Supporting Information

Singlet-triplet gaps of cobalt nitrosyls: Insights from tropocoronand complexes

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Contents

Spectra for Co(TC-3,3)(NO)

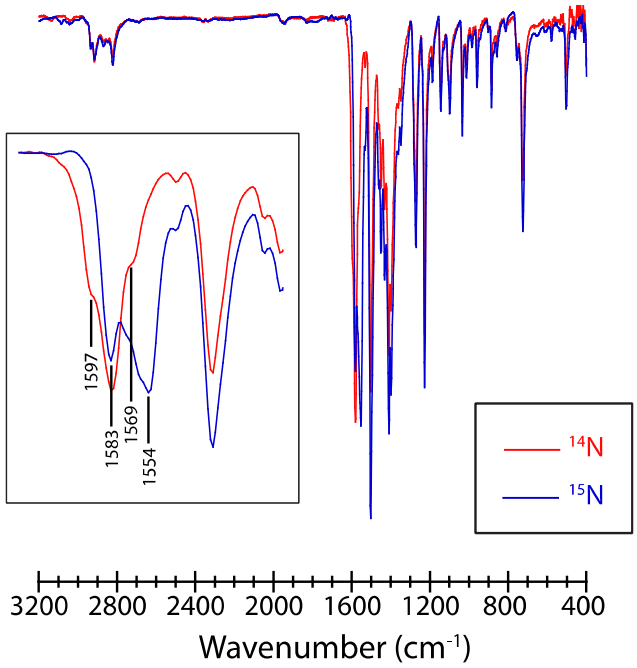


Figure S1. IR spectra (KBr disc) of Co(TC-3,3)(NO) (red) and [Co(TC-3,3)(^{15}NO)] (blue). Inset shows magnification of the nitrosyl stretching region.

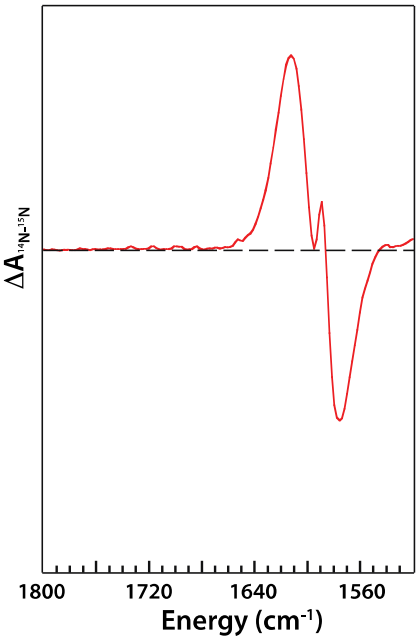


Figure S2. Difference IR spectrum for Co(TC-3,3)(NO) and [Co(TC-3,3)(^{15}NO)] in CH_2Cl_2.

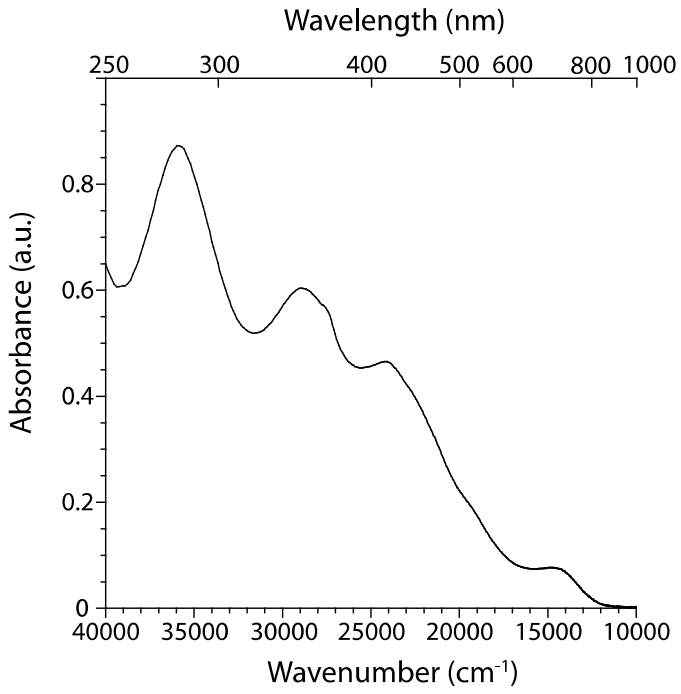


Figure S3. Electronic absorption spectrum of [Co(TC-3,3)(NO)] in CH_2Cl_2.

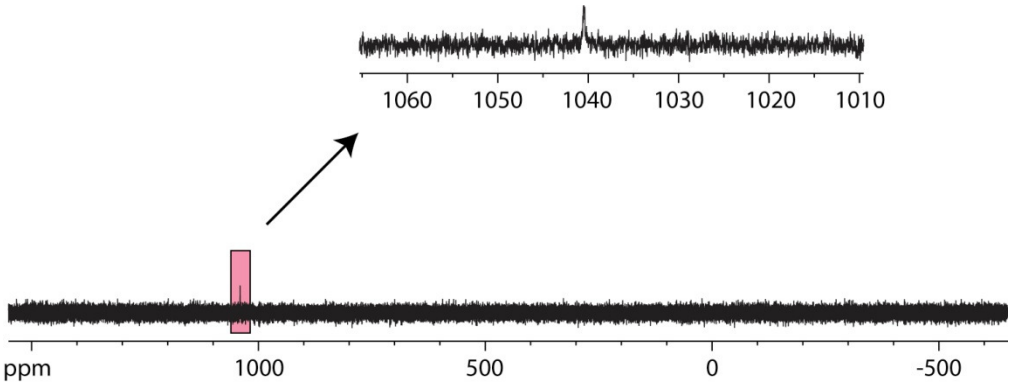


Figure S4. 50.7 ^{15}N NMR spectrum of [Co(TC-3,3)(^{15}NO)] in CD_2Cl_2.

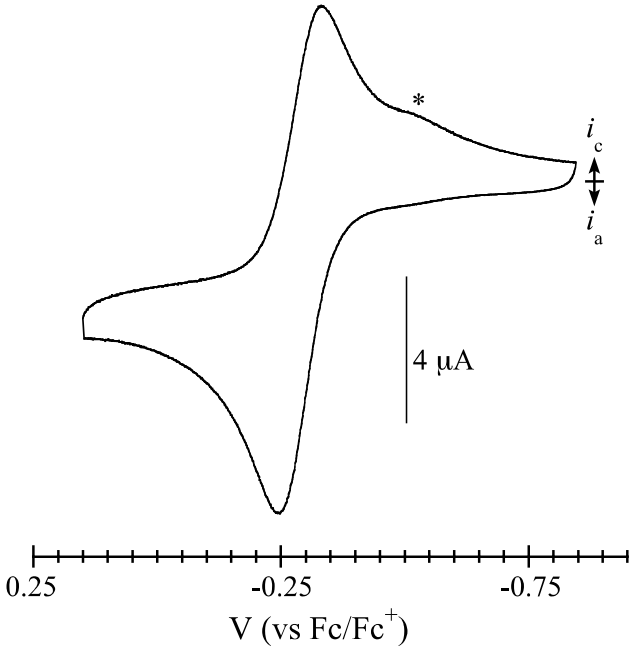
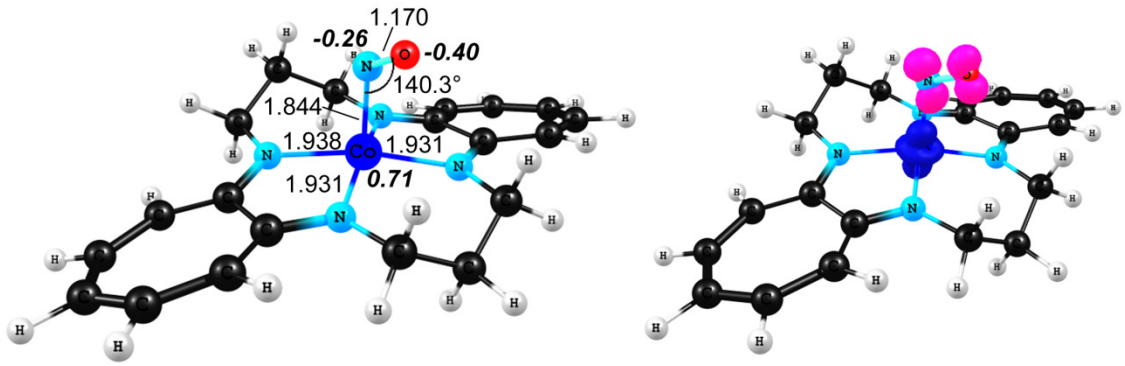


