.071872	0.000000
C	-1.604355	-1.305267	0.000000
C	-0.431891	-2.056913	0.000000
C	0.789472	-1.407889	0.000000
C	0.854032	-0.015751	0.000000
O	-0.555071	-3.416663	0.000000
O	-0.367737	2.091435	0.000000
C	0.850117	2.796759	0.000000
H	1.824581	0.460084	0.000000
H	-2.449873	0.664308	0.000000
H	-2.557470	-1.817882	0.000000

H	1.712015	-1.979338	0.000000
H	0.590779	3.853123	0.000000
H	1.444476	2.574536	0.893028
H	1.444476	2.574536	-0.893028
H	0.315154	-3.818059	0.000000

p-methoxyphenol, *cis* S_1

C	1.326446	0.000234	-0.618166
C	0.052732	0.000320	0.001694
C	-0.016674	0.000252	1.411899
C	1.187869	0.000204	2.136277
C	2.466297	-0.001441	1.522576
C	2.539591	0.001123	0.112537
O	1.086955	0.000722	3.473952
O	1.287017	0.000298	-1.953875
C	2.490515	-0.000451	-2.703169
H	3.497354	0.002397	-0.383266
H	-0.829065	-0.001260	-0.620893
H	-0.955485	0.001103	1.944974
H	3.363958	-0.000838	2.128346
H	2.189279	-0.000945	-3.747344
H	3.080344	0.893820	-2.491117
H	3.079929	-0.894738	-2.490078
H	1.966468	-0.000817	3.862653

p-methoxyphenol, *trans* S_0

C	-0.654783	1.300329	0.000000
C	-1.884643	0.669470	0.000000
C	-1.960956	-0.720172	0.000000
C	-0.793019	-1.462854	0.000000
C	0.444726	-0.832089	0.000000
C	0.521051	0.556235	0.000000
O	-3.147656	-1.395785	0.000000
H	1.338449	-1.440523	0.000000
O	1.680257	1.270309	0.000000
H	-0.586584	2.380479	0.000000
H	-2.791779	1.265293	0.000000
H	-3.873406	-0.770198	0.000000
H	-0.857542	-2.543220	0.000000
C	2.894036	0.557057	0.000000
H	3.684132	1.304487	0.000000
H	2.993854	-0.069418	0.892869
H	2.993854	-0.069418	-0.892869

p-methoxyphenol, *trans* S_1

C	0.123420	-0.064102	-1.389958
C	-1.276449	-0.007929	-1.217404
C	-1.781121	0.028870	0.101798
C	-0.958096	0.046090	1.247252
C	0.443887	0.025140	1.077284
C	0.953933	-0.030270	-0.241024
O	-3.103397	0.055967	0.326404
H	1.096820	0.049766	1.935188
O	2.261489	-0.061894	-0.514806
H	0.586608	-0.106489	-2.364129
H	-1.951487	-0.012379	-2.063884
H	-3.571584	0.038298	-0.513319
H	-1.417946	0.070014	2.223901
C	3.210561	-0.006556	0.537152
H	4.184805	-0.060379	0.058822
H	3.121364	0.931392	1.089168
H	3.087983	-0.851229	1.218254

1-naphthol, *cis* S_0

C	0.829178	1.516602	0.013851
C	0.525938	0.123523	-0.001733
C	-0.840479	-0.265946	-0.005573
C	-1.853127	0.721254	-0.016026
C	-1.518536	2.045171	-0.019641
C	-0.172278	2.448949	-0.002123
C	1.520478	-0.885235	-0.017108
C	1.184270	-2.209187	-0.017024
C	-0.170814	-2.596226	-0.006826
C	-1.152227	-1.648062	-0.004411
O	2.109643	1.971592	0.028328
H	-2.196122	-1.940227	-0.003115
H	-0.427962	-3.648154	-0.005805
H	1.959891	-2.964355	-0.030867
H	2.574426	-0.628517	-0.044493
H	-2.890886	0.411057	-0.022042
H	-2.293090	2.801851	-0.030029
H	0.092589	3.498068	0.007064
H	2.719118	1.247853	0.177572

1-naphthol, *cis* S_1

C	0.870041	1.464260	0.019719
C	0.538240	0.090413	-0.055840

C	-0.849955	-0.247089	0.013440
C	-1.792253	0.797572	-0.017008
C	-1.421815	2.165783	-0.029367
C	-0.102684	2.506124	-0.032097
C	1.500458	-0.930459	-0.127214
C	1.091459	-2.294346	-0.054484
C	-0.233851	-2.617293	0.040012
C	-1.224478	-1.600639	0.056792
O	2.137212	1.865368	0.144136
H	-2.273261	-1.859056	0.125163
H	-0.537811	-3.654888	0.097500
H	1.844582	-3.071539	-0.080167
H	2.547908	-0.715909	-0.307584
H	-2.845344	0.541626	-0.025034
H	-2.188900	2.927742	-0.058954
H	0.240460	3.531558	-0.023781
H	2.699992	1.100761	0.314749

1-naphthol, *trans* S_0

C	-0.712349	-0.538113	0.000000
C	-0.670858	-1.953294	0.000000
C	0.520177	-2.621842	0.000000
C	1.736386	-1.908793	0.000000
C	1.734833	-0.542314	0.000000
C	0.514394	0.172015	0.000000
H	-1.606744	-2.500363	0.000000
H	0.534875	-3.704945	0.000000
H	2.674375	-2.449969	0.000000
H	2.663671	0.012012	0.000000
C	-1.936662	0.176064	0.000000
C	-1.934078	1.539508	0.000000
C	-0.722266	2.259945	0.000000
C	0.473517	1.594312	0.000000
H	-2.868491	-0.376394	0.000000
H	-2.868210	2.087377	0.000000
H	-0.741416	3.344774	0.000000
O	1.674569	2.230856	0.000000
H	1.534288	3.179153	0.000000

1-naphthol, *trans* S_1

C	-0.941854	-0.392516	0.000000
C	-1.304364	-1.746245	0.000000
C	-0.313070	-2.765667	0.000000
C	1.012175	-2.425642	0.000000

C	1.415857	-1.061346	0.000000
C	0.451730	-0.044009	0.000000
H	-2.354470	-2.011301	0.000000
H	-0.614491	-3.805077	0.000000
H	1.773243	-3.196178	0.000000
H	2.465863	-0.806019	0.000000
C	-1.891147	0.644606	0.000000
C	-1.519924	2.013958	0.000000
C	-0.202466	2.363316	0.000000
C	0.783314	1.326628	0.000000
H	-2.943708	0.386951	0.000000
H	-2.289210	2.775018	0.000000
H	0.109629	3.401623	0.000000
O	2.089155	1.643392	0.000000
H	2.198059	2.597580	0.000000

2-naphthol, *cis* S_0

C	0.595314	2.005969	0.000000
C	0.618104	0.591945	0.000000
C	-0.608142	-0.119569	0.000000
C	-1.818998	0.614280	0.000000
C	-1.809115	1.980795	0.000000
C	-0.588772	2.687823	0.000000
C	1.828660	-0.145663	0.000000
C	1.827919	-1.507312	0.000000
C	0.602019	-2.211611	0.000000
C	-0.586726	-1.535408	0.000000
H	-1.528444	-2.076063	0.000000
H	1.537751	2.542295	0.000000
H	-0.596096	3.770623	0.000000
H	-2.743660	2.528355	0.000000
H	-2.759259	0.074377	0.000000
H	2.769370	0.393156	0.000000
H	2.749383	-2.074773	0.000000
O	0.694854	-3.567850	0.000000
H	-0.184170	-3.951359	0.000000

2-naphthol, *cis* S_1

C	0.601059	1.986360	0.000000
C	0.644524	0.585488	0.000000
C	-0.627040	-0.118223	0.000000
C	-1.829442	0.605946	0.000000
C	-1.838315	2.014181	0.000000
C	-0.625689	2.681974	0.000000

C	1.846623	-0.150834	0.000000
C	1.876937	-1.552969	0.000000
C	0.656183	-2.215349	0.000000
C	-0.583199	-1.518025	0.000000
H	-1.508355	-2.087286	0.000000
H	1.528810	2.545923	0.000000
H	-0.607210	3.765539	0.000000
H	-2.771865	2.558683	0.000000
H	-2.765840	0.059514	0.000000
H	2.781127	0.397956	0.000000
H	2.799038	-2.113883	0.000000
O	0.662025	-3.555688	0.000000
H	-0.239360	-3.889298	0.000000

2-naphthol, *trans* S_0

C	0.508357	2.008204	0.000000
C	0.536952	0.592684	0.000000
C	-0.686860	-0.126040	0.000000
C	-1.901735	0.604818	0.000000
C	-1.896733	1.970086	0.000000
C	-0.678060	2.683435	0.000000
C	1.747697	-0.137877	0.000000
C	1.747794	-1.502401	0.000000
C	0.525104	-2.212387	0.000000
C	-0.664393	-1.538394	0.000000
H	-1.591967	-2.097355	0.000000
H	1.448396	2.548819	0.000000
H	-0.690859	3.766218	0.000000
H	-2.833216	2.514356	0.000000
H	-2.838862	0.059981	0.000000
H	2.687826	0.401869	0.000000
H	2.685516	-2.048869	0.000000
O	0.499750	-3.572968	0.000000
H	1.395304	-3.914178	0.000000

2-naphthol, *trans* S_1

C	0.512669	1.990663	0.000000
C	0.558929	0.590202	0.000000
C	-0.707895	-0.118301	0.000000
C	-1.911096	0.601924	0.000000
C	-1.924306	2.011888	0.000000
C	-0.716761	2.683687	0.000000
C	1.763711	-0.140806	0.000000
C	1.796017	-1.545102	0.000000

C	0.572773	-2.209607	0.000000
C	-0.664738	-1.518922	0.000000
H	-1.573629	-2.107377	0.000000
H	1.439027	2.552746	0.000000
H	-0.701520	3.767297	0.000000
H	-2.860393	2.552265	0.000000
H	-2.845348	0.052257	0.000000
H	2.697059	0.410027	0.000000
H	2.730848	-2.090270	0.000000
O	0.477716	-3.547101	0.000000
H	1.356935	-3.935463	0.000000

5-methoxysalicylic acid S_0

C	2.272840	-0.166110	0.000000
C	1.562782	-1.338568	0.000000
C	0.160269	-1.333433	0.000000
C	-0.506557	-0.129831	0.000000
C	0.212277	1.080477	0.000000
C	1.613050	1.068956	0.000000
O	-0.433283	-2.555658	0.000000
C	-1.841277	-2.599721	0.000000
C	-0.484343	2.367686	0.000000
O	-1.821285	2.283563	0.000000
O	2.367255	2.175247	0.000000
O	0.072386	3.452114	0.000000
H	-2.111069	-3.653185	0.000000
H	-2.258398	-2.121260	-0.892577
H	-2.258398	-2.121260	0.892577
H	-1.585188	-0.080314	0.000000
H	3.354792	-0.168612	0.000000
H	2.072664	-2.293732	0.000000
H	1.769274	2.946116	0.000000
H	-2.157774	3.187522	0.000000

5-methoxysalicylic acid S_1

C	2.172361	-0.134474	0.000000
C	1.726380	-1.455296	0.000000
C	0.337331	-1.680945	0.000000
C	-0.599956	-0.616658	0.000000
C	-0.164946	0.706215	0.000000
C	1.269800	0.930612	0.000000
O	-0.032424	-2.961178	0.000000
C	-1.408202	-3.315742	0.000000
C	-1.040802	1.836633	0.000000

O	-2.364135	1.548269	0.000000
O	1.721161	2.166719	0.000000
O	-0.659245	3.027734	0.000000
H	-1.428307	-4.401882	0.000000
H	-1.908274	-2.939135	-0.894330
H	-1.908274	-2.939135	0.894330
H	-1.661387	-0.814295	0.000000
H	3.228252	0.101403	0.000000
H	2.403662	-2.295623	0.000000
H	0.910953	2.772005	0.000000
H	-2.821896	2.395550	0.000000

m-dimethoxybenzene, *trans* S_0

C	0.000000	-0.705948	-0.173781
C	0.000000	0.705948	-0.173781
C	0.000000	1.385864	1.031483
C	0.000000	0.688501	2.239424
C	0.000000	-0.688501	2.239424
C	0.000000	-1.385864	1.031483
O	0.000000	1.290965	-1.393415
H	0.000000	2.466955	1.045149
H	0.000000	1.238499	3.171725
H	0.000000	-1.238499	3.171725
H	0.000000	-2.466955	1.045149
O	0.000000	-1.290965	-1.393415
C	0.000000	-2.697537	-1.451916
H	0.000000	-2.953195	-2.509065
H	0.892643	-3.121230	-0.979792
H	-0.892642	-3.121230	-0.979792
C	0.000000	2.697537	-1.451916
H	0.000000	2.953195	-2.509065
H	-0.892642	3.121230	-0.979792
H	0.892643	3.121230	-0.979792

m-dimethoxybenzene, *trans* S_1

C	-0.112151	-1.064444	-1.443656
C	-0.240357	0.159830	-0.707865
C	-0.240357	0.159830	0.707865
C	-0.112151	-1.064444	1.443656
C	0.274496	-2.189662	0.704489
C	0.274496	-2.189662	-0.704489
O	-0.194224	1.370588	-1.286950
C	-0.018547	1.456777	-2.690454
O	-0.194224	1.370588	1.286950

C	-0.018547	1.456777	2.690454
H	-0.337937	-1.128803	2.497503
H	0.551139	-3.101592	1.222007
H	0.551139	-3.101592	-1.222007
H	-0.337937	-1.128803	-2.497503
H	0.041866	2.519216	-2.912676
H	0.899871	0.957603	-3.006360
H	-0.871065	1.022926	-3.219156
H	0.041866	2.519216	2.912676
H	-0.871065	1.022926	3.219156
H	0.899871	0.957603	3.006360

3P-propionic acid, *gauche* S_0

C	-1.001615	0.877957	-1.163588
C	-0.377923	0.680475	0.066174
C	-1.043854	-0.057870	1.040202
C	-2.302163	-0.587105	0.789234
C	-2.912586	-0.385617	-0.439757
C	-2.258413	0.350445	-1.417739
C	1.006041	1.228595	0.313552
C	2.106132	0.311059	-0.224207
C	2.276999	-0.945147	0.591312
O	2.020850	-1.062780	1.759679
O	2.802616	-1.948915	-0.133507
H	1.923263	0.038761	-1.264294
H	3.072961	0.823819	-0.197072
H	1.163328	1.383542	1.381665
H	1.104447	2.200128	-0.174990
H	-0.565015	-0.224960	1.997492
H	-2.806179	-1.159580	1.558469
H	-3.895003	-0.797793	-0.634711
H	-2.728956	0.517087	-2.379147
H	-0.498858	1.458431	-1.930363
H	2.913937	-2.700554	0.461606

3P-propionic acid, *gauche* S_1

C	-1.000003	0.957072	-1.180010
C	-0.364258	0.713874	0.070607
C	-1.034641	-0.070238	1.051571
C	-2.312153	-0.621068	0.780644
C	-2.926939	-0.384767	-0.472542
C	-2.271992	0.397038	-1.455716
C	1.017497	1.225113	0.312489
C	2.102783	0.277472	-0.224262

C	2.282937	-0.951624	0.629502
O	2.071922	-1.021714	1.810788
O	2.765968	-1.988382	-0.077503
H	1.891335	-0.022724	-1.250911
H	3.071481	0.787591	-0.233822
H	1.185572	1.377628	1.380240
H	1.139215	2.189115	-0.189079
H	-0.546774	-0.256171	1.998879
H	-2.811205	-1.223556	1.526557
H	-3.901661	-0.804308	-0.682796
H	-2.744097	0.568435	-2.413264
H	-0.504501	1.571282	-1.921136
H	2.889523	-2.720076	0.539763

3P-propionic acid, *anti* S_0

C	1.444628	-0.438974	0.000000
C	0.542706	0.793252	0.000000
C	2.910438	-0.097015	0.000000
H	1.244903	-1.068411	0.871260
H	1.244903	-1.068411	-0.871260
C	-0.913249	0.403354	0.000000
H	0.770485	1.405498	0.874095
H	0.770485	1.405498	-0.874095
C	-1.594853	0.197345	1.196039
C	-2.922397	-0.205464	1.198904
C	-3.590258	-0.409381	0.000000
C	-2.922397	-0.205464	-1.198904
C	-1.594853	0.197345	-1.196039
H	-1.080788	0.360447	2.137365
H	-3.437253	-0.356623	2.139946
H	-4.627482	-0.721048	0.000000
H	-3.437253	-0.356623	-2.139946
H	-1.080788	0.360447	-2.137365
O	3.679184	-1.203607	0.000000
O	3.378260	1.009327	0.000000
H	4.598420	-0.910168	0.000000

3P-propionic acid, *anti* S_1

C	1.449721	-0.424782	0.000000
C	0.559268	0.824870	0.000000
C	2.917957	-0.093357	0.000000
H	1.241345	-1.048916	0.872563
H	1.241345	-1.048916	-0.872563
C	-0.886617	0.459936	0.000000

H	0.798754	1.428458	0.878371
H	0.798754	1.428458	-0.878371
C	-1.571538	0.241367	1.228302
C	-2.910289	-0.223234	1.229706
C	-3.575506	-0.448635	0.000000
C	-2.910289	-0.223234	-1.229706
C	-1.571538	0.241367	-1.228302
H	-1.060187	0.431762	2.163319
H	-3.423001	-0.402029	2.164486
H	-4.601049	-0.793454	0.000000
H	-3.423001	-0.402029	-2.164486
H	-1.060187	0.431762	-2.163319
O	3.676595	-1.206444	0.000000
O	3.393570	1.009587	0.000000
H	4.598519	-0.921375	0.000000

fluorine S_0

C	0.000000	0.000000	-1.788917
C	0.000000	1.178221	-0.846844
C	0.000000	0.733667	0.480369
C	0.000000	-0.733667	0.480369
C	0.000000	1.642494	1.528146
C	0.000000	2.999838	1.236696
C	0.000000	3.441299	-0.082271
C	0.000000	2.530596	-1.133132
H	0.000000	2.880854	-2.159075
H	0.000000	4.504035	-0.291399
H	0.000000	3.723201	2.042810
H	0.000000	1.303236	2.557366
C	0.000000	-1.642494	1.528146
C	0.000000	-2.999838	1.236696
C	0.000000	-3.441299	-0.082271
C	0.000000	-2.530596	-1.133132
C	0.000000	-1.178221	-0.846844
H	0.000000	-1.303236	2.557366
H	0.000000	-3.723201	2.042810
H	0.000000	-4.504035	-0.291399
H	0.000000	-2.880854	-2.159075
H	-0.880062	0.000000	-2.438198
H	0.880062	0.000000	-2.438198

fluorine S_1

C	0.000000	0.000000	-1.867246
C	0.000000	1.176935	-0.918246

C	0.000000	0.693672	0.451614
C	0.000000	-0.693672	0.451614
C	0.000000	1.636972	1.534128
C	0.000000	2.972540	1.229081
C	0.000000	3.427328	-0.107100
C	0.000000	2.517256	-1.182477
H	0.000000	2.885357	-2.201926
H	0.000000	4.491769	-0.305302
H	0.000000	3.706021	2.026550
H	0.000000	1.291996	2.560269
C	0.000000	-1.636972	1.534128
C	0.000000	-2.972540	1.229081
C	0.000000	-3.427328	-0.107100
C	0.000000	-2.517256	-1.182477
C	0.000000	-1.176935	-0.918246
H	0.000000	-1.291996	2.560269
H	0.000000	-3.706021	2.026550
H	0.000000	-4.491769	-0.305302
H	0.000000	-2.885357	-2.201926
H	-0.879159	0.000000	-2.520807
H	0.879159	0.000000	-2.520807

phenanthrene S_0

C	0.727605	0.000000	-0.348543
C	-0.727605	0.000000	-0.348543
C	-1.414337	0.000000	0.885060
C	-0.673364	0.000000	2.112335
C	0.673364	0.000000	2.112335
C	1.414337	0.000000	0.885060
C	-1.492235	0.000000	-1.530841
C	-2.821886	0.000000	0.899714
H	-1.224114	0.000000	3.046024
H	1.224114	0.000000	3.046024
C	1.492235	0.000000	-1.530841
C	2.864988	0.000000	-1.494209
C	3.540450	0.000000	-0.267866
C	2.821886	0.000000	0.899714
H	1.000295	0.000000	-2.493885
H	3.426500	0.000000	-2.420336
H	4.623125	0.000000	-0.243706
H	3.331975	0.000000	1.856345
C	-3.540450	0.000000	-0.267866
C	-2.864988	0.000000	-1.494209
H	-1.000295	0.000000	-2.493885
H	-3.426500	0.000000	-2.420336

H	-4.623125	0.000000	-0.243706
H	-3.331975	0.000000	1.856345

phenanthrene S_1

C	0.710306	0.000000	-0.388439
C	-0.710306	0.000000	-0.388439
C	-1.430443	0.000000	0.882816
C	-0.692884	0.000000	2.079108
C	0.692884	0.000000	2.079108
C	1.430443	0.000000	0.882816
C	-1.491145	0.000000	-1.568723
C	-2.834017	0.000000	0.884005
H	-1.228274	0.000000	3.021438
H	1.228274	0.000000	3.021438
C	1.491145	0.000000	-1.568723
C	2.876107	0.000000	-1.524931
C	3.559650	0.000000	-0.298870
C	2.834017	0.000000	0.884005
H	1.007800	0.000000	-2.535589
H	3.435321	0.000000	-2.452159
H	4.641289	0.000000	-0.276940
H	3.349906	0.000000	1.837323
C	-3.559650	0.000000	-0.298870
C	-2.876107	0.000000	-1.524931
H	-1.007800	0.000000	-2.535589
H	-3.435321	0.000000	-2.452159
H	-4.641289	0.000000	-0.276940
H	-3.349906	0.000000	1.837323

2,4,6,8-decatetraene S_0

C	-2.586709	-5.003423	0.000000
C	-2.461332	-3.515122	0.000000
C	-1.309287	-2.843463	0.000000
C	-1.207860	-1.396783	0.000000
C	-0.050266	-0.721317	0.000000
C	0.050266	0.721317	0.000000
C	1.207860	1.396783	0.000000
C	1.309287	2.843463	0.000000
C	2.461332	3.515122	0.000000
C	2.586709	5.003423	0.000000
H	-0.372781	-3.397905	0.000000
H	-2.142904	-0.840442	0.000000
H	0.884631	-1.277875	0.000000
H	-0.884631	1.277875	0.000000

H	2.142904	0.840442	0.000000
H	0.372781	3.397905	0.000000
H	3.391958	2.951394	0.000000
H	-3.391958	-2.951394	0.000000
H	1.608657	5.487268	0.000000
H	3.138404	5.350363	0.878211
H	3.138404	5.350363	-0.878211
H	-1.608657	-5.487268	0.000000
H	-3.138404	-5.350363	0.878211
H	-3.138404	-5.350363	-0.878211

2,4,6,8-decatetraene S_1

C	-2.573564	-5.012489	0.000000
C	-2.510593	-3.528600	0.000000
C	-1.351412	-2.805981	0.000000
C	-1.265896	-1.401692	0.000000
C	-0.052793	-0.692103	0.000000
C	0.052793	0.692103	0.000000
C	1.265896	1.401692	0.000000
C	1.351412	2.805981	0.000000
C	2.510593	3.528600	0.000000
C	2.573564	5.012489	0.000000
H	-0.411037	-3.356117	0.000000
H	-2.191544	-0.830581	0.000000
H	0.867800	-1.272427	0.000000
H	-0.867800	1.272427	0.000000
H	2.191544	0.830581	0.000000
H	0.411037	3.356117	0.000000
H	3.456437	2.991480	0.000000
H	-3.456437	-2.991480	0.000000
H	1.576476	5.457103	0.000000
H	3.114139	5.392648	0.875916
H	3.114139	5.392648	-0.875916
H	-1.576476	-5.457103	0.000000
H	-3.114139	-5.392648	0.875916
H	-3.114139	-5.392648	-0.875916

tetracene S_0

C	3.693077	1.402433	0.000000
C	2.432938	0.719694	0.000000
C	2.432938	-0.719694	0.000000
C	3.693077	-1.402433	0.000000
C	4.858787	-0.714479	0.000000
C	4.858787	0.714479	0.000000

C	1.229444	1.397567	0.000000
C	0.000000	0.718485	0.000000
C	0.000000	-0.718485	0.000000
C	1.229444	-1.397567	0.000000
C	-1.229444	1.397567	0.000000
C	-2.432938	0.719694	0.000000
C	-2.432938	-0.719694	0.000000
C	-1.229444	-1.397567	0.000000
C	-3.693077	1.402433	0.000000
C	-4.858787	0.714479	0.000000
C	-4.858787	-0.714479	0.000000
C	-3.693077	-1.402433	0.000000
H	-3.691569	-2.486555	0.000000
H	-5.803998	-1.243103	0.000000
H	-5.803998	1.243103	0.000000
H	-3.691569	2.486555	0.000000
H	-1.229490	-2.482607	0.000000
H	-1.229490	2.482607	0.000000
H	1.229490	-2.482607	0.000000
H	1.229490	2.482607	0.000000
H	3.691569	-2.486555	0.000000
H	5.803998	-1.243103	0.000000
H	5.803998	1.243103	0.000000
H	3.691569	2.486555	0.000000

tetracene S_1

C	3.691965	1.391948	0.000000
C	2.464241	0.715861	0.000000
C	2.464241	-0.715861	0.000000
C	3.691965	-1.391948	0.000000
C	4.891172	-0.696456	0.000000
C	4.891172	0.696456	0.000000
C	1.223946	1.394742	0.000000
C	0.000000	0.725030	0.000000
C	0.000000	-0.725030	0.000000
C	1.223946	-1.394742	0.000000
C	-1.223946	1.394742	0.000000
C	-2.464241	0.715861	0.000000
C	-2.464241	-0.715861	0.000000
C	-1.223946	-1.394742	0.000000
C	-3.691965	1.391948	0.000000
C	-4.891172	0.696456	0.000000
C	-4.891172	-0.696456	0.000000
C	-3.691965	-1.391948	0.000000
H	-3.694051	-2.476109	0.000000

H	-5.828756	-1.237944	0.000000
H	-5.828756	1.237944	0.000000
H	-3.694051	2.476109	0.000000
H	-1.227118	-2.479952	0.000000
H	-1.227118	2.479952	0.000000
H	1.227118	-2.479952	0.000000
H	1.227118	2.479952	0.000000
H	3.694051	-2.476109	0.000000
H	5.828756	-1.237944	0.000000
H	5.828756	1.237944	0.000000
H	3.694051	2.476109	0.000000

perylene S_0

C	0.020457	1.470072	-2.411257
C	0.010909	0.738598	-1.244129
C	0.014165	1.435531	-0.000001
C	0.034466	2.856861	0.000001
C	0.043357	3.555984	-1.227677
C	0.036684	2.872513	-2.407520
C	0.044072	3.555970	1.227683
C	0.038085	2.872485	2.407522
C	0.021645	1.470047	2.411253
C	0.011249	0.738591	1.244122
C	-0.010909	-0.738598	-1.244129
C	-0.014165	-1.435531	-0.000001
C	-0.011249	-0.738591	1.244122
C	-0.034466	-2.856861	0.000001
C	-0.044072	-3.555970	1.227683
C	-0.038085	-2.872485	2.407522
C	-0.021645	-1.470047	2.411253
C	-0.020457	-1.470072	-2.411257
C	-0.036684	-2.872513	-2.407520
C	-0.043357	-3.555984	-1.227677
H	0.057468	4.639517	1.212885
H	0.046179	3.405013	3.350428
H	0.018459	0.970035	3.369459
H	-0.057468	-4.639517	1.212885
H	-0.046179	-3.405013	3.350428
H	-0.018459	-0.970035	3.369459
H	-0.056710	-4.639531	-1.212874
H	-0.044105	-3.405052	-3.350424
H	-0.016699	-0.970076	-3.369469
H	0.056710	4.639531	-1.212874
H	0.044105	3.405052	-3.350424
H	0.016699	0.970076	-3.369469

perylene S_1

C	-0.005324	1.464949	-2.441539
C	-0.006132	0.717493	-1.235824
C	0.011180	1.415581	-0.000002
C	0.006750	2.845701	0.000000
C	0.008250	3.535384	-1.226021
C	-0.000608	2.843944	-2.426471
C	0.008418	3.535383	1.226019
C	-0.000268	2.843940	2.426471
C	-0.005034	1.464946	2.441537
C	-0.006057	0.717492	1.235822
C	0.006132	-0.717493	-1.235824
C	-0.011180	-1.415581	-0.000002
C	0.006057	-0.717492	1.235822
C	-0.006750	-2.845701	0.000000
C	-0.008418	-3.535383	1.226019
C	0.000268	-2.843940	2.426471
C	0.005034	-1.464946	2.441537
C	0.005324	-1.464949	-2.441539
C	0.000608	-2.843944	-2.426471
C	-0.008250	-3.535384	-1.226021
H	0.011676	4.619057	1.218371
H	-0.003034	3.388968	3.362398
H	-0.023248	0.957508	3.394608
H	-0.011676	-4.619057	1.218371
H	0.003034	-3.388968	3.362398
H	0.023248	-0.957508	3.394608
H	-0.011493	-4.619058	-1.218371
H	0.003556	-3.388972	-3.362398
H	0.023741	-0.957512	-3.394606
H	0.011493	4.619058	-1.218371
H	-0.003556	3.388972	-3.362398
H	-0.023741	0.957512	-3.394606

CIS/TZVP geometries – Group I

pyrazine S_0

C	1.119913	-0.691798	0.000000
C	1.119913	0.691798	0.000000
N	0.000000	1.382381	0.000000
C	-1.119913	0.691798	0.000000
C	-1.119913	-0.691798	0.000000

N	0.000000	-1.382381	0.000000
H	-2.041739	-1.243106	0.000000
H	2.041739	-1.243106	0.000000
H	2.041739	1.243106	0.000000
H	-2.041739	1.243106	0.000000

pyrazine S_1

C	-1.175508	0.652729	0.000000
C	-1.128640	-0.730686	0.000000
N	0.045453	-1.348772	0.000000
C	1.175508	-0.652729	0.000000
C	1.128640	0.730686	0.000000
N	-0.045453	1.348772	0.000000
H	2.043899	1.289942	0.000000
H	-2.125909	1.149788	0.000000
H	-2.043899	-1.289942	0.000000
H	2.125909	-1.149788	0.000000

2,6-difluoropyridine S_0

C	1.106153	0.000000	-0.870702
N	0.000000	0.000000	-1.552051
C	-1.106153	0.000000	-0.870702
C	-1.196102	0.000000	0.503126
C	0.000000	0.000000	1.192910
C	1.196102	0.000000	0.503126
F	-2.208601	0.000000	-1.575047
H	-2.150344	0.000000	0.989051
H	0.000000	0.000000	2.266705
H	2.150344	0.000000	0.989051
F	2.208601	0.000000	-1.575047

2,6-difluoropyridine S_1

C	-1.094635	0.000000	-0.335202
N	0.000000	0.000000	-1.081589
C	1.094635	0.000000	-0.335202
C	1.185118	0.000000	1.070084
C	0.000000	0.000000	1.833574
C	-1.185118	0.000000	1.070084
F	2.209290	0.000000	-0.997560
H	2.162145	0.000000	1.510722
H	0.000000	0.000000	2.901220
H	-2.162145	0.000000	1.510722
F	-2.209290	0.000000	-0.997560

2-fluoropyridine S_0

C	-1.309124	0.498341	0.000000
N	-1.353954	-0.791334	0.000000
C	-0.196510	-1.438978	0.000000
C	1.023665	-0.806413	0.000000
C	1.035391	0.581675	0.000000
C	-0.156476	1.264635	0.000000
H	-0.260198	-2.511213	0.000000
H	1.933180	-1.374460	0.000000
H	1.964772	1.120155	0.000000
H	-0.215835	2.334603	0.000000
F	-2.464921	1.122979	0.000000

2-fluoropyridine S_1

C	-1.325639	0.481428	0.000000
N	-1.422900	-0.823849	0.000000
C	-0.223731	-1.450704	0.000000
C	1.031191	-0.785145	0.000000
C	1.098819	0.608280	0.000000
C	-0.150842	1.271306	0.000000
H	-0.251064	-2.522886	0.000000
H	1.919696	-1.386593	0.000000
H	2.025727	1.141107	0.000000
H	-0.250963	2.338016	0.000000
F	-2.450305	1.129032	0.000000

2-hydroxypyridine S_0

C	-0.971433	0.745298	0.000000
C	-0.957184	-0.648367	0.000000
N	0.132768	-1.363847	0.000000
C	1.297731	-0.727519	0.000000
C	1.414289	0.638744	0.000000
C	0.239091	1.385216	0.000000
O	-2.125226	-1.292532	0.000000
H	2.171361	-1.353384	0.000000
H	2.378509	1.107778	0.000000
H	0.278336	2.459081	0.000000
H	-1.905024	1.271527	0.000000
H	-1.953217	-2.221994	0.000000

2-hydroxypyridine S_1

C	-0.981827	0.757327	0.000000
C	-0.956167	-0.657276	0.000000
N	0.127867	-1.440522	0.000000
C	1.287950	-0.765365	0.000000
C	1.390606	0.649685	0.000000
C	0.248966	1.452672	0.000000
O	-2.105502	-1.279928	0.000000
H	2.184318	-1.355455	0.000000
H	2.372794	1.082273	0.000000
H	0.298822	2.520901	0.000000
H	-1.933929	1.248847	0.000000
H	-1.933898	-2.213157	0.000000

2-pyridone S_0

C	-1.241952	0.697150	0.000000
N	-1.136492	-0.679731	0.000000
C	0.035177	-1.372205	0.000000
C	1.210510	-0.738471	0.000000
C	1.193286	0.697565	0.000000
C	0.043613	1.383143	0.000000
H	-2.002652	-1.169462	0.000000
H	-0.055119	-2.440944	0.000000
H	2.130781	-1.285554	0.000000
H	2.128556	1.227357	0.000000
H	0.011074	2.454429	0.000000
O	-2.316783	1.226734	0.000000

2-pyridone S_1

C	-1.410538	0.098867	0.000000
N	-0.731474	-1.155873	0.000000
C	0.607078	-1.241950	0.000000
C	1.403725	-0.074996	0.000000
C	0.823594	1.174654	0.000000
C	-0.594628	1.265035	0.000000
H	-1.313625	-1.962335	0.000000
H	1.040917	-2.221883	0.000000
H	2.468346	-0.201082	0.000000
H	1.423676	2.061748	0.000000
H	-1.107460	2.205529	0.000000
O	-2.609610	0.052276	0.000000