Figure S5. Cyclic voltammogram of Co(TC-3,3)(NO) at a glassy carbon electrode in CH_2Cl_2. The scan rate is 50 mV/s. The asterisk corresponds to the cathodic wave of $[Co^{III}(TC\text{-}3,3)]^+$ formed by dissociation of NO from $[Co^{III}(TC\text{-}3,3)(NO)]^+$.

Highlights of computational results

A



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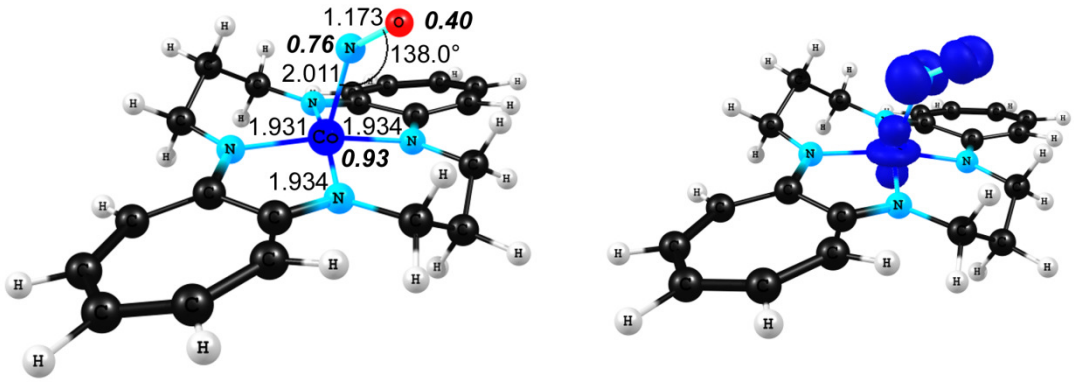
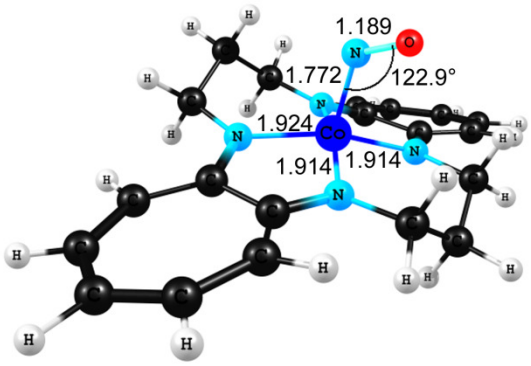


Figure S6. Selected optimized B3LYP results for Co(TC-3,3)(NO): bond distances (Å) and angles (deg); Mulliken spin populations (bold italic) and spin density plot.: (**A**) Low-spin, $M_S = 0$ broken-symmetry solution; (**B**) Triplet solution (T1, $M_S = 1$). Color code for atoms: C (black), H (ivory), N (cyan), O (red), and Co (dark blue). Majority and minority spin densities are indicated in blue and magenta, respectively.

A



B

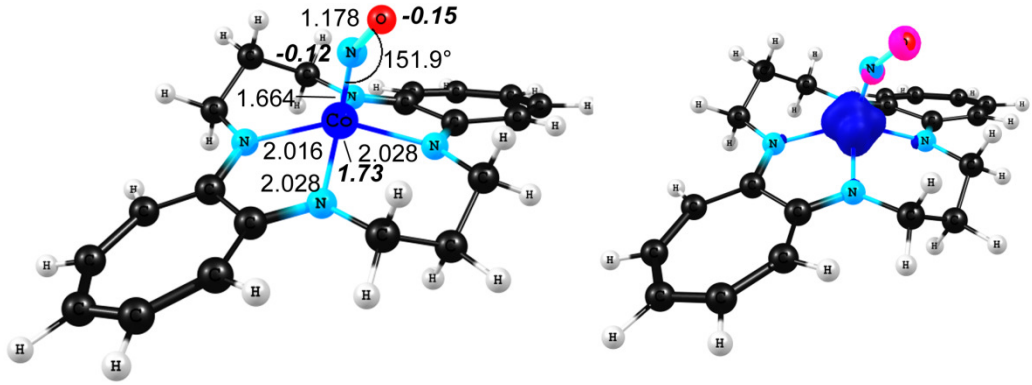


Figure S7. Selected optimized PW91 results for Co(TC-3,3)(NO): (**A**) Low-spin, $M_S = 0$ closed-shell solution; (**B**) Triplet solution (T2, $M_S = 1$). The content has been organized in the same style as Figure S6.

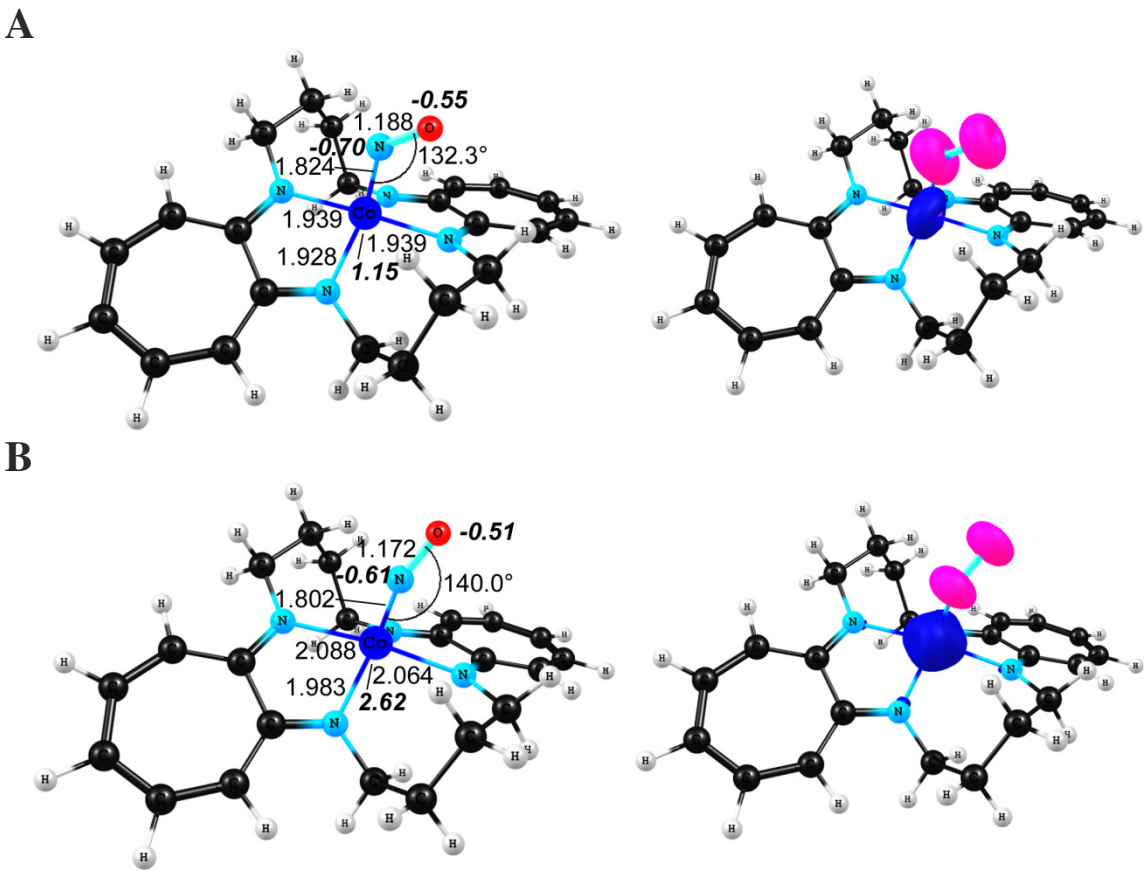
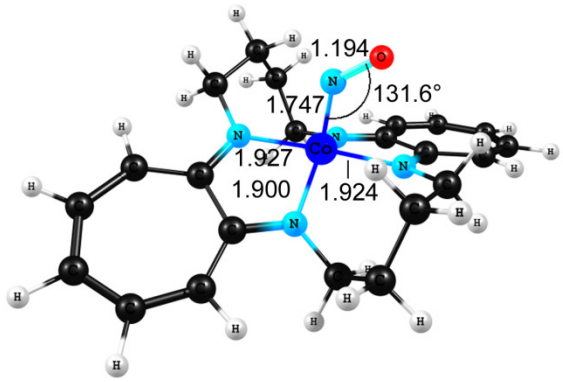


Figure S8. Selected optimized B3LYP results for Co(TC-4,4)(NO). (**A**) Low-spin, M_S = 0 broken-symmetry solution; (**B**) Triplet solution (T2, M_S = 1). The content has been organized in the same style as Figure S6.

A



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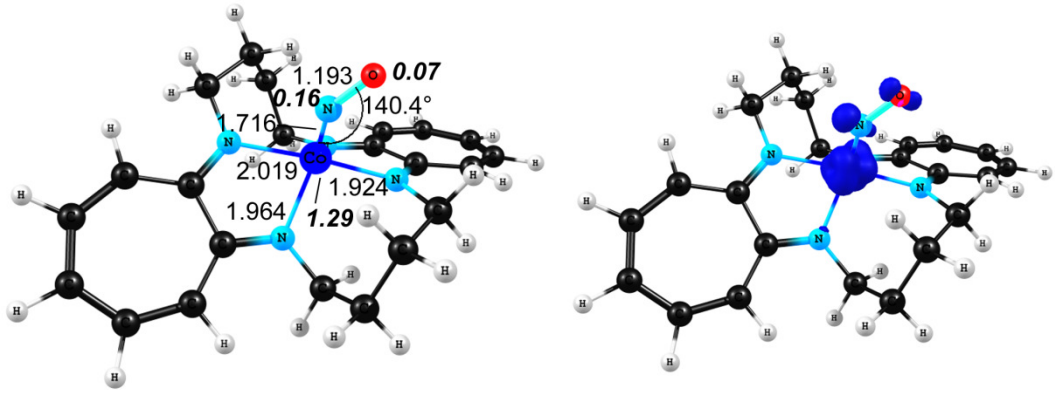


Figure S9. Selected optimized PW91 results for Co(TC-4,4)(NO): (**A**) Low-spin, $M_S = 0$ closed-shell solution; (**B**) Triplet solution (T1, $M_S = 1$). The content has been organized in the same style as Figure S6.

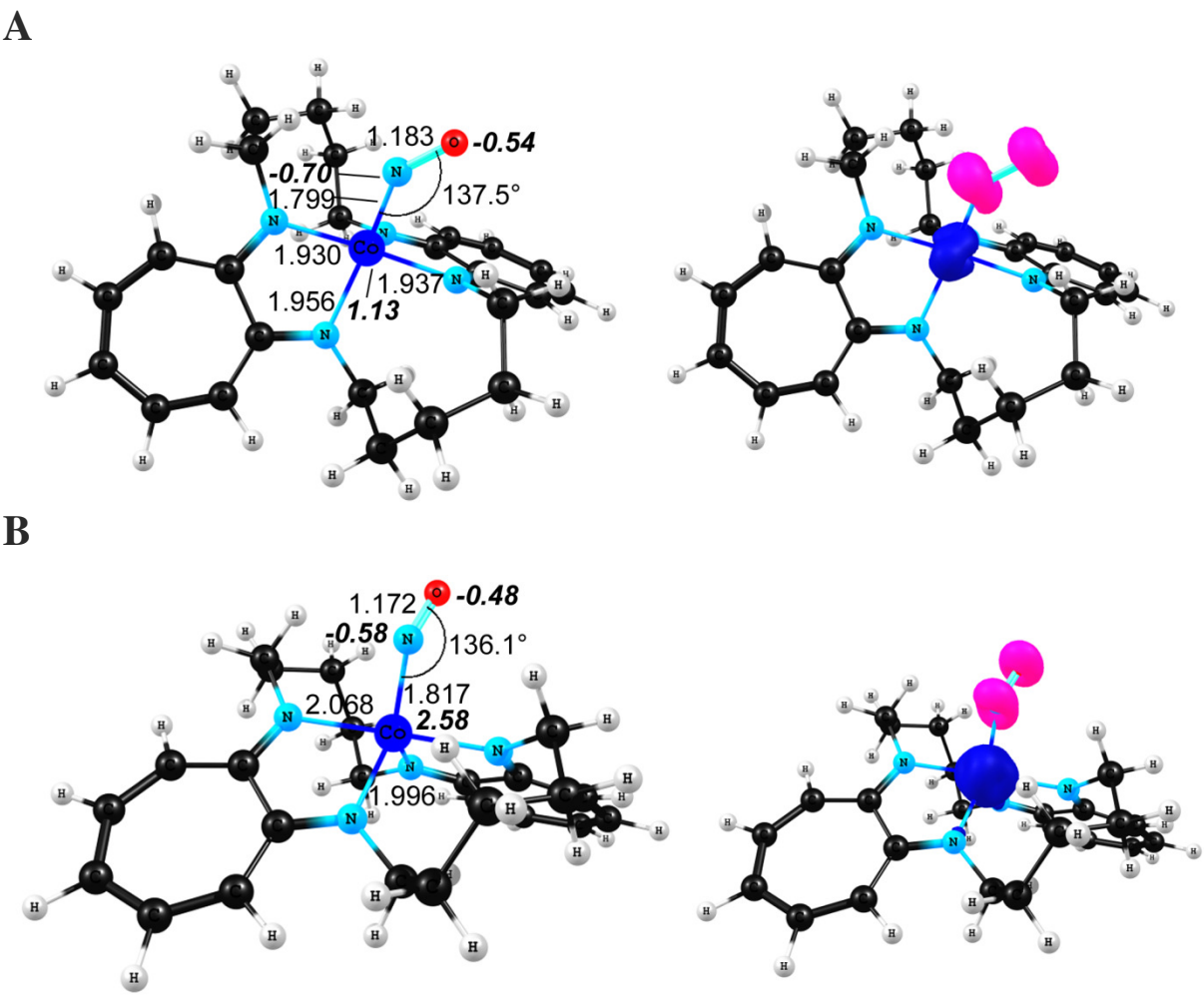


Figure S10. Selected optimized B3LYP results for Co(TC-5,5)(NO). (**A**) Low-spin, M_S = 0 broken-symmetry solution; (**B**) Triplet solution (T2, M_S = 1). The content has been organized in the same style as Figure S6.