2-methylpyrimidine S_0

C	0.000341	1.955396	0.000000

C	-1.164690	1.214686	0.000000
N	-1.164939	-0.099229	0.000000
C	0.011723	-0.705935	0.000000
N	1.179861	-0.091881	0.000000
C	1.168043	1.226665	0.000000
H	-2.127556	1.694539	0.000000
H	2.127510	1.712849	0.000000
H	-0.004715	3.027129	0.000000
C	0.004248	-2.205887	0.000000
H	1.014683	-2.585839	0.000000
H	-0.522259	-2.571247	0.873902
H	-0.522259	-2.571247	-0.873902

2-methylpyrimidine S_1

C	-0.000859	1.998572	0.000000
C	-1.182733	1.283941	0.000000
N	-1.090912	-0.072114	0.000000
C	0.013938	-0.777868	0.000000
N	1.107408	-0.075282	0.000000
C	1.178976	1.284852	0.000000
H	-2.157172	1.724546	0.000000
H	2.151017	1.730882	0.000000
H	-0.003540	3.072205	0.000000
C	0.003281	-2.267701	0.000000
H	1.017097	-2.639613	0.000000
H	-0.518251	-2.631214	0.877045
H	-0.518251	-2.631214	-0.877045

5-methylpyrimidine S_0

C	0.872829	0.841051	0.000000
C	-0.354774	0.209043	0.000000
C	-0.290663	-1.174606	0.000000
N	0.843292	-1.840779	0.000000
C	1.947262	-1.123002	0.000000
N	2.018878	0.187467	0.000000
H	2.876173	-1.661892	0.000000
H	-1.191396	-1.764891	0.000000
H	0.936849	1.915460	0.000000
C	-1.661555	0.956996	0.000000
H	-1.491834	2.026348	0.000000
H	-2.252531	0.714393	-0.876214
H	-2.252531	0.714393	0.876214

5-methylpyrimidine S_1

C	0.838161	0.869041	0.000000
C	-0.372646	0.227326	0.000000
C	-0.337977	-1.175467	0.000000
N	0.873369	-1.766804	0.000000
C	2.030494	-1.167487	0.000000
N	1.991898	0.133052	0.000000
H	2.951141	-1.712024	0.000000
H	-1.209396	-1.796099	0.000000
H	0.940793	1.934420	0.000000
C	-1.675996	0.972888	0.000000
H	-1.508575	2.041946	0.000000
H	-2.260637	0.719608	-0.877124
H	-2.260637	0.719608	0.877124

7-azaindole S_0

N	-0.631860	1.828575	0.000000
C	-0.668599	0.467496	0.000000
C	0.654924	0.003603	0.000000
C	1.500305	1.170502	0.000000
C	0.679874	2.236844	0.000000
C	0.835614	-1.370110	0.000000
C	-0.291553	-2.163463	0.000000
C	-1.552479	-1.567733	0.000000
N	-1.757231	-0.269597	0.000000
H	-2.432837	-2.184826	0.000000
H	1.817918	-1.806457	0.000000
H	-0.213950	-3.233638	0.000000
H	-1.432420	2.412693	0.000000
H	2.569225	1.197723	0.000000
H	0.923089	3.278389	0.000000

7-azaindole S_1

N	-0.626758	1.862105	0.000000
C	-0.682955	0.472899	0.000000
C	0.671037	0.009565	0.000000
C	1.482620	1.130654	0.000000
C	0.645619	2.274435	0.000000
C	0.876014	-1.408330	0.000000
C	-0.287884	-2.173277	0.000000
C	-1.538514	-1.587141	0.000000
N	-1.769776	-0.217416	0.000000
H	-2.423589	-2.192650	0.000000
H	1.855243	-1.843365	0.000000

H	-0.229727	-3.245316	0.000000
H	-1.434720	2.440264	0.000000
H	2.551580	1.168095	0.000000
H	0.911821	3.309497	0.000000

7-hydroxyquinoline, *cis* S_0

N	0.448850	1.957454	0.000000
C	0.424250	0.605537	0.000000
C	-0.777931	-0.119356	0.000000
C	-1.984427	0.609940	0.000000
C	-1.941319	1.964871	0.000000
C	-0.676064	2.591236	0.000000
C	1.657509	-0.089854	0.000000
C	1.672064	-1.445060	0.000000
C	0.463064	-2.185875	0.000000
C	-0.721188	-1.537287	0.000000
H	-0.620488	3.666412	0.000000
H	-1.639742	-2.095745	0.000000
H	0.519586	-3.257296	0.000000
O	2.803899	-2.176314	0.000000
H	2.564260	0.486687	0.000000
H	-2.923051	0.085126	0.000000
H	-2.834048	2.560003	0.000000
H	3.564777	-1.620468	0.000000

7-hydroxyquinoline, *cis* S_1

N	0.470301	1.964486	0.000000
C	0.436670	0.624204	0.000000
C	-0.797632	-0.140284	0.000000
C	-1.986618	0.590565	0.000000
C	-1.916261	1.990922	0.000000
C	-0.680099	2.624593	0.000000
C	1.628014	-0.078832	0.000000
C	1.652920	-1.509716	0.000000
C	0.488411	-2.239210	0.000000
C	-0.724648	-1.548870	0.000000
H	-0.618657	3.696139	0.000000
H	-1.642834	-2.107123	0.000000
H	0.526542	-3.309891	0.000000
O	2.819341	-2.148828	0.000000
H	2.551201	0.471595	0.000000
H	-2.936741	0.091029	0.000000
H	-2.815945	2.576407	0.000000
H	3.546032	-1.547177	0.000000

7-hydroxyquinoline, *trans* S_0

N	0.500186	2.028408	0.000000
C	0.472565	0.673141	0.000000
C	-0.735908	-0.045026	0.000000
C	-1.941678	0.691117	0.000000
C	-1.891738	2.043350	0.000000
C	-0.620211	2.664855	0.000000
C	1.700277	-0.022838	0.000000
C	1.710500	-1.378882	0.000000
C	0.498150	-2.111328	0.000000
C	-0.687645	-1.457882	0.000000
H	-0.561429	3.740018	0.000000
H	-1.607484	-2.014186	0.000000
H	0.526707	-3.186750	0.000000
O	2.899113	-2.018022	0.000000
H	2.617171	0.532400	0.000000
H	-2.882506	0.170190	0.000000
H	-2.780959	2.643755	0.000000
H	2.784870	-2.952301	0.000000

7-hydroxyquinoline, *trans* S_1

N	0.514428	2.033436	0.000004
C	0.476196	0.697918	0.000055
C	-0.759535	-0.058951	0.000119
C	-1.945953	0.675837	0.000076
C	-1.870844	2.077102	-0.000006
C	-0.635712	2.702245	-0.000055
C	1.668681	-0.010994	0.000067
C	1.686379	-1.440274	0.000015
C	0.520208	-2.165076	-0.000049
C	-0.693976	-1.465110	0.000000
H	-0.565969	3.773147	-0.000103
H	-1.614071	-2.020299	-0.000036
H	0.533448	-3.238742	-0.000116
O	2.898388	-1.988881	-0.000012
H	2.603000	0.514352	0.000077
H	-2.897960	0.179712	0.000075
H	-2.768481	2.665718	-0.000042
H	2.851774	-2.931157	-0.000070

2-hydroxyquinoline, enol S_0

C	0.425688	1.898267	0.000000

C	0.478705	0.485722	0.000000
C	-0.710099	-0.255204	0.000000
C	-1.943661	0.435259	0.000000
C	-1.967830	1.792334	0.000000
C	-0.769220	2.539827	0.000000
C	1.692033	-0.247997	0.000000
C	1.660753	-1.595149	0.000000
C	0.387180	-2.237292	0.000000
N	-0.725674	-1.611628	0.000000
O	0.320230	-3.574717	0.000000
H	1.345371	2.455346	0.000000
H	-0.811112	3.612820	0.000000
H	-2.909427	2.309886	0.000000
H	-2.846098	-0.144971	0.000000
H	2.630787	0.275866	0.000000
H	2.563145	-2.178231	0.000000
H	1.179228	-3.960139	0.000000

2-hydroxyquinoline, enol S_1

C	0.437383	1.880614	0.000000
C	0.532426	0.492735	0.000000
C	-0.714876	-0.268715	0.000000
C	-1.950696	0.432492	0.000000
C	-1.999654	1.827617	0.000000
C	-0.816175	2.539123	0.000000
C	1.722290	-0.234367	0.000000
C	1.683288	-1.632124	0.000000
C	0.441086	-2.238072	0.000000
N	-0.729121	-1.584053	0.000000
O	0.297554	-3.556769	0.000000
H	1.333812	2.472574	0.000000
H	-0.830694	3.612798	0.000000
H	-2.943502	2.336111	0.000000
H	-2.847109	-0.156950	0.000000
H	2.664453	0.280869	0.000000
H	2.583064	-2.216622	0.000000
H	1.136464	-3.987240	0.000000

2-hydroxyquinoline, keto S_0

N	0.557934	1.701681	0.000000
C	0.596423	0.324358	0.000000
C	-0.603739	-0.380800	0.000000
C	-1.834210	0.384230	0.000000
C	-1.832040	1.713520	0.000000

C	-0.576265	2.472927	0.000000
C	1.808695	-0.361181	0.000000
C	1.812486	-1.734032	0.000000
C	0.620069	-2.452757	0.000000
C	-0.572477	-1.774567	0.000000
H	-1.501336	-2.315671	0.000000
H	0.635981	-3.525783	0.000000
H	2.750555	-2.257420	0.000000
H	2.733291	0.186567	0.000000
H	-2.765034	-0.154132	0.000000
H	-2.732678	2.294488	0.000000
O	-0.510461	3.667595	0.000000
H	1.412827	2.210997	0.000000

2-hydroxyquinoline, keto S_1

N	0.573337	1.684186	0.000000
C	0.618970	0.343240	0.000000
C	-0.663857	-0.382218	0.000000
C	-1.842858	0.357893	0.000000
C	-1.839924	1.747512	0.000000
C	-0.609775	2.471645	0.000000
C	1.828084	-0.352758	0.000000
C	1.837967	-1.729227	0.000000
C	0.613152	-2.441544	0.000000
C	-0.592550	-1.794648	0.000000
H	-1.507769	-2.355536	0.000000
H	0.637013	-3.515060	0.000000
H	2.767660	-2.263762	0.000000
H	2.748330	0.202412	0.000000
H	-2.778794	-0.168305	0.000000
H	-2.743304	2.321940	0.000000
O	-0.462726	3.660389	0.000000
H	1.417043	2.213851	0.000000

dibenzofuran S_0

C	1.718334	0.000000	-1.350759
C	0.728115	0.000000	-0.381192
C	1.087410	0.000000	0.958201
C	2.395811	0.000000	1.385032
C	3.369716	0.000000	0.405652
C	3.037489	0.000000	-0.946699
C	-0.728115	0.000000	-0.381192
C	-1.087410	0.000000	0.958201
O	0.000000	0.000000	1.767801

C	-1.718334	0.000000	-1.350759
C	-3.037489	0.000000	-0.946699
C	-3.369716	0.000000	0.405652
C	-2.395811	0.000000	1.385032
H	-2.639875	0.000000	2.429762
H	-4.404459	0.000000	0.693725
H	-3.820003	0.000000	-1.682073
H	-1.468269	0.000000	-2.395383
H	1.468269	0.000000	-2.395383
H	3.820003	0.000000	-1.682073
H	4.404459	0.000000	0.693725
H	2.639875	0.000000	2.429762

dibenzofuran S_1

C	0.000000	1.722768	-1.525625
C	0.000000	0.712647	-0.565651
C	0.000000	1.088521	0.801328
C	0.000000	2.393449	1.249251
C	0.000000	3.392963	0.266794
C	0.000000	3.056541	-1.086778
C	0.000000	-0.712647	-0.565651
C	0.000000	-1.088521	0.801328
O	0.000000	0.000000	1.584247
C	0.000000	-1.722768	-1.525625
C	0.000000	-3.056541	-1.086778
C	0.000000	-3.392963	0.266794
C	0.000000	-2.393449	1.249251
H	0.000000	-2.620960	2.296993
H	0.000000	-4.424784	0.558812
H	0.000000	-3.842027	-1.818726
H	0.000000	-1.499035	-2.574811
H	0.000000	1.499035	-2.574811
H	0.000000	3.842027	-1.818726
H	0.000000	4.424784	0.558812
H	0.000000	2.620960	2.296993

pyrrolo[3,2-*h*]quinoline S_0

C	0.140550	-0.680697	0.000000
N	0.072872	-2.023730	0.000000
C	1.183915	-2.690122	0.000000
C	2.454471	-2.087718	0.000000
C	2.529441	-0.729249	0.000000
C	1.348012	0.033963	0.000000
H	1.103388	-3.763242	0.000000

H	3.336225	-2.699234	0.000000
H	3.482648	-0.231783	0.000000
C	-1.050396	0.086367	0.000000
C	-1.050804	1.465630	0.000000
C	0.187734	2.165436	0.000000
C	1.342504	1.467603	0.000000
H	0.199369	3.239769	0.000000
H	2.287340	1.979665	0.000000
C	-2.423916	1.874093	0.000000
C	-3.164226	0.741294	0.000000
N	-2.338764	-0.344906	0.000000
H	-2.610639	-1.298160	0.000000
H	-2.802877	2.874236	0.000000
H	-4.226836	0.620786	0.000000

pyrrolo[3,2-*h*]quinoline S_1

C	0.141493	-0.701806	0.000000
N	0.047222	-2.010593	0.000000
C	1.206849	-2.717387	0.000000
C	2.438365	-2.128044	0.000000
C	2.545718	-0.721129	0.000000
C	1.373697	0.035500	0.000000
H	1.102657	-3.785349	0.000000
H	3.322482	-2.736627	0.000000
H	3.507440	-0.244309	0.000000
C	-1.032543	0.088490	0.000000
C	-1.054076	1.527488	0.000000
C	0.140071	2.204396	0.000000
C	1.332174	1.448153	0.000000
H	0.184919	3.276043	0.000000
H	2.268036	1.976361	0.000000
C	-2.446691	1.893162	0.000000
C	-3.154980	0.748762	0.000000
N	-2.302364	-0.340130	0.000000
H	-2.556471	-1.300265	0.000000
H	-2.849698	2.883067	0.000000
H	-4.214310	0.604214	0.000000

carbazole S_0

C	1.123087	0.000000	-0.888285
N	0.000000	0.000000	-1.684939
C	-1.123087	0.000000	-0.888285
C	-0.726771	0.000000	0.452157
C	0.726771	0.000000	0.452157

C	-1.690284	0.000000	1.450594
C	-3.022065	0.000000	1.098381
C	-3.398744	0.000000	-0.244270
C	-2.460519	0.000000	-1.252872
C	2.460519	0.000000	-1.252872
C	3.398744	0.000000	-0.244270
C	3.022065	0.000000	1.098381
C	1.690284	0.000000	1.450594
H	-2.758587	0.000000	-2.285235
H	-4.442747	0.000000	-0.498316
H	-3.778253	0.000000	1.860774
H	-1.404373	0.000000	2.486477
H	1.404373	0.000000	2.486477
H	3.778253	0.000000	1.860774
H	4.442747	0.000000	-0.498316
H	2.758587	0.000000	-2.285235
H	0.000000	0.000000	-2.674830

carbazole S_1

C	1.126687	0.000000	-0.893671
N	0.000000	0.000000	-1.682595
C	-1.126687	0.000000	-0.893671
C	-0.692299	0.000000	0.482288
C	0.692299	0.000000	0.482288
C	-1.672236	0.000000	1.521290
C	-2.997196	0.000000	1.159453
C	-3.389362	0.000000	-0.185096
C	-2.447623	0.000000	-1.235818
C	2.447623	0.000000	-1.235818
C	3.389362	0.000000	-0.185096
C	2.997196	0.000000	1.159453
C	1.672236	0.000000	1.521290
H	-2.768922	0.000000	-2.260174
H	-4.435875	0.000000	-0.425957
H	-3.757298	0.000000	1.918088
H	-1.371639	0.000000	2.551181
H	1.371639	0.000000	2.551181
H	3.757298	0.000000	1.918088
H	4.435875	0.000000	-0.425957
H	2.768922	0.000000	-2.260174
H	0.000000	0.000000	-2.673198

tryptamine, A-ph S_0

C	-2.112375	0.130567	0.880029

N	-1.243455	0.126344	1.945278
C	0.035250	0.044752	1.468184
C	-0.037905	-0.011212	0.073385
C	-1.439573	0.044297	-0.282959
C	1.249389	0.020734	2.147315
C	2.395376	-0.057776	1.396872
C	2.346134	-0.110030	-0.002566
C	1.144592	-0.087517	-0.665019
C	-2.020046	0.000579	-1.665915
C	-1.994447	-1.393566	-2.292389
N	-2.504266	-1.348706	-3.654683
H	1.290792	0.063848	3.220471
H	3.349692	-0.077730	1.890183
H	3.263265	-0.167392	-0.558757
H	1.118042	-0.124522	-1.738678
H	-1.502655	0.204822	2.897122
H	-3.167933	0.200202	1.044532
H	-1.482662	0.679741	-2.319151
H	-3.047401	0.353172	-1.632052
H	-2.546940	-2.078378	-1.649099
H	-0.973214	-1.753710	-2.329969
H	-3.472399	-1.100133	-3.670605
H	-2.414673	-2.236007	-4.104159

tryptamine, A-ph S_1

C	-2.136292	0.113816	0.883141
N	-1.279456	0.098157	1.919516
C	0.027855	0.042913	1.466354
C	-0.040246	0.026632	0.043889
C	-1.386123	0.068560	-0.316408
C	1.201812	-0.005973	2.164102
C	2.416314	-0.066308	1.382552
C	2.383283	-0.079606	0.005520
C	1.177619	-0.033787	-0.705898
C	-1.971140	0.023240	-1.691210
C	-2.007229	-1.394952	-2.267598
N	-2.560154	-1.379988	-3.611970
H	1.239082	-0.000864	3.236424
H	3.357897	-0.100340	1.896893
H	3.308660	-0.122865	-0.537984
H	1.167058	-0.027440	-1.778556
H	-1.543796	0.140435	2.874824
H	-3.194395	0.178565	1.020749
H	-1.395856	0.651530	-2.361076
H	-2.980349	0.426365	-1.667455

H	-2.555767	-2.042184	-1.583041
H	-0.994562	-1.776857	-2.321637
H	-3.531301	-1.143644	-3.604135
H	-2.470344	-2.273027	-4.049665

tryptamine, A-py S_0

C	-2.105244	0.105561	0.857924
N	-1.246277	0.114955	1.930794
C	0.037411	0.045045	1.465916
C	-0.022248	-0.017636	0.070506
C	-1.421230	0.021756	-0.298771
C	1.245109	0.036787	2.156652
C	2.399365	-0.032483	1.418075
C	2.364125	-0.091410	0.018598
C	1.168619	-0.084907	-0.655060
C	-1.998567	-0.028524	-1.683109
C	-1.959752	-1.421088	-2.311421
N	-2.531092	-1.388790	-3.649944
H	1.275430	0.084570	3.229974
H	3.348924	-0.040242	1.920772
H	3.287097	-0.142053	-0.528567
H	1.153950	-0.129143	-1.728719
H	-1.515322	0.191768	2.880071
H	-3.163012	0.164700	1.011555
H	-1.459723	0.664635	-2.325438
H	-3.028357	0.308603	-1.664261
H	-2.556324	-2.094357	-1.706688
H	-0.938922	-1.800966	-2.292539
H	-1.971363	-0.837779	-4.268351
H	-2.592684	-2.306612	-4.038860

tryptamine, A-py S_1

C	-2.128327	0.083400	0.862836
N	-1.280994	0.077969	1.906083
C	0.031046	0.039471	1.465050
C	-0.023727	0.021998	0.042332
C	-1.366809	0.047778	-0.330037
C	1.199040	0.007114	2.174364
C	2.421271	-0.037451	1.403899
C	2.401687	-0.052063	0.027006
C	1.201725	-0.022851	-0.695902
C	-1.946471	-0.001052	-1.706770
C	-1.973281	-1.418973	-2.284738
N	-2.575784	-1.411725	-3.607969

H	1.226181	0.013710	3.246924
H	3.358348	-0.058840	1.927120
H	3.332670	-0.083966	-0.507685
H	1.202116	-0.020396	-1.768633
H	-1.554628	0.115430	2.859052
H	-3.188585	0.132858	0.989699
H	-1.365020	0.639484	-2.363981
H	-2.958209	0.388433	-1.699269
H	-2.577900	-2.048846	-1.641900
H	-0.963031	-1.825975	-2.271947
H	-2.001902	-0.922184	-4.263982
H	-2.699506	-2.340943	-3.952452

tryptamine, A-up S_0

C	-2.104477	0.121018	0.868686
N	-1.243724	0.106309	1.939744
C	0.038851	0.036822	1.471429
C	-0.023303	-0.000483	0.075434
C	-1.422539	0.054796	-0.290591
C	1.247611	0.008422	2.159902
C	2.399936	-0.055511	1.418053
C	2.362077	-0.089747	0.017716
C	1.165766	-0.063103	-0.653695
C	-1.997157	0.023693	-1.676451
C	-1.964853	-1.367089	-2.326116
N	-2.485301	-1.426498	-3.680598
H	1.280015	0.036666	3.233829
H	3.350278	-0.078939	1.918735
H	3.283744	-0.137962	-0.531759
H	1.149266	-0.089499	-1.727900
H	-1.510809	0.164346	2.890923
H	-3.161587	0.182739	1.026143
H	-1.456947	0.722294	-2.311319
H	-3.025964	0.371643	-1.644852
H	-2.533791	-2.057024	-1.713232
H	-0.947889	-1.741078	-2.340254
H	-1.959624	-0.845445	-4.300751
H	-3.438341	-1.128461	-3.719835

tryptamine, A-up S_1

C	-2.125635	0.092663	0.871536
N	-1.276478	0.065080	1.913226
C	0.034777	0.029268	1.469906
C	-0.021736	0.035712	0.046925

C	-1.365216	0.076333	-0.323111
C	1.203657	-0.015802	2.176559
C	2.424813	-0.052062	1.404258
C	2.403239	-0.044685	0.027452
C	1.202206	-0.000380	-0.692995
C	-1.941264	0.047637	-1.701128
C	-2.004048	-1.373901	-2.290150
N	-2.549481	-1.459120	-3.630423
H	1.232285	-0.025607	3.249082
H	3.362350	-0.085556	1.925936
H	3.333129	-0.072099	-0.509288
H	1.201492	0.014208	-1.765669
H	-1.548626	0.084607	2.867187
H	-3.185431	0.142056	1.002154
H	-1.343595	0.674993	-2.355910
H	-2.942293	0.470799	-1.685549
H	-2.600649	-2.002238	-1.638464
H	-1.006860	-1.798017	-2.299245
H	-1.999919	-0.943605	-4.286384
H	-3.485496	-1.112362	-3.672683

tryptamine, Ph-out S_0

C	0.026935	0.000649	0.095941
C	0.055720	0.067663	1.492276
C	1.248330	0.096098	2.209252
C	2.418572	0.060568	1.494723
C	2.413972	-0.003977	0.094496
C	1.234660	-0.034709	-0.606083
N	-1.238434	0.100274	1.931027
H	1.254141	0.146671	3.282877
H	3.357430	0.082392	2.016882
H	3.349464	-0.030361	-0.432740
H	1.238662	-0.096206	-1.677954
C	-1.365652	-0.000371	-0.302310
C	-2.074663	0.068835	0.841515
H	-1.528236	0.180461	2.873938
H	-3.136276	0.107095	0.975000
C	-1.924324	-0.050659	-1.698328
H	-1.284511	0.515551	-2.366488
C	-2.104248	-1.457456	-2.271349
H	-2.894116	0.437353	-1.702529
H	-2.567170	-1.367263	-3.248725
N	-0.833706	-2.142180	-2.445820
H	-2.799610	-2.008021	-1.636311
H	-0.402290	-2.333549	-1.565090

H	-0.959680	-3.014747	-2.914989

tryptamine, Ph-out S_1

C	0.034878	0.015460	0.070572
C	0.055523	0.056330	1.496017
C	1.206175	0.094099	2.231389
C	2.448281	0.095276	1.493371
C	2.461170	0.050805	0.116944
C	1.280031	0.003720	-0.634291
N	-1.265984	0.051020	1.906939
H	1.205671	0.129871	3.303911
H	3.371871	0.127511	2.039382
H	3.404481	0.047577	-0.396644
H	1.305119	-0.050565	-1.704836
C	-1.300019	-0.002284	-0.333072
C	-2.090618	0.017573	0.844941
H	-1.561776	0.083971	2.853429
H	-3.154350	0.029849	0.949742
C	-1.862222	-0.038582	-1.720096
H	-1.177153	0.448750	-2.403283
C	-2.149617	-1.450916	-2.241475
H	-2.791265	0.525059	-1.732507
H	-2.667351	-1.359515	-3.190235
N	-0.921750	-2.189051	-2.472299
H	-2.830576	-1.950492	-1.550672
H	-0.406718	-2.322086	-1.626278
H	-1.108813	-3.089260	-2.861736

tryptamine, Ph-up S_0

C	-2.053068	0.011825	0.813050
N	-1.228051	0.015327	1.911007
C	0.070165	0.039241	1.485406
C	0.055080	0.042291	0.087042
C	-1.331968	0.019705	-0.325650
C	1.255109	0.062812	2.214886
C	2.432922	0.094535	1.512899
C	2.443012	0.104302	0.111311
C	1.270686	0.078686	-0.600505
C	-1.870381	0.000761	-1.730029
C	-2.137522	-1.403345	-2.295505
N	-0.993516	-2.285823	-2.416783
H	1.249617	0.058369	3.289637
H	3.365792	0.113934	2.045483
H	3.383390	0.133522	-0.406930

H	1.292156	0.089460	-1.674580
H	-1.528910	0.030461	2.853834
H	-3.116410	0.008418	0.937905
H	-1.181640	0.525233	-2.386725
H	-2.802544	0.557835	-1.761978
H	-2.583962	-1.298352	-3.279408
H	-2.874757	-1.898019	-1.672311
H	-0.557038	-2.441633	-1.532007
H	-0.304510	-1.909917	-3.034990

tryptamine, Ph-up S_1

C	-2.072536	-0.027096	0.821624
N	-1.255496	-0.018843	1.888536
C	0.068254	0.036137	1.488124
C	0.056772	0.064292	0.063267
C	-1.273847	0.025511	-0.350676
C	1.213651	0.055668	2.233212
C	2.458852	0.117643	1.504208
C	2.482006	0.147242	0.127998
C	1.305570	0.119349	-0.632486
C	-1.817730	0.012675	-1.742561
C	-2.167180	-1.396065	-2.263251
N	-1.062187	-2.319474	-2.404276
H	1.206426	0.032759	3.305921
H	3.378536	0.139004	2.057296
H	3.428532	0.192888	-0.377530
H	1.341487	0.150242	-1.703953
H	-1.557645	-0.038646	2.833528
H	-3.136752	-0.048773	0.919947
H	-1.100365	0.473636	-2.413447
H	-2.718798	0.621110	-1.777214
H	-2.644297	-1.289286	-3.231633
H	-2.901849	-1.845725	-1.604005
H	-0.590706	-2.467524	-1.536110
H	-0.387039	-1.987116	-3.061429

tryptamine, Py-out S_0

C	0.530159	0.447303	0.239489
C	0.604614	0.539816	1.632815
C	1.817648	0.511437	2.313272
C	2.962660	0.391330	1.566563
C	2.912859	0.302085	0.169347
C	1.711948	0.329177	-0.494552
N	-0.672343	0.657813	2.107157

H	1.859253	0.583164	3.384877
H	3.916122	0.367014	2.061265
H	3.828881	0.212427	-0.384423
H	1.686429	0.262541	-1.566674
C	-0.871071	0.520118	-0.118309
C	-1.541544	0.649261	1.042438
H	-0.930094	0.764457	3.056739
H	-2.596092	0.738232	1.202418
C	-1.460785	0.458438	-1.498260
H	-0.912788	1.129435	-2.154063
C	-1.457013	-0.938888	-2.120731
H	-2.484747	0.812569	-1.464735
H	-0.430323	-1.295106	-2.205321
N	-2.310126	-1.848713	-1.373415
H	-1.851460	-0.863606	-3.128540
H	-2.356640	-2.742080	-1.817553
H	-1.955526	-1.988223	-0.449783

tryptamine, Py-out S_1

C	0.531075	0.461432	0.217959
C	0.608923	0.532285	1.638165
C	1.787664	0.508267	2.330470
C	2.996690	0.412575	1.543760
C	2.954841	0.347121	0.168720
C	1.744007	0.367874	-0.536416
N	-0.694351	0.618877	2.097226
H	1.832224	0.562703	3.401088
H	3.941443	0.394448	2.053104
H	3.876444	0.279056	-0.378663
H	1.727604	0.324526	-1.608036
C	-0.817842	0.507778	-0.135123
C	-1.558598	0.601981	1.067470
H	-0.952537	0.685507	3.052949
H	-2.616550	0.661235	1.207388
C	-1.414525	0.456920	-1.506782
H	-0.824837	1.083023	-2.169189
C	-1.477662	-0.953212	-2.101710
H	-2.418809	0.865201	-1.479718
H	-0.466847	-1.353631	-2.171975
N	-2.377413	-1.807538	-1.343637
H	-1.864506	-0.875014	-3.111673
H	-2.505839	-2.685481	-1.802322
H	-2.010610	-1.995944	-0.433065

tryptamine, Py-up S_0

C	-2.100904	0.258932	0.902488
N	-1.228159	0.248627	1.964334
C	0.044387	0.106483	1.484836
C	-0.036683	0.017749	0.091999
C	-1.437490	0.117881	-0.261092
C	1.259120	0.053866	2.161153
C	2.398607	-0.086571	1.410030
C	2.342240	-0.172469	0.012661
C	1.140007	-0.121654	-0.646810
C	-2.028312	0.067610	-1.639615
C	-2.012519	-1.326532	-2.287700
N	-2.794981	-2.348198	-1.619362
H	1.305813	0.122491	3.232719
H	3.353216	-0.130298	1.901119
H	3.254332	-0.279259	-0.544418
H	1.109830	-0.186578	-1.718878
H	-1.479738	0.360762	2.914933
H	-3.152050	0.375393	1.068577
H	-1.490733	0.754612	-2.288880
H	-3.054314	0.423351	-1.599280
H	-0.991775	-1.683936	-2.358430
H	-2.378663	-1.236073	-3.305117
H	-3.760205	-2.092748	-1.571234
H	-2.472505	-2.493819	-0.685141

tryptamine, Py-up S_1

C	-2.127658	0.238335	0.927590
N	-1.258450	0.234501	1.954189
C	0.039169	0.107255	1.489042
C	-0.047725	0.032135	0.069100
C	-1.396290	0.114556	-0.278112
C	1.219521	0.050739	2.175206
C	2.422071	-0.084521	1.384523
C	2.371763	-0.152926	0.009868
C	1.159170	-0.097547	-0.689405
C	-1.998272	0.067389	-1.646203
C	-2.020432	-1.339758	-2.272379
N	-2.827556	-2.331506	-1.591433
H	1.270287	0.106436	3.245513
H	3.367822	-0.130519	1.890050
H	3.288092	-0.250652	-0.541693
H	1.137565	-0.141972	-1.760868
H	-1.509149	0.318607	2.910461
H	-3.180740	0.347756	1.074572

H	-1.435374	0.724662	-2.303398
H	-3.012607	0.455941	-1.606887
H	-1.006637	-1.717433	-2.333420
H	-2.383459	-1.251094	-3.290616
H	-3.785009	-2.051535	-1.533117
H	-2.497579	-2.499218	-0.663670

porphycene S_0

C	2.693304	-2.865313	-0.004806
C	2.066720	-1.629182	-0.001041
N	0.735020	-1.849623	-0.000954
C	0.468725	-3.166100	-0.004886
C	1.689611	-3.833095	-0.007483
C	-0.850660	-3.746147	-0.008613
C	-2.080066	-3.200688	-0.010267
C	-2.530238	-1.821402	-0.006917
H	0.006481	-1.157697	0.002886
N	-1.770839	-0.765058	0.003704
C	-3.932037	-1.440934	-0.013463
C	-3.961890	-0.093966	-0.007730
C	-2.588363	0.330941	0.006036
C	-2.051217	1.589614	-0.009494
C	-2.690312	2.898568	-0.000935
C	-1.727168	3.823691	0.004475
C	-0.432299	3.147555	0.003653
N	-0.723888	1.817740	-0.005326
C	0.788788	3.731538	0.007389
C	2.103376	3.155622	0.006157
C	2.540853	1.873341	0.003680
C	3.946504	1.472367	0.004038
C	3.971758	0.137013	0.002890
C	2.571787	-0.286085	0.001999
N	1.770565	0.730503	0.002463
H	-0.000017	1.118851	-0.005061
H	-1.847793	4.887317	0.010480
H	-3.747691	3.058649	-0.002861
H	0.772501	4.805497	0.013174
H	2.889043	3.890346	0.007971
H	4.780213	2.145059	0.005111
H	4.824204	-0.509624	0.002785
H	3.749346	-3.036711	-0.005812
H	1.819884	-4.895208	-0.011193
H	-0.825030	-4.821457	-0.012383
H	-2.890473	-3.907884	-0.015584
H	-4.764119	-2.115035	-0.021813