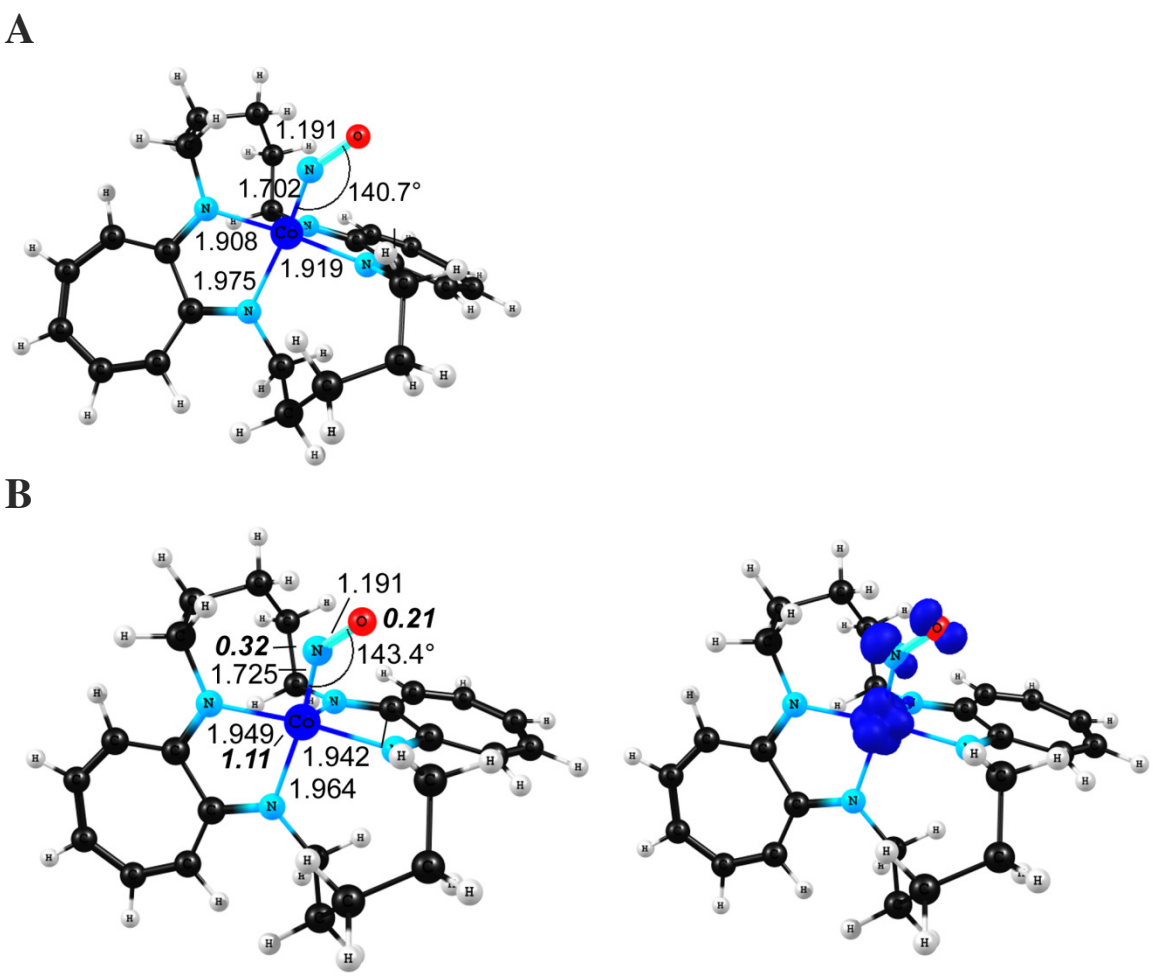


Figure S11. Selected optimized PW91 results for Co(TC-5,5)(NO): (**A**) Low-spin, M_S = 0 closed-shell solution; (**B**) Triplet solution (T1, M_S = 1). The content has been organized in the same style as Figure S6.

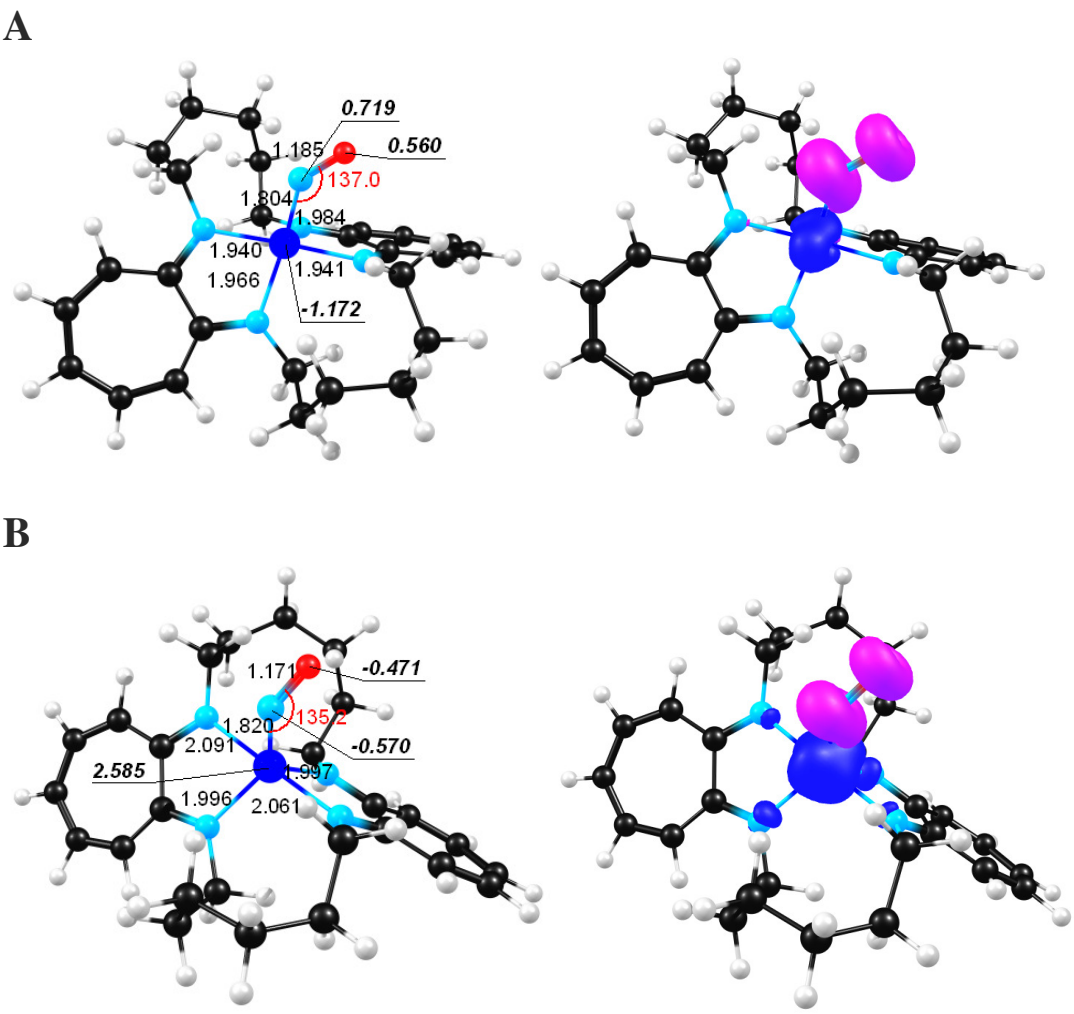
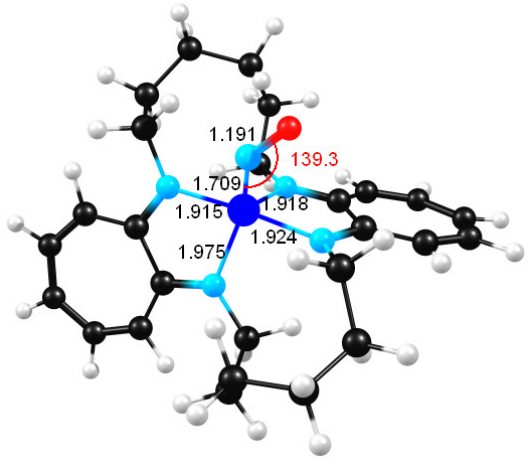


Figure S12. Selected optimized B3LYP results for Co(TC-6,6)(NO): (**A**) Low-spin, M_S = 0 closed-shell solution; (**B**) Triplet solution (T1, M_S = 1). The content has been organized in the same style as Figure S6.

A



B

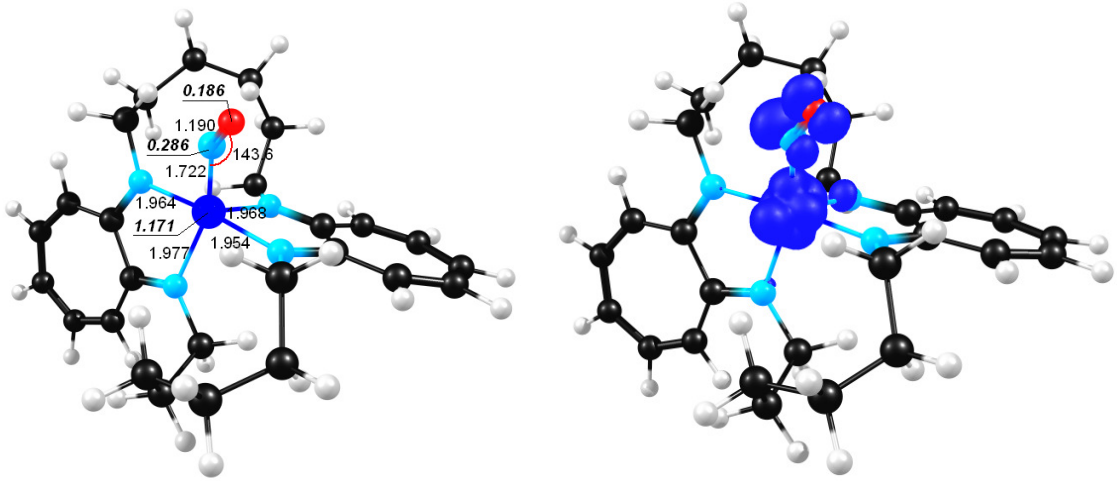


Figure S13. Selected optimized PW91 results for Co(TC-6,6)(NO): (**A**) Low-spin, M_S = 0 closed-shell solution; (**B**) Triplet solution (T2, M_S = 1). The content has been organized in the same style as Figure S6.

Optimized Cartesian coordinates (Å)

Co(TC-3,3)(NO), B3LYP, *S* = 0

Co	0.000000	0.006548	0.183084
N	-1.443615	1.287730	0.018814
N	-1.457485	-1.219230	-0.113985
N	0.000018	-0.091326	1.966978
N	1.443607	1.287743	0.018806
N	1.457484	-1.219219	-0.114011
O	0.000016	-1.138042	2.499458
C	-2.645924	0.789674	-0.250726
C	-3.746439	1.601782	-0.632937
C	-5.088349	1.301222	-0.815475
C	-5.772540	0.103231	-0.629623
C	-5.200590	-1.108843	-0.255870
C	-3.869739	-1.451566	-0.058934
C	-2.677840	-0.687870	-0.165584
C	-1.277343	2.730087	0.141830
C	-0.000011	3.096499	0.887846
C	-1.286520	-2.664423	-0.101151
C	0.000005	-3.093863	-0.798776
C	2.645920	0.789689	-0.250722
C	3.746442	1.601792	-0.632932
C	5.088352	1.301227	-0.815460
C	5.772537	0.103231	-0.629609
C	5.200579	-1.108844	-0.255874
C	3.869724	-1.451562	-0.058954
C	2.677835	-0.687855	-0.165594
C	1.277324	2.730099	0.141832
C	1.286548	-2.664413	-0.101191
H	-3.493239	2.634448	-0.833286
H	-5.698081	2.144947	-1.128837
H	-6.846495	0.118483	-0.778553
H	-5.899263	-1.927782	-0.103868
H	-3.721681	-2.481171	0.237259
H	-2.130511	3.153340	0.685720
H	-1.267197	3.206723	-0.851736
H	-0.000010	2.617068	1.870098
H	-0.000017	4.179226	1.051117
H	-2.118652	-3.146714	-0.620838
H	-1.286270	-3.036876	0.933630
H	0.000010	-4.187457	-0.864201
H	-0.000013	-2.707805	-1.823587
H	3.493247	2.634458	-0.833291
H	5.698089	2.144951	-1.128816
H	6.846493	0.118480	-0.778532
H	5.899246	-1.927789	-0.103880
H	3.721651	-2.481174	0.237211
H	2.130488	3.153356	0.685727
H	1.267179	3.206740	-0.851732
H	2.118677	-3.146672	-0.620914
H	1.286343	-3.036885	0.933583

Co(TC-3,3)(NO), B3LYP, M_S = 0

Co	0.000000	0.009161	0.185437
N	-1.446487	1.289785	0.027625
N	-1.459665	-1.218870	-0.116849
N	0.000006	-0.128030	2.024594
N	1.446489	1.289782	0.027621
N	1.459661	-1.218874	-0.116860
O	-0.000002	-1.161219	2.572781
C	-2.646919	0.791971	-0.251161
C	-3.746023	1.604557	-0.636903
C	-5.087401	1.304563	-0.824340
C	-5.772711	0.106460	-0.642997
C	-5.202154	-1.106661	-0.270401
C	-3.871981	-1.450392	-0.070595
C	-2.679361	-0.686548	-0.170740
C	-1.278342	2.732064	0.145401
C	0.000005	3.099791	0.889868
C	-1.287891	-2.663889	-0.115762
C	-0.000010	-3.087598	-0.815488
C	2.646919	0.791966	-0.251166
C	3.746024	1.604553	-0.636902
C	5.087403	1.304561	-0.824334
C	5.772713	0.106457	-0.642991
C	5.202154	-1.106664	-0.270401
C	3.871981	-1.450397	-0.070602
C	2.679360	-0.686554	-0.170749
C	1.278349	2.732061	0.145399
C	1.287883	-2.663894	-0.115781
H	-3.492074	2.637641	-0.834436
H	-5.695872	2.149034	-1.138379
H	-6.846222	0.122350	-0.795326
H	-5.901553	-1.925856	-0.122679
H	-3.724966	-2.480973	0.223107
H	-2.130783	3.158698	0.687918
H	-1.267212	3.206009	-0.849463
H	0.000005	2.624674	1.874537
H	0.000007	4.182969	1.050573
H	-2.119137	-3.143334	-0.639898
H	-1.288881	-3.046134	0.915843
H	-0.000013	-4.180699	-0.889020
H	-0.000017	-2.694356	-1.837512
H	3.492075	2.637638	-0.834430
H	5.695875	2.149033	-1.138367
H	6.846225	0.122348	-0.795313
H	5.901553	-1.925859	-0.122676
H	3.724967	-2.480978	0.223101
H	2.130794	3.158692	0.687914
H	1.267219	3.206006	-0.849465
H	2.119118	-3.143337	-0.639935
H	1.288890	-3.046147	0.915822

Co(TC-3,3)(NO), B3LYP, S = 1

Co	0.000003	0.032837	0.087534
N	-1.448233	1.307547	0.001650
N	-1.462183	-1.199672	-0.202383
N	-0.000005	-0.406544	2.050388
N	1.448225	1.307572	0.001656