H	-4.824705	0.540230	-0.009669

porphycene S_1

C	2.695503	-2.885387	-0.004003
C	2.070031	-1.614288	-0.002370
N	0.728080	-1.841668	-0.005012
C	0.458937	-3.152375	-0.007953
C	1.707165	-3.830127	-0.007375
C	-0.834740	-3.745531	-0.010952
C	-2.079611	-3.190545	-0.011496
C	-2.532819	-1.833181	-0.009408
H	-0.001852	-1.146407	-0.004891
N	-1.771229	-0.751648	-0.006571
C	-3.930135	-1.456721	-0.009935
C	-3.965426	-0.106939	-0.007396
C	-2.593123	0.319332	-0.005642
C	-2.072512	1.615045	-0.001294
C	-2.698026	2.886310	0.000311
C	-1.709698	3.830895	0.003400
C	-0.461311	3.153250	0.003384
N	-0.730853	1.842226	0.000579
C	0.831792	3.745990	0.006268
C	2.077156	3.190879	0.006777
C	2.529918	1.834024	0.004961
C	3.927634	1.457413	0.006474
C	3.963000	0.107925	0.003872
C	2.590361	-0.318563	0.000682
N	1.768504	0.752195	0.001447
H	-0.001260	1.146742	0.000360
H	-1.829033	4.894304	0.005546
H	-3.753994	3.055890	-0.000487
H	0.803407	4.820207	0.008098
H	2.882546	3.903741	0.009307
H	4.757010	2.135346	0.009143
H	4.824306	-0.527315	0.004106
H	3.751508	-3.054801	-0.002778
H	1.826278	-4.893548	-0.009281
H	-0.806070	-4.819730	-0.012850
H	-2.885021	-3.903415	-0.013772
H	-4.759696	-2.134436	-0.011889
H	-4.826851	0.528146	-0.006759

porphine S_0

N	-0.000001	2.042314	0.023541

N	0.000000	0.000000	2.089283
C	0.000001	2.828326	1.056648
C	0.000005	4.241536	0.664795
C	-0.000002	2.405611	2.427989
C	-0.000002	1.128736	2.854355
C	-0.000005	0.664705	4.241744
H	0.000007	5.072830	1.339905
H	-0.000004	3.174081	3.176654
H	-0.000007	1.320750	5.087397
H	0.000002	0.000000	1.097020
N	-0.000001	-2.042314	0.023541
N	0.000004	0.000000	-2.099306
C	0.000001	-2.828326	1.056648
C	0.000002	-2.859196	-1.094559
C	0.000002	2.859196	-1.094559
C	0.000005	-4.241536	0.664795
C	0.000006	-4.254021	-0.667305
C	0.000006	4.254021	-0.667305
C	-0.000002	-2.405611	2.427989
C	0.000002	-2.449038	-2.377176
C	0.000002	2.449038	-2.377176
C	-0.000002	-1.128736	2.854355
C	-0.000001	-1.110260	-2.871546
C	-0.000001	1.110260	-2.871546
C	-0.000005	-0.664705	4.241744
C	-0.000010	-0.695568	-4.195676
C	-0.000010	0.695568	-4.195676
H	0.000007	-5.072830	1.339905
H	0.000009	-5.100349	-1.324015
H	0.000009	5.100349	-1.324015
H	-0.000004	-3.174081	3.176654
H	0.000005	-3.210066	-3.135666
H	0.000005	3.210066	-3.135666
H	-0.000007	-1.320750	5.087397
H	-0.000015	-1.343120	-5.047561
H	-0.000015	1.343120	-5.047561
H	0.000011	0.000000	-1.106047

porphine S_1

N	0.000054	2.041297	-0.002699
N	-0.000046	-0.000004	2.091690
C	0.000012	2.844784	1.072619
C	0.000047	4.246404	0.664600
C	0.000036	2.429051	2.399730
C	0.000017	1.119249	2.860882

C	-0.000003	0.679450	4.216848
H	0.000314	5.084797	1.330910
H	0.000136	3.193311	3.153288
H	-0.000061	1.331464	5.065287
H	-0.000167	-0.000159	1.098371
N	-0.000006	-2.041301	-0.002670
N	0.000164	-0.000033	-2.097258
C	-0.000044	-2.844705	1.072636
C	-0.000014	-2.844688	-1.078097
C	0.000015	2.844708	-1.078054
C	-0.000052	-4.246274	0.664672
C	0.000010	-4.246251	-0.670201
C	-0.000131	4.246376	-0.670199
C	-0.000064	-2.428952	2.399838
C	-0.000012	-2.428970	-2.405285
C	-0.000003	2.429004	-2.405207
C	0.000013	-1.119300	2.861081
C	0.000011	-1.119310	-2.866621
C	0.000018	1.119293	-2.866460
C	0.000018	-0.679327	4.216947
C	-0.000061	-0.679361	-4.222506
C	0.000007	0.679456	-4.222402
H	-0.000094	-5.084998	1.330569
H	0.000074	-5.084993	-1.336104
H	-0.000442	5.084761	-1.336543
H	-0.000262	-3.193464	3.153146
H	0.000053	-3.193672	-3.158408
H	0.000034	3.193486	-3.158554
H	0.000021	-1.331181	5.065513
H	-0.000143	-1.331556	-5.070807
H	0.000142	1.331783	-5.070605
H	0.000407	-0.000175	-1.103946

chlorin S_0

C	0.000000	4.236937	0.732878
C	0.000000	2.855212	1.209525
N	0.000000	2.078559	0.073814
C	0.000000	2.833890	-1.050294
C	0.000000	4.227526	-0.595589
C	0.000000	2.436490	2.480368
C	0.000000	1.059708	2.917346
N	0.000000	0.030837	2.125441
C	0.000000	-1.088571	2.938465
C	0.000000	-0.670963	4.325197
C	0.000000	0.668192	4.319290

C	0.000000	-2.373527	2.512413
C	0.000000	-2.865591	1.185520
N	0.000000	-2.092758	0.057725
C	0.000000	-2.865535	-1.040934
C	0.000000	-4.189610	-0.623408
C	0.000000	-4.185360	0.769102
C	0.000000	-2.384596	-2.401244
C	0.000000	-1.126842	-2.845181
C	0.000000	-0.755094	-4.320351
C	0.000000	0.774552	-4.281953
C	0.000000	1.063396	-2.794841
N	0.000000	0.016071	-2.052804
C	0.000000	2.419049	-2.336801
H	0.873747	-1.153303	-4.820031
H	0.000000	-3.163832	-3.141468
H	0.000000	-5.042093	-1.269569
H	0.000000	-1.329091	5.170707
H	0.000000	1.337886	5.155004
H	0.873121	1.213998	-4.750431
H	0.000000	-3.134138	3.272242
H	0.000000	3.189702	3.245081
H	0.000000	3.182919	-3.090369
H	0.000000	-5.037027	1.417859
H	0.000000	5.088918	1.381023
H	0.000000	5.067246	-1.258948
H	-0.873121	1.213998	-4.750431
H	-0.873748	-1.153303	-4.820031
H	0.000000	1.086976	0.089271
H	0.000000	-1.101228	0.056114

chlorin S_1

C	0.000212	4.202302	0.742931
C	0.000276	2.851816	1.190864
N	0.000064	2.075799	0.061848
C	-0.000046	2.838515	-1.051235
C	0.000162	4.197542	-0.616607
C	0.000364	2.395111	2.494751
C	0.000275	1.065828	2.917674
N	0.000113	-0.009624	2.114977
C	0.000033	-1.082887	2.920492
C	-0.000116	-0.675656	4.317657
C	0.000222	0.662266	4.315875
C	-0.000174	-2.413282	2.501095
C	-0.000226	-2.873386	1.198409
N	-0.000097	-2.100559	0.067230

C	-0.000096	-2.866346	-1.043704
C	-0.000276	-4.224213	-0.605282
C	-0.000419	-4.225136	0.754236
C	0.000149	-2.417480	-2.368251
C	0.000318	-1.110328	-2.809767
C	0.001029	-0.782260	-4.289818
C	-0.000876	0.745801	-4.291813
C	-0.000265	1.077729	-2.812612
N	0.000026	-0.015317	-2.041908
C	-0.000237	2.386014	-2.374558
H	0.875490	-1.202348	-4.772155
H	0.000234	-3.186286	-3.117252
H	-0.000257	-5.070787	-1.259446
H	-0.000540	-1.340144	5.157590
H	0.000426	1.328955	5.154067
H	0.871525	1.167011	-4.776858
H	-0.000266	-3.166509	3.266059
H	0.000434	3.150280	3.257806
H	-0.000486	3.152824	-3.125611
H	-0.000673	-5.075337	1.404531
H	0.000081	5.054311	1.390852
H	0.000334	5.042256	-1.273177
H	-0.875311	1.164614	-4.775308
H	-0.871331	-1.204753	-4.773820
H	-0.000064	1.083332	0.070471
H	-0.000014	-1.108070	0.072957

Zn-tetraphenylporphine S_0

C	-3.993804	-3.868162	1.093851
C	-3.477445	-3.381828	-0.098931
C	-3.963839	-3.901804	-1.289958
C	-4.943191	-4.879008	-1.290596
C	-5.451288	-5.353436	-0.095830
C	-4.973127	-4.845217	1.097526
C	-2.411301	-2.320942	-0.100723
C	-2.797102	-1.003893	-0.129261
N	-1.990555	0.089228	-0.136279
C	-2.780867	1.196890	-0.165847
C	-4.182837	0.769931	-0.178622
C	-4.192847	-0.556877	-0.156701
C	-2.374554	2.505568	-0.181984
C	-3.423191	3.583272	-0.214533
C	-3.898714	4.074911	-1.421834
C	-4.861390	5.067950	-1.453930
C	-5.363165	5.586834	-0.275031

C	-4.895766	5.106765	0.934081
C	-3.932763	4.113939	0.961987
C	-1.057555	-2.757507	-0.070863
N	0.017070	-1.979853	-0.067042
C	1.131041	-2.796360	-0.033684
C	0.680728	-4.169799	-0.015831
C	-0.657480	-4.151320	-0.038981
C	2.434357	-2.387521	-0.020725
C	3.498235	-3.449760	0.015871
C	4.014414	-3.970769	-1.160350
C	4.992794	-4.947862	-1.127594
C	5.468745	-5.413938	0.083619
C	4.960853	-4.897512	1.260972
C	3.982639	-3.920327	1.226379
C	-1.012097	2.923624	-0.169151
N	0.049591	2.129411	-0.140643
C	1.175818	2.928870	-0.138126
C	0.748513	4.307238	-0.167754
C	-0.591325	4.309332	-0.186688
C	2.474029	2.498305	-0.112224
C	3.553916	3.544944	-0.116403
C	4.075394	4.013940	-1.311931
C	5.068574	4.976528	-1.316765
C	5.553745	5.480014	-0.124345
C	5.040275	5.015545	1.072096
C	4.047157	4.052923	1.075215
C	2.906616	1.142126	-0.081192
N	2.095554	0.058347	-0.071209
C	2.888683	-1.035513	-0.039793
C	4.246663	-0.639116	-0.029572
C	4.257626	0.723930	-0.055742
H	5.113763	1.363045	-0.057287
H	1.398646	5.155535	-0.173137
H	-5.022989	1.429676	-0.201394
H	-5.042679	-1.204457	-0.157695
H	5.092153	-1.291760	-0.006006
H	-1.243145	5.155048	-0.210186
H	-1.323048	-4.986601	-0.035191
H	1.317692	-5.027640	0.010635
H	-3.513041	3.676421	-2.342261
H	-5.218009	5.434640	-2.398992
H	-6.111318	6.357592	-0.298300
H	-5.279522	5.503524	1.856090
H	-3.573241	3.746425	1.905596
H	3.702948	3.624815	-2.241528
H	5.461733	5.331429	-2.251642

H	6.325588	6.227315	-0.127422
H	5.411373	5.400929	2.003917
H	3.652606	3.694268	2.007941
H	3.649451	-3.610622	-2.104489
H	5.381633	-5.343311	-2.047898
H	6.228992	-6.172592	0.109762
H	5.324539	-5.253802	2.207188
H	3.592972	-3.520791	2.144437
H	-3.573422	-3.537853	-2.222618
H	-5.307482	-5.268314	-2.223621
H	-6.212639	-6.111516	-0.094654
H	-5.361103	-5.207931	2.031721
H	-3.626666	-3.477759	2.025286
Zn	0.048469	0.074087	-0.103258

Zn-tetraphenylporphine S_1

C	-3.994186	-3.991565	1.193058
C	-3.492014	-3.493210	-0.000028
C	-3.994192	-3.991684	-1.193060
C	-4.974370	-4.967858	-1.194496
C	-5.467148	-5.458762	0.000075
C	-4.974359	-4.967744	1.194595
C	-2.427179	-2.433447	-0.000084
C	-2.851542	-1.093644	-0.000091
N	-2.049390	0.000806	-0.000092
C	-2.850369	1.096168	-0.000051
C	-4.226596	0.675547	-0.000041
C	-4.227307	-0.671554	-0.000049
C	-2.424578	2.435445	-0.000025
C	-3.488242	3.496382	0.000007
C	-3.989883	3.995359	-1.193039
C	-4.969016	4.972582	-1.194496
C	-5.461247	5.464061	0.000064
C	-4.969017	4.972511	1.194597
C	-3.989882	3.995292	1.193084
C	-1.097832	-2.853120	-0.000094
N	-0.001152	-2.053295	-0.000121
C	1.094712	-2.854332	-0.000105
C	0.667173	-4.239148	-0.000051
C	-0.671824	-4.238410	-0.000061
C	2.424457	-2.436108	-0.000103
C	3.488160	-3.497005	-0.000034
C	3.989803	-3.996024	-1.193062
C	4.969041	-4.973141	-1.194484
C	5.461362	-5.464487	0.000093

C	4.969079	-4.972949	1.194608
C	3.989837	-3.995835	1.193059
C	-1.094718	2.853732	-0.000028
N	0.001076	2.052754	-0.000066
C	1.097774	2.852563	-0.000025
C	0.671796	4.237799	0.000021
C	-0.667261	4.238511	0.000022
C	2.427139	2.432841	-0.000027
C	3.491972	3.492603	0.000005
C	3.994205	3.990979	-1.193042
C	4.974568	4.966968	-1.194498
C	5.467414	5.457829	0.000063
C	4.974535	4.966930	1.194595
C	3.994176	3.990939	1.193083
C	2.851516	1.093074	-0.000048
N	2.049352	-0.001416	-0.000100
C	2.850313	-1.096721	-0.000129
C	4.226495	-0.676153	-0.000044
C	4.227251	0.670982	-0.000081
H	5.075064	1.321011	-0.000201
H	1.323906	5.083967	0.000058
H	-5.073696	1.326503	-0.000043
H	-5.075128	-1.321574	-0.000006
H	5.073618	-1.327087	0.000113
H	-1.318468	5.085377	0.000057
H	-1.324271	-5.084317	-0.000051
H	1.318687	-5.085773	0.000008
H	-3.611692	3.616790	-2.124796
H	-5.345724	5.348274	-2.128097
H	-6.221626	6.223061	0.000087
H	-5.345732	5.348143	2.128219
H	-3.611683	3.616676	2.124818
H	3.615470	3.612957	-2.124800
H	5.351765	5.342171	-2.128099
H	6.228795	6.215824	0.000086
H	5.351703	5.342108	2.128218
H	3.615421	3.612881	2.124817
H	3.611508	-3.617595	-2.124833
H	5.345813	-5.348803	-2.128073
H	6.221871	-6.223357	0.000143
H	5.345885	-5.348456	2.128245
H	3.611567	-3.617262	2.124781
H	-3.615612	-3.613532	-2.124828
H	-5.351496	-5.343152	-2.128090
H	-6.228389	-6.216897	0.000116
H	-5.351471	-5.342954	2.128228

H	-3.615609	-3.613314	2.124786
Zn	-0.000017	-0.000581	-0.000114

tetraphenylporphine S_0

C	0.238368	4.740425	-0.121451
C	-0.309614	3.399101	-0.336874
N	0.739952	2.541011	-0.146940
C	1.891504	3.212075	0.165502
C	1.527196	4.630932	0.172670
C	3.115810	2.702290	0.417097
C	3.427307	1.287230	0.397428
N	2.595364	0.323091	0.142676
C	3.320041	-0.861851	0.233845
C	4.703976	-0.542905	0.573697
C	4.777042	0.780313	0.675926
C	2.847094	-2.113322	0.043308
C	1.493629	-2.472155	-0.294369
N	0.464840	-1.608019	-0.483873
C	-0.668949	-2.288393	-0.788322
C	-0.351783	-3.637465	-0.793562
C	0.997976	-3.752120	-0.485604
C	-1.958817	-1.705029	-1.054140
C	-2.260497	-0.387848	-1.039776
N	-1.387821	0.661555	-0.766433
C	-2.081888	1.755218	-0.860224
C	-3.481921	1.481577	-1.208590
C	-3.584878	0.160905	-1.317894
C	-1.587025	3.101787	-0.656102
H	-4.454926	-0.410262	-1.560943
C	-3.049202	-2.689607	-1.373697
H	-1.030724	-4.435809	-0.997927
H	0.531672	-0.620360	-0.408687
H	5.489886	-1.254533	0.708702
H	5.632365	1.375624	0.911044
H	-4.247597	2.214367	-1.342800
C	3.794799	-3.271073	0.191264
C	4.233275	3.655620	0.737036
C	-2.564796	4.232920	-0.812232
H	1.561134	-4.655903	-0.407409
H	2.213792	5.421453	0.384353
H	-0.335786	5.638048	-0.197436
H	0.674005	1.554799	-0.225617
C	4.493304	-3.752780	-0.904643
C	5.366075	-4.817056	-0.769166
C	5.546493	-5.414614	0.464316

C	4.849167	-4.942774	1.560645
C	3.976889	-3.878158	1.423758
H	4.355947	-3.291644	-1.865272
H	5.904235	-5.177208	-1.626610
H	6.224864	-6.240949	0.570268
H	4.982894	-5.401632	2.522982
H	3.436265	-3.515311	2.278387
C	-3.271578	-3.093441	-2.680847
C	-4.274482	-3.999027	-2.975433
C	-5.063809	-4.514484	-1.964418
C	-4.844394	-4.120260	-0.657942
C	-3.841094	-3.214511	-0.364570
H	-2.660106	-2.695966	-3.469833
H	-4.438318	-4.299928	-3.993846
H	-5.843185	-5.217767	-2.192885
H	-5.452768	-4.516405	0.134200
H	-3.673026	-2.912095	0.652608
C	-2.757309	4.839336	-2.045406
C	-3.660345	5.877077	-2.192089
C	-4.389085	6.321997	-1.104910
C	-4.207891	5.724002	0.128192
C	-3.303176	4.687204	0.271234
H	-2.196207	4.496273	-2.895269
H	-3.793011	6.336714	-3.154326
H	-5.091896	7.126772	-1.217690
H	-4.769736	6.062847	0.979237
H	-3.167500	4.226356	1.232484
C	5.031570	4.177071	-0.271089
C	6.063673	5.050491	0.021826
C	6.314899	5.413802	1.331743
C	5.528130	4.898735	2.344986
C	4.496742	4.025788	2.048169
H	4.842931	3.897079	-1.291292
H	6.669659	5.445700	-0.772746
H	7.116328	6.091715	1.560812
H	5.715743	5.175092	3.366352
H	3.889810	3.627993	2.840739

tetraphenylporphine S_1

C	-0.677738	4.212363	0.000219
C	-1.122135	2.857072	0.000110
N	0.000099	2.084468	0.000049
C	1.122126	2.856993	0.000146
C	0.677867	4.212357	0.000249
C	2.446583	2.416638	0.000106

C	2.853458	1.077393	0.000044
N	2.048154	-0.000776	0.000081
C	2.853450	-1.078998	0.000020
C	4.254145	-0.667174	-0.000081
C	4.254145	0.665544	-0.000112
C	2.446563	-2.418153	0.000086
C	1.122102	-2.858537	0.000179
N	0.000072	-2.086054	0.000081
C	-1.122177	-2.858627	0.000206
C	-0.677795	-4.213863	0.000431
C	0.677856	-4.213855	0.000407
C	-2.446446	-2.418227	0.000134
C	-2.853518	-1.078927	0.000044
N	-2.048130	-0.000774	0.000101
C	-2.853459	1.077376	0.000002
C	-4.253989	0.665664	-0.000185
C	-4.254034	-0.667170	-0.000121
C	-2.446358	2.416701	0.000038
H	-5.097063	-1.323498	-0.000184
C	-3.507496	-3.481551	0.000090
H	-1.322466	-5.065111	0.000584
H	0.000067	-1.093308	-0.000064
H	5.097035	-1.323682	-0.000106
H	5.097089	1.321980	-0.000275
H	-5.097034	1.321968	-0.000377
C	3.507487	-3.481574	-0.000055
C	3.507551	3.480028	0.000085
C	-3.507414	3.480022	-0.000047
H	1.322590	-5.065046	0.000535
H	1.322891	5.063325	0.000338
H	-1.322699	5.063388	0.000266
H	0.000096	1.091723	-0.000042
C	4.006015	-3.982115	-1.193557
C	4.984059	-4.960377	-1.194966
C	5.475995	-5.451982	-0.000305
C	4.984489	-4.960249	1.194482
C	4.006446	-3.981986	1.193321
H	3.627887	-3.602582	-2.124925
H	5.360508	-5.336408	-2.128509
H	6.235886	-6.211471	-0.000400
H	5.361264	-5.336190	2.127929
H	3.628645	-3.602362	2.124784
C	-4.006077	-3.982104	-1.193378
C	-4.984231	-4.960257	-1.194696
C	-5.476161	-5.451758	0.000009
C	-4.984621	-4.959964	1.194754

C	-4.006462	-3.981816	1.193517
H	-3.627911	-3.602680	-2.124774
H	-5.360748	-5.336304	-2.128204
H	-6.236056	-6.211243	-0.000022
H	-5.361450	-5.335775	2.128231
H	-3.628571	-3.602194	2.124944
C	-4.006107	3.980421	-1.193534
C	-4.984590	4.958246	-1.194892
C	-5.476694	5.449622	-0.000208
C	-4.985008	4.958022	1.194557
C	-4.006507	3.980214	1.193358
H	-3.627805	3.601099	-2.124915
H	-5.361109	5.334252	-2.128417
H	-6.236765	6.208931	-0.000270
H	-5.361884	5.333823	2.128019
H	-3.628483	3.600765	2.124801
C	4.006252	3.980539	-1.193360
C	4.984540	4.958560	-1.194662
C	5.476483	5.450026	0.000053
C	4.984840	4.958299	1.194783
C	4.006567	3.980264	1.193514
H	3.628099	3.601136	-2.124769
H	5.361097	5.334585	-2.128164
H	6.236399	6.209490	0.000040
H	5.361609	5.334143	2.128273
H	3.628685	3.600619	2.124935

CIS/TZVP geometries – Group II

tetrafluorobenzene S_0

C	-1.184138	0.687535	0.000000
C	-1.184138	-0.687535	0.000000
C	0.000000	-1.385263	0.000000
C	1.184138	-0.687535	0.000000
C	1.184138	0.687535	0.000000
C	0.000000	1.385263	0.000000
F	-2.327895	-1.338482	0.000000
H	0.000000	-2.457630	0.000000
F	2.327895	-1.338482	0.000000
F	2.327895	1.338482	0.000000
H	0.000000	2.457630	0.000000
F	-2.327895	1.338482	0.000000

tetrafluorobenzene S_1

C	1.163878	-0.704358	0.096236
C	1.163878	0.704358	0.096236
C	0.000000	1.451411	0.288401
C	-1.163878	0.704358	0.096236
C	-1.163878	-0.704358	0.096236
C	0.000000	-1.451411	0.288401
F	2.296001	1.310623	-0.150438
H	0.000000	2.496649	0.518126
F	-2.296001	1.310623	-0.150438
F	-2.296001	-1.310623	-0.150438
H	0.000000	-2.496649	0.518126
F	2.296001	-1.310623	-0.150438

benzonitrile S_0

C	0.000000	0.000000	-1.045841
C	-1.203930	0.000000	-0.356787
C	-1.199689	0.000000	1.023288
C	0.000000	0.000000	1.712111
C	1.199689	0.000000	1.023288
C	1.203930	0.000000	-0.356787
H	-2.129423	0.000000	-0.900005
H	-2.129730	0.000000	1.559299
H	0.000000	0.000000	2.786056
H	2.129730	0.000000	1.559299
H	2.129423	0.000000	-0.900005
C	0.000000	0.000000	-2.487747
N	0.000000	0.000000	-3.616159

benzonitrile S_1

C	0.000000	0.000000	-1.089630
C	-1.219457	0.000000	-0.371095
C	-1.211706	0.000000	1.039983
C	0.000000	0.000000	1.753539
C	1.211706	0.000000	1.039983
C	1.219457	0.000000	-0.371095
H	-2.150596	0.000000	-0.901941
H	-2.146503	0.000000	1.565245
H	0.000000	0.000000	2.824748
H	2.146503	0.000000	1.565245
H	2.150596	0.000000	-0.901941
C	0.000000	0.000000	-2.510024
N	0.000000	0.000000	-3.643018

o-fluorophenol, *cis* S_0

C	0.325180	1.444103	0.000000
C	-0.870657	0.773818	0.000000
C	-0.946457	-0.603976	0.000000
C	0.231893	-1.324813	0.000000
C	1.446673	-0.666489	0.000000
C	1.500275	0.715269	0.000000
F	-2.020305	1.454497	0.000000
O	-2.124930	-1.254443	0.000000
H	0.177981	-2.396702	0.000000
H	2.355210	-1.238854	0.000000
H	2.445116	1.224109	0.000000
H	0.323962	2.517486	0.000000
H	-2.843929	-0.644025	0.000000

o-fluorophenol, *cis* S_1

C	1.232849	-0.209328	-0.749934
C	0.007874	0.041548	-0.093731
C	-0.029581	-0.018457	1.362581
C	1.146866	0.117642	2.079403
C	2.345430	0.129461	1.394763
C	2.379746	-0.075140	-0.010011
F	-0.813199	0.979989	-0.641996
O	-1.163527	-0.292113	1.986872
H	1.117515	0.069892	3.153031
H	3.268801	0.219667	1.933762
H	3.335130	-0.113945	-0.502429
H	1.267751	-0.362366	-1.812282
H	-1.840274	-0.486851	1.349911

o-fluorophenol, *trans* S_0

C	0.286179	1.255124	0.000000
C	-0.940035	0.612370	0.000000
C	-0.956084	-0.768483	0.000000
C	0.227837	-1.486829	0.000000
C	1.439322	-0.829822	0.000000
C	1.464103	0.555418	0.000000
O	-2.051273	1.373105	0.000000
H	-1.900238	-1.284372	0.000000
H	0.193289	-2.559997	0.000000
H	2.359873	-1.381413	0.000000
H	2.388546	1.101146	0.000000
F	0.313218	2.577822	0.000000

H	-2.824746	0.835932	0.000000

o-fluorophenol, *trans* S_1

C	0.820928	1.032082	0.083764
C	-0.579335	0.973500	0.068808
C	-1.260560	-0.297462	0.114992
C	-0.473477	-1.429403	-0.054454
C	0.930447	-1.339056	-0.072774
C	1.606158	-0.113538	0.127140
O	-1.251338	2.094500	-0.113164
H	-2.291343	-0.345571	0.411485
H	-0.929898	-2.397768	-0.136018
H	1.504609	-2.236789	-0.207124
H	2.670395	-0.048540	0.217912
F	1.391368	2.209689	-0.049520
H	-2.137985	1.898356	-0.391048

m-fluorophenol, *cis* S_0

C	0.308876	1.402711	0.000000
C	-0.921832	0.784396	0.000000
C	-0.962043	-0.598087	0.000000
C	0.212078	-1.334709	0.000000
C	1.421878	-0.675592	0.000000
C	1.491797	0.708482	0.000000
O	-2.124270	-1.278725	0.000000
F	0.338038	2.726550	0.000000
H	0.157500	-2.405823	0.000000
H	2.331233	-1.247179	0.000000
H	2.426578	1.233596	0.000000
H	-1.816511	1.379223	0.000000
H	-2.863322	-0.694842	0.000000

m-fluorophenol, *cis* S_1

C	1.229195	-0.017390	-0.689376
C	-0.027911	0.028632	-0.097249
C	-0.023573	0.020605	1.325334
C	1.163944	-0.000168	2.081553
C	2.415114	0.072902	1.437725
C	2.432577	-0.028787	0.029556
O	-1.165839	0.000388	1.997114
F	1.297193	-0.055165	-2.006427
H	1.077799	-0.067882	3.148122
H	3.326112	0.093145	1.997295

H	3.352393	-0.095143	-0.518487
H	-0.920463	0.170344	-0.672290
H	-1.901181	-0.121481	1.417080

m-fluorophenol, *trans* S_0

C	0.266447	1.294683	0.000000
C	-0.943865	0.622491	0.000000
C	-0.978756	-0.761539	0.000000
C	0.208644	-1.470495	0.000000
C	1.428177	-0.824808	0.000000
C	1.420392	0.552891	0.000000
O	-2.061309	1.374466	0.000000
H	-1.920678	-1.280058	0.000000
H	0.179270	-2.544149	0.000000
H	2.357833	-1.358921	0.000000
F	2.577825	1.194661	0.000000
H	0.299091	2.366180	0.000000
H	-2.833072	0.834606	0.000000

m-fluorophenol, *trans* S_1

C	1.068035	-0.016680	0.000000
C	0.322588	1.186064	0.000000
C	-1.091036	1.205139	0.000000
C	-1.810835	-0.005637	0.000000
C	-1.080795	-1.217337	0.000000
C	0.319472	-1.190648	0.000000
O	1.025558	2.309694	0.000000
H	-1.601529	2.150321	0.000000
H	-2.880456	-0.013064	0.000000
H	-1.576751	-2.168183	0.000000
F	0.961768	-2.343653	0.000000
H	2.136969	-0.011188	0.000000
H	0.465863	3.069318	0.000000

p-fluorophenol S_0

C	0.268541	1.305214	0.000000
C	-0.945827	0.640376	0.000000
C	-0.973711	-0.740460	0.000000
C	0.209283	-1.460937	0.000000
C	1.401166	-0.784719	0.000000
C	1.447884	0.590943	0.000000
O	-2.069663	1.394879	0.000000
H	-1.913493	-1.263655	0.000000

H	0.203102	-2.534109	0.000000
F	2.539792	-1.471715	0.000000
H	2.397596	1.090898	0.000000
H	0.276378	2.378161	0.000000
H	-2.841068	0.855113	0.000000

p-fluorophenol S_1

C	1.253911	0.674251	0.000000
C	0.022604	1.363750	0.000000
C	-1.231598	0.701503	0.000000
C	-1.241574	-0.700958	0.000000
C	-0.005779	-1.365169	0.000000
C	1.240989	-0.729674	0.000000
O	0.086377	2.683763	0.000000
H	-2.141540	1.269950	0.000000
H	-2.147048	-1.272262	0.000000
F	-0.024440	-2.675399	0.000000
H	2.136479	-1.315970	0.000000
H	2.162611	1.240397	0.000000
H	-0.774296	3.071413	0.000000

phenylacetylene S_0

C	1.199604	0.000000	-0.013134
C	0.000000	0.000000	-0.714140
C	-1.199604	0.000000	-0.013134
C	-1.197000	0.000000	1.367308
C	0.000000	0.000000	2.060171
C	1.197000	0.000000	1.367308
C	0.000000	0.000000	-2.154070
C	0.000000	0.000000	-3.337778
H	-2.126836	0.000000	-0.553597
H	-2.128742	0.000000	1.901356
H	0.000000	0.000000	3.134206
H	2.128742	0.000000	1.901356
H	2.126836	0.000000	-0.553597
H	0.000000	0.000000	-4.392274

phenylacetylene S_1

C	1.240007	0.000000	-0.004572
C	0.000000	0.000000	-0.749582
C	-1.240007	0.000000	-0.004572
C	-1.218229	0.000000	1.358853
C	0.000000	0.000000	2.061997

C	1.218229	0.000000	1.358853
C	0.000000	0.000000	-2.118564
C	0.000000	0.000000	-3.350419
H	-2.165002	0.000000	-0.547583
H	-2.142240	0.000000	1.906256
H	0.000000	0.000000	3.135295
H	2.142240	0.000000	1.906256
H	2.165002	0.000000	-0.547583
H	0.000000	0.000000	-4.404634

aniline S_0

C	0.914102	0.035741	0.000000
C	0.205928	0.040823	1.195653
C	-1.174574	0.042175	1.189750
C	-1.879108	0.043237	0.000000
C	-1.174574	0.042175	-1.189750
C	0.205928	0.040823	-1.195653
H	0.738958	0.046205	2.129681
H	-2.952648	0.044134	0.000000
H	-1.702722	0.044109	2.125929
H	-1.702722	0.044109	-2.125929
H	0.738958	0.046205	-2.129681
N	2.308240	0.083285	0.000000
H	2.737123	-0.276505	-0.822090
H	2.737123	-0.276505	0.822090

aniline S_1

C	0.907674	-0.034655	0.000000
C	0.218746	-0.008286	1.242442
C	-1.185796	0.045329	1.230458
C	-1.864187	0.071200	0.000000
C	-1.185796	0.045329	-1.230458
C	0.218746	-0.008286	-1.242442
H	0.777265	-0.029618	2.158010
H	-2.937506	0.112083	0.000000
H	-1.738728	0.066448	2.147942
H	-1.738728	0.066448	-2.147942
H	0.777265	-0.029618	-2.158010
N	2.244756	-0.085869	0.000000
H	2.753139	-0.105262	-0.850465
H	2.753139	-0.105262	0.850465

catechol S_0

C	0.467510	1.270066	0.000000
C	-0.744621	0.619153	0.000000
C	-0.795681	-0.768410	0.000000
C	0.376866	-1.489606	0.000000
C	1.598242	-0.836258	0.000000
C	1.646443	0.541422	0.000000
O	-1.948807	1.255143	0.000000
O	-1.977527	-1.417535	0.000000
H	0.319349	-2.561585	0.000000
H	2.506161	-1.409516	0.000000
H	2.589208	1.054946	0.000000
H	0.494297	2.345936	0.000000
H	-1.845198	2.190711	0.000000
H	-2.686243	-0.794467	0.000000

catechol S_1

C	0.469694	1.333616	0.000000
C	-0.755959	0.631002	0.000000
C	-0.804486	-0.776122	0.000000
C	0.383474	-1.553739	0.000000
C	1.593490	-0.856463	0.000000
C	1.638262	0.554716	0.000000
O	-1.947913	1.252820	0.000000
O	-1.970974	-1.409238	0.000000
H	0.318142	-2.621104	0.000000
H	2.519690	-1.398053	0.000000
H	2.595423	1.039844	0.000000
H	0.494518	2.404981	0.000000
H	-1.845913	2.189925	0.000000
H	-2.687449	-0.792185	0.000000

resorcinol, isomer 1 S_0

C	0.072561	1.140292	0.000000
C	-1.133734	0.459619	0.000000
C	-1.164461	-0.921551	0.000000
C	0.035206	-1.615144	0.000000
C	1.245694	-0.961240	0.000000
C	1.253816	0.426430	0.000000
O	-2.255072	1.209193	0.000000
H	-2.101948	-1.447832	0.000000
H	0.018083	-2.689528	0.000000
H	2.175947	-1.494624	0.000000
O	2.454103	1.039360	0.000000
H	0.066654	2.214950	0.000000