N	1.462206	-1.199649	-0.202367
O	-0.000094	-1.363667	2.729104
C	-2.656724	0.811277	-0.243870
C	-3.771565	1.626554	-0.577204
C	-5.118361	1.326175	-0.714968
C	-5.793854	0.123392	-0.523415
C	-5.206942	-1.094449	-0.196664
C	-3.868248	-1.438014	-0.059565
C	-2.684013	-0.668363	-0.192342
C	-1.280297	2.747682	0.142236
C	-0.000028	3.103036	0.889807
C	-1.289447	-2.644596	-0.215140
C	0.000044	-3.063113	-0.916207
C	2.656730	0.811309	-0.243839
C	3.771581	1.626575	-0.577183
C	5.118373	1.326183	-0.714949
C	5.793859	0.123392	-0.523403
C	5.206939	-1.094448	-0.196662
C	3.868243	-1.438000	-0.059559
C	2.684022	-0.668332	-0.192315
C	1.280257	2.747705	0.142249
C	1.289514	-2.644572	-0.215122
H	-3.527301	2.662468	-0.772282
H	-5.740643	2.173142	-0.992962
H	-6.872784	0.139781	-0.630594
H	-5.898075	-1.918056	-0.035753
H	-3.705997	-2.474044	0.205433
H	-2.129271	3.166153	0.695595
H	-1.272076	3.238630	-0.844299
H	-0.000029	2.615323	1.868830
H	-0.000039	4.183593	1.067952
H	-2.120690	-3.118569	-0.745224
H	-1.295339	-3.037709	0.812989
H	0.000059	-4.155631	-0.996195
H	0.000047	-2.665418	-1.936603
H	3.527325	2.662485	-0.772289
H	5.740663	2.173142	-0.992948
H	6.872788	0.139772	-0.630591
H	5.898063	-1.918066	-0.035774
H	3.705966	-2.474037	0.205400
H	2.129213	3.166194	0.695623
H	1.272036	3.238657	-0.844284
H	2.120789	-3.118511	-0.745189
H	1.295403	-3.037684	0.813007

Co(TC-3,3)(NO), B3LYP, M_S = 1

Co	0.000000	-0.032196	0.572963
N	-1.472953	1.305757	0.130939
N	-1.488978	-1.238011	-0.092260
N	-0.000002	-0.406503	2.293391
N	1.472953	1.305757	0.130939
N	1.488979	-1.238012	-0.092258
O	-0.000009	-1.193645	3.155834
C	-2.634091	0.811623	-0.272273
C	-3.693038	1.636509	-0.742221
C	-5.008722	1.356094	-1.077957
C	-5.717486	0.159772	-1.006477

C	-5.193595	-1.068605	-0.618989
C	-3.891040	-1.427761	-0.298792
C	-2.685282	-0.679691	-0.244143
C	-1.288503	2.746603	0.228922
C	0.000000	3.114435	0.964231
C	-1.304910	-2.680666	-0.149944
C	0.000001	-3.067754	-0.852848
C	2.634091	0.811622	-0.272272
C	3.693039	1.636509	-0.742221
C	5.008722	1.356094	-1.077957
C	5.717486	0.159772	-1.006476
C	5.193596	-1.068605	-0.618987
C	3.891042	-1.427761	-0.298789
C	2.685283	-0.679691	-0.244142
C	1.288503	2.746603	0.228922
C	1.304912	-2.680666	-0.149941
H	-3.421078	2.676055	-0.870466
H	-5.576507	2.216567	-1.423405
H	-6.769745	0.190505	-1.266795
H	-5.906582	-1.888260	-0.574519
H	-3.779274	-2.472699	-0.040820
H	-2.134917	3.201257	0.762319
H	-1.269260	3.204380	-0.773128
H	0.000000	2.656863	1.958567
H	0.000000	4.199022	1.117679
H	-2.119706	-3.160453	-0.700888
H	-1.315949	-3.104794	0.865825
H	0.000001	-4.157458	-0.971908
H	0.000002	-2.634632	-1.858377
H	3.421078	2.676055	-0.870467
H	5.576508	2.216567	-1.423405
H	6.769746	0.190505	-1.266795
H	5.906583	-1.888259	-0.574517
H	3.779275	-2.472699	-0.040816
H	2.134918	3.201257	0.762317
H	1.269260	3.204379	-0.773129
H	2.119709	-3.160453	-0.700884
H	1.315948	-3.104793	0.865827

Co(TC-3,3)(NO), PW91, *S* = 0

Co	0.000000	-0.003992	0.280136
N	-1.422170	1.276185	0.081482
N	-1.442616	-1.213215	-0.067660
N	0.000001	-0.173292	2.043759
N	1.422169	1.276185	0.081481
N	1.442615	-1.213215	-0.067663
O	0.000002	-1.229258	2.590731
C	-2.622930	0.793893	-0.265952
C	-3.691942	1.632615	-0.682225
C	-5.027969	1.347099	-0.954375
C	-5.726539	0.143065	-0.838167
C	-5.186470	-1.085360	-0.447884
C	-3.868288	-1.440914	-0.169979
C	-2.668013	-0.678547	-0.196405
C	-1.266830	2.713693	0.262518
C	0.000000	3.050590	1.036884
C	-1.278702	-2.658136	-0.024840

C	-0.000001	-3.107388	-0.722265
C	2.622929	0.793893	-0.265952
C	3.691941	1.632616	-0.682225
C	5.027968	1.347099	-0.954375
C	5.726539	0.143065	-0.838165
C	5.186470	-1.085359	-0.447883
C	3.868287	-1.440914	-0.169980
C	2.668013	-0.678546	-0.196406
C	1.266830	2.713693	0.262517
C	1.278703	-2.658136	-0.024844
H	-3.415326	2.675386	-0.836487
H	-5.618041	2.207098	-1.283375
H	-6.795689	0.167150	-1.054990
H	-5.903876	-1.905104	-0.350267
H	-3.745818	-2.479821	0.133404
H	-2.139976	3.106475	0.812467
H	-1.245146	3.234480	-0.716871
H	0.000000	2.515518	1.997757
H	0.000000	4.129682	1.253896
H	-2.124040	-3.149646	-0.527952
H	-1.268603	-3.003940	1.026018
H	0.000000	-4.207953	-0.765582
H	-0.000002	-2.736230	-1.759243
H	3.415326	2.675386	-0.836489
H	5.618042	2.207098	-1.283375
H	6.795689	0.167150	-1.054988
H	5.903875	-1.905104	-0.350266
H	3.745817	-2.479821	0.133402
H	2.139975	3.106476	0.812465
H	1.245144	3.234480	-0.716872
H	2.124040	-3.149645	-0.527959
H	1.268607	-3.003942	1.026014

Co(TC-3,3)(NO), PW91, *S* = 1

Co	-0.000220	0.010524	0.222809
N	-1.421785	1.284290	0.066488
N	-1.447160	-1.201726	-0.129788
N	0.002121	-0.401601	2.032229
N	1.421072	1.284347	0.067326
N	1.445699	-1.201373	-0.132910
O	0.010504	-1.346728	2.775561
C	-2.629761	0.807541	-0.265293
C	-3.708213	1.656345	-0.640361
C	-5.046107	1.375293	-0.901350
C	-5.741932	0.166747	-0.805054
C	-5.195635	-1.068809	-0.449438
C	-3.873714	-1.428076	-0.194896
C	-2.674384	-0.664107	-0.224945
C	-1.268681	2.716437	0.291159
C	-0.000866	3.032334	1.073305
C	-1.282850	-2.646377	-0.058443
C	-0.001631	-3.112169	-0.741455
C	2.628944	0.807875	-0.264930
C	3.707703	1.657082	-0.638622
C	5.045447	1.376191	-0.899946
C	5.740950	0.167151	-0.805887
C	5.194258	-1.068913	-0.453110