H	-3.022983	0.663973	0.000000
H	2.356134	1.976094	0.000000

resorcinol, isomer 1 S_1

C	-0.004473	1.039645	0.119709
C	-1.191854	0.300811	0.017841
C	-1.198644	-1.112275	-0.033723
C	0.000507	-1.836874	0.114115
C	1.202607	-1.105645	-0.022701
C	1.188412	0.303105	0.021506
O	-2.329001	0.995699	-0.029681
H	-2.136032	-1.621482	-0.173032
H	0.002543	-2.906059	0.132206
H	2.147673	-1.594126	-0.162845
O	2.372089	0.915617	-0.038927
H	-0.025779	2.103028	0.246005
H	-3.080075	0.425852	-0.046472
H	2.263020	1.848827	-0.124352

resorcinol, isomer 2 S_0

C	1.191286	0.000000	-0.541124
C	0.000000	0.000000	-1.238879
C	-1.191286	0.000000	-0.541124
C	-1.203479	0.000000	0.845905
C	0.000000	0.000000	1.521843
C	1.203479	0.000000	0.845905
O	-2.327452	0.000000	-1.266717
O	2.327452	0.000000	-1.266717
H	-2.134133	0.000000	1.384177
H	0.000000	0.000000	2.596331
H	2.134133	0.000000	1.384177
H	0.000000	0.000000	-2.310912
H	-3.084478	0.000000	-0.706673
H	3.084478	0.000000	-0.706673

resorcinol, isomer 2 S_1

C	1.194456	0.000000	-0.326711
C	0.000000	0.000000	-1.062097
C	-1.194456	0.000000	-0.326711
C	-1.208921	0.000000	1.087762
C	0.000000	0.000000	1.814857
C	1.208921	0.000000	1.087762
O	-2.331630	0.000000	-1.026423

O	2.331630	0.000000	-1.026423
H	-2.152973	0.000000	1.601482
H	0.000000	0.000000	2.884567
H	2.152973	0.000000	1.601482
H	0.000000	0.000000	-2.131084
H	-3.084102	0.000000	-0.458774
H	3.084102	0.000000	-0.458774

resorcinol, isomer 3 S_0

C	1.196800	0.000000	-0.287090
C	0.000000	0.000000	-0.984729
C	-1.196800	0.000000	-0.287090
C	-1.206556	0.000000	1.094951
C	0.000000	0.000000	1.766625
C	1.206556	0.000000	1.094951
O	-2.386886	0.000000	-0.921889
O	2.386886	0.000000	-0.921889
H	-2.143470	0.000000	1.616551
H	0.000000	0.000000	2.841170
H	2.143470	0.000000	1.616551
H	0.000000	0.000000	-2.061987
H	2.275681	0.000000	-1.856823
H	-2.275681	0.000000	-1.856823

resorcinol, isomer 3 S_1

C	-0.032943	-0.303105	1.189630
C	-0.158965	-1.047721	0.000000
C	-0.032943	-0.303105	-1.189630
C	0.114075	1.098345	-1.197979
C	0.043291	1.835151	0.000000
C	0.114075	1.098345	1.197979
O	-0.032943	-0.911755	-2.375722
O	-0.032943	-0.911755	2.375722
H	0.283384	1.574999	-2.144727
H	0.100286	2.902975	0.000000
H	0.283384	1.574999	2.144727
H	-0.563801	-2.043488	0.000000
H	0.072143	-1.844434	2.269995
H	0.072143	-1.844434	-2.269995

hydroquinone, *cis* S_0

C	-0.694287	0.000000	1.084628
C	0.694287	0.000000	1.084628

C	1.387977	0.000000	-0.103938
C	0.687607	0.000000	-1.300157
C	-0.687607	0.000000	-1.300157
C	-1.387977	0.000000	-0.103938
O	2.743743	0.000000	-0.170091
O	-2.743743	0.000000	-0.170091
H	1.234548	0.000000	-2.223739
H	-1.234548	0.000000	-2.223739
H	-1.222271	0.000000	2.022185
H	1.222271	0.000000	2.022185
H	-3.123003	0.000000	0.691402
H	3.123003	0.000000	0.691402

hydroquinone, *cis* S_1

C	0.700238	0.000000	-1.128155
C	-0.700238	0.000000	-1.128155
C	-1.376455	0.000000	0.116264
C	-0.700927	0.000000	1.348985
C	0.700927	0.000000	1.348985
C	1.376455	0.000000	0.116264
O	-2.701442	0.000000	0.160713
O	2.701442	0.000000	0.160713
H	-1.273723	0.000000	2.253690
H	1.273723	0.000000	2.253690
H	1.260068	0.000000	-2.044018
H	-1.260068	0.000000	-2.044018
H	3.072490	0.000000	-0.706708
H	-3.072490	0.000000	-0.706708

hydroquinone, *trans* S_0

C	0.016827	1.379574	0.000000
C	-1.191033	0.712685	0.000000
C	-1.202153	-0.669565	0.000000
C	-0.016827	-1.379574	0.000000
C	1.191033	-0.712685	0.000000
C	1.202153	0.669565	0.000000
O	-2.325987	1.457698	0.000000
H	-2.137135	-1.202344	0.000000
H	-0.022892	-2.452866	0.000000
O	2.325987	-1.457698	0.000000
H	2.137135	1.202344	0.000000
H	0.022892	2.452866	0.000000
H	-3.089595	0.907335	0.000000
H	3.089595	-0.907335	0.000000

hydroquinone, *trans* S_1

C	1.251077	0.672915	0.000000
C	0.030374	1.375869	0.000000
C	-1.225420	0.728121	0.000000
C	-1.251077	-0.672915	0.000000
C	-0.030374	-1.375869	0.000000
C	1.225420	-0.728121	0.000000
O	0.110451	2.699301	0.000000
H	-2.130424	1.304964	0.000000
H	-2.166249	-1.229198	0.000000
O	-0.110451	-2.699301	0.000000
H	2.130424	-1.304964	0.000000
H	2.166249	1.229198	0.000000
H	-0.747260	3.092448	0.000000
H	0.747260	-3.092448	0.000000

salicylic acid S_0

C	1.093627	1.588646	0.000000
C	1.127369	0.195888	0.000000
C	-0.075113	-0.517079	0.000000
C	-1.286005	0.182690	0.000000
C	-1.313018	1.551093	0.000000
C	-0.107059	2.248848	0.000000
O	2.325075	-0.378241	0.000000
C	-0.049343	-1.987996	0.000000
O	-1.241992	-2.558694	0.000000
O	0.948983	-2.647176	0.000000
H	-2.201736	-0.374296	0.000000
H	2.026205	2.118696	0.000000
H	-2.247714	2.077601	0.000000
H	-0.114209	3.323476	0.000000
H	2.238825	-1.325075	0.000000
H	-1.123895	-3.498384	0.000000

salicylic acid S_1

C	1.001698	1.905713	0.000000
C	0.977776	0.507266	0.000000
C	-0.292801	-0.244894	0.000000
C	-1.455409	0.521609	0.000000
C	-1.400843	1.928497	0.000000
C	-0.188620	2.634168	0.000000
O	2.098957	-0.136861	0.000000

C	-0.251298	-1.669106	0.000000
O	-1.437990	-2.272396	0.000000
O	0.774064	-2.333830	0.000000
H	-2.409297	0.034384	0.000000
H	1.962117	2.383487	0.000000
H	-2.326280	2.472604	0.000000
H	-0.178486	3.704999	0.000000
H	1.925485	-1.091951	0.000000
H	-1.288493	-3.206744	0.000000

o-cresol, *cis* S_0

C	1.953582	0.508840	0.000000
C	0.725628	1.140762	0.000000
C	-0.463501	0.427608	0.000000
C	-0.387461	-0.960492	0.000000
C	0.834770	-1.606857	0.000000
C	2.002252	-0.872739	0.000000
C	-1.798694	1.132588	0.000000
O	-1.491859	-1.745608	0.000000
H	0.850118	-2.680200	0.000000
H	2.948544	-1.381477	0.000000
H	2.858135	1.087377	0.000000
H	0.685051	2.215270	0.000000
H	-2.280713	-1.233656	0.000000
H	-2.386964	0.881678	0.879051
H	-1.661925	2.205235	0.000000
H	-2.386964	0.881678	-0.879051

o-cresol, *cis* S_1

C	1.863404	-0.090020	-0.778872
C	0.626277	-0.076173	-1.449966
C	-0.579992	-0.051570	-0.715366
C	-0.473756	0.067851	0.698409
C	0.766211	0.081460	1.378052
C	1.943936	-0.021257	0.624079
C	-1.898817	-0.030045	-1.428030
O	-1.550023	0.157789	1.470448
H	0.765751	0.168304	2.445230
H	2.900498	-0.030878	1.107413
H	2.768356	-0.149311	-1.353443
H	0.598008	-0.134095	-2.520051
H	-2.344663	0.177471	0.964253
H	-2.698760	-0.503537	-0.865439
H	-2.218153	0.984752	-1.670219

H	-1.818857	-0.570231	-2.364087

o-cresol, *trans* S_0

C	2.406282	0.000015	0.030402
C	1.239505	-0.000039	-0.709937
C	0.033141	-0.000011	-0.015299
C	0.005166	0.000067	1.364752
C	1.189434	0.000108	2.081673
C	2.395564	0.000094	1.416657
C	1.248036	-0.000116	-2.216621
O	-1.103075	-0.000063	-0.754260
H	-0.939284	0.000092	1.881211
H	1.159203	0.000173	3.155566
H	3.319946	0.000134	1.963038
H	3.348096	-0.000007	-0.488304
H	-1.863845	-0.000048	-0.199741
H	2.264170	-0.000067	-2.589972
H	0.738240	-0.872407	-2.609558
H	0.738128	0.872074	-2.609636

o-cresol, *trans* S_1

C	2.425238	0.147782	-0.006540
C	1.221256	0.025504	-0.743477
C	0.010122	-0.068031	-0.010879
C	-0.034312	-0.095589	1.405201
C	1.176092	0.006760	2.102932
C	2.390506	0.111938	1.393837
C	1.251286	0.007149	-2.237016
O	-1.118154	-0.153692	-0.706555
H	-0.979589	-0.133749	1.911996
H	1.185991	-0.000489	3.175098
H	3.308392	0.178059	1.946821
H	3.359666	0.231676	-0.524919
H	-1.857958	-0.271529	-0.133098
H	1.873376	-0.813829	-2.591035
H	0.267043	-0.096612	-2.666238
H	1.699733	0.924652	-2.616148

m-cresol, *cis* S_0

C	1.155694	0.009572	2.075526
C	2.358090	0.040568	1.408482
C	2.408380	0.038989	0.021972
C	1.238914	0.005971	-0.713063

C	0.022551	-0.025385	-0.039381
C	-0.018903	-0.023618	1.339707
C	1.260787	0.003870	-2.221798
O	-1.182584	-0.053460	2.026759
H	1.104922	0.010392	3.147311
H	3.272694	0.066344	1.972239
H	3.358432	0.063470	-0.478606
H	-0.897313	-0.051320	-0.599850
H	-1.919412	-0.075991	1.440930
H	2.275697	0.026257	-2.596614
H	0.776973	-0.883740	-2.615404
H	0.737379	0.867452	-2.618260

m-cresol, *cis* S_1

C	1.162473	0.007249	2.108918
C	2.399564	0.043749	1.440449
C	2.408844	0.032910	0.033459
C	1.220582	0.006939	-0.736315
C	-0.018232	-0.035591	-0.068394
C	-0.022724	-0.020406	1.345147
C	1.264947	0.006342	-2.231823
O	-1.165176	-0.041866	2.020648
H	1.084672	0.005909	3.177618
H	3.319193	0.065591	1.988652
H	3.350958	0.052027	-0.481779
H	-0.945387	-0.046980	-0.610559
H	-1.905298	-0.073580	1.436400
H	2.281699	0.046853	-2.600445
H	0.793400	-0.888635	-2.634677
H	0.722767	0.858859	-2.637360

m-cresol, *trans* S_0

C	-1.187231	-1.093515	0.000000
C	0.196136	-1.201986	0.000000
C	0.961655	-0.047565	0.000000
C	0.358963	1.195564	0.000000
C	-1.021092	1.303628	0.000000
C	-1.783689	0.152585	0.000000
C	0.871632	-2.551457	0.000000
O	1.167379	2.279404	0.000000
H	-1.491825	2.271080	0.000000
H	-2.855460	0.231208	0.000000
H	-1.796309	-1.978245	0.000000
H	2.034933	-0.097726	0.000000

H	0.663606	3.074871	0.000000
H	0.144098	-3.352716	0.000000
H	1.501145	-2.668304	-0.875498
H	1.501145	-2.668304	0.875498

m-cresol, *trans* S_1

C	-1.201533	-1.058420	0.000000
C	0.201834	-1.222914	0.000000
C	1.012793	-0.071485	0.000000
C	0.397002	1.196333	0.000000
C	-1.008891	1.360680	0.000000
C	-1.816928	0.211920	0.000000
C	0.828207	-2.582602	0.000000
O	1.204199	2.249642	0.000000
H	-1.432656	2.347532	0.000000
H	-2.885040	0.292679	0.000000
H	-1.823868	-1.933691	0.000000
H	2.083098	-0.125820	0.000000
H	0.714884	3.056216	0.000000
H	0.079687	-3.364566	0.000000
H	1.461846	-2.720244	-0.874210
H	1.461846	-2.720244	0.874210

p-cresol S_0

C	0.705667	0.058977	-1.177256
C	-0.670230	0.054414	-1.185551
C	-1.365325	-0.000781	0.012240
C	-0.669488	-0.050562	1.200402
C	0.717915	-0.045092	1.189588
C	1.431460	0.009372	0.009436
O	-2.717960	-0.003015	-0.047445
C	2.941057	0.015508	-0.007295
H	-1.197737	-0.093685	2.137152
H	1.241093	-0.084498	2.128053
H	1.229670	0.102148	-2.115895
H	-1.220022	0.092980	-2.106708
H	-3.092423	-0.041786	0.815515
H	3.331426	-0.835424	-0.555880
H	3.325150	0.914008	-0.479084
H	3.341307	-0.027187	0.998027

p-cresol S_1

C	0.722126	-0.070978	-1.228435

C	-0.680210	-0.052273	-1.232496
C	-1.355860	-0.003644	0.006336
C	-0.672866	0.040529	1.240756
C	0.729087	-0.015972	1.227400
C	1.427821	-0.032042	-0.007957
O	-2.679777	0.013095	-0.041239
C	2.919183	0.036281	-0.004364
H	-1.226062	0.087150	2.159935
H	1.282255	-0.008346	2.146007
H	1.265342	-0.098209	-2.152376
H	-1.255913	-0.073743	-2.135395
H	-3.052659	0.049146	0.824846
H	3.334868	-0.335316	-0.932428
H	3.246114	1.067337	0.123819
H	3.328102	-0.537633	0.820882

o-methoxyphenol S_0

C	2.024329	-0.094988	0.000000
C	0.876286	0.688136	0.000000
C	-0.363146	0.089479	0.000000
C	-0.463813	-1.301900	0.000000
C	0.674159	-2.070476	0.000000
C	1.923091	-1.466269	0.000000
O	-1.555241	0.737082	0.000000
O	-1.672254	-1.898715	0.000000
H	0.572158	-3.139133	0.000000
H	2.807280	-2.075608	0.000000
H	2.986797	0.380851	0.000000
H	0.966004	1.756395	0.000000
C	-1.586018	2.136320	0.000000
H	-2.347891	-1.239641	0.000000
H	-2.627380	2.419180	0.000000
H	-1.107181	2.539644	0.885625
H	-1.107181	2.539644	-0.885625

o-methoxyphenol S_1

C	2.506247	-0.000104	0.074940
C	1.391585	-0.245299	-0.742452
C	0.126445	-0.175283	-0.111179
C	0.022083	-0.063521	1.293084
C	1.172128	-0.023698	2.124873
C	2.399151	0.117331	1.476938
O	-1.050863	-0.173430	-0.753322
O	-1.169131	0.049162	1.863273

H	1.058749	-0.013942	3.188380
H	3.292397	0.286121	2.047933
H	3.479140	0.075871	-0.373800
H	1.495670	-0.439488	-1.788058
C	-1.103712	0.099761	-2.134909
H	-1.848722	0.006661	1.205981
H	-2.150152	0.112804	-2.396250
H	-0.658174	1.061757	-2.355536
H	-0.604280	-0.674713	-2.701814

m-methoxyphenol, isomer 1 S_0

C	0.917996	1.432600	0.000000
C	-0.262252	0.701223	0.000000
C	-0.222765	-0.683424	0.000000
C	1.006652	-1.330571	0.000000
C	2.185569	-0.617352	0.000000
C	2.121483	0.765120	0.000000
H	-1.123415	-1.266340	0.000000
O	1.087514	-2.678367	0.000000
H	3.121906	-1.139975	0.000000
H	3.034685	1.331514	0.000000
H	0.866904	2.503725	0.000000
O	-1.400171	1.416381	0.000000
H	0.231870	-3.070995	0.000000
C	-2.640549	0.770802	0.000000
H	-3.386675	1.550230	0.000000
H	-2.769375	0.157714	-0.885925
H	-2.769375	0.157714	0.885925

m-methoxyphenol, isomer 1 S_1

C	1.163582	0.010557	-0.614379
C	-0.034907	-0.058432	0.130581
C	-0.024256	-0.185150	1.532414
C	1.237960	-0.018865	2.140729
C	2.437870	0.039228	1.407440
C	2.421461	-0.138380	0.012253
H	-0.896947	-0.397966	2.113299
O	1.340437	0.085443	3.466679
H	3.346081	0.224556	1.949149
H	3.325801	-0.150794	-0.558308
H	1.076489	0.174699	-1.671681
O	-1.148358	-0.005165	-0.592674
H	0.489710	0.197026	3.859806
C	-2.407791	0.045613	0.027633

H	-3.128409	0.134057	-0.769871
H	-2.605272	-0.861008	0.586679
H	-2.485141	0.904580	0.682990

m-methoxyphenol, isomer 2 S_0

C	0.341951	2.144885	0.000000
C	-0.829668	1.432392	0.000000
C	-0.778998	0.039099	0.000000
C	0.437163	-0.613611	0.000000
C	1.609156	0.132467	0.000000
C	1.576877	1.509349	0.000000
O	-1.965699	-0.588882	0.000000
C	-2.020197	-1.987484	0.000000
O	2.764566	-0.566109	0.000000
H	0.517865	-1.680898	0.000000
H	2.488041	2.080103	0.000000
H	0.305750	3.218826	0.000000
H	-1.785647	1.918256	0.000000
H	-3.067264	-2.248228	0.000000
H	-1.550188	-2.402085	-0.885265
H	-1.550188	-2.402085	0.885265
H	3.506470	0.014015	0.000000

m-methoxyphenol, isomer 2 S_1

C	1.241059	-0.129770	-0.692806
C	0.064815	0.004758	0.084846
C	0.117122	-0.054271	1.495691
C	1.340160	-0.161000	2.182547
C	2.496844	-0.016978	1.398028
C	2.459827	0.040633	-0.012379
O	-1.063856	-0.009893	2.103233
C	-1.147163	0.041819	3.505004
O	3.654411	0.055758	2.057833
H	1.426152	-0.249620	3.242628
H	3.378359	0.196432	-0.550782
H	1.198258	-0.141059	-1.761320
H	-0.896384	0.147823	-0.370217
H	-2.198782	0.096786	3.737940
H	-0.726791	-0.849351	3.954432
H	-0.643900	0.919123	3.893022
H	4.385000	0.108810	1.464198

p-methoxyphenol, *cis* S_0

C	-0.298711	0.723305	0.000000
C	-1.527514	0.068988	0.000000
C	-1.593806	-1.300349	0.000000
C	-0.428303	-2.056247	0.000000
C	0.785905	-1.416852	0.000000
C	0.856106	-0.025657	0.000000
O	-0.558227	-3.407131	0.000000
O	-0.347579	2.074966	0.000000
C	0.841437	2.806298	0.000000
H	1.821829	0.438720	0.000000
H	-2.423770	0.659684	0.000000
H	-2.541872	-1.803711	0.000000
H	1.698903	-1.986567	0.000000
H	0.559287	3.848109	0.000000
H	1.435709	2.601162	0.885190
H	1.435709	2.601162	-0.885190
H	0.284896	-3.825860	0.000000

p-methoxyphenol, *cis* S_1

C	1.339739	-0.018753	-0.618621
C	0.070333	-0.074564	0.009632
C	-0.002847	0.041004	1.403861
C	1.184375	0.001539	2.140907
C	2.460895	-0.086867	1.520597
C	2.539540	0.028111	0.127327
O	1.087181	0.038309	3.464040
O	1.305553	-0.010335	-1.937826
C	2.483141	0.020315	-2.707350
H	3.491142	0.071585	-0.358362
H	-0.802971	-0.121466	-0.607952
H	-0.936471	0.121089	1.922898
H	3.345255	-0.170379	2.123575
H	2.162497	0.020306	-3.736668
H	3.053543	0.918083	-2.506336
H	3.092546	-0.854524	-2.518708
H	1.940079	0.076533	3.865987

p-methoxyphenol, *trans* S_0

C	-0.647981	1.287485	0.000000
C	-1.876955	0.665909	0.000000
C	-1.961395	-0.716734	0.000000
C	-0.803908	-1.460215	0.000000
C	0.434333	-0.837245	0.000000
C	0.520366	0.542507	0.000000

O	-3.146795	-1.378584	0.000000
H	1.315237	-1.447485	0.000000
O	1.676511	1.245533	0.000000
H	-0.578076	2.358525	0.000000
H	-2.772591	1.262654	0.000000
H	-3.868868	-0.774815	0.000000
H	-0.870223	-2.531554	0.000000
C	2.896467	0.566097	0.000000
H	3.666472	1.322448	0.000000
H	3.008698	-0.052274	0.885174
H	3.008698	-0.052274	-0.885174

p-methoxyphenol, *trans* S_1

C	0.120651	0.012804	-1.376018
C	-1.267810	-0.081315	-1.209453
C	-1.786885	0.028199	0.092178
C	-0.957699	0.114116	1.232693
C	0.430558	-0.000204	1.078395
C	0.958162	-0.008949	-0.230204
O	-3.095298	0.049384	0.313635
H	1.069359	-0.023196	1.935307
O	2.250766	-0.034396	-0.495034
H	0.582249	0.021538	-2.342210
H	-1.928651	-0.160857	-2.051722
H	-3.577215	0.013642	-0.496757
H	-1.416479	0.207691	2.196061
C	3.212893	-0.024850	0.532049
H	4.171022	-0.050638	0.038397
H	3.135829	0.876738	1.126474
H	3.109339	-0.895399	1.166910

1-naphthol, *cis* S_0

C	0.828491	1.506092	-0.013623
C	0.520593	0.114978	-0.021618
C	-0.833569	-0.268582	-0.000295
C	-1.845770	0.722764	-0.008407
C	-1.510248	2.034122	-0.031533
C	-0.157839	2.434169	-0.027277
C	1.517021	-0.894694	-0.057641
C	1.179636	-2.207279	-0.043631
C	-0.178090	-2.592671	0.000146
C	-1.151130	-1.650689	0.016278
O	2.114053	1.938882	-0.030015
H	-2.185926	-1.939820	0.039012

H	-0.433402	-3.635968	0.012047
H	1.944882	-2.960188	-0.076174
H	2.555261	-0.627767	-0.121043
H	-2.875813	0.418325	0.000690
H	-2.275049	2.788389	-0.041798
H	0.106127	3.474250	-0.025744
H	2.680783	1.345696	0.430623

1-naphthol, *cis* S_1

C	0.880234	1.459042	0.009613
C	0.545924	0.095420	-0.041875
C	-0.856283	-0.244991	0.020859
C	-1.797918	0.786952	-0.006504
C	-1.417604	2.149965	-0.019077
C	-0.100731	2.485725	-0.032532
C	1.485595	-0.938433	-0.094906
C	1.080130	-2.296234	-0.050777
C	-0.244470	-2.617973	0.024669
C	-1.219813	-1.594874	0.045796
O	2.145355	1.881578	0.071019
H	-2.260837	-1.854681	0.093693
H	-0.555795	-3.644665	0.057223
H	1.828954	-3.064771	-0.080883
H	2.533847	-0.732366	-0.208758
H	-2.842623	0.537684	0.001732
H	-2.174793	2.909640	-0.042306
H	0.234308	3.504187	-0.031126
H	2.736519	1.178786	0.284121

1-naphthol, *trans* S_0

C	-0.706760	-0.534195	0.000000
C	-0.666913	-1.950873	0.000000
C	0.515852	-2.613177	0.000000
C	1.734093	-1.899086	0.000000
C	1.731050	-0.542901	0.000000
C	0.508001	0.171096	0.000000
H	-1.594289	-2.494039	0.000000
H	0.531613	-3.687553	0.000000
H	2.664219	-2.436281	0.000000
H	2.651756	0.005805	0.000000
C	-1.934763	0.178808	0.000000
C	-1.931683	1.530726	0.000000
C	-0.717277	2.254205	0.000000
C	0.466876	1.594177	0.000000

H	-2.858888	-0.368686	0.000000
H	-2.858148	2.074579	0.000000
H	-0.737544	3.329886	0.000000
O	1.660350	2.226588	0.000000
H	1.542465	3.160912	0.000000

1-naphthol, *trans* S_1

C	-0.948639	-0.386186	0.000000
C	-1.297413	-1.740220	0.000000
C	-0.313119	-2.755328	0.000000
C	1.011271	-2.415982	0.000000
C	1.405507	-1.055324	0.000000
C	0.452552	-0.035467	0.000000
H	-2.337181	-2.010739	0.000000
H	-0.615081	-3.785185	0.000000
H	1.769017	-3.176599	0.000000
H	2.447367	-0.804653	0.000000
C	-1.898634	0.640295	0.000000
C	-1.520670	2.001942	0.000000
C	-0.201262	2.345602	0.000000
C	0.786334	1.326326	0.000000
H	-2.942693	0.388221	0.000000
H	-2.278897	2.761232	0.000000
H	0.104490	3.376276	0.000000
O	2.088804	1.645320	0.000000
H	2.212566	2.579543	0.000000

2-naphthol, *cis* S_0

C	0.591233	2.004377	0.000000
C	0.611060	0.589171	0.000000
C	-0.603313	-0.115912	0.000000
C	-1.815700	0.617632	0.000000
C	-1.804818	1.974062	0.000000
C	-0.583146	2.682696	0.000000
C	1.823392	-0.150263	0.000000
C	1.821859	-1.501116	0.000000
C	0.592995	-2.204478	0.000000
C	-0.584666	-1.535193	0.000000
H	-1.517847	-2.071584	0.000000
H	1.525610	2.536368	0.000000
H	-0.590783	3.756672	0.000000
H	-2.731395	2.518146	0.000000
H	-2.748489	0.083347	0.000000
H	2.756862	0.382790	0.000000

H	2.734518	-2.065588	0.000000
O	0.688112	-3.551406	0.000000
H	-0.165495	-3.949713	0.000000

2-naphthol, *cis* S_1

C	0.598786	1.987485	0.000000
C	0.643804	0.591484	0.000000
C	-0.619154	-0.122601	0.000000
C	-1.818235	0.605736	0.000000
C	-1.825282	2.013154	0.000000
C	-0.627984	2.686870	0.000000
C	1.834053	-0.145910	0.000000
C	1.851192	-1.551215	0.000000
C	0.655896	-2.220008	0.000000
C	-0.578977	-1.513546	0.000000
H	-1.497951	-2.074006	0.000000
H	1.517508	2.544434	0.000000
H	-0.610812	3.760682	0.000000
H	-2.756378	2.545415	0.000000
H	-2.750653	0.071084	0.000000
H	2.768600	0.384303	0.000000
H	2.772065	-2.099162	0.000000
O	0.659968	-3.558935	0.000000
H	-0.216434	-3.905256	0.000000

2-naphthol, *trans* S_0

C	0.504333	2.007410	0.000000
C	0.531795	0.589629	0.000000
C	-0.679879	-0.123966	0.000000
C	-1.897752	0.606258	0.000000
C	-1.892738	1.960708	0.000000
C	-0.672417	2.677477	0.000000
C	1.743480	-0.140839	0.000000
C	1.744720	-1.495550	0.000000
C	0.521154	-2.204992	0.000000
C	-0.658612	-1.538242	0.000000
H	-1.578142	-2.092517	0.000000
H	1.435871	2.544454	0.000000
H	-0.686965	3.751410	0.000000
H	-2.821546	2.500992	0.000000
H	-2.826903	0.066180	0.000000
H	2.676044	0.393776	0.000000
H	2.673996	-2.038112	0.000000
O	0.504890	-3.557187	0.000000

H	1.378682	-3.906887	0.000000

2-naphthol, *trans* S_1

C	0.510035	1.992893	0.000000
C	0.561055	0.597044	0.000000
C	-0.698192	-0.124197	0.000000
C	-1.899384	0.598865	0.000000
C	-1.912600	2.006577	0.000000
C	-0.719545	2.686464	0.000000
C	1.754282	-0.132776	0.000000
C	1.776587	-1.541263	0.000000
C	0.581140	-2.213032	0.000000
C	-0.655177	-1.514442	0.000000
H	-1.557504	-2.095856	0.000000
H	1.426258	2.554166	0.000000
H	-0.707732	3.760372	0.000000
H	-2.846482	2.534084	0.000000
H	-2.828844	0.059447	0.000000
H	2.686846	0.400974	0.000000
H	2.710635	-2.071555	0.000000
O	0.483039	-3.547630	0.000000
H	1.335581	-3.950127	0.000000

5-methoxysalicylic acid S_0

C	2.259664	-0.164748	0.000000
C	1.548458	-1.326558	0.000000
C	0.148156	-1.317063	0.000000
C	-0.503156	-0.118564	0.000000
C	0.220348	1.090337	0.000000
C	1.606265	1.071773	0.000000
O	-0.444646	-2.531836	0.000000
C	-1.839651	-2.611681	0.000000
C	-0.487594	2.381298	0.000000
O	-1.807438	2.286516	0.000000
O	2.376652	2.158917	0.000000
O	0.051173	3.448783	0.000000
H	-2.084726	-3.662574	0.000000
H	-2.263604	-2.148203	-0.885320
H	-2.263604	-2.148203	0.885320
H	-1.570886	-0.065143	0.000000
H	3.332419	-0.172294	0.000000
H	2.052112	-2.274751	0.000000
H	1.839618	2.942327	0.000000
H	-2.169541	3.161668	0.000000

5-methoxysalicylic acid S_1

C	2.165277	-0.131319	0.000000
C	1.708264	-1.441446	0.000000
C	0.313963	-1.667898	0.000000
C	-0.612338	-0.604042	0.000000
C	-0.175213	0.718484	0.000000
C	1.276347	0.938930	0.000000
O	-0.046739	-2.935724	0.000000
C	-1.401140	-3.325123	0.000000
C	-1.052562	1.843584	0.000000
O	-2.353880	1.547729	0.000000
O	1.746846	2.151748	0.000000
O	-0.692993	3.009664	0.000000
H	-1.395443	-4.402825	0.000000
H	-1.907274	-2.965604	-0.886753
H	-1.907274	-2.965604	0.886753
H	-1.662613	-0.800821	0.000000
H	3.213869	0.094569	0.000000
H	2.372190	-2.280982	0.000000
H	1.016360	2.784363	0.000000
H	-2.833594	2.363095	0.000000

m-dimethoxybenzene, *trans* S_0

C	0.000000	-0.703933	-0.158156
C	0.000000	0.703933	-0.158156
C	0.000000	1.378328	1.039280
C	0.000000	0.683603	2.247728
C	0.000000	-0.683603	2.247728
C	0.000000	-1.378328	1.039280
O	0.000000	1.289453	-1.368165
H	0.000000	2.449697	1.054671
H	0.000000	1.232010	3.170954
H	0.000000	-1.232010	3.170954
H	0.000000	-2.449697	1.054671
O	0.000000	-1.289453	-1.368165
C	0.000000	-2.682344	-1.461782
H	0.000000	-2.913927	-2.515844
H	0.885146	-3.113274	-1.004333
H	-0.885146	-3.113274	-1.004333
C	0.000000	2.682344	-1.461782
H	0.000000	2.913927	-2.515844
H	-0.885146	3.113274	-1.004333
H	0.885146	3.113274	-1.004333

m-dimethoxybenzene, *trans* S_1

C	-0.115071	-1.078424	-1.434195
C	-0.175187	0.148375	-0.708193
C	-0.175187	0.148375	0.708193
C	-0.115071	-1.078424	1.434195
C	0.226494	-2.217676	0.704365
C	0.226494	-2.217676	-0.704365
O	-0.197561	1.340984	-1.286013
C	-0.024229	1.470661	-2.674599
O	-0.197561	1.340984	1.286013
C	-0.024229	1.470661	2.674599
H	-0.229252	-1.108238	2.495750
H	0.455128	-3.132457	1.219562
H	0.455128	-3.132457	-1.219562
H	-0.229252	-1.108238	-2.495750
H	-0.051110	2.529948	-2.875643
H	0.929286	1.065172	-2.990190
H	-0.825407	0.984095	-3.216971
H	-0.051110	2.529948	2.875643
H	-0.825407	0.984095	3.216971
H	0.929286	1.065172	2.990190

3P-propionic acid, *gauche* S_0

C	-1.018021	0.861276	-1.164967
C	-0.397370	0.650286	0.059378
C	-1.082372	-0.061790	1.032334
C	-2.351993	-0.554066	0.785735
C	-2.957293	-0.341375	-0.437660
C	-2.284689	0.369590	-1.414916
C	0.995530	1.187637	0.312704
C	2.111784	0.286715	-0.223537
C	2.335657	-0.959367	0.594764
O	2.049601	-1.099008	1.734114
O	2.952531	-1.908855	-0.100940
H	1.933497	-0.000289	-1.251375
H	3.058869	0.820262	-0.208106
H	1.144615	1.341492	1.372836
H	1.092583	2.154761	-0.167277
H	-0.617631	-0.238057	1.984171
H	-2.867193	-1.102766	1.552693
H	-3.943778	-0.722057	-0.627755
H	-2.748186	0.546521	-2.368162
H	-0.509399	1.421714	-1.929951

H	3.103269	-2.652645	0.465928

3P-propionic acid, *gauche* S_1

C	-1.041781	0.950698	-1.176418
C	-0.385401	0.671311	0.048043
C	-1.061136	-0.094313	1.029660
C	-2.354269	-0.598284	0.782605
C	-2.987271	-0.331379	-0.447897
C	-2.330344	0.438786	-1.428954
C	1.009381	1.175856	0.283645
C	2.109485	0.239788	-0.240338
C	2.358963	-0.959419	0.638422
O	2.105320	-1.037767	1.791306
O	2.961170	-1.942513	-0.021796
H	1.897963	-0.099777	-1.245152
H	3.055818	0.773493	-0.282132
H	1.168639	1.344492	1.340788
H	1.123473	2.129853	-0.220417
H	-0.571801	-0.302547	1.960370
H	-2.852017	-1.185523	1.528726
H	-3.970197	-0.715475	-0.640060
H	-2.814745	0.640949	-2.364097
H	-0.553269	1.555808	-1.916082
H	3.132032	-2.654047	0.579779

3P-propionic acid, *anti* S_0

C	1.461421	-0.448419	0.000000
C	0.542169	0.772932	0.000000
C	2.923152	-0.086839	0.000000
H	1.279830	-1.075736	0.866125
H	1.279830	-1.075736	-0.866125
C	-0.918444	0.380759	0.000000
H	0.760276	1.383126	0.867163
H	0.760276	1.383126	-0.867163
C	-1.602569	0.186550	1.191153
C	-2.931039	-0.196760	1.193658
C	-3.600406	-0.391097	0.000000
C	-2.931039	-0.196760	-1.193658
C	-1.602569	0.186550	-1.191153
H	-1.095425	0.342484	2.126930
H	-3.443576	-0.338634	2.127416
H	-4.633462	-0.685614	0.000000
H	-3.443576	-0.338634	-2.127416
H	-1.095425	0.342484	-2.126930

O	3.698834	-1.167953	0.000000
O	3.369472	1.008237	0.000000
H	4.605110	-0.892744	0.000000

3P-propionic acid, *anti* S_1

C	1.474277	-0.437697	0.000000
C	0.560049	0.794021	0.000000
C	2.936653	-0.078407	0.000000
H	1.289412	-1.061835	0.867040
H	1.289412	-1.061835	-0.867040
C	-0.892946	0.420996	0.000000
H	0.783558	1.399387	0.870100
H	0.783558	1.399387	-0.870100
C	-1.582872	0.222275	1.220681
C	-2.924421	-0.209393	1.222649
C	-3.593139	-0.421650	0.000000
C	-2.924421	-0.209393	-1.222649
C	-1.582872	0.222275	-1.220681
H	-1.076911	0.401859	2.149943
H	-3.436968	-0.371199	2.150315
H	-4.616140	-0.744428	0.000000
H	-3.436968	-0.371199	-2.150315
H	-1.076911	0.401859	-2.149943
O	3.709384	-1.161190	0.000000
O	3.384355	1.015948	0.000000
H	4.616536	-0.888623	0.000000

fluorine S_0

C	0.000000	0.000000	-1.789671
C	0.000000	1.178032	-0.841661
C	0.000000	0.736387	0.478887
C	0.000000	-0.736387	0.478887
C	0.000000	1.642459	1.522693
C	0.000000	2.995467	1.232637
C	0.000000	3.434957	-0.081028
C	0.000000	2.525709	-1.127216
H	0.000000	2.873810	-2.144530
H	0.000000	4.488733	-0.289808
H	0.000000	3.712104	2.032966
H	0.000000	1.310078	2.544376
C	0.000000	-1.642459	1.522693
C	0.000000	-2.995467	1.232637
C	0.000000	-3.434957	-0.081028
C	0.000000	-2.525709	-1.127216

C	0.000000	-1.178032	-0.841661
H	0.000000	-1.310078	2.544376
H	0.000000	-3.712104	2.032966
H	0.000000	-4.488733	-0.289808
H	0.000000	-2.873810	-2.144530
H	-0.874918	0.000000	-2.432470
H	0.874918	0.000000	-2.432470

fluorine S_1

C	0.000000	0.000000	-1.870905
C	0.000000	1.175814	-0.915451
C	0.000000	0.694047	0.447338
C	0.000000	-0.694047	0.447338
C	0.000000	1.634503	1.525762
C	0.000000	2.966107	1.227864
C	0.000000	3.421047	-0.104723
C	0.000000	2.512768	-1.174724
H	0.000000	2.880863	-2.184897
H	0.000000	4.476613	-0.302311
H	0.000000	3.690130	2.021693
H	0.000000	1.294884	2.544131
C	0.000000	-1.634503	1.525762
C	0.000000	-2.966107	1.227864
C	0.000000	-3.421047	-0.104723
C	0.000000	-2.512768	-1.174724
C	0.000000	-1.175814	-0.915451
H	0.000000	-1.294884	2.544131
H	0.000000	-3.690130	2.021693
H	0.000000	-4.476613	-0.302311
H	0.000000	-2.880863	-2.184897
H	-0.874325	0.000000	-2.517068
H	0.874325	0.000000	-2.517068

phenanthrene S_0

C	0.729575	0.000000	-0.346734
C	-0.729575	0.000000	-0.346734
C	-1.410497	0.000000	0.877087
C	-0.667571	0.000000	2.108929
C	0.667571	0.000000	2.108929
C	1.410497	0.000000	0.877087
C	-1.495287	0.000000	-1.528349
C	-2.816605	0.000000	0.895209
H	-1.214077	0.000000	3.034265
H	1.214077	0.000000	3.034265

C	1.495287	0.000000	-1.528349
C	2.859365	0.000000	-1.490136
C	3.533281	0.000000	-0.263524
C	2.816605	0.000000	0.895209
H	1.011373	0.000000	-2.484005
H	3.418411	0.000000	-2.407475
H	4.607118	0.000000	-0.239052
H	3.322002	0.000000	1.843877
C	-3.533281	0.000000	-0.263524
C	-2.859365	0.000000	-1.490136
H	-1.011373	0.000000	-2.484005
H	-3.418411	0.000000	-2.407475
H	-4.607118	0.000000	-0.239052
H	-3.322002	0.000000	1.843877

phenanthrene S_1

C	0.727112	0.000000	-0.390335
C	-0.727112	0.000000	-0.390335
C	-1.425656	0.000000	0.877054
C	-0.699281	0.000000	2.065882
C	0.699281	0.000000	2.065882
C	1.425656	0.000000	0.877054
C	-1.492614	0.000000	-1.551215
C	-2.842978	0.000000	0.874656
H	-1.224763	0.000000	3.002564
H	1.224763	0.000000	3.002564
C	1.492614	0.000000	-1.551215
C	2.881748	0.000000	-1.518431
C	3.556006	0.000000	-0.296327
C	2.842978	0.000000	0.874656
H	1.015524	0.000000	-2.510392
H	3.433179	0.000000	-2.439454
H	4.629441	0.000000	-0.273508
H	3.356462	0.000000	1.818545
C	-3.556006	0.000000	-0.296327
C	-2.881748	0.000000	-1.518431
H	-1.015524	0.000000	-2.510392
H	-3.433179	0.000000	-2.439454
H	-4.629441	0.000000	-0.273508
H	-3.356462	0.000000	1.818545

2,4,6,8-decatetraene S_0

C	-2.585127	-5.001881	0.000000
C	-2.451256	-3.508803	0.000000

C	-1.306844	-2.847380	0.000000
C	-1.201272	-1.390661	0.000000
C	-0.052409	-0.726658	0.000000
C	0.052409	0.726658	0.000000
C	1.201272	1.390661	0.000000
C	1.306844	2.847380	0.000000
C	2.451256	3.508803	0.000000
C	2.585127	5.001881	0.000000
H	-0.377916	-3.395494	0.000000
H	-2.128690	-0.840485	0.000000
H	0.874980	-1.276820	0.000000
H	-0.874980	1.276820	0.000000
H	2.128690	0.840485	0.000000
H	0.377916	3.395494	0.000000
H	3.374662	2.950132	0.000000
H	-3.374662	-2.950132	0.000000
H	1.616092	5.486508	0.000000
H	3.134544	5.340033	0.873820
H	3.134544	5.340033	-0.873820
H	-1.616092	-5.486508	0.000000
H	-3.134544	-5.340033	0.873820
H	-3.134544	-5.340033	-0.873820

2,4,6,8-decatetraene S_1

C	-2.568345	-5.009460	0.000000
C	-2.503345	-3.517927	0.000000
C	-1.353064	-2.800485	0.000000
C	-1.265471	-1.393190	0.000000
C	-0.055924	-0.691385	0.000000
C	0.055924	0.691385	0.000000
C	1.265471	1.393190	0.000000
C	1.353064	2.800485	0.000000
C	2.503345	3.517927	0.000000
C	2.568345	5.009460	0.000000
H	-0.419752	-3.343306	0.000000
H	-2.181927	-0.825749	0.000000
H	0.853646	-1.270543	0.000000
H	-0.853646	1.270543	0.000000
H	2.181927	0.825749	0.000000
H	0.419752	3.343306	0.000000
H	3.444470	2.990216	0.000000
H	-3.444470	-2.990216	0.000000
H	1.577593	5.449537	0.000000
H	3.103418	5.381666	0.872708
H	3.103418	5.381666	-0.872708

H	-1.577593	-5.449537	0.000000
H	-3.103418	-5.381666	0.872708
H	-3.103418	-5.381666	-0.872708

tetracene S_0

C	3.691873	1.402323	0.000000
C	2.422048	0.717717	0.000000
C	2.422048	-0.717717	0.000000
C	3.691873	-1.402323	0.000000
C	4.843459	-0.720115	0.000000
C	4.843459	0.720115	0.000000
C	1.229971	1.392474	0.000000
C	0.000000	0.712265	0.000000
C	0.000000	-0.712265	0.000000
C	1.229971	-1.392474	0.000000
C	-1.229971	1.392474	0.000000
C	-2.422048	0.717717	0.000000
C	-2.422048	-0.717717	0.000000
C	-1.229971	-1.392474	0.000000
C	-3.691873	1.402323	0.000000
C	-4.843459	0.720115	0.000000
C	-4.843459	-0.720115	0.000000
C	-3.691873	-1.402323	0.000000
H	-3.691500	-2.477182	0.000000
H	-5.783038	-1.240832	0.000000
H	-5.783038	1.240832	0.000000
H	-3.691500	2.477182	0.000000
H	-1.229010	-2.467879	0.000000
H	-1.229010	2.467879	0.000000
H	1.229010	-2.467879	0.000000
H	1.229010	2.467879	0.000000
H	3.691500	-2.477182	0.000000
H	5.783038	-1.240832	0.000000
H	5.783038	1.240832	0.000000
H	3.691500	2.477182	0.000000

tetracene S_1

C	3.685273	1.388742	0.000000
C	2.456465	0.713753	0.000000
C	2.456465	-0.713753	0.000000
C	3.685273	-1.388742	0.000000
C	4.875019	-0.697487	0.000000
C	4.875019	0.697487	0.000000
C	1.220803	1.392516	0.000000

C	0.000000	0.725795	0.000000
C	0.000000	-0.725795	0.000000
C	1.220803	-1.392516	0.000000
C	-1.220803	1.392516	0.000000
C	-2.456465	0.713753	0.000000
C	-2.456465	-0.713753	0.000000
C	-1.220803	-1.392516	0.000000
C	-3.685273	1.388742	0.000000
C	-4.875019	0.697487	0.000000
C	-4.875019	-0.697487	0.000000
C	-3.685273	-1.388742	0.000000
H	-3.690248	-2.463627	0.000000
H	-5.805447	-1.233683	0.000000
H	-5.805447	1.233683	0.000000
H	-3.690248	2.463627	0.000000
H	-1.225399	-2.467908	0.000000
H	-1.225399	2.467908	0.000000
H	1.225399	-2.467908	0.000000
H	1.225399	2.467908	0.000000
H	3.690248	-2.463627	0.000000
H	5.805447	-1.233683	0.000000
H	5.805447	1.233683	0.000000
H	3.690248	2.463627	0.000000

perylene S_0

C	0.051437	1.467800	-2.402395
C	0.019534	0.741925	-1.245358
C	0.013711	1.439045	-0.000029
C	0.034623	2.849370	-0.000030
C	0.062211	3.551049	-1.227122
C	0.073404	2.872795	-2.397424
C	0.024990	3.551583	1.227010
C	0.001543	2.873801	2.397416
C	-0.009507	1.468692	2.402458
C	0.002714	0.742193	1.245413
C	-0.019534	-0.741925	-1.245358
C	-0.013711	-1.439045	-0.000029
C	-0.002714	-0.742193	1.245413
C	-0.034623	-2.849370	-0.000030
C	-0.024990	-3.551583	1.227010
C	-0.001543	-2.873801	2.397416
C	0.009507	-1.468692	2.402458
C	-0.051437	-1.467800	-2.402395
C	-0.073404	-2.872795	-2.397424
C	-0.062211	-3.551049	-1.227122

H	0.036989	4.625822	1.212378
H	-0.007667	3.400842	3.333391
H	-0.026538	0.979283	3.354326
H	-0.036989	-4.625822	1.212378
H	0.007667	-3.400842	3.333391
H	0.026538	-0.979283	3.354326
H	-0.076894	-4.625256	-1.212537
H	-0.097795	-3.399394	-3.333375
H	-0.062001	-0.977921	-3.354120
H	0.076894	4.625256	-1.212537
H	0.097795	3.399394	-3.333375
H	0.062001	0.977921	-3.354120

perylene S_1

C	-0.005126	1.464236	-2.433756
C	-0.005965	0.718628	-1.232950
C	0.012929	1.413482	0.000000
C	0.006558	2.841563	0.000000
C	0.008812	3.529821	-1.223424
C	-0.000748	2.840933	-2.417294
C	0.008868	3.529821	1.223419
C	-0.000589	2.840932	2.417292
C	-0.004943	1.464237	2.433757
C	-0.005922	0.718627	1.232951
C	0.005965	-0.718628	-1.232950
C	-0.012929	-1.413482	0.000000
C	0.005922	-0.718627	1.232951
C	-0.006558	-2.841563	0.000000
C	-0.008868	-3.529821	1.223419
C	0.000589	-2.840932	2.417292
C	0.004943	-1.464237	2.433757
C	0.005126	-1.464236	-2.433756
C	0.000748	-2.840933	-2.417294
C	-0.008812	-3.529821	-1.223424
H	0.011658	4.604214	1.218676
H	-0.003610	3.381279	3.345700
H	-0.025155	0.966102	3.379705
H	-0.011658	-4.604214	1.218676
H	0.003610	-3.381279	3.345700
H	0.025155	-0.966102	3.379705
H	-0.011614	-4.604213	-1.218680
H	0.003848	-3.381279	-3.345703
H	0.025477	-0.966099	-3.379699
H	0.011614	4.604213	-1.218680
H	-0.003848	3.381279	-3.345703

H	-0.025477	0.966099	-3.379699

CC2/TZVP geometries – Group I

pyrazine S_0

C	1.132312	-0.696476	-0.000010
C	1.132312	0.696476	0.000009
N	0.000000	1.417550	0.000034
C	-1.132312	0.696476	0.000008
C	-1.132312	-0.696476	-0.000005
N	0.000000	-1.417550	-0.000031
H	-2.063169	-1.251290	0.000030
H	2.063169	-1.251290	0.000014
H	2.063169	1.251290	-0.000015
H	-2.063169	1.251290	-0.000033

pyrazine S_1

C	-1.221966	0.696174	0.095215
C	-1.116217	-0.752525	0.001529
N	0.024588	-1.353955	-0.002941
C	1.222069	-0.695840	-0.111868
C	1.116279	0.752896	-0.017983
N	-0.024476	1.354371	-0.013466
H	2.037554	1.325435	0.035557
H	-2.139277	1.188962	-0.192179
H	-2.037373	-1.325270	-0.051791
H	2.139454	-1.188466	0.175601

2,6-difluoropyridine S_0

C	1.116685	-0.007903	-0.874860
N	0.000002	-0.008794	-1.579366
C	-1.116690	-0.007917	-0.874847
C	-1.205210	0.020919	0.509832
C	0.000059	-0.014327	1.205917
C	1.205275	0.021004	0.509830
F	-2.251262	-0.015093	-1.592732
H	-2.166392	0.004172	1.000970
H	-0.000151	0.009323	2.287500
H	2.166446	0.004281	1.000953
F	2.251238	-0.015100	-1.592776

2,6-difluoropyridine S_1

C	-1.088394	0.067505	-0.335738
N	-0.000012	0.299896	-1.096388
C	1.088393	0.067217	-0.335890
C	1.167565	-0.033359	1.071112
C	0.000203	0.310270	1.850896
C	-1.167366	-0.033020	1.071275
F	2.223806	-0.093369	-1.017477
H	2.088249	-0.387428	1.517333
H	0.000234	0.198078	2.923963
H	-2.088055	-0.386815	1.517705
F	-2.223919	-0.092764	-1.017172

2-fluoropyridine S_0

C	-1.315242	0.503842	-0.002550
N	-1.378092	-0.809457	-0.005316
C	-0.194903	-1.455969	-0.011208
C	1.033990	-0.809937	0.018311
C	1.047974	0.585735	-0.020778
C	-0.156749	1.275184	0.018141
H	-0.256586	-2.537307	-0.002495
H	1.950431	-1.382943	-0.005071
H	1.983461	1.129554	-0.002644
H	-0.214695	2.353990	0.003091
F	-2.499601	1.147300	-0.000851

2-fluoropyridine S_1

C	-1.328210	0.566339	0.056675
N	-1.263248	-0.744195	0.169861
C	-0.195189	-1.550472	-0.228877
C	1.026232	-0.803185	-0.021075
C	1.039699	0.574547	0.034738
C	-0.170318	1.345349	0.045327
H	-0.265056	-2.597210	0.033767
H	1.939439	-1.379722	0.072588
H	1.991896	1.087476	0.085546
H	-0.226927	2.390701	-0.221054
F	-2.547534	1.109682	0.014692

2-hydroxypyridine S_0

C	-0.982106	0.753709	0.021568
C	-0.971751	-0.645112	-0.003482
N	0.130422	-1.391271	-0.004135

C	1.309236	-0.737579	-0.011748
C	1.419825	0.644552	0.015711
C	0.242948	1.399259	-0.022718
O	-2.163094	-1.297231	-0.000328
H	2.190151	-1.368457	-0.002627
H	2.393116	1.114143	-0.012308
H	0.283761	2.480930	-0.006174
H	-1.921527	1.288070	0.006512
H	-1.930980	-2.241014	-0.002406

2-hydroxypyridine S_1

C	-0.991824	0.769006	-0.002048
C	-0.974892	-0.632270	-0.087292
N	0.120764	-1.455874	-0.257855
C	1.276550	-0.774094	-0.008828
C	1.379796	0.644219	0.054547
C	0.253583	1.472110	-0.212144
O	-2.130508	-1.298795	0.080236
H	2.174341	-1.376006	0.070484
H	2.351876	1.075552	0.263445
H	0.310303	2.546897	-0.135154
H	-1.909272	1.268033	0.281770
H	-1.860668	-2.239331	0.021958

2-pyridone S_0

C	-1.248997	0.720313	-0.007055
N	-1.133194	-0.687822	0.035222
C	0.035472	-1.390355	-0.011605
C	1.230131	-0.731593	0.001251
C	1.209981	0.688579	-0.022468
C	0.033481	1.385575	0.039132
H	-2.020431	-1.177107	-0.002802
H	-0.056199	-2.467886	-0.006811
H	2.153364	-1.287962	-0.051143
H	2.147770	1.230931	-0.011825
H	0.014142	2.466617	0.023221
O	-2.365518	1.250720	-0.052479

2-pyridone S_1

C	-1.314200	0.118032	0.000001
N	-0.749905	-1.124015	-0.000001
C	0.647505	-1.254548	0.000005
C	1.416959	-0.087429	0.000000

C	0.836955	1.160651	-0.000007
C	-0.627768	1.267426	0.000009
H	-1.342656	-1.941777	-0.000010
H	1.030665	-2.262269	0.000016
H	2.494042	-0.197860	0.000002
H	1.433461	2.062545	-0.000029
H	-1.138047	2.219314	0.000035
O	-2.739501	0.013261	-0.000021

2-methylpyrimidine S_0

C	0.000075	1.965544	0.000008
C	-1.178402	1.227299	-0.000006
N	-1.194000	-0.112814	-0.000020
C	0.010164	-0.720009	-0.000019
N	1.207895	-0.105487	-0.000017
C	1.182223	1.237436	-0.000005
H	-2.147131	1.715125	-0.000003
H	2.147849	1.731041	-0.000006
H	-0.004421	3.046736	0.000034
C	0.002807	-2.217025	0.000004
H	1.022014	-2.594181	0.000010
H	-0.524542	-2.586819	0.879243
H	-0.524541	-2.586845	-0.879224

2-methylpyrimidine S_1

C	-0.013075	2.013633	0.042691
C	-1.164813	1.275896	-0.013216
N	-1.175471	-0.106484	-0.104208
C	0.009189	-0.787737	-0.024946
N	1.094488	-0.071623	0.019272
C	1.222304	1.307619	-0.081878
H	-2.142924	1.738512	0.032564
H	2.198046	1.724258	0.113759
H	-0.032675	3.094219	0.103190
C	0.010782	-2.271853	0.015272
H	1.029905	-2.649598	0.058460
H	-0.547447	-2.612724	0.887158
H	-0.487919	-2.654053	-0.875431

5-methylpyrimidine S_0

C	0.873400	0.856727	-0.000052
C	-0.362588	0.212922	-0.000036
C	-0.305203	-1.181890	-0.000024

N	0.843530	-1.873866	0.000047
C	1.961205	-1.131710	0.000033
N	2.047600	0.204749	-0.000035
H	2.898275	-1.675121	0.000096
H	-1.217695	-1.771427	-0.000135
H	0.929045	1.941415	-0.000059
C	-1.663765	0.959118	0.000029
H	-1.491982	2.035254	0.000035
H	-2.255949	0.711917	-0.881659
H	-2.255875	0.711895	0.881760

5-methylpyrimidine S_1

C	0.843957	0.855065	-0.042151
C	-0.381205	0.240939	-0.000252
C	-0.366549	-1.195932	-0.094792
N	0.880869	-1.769674	0.055378
C	2.038319	-1.177702	0.036737
N	2.053249	0.180802	-0.063505
H	2.961839	-1.732028	0.109494
H	-1.226427	-1.822869	0.091291
H	0.927893	1.936051	-0.030512
C	-1.679913	0.980960	0.024932
H	-1.512608	2.057927	0.020188
H	-2.282980	0.721734	-0.847442
H	-2.255711	0.726950	0.917160

7-azaindole S_0

N	-0.633428	1.844450	-0.027670
C	-0.672231	0.471758	0.000315
C	0.671684	0.008041	0.072066
C	1.512841	1.161908	0.043283
C	0.681570	2.257594	0.029873
C	0.849985	-1.378569	0.002932
C	-0.290569	-2.172746	0.019239
C	-1.565530	-1.581934	-0.002075
N	-1.789631	-0.258675	-0.007221
H	-2.451646	-2.206672	0.002838
H	1.838502	-1.822788	0.014148
H	-0.212525	-3.251810	-0.012919
H	-1.452167	2.431210	0.031550
H	2.589458	1.190436	0.084744
H	0.923706	3.307799	0.012064

7-azaindole S_1

N	-0.604342	1.878510	0.006554
C	-0.658562	0.440528	0.093263
C	0.664695	-0.005829	0.164623
C	1.485353	1.143227	-0.006317
C	0.651201	2.313655	-0.041672
C	0.900452	-1.415664	0.023219
C	-0.294972	-2.178317	-0.028143
C	-1.552001	-1.595754	-0.028866
N	-1.817124	-0.214022	0.004268
H	-2.438550	-2.218403	-0.046871
H	1.876955	-1.859475	0.160369
H	-0.242297	-3.259656	-0.086476
H	-1.445654	2.447954	0.027168
H	2.561413	1.164074	-0.106726
H	0.913563	3.358995	-0.041397

7-hydroxyquinoline, *cis* S_0

N	0.478954	1.977243	-0.005393
C	0.435679	0.608774	-0.015798
C	-0.787677	-0.126213	0.046304
C	-1.994269	0.603444	-0.010172
C	-1.946887	1.979728	-0.000400
C	-0.686149	2.612810	-0.001503
C	1.664310	-0.087965	0.035419
C	1.677086	-1.465562	-0.010129
C	0.469709	-2.202270	0.018132
C	-0.734362	-1.541912	-0.005491
H	-0.630733	3.697094	0.000162
H	-1.661583	-2.104490	0.006617
H	0.520898	-3.283302	-0.010301
O	2.827314	-2.210121	-0.011445
H	2.580309	0.493511	0.026423
H	-2.940802	0.073152	-0.005746
H	-2.850151	2.575911	-0.021860
H	3.578355	-1.599823	-0.034820

7-hydroxyquinoline, *cis* S_1

N	0.508421	1.984892	0.122155
C	0.452050	0.635444	0.090359
C	-0.792009	-0.152511	0.001136
C	-2.002126	0.590132	-0.034439
C	-1.925829	1.991351	-0.047087
C	-0.683099	2.649226	0.031982

C	1.645464	-0.081135	-0.049706
C	1.655849	-1.501603	-0.013840
C	0.475555	-2.269384	0.000822
C	-0.735590	-1.562560	0.060039
H	-0.629445	3.729957	0.070508
H	-1.671810	-2.110917	0.083554
H	0.529153	-3.346725	0.057995
O	2.829330	-2.170305	-0.032811
H	2.578079	0.473596	-0.105569
H	-2.952832	0.078930	-0.131134
H	-2.834098	2.582832	-0.063584
H	3.552938	-1.521209	-0.040383

7-hydroxyquinoline, *trans* S_0

N	0.528693	2.049916	0.006179
C	0.483208	0.679429	0.018282
C	-0.745498	-0.049706	-0.045458
C	-1.950998	0.684222	0.009598
C	-1.898317	2.059085	-0.000097
C	-0.633416	2.687776	0.000762
C	1.708784	-0.016778	-0.029001
C	1.718507	-1.394511	0.014513
C	0.507294	-2.124780	-0.020298
C	-0.698802	-1.462474	0.005620
H	-0.575237	3.772051	-0.001960
H	-1.626537	-2.024181	-0.010476
H	0.533364	-3.209732	0.007502
O	2.934771	-2.028297	0.018112
H	2.633987	0.544563	-0.014646
H	-2.899209	0.156830	0.004322
H	-2.799140	2.659050	0.020362
H	2.778524	-2.982444	0.016682

7-hydroxyquinoline, *trans* S_1

N	0.552286	2.061080	-0.103761
C	0.494068	0.715171	-0.083634
C	-0.747967	-0.068759	0.006441
C	-1.958116	0.672108	0.025127
C	-1.881812	2.074321	0.039401
C	-0.641490	2.728698	-0.022917
C	1.691274	-0.004538	0.040472
C	1.695023	-1.422026	0.012412
C	0.510328	-2.193045	0.012815
C	-0.697285	-1.480656	-0.052548

H	-0.583681	3.809547	-0.050677
H	-1.636291	-2.024510	-0.080138
H	0.545716	-3.272621	-0.063352
O	2.918634	-1.990813	0.033558
H	2.634257	0.526757	0.086773
H	-2.910075	0.161172	0.112358
H	-2.790879	2.664926	0.052297
H	2.805989	-2.956789	0.035373

2-hydroxyquinoline, enol S_0

C	0.435920	1.902880	-0.008012
C	0.488062	0.490456	0.042669
C	-0.724323	-0.258442	-0.025892
C	-1.955898	0.434253	0.016119
C	-1.979370	1.812787	-0.013757
C	-0.778418	2.554728	0.011997
C	1.700007	-0.240076	-0.010578
C	1.665927	-1.610784	0.008764
C	0.397134	-2.252443	-0.005002
N	-0.755064	-1.626855	-0.010198
O	0.311858	-3.615276	-0.001913
H	1.364552	2.463746	0.005182
H	-0.813339	3.636854	-0.014973
H	-2.929022	2.333760	0.003534
H	-2.867164	-0.150752	0.003893
H	2.647155	0.288350	0.001275
H	2.580687	-2.192663	-0.014867
H	1.211293	-3.970524	0.011759

2-hydroxyquinoline, enol S_1

C	0.444754	1.885534	0.059552
C	0.529263	0.490921	-0.019263
C	-0.743674	-0.263215	0.035368
C	-1.970178	0.433298	-0.046106
C	-2.015635	1.836054	-0.000434
C	-0.804491	2.550129	0.013096
C	1.739646	-0.231138	-0.014120
C	1.696388	-1.641224	-0.113643
C	0.418892	-2.245540	0.011204
N	-0.773552	-1.622820	0.039256
O	0.299548	-3.588960	0.095275
H	1.358758	2.470271	0.061775
H	-0.817578	3.633663	0.038352
H	-2.960702	2.359459	-0.048019

H	-2.875619	-0.161631	-0.058100
H	2.682986	0.302163	-0.032013
H	2.596198	-2.243015	-0.075036
H	1.194994	-3.963949	0.052855

2-hydroxyquinoline, keto S_0

N	0.559103	1.705863	0.051021
C	0.600113	0.326298	-0.003773
C	-0.618020	-0.385197	0.055942
C	-1.837254	0.371432	0.014986
C	-1.831206	1.729669	0.025944
C	-0.592506	2.495760	-0.017353
C	1.821096	-0.362996	0.027862
C	1.827211	-1.748349	-0.021586
C	0.623893	-2.469610	0.000231
C	-0.582803	-1.789625	-0.009052
H	-1.520892	-2.333599	0.000757
H	0.639377	-3.551076	-0.038897
H	2.773211	-2.275512	-0.015145
H	2.752478	0.192422	0.019244
H	-2.779010	-0.167614	0.027594
H	-2.746823	2.304879	-0.004553
O	-0.513764	3.728029	-0.084819
H	1.427394	2.225992	-0.024727

2-hydroxyquinoline, keto S_1

N	0.551573	1.713787	-0.083991
C	0.589791	0.314377	0.009527
C	-0.661439	-0.386310	-0.043069
C	-1.854349	0.331961	0.009255
C	-1.837641	1.786539	-0.013238
C	-0.637419	2.377512	-0.001731
C	1.811086	-0.355651	-0.027324
C	1.843645	-1.745092	0.019920
C	0.633410	-2.464352	-0.003649
C	-0.580888	-1.809580	0.017450
H	-1.507857	-2.372741	0.008002
H	0.655219	-3.547307	0.028100
H	2.792897	-2.264875	0.001007
H	2.735090	0.215162	-0.027849
H	-2.804832	-0.187637	-0.018923
H	-2.745355	2.370975	0.029464
O	-0.390372	3.792518	0.014386
H	1.407441	2.230724	0.082663

dibenzofuran S_0

C	1.718043	-0.024648	-1.363835
C	0.721693	0.023729	-0.383141
C	1.096909	-0.015936	0.971151
C	2.415858	0.027937	1.399705
C	3.391199	-0.011217	0.405086
C	3.048707	0.008091	-0.957621
C	-0.721882	-0.023801	-0.383134
C	-1.097087	0.015987	0.971159
O	-0.000086	0.000102	1.809526
C	-1.718234	0.024545	-1.363825
C	-3.048897	-0.008251	-0.957607
C	-3.391377	0.011223	0.405097
C	-2.416030	-0.027955	1.399715
H	-2.667901	-0.022244	2.452049
H	-4.436061	-0.013071	0.689327
H	-3.835704	0.022209	-1.700924
H	-1.460049	0.022348	-2.416237
H	1.459858	-0.022315	-2.416247
H	3.835511	-0.022600	-1.700933
H	4.435890	0.013320	0.689268
H	2.667689	0.022032	2.452047

dibenzofuran S_1

C	1.729871	-0.039130	-1.384414
C	0.708804	0.019534	-0.417123
C	1.112701	-0.030178	0.960803
C	2.416453	0.026759	1.416851
C	3.428889	-0.016299	0.418547
C	3.077187	0.002703	-0.939634
C	-0.708818	-0.020191	-0.417100
C	-1.112705	0.030118	0.960789
O	0.000018	0.000068	1.779282
C	-1.729867	0.038449	-1.384413
C	-3.077196	-0.002555	-0.939628
C	-3.428894	0.016658	0.418547
C	-2.416452	-0.026410	1.416855
H	-2.645944	-0.029657	2.474263
H	-4.470111	-0.025096	0.707648
H	-3.865392	0.015351	-1.683315
H	-1.501495	0.037635	-2.443095
H	1.501501	-0.039000	-2.443094
H	3.865397	-0.014413	-1.683326

H	4.470113	0.025388	0.707632
H	2.645941	0.030266	2.474259

pyrrolo[3,2-*h*]quinoline S_0

C	0.131210	-0.683975	0.021407
N	0.043007	-2.043064	0.016264
C	1.193811	-2.712924	0.011867
C	2.462022	-2.103807	-0.000977
C	2.543456	-0.724555	0.008691
C	1.360885	0.041597	-0.030531
H	1.112486	-3.795250	0.012985
H	3.353301	-2.718225	0.013883
H	3.505880	-0.223170	-0.002156
C	-1.050335	0.084428	-0.045043
C	-1.058400	1.492509	0.018439
C	0.179754	2.185273	-0.015664
C	1.354018	1.470487	0.000452
H	0.199724	3.269103	0.008564
H	2.307227	1.988009	-0.022208
C	-2.427724	1.894257	0.014446
C	-3.185496	0.741919	0.006450
N	-2.346368	-0.350145	-0.021679
H	-2.609014	-1.325280	-0.035366
H	-2.813930	2.900546	0.039352
H	-4.255501	0.612271	0.000820

pyrrolo[3,2-*h*]quinoline S_1

C	0.120810	-0.687139	0.056770
N	-0.016071	-2.042845	0.067359
C	1.168716	-2.733270	0.023155
C	2.428846	-2.115388	-0.023292
C	2.561146	-0.713162	0.016754
C	1.368382	0.066649	-0.006102
H	1.086146	-3.813833	0.014909
H	3.313957	-2.741472	-0.040931
H	3.532626	-0.235282	-0.030612
C	-1.018342	0.095400	-0.046268
C	-1.053095	1.536047	0.006885
C	0.174006	2.246321	-0.019361
C	1.347563	1.488258	0.016892
H	0.199115	3.327717	0.016354
H	2.306119	1.998250	0.003163
C	-2.408797	1.890515	-0.003297
C	-3.166350	0.697653	-0.010061

N	-2.327276	-0.364451	-0.037860
H	-2.549547	-1.352946	-0.021092
H	-2.830059	2.883790	0.024161
H	-4.237883	0.569187	-0.007525

carbazole S_0

C	1.129525	0.016007	-0.900599
N	0.000017	-0.000036	-1.699881
C	-1.129486	-0.016188	-0.900590
C	-0.720604	0.021537	0.457585
C	0.720646	-0.021463	0.457586
C	-1.690343	-0.031159	1.465330
C	-3.033499	0.002941	1.108236
C	-3.418791	-0.008701	-0.244278
C	-2.475948	0.034849	-1.266056
C	2.475986	-0.035086	-1.266063
C	3.418834	0.008432	-0.244289
C	3.033543	-0.002742	1.108229
C	1.690387	0.031471	1.465314
H	-2.780872	0.030329	-2.306207
H	-4.471932	0.017504	-0.496668
H	-3.795254	-0.031753	1.877155
H	-1.397803	-0.032583	2.509260
H	1.397853	0.033086	2.509246
H	3.795297	0.032309	1.877133
H	4.471964	-0.018286	-0.496670
H	2.780911	-0.030442	-2.306213
H	0.000031	-0.001168	-2.708311

carbazole S_1

C	1.149322	-0.033060	-0.883628
N	-0.000015	-0.000079	-1.659642
C	-1.149333	0.033046	-0.883614
C	-0.712461	-0.019598	0.489690
C	0.712489	0.019636	0.489674
C	-1.703266	0.036732	1.485445
C	-3.063017	-0.003389	1.083400
C	-3.457134	0.016308	-0.258328
C	-2.471840	-0.025599	-1.286885
C	2.471835	0.025388	-1.286897
C	3.457115	-0.016461	-0.258335
C	3.063014	0.003427	1.083397
C	1.703271	-0.036619	1.485445
H	-2.749337	-0.020023	-2.334688