C	3.872102	−1.428293	−0.199354
C	2.673213	−0.663799	−0.227278
C	1.268117	2.716377	0.293143
C	1.282024	−2.646297	−0.063239
H	−3.435279	2.702920	−0.773833
H	−5.641980	2.241641	−1.201978
H	−6.813654	0.194401	−1.008051
H	−5.910701	−1.891707	−0.361859
H	−3.745996	−2.472922	0.083961
H	−2.140064	3.092133	0.855027
H	−1.248572	3.265609	−0.672260
H	−0.001603	2.476564	2.022427
H	−0.000963	4.105829	1.317078
H	−2.124708	−3.149483	−0.556155
H	−1.282146	−2.967144	1.000370
H	−0.001471	−4.213501	−0.752975
H	−0.003716	−2.773849	−1.789829
H	3.435075	2.703966	−0.770236
H	5.641630	2.242919	−1.198844
H	6.812715	0.194937	−1.008638
H	5.908991	−1.892298	−0.367483
H	3.744024	−2.473794	0.076816
H	2.138730	3.091215	0.858761
H	1.249835	3.266291	−0.669873
H	2.122151	−3.148053	−0.565254
H	1.286081	−2.968765	0.995040

Co(TC-3,3)(NO), PW91, M_S = 1

Co	0.000002	−0.016249	0.564980
N	−1.452689	1.303895	0.105755
N	−1.477937	−1.224758	−0.119622
N	−0.000085	−0.477480	2.164129
N	1.452733	1.303889	0.105754
N	1.477972	−1.224766	−0.119571
O	−0.000377	−1.299101	3.008330
C	−2.634723	0.815835	−0.272602
C	−3.702315	1.654898	−0.702942
C	−5.025580	1.375899	−1.033780
C	−5.729427	0.170640	−0.973976
C	−5.201759	−1.068792	−0.602010
C	−3.892723	−1.427594	−0.292862
C	−2.685910	−0.671778	−0.250403
C	−1.282378	2.742777	0.248639
C	0.000023	3.092791	1.000508
C	−1.298024	−2.667916	−0.135406
C	0.000026	−3.073417	−0.838462
C	2.634760	0.815820	−0.272587
C	3.702363	1.654872	−0.702924
C	5.025632	1.375870	−1.033737
C	5.729482	0.170607	−0.973911
C	5.201800	−1.068821	−0.601938
C	3.892753	−1.427615	−0.292798
C	2.685940	−0.671792	−0.250358
C	1.282433	2.742768	0.248656
C	1.298046	−2.667920	−0.135343
H	−3.429156	2.704155	−0.816119
H	−5.603592	2.244578	−1.362185

H	-6.790096	0.201970	-1.228706
H	-5.919110	-1.893565	-0.560733
H	-3.772512	-2.481016	-0.039714
H	-2.141903	3.176674	0.793523
H	-1.261258	3.231485	-0.746752
H	0.000012	2.595531	1.982463
H	0.000024	4.177886	1.189818
H	-2.127269	-3.167819	-0.662128
H	-1.295011	-3.059124	0.900782
H	0.000026	-4.170949	-0.938985
H	0.000053	-2.653689	-1.856565
H	3.429213	2.704124	-0.816131
H	5.603655	2.244541	-1.362146
H	6.790159	0.201930	-1.228628
H	5.919150	-1.893602	-0.560645
H	3.772548	-2.481037	-0.039635
H	2.141947	3.176648	0.793566
H	1.261335	3.231500	-0.746721
H	2.127311	-3.167843	-0.662015
H	1.294973	-3.059115	0.900850

Co(TC-4,4)(NO), B3LYP, *S* = 0

Co	-0.021063	0.019755	0.229617
N	0.040316	0.127443	1.989926
N	1.451627	-1.257466	0.160395
N	-1.385381	-1.129871	-0.464624
N	-1.514623	1.294059	0.207323
N	1.344390	1.176248	-0.443481
O	0.740473	-0.492685	2.703413
C	2.584682	0.690327	-0.513025
C	3.695775	1.486363	-0.889128
C	5.042441	1.188606	-1.043959
C	5.724076	-0.008378	-0.857593
C	5.151386	-1.208337	-0.445885
C	3.836084	-1.522264	-0.137018
C	2.643340	-0.746045	-0.149713
C	1.412828	-2.635773	0.678900
C	0.042947	-3.160596	1.120652
C	-0.903737	-3.539934	-0.022623
C	-1.044154	-2.420794	-1.056113
C	0.988459	2.481407	-0.992667
C	0.845040	3.572573	0.070215
C	-0.111681	3.182340	1.202779
C	-1.480428	2.661822	0.751565
C	-2.702912	0.773434	-0.093664
C	-2.635196	-0.655249	-0.486924
C	-3.904872	1.537026	-0.049804
C	-5.222997	1.212356	-0.328458
C	-5.791944	0.009068	-0.739401
C	-5.101311	-1.175261	-0.959753
C	-3.745736	-1.457155	-0.844825
H	3.459283	2.527794	-1.061827
H	5.655316	2.035348	-1.343026
H	6.793359	-0.004744	-1.037391
H	5.841017	-2.043175	-0.347783
H	3.698226	-2.556042	0.142766
H	2.085859	-2.697466	1.542645

H	1.811702	-3.324747	-0.079717
H	-0.439141	-2.446736	1.786778
H	0.231172	-4.053344	1.726594
H	-0.529860	-4.434344	-0.535993
H	-1.884023	-3.798208	0.391897
H	-0.085719	-2.290068	-1.563755
H	-1.762126	-2.700671	-1.831581
H	0.029226	2.359090	-1.501811
H	1.700550	2.790393	-1.762347
H	1.825172	3.814531	0.494804
H	0.481337	4.481195	-0.426094
H	0.356866	2.455910	1.865601
H	-0.302370	4.071695	1.813457
H	-1.887437	3.365240	0.009651
H	-2.152214	2.706222	1.618458
H	-3.770493	2.570344	0.233972
H	-5.919488	2.038080	-0.205267
H	-6.865483	-0.005442	-0.891246
H	-5.710730	-2.025941	-1.254451
H	-3.501960	-2.492928	-1.039408

Co(TC-4,4)(NO), B3LYP, M_S = 0

Co	-0.024842	0.015562	0.364344
N	0.064837	0.055802	2.186120
N	1.467341	-1.218064	0.266509
N	-1.307934	-1.090287	-0.555609
N	-1.523849	1.244618	0.346097
N	1.261444	1.154140	-0.524119
O	0.719336	-0.553045	2.968137
C	2.512921	0.703421	-0.602557
C	3.580321	1.480650	-1.117162
C	4.930913	1.208283	-1.283447
C	5.663147	0.068316	-0.970358
C	5.151204	-1.090246	-0.394124
C	3.855117	-1.414510	-0.020263
C	2.634714	-0.691105	-0.103925
C	1.435514	-2.584934	0.803519
C	0.035673	-3.143804	1.077176
C	-0.785998	-3.497790	-0.169366
C	-0.895608	-2.343840	-1.174979
C	0.833696	2.428354	-1.088234
C	0.722104	3.544716	-0.041134
C	-0.087654	3.152497	1.202577
C	-1.487441	2.589303	0.934195
C	-2.692217	0.723845	-0.026183
C	-2.568367	-0.649809	-0.579178
C	-3.916711	1.435072	0.103799
C	-5.217682	1.111387	-0.250258
C	-5.732558	-0.034836	-0.849837
C	-4.998445	-1.157202	-1.213955
C	-3.640761	-1.421209	-1.088502
H	3.297683	2.479696	-1.421303
H	5.501957	2.027497	-1.713216
H	6.726527	0.088595	-1.181311
H	5.878569	-1.874835	-0.200937
H	3.764659	-2.401189	0.410322
H	2.001664	-2.611426	1.743310