H	-4.506760	-0.024475	-0.516679
H	-3.827823	0.013041	1.851786
H	-1.442265	0.029534	2.536754
H	1.442224	-0.029228	2.536743
H	3.827859	-0.012911	1.851744
H	4.506753	0.024329	-0.516648
H	2.749365	0.019439	-2.334688
H	0.000004	0.000565	-2.675006

tryptamine, A-ph S_0

C	-2.153233	0.159997	0.898065
N	-1.269424	0.088138	1.961600
C	0.018036	0.040116	1.469308
C	-0.077636	-0.026918	0.053543
C	-1.465396	0.094782	-0.291804
C	1.238699	-0.057727	2.140673
C	2.390600	-0.091009	1.364492
C	2.322802	-0.130965	-0.042503
C	1.105013	-0.049490	-0.703877
C	-2.032992	0.033456	-1.669585
C	-1.943732	-1.371639	-2.259071
N	-2.425069	-1.370124	-3.643133
H	1.294853	-0.033562	3.223083
H	3.355848	-0.156841	1.851611
H	3.242444	-0.152639	-0.614452
H	1.064770	-0.068765	-1.787367
H	-1.509317	0.293308	2.919268
H	-3.213963	0.253070	1.075620
H	-1.500406	0.719099	-2.334494
H	-3.081430	0.348489	-1.652921
H	-2.487698	-2.056920	-1.595426
H	-0.899396	-1.688415	-2.263693
H	-3.418138	-1.158240	-3.653453
H	-2.322641	-2.294819	-4.048112

tryptamine, A-ph S_1

C	-2.220468	0.196745	0.898833
N	-1.324159	0.128626	1.892948
C	0.013421	0.106450	1.404003
C	-0.075426	0.228265	0.008377
C	-1.467114	0.243293	-0.323945
C	1.172221	-0.226160	2.110132
C	2.368861	-0.215556	1.293873
C	2.311688	-0.126980	-0.083405

C	1.083947	0.024305	-0.798841
C	-2.026003	0.114270	-1.683314
C	-1.893484	-1.345583	-2.153360
N	-2.409151	-1.472584	-3.514283
H	1.207990	-0.274708	3.190789
H	3.329261	-0.351200	1.778057
H	3.238994	-0.163360	-0.644822
H	1.070782	0.221833	-1.863768
H	-1.554241	0.142191	2.881481
H	-3.273440	0.354469	1.075782
H	-1.466844	0.740938	-2.380883
H	-3.078880	0.409859	-1.703446
H	-2.391304	-1.992906	-1.418792
H	-0.831889	-1.598305	-2.151431
H	-3.423767	-1.458095	-3.507420
H	-2.128421	-2.363424	-3.909232

tryptamine, A-py S_0

C	-2.145768	0.137033	0.873374
N	-1.271835	0.083093	1.945508
C	0.020567	0.043113	1.466837
C	-0.060330	-0.036357	0.050274
C	-1.445855	0.067870	-0.309323
C	1.234948	-0.037473	2.151774
C	2.395589	-0.064902	1.388671
C	2.343158	-0.116051	-0.018582
C	1.131482	-0.052700	-0.692927
C	-2.012443	-0.001821	-1.687393
C	-1.907182	-1.404300	-2.279985
N	-2.500247	-1.428761	-3.620300
H	1.278962	-0.005175	3.234532
H	3.356098	-0.117550	1.886582
H	3.268960	-0.133144	-0.580712
H	1.104332	-0.084472	-1.776555
H	-1.524105	0.285846	2.900498
H	-3.209254	0.220109	1.038504
H	-1.482331	0.700404	-2.341201
H	-3.064304	0.292798	-1.683509
H	-2.471833	-2.089934	-1.645402
H	-0.857597	-1.723837	-2.250551
H	-1.950269	-0.842457	-4.240827
H	-2.460830	-2.368946	-4.000170

tryptamine, A-py S_1

C	-2.213633	0.153099	0.873657
N	-1.329203	0.094557	1.876563
C	0.014827	0.101502	1.400496
C	-0.060965	0.227903	0.005473
C	-1.448235	0.216404	-0.341148
C	1.173405	-0.213931	2.118072
C	2.375252	-0.180851	1.312242
C	2.332632	-0.083781	-0.065440
C	1.109422	0.048723	-0.793159
C	-1.996547	0.078269	-1.702876
C	-1.853681	-1.383857	-2.165804
N	-2.422010	-1.526432	-3.504670
H	1.201260	-0.259940	3.199026
H	3.333238	-0.302156	1.805229
H	3.267005	-0.102791	-0.615878
H	1.104422	0.263942	-1.854914
H	-1.570171	0.100586	2.862408
H	-3.273149	0.278249	1.036786
H	-1.431081	0.715669	-2.388435
H	-3.051456	0.355938	-1.744466
H	-2.422357	-2.019120	-1.482914
H	-0.795730	-1.659224	-2.081357
H	-1.814788	-1.072489	-4.180161
H	-2.458543	-2.507886	-3.759624

tryptamine, A-up S_0

C	-2.144987	0.153065	0.884295
N	-1.270022	0.070931	1.953588
C	0.021689	0.034848	1.472623
C	-0.060937	-0.010702	0.054865
C	-1.446174	0.111303	-0.300771
C	1.236288	-0.069297	2.153988
C	2.395627	-0.087879	1.388694
C	2.341314	-0.108049	-0.019243
C	1.129504	-0.020481	-0.690555
C	-2.007825	0.055666	-1.681336
C	-1.908015	-1.350028	-2.290966
N	-2.414370	-1.488285	-3.655497
H	1.281864	-0.062149	3.237112
H	3.356279	-0.158765	1.884027
H	3.266292	-0.121316	-0.582716
H	1.101097	-0.029878	-1.774574
H	-1.520531	0.249058	2.913958
H	-3.207760	0.237115	1.053857
H	-1.477097	0.760322	-2.331449

H	-3.058940	0.361277	-1.668717
H	-2.456368	-2.044572	-1.651238
H	-0.865183	-1.672140	-2.280597
H	-1.904431	-0.866367	-4.275176
H	-3.386071	-1.195766	-3.690926

tryptamine, A-up S_1

C	-2.214751	0.168285	0.883544
N	-1.324386	0.079913	1.882034
C	0.016835	0.092087	1.405242
C	-0.061922	0.254683	0.013445
C	-1.451285	0.270521	-0.330193
C	1.175745	-0.243089	2.110932
C	2.376796	-0.198111	1.304309
C	2.329909	-0.068191	-0.069953
C	1.105414	0.091643	-0.790529
C	-1.989329	0.143196	-1.692249
C	-1.889783	-1.346817	-2.140028
N	-2.330129	-1.616013	-3.496459
H	1.204597	-0.322421	3.189948
H	3.334835	-0.340699	1.791245
H	3.261951	-0.079634	-0.624547
H	1.100435	0.327493	-1.847932
H	-1.562888	0.058027	2.868404
H	-3.270869	0.305622	1.058815
H	-1.393931	0.744061	-2.383874
H	-3.033718	0.462609	-1.744451
H	-2.484845	-1.951228	-1.452625
H	-0.847518	-1.652702	-2.035571
H	-1.758643	-1.110122	-4.164506
H	-3.291294	-1.321189	-3.631778

tryptamine, Ph-out S_0

C	-0.015055	-0.036602	0.060616
C	0.035322	0.051111	1.478580
C	1.236786	0.004010	2.189159
C	2.412478	0.009736	1.449364
C	2.388934	-0.043967	0.041060
C	1.191690	-0.022270	-0.660956
N	-1.266537	0.060681	1.932946
H	1.257194	0.039080	3.272587
H	3.364060	-0.013682	1.966528
H	3.326288	-0.036556	-0.501939
H	1.179275	-0.073744	-1.742827

C	-1.396948	0.033513	-0.325935
C	-2.120365	0.092360	0.844747
H	-1.541227	0.263082	2.881908
H	-3.187411	0.167972	0.990428
C	-1.952041	-0.025578	-1.711818
H	-1.323195	0.556600	-2.391250
C	-2.055105	-1.452928	-2.245992
H	-2.950357	0.421849	-1.719988
H	-2.481857	-1.426280	-3.251468
N	-0.725337	-2.058559	-2.338510
H	-2.750277	-2.010678	-1.602629
H	-0.349112	-2.200246	-1.405347
H	-0.792228	-2.974793	-2.770053

tryptamine, Ph-out S_1

C	-0.014032	0.159474	0.014538
C	0.022384	0.119830	1.416656
C	1.161465	-0.151952	2.185910
C	2.386350	-0.127208	1.418556
C	2.389709	-0.086428	0.037474
C	1.186620	-0.040735	-0.737073
N	-1.332827	0.139592	1.859250
H	1.156743	-0.128058	3.268120
H	3.330266	-0.184151	1.949165
H	3.341894	-0.105644	-0.481251
H	1.212276	0.133392	-1.806028
C	-1.391940	0.158381	-0.368533
C	-2.186457	0.159323	0.832685
H	-1.598512	0.195413	2.837015
H	-3.250627	0.285320	0.960641
C	-1.954394	-0.024570	-1.723341
H	-1.318948	0.464205	-2.464932
C	-2.031074	-1.522587	-2.082359
H	-2.959106	0.403632	-1.768517
H	-2.691758	-1.627951	-2.945665
N	-0.709668	-2.014212	-2.447577
H	-2.499696	-2.050594	-1.238535
H	-0.033085	-1.808053	-1.711329
H	-0.730592	-3.022295	-2.565659

tryptamine, Ph-up S_0

C	-2.105790	0.049529	0.813440
N	-1.262551	-0.013270	1.907953
C	0.043482	0.024794	1.470590

C	0.008781	0.011919	0.049167
C	-1.368538	0.069484	-0.350457
C	1.238570	-0.037373	2.190869
C	2.422036	0.027679	1.466784
C	2.415095	0.052556	0.057490
C	1.223695	0.094767	-0.652765
C	-1.902146	0.021984	-1.743939
C	-2.073004	-1.417587	-2.257698
N	-0.859156	-2.226403	-2.302565
H	1.247139	-0.059535	3.274737
H	3.368186	-0.007110	1.992839
H	3.357503	0.110890	-0.473381
H	1.231971	0.122908	-1.736450
H	-1.553123	0.115126	2.865074
H	-3.175952	0.083835	0.951252
H	-1.227069	0.563272	-2.415397
H	-2.871038	0.530195	-1.787397
H	-2.501789	-1.392195	-3.262627
H	-2.791099	-1.929740	-1.612679
H	-0.432308	-2.254484	-1.381131
H	-0.179248	-1.791612	-2.918647

tryptamine, Ph-up S_1

C	-2.188868	0.173502	0.833036
N	-1.334748	0.126101	1.860751
C	0.019169	0.115961	1.419327
C	-0.016505	0.199430	0.019401
C	-1.393926	0.206727	-0.365044
C	1.160116	-0.173206	2.179782
C	2.383861	-0.129626	1.413228
C	2.388024	-0.048948	0.034112
C	1.184524	0.021704	-0.739490
C	-1.934424	0.020821	-1.716958
C	-1.957079	-1.508319	-2.077983
N	-0.674375	-2.126538	-2.306753
H	1.155902	-0.181320	3.262187
H	3.327908	-0.206491	1.941183
H	3.340934	-0.049821	-0.483843
H	1.215202	0.267372	-1.794984
H	-1.601491	0.156385	2.839073
H	-3.253228	0.294203	0.964689
H	-1.314580	0.533525	-2.455640
H	-2.959081	0.399626	-1.778510
H	-2.566657	-1.616695	-2.977403
H	-2.466395	-2.035088	-1.268376

H	-0.032432	-1.962742	-1.530737
H	-0.228190	-1.726953	-3.125958

tryptamine, Py-out S_0

C	0.475627	0.435031	0.195963
C	0.559148	0.516085	1.612907
C	1.768763	0.390655	2.299321
C	2.927839	0.312117	1.537226
C	2.874139	0.255481	0.130386
C	1.666736	0.365848	-0.546011
N	-0.731189	0.605446	2.091245
H	1.813386	0.428196	3.381898
H	3.885202	0.224258	2.036243
H	3.798938	0.198083	-0.430697
H	1.639841	0.332194	-1.629311
C	-0.905161	0.593663	-0.163830
C	-1.602924	0.685221	1.018885
H	-0.976359	0.817149	3.046253
H	-2.663995	0.797673	1.180793
C	-1.478622	0.510172	-1.538839
H	-0.942526	1.186132	-2.212505
C	-1.399123	-0.913105	-2.089635
H	-2.527518	0.816167	-1.520410
H	-0.342461	-1.192526	-2.196102
N	-2.155190	-1.815814	-1.219816
H	-1.852556	-0.940916	-3.082740
H	-2.123867	-2.759220	-1.593350
H	-1.708107	-1.847990	-0.307856

tryptamine, Py-out S_1

C	0.418701	0.627579	0.133455
C	0.489639	0.577264	1.530944
C	1.612002	0.158281	2.266738
C	2.805995	0.055297	1.460353
C	2.777542	0.121579	0.079871
C	1.566779	0.320438	-0.659851
N	-0.848350	0.729488	2.013114
H	1.646460	0.188384	3.348371
H	3.752070	-0.121936	1.960184
H	3.708341	0.003243	-0.464234
H	1.588024	0.528042	-1.723036
C	-0.965203	0.778355	-0.208658
C	-1.718369	0.849753	1.013041
H	-1.085194	0.768159	2.998881

H	-2.773646	1.012449	1.165066
C	-1.560560	0.586448	-1.546844
H	-1.103153	1.271105	-2.267578
C	-1.288326	-0.863778	-1.994404
H	-2.637231	0.764044	-1.512224
H	-0.239559	-0.941320	-2.294453
N	-1.638545	-1.784314	-0.908171
H	-1.917746	-1.082717	-2.858040
H	-1.729367	-2.724958	-1.280167
H	-0.860311	-1.820895	-0.252369

tryptamine, Py-up S_0

C	-2.158818	0.286381	0.881282
N	-1.285278	0.196574	1.951457
C	0.002088	0.088421	1.468600
C	-0.086538	0.006629	0.052527
C	-1.466726	0.178460	-0.303760
C	1.211957	-0.052680	2.151546
C	2.367182	-0.147676	1.385785
C	2.308244	-0.206558	-0.020774
C	1.100610	-0.081282	-0.693726
C	-2.035239	0.109682	-1.679885
C	-1.950835	-1.313220	-2.258695
N	-2.632486	-2.341982	-1.480373
H	1.260371	-0.015267	3.233905
H	3.324806	-0.248372	1.881799
H	3.230230	-0.279327	-0.584524
H	1.070013	-0.119009	-1.776760
H	-1.523267	0.418427	2.905971
H	-3.215870	0.427531	1.048990
H	-1.503709	0.800675	-2.343958
H	-3.084626	0.422317	-1.661190
H	-0.901809	-1.603979	-2.341378
H	-2.368141	-1.317214	-3.268213
H	-3.617687	-2.108915	-1.393249
H	-2.255949	-2.349995	-0.536489

tryptamine, Py-up S_1

C	-2.271255	0.416939	0.872478
N	-1.389256	0.314942	1.873585
C	-0.057858	0.149488	1.392646
C	-0.134158	0.193461	-0.008424
C	-1.517397	0.336432	-0.349038
C	1.065382	-0.249340	2.125202

C	2.264005	-0.361063	1.320891
C	2.226707	-0.317063	-0.058621
C	1.016171	-0.117768	-0.794903
C	-2.101715	0.178412	-1.693059
C	-1.855740	-1.271208	-2.200011
N	-2.231265	-2.332829	-1.282209
H	1.092944	-0.239481	3.207188
H	3.209354	-0.538518	1.821043
H	3.153880	-0.440659	-0.607499
H	1.033721	0.056323	-1.863827
H	-1.618808	0.389105	2.859581
H	-3.311372	0.655826	1.032616
H	-1.627673	0.872937	-2.394637
H	-3.176104	0.382121	-1.670358
H	-0.792606	-1.383549	-2.409042
H	-2.403798	-1.397525	-3.135487
H	-3.177755	-2.207653	-0.937855
H	-1.606883	-2.339698	-0.481344

porphycene S_0

C	-3.443303	1.914343	-0.001322
C	-2.412824	0.916434	-0.001417
N	-1.214195	1.564133	-0.001513
C	-1.399770	2.918984	-0.001582
C	-2.818154	3.149631	-0.001468
C	-0.372394	3.885827	-0.001672
C	1.017453	3.732163	-0.001602
C	1.831359	2.574455	-0.001448
H	-0.223446	1.162588	-0.001703
N	1.397588	1.278350	-0.001610
C	3.283961	2.608116	-0.001164
C	3.709484	1.299806	-0.001079
C	2.505620	0.495081	-0.001506
C	2.412861	-0.916435	-0.001143
C	3.443339	-1.914348	-0.001262
C	2.818189	-3.149633	-0.001432
C	1.399807	-2.918986	-0.001528
N	1.214229	-1.564134	-0.001331
C	0.372430	-3.885828	-0.001518
C	-1.017417	-3.732162	-0.001448
C	-1.831322	-2.574454	-0.001301
C	-3.283927	-2.608119	-0.001282
C	-3.709448	-1.299807	-0.001302
C	-2.505585	-0.495083	-0.001212
N	-1.397553	-1.278350	-0.001311

H	0.223483	-1.162585	-0.001269
H	3.290714	-4.130971	-0.001389
H	4.513395	-1.714241	-0.001057
H	0.735559	-4.918223	-0.001564
H	-1.583281	-4.669628	-0.001707
H	-3.898122	-3.508744	-0.001275
H	-4.734265	-0.930071	-0.001418
H	-4.513359	1.714236	-0.001198
H	-3.290683	4.130967	-0.001516
H	-0.735524	4.918222	-0.001979
H	1.583316	4.669630	-0.001340
H	3.898157	3.508741	-0.000989
H	4.734301	0.930070	-0.000758

porphycene S_1

C	-3.465924	1.905468	0.000137
C	-2.441130	0.907580	0.000149
N	-1.235320	1.554219	-0.000123
C	-1.419358	2.910930	-0.000047
C	-2.834942	3.143522	0.000064
C	-0.389590	3.883386	0.000093
C	1.002879	3.742032	0.000034
C	1.847362	2.596972	0.000127
H	-0.258778	1.148585	-0.000221
N	1.415076	1.287634	-0.000267
C	3.287030	2.636969	0.000173
C	3.726745	1.323238	-0.000189
C	2.544340	0.509564	-0.000484
C	2.441130	-0.907581	0.000133
C	3.465925	-1.905468	0.000277
C	2.834940	-3.143523	0.000098
C	1.419359	-2.910930	-0.000164
N	1.235319	-1.554218	-0.000292
C	0.389590	-3.883387	-0.000180
C	-1.002878	-3.742032	0.000016
C	-1.847358	-2.596970	0.000002
C	-3.287029	-2.636968	0.000007
C	-3.726743	-1.323239	-0.000119
C	-2.544338	-0.509564	-0.000183
N	-1.415076	-1.287633	0.000029
H	0.258775	-1.148588	-0.000178
H	3.305004	-4.126042	0.000216
H	4.536219	-1.707192	0.000679
H	0.757052	-4.913829	-0.000176
H	-1.555207	-4.688018	0.000026

H	-3.897453	-3.540294	0.000105
H	-4.756182	-0.966321	-0.000235
H	-4.536220	1.707199	0.000199
H	-3.305012	4.126038	0.000095
H	-0.757048	4.913828	0.000121
H	1.555201	4.688021	0.000163
H	3.897454	3.540294	0.000420
H	4.756183	0.966320	-0.000503

porphine S_0

N	-0.000673	-2.016906	-0.000407
N	2.124854	0.000830	-0.000362
C	1.084459	-2.848978	-0.000804
C	0.683636	-4.249976	-0.000963
C	2.427230	-2.441751	-0.000827
C	2.903545	-1.127012	-0.000544
C	4.270451	-0.690061	-0.000400
H	1.361468	-5.103595	-0.001337
H	3.187716	-3.227824	-0.000999
H	5.130837	-1.357422	-0.000421
H	1.100525	0.002140	-0.000394
N	0.000611	2.016997	-0.000165
N	-2.124930	-0.000749	0.000231
C	1.085271	2.849731	-0.000177
C	-1.084527	2.849064	-0.000091
C	-1.085339	-2.849640	-0.000193
C	0.683647	4.250476	-0.000178
C	-0.683707	4.250061	-0.000151
C	-0.683713	-4.250382	-0.000549
C	2.428191	2.442964	-0.000073
C	-2.427286	2.441823	0.000137
C	-2.428270	-2.442879	0.000103
C	2.904360	1.128167	-0.000170
C	-2.903628	1.127095	0.000496
C	-2.904439	-1.128083	0.000597
C	4.270969	0.690377	-0.000138
C	-4.270533	0.690149	0.001060
C	-4.271047	-0.690291	0.001166
H	1.360978	5.104494	-0.000260
H	-1.361558	5.103664	-0.000129
H	-1.361045	-5.104399	-0.000570
H	3.188535	3.229165	0.000085
H	-3.187770	3.227897	0.000173
H	-3.188594	-3.229104	0.000571
H	5.131852	1.357075	-0.000115

H	-5.130935	1.357481	0.001422
H	-5.131904	-1.357022	0.001462
H	-1.100601	-0.002017	-0.000074

porphine S_1

N	0.000000	-2.042770	-0.000007
N	2.120309	0.000001	-0.000005
C	1.090183	-2.882272	0.000020
C	0.686908	-4.274771	0.000010
C	2.435181	-2.451582	0.000038
C	2.903544	-1.130610	0.000022
C	4.269331	-0.691926	0.000017
H	1.362144	-5.130325	-0.000004
H	3.203591	-3.229939	0.000072
H	5.130677	-1.357872	0.000021
H	1.098450	0.000002	-0.000028
N	0.000001	2.042768	-0.000014
N	-2.120309	0.000000	0.000008
C	1.090183	2.882272	-0.000022
C	-1.090182	2.882272	0.000017
C	-1.090183	-2.882273	-0.000019
C	0.686908	4.274772	-0.000013
C	-0.686907	4.274772	0.000028
C	-0.686908	-4.274773	-0.000001
C	2.435181	2.451583	-0.000030
C	-2.435180	2.451583	0.000028
C	-2.435182	-2.451583	-0.000036
C	2.903544	1.130611	-0.000007
C	-2.903544	1.130611	0.000007
C	-2.903545	-1.130611	-0.000019
C	4.269331	0.691925	-0.000002
C	-4.269331	0.691925	0.000002
C	-4.269332	-0.691926	-0.000016
H	1.362143	5.130326	-0.000040
H	-1.362142	5.130327	0.000058
H	-1.362143	-5.130327	0.000014
H	3.203590	3.229941	-0.000090
H	-3.203589	3.229942	0.000070
H	-3.203592	-3.229942	-0.000084
H	5.130676	1.357871	-0.000021
H	-5.130676	1.357872	0.000015
H	-5.130678	-1.357872	-0.000025
H	-1.098451	0.000000	0.000035

chlorin S_0

C	-0.077908	-4.264318	0.921875
C	-0.070915	-2.903863	1.367143
N	-0.031485	-2.115759	0.248919
C	-0.003524	-2.885448	-0.888732
C	-0.034765	-4.250847	-0.460600
C	-0.080493	-2.426964	2.686036
C	-0.041414	-1.086594	3.084538
N	0.000290	0.000014	2.252061
C	0.041872	1.086477	3.084745
C	0.027803	0.681392	4.487916
C	-0.027655	-0.681755	4.487788
C	0.081036	2.426901	2.686424
C	0.071115	2.903883	1.367562
N	0.031075	2.115732	0.249383
C	0.003395	2.885369	-0.888300
C	0.034944	4.250784	-0.460216
C	0.078270	4.264318	0.922252
C	-0.052808	2.418470	-2.208109
C	-0.062330	1.098775	-2.658397
C	-0.204216	0.736019	-4.128196
C	0.203883	-0.735658	-4.128318
C	0.061916	-1.098693	-2.658604
N	-0.000313	-0.000036	-1.866708
C	0.052550	-2.418457	-2.208516
H	-1.256686	0.858973	-4.433110
H	-0.094007	3.198046	-2.974376
H	0.024865	5.106624	-1.133606
H	0.054598	1.359682	5.340706
H	-0.054755	-1.360199	5.340446
H	-0.410556	-1.370445	-4.781807
H	0.111525	3.185902	3.473198
H	-0.110595	-3.186056	3.472738
H	0.093922	-3.197938	-2.974868
H	0.109420	5.130297	1.581439
H	-0.108893	-5.130263	1.581116
H	-0.024617	-5.106723	-1.133942
H	1.256370	-0.858561	-4.433192
H	0.410259	1.370929	-4.781531
H	-0.011888	-1.094045	0.281994
H	0.010717	1.094035	0.282836

chlorin S_1

C	-0.092030	-4.271878	0.921706
C	-0.079824	-2.909381	1.364025

N	-0.028069	-2.122512	0.241597
C	0.001720	-2.901576	-0.895768
C	-0.039383	-4.263350	-0.465664
C	-0.096280	-2.434293	2.688453
C	-0.048644	-1.088044	3.094971
N	0.000070	-0.000022	2.259476
C	0.048980	1.087874	3.095139
C	0.032973	0.681507	4.498843
C	-0.032256	-0.681902	4.498741
C	0.096521	2.434175	2.688781
C	0.079766	2.909365	1.364389
N	0.027924	2.122497	0.241958
C	-0.001914	2.901562	-0.895396
C	0.039082	4.263336	-0.465275
C	0.091790	4.271866	0.922094
C	-0.066030	2.429066	-2.219545
C	-0.079013	1.099708	-2.659703
C	-0.232653	0.727267	-4.121192
C	0.232473	-0.726922	-4.121304
C	0.078857	-1.099569	-2.659869
N	-0.000032	0.000014	-1.857001
C	0.065743	-2.428986	-2.219887
H	-1.295803	0.800549	-4.407289
H	-0.114098	3.202471	-2.990929
H	0.029663	5.121694	-1.135250
H	0.064612	1.359585	5.351417
H	-0.063625	-1.360123	5.351211
H	-0.340423	-1.385802	-4.788687
H	0.135893	3.194057	3.473757
H	-0.135388	-3.194262	3.473360
H	0.113920	-3.202308	-2.991345
H	0.130994	5.135727	1.583579
H	-0.131304	-5.135735	1.583193
H	-0.030086	-5.121710	-1.135637
H	1.295621	-0.800169	-4.407424
H	0.340234	1.386243	-4.788489
H	-0.003863	-1.101864	0.264203
H	0.003885	1.101845	0.264747

Zn-tetraphenylporphine S_0

C	-3.649443	4.475233	1.081245
C	-3.548912	3.549288	-0.000140
C	-4.475322	3.650398	-1.081060
C	-5.478980	4.655125	-1.081409
C	-5.572391	5.572742	0.000858

C	-4.654296	5.478764	1.082674
C	-2.486693	2.486821	-0.000602
C	-1.127779	2.908162	-0.046502
N	0.000134	2.062098	0.014476
C	1.128134	2.908065	-0.046308
C	0.696481	4.303524	-0.177995
C	-0.695990	4.303621	-0.177721
C	2.487009	2.486578	-0.000553
C	3.549339	3.548933	0.000088
C	4.475444	3.650444	-1.081056
C	5.478309	4.655964	-1.081924
C	5.571871	5.573339	0.000535
C	4.654157	5.478886	1.082633
C	3.650046	4.474612	1.081682
C	-2.908152	1.127964	0.045498
N	-2.062179	-0.000038	-0.014997
C	-2.908288	-1.127935	0.045623
C	-4.303718	-0.696129	0.177056
C	-4.303683	0.696353	0.176438
C	-2.486960	-2.486853	0.000130
C	-3.549353	-3.549148	0.000087
C	-4.474970	-3.650399	-1.081500
C	-5.478353	-4.655401	-1.082676
C	-5.572807	-5.572631	-0.000172
C	-4.655534	-5.478485	1.082326
C	-3.650874	-4.474758	1.081660
C	2.908338	1.127674	0.045373
N	2.062236	-0.000241	-0.014986
C	2.908216	-1.128225	0.045784
C	4.303722	-0.696566	0.176865
C	4.303792	0.695916	0.176660
C	2.486756	-2.487098	0.000134
C	3.549045	-3.549498	-0.000020
C	4.474928	-3.650450	-1.081409
C	5.478790	-4.654973	-1.082246
C	5.573046	-5.572430	0.000082
C	4.655477	-5.478611	1.082358
C	3.650358	-4.475344	1.081373
C	1.127837	-2.908471	-0.045475
N	-0.000079	-2.062384	0.015180
C	-1.128079	-2.908370	-0.045337
C	-0.696428	-4.303878	-0.176475
C	0.696048	-4.303971	-0.176243
H	1.360249	-5.171261	-0.287680
H	5.170855	-1.360825	0.289203
H	1.360740	5.170561	-0.291023

H	-1.360190	5.170889	-0.289336
H	-1.360694	-5.170968	-0.289065
H	5.170972	1.360121	0.288942
H	-5.170918	1.360669	0.287659
H	-5.170794	-1.360275	0.290462
H	4.395036	2.945370	-1.926017
H	6.181530	4.726904	-1.927993
H	6.350969	6.352802	0.000840
H	4.723613	6.182637	1.928384
H	2.945366	4.392872	1.926845
H	4.393511	-2.945793	-1.926623
H	6.182518	-4.724809	-1.927985
H	6.352275	-6.351761	-0.000074
H	4.726066	-6.181829	1.928458
H	2.945263	-4.394610	1.926285
H	-4.393876	-2.945432	-1.926486
H	-6.181369	-4.725964	-1.928947
H	-6.352118	-6.351882	-0.000245
H	-4.725856	-6.181952	1.928242
H	-2.946479	-4.393311	1.927088
H	-4.394285	2.945899	-1.926442
H	-6.183207	4.724998	-1.926728
H	-6.351437	6.352257	0.001058
H	-4.724241	6.182089	1.928738
H	-2.943777	4.394533	1.925685
Zn	0.000029	-0.000145	-0.000013

Zn-tetraphenylporphine S_1

C	-3.559097	4.578152	0.997228
C	-3.549605	3.555317	-0.000076
C	-4.568772	3.563345	-1.001786
C	-5.565765	4.573484	-1.010941
C	-5.567191	5.587097	-0.012853
C	-4.560710	5.584633	0.991522
C	-2.496084	2.491798	0.004914
C	-1.131607	2.898022	-0.077217
N	0.000043	2.049956	0.040706
C	1.131692	2.898033	-0.077197
C	0.697645	4.276564	-0.308252
C	-0.697563	4.276552	-0.308291
C	2.496157	2.491801	0.004967
C	3.549689	3.555309	0.000007
C	4.568830	3.563386	-1.001730
C	5.565661	4.573683	-1.011024
C	5.566959	5.587401	-0.013041

C	4.560611	5.584783	0.991467
C	3.559156	4.578146	0.997309
C	-2.933463	1.129736	0.098775
N	-2.087254	-0.000013	-0.025652
C	-2.933468	-1.129764	0.098685
C	-4.310098	-0.699690	0.331221
C	-4.310104	0.699650	0.331226
C	-2.496092	-2.491826	0.004779
C	-3.549616	-3.555342	-0.000159
C	-4.568869	-3.563327	-1.001782
C	-5.565911	-4.573418	-1.010846
C	-5.567291	-5.587035	-0.012761
C	-4.560778	-5.584559	0.991583
C	-3.559051	-4.578191	0.997131
C	2.933518	1.129728	0.098843
N	2.087315	-0.000024	-0.025544
C	2.933513	-1.129785	0.098830
C	4.310140	-0.699705	0.331306
C	4.310140	0.699637	0.331343
C	2.496146	-2.491850	0.004902
C	3.549673	-3.555363	-0.000040
C	4.568900	-3.563378	-1.001689
C	5.565837	-4.573571	-1.010853
C	5.567116	-5.587284	-0.012866
C	4.560652	-5.584757	0.991527
C	3.559087	-4.578228	0.997235
C	1.131679	-2.898074	-0.077293
N	0.000034	-2.049996	0.040615
C	-1.131620	-2.898050	-0.077388
C	-0.697577	-4.276582	-0.308445
C	0.697632	-4.276588	-0.308448
H	1.359535	-5.132532	-0.495025
H	5.165099	-1.363677	0.515290
H	1.359552	5.132537	-0.494679
H	-1.359470	5.132501	-0.494828
H	-1.359487	-5.132552	-0.494873
H	5.165083	1.363600	0.515428
H	-5.165068	1.363619	0.515197
H	-5.165031	-1.363665	0.515316
H	4.560918	2.785041	-1.783705
H	6.337709	4.573089	-1.798034
H	6.342932	6.369996	-0.018706
H	4.559517	6.361651	1.773716
H	2.787273	4.567487	1.785437
H	4.560958	-2.785084	-1.783715
H	6.337999	-4.572886	-1.797752

H	6.343158	-6.369811	-0.018442
H	4.559561	-6.361601	1.773799
H	2.787049	-4.567700	1.785212
H	-4.560867	-2.785092	-1.783866
H	-6.338067	-4.572737	-1.797750
H	-6.343450	-6.369447	-0.018224
H	-4.559798	-6.361293	1.773965
H	-2.786858	-4.567812	1.784959
H	-4.560736	2.785109	-1.783869
H	-6.337829	4.572860	-1.797936
H	-6.343399	6.369460	-0.018299
H	-4.559618	6.361514	1.773759
H	-2.787083	4.567634	1.785230
Zn	0.000174	-0.000020	0.005686

tetraphenylporphine S_0

C	-2.958596	4.476938	1.417891
C	-3.433628	3.339426	0.729757
C	-4.803847	3.259484	0.402912
C	-5.680581	4.282053	0.779368
C	-5.203710	5.395879	1.483466
C	-3.841326	5.489384	1.802719
C	-2.494273	2.281443	0.342264
C	-1.198909	2.696375	-0.165891
N	-0.060422	2.075585	0.156618
C	0.935040	2.830165	-0.448173
C	0.376107	3.964953	-1.175917
C	-0.982103	3.877282	-1.001714
C	2.281207	2.494074	-0.342558
C	3.339314	3.433382	-0.729821
C	4.477119	2.958189	-1.417362
C	5.489599	3.840885	-1.802179
C	5.396245	5.203239	-1.482739
C	4.282102	5.680269	-0.779251
C	3.259108	4.803709	-0.403518
C	-2.830266	0.935224	0.447848
N	-2.075566	-0.060192	-0.156875
C	-2.696161	-1.198739	0.165745
C	-3.877380	-0.982003	1.001134
C	-3.964475	0.376111	1.176372
C	-2.281213	-2.494076	-0.342552
C	-3.339316	-3.433385	-0.729824
C	-4.477116	-2.958192	-1.417373
C	-5.489592	-3.840888	-1.802198
C	-5.396239	-5.203243	-1.482761

C	-4.282102	-5.680272	-0.779263
C	-3.259113	-4.803712	-0.403520
C	2.696147	1.198744	0.165761
N	2.075562	0.060192	-0.156864
C	2.830251	-0.935216	0.447884
C	3.964443	-0.376094	1.176427
C	3.877339	0.982019	1.001190
C	2.494262	-2.281437	0.342306
C	3.433634	-3.339416	0.729769
C	4.803845	-3.259462	0.402894
C	5.680592	-4.282036	0.779310
C	5.203742	-5.395874	1.483402
C	3.841368	-5.489387	1.802691
C	2.958624	-4.476939	1.417901
C	1.198901	-2.696377	-0.165849
N	0.060413	-2.075572	0.156627
C	-0.935046	-2.830171	-0.448143
C	-0.376109	-3.964982	-1.175850
C	0.982100	-3.877313	-1.001633
H	1.756446	-4.518823	-1.422778
H	4.665270	-0.927636	1.801201
H	0.927942	4.667160	-1.798878
H	-1.756449	4.518769	-1.422898
H	-0.927939	-4.667204	-1.798798
H	4.519853	1.756366	1.420803
H	-4.665302	0.927657	1.801141
H	-4.519926	-1.756343	1.420711
H	4.540356	1.897567	-1.671617
H	6.356422	3.466371	-2.350797
H	6.193872	5.889573	-1.774686
H	4.216506	6.736856	-0.510754
H	2.405059	5.164021	0.173462
H	5.163786	-2.406204	-0.175477
H	6.737264	-4.216182	0.511217
H	5.890270	-6.193050	1.776124
H	3.466849	-6.356405	2.350998
H	1.898119	-4.539944	1.672701
H	-4.540352	-1.897570	-1.671628
H	-6.356416	-3.466373	-2.350816
H	-6.193861	-5.889578	-1.774718
H	-4.216508	-6.736859	-0.510764
H	-2.405071	-5.164023	0.173472
H	-5.163805	2.406240	-0.175470
H	-6.737261	4.216206	0.511305
H	-5.890229	6.193048	1.776225
H	-3.466790	6.356397	2.351021

H	-1.898083	4.539938	1.672662

tetraphenylporphine S_1

C	-4.358744	-0.086474	0.309902
C	-3.073394	-0.729534	0.070998
N	-2.124662	0.303280	-0.060583
C	-2.746162	1.560461	0.070933
C	-4.160157	1.303094	0.310018
C	-2.114204	2.836207	-0.024936
C	-0.699634	3.056521	-0.151345
N	0.293360	2.053310	-0.013922
C	1.527436	2.738573	-0.151133
C	1.300475	4.167913	-0.412506
C	-0.081726	4.365235	-0.412698
C	2.823808	2.131157	-0.024537
C	3.073349	0.729508	0.071236
N	2.124633	-0.303305	-0.060514
C	2.746113	-1.560487	0.071124
C	4.160079	-1.303122	0.310425
C	4.358664	0.086441	0.310350
C	2.114174	-2.836229	-0.024829
C	0.699604	-3.056546	-0.151317
N	-0.293398	-2.053348	-0.013930
C	-1.527471	-2.738608	-0.151258
C	-1.300492	-4.167939	-0.412675
C	0.081709	-4.365251	-0.412761
C	-2.823842	-2.131192	-0.024763
H	0.617373	-5.302614	-0.616584
C	3.005826	-4.040475	0.004036
H	4.916277	-2.076199	0.495911
H	1.104964	-0.157398	-0.125363
H	2.077058	4.917989	-0.616063
H	-0.617373	5.302604	-0.616544
H	-2.077056	-4.918006	-0.616337
C	4.016871	3.037661	0.005086
C	-3.005830	4.040469	0.004040
C	-4.016900	-3.037698	0.005010
H	5.301211	0.616755	0.495449
H	-4.916383	2.076170	0.495397
H	-5.301323	-0.616792	0.494831
H	-1.104977	0.157370	-0.125214
C	5.053122	2.915657	-0.970314
C	6.178197	3.781956	-0.941493
C	6.286978	4.779817	0.065497
C	5.260037	4.908267	1.041572

C	4.132334	4.046989	1.009648
H	4.960782	2.152252	-1.761514
H	6.964523	3.682934	-1.707832
H	7.160616	5.451240	0.088496
H	5.340245	5.675377	1.829252
H	3.341707	4.138222	1.773706
C	4.034570	-4.212972	-0.971685
C	4.874010	-5.358206	-0.941887
C	4.699753	-6.346756	0.065088
C	3.678150	-6.183037	1.041483
C	2.834805	-5.041884	1.008591
H	4.157415	-3.455451	-1.764394
H	5.658116	-5.481681	-1.706949
H	5.350279	-7.236083	0.087321
H	3.542607	-6.940734	1.830693
H	2.048690	-4.909755	1.771328
C	-5.053220	-2.915745	-0.970319
C	-6.178287	-3.782050	-0.941375
C	-6.287023	-4.779813	0.065717
C	-5.259991	-4.908240	1.041699
C	-4.132296	-4.046955	1.009651
H	-4.960955	-2.152359	-1.761547
H	-6.964623	-3.683131	-1.707715
H	-7.160728	-5.451141	0.088900
H	-5.340099	-5.675364	1.829374
H	-3.341635	-4.138117	1.773682
C	-4.034639	4.213029	-0.971600
C	-4.873937	5.358366	-0.941799
C	-4.699593	6.346865	0.065210
C	-3.677889	6.183110	1.041495
C	-2.834692	5.041849	1.008607
H	-4.157703	3.455429	-1.764199
H	-5.657945	5.482001	-1.706935
H	-5.350194	7.236132	0.087615
H	-3.542090	6.940914	1.830559
H	-2.048656	4.909572	1.771400

CC2/TZVP geometries – Group II

tetrafluorobenzene S_0

C	-1.194054	0.695303	0.022817
C	-1.194055	-0.695303	-0.022808
C	0.000000	-1.399322	0.021462
C	1.194055	-0.695303	-0.022812

C	1.194054	0.695303	0.022820
C	0.000000	1.399321	-0.021484
F	-2.362659	-1.359184	-0.025382
H	0.000000	-2.479980	-0.001106
F	2.362659	-1.359184	-0.025398
F	2.362658	1.359184	0.025449
H	0.000000	2.479980	0.001009
F	-2.362658	1.359184	0.025434

tetrafluorobenzene S_1

C	1.166960	-0.711234	0.115373
C	1.166964	0.711234	0.115387
C	-0.000001	1.469124	0.373482
C	-1.166962	0.711232	0.115379
C	-1.166961	-0.711236	0.115381
C	0.000001	-1.469121	0.373493
F	2.306126	1.327556	-0.233182
H	-0.000002	2.530999	0.560300
F	-2.306119	1.327551	-0.233212
F	-2.306108	-1.327560	-0.233235
H	0.000002	-2.530989	0.560350
F	2.306101	-1.327555	-0.233265

benzonitrile S_0

C	-0.000010	0.025790	-1.056730
C	-1.214659	-0.010425	-0.359015
C	-1.208794	0.016785	1.032265
C	0.000001	-0.020520	1.727824
C	1.208787	0.016910	1.032253
C	1.214639	-0.010625	-0.359021
H	-2.147214	0.003873	-0.908478
H	-2.146928	-0.004919	1.572103
H	0.000006	-0.009214	2.810409
H	2.146936	-0.004016	1.572095
H	2.147195	0.002979	-0.908499
C	0.000005	0.012533	-2.487537
N	0.000036	0.008606	-3.667663

benzonitrile S_1

C	-0.000029	-0.036809	-1.108243
C	-1.236835	0.045478	-0.374399
C	-1.226562	-0.019502	1.052690
C	-0.000163	0.009101	1.773846

C	1.226300	-0.019619	1.052803
C	1.236711	0.045379	-0.374285
H	-2.172328	0.091909	-0.915700
H	-2.169219	-0.029871	1.583773
H	-0.000217	-0.032688	2.853597
H	2.168906	-0.030117	1.583973
H	2.172261	0.091773	-0.915491
C	0.000023	-0.051767	-2.512719
N	0.000050	-0.073472	-3.699667

o-fluorophenol, *cis* S_0

C	0.326477	1.456627	-0.021519
C	-0.874486	0.775240	0.033162
C	-0.951262	-0.616225	-0.015326
C	0.237272	-1.340415	0.030029
C	1.459919	-0.673735	-0.015721
C	1.510642	0.719859	0.013834
F	-2.056405	1.459990	0.030688
O	-2.146838	-1.276476	-0.008118
H	0.182577	-2.421179	0.013940
H	2.376533	-1.248459	0.004271
H	2.461310	1.234633	-0.018833
H	0.322177	2.538366	-0.007999
H	-2.847907	-0.608244	-0.038407

o-fluorophenol, *cis* S_1

C	0.302974	1.489119	0.102234
C	-0.938492	0.812242	0.192136
C	-0.945101	-0.621953	0.031399
C	0.244019	-1.384825	0.040711
C	1.480284	-0.699325	-0.101628
C	1.495152	0.707352	-0.006532
F	-2.068415	1.442358	-0.337210
O	-2.127061	-1.262108	-0.057082
H	0.181765	-2.455589	0.185471
H	2.408885	-1.249076	-0.151811
H	2.439626	1.231203	-0.096475
H	0.347993	2.565400	0.193737
H	-2.821621	-0.574818	0.005050

o-fluorophenol, *trans* S_0

C	0.290603	1.263513	-0.027360
C	-0.948119	0.618122	0.019812

C	-0.964891	-0.774925	-0.029574
C	0.226259	-1.499904	0.017661
C	1.449488	-0.836866	-0.014132
C	1.479614	0.558352	0.019614
O	-2.068790	1.401062	0.020688
H	-1.919436	-1.290406	-0.010639
H	0.190378	-2.581139	-0.004394
H	2.376085	-1.393962	0.016100
H	2.410892	1.108933	0.004459
F	0.312871	2.613839	-0.031886
H	-2.836768	0.813317	0.026569

o-fluorophenol, *trans* S_1

C	0.294895	1.287805	0.095768
C	-0.955703	0.625840	0.108497
C	-1.039322	-0.813402	0.094419
C	0.189944	-1.496213	-0.063220
C	1.432035	-0.802405	-0.090294
C	1.530360	0.580257	0.199641
O	-2.056134	1.392181	-0.076599
H	-1.928494	-1.313168	0.464227
H	0.194090	-2.572188	-0.188346
H	2.336746	-1.373430	-0.264048
H	2.468291	1.110446	0.252191
F	0.309563	2.598346	-0.221036
H	-2.776280	0.775930	-0.311199

m-fluorophenol, *cis* S_0

C	0.308648	1.409675	-0.023069
C	-0.931100	0.787517	0.018043
C	-0.968301	-0.606849	-0.019208
C	0.213980	-1.347056	0.032204
C	1.435081	-0.683214	-0.009772
C	1.503172	0.710917	0.017374
O	-2.146108	-1.307839	-0.023519
F	0.337613	2.765365	-0.038051
H	0.158983	-2.426885	0.017132
H	2.351843	-1.257969	0.016256
H	2.443747	1.242233	-0.008836
H	-1.833571	1.386286	-0.005438
H	-2.876203	-0.674725	-0.058210

m-fluorophenol, *cis* S_1

C	1.224275	-0.033628	-0.691728
C	-0.062016	0.008299	-0.107548
C	-0.029965	0.041815	1.325962
C	1.163384	0.015364	2.089714
C	2.436873	0.166402	1.443089
C	2.439547	-0.042887	0.032538
O	-1.189248	-0.020221	2.030759
F	1.304777	-0.121802	-2.039260
H	1.078521	-0.132201	3.158525
H	3.355345	0.146798	2.008183
H	3.360929	-0.165429	-0.522219
H	-0.923965	0.341062	-0.673169
H	-1.903100	-0.203573	1.395101

m-fluorophenol, *trans* S_0

C	0.267796	1.306157	-0.019020
C	-0.950866	0.628838	0.018027
C	-0.987391	-0.765850	-0.034547
C	0.206542	-1.483723	0.012412
C	1.437077	-0.832517	-0.017528
C	1.429642	0.555214	0.019376
O	-2.082116	1.402924	0.024855
H	-1.938543	-1.285652	-0.016940
H	0.176052	-2.565336	-0.012938
H	2.373178	-1.371644	0.008878
F	2.614701	1.212798	0.031407
H	0.301813	2.386270	0.005159
H	-2.847888	0.812529	0.038721

m-fluorophenol, *trans* S_1

C	1.097301	-0.014641	-0.008205
C	0.335759	1.187092	0.017814
C	-1.090132	1.213243	-0.041429
C	-1.832169	-0.004974	0.115956
C	-1.091051	-1.223342	-0.015078
C	0.321163	-1.198751	0.003039
O	1.050622	2.341959	-0.014853
H	-1.597591	2.161829	-0.176782
H	-2.910409	-0.009152	0.079275
H	-1.589800	-2.180804	-0.086270
F	0.971378	-2.383820	-0.046971
H	2.166164	-0.016559	0.136900
H	0.426460	3.082103	0.062668

p-fluorophenol S_0

C	0.270997	1.319382	0.020482
C	-0.951683	0.648459	-0.025603
C	-0.984004	-0.745117	0.028366
C	0.204996	-1.473821	-0.011809
C	1.406945	-0.787278	0.022726
C	1.460613	0.599064	-0.014032
O	-2.087825	1.421607	-0.031483
H	-1.933395	-1.269065	0.009655
H	0.199555	-2.555071	0.011900
F	2.568325	-1.491260	0.024185
H	2.418764	1.100486	0.004759
H	0.279349	2.400940	-0.002426
H	-2.852656	0.831663	-0.069371

p-fluorophenol S_1

C	1.272486	0.684500	-0.018224
C	0.028721	1.366021	0.033943
C	-1.243384	0.715265	-0.047389
C	-1.258412	-0.706988	0.020053
C	-0.005503	-1.369073	-0.031544
C	1.259879	-0.742160	0.026463
O	0.099179	2.719698	0.056930
H	-2.156247	1.293654	0.018664
H	-2.170250	-1.284455	-0.004108
F	-0.029298	-2.713960	-0.053220
H	2.159332	-1.336647	-0.020517
H	2.188702	1.255354	0.010283
H	-0.809098	3.065682	0.043400

phenylacetylene S_0

C	1.210406	0.018728	-0.013252
C	0.000015	-0.016217	-0.723134
C	-1.210386	0.018729	-0.013267
C	-1.207061	-0.018298	1.378197
C	-0.000003	0.014483	2.077112
C	1.207064	-0.018299	1.378212
C	0.000017	0.001361	-2.150600
C	-0.000034	-0.014615	-3.371679
H	-2.144618	0.007450	-0.560781
H	-2.146478	0.000746	1.916861
H	-0.000010	-0.005522	3.159771
H	2.146474	0.000747	1.916889

H	2.144647	0.007448	-0.560753
H	-0.000033	-0.002858	-4.433597

phenylacetylene S_1

C	1.239804	-0.057202	-0.028718
C	-0.000065	0.008134	-0.764307
C	-1.239973	-0.057345	-0.028796
C	-1.230322	0.024109	1.398690
C	-0.000151	0.001046	2.111689
C	1.230059	0.024282	1.398764
C	-0.000021	0.023336	-2.162320
C	0.000001	0.044640	-3.390638
H	-2.174053	-0.086342	-0.574023
H	-2.169204	0.032721	1.936624
H	-0.000191	0.042889	3.192424
H	2.168905	0.033105	1.936759
H	2.173915	-0.086162	-0.573895
H	0.000033	0.059497	-4.452932

aniline S_0

C	0.922330	0.022617	0.000000
C	0.208862	0.065117	1.204279
C	-1.182526	0.026753	1.201552
C	-1.889537	0.055861	0.000000
C	-1.182525	0.026744	-1.201552
C	0.208862	0.065126	-1.204278
H	0.749070	0.056510	2.144737
H	-2.971272	0.029320	0.000000
H	-1.714716	0.045194	2.144929
H	-1.714716	0.045150	-2.144929
H	0.749071	0.056551	-2.144736
N	2.323920	0.098014	0.000001
H	2.746592	-0.296470	-0.829522
H	2.746592	-0.296478	0.829520

aniline S_1

C	0.905082	-0.039080	-0.000017
C	0.225917	-0.053362	1.252461
C	-1.197092	0.086255	1.245296
C	-1.876271	0.076713	0.000004
C	-1.197109	0.086244	-1.245298
C	0.225902	-0.053351	-1.252479
H	0.794491	-0.076235	2.173740

H	-2.959387	0.118248	0.000013
H	-1.756541	0.078281	2.170241
H	-1.756566	0.078274	-2.170238
H	0.794467	-0.076159	-2.173766
N	2.264733	-0.196898	-0.000002
H	2.766229	-0.014494	-0.859000
H	2.766136	-0.014455	0.859044

catechol S_0

C	0.470329	1.282780	0.005144
C	-0.748522	0.620160	-0.055463
C	-0.799587	-0.778209	0.011580
C	0.383199	-1.506985	-0.022058
C	1.609756	-0.844023	0.022321
C	1.657491	0.547701	-0.013749
O	-1.981236	1.245517	-0.086658
O	-2.000450	-1.431782	0.005062
H	0.325002	-2.587596	0.002942
H	2.526478	-1.418925	0.009909
H	2.606743	1.065735	0.021265
H	0.493081	2.367053	-0.028964
H	-1.852255	2.188324	0.080298
H	-2.688591	-0.749173	0.048671

catechol S_1

C	0.460556	1.364438	-0.122967
C	-0.774501	0.630263	-0.208979
C	-0.805872	-0.788320	-0.136873
C	0.392814	-1.567824	-0.170028
C	1.569421	-0.850525	0.113800
C	1.615538	0.569773	0.070586
O	-1.981314	1.244583	0.009756
O	-1.979784	-1.415884	0.104727
H	0.348987	-2.642560	-0.259941
H	2.495838	-1.386320	0.282781
H	2.571432	1.057463	0.225612
H	0.527000	2.385230	-0.481929
H	-1.777840	2.116573	0.407413
H	-2.662275	-0.716889	0.166043

resorcinol, isomer 1 S_0

C	0.075430	1.148970	-0.039355
C	-1.139441	0.466397	0.011987

C	-1.172002	-0.926346	-0.026347
C	0.032671	-1.629925	0.014669
C	1.253980	-0.968819	-0.024041
C	1.264923	0.427135	0.010454
O	-2.274976	1.239077	0.019863
H	-2.119339	-1.452384	0.004594
H	0.013507	-2.712383	-0.001478
H	2.190872	-1.507832	0.002664
O	2.491871	1.042073	0.011476
H	0.071811	2.232997	-0.025902
H	-3.036782	0.643602	0.026030
H	2.347585	1.997750	0.043667

resorcinol, isomer 1 S_1

C	0.000719	1.062144	0.208484
C	-1.181428	0.315357	0.033336
C	-1.183734	-1.104907	-0.034234
C	-0.005628	-1.848836	0.330327
C	1.192121	-1.109919	-0.000012
C	1.186865	0.302553	0.042198
O	-2.338662	1.020313	-0.110210
H	-2.076294	-1.612944	-0.390618
H	-0.007863	-2.927004	0.263024
H	2.096971	-1.609420	-0.326880
O	2.394527	0.912739	-0.123122
H	-0.013626	2.108479	0.480091
H	-3.074543	0.388038	-0.101302
H	2.221567	1.859529	-0.251435

resorcinol, isomer 2 S_0

C	1.199695	0.012450	-0.546893
C	-0.000001	-0.034398	-1.249910
C	-1.199698	0.012476	-0.546897
C	-1.211472	-0.027520	0.849654
C	0.000004	0.013835	1.534709
C	1.211465	-0.027869	0.849649
O	-2.350874	0.017801	-1.294862
O	2.350870	0.018305	-1.294858
H	-2.150318	0.001059	1.390829
H	0.000004	-0.005296	2.617275
H	2.150329	-0.000024	1.390830
H	0.000001	-0.015283	-2.331208
H	-3.100525	0.030478	-0.684403
H	3.100518	0.030994	-0.684395

resorcinol, isomer 2 S_1

C	1.178491	-0.040905	-0.339129
C	-0.000078	-0.224576	-1.086385
C	-1.178641	-0.041110	-0.339072
C	-1.176775	0.008963	1.080547
C	0.000007	-0.404094	1.816302
C	1.176685	0.009162	1.080490
O	-2.334157	0.130889	-1.038564
O	2.333944	0.131288	-1.038676
H	-2.045077	0.409853	1.598019
H	0.000029	-0.335998	2.895338
H	2.044945	0.410189	1.597926
H	-0.000090	-0.355401	-2.156871
H	-3.068138	0.131650	-0.404253
H	3.067951	0.132216	-0.404395

resorcinol, isomer 3 S_0

C	1.205202	-0.007510	-0.288981
C	-0.000049	0.052436	-0.990823
C	-1.205296	-0.007353	-0.288961
C	-1.214489	0.022594	1.103628
C	-0.000031	-0.015612	1.783592
C	1.214422	0.022428	1.103608
O	-2.421473	-0.004083	-0.927192
O	2.421369	-0.004383	-0.927231
H	-2.159798	-0.007413	1.627611
H	-0.000023	-0.004421	2.866309
H	2.159736	-0.007702	1.627576
H	-0.000058	0.050234	-2.077520
H	2.263039	-0.056339	-1.879511
H	-2.263168	-0.056080	-1.879473

resorcinol, isomer 3 S_1

C	-0.025281	-0.305189	1.188623
C	-0.126022	-1.087051	0.000000
C	-0.025282	-0.305190	-1.188622
C	0.029588	1.110182	-1.200239
C	-0.174391	1.857384	0.000000
C	0.029591	1.110182	1.200240
O	0.080079	-0.915946	-2.403758
O	0.080091	-0.915943	2.403759
H	0.231907	1.597605	-2.146462

H	-0.122737	2.934961	0.000000
H	0.231911	1.597606	2.146462
H	-0.662995	-2.034395	-0.000002
H	0.262967	-1.854733	2.226560
H	0.262986	-1.854730	-2.226560

hydroquinone, *cis* S_0

C	-0.697930	0.025648	1.094290
C	0.697931	-0.025667	1.094289
C	1.396065	0.020265	-0.109318
C	0.694083	-0.018529	-1.315155
C	-0.694083	0.018525	-1.315155
C	-1.396065	-0.020268	-0.109318
O	2.771401	0.009918	-0.181177
O	-2.771400	-0.009893	-0.181177
H	1.246101	-0.000221	-2.245784
H	-1.246101	0.000207	-2.245784
H	-1.233454	0.008025	2.037625
H	1.233455	-0.008043	2.037624
H	-3.116952	-0.064001	0.719809
H	3.116951	0.064036	0.719809

hydroquinone, *cis* S_1

C	0.707425	-0.061906	-1.136999
C	-0.707610	0.062018	-1.136956
C	-1.378069	-0.016046	0.122875
C	-0.712666	0.014026	1.370218
C	0.712654	-0.014073	1.370176
C	1.377972	0.016090	0.122787
O	-2.735563	-0.017089	0.168521
O	2.735469	0.017135	0.168337
H	-1.291558	-0.040389	2.280386
H	1.291599	0.040365	2.280309
H	1.277410	-0.053933	-2.058016
H	-1.277654	0.053933	-2.057936
H	3.061796	0.023877	-0.746338
H	-3.061954	-0.023595	-0.746132

hydroquinone, *trans* S_0

C	0.021575	1.393440	0.014949
C	-1.196308	0.719522	-0.025689
C	-1.213846	-0.674875	0.023364
C	-0.021562	-1.393444	-0.015002

C	1.196319	-0.719538	0.025717
C	1.213855	0.674860	-0.023380
O	-2.342034	1.483919	-0.023517
H	-2.159116	-1.207273	0.007812
H	-0.028608	-2.475270	0.009726
O	2.342043	-1.483929	0.023904
H	2.159106	1.207289	-0.007699
H	0.028560	2.475264	-0.009777
H	-3.099116	0.884570	-0.063949
H	3.099132	-0.884534	0.063542

hydroquinone, *trans* S_1

C	1.267059	0.678625	0.001008
C	0.034279	1.376834	0.037810
C	-1.239932	0.743316	-0.054752
C	-1.266908	-0.678528	-0.001153
C	-0.034129	-1.376739	-0.037923
C	1.240085	-0.743221	0.054599
O	0.125709	2.731480	0.062467
H	-2.145340	1.327952	0.052777
H	-2.189664	-1.240562	-0.001734
O	-0.125559	-2.731387	-0.062470
H	2.145492	-1.327859	-0.052936
H	2.189815	1.240659	0.001584
H	-0.775276	3.087186	-0.012512
H	0.775422	-3.087083	0.012607

salicylic acid S_0

C	1.103972	1.598226	0.015859
C	1.131325	0.198111	-0.007634
C	-0.085564	-0.518278	0.067541
C	-1.302179	0.184809	0.008195
C	-1.319639	1.568964	0.017878
C	-0.107212	2.270415	-0.022229
O	2.339945	-0.403573	-0.011982
C	-0.042220	-1.978721	0.017293
O	-1.257552	-2.575346	-0.007099
O	0.999789	-2.647419	0.000618
H	-2.226376	-0.376559	0.030884
H	2.046519	2.129422	-0.012323
H	-2.261095	2.100866	-0.015125
H	-0.110354	3.353590	-0.022040
H	2.161151	-1.373934	-0.013168
H	-1.070384	-3.530558	-0.033660

salicylic acid S_1

C	0.998588	1.934591	0.043317
C	0.982717	0.551326	0.147177
C	-0.267035	-0.145494	0.064688
C	-1.432519	0.547063	-0.011876
C	-1.409798	1.991682	-0.096172
C	-0.225602	2.666257	-0.014143
O	2.112436	-0.166972	0.231590
C	-0.182514	-1.631533	0.182477
O	-1.350834	-2.310645	0.266262
O	0.817667	-2.238680	-0.467132
H	-2.379487	0.021420	-0.043479
H	1.953705	2.444509	0.083782
H	-2.352322	2.524809	-0.109277
H	-0.199795	3.747515	-0.059195
H	1.584109	-1.562092	-0.274719
H	-1.138737	-3.236810	0.056702

o-cresol, *cis* S_0

C	1.965914	0.514882	-0.005295
C	0.729339	1.154708	0.029687
C	-0.467740	0.435910	-0.029869
C	-0.391334	-0.963734	0.015080
C	0.837657	-1.619316	-0.033779
C	2.014624	-0.879009	0.007904
C	-1.803682	1.125590	-0.028619
O	-1.516435	-1.756197	-0.006205
H	0.851680	-2.701760	-0.025567
H	2.967835	-1.392115	-0.016472
H	2.878399	1.096002	0.027272
H	0.684778	2.238327	0.019293
H	-2.288640	-1.190391	0.128009
H	-2.388597	0.874831	0.861645
H	-1.676626	2.206969	-0.037928
H	-2.395378	0.855603	-0.907810

o-cresol, *cis* S_1

C	1.881299	-0.096475	-0.780467
C	0.632778	-0.066505	-1.467391
C	-0.592989	-0.100484	-0.722253
C	-0.470960	0.073440	0.700175
C	0.768770	0.053645	1.400387

C	1.968664	0.017614	0.632335
C	-1.909867	-0.026204	-1.420838
O	-1.578423	0.167068	1.483584
H	0.764037	0.154038	2.476232
H	2.932535	-0.006557	1.120650
H	2.794265	-0.152601	-1.361131
H	0.606060	-0.148196	-2.546180
H	-2.356181	0.154479	0.901106
H	-2.724190	-0.494592	-0.857576
H	-2.210974	1.007005	-1.642354
H	-1.855402	-0.555164	-2.373869

o-cresol, *trans* S_0

C	2.422255	0.025429	0.028315
C	1.246048	-0.022810	-0.720026
C	0.031003	0.016422	-0.022156
C	-0.003501	-0.034131	1.370317
C	1.187366	0.013069	2.094071
C	2.406968	-0.006658	1.423520
C	1.246715	-0.010587	-2.220625
O	-1.113672	0.015595	-0.787335
H	-0.958291	-0.022708	1.886845
H	1.155287	-0.010483	3.176123
H	3.336127	0.023149	1.977778
H	3.370675	0.013857	-0.497589
H	-1.871439	0.022124	-0.186239
H	2.266920	-0.029237	-2.602688
H	0.709485	-0.873511	-2.617009
H	0.746757	0.880479	-2.603331

o-cresol, *trans* S_1

C	2.430624	0.285876	-0.006912
C	1.218001	0.081171	-0.756480
C	0.003830	0.006533	-0.017479
C	-0.057267	-0.106211	1.414608
C	1.176525	-0.055176	2.113621
C	2.398353	0.075358	1.396444
C	1.257113	-0.031206	-2.241454
O	-1.145766	-0.086857	-0.737911
H	-1.004909	0.028526	1.923820
H	1.196112	-0.139102	3.192188
H	3.327956	0.070656	1.953492
H	3.372588	0.380864	-0.530096
H	-1.848896	-0.339336	-0.113506

H	1.929703	-0.840509	-2.544742
H	0.272388	-0.220723	-2.663015
H	1.652328	0.890135	-2.682598

m-cresol, *cis* S_0

C	1.156771	-0.043478	2.087580
C	2.372588	-0.007574	1.413444
C	2.415126	-0.019666	0.018714
C	1.233435	0.032687	-0.723730
C	0.012803	-0.006625	-0.042648
C	-0.025897	0.016865	1.351091
C	1.261216	0.003489	-2.228231
O	-1.204927	0.024997	2.056910
H	1.107329	-0.035031	3.168426
H	3.295125	-0.037273	1.980347
H	3.370081	0.007452	-0.492525
H	-0.916797	0.027980	-0.604725
H	-1.931495	0.077027	1.420868
H	2.180752	0.447731	-2.609086
H	1.207869	-1.022522	-2.598297
H	0.418316	0.553310	-2.648190

m-cresol, *cis* S_1

C	1.163392	-0.001265	2.133670
C	2.417368	0.067233	1.451860
C	2.419079	0.009628	0.031046
C	1.221292	0.031496	-0.753016
C	-0.029634	-0.091271	-0.070883
C	-0.022704	-0.002920	1.358009
C	1.262644	0.019616	-2.244084
O	-1.191897	-0.013380	2.050650
H	1.084740	0.009615	3.211595
H	3.347105	0.045853	2.001604
H	3.369113	0.010858	-0.492039
H	-0.968017	-0.051644	-0.613736
H	-1.915435	-0.060387	1.403795
H	2.283088	0.117160	-2.615076
H	0.842478	-0.911251	-2.641828
H	0.669663	0.840028	-2.661630

m-cresol, *trans* S_0

C	-1.146116	-1.135567	-0.016245
C	-1.197632	0.261383	0.023644

C	-0.001995	0.981274	-0.016476
C	1.223432	0.320394	0.023272
C	1.271949	-1.073835	-0.024708
C	0.080975	-1.795185	0.012201
C	-2.512956	0.993316	0.013398
O	2.354371	1.101574	0.032135
H	2.227495	-1.587410	-0.006372
H	0.114578	-2.877562	-0.011499
H	-2.065566	-1.708061	0.007671
H	-0.008627	2.065066	0.003542
H	3.121687	0.513226	0.037837
H	-3.349535	0.295162	0.019643
H	-2.605568	1.640931	0.886865
H	-2.600819	1.620506	-0.875070

m-cresol, *trans* S_1

C	-1.206683	-1.065166	0.027831
C	0.207611	-1.242890	-0.057409
C	1.031767	-0.070948	0.007228
C	0.401723	1.202468	-0.030378
C	-1.012945	1.380756	0.041904
C	-1.833148	0.215724	-0.006463
C	0.831338	-2.597514	-0.014544
O	1.233083	2.277302	-0.045279
H	-1.436515	2.377700	0.012012
H	-2.909875	0.296357	0.039122
H	-1.835604	-1.948140	0.058266
H	2.111655	-0.126922	-0.017915
H	0.683095	3.078038	-0.031734
H	0.084480	-3.382815	-0.135414
H	1.577203	-2.712347	-0.806943
H	1.349458	-2.766299	0.936802

p-cresol S_0

C	0.713270	0.002969	-1.192326
C	-0.676918	-0.032340	-1.201559
C	-1.373517	0.012004	0.005781
C	-0.672641	-0.031390	1.209924
C	0.721585	0.009523	1.198896
C	1.441299	-0.026180	0.003279
O	-2.746927	0.008798	-0.059135
C	2.945183	0.027285	-0.003972
H	-1.209366	-0.019110	2.153296
H	1.252703	-0.012029	2.144161

H	1.243266	-0.019696	-2.138349
H	-1.231718	-0.021257	-2.131026
H	-3.086883	0.040498	0.845431
H	3.353626	-0.559652	-0.827413
H	3.303437	1.052703	-0.117968
H	3.355158	-0.366750	0.926280

p-cresol S_1

C	0.734126	-0.101607	-1.244035
C	-0.690532	-0.015610	-1.251585
C	-1.361670	-0.017089	-0.002498
C	-0.685599	0.051497	1.254374
C	0.734388	-0.060035	1.243257
C	1.436692	-0.033054	-0.003856
O	-2.718053	0.018526	-0.053623
C	2.926098	0.046801	-0.000990
H	-1.252187	0.046169	2.178050
H	1.294540	-0.039490	2.169028
H	1.289288	-0.093978	-2.172603
H	-1.271662	-0.020640	-2.162663
H	-3.046789	0.053562	0.860093
H	3.345646	-0.422155	-0.892202
H	3.255388	1.091358	0.010993
H	3.341873	-0.438877	0.883549

o-methoxyphenol S_0

C	2.024701	-0.080278	-0.016249
C	0.866228	0.704072	0.018397
C	-0.378314	0.084600	-0.035305
C	-0.471865	-1.317573	0.024666
C	0.680678	-2.088220	-0.020003
C	1.931215	-1.467575	0.016218
O	-1.600515	0.716326	-0.043060
O	-1.696908	-1.923682	0.021616
H	0.584262	-3.166313	-0.000967
H	2.827865	-2.073217	-0.006059
H	2.992084	0.404191	0.011684
H	0.947825	1.781878	-0.005561
C	-1.577812	2.140381	-0.008426
H	-2.353129	-1.208360	0.046258
H	-2.617841	2.452201	-0.007687
H	-1.084013	2.498149	0.897167
H	-1.073139	2.543127	-0.888601

o-methoxyphenol S_1

C	2.467351	0.064215	0.040079
C	1.368095	-0.298288	-0.772034
C	0.096112	-0.320988	-0.091524
C	0.014257	-0.192795	1.321773
C	1.190243	-0.146576	2.143715
C	2.367027	0.198649	1.451311
O	-1.108650	-0.120956	-0.717322
O	-1.180897	0.087201	1.899650
H	1.106348	-0.159135	3.219785
H	3.252618	0.492445	2.003306
H	3.425386	0.265532	-0.428490
H	1.505046	-0.696535	-1.768957
C	-1.069365	0.137492	-2.133823
H	-1.840667	0.095214	1.177283
H	-2.102022	0.310010	-2.420256
H	-0.457069	1.013313	-2.343051
H	-0.675255	-0.728809	-2.663365

m-methoxyphenol, isomer 1 S_0

C	0.929806	1.452917	-0.023685
C	-0.264104	0.725422	-0.010247
C	-0.236526	-0.670829	-0.072149
C	0.995096	-1.330410	0.002475
C	2.190174	-0.620240	-0.016015
C	2.140094	0.772833	0.024059
H	-1.148217	-1.254325	-0.078146
O	1.076610	-2.702881	-0.005806
H	3.127845	-1.157225	0.023769
H	3.064944	1.336173	0.024184
H	0.882862	2.532924	0.009431
O	-1.412635	1.468514	-0.016259
H	0.180051	-3.057090	0.067193
C	-2.639242	0.748413	0.020047
H	-3.420516	1.502480	0.013984
H	-2.747942	0.107920	-0.858389
H	-2.718185	0.145568	0.927907

m-methoxyphenol, isomer 1 S_1

C	0.928429	1.434202	0.006914
C	-0.275520	0.688908	0.028377
C	-0.314487	-0.744911	0.027937
C	0.983366	-1.339298	0.008279

C	2.197099	-0.609945	-0.014318
C	2.199776	0.800965	0.182158
H	-1.136655	-1.290252	0.483434
O	1.104697	-2.695222	-0.104013
H	3.112804	-1.165761	-0.175746
H	3.115723	1.369972	0.147766
H	0.844283	2.506123	-0.125901
O	-1.399338	1.453622	-0.067252
H	0.223361	-3.032733	-0.339520
C	-2.658226	0.768885	-0.020432
H	-3.401550	1.513153	-0.288522
H	-2.670752	-0.053726	-0.735214
H	-2.853008	0.396021	0.986052

m-methoxyphenol, isomer 2 S_0

C	0.346150	2.162963	-0.022800
C	-0.842167	1.450969	0.027551
C	-0.802992	0.050069	0.008549
C	0.417739	-0.622007	0.058036
C	1.601175	0.118224	-0.009201
C	1.580884	1.508960	0.017226
O	-2.019459	-0.572909	0.014667
C	-2.004016	-1.996764	-0.018648
O	2.767441	-0.609966	-0.021135
H	0.491932	-1.699392	0.053748
H	2.506358	2.071826	-0.027155
H	0.319488	3.245500	-0.017418
H	-1.802534	1.947550	-0.000372
H	-3.046826	-2.299204	-0.010876
H	-1.519803	-2.365293	-0.925614
H	-1.499319	-2.405733	0.859280
H	3.505039	0.015298	-0.010498

m-methoxyphenol, isomer 2 S_1

C	1.254741	-0.347933	-0.713657
C	0.071258	-0.041443	0.065704
C	0.105540	-0.118570	1.476557
C	1.319118	-0.321221	2.191607
C	2.465545	-0.042362	1.423886
C	2.433348	0.056125	0.006340
O	-1.103043	0.033179	2.077548
C	-1.111674	0.090778	3.509999
O	3.632231	0.140394	2.106581
H	1.395169	-0.485638	3.253464

H	3.299450	0.458386	-0.513884
H	1.225129	-0.242029	-1.789009
H	-0.847283	0.293628	-0.402975
H	-2.152298	0.231287	3.784507
H	-0.740387	-0.841133	3.936353
H	-0.510355	0.929152	3.862644
H	4.348641	0.207402	1.456225

p-methoxyphenol, *cis* S_0

C	-0.321112	0.738440	-0.010933
C	-1.554235	0.074749	0.016107
C	-1.611073	-1.309127	-0.023772
C	-0.431378	-2.057028	0.022512
C	0.794713	-1.403923	-0.014899
C	0.857210	-0.006145	0.038868
O	-0.555998	-3.428738	0.008140
O	-0.386370	2.108503	-0.004224
C	0.858921	2.793980	-0.023589
H	1.827047	0.469960	0.025297
H	-2.460992	0.665521	-0.008026
H	-2.562876	-1.824260	-0.013891
H	1.716734	-1.975923	0.005936
H	0.611990	3.851506	-0.018535
H	1.455650	2.555330	0.860380
H	1.429498	2.555397	-0.924677
H	0.330640	-3.807871	0.074768

p-methoxyphenol, *cis* S_1

C	-0.323419	0.719129	0.014513
C	-1.599691	0.096717	0.030380
C	-1.664241	-1.327664	-0.023676
C	-0.448886	-2.044776	0.008319
C	0.835011	-1.423263	-0.049641
C	0.905014	-0.010205	0.084157
O	-0.546356	-3.400493	-0.007327
O	-0.369628	2.072427	0.026775
C	0.869624	2.796992	-0.023463
H	1.861623	0.487413	0.107173
H	-2.481378	0.717183	-0.039024
H	-2.600460	-1.865807	0.002119
H	1.731456	-2.031428	-0.019897
H	0.586227	3.843652	0.015798
H	1.491814	2.546829	0.834994
H	1.397714	2.583190	-0.952071

H	0.355577	-3.759878	-0.009128

p-methoxyphenol, *trans* S_0

C	-0.657412	1.310628	0.020688
C	-1.890500	0.672571	-0.029652
C	-1.959809	-0.722148	0.017253
C	-0.786334	-1.466287	-0.013940
C	0.455263	-0.829618	0.036042
C	0.524600	0.565712	-0.008122
O	-3.152284	-1.411891	0.004179
H	1.348870	-1.437001	0.025278
O	1.686223	1.295629	0.000244
H	-0.592986	2.390901	-0.003161
H	-2.800487	1.263780	-0.022324
H	-3.869445	-0.764734	0.032825
H	-0.846681	-2.546794	0.007954
C	2.896001	0.548493	-0.014168
H	3.694774	1.284256	-0.008366
H	2.979580	-0.086639	0.871146
H	2.972039	-0.067078	-0.913891

p-methoxyphenol, *trans* S_1

C	-0.664374	1.347815	0.020070
C	-1.934372	0.705965	-0.054437
C	-1.950806	-0.715242	0.018602
C	-0.782774	-1.515355	-0.010253
C	0.487752	-0.879202	0.074639
C	0.510579	0.545276	-0.003891
O	-3.129516	-1.391707	0.019202
H	1.391592	-1.466098	0.034820
O	1.657920	1.264280	-0.010306
H	-0.556977	2.422754	-0.007641
H	-2.856838	1.267175	0.033139
H	-3.842165	-0.734801	-0.043778
H	-0.884498	-2.591257	-0.006142
C	2.904905	0.550626	-0.015790
H	3.670145	1.318666	0.027408
H	2.974142	-0.098393	0.856172
H	3.005276	-0.030521	-0.931815

1-naphthol, *cis* S_0

C	0.832471	1.514057	0.020374
C	0.530042	0.123724	-0.044874

C	-0.845962	-0.268885	0.027338
C	-1.857944	0.719539	-0.027105
C	-1.520341	2.055127	-0.025232
C	-0.171222	2.457310	-0.036356
C	1.527917	-0.882740	-0.043504
C	1.186771	-2.218316	-0.055142
C	-0.167280	-2.606598	0.020460
C	-1.159178	-1.651080	0.006273
O	2.129384	1.969079	0.027869
H	-2.202985	-1.944791	0.038523
H	-0.426499	-3.658222	0.012046
H	1.964543	-2.972034	-0.068241
H	2.576874	-0.617169	-0.124834
H	-2.896411	0.409722	-0.005325
H	-2.295150	2.811299	-0.062388
H	0.098655	3.505407	-0.008121
H	2.696324	1.254578	0.348232

1-naphthol, *cis* S_1

C	0.857354	1.459218	0.030466
C	0.531592	0.087472	-0.130319
C	-0.853595	-0.245732	0.005918
C	-1.792384	0.814882	-0.044926
C	-1.427730	2.185885	-0.032562
C	-0.097674	2.523032	-0.028411
C	1.526567	-0.915445	-0.187587
C	1.116232	-2.285509	-0.069641
C	-0.213527	-2.604282	0.093376
C	-1.230855	-1.609161	0.040720
O	2.125363	1.821133	0.252697
H	-2.274444	-1.872168	0.169690
H	-0.503452	-3.644871	0.190473
H	1.868908	-3.065310	-0.055130
H	2.535038	-0.681492	-0.518546
H	-2.846551	0.555056	-0.061167
H	-2.193325	2.948952	-0.084089
H	0.258572	3.544684	0.004328
H	2.613913	0.983645	0.424689

1-naphthol, *trans* S_0

C	-0.717001	-0.541062	0.026701
C	-0.676689	-1.957218	-0.007484
C	0.524530	-2.631748	0.016845
C	1.741272	-1.917371	-0.018909

C	1.740910	-0.538935	0.002368
C	0.518809	0.174260	-0.033992
H	-1.613536	-2.503899	0.008608
H	0.536529	-3.714917	-0.000744
H	2.681083	-2.455756	0.001902
H	2.670781	0.014195	-0.012662
C	-1.941548	0.172683	-0.012254
C	-1.940344	1.548488	0.009823
C	-0.726812	2.267886	-0.024812
C	0.476450	1.594715	0.015375
H	-2.874151	-0.379356	0.007779
H	-2.875741	2.094349	-0.014023
H	-0.739549	3.352963	0.004282
O	1.691507	2.234057	0.028264
H	1.523511	3.186657	0.002934

1-naphthol, *trans* S_1

C	-0.734021	-0.565861	0.034501
C	-0.690677	-1.970513	0.006734
C	0.528810	-2.669930	0.035885
C	1.750442	-1.939216	-0.026973
C	1.755765	-0.537321	-0.011047
C	0.547942	0.190200	-0.039848
H	-1.628850	-2.516220	0.025043
H	0.539393	-3.751607	0.015796
H	2.694122	-2.470928	-0.016602
H	2.695325	0.000262	-0.039388
C	-1.936643	0.164871	-0.025566
C	-1.945635	1.573522	-0.002426
C	-0.735003	2.305944	-0.026718
C	0.488126	1.599002	0.028610
H	-2.878252	-0.373851	-0.018206
H	-2.889864	2.102864	-0.028185
H	-0.740069	3.388065	0.038616
O	1.682804	2.261401	0.062068
H	1.496297	3.209305	-0.012295

2-naphthol, *cis* S_0

C	0.601006	2.009624	-0.013179
C	0.623307	0.595128	0.034783
C	-0.612203	-0.121877	-0.020034
C	-1.824494	0.611000	0.014936
C	-1.815331	1.989081	-0.016329
C	-0.593818	2.696460	0.008046

C	1.835157	-0.141148	-0.005104
C	1.833461	-1.514835	0.021541
C	0.607160	-2.216839	-0.009588
C	-0.591362	-1.537604	0.028672
H	-1.532585	-2.080862	0.020186
H	1.543753	2.546616	-0.005061
H	-0.598441	3.779179	-0.021273
H	-2.751352	2.534427	0.001139
H	-2.764691	0.069589	0.004560
H	2.776458	0.397758	0.006283
H	2.755524	-2.081851	-0.001940
O	0.702744	-3.586098	-0.007995
H	-0.194303	-3.947741	-0.039644

2-naphthol, *cis* S_1

C	0.610578	1.996912	0.012878
C	0.654584	0.587455	-0.029321
C	-0.642389	-0.124581	0.030921
C	-1.845740	0.603479	-0.000782
C	-1.850045	2.012955	0.033834
C	-0.614514	2.690632	-0.012794
C	1.860958	-0.141962	0.011854
C	1.888644	-1.550035	-0.032145
C	0.641114	-2.215407	0.003165
C	-0.595159	-1.528262	-0.042694
H	-1.520779	-2.099474	-0.051871
H	1.541740	2.553071	-0.010665
H	-0.598882	3.774606	-0.004226
H	-2.780471	2.563558	0.004920
H	-2.782268	0.054837	0.011296
H	2.794053	0.411669	0.006631
H	2.804192	-2.120725	0.023128
O	0.674185	-3.571178	0.005880
H	-0.239809	-3.897542	0.039990

2-naphthol, *trans* S_0

C	0.514175	2.011873	-0.012637
C	0.541739	0.596333	0.034265
C	-0.691304	-0.127881	-0.021640
C	-1.907231	0.601902	0.014524
C	-1.902738	1.979071	-0.015361
C	-0.683181	2.692424	0.009899
C	1.753909	-0.133569	-0.006667
C	1.752431	-1.510073	0.022683

C	0.529358	-2.217726	-0.015178
C	-0.669975	-1.540531	0.020961
H	-1.598259	-2.100046	0.007478
H	1.454623	2.552968	-0.003520
H	-0.692630	3.775181	-0.018313
H	-2.840716	2.521068	0.002886
H	-2.844605	0.056072	0.003265
H	2.694895	0.405800	0.008667
H	2.689929	-2.057290	-0.002060
O	0.494305	-3.591065	-0.017917
H	1.405285	-3.914507	-0.011335

2-naphthol, *trans* S_1

C	0.521579	1.996127	0.013275
C	0.566382	0.588313	-0.029091
C	-0.725581	-0.123639	0.035726
C	-1.928234	0.600326	-0.001651
C	-1.936550	2.011488	0.028335
C	-0.705289	2.688628	-0.015403
C	1.777913	-0.136328	0.010402
C	1.809766	-1.544316	-0.045586
C	0.555668	-2.210453	0.008233
C	-0.679333	-1.530137	-0.023776
H	-1.590504	-2.118050	-0.022098
H	1.451759	2.554286	-0.009427
H	-0.689689	3.772769	-0.009160
H	-2.868240	2.559814	-0.003830
H	-2.863048	0.049041	0.012686
H	2.708599	0.421643	0.007490
H	2.734753	-2.101371	0.040379
O	0.477438	-3.563567	0.019039
H	1.382620	-3.914576	-0.015543

5-methoxysalicylic acid S_0

C	2.282492	-0.166885	-0.023695
C	1.571678	-1.349125	0.024437
C	0.165372	-1.345722	-0.001997
C	-0.512790	-0.136877	0.025782
C	0.206397	1.076049	-0.055626
C	1.613915	1.066630	0.002526
O	-0.424657	-2.579793	0.023314
C	-1.847978	-2.589205	-0.017007
C	-0.485273	2.360885	-0.007692
O	-1.839146	2.271660	-0.006841

O	2.369413	2.188871	-0.010503
O	0.081259	3.461747	0.021972
H	-2.134179	-3.636328	0.004188
H	-2.219268	-2.122727	-0.932645
H	-2.269168	-2.077552	0.851691
H	-1.590849	-0.087985	0.015339
H	3.364708	-0.166792	-0.008190
H	2.084836	-2.302742	0.018332
H	1.734137	2.942519	0.009751
H	-2.150877	3.193370	0.031168

5-methoxysalicylic acid S_1

C	2.187631	-0.128980	0.027036
C	1.744198	-1.468066	-0.010913
C	0.357863	-1.699836	-0.010516
C	-0.593271	-0.629631	-0.071658
C	-0.166608	0.689066	0.061304
C	1.275589	0.924428	-0.016495
O	-0.017786	-2.997015	-0.021697
C	-1.422620	-3.307417	0.011576
C	-1.032894	1.819337	0.039083
O	-2.377376	1.554908	0.030408
O	1.695296	2.187933	-0.055144
O	-0.615984	3.032465	0.033125
H	-1.468847	-4.391139	0.004379
H	-1.922946	-2.907775	-0.869796
H	-1.878131	-2.916032	0.920544
H	-1.653945	-0.828169	-0.122126
H	3.243340	0.111176	0.012432
H	2.426162	-2.303559	0.053525
H	0.788304	2.756918	-0.023397
H	-2.795923	2.432169	0.008329

m-dimethoxybenzene, *trans* S_0

C	0.019326	-0.707497	-0.186559
C	-0.020036	0.707822	-0.186514
C	0.039539	1.393667	1.023335
C	-0.004763	0.692761	2.235662
C	0.005574	-0.692530	2.235614
C	-0.039523	-1.393388	1.023302
O	-0.016384	1.287036	-1.421220
H	0.033566	2.474189	1.037364
H	0.028143	1.242611	3.167497
H	-0.026756	-1.242409	3.167458

H	-0.033551	-2.473912	1.037276
O	0.014884	-1.286661	-1.421275
C	0.017920	-2.709550	-1.443775
H	0.018126	-2.982230	-2.494889
H	0.910732	-3.111911	-0.959257
H	-0.874543	-3.114070	-0.960411
C	-0.018190	2.709928	-1.443654
H	-0.018556	2.982670	-2.494750
H	-0.910459	3.113082	-0.958791
H	0.874814	3.113592	-0.960574

m-dimethoxybenzene, *trans* S_1

C	-0.223104	-1.078765	-1.451238
C	-0.292630	0.173334	-0.712389
C	-0.339888	0.166958	0.703597
C	-0.168738	-1.060484	1.447456
C	0.287677	-2.161056	0.704633
C	0.332064	-2.142912	-0.714057
O	-0.005374	1.388862	-1.265630
C	0.035790	1.441301	-2.698036
O	-0.314923	1.393509	1.286864
C	-0.030670	1.433942	2.696271
H	-0.485603	-1.163893	2.476520
H	0.604175	-3.061977	1.220592
H	0.718757	-3.017015	-1.229684
H	-0.372337	-1.135397	-2.518251
H	0.187619	2.489133	-2.938708
H	0.860203	0.842972	-3.085745
H	-0.907999	1.095128	-3.121253
H	0.004925	2.490034	2.944763
H	-0.824401	0.946782	3.262153
H	0.924710	0.955905	2.908954

3P-propionic acid, *gauche* S_0

C	-0.906288	0.830637	-1.167266
C	-0.294276	0.714904	0.085774
C	-0.939629	-0.022023	1.084427
C	-2.139529	-0.680868	0.816270
C	-2.747363	-0.547073	-0.431171
C	-2.103714	0.172241	-1.438665
C	1.047757	1.344597	0.340041
C	2.175173	0.443833	-0.186575
C	2.121135	-0.874902	0.534991
O	2.197085	-1.008483	1.745818

O	1.947264	-1.923144	-0.315289
H	2.071474	0.282057	-1.258679
H	3.146873	0.898622	0.016495
H	1.193612	1.496714	1.410840
H	1.111352	2.315917	-0.155001
H	-0.473300	-0.116930	2.058787
H	-2.631929	-1.241133	1.601908
H	-3.680227	-1.056182	-0.639089
H	-2.569888	0.278953	-2.410655
H	-0.416482	1.403484	-1.948323
H	1.890910	-2.711240	0.255373

3P-propionic acid, *gauche* S_1

C	-0.827279	0.840778	-1.215723
C	-0.265847	0.762556	0.102832
C	-0.919917	-0.045207	1.095831
C	-2.159817	-0.691555	0.797996
C	-2.690898	-0.630448	-0.526102
C	-2.068145	0.193590	-1.511925
C	1.066597	1.367160	0.381580
C	2.201424	0.448943	-0.127260
C	2.074290	-0.876353	0.569854
O	2.243058	-1.053311	1.765632
O	1.693259	-1.869126	-0.280497
H	2.128335	0.314642	-1.205436
H	3.170950	0.880858	0.126233
H	1.199369	1.514504	1.455783
H	1.159083	2.336607	-0.116312
H	-0.491501	-0.112915	2.088347
H	-2.653988	-1.288317	1.552853
H	-3.614454	-1.142875	-0.760467
H	-2.492647	0.264656	-2.504382
H	-0.334829	1.445263	-1.968131
H	1.582965	-2.659459	0.279294

3P-propionic acid, *anti* S_0

C	1.437268	-0.440757	-0.000041
C	0.547009	0.797733	-0.000009
C	2.903407	-0.099426	0.000014
H	1.230634	-1.062598	0.874405
H	1.230683	-1.062514	-0.874559
C	-0.904329	0.405838	0.000000
H	0.774403	1.405464	0.877432
H	0.774385	1.405496	-0.877432

C	-1.593819	0.219419	1.202504
C	-2.914676	-0.226306	1.205306
C	-3.593178	-0.404723	0.000011
C	-2.914649	-0.226418	-1.205286
C	-1.593852	0.219487	-1.202496
H	-1.075039	0.375941	2.142806
H	-3.435809	-0.362484	2.145162
H	-4.621477	-0.744005	0.000015
H	-3.435679	-0.362963	-2.145146
H	-1.075183	0.376337	-2.142804
O	3.670184	-1.228858	0.000019
O	3.380635	1.021704	0.000049
H	4.591920	-0.915049	0.000049

3P-propionic acid, *anti* S_1

C	1.439050	-0.422540	0.000239
C	0.569694	0.837939	0.000186
C	2.910513	-0.104463	-0.000213
H	1.220157	-1.037710	0.876190
H	1.219701	-1.038101	-0.875323
C	-0.876785	0.482880	0.000084
H	0.813220	1.436636	0.880984
H	0.813344	1.436651	-0.880568
C	-1.574884	0.283647	1.238564
C	-2.897479	-0.260317	1.239121
C	-3.578138	-0.460685	-0.000109
C	-2.897309	-0.260297	-1.239242
C	-1.574711	0.283658	-1.238495
H	-1.066863	0.488011	2.173432
H	-3.412487	-0.437102	2.173704
H	-4.594506	-0.832019	-0.000182
H	-3.412191	-0.437060	-2.173899
H	-1.066556	0.488022	-2.173290
O	3.658191	-1.246495	-0.000125
O	3.405437	1.008881	-0.000616
H	4.585230	-0.948377	-0.000442

fluorine S_0

C	0.000144	-0.000004	-1.796462
C	-0.022764	1.178508	-0.853528
C	0.018471	0.731286	0.481328
C	-0.017956	-0.731281	0.481334
C	-0.020053	1.643949	1.536366
C	0.013302	3.007220	1.242973

C	-0.012488	3.452072	-0.083605
C	0.017614	2.538451	-1.140788
H	0.005715	2.890330	-2.166707
H	0.010580	4.515096	-0.291436
H	-0.008213	3.730731	2.049124
H	-0.008691	1.304751	2.566257
C	0.020392	-1.643958	1.536367
C	-0.013591	-3.007214	1.242974
C	0.011967	-3.452076	-0.083605
C	-0.017607	-2.538441	-1.140790
C	0.023138	-1.178510	-0.853523
H	0.009501	-1.304757	2.566261
H	0.007595	-3.730735	2.049125
H	-0.011827	-4.515084	-0.291436
H	-0.005460	-2.890321	-2.166705
H	-0.883317	-0.019887	-2.441710
H	0.883546	0.019875	-2.441791

fluorine S_1

C	-0.000040	-0.000005	-1.828953
C	-0.024477	1.166821	-0.879148
C	0.029077	0.707165	0.475425
C	-0.029142	-0.707213	0.475374
C	-0.012449	1.613518	1.567608
C	0.020713	2.986995	1.264376
C	-0.015106	3.438194	-0.072980
C	0.018278	2.540883	-1.164176
H	-0.005704	2.906470	-2.183393
H	-0.004072	4.505159	-0.263688
H	0.002426	3.717710	2.063970
H	0.015824	1.256166	2.589086
C	0.012403	-1.613586	1.567472
C	-0.020699	-2.986966	1.264332
C	0.015168	-3.438167	-0.072968
C	-0.018262	-2.540828	-1.164075
C	0.024299	-1.166874	-0.879124
H	-0.015777	-1.256211	2.588954
H	-0.002505	-3.717649	2.063960
H	0.004235	-4.505126	-0.263719
H	0.005784	-2.906416	-2.183299
H	-0.882643	-0.020516	-2.482573
H	0.882666	0.020477	-2.482443

phenanthrene S_0

C	0.725016	-0.020753	-0.350497
C	-0.725013	0.020339	-0.350505
C	-1.418401	-0.023214	0.892901
C	-0.681207	0.011950	2.117636
C	0.681200	-0.012164	2.117642
C	1.418403	0.022880	0.892908
C	-1.491028	-0.022899	-1.537101
C	-2.830421	0.017433	0.906310
H	-1.231757	-0.003197	3.052653
H	1.231741	0.003080	3.052664
C	1.491018	0.022616	-1.537095
C	2.873368	-0.010422	-1.500676
C	3.552324	0.011179	-0.270231
C	2.830433	-0.017377	0.906311
H	0.997581	0.021305	-2.500151
H	3.433689	0.015855	-2.427611
H	4.635029	-0.012088	-0.246743
H	3.341131	-0.006896	1.863585
C	-3.552324	-0.010812	-0.270233
C	-2.873365	0.010654	-1.500679
H	-0.997578	-0.021781	-2.500150
H	-3.433697	-0.015432	-2.427614
H	-4.635017	0.012963	-0.246724
H	-3.341124	0.006780	1.863579

phenanthrene S_1

C	0.711336	-0.013540	-0.388781
C	-0.711347	0.013685	-0.388781
C	-1.436624	-0.022723	0.891556
C	-0.700431	0.019324	2.088669
C	0.700446	-0.019530	2.088668
C	1.436635	0.022618	0.891555
C	-1.491215	-0.058091	-1.572937
C	-2.843381	0.035882	0.889914
H	-1.237507	0.010239	3.032157
H	1.237524	-0.010415	3.032155
C	1.491211	0.058408	-1.572923
C	2.888898	0.011088	-1.534368
C	3.574882	0.004340	-0.305840
C	2.843384	-0.036123	0.889888
H	1.002281	0.086585	-2.538340
H	3.445326	0.051253	-2.463197
H	4.656710	-0.033027	-0.283890
H	3.360650	-0.044511	1.844061
C	-3.574878	-0.004372	-0.305821

C	-2.888907	-0.010946	-1.534355
H	-1.002291	-0.085909	-2.538366
H	-3.445349	-0.051160	-2.463174
H	-4.656705	0.033023	-0.283863
H	-3.360647	0.043904	1.844090

2,4,6,8-decatetraene S_0

C	-2.588135	-5.006750	-0.008319
C	-2.475492	-3.517110	-0.005991
C	-1.311313	-2.839386	0.028122
C	-1.215988	-1.399751	0.031986
C	-0.046572	-0.717349	-0.043219
C	0.046614	0.717272	-0.042290
C	1.216240	1.399564	0.030617
C	1.311561	2.839203	0.028564
C	2.475636	3.516976	-0.008036
C	2.588280	5.006617	-0.008464
H	-0.376700	-3.396888	0.038949
H	-2.148467	-0.839151	0.061315
H	0.886333	-1.277422	-0.070649
H	-0.886363	1.277383	-0.066257
H	2.148792	0.838921	0.056590
H	0.376987	3.396690	0.043027
H	3.404285	2.950978	-0.026518
H	-3.404194	-2.951091	-0.020789
H	1.603546	5.474136	0.011162
H	3.149210	5.357809	0.860634
H	3.117431	5.361014	-0.895887
H	-1.603345	-5.474292	0.007651
H	-3.146453	-5.359250	0.861931
H	-3.119946	-5.359818	-0.894680

2,4,6,8-decatetraene S_1

C	-2.572020	-5.015465	0.016090
C	-2.528879	-3.530134	-0.006184
C	-1.360502	-2.795016	-0.012443
C	-1.279565	-1.396130	-0.069460
C	-0.056911	-0.687150	-0.079545
C	0.057220	0.687437	0.078955
C	1.279834	1.396485	0.068716
C	1.360625	2.795406	0.012327
C	2.528926	3.530643	0.005762
C	2.571903	5.015986	-0.015942
H	-0.419167	-3.344526	0.002516

H	-2.203813	-0.819801	-0.059353
H	0.859516	-1.270727	-0.161764
H	-0.859214	1.270963	0.161501
H	2.204112	0.820225	0.057609
H	0.419232	3.344837	-0.001847
H	3.476872	2.996052	0.023250
H	-3.476763	-2.995452	-0.024310
H	1.566329	5.438422	-0.037900
H	3.088577	5.417086	0.863704
H	3.118008	5.391151	-0.889014
H	-1.566503	-5.437990	0.038987
H	-3.118827	-5.390220	0.888896
H	-3.088055	-5.416882	-0.863789

tetracene S_0

C	3.697460	1.406324	-0.010274
C	2.445456	0.722233	0.032128
C	2.445460	-0.722235	-0.032143
C	3.697468	-1.406320	0.010254
C	4.878973	-0.711782	-0.011127
C	4.878969	0.711792	0.011119
C	1.230844	1.406856	-0.012165
C	0.000469	0.724335	-0.031617
C	0.000470	-0.724351	0.031506
C	1.230851	-1.406864	0.012139
C	-1.230160	1.405441	0.005839
C	-2.445787	0.722275	-0.024558
C	-2.445790	-0.722283	0.024522
C	-1.230164	-1.405454	-0.005854
C	-3.697621	1.406465	0.022612
C	-4.878977	0.711912	-0.007678
C	-4.878984	-0.711900	0.007645
C	-3.697632	-1.406464	-0.022562
H	-3.695570	-2.491550	-0.018955
H	-5.821429	-1.245705	-0.019758
H	-5.821421	1.245727	0.019591
H	-3.695549	2.491551	0.019198
H	-1.232261	-2.492539	0.007411
H	-1.232253	2.492528	-0.007291
H	1.231283	-2.494059	0.011842
H	1.231267	2.494050	-0.011792
H	3.696011	-2.491377	0.000133
H	5.821314	-1.245914	0.014029
H	5.821307	1.245929	-0.014019
H	3.695996	2.491381	-0.000172

tetracene S_1

C	3.700743	1.398915	-0.018765
C	2.472418	0.721041	0.025104
C	2.472418	-0.721043	-0.025195
C	3.700740	-1.398921	0.018693
C	4.911153	-0.697736	-0.013082
C	4.911150	0.697733	0.013262
C	1.228462	1.398181	-0.012284
C	-0.000674	0.726742	0.035428
C	-0.000676	-0.726735	-0.035573
C	1.228456	-1.398177	0.012165
C	-1.229291	1.400327	0.014837
C	-2.471889	0.720945	-0.035040
C	-2.471886	-0.720937	0.035040
C	-1.229291	-1.400321	-0.014855
C	-3.700515	1.398486	0.007700
C	-4.911091	0.697673	-0.014370
C	-4.911086	-0.697679	0.014512
C	-3.700508	-1.398482	-0.007775
H	-3.701754	-2.484109	0.007726
H	-5.847421	-1.242687	-0.005949
H	-5.847423	1.242676	0.006356
H	-3.701769	2.484108	-0.008138
H	-1.230000	-2.488628	-0.021784
H	-1.230004	2.488633	0.021926
H	1.230823	-2.486452	0.004762
H	1.230832	2.486455	-0.004833
H	3.701376	-2.484613	0.009215
H	5.847662	-1.242290	0.010515
H	5.847667	1.242287	-0.010049
H	3.701378	2.484609	-0.009552

perylene S_0

C	-0.246293	1.460286	-2.409583
C	-0.047902	0.731711	-1.239451
C	-0.006235	1.433285	0.002568
C	0.057814	2.865107	-0.002361
C	-0.115221	3.559864	-1.223052
C	-0.243599	2.864518	-2.406883
C	0.175778	3.557180	1.226262
C	0.347454	2.857714	2.402365
C	0.265595	1.455820	2.412865
C	0.095061	0.727514	1.238448

C	0.048113	-0.731704	-1.239440
C	0.006272	-1.433277	0.002573
C	-0.095142	-0.727505	1.238441
C	-0.057808	-2.865097	-0.002361
C	-0.175766	-3.557175	1.226261
C	-0.347442	-2.857714	2.402366
C	-0.265637	-1.455816	2.412860
C	0.246406	-1.460294	-2.409579
C	0.243542	-2.864527	-2.406893
C	0.115126	-3.559862	-1.223060
H	0.209940	4.641505	1.215909
H	0.469950	3.389517	3.338662
H	0.383709	0.937095	3.356110
H	-0.209818	-4.641504	1.215918
H	-0.469831	-3.389519	3.338677
H	-0.383831	-0.937094	3.356096
H	0.091204	-4.644489	-1.217335
H	0.391648	-3.399329	-3.337783
H	0.350062	-0.945610	-3.356753
H	-0.091499	4.644495	-1.217314
H	-0.391897	3.399307	-3.337749
H	-0.349753	0.945599	-3.356777

perylene S_1

C	0.020386	1.465986	-2.455490
C	-0.018081	0.715380	-1.240064
C	0.020600	1.418238	-0.000003
C	-0.022910	2.856830	0.000002
C	0.018043	3.547303	-1.229671
C	-0.014018	2.850374	-2.439297
C	0.018394	3.547300	1.229665
C	-0.013239	2.850370	2.439302
C	0.021109	1.465981	2.455481
C	-0.017882	0.715385	1.240065
C	0.018076	-0.715380	-1.240063
C	-0.020599	-1.418238	-0.000003
C	0.017887	-0.715386	1.240066
C	0.022909	-2.856831	0.000002
C	-0.018392	-3.547300	1.229665
C	0.013239	-2.850370	2.439302
C	-0.021108	-1.465981	2.455481
C	-0.020386	-1.465986	-2.455490
C	0.014017	-2.850374	-2.439297
C	-0.018046	-3.547303	-1.229671
H	0.001171	4.632554	1.221336

H	0.008460	3.397393	3.375060
H	-0.001842	0.953742	3.407547
H	-0.001160	-4.632554	1.221337
H	-0.008463	-3.397393	3.375060
H	0.001838	-0.953742	3.407548
H	-0.000811	-4.632558	-1.221326
H	-0.007285	-3.397391	-3.375068
H	0.003001	-0.953743	-3.407545
H	0.000800	4.632558	-1.221326
H	0.007284	3.397391	-3.375068
H	-0.002992	0.953743	-3.407545