H	1.944728	-3.262419	0.104367
H	-0.523436	-2.456622	1.712267
H	0.170967	-4.054511	1.670287
H	-0.333200	-4.354395	-0.683575
H	-1.786819	-3.811940	0.145980
H	0.086805	-2.164685	-1.616398
H	-1.555715	-2.622131	-2.001375
H	-0.150785	2.259892	-1.530644
H	1.484335	2.746268	-1.907824
H	1.723646	3.853411	0.277308
H	0.262679	4.415663	-0.525316
H	0.478194	2.451265	1.815295
H	-0.224937	4.049722	1.816098
H	-2.018686	3.289960	0.274862
H	-2.035932	2.576579	1.886111
H	-3.823808	2.409548	0.561119
H	-5.947154	1.883189	-0.017757
H	-6.800342	-0.058618	-1.036805
H	-5.572086	-1.968949	-1.654125
H	-3.357615	-2.408195	-1.428919

Co(TC-4,4)(NO), B3LYP, *S* = 1

Co	-0.013862	0.012474	0.481901
N	0.316914	0.182532	2.308097
N	-1.532804	1.188401	0.447424
N	1.246479	1.103183	-0.583252
N	1.515556	-1.208661	0.394228
N	-1.202197	-1.058215	-0.624530
O	-0.322614	-0.205017	3.218735
C	-2.475891	-0.670307	-0.651102
C	-3.509824	-1.452141	-1.227934
C	-4.867348	-1.221309	-1.387828
C	-5.644772	-0.127587	-1.015467
C	-5.185356	1.010604	-0.363510
C	-3.907538	1.350214	0.062990
C	-2.668191	0.667781	-0.025636
C	-1.508108	2.561608	0.963112
C	-0.102422	3.157587	1.115023
C	0.640214	3.494913	-0.188914
C	0.772485	2.335743	-1.192591
C	-0.729920	-2.297553	-1.226238
C	-0.652942	-3.459097	-0.218842
C	0.066463	-3.123050	1.097351
C	1.484669	-2.560367	0.951105
C	2.665678	-0.674476	-0.021443
C	2.499130	0.676310	-0.639041
C	3.903456	-1.350194	0.121758
C	5.192442	-1.028510	-0.290542
C	5.667815	0.080215	-0.977063
C	4.900737	1.167536	-1.395597
C	3.548708	1.421687	-1.244778
H	-3.181297	-2.408327	-1.613209
H	-5.403392	-2.028851	-1.880164
H	-6.703380	-0.172417	-1.246114
H	-5.942734	1.757228	-0.138244
H	-3.860204	2.302829	0.572027
H	-2.008790	2.598968	1.941355

H	-2.083507	3.213235	0.292417
H	0.515779	2.506737	1.735484
H	-0.217812	4.087496	1.683147
H	0.129554	4.321348	-0.699187
H	1.638715	3.860244	0.074686
H	-0.213347	2.116708	-1.610519
H	1.395766	2.653878	-2.034280
H	0.269668	-2.093193	-1.612839
H	-1.338885	-2.593507	-2.086192
H	-1.665154	-3.802954	0.020136
H	-0.145207	-4.297411	-0.711339
H	-0.546488	-2.442553	1.693325
H	0.141448	-4.043042	1.687149
H	2.062994	-3.240210	0.310472
H	1.971659	-2.574511	1.937801
H	3.841971	-2.289515	0.654047
H	5.941855	-1.770288	-0.025222
H	6.728974	0.109660	-1.198452
H	5.448060	1.951196	-1.913940
H	3.234401	2.372249	-1.656179

Co(TC-4,4)(NO), B3LYP, M_S = 1

Co	0.014222	0.008410	0.490097
N	-0.082471	0.022682	2.289501
N	-1.589757	1.295104	0.308503
N	1.338680	1.106091	-0.496595
N	1.640866	-1.290706	0.324913
N	-1.254735	-1.085002	-0.545166
O	-0.848752	-0.196375	3.148786
C	-2.523464	-0.674448	-0.607003
C	-3.561696	-1.496697	-1.103928
C	-4.923193	-1.281830	-1.286882
C	-5.695876	-0.157552	-1.030656
C	-5.231321	1.044929	-0.500945
C	-3.956585	1.416510	-0.107662
C	-2.711026	0.726973	-0.110780
C	-1.587210	2.683405	0.769447
C	-0.184696	3.214096	1.094563
C	0.717662	3.514170	-0.113478
C	0.895051	2.353884	-1.106876
C	-0.791333	-2.323642	-1.161734
C	-0.647502	-3.499335	-0.182032
C	0.224225	-3.221604	1.053198
C	1.632148	-2.681774	0.770394
C	2.774378	-0.718525	-0.051618
C	2.605489	0.692130	-0.530559
C	4.021132	-1.408175	-0.019156
C	5.307589	-1.033374	-0.369462
C	5.791141	0.172998	-0.872371
C	5.026552	1.301462	-1.135460
C	3.661537	1.518294	-0.986178
H	-3.241862	-2.492269	-1.382414
H	-5.459515	-2.136488	-1.691362
H	-6.754388	-0.221325	-1.257678
H	-5.984252	1.817710	-0.367540
H	-3.900435	2.426057	0.276297
H	-2.210880	2.779602	1.670171

H	-2.041451	3.336216	0.009080
H	0.319490	2.524248	1.774767
H	-0.312883	4.145743	1.656568
H	0.303341	4.363825	-0.670878
H	1.698101	3.832275	0.257571
H	-0.071952	2.142809	-1.570106
H	1.559618	2.667257	-1.918094
H	0.190104	-2.103874	-1.587128
H	-1.429674	-2.620839	-1.999607
H	-1.638881	-3.820523	0.156134
H	-0.220322	-4.340471	-0.742199
H	-0.298139	-2.549950	1.737548
H	0.340263	-4.164636	1.598739
H	2.109630	-3.329096	0.018764
H	2.230865	-2.785821	1.687741
H	3.953979	-2.423049	0.348492
H	6.054566	-1.809842	-0.222673
H	6.855705	0.236963	-1.068883
H	5.575311	2.160767	-1.513185
H	3.353603	2.520105	-1.256062

Co(TC-4,4)(NO), PW91, *S* = 0

Co	-0.026252	0.019840	0.340464
N	0.082289	0.057175	2.084001
N	1.437700	-1.223757	0.235973
N	-1.307717	-1.085694	-0.523579
N	-1.503440	1.256476	0.322035
N	1.257097	1.142761	-0.501119
O	0.771244	-0.548158	2.847981
C	2.520163	0.690715	-0.581203
C	3.593111	1.490584	-1.057856
C	4.947507	1.211602	-1.225615
C	5.665443	0.045298	-0.955261
C	5.137818	-1.139059	-0.430944
C	3.833368	-1.464699	-0.073427
C	2.624572	-0.710071	-0.127833
C	1.400620	-2.591376	0.777464
C	0.006937	-3.132936	1.107259
C	-0.843112	-3.499219	-0.115106
C	-0.922451	-2.354524	-1.132313
C	0.851776	2.432308	-1.049484
C	0.777639	3.538070	0.010498
C	-0.064009	3.142069	1.230576
C	-1.461037	2.604616	0.905694
C	-2.687497	0.746582	-0.049789
C	-2.579769	-0.643480	-0.544909
C	-3.898659	1.493108	0.031801
C	-5.209201	1.164686	-0.301146
C	-5.739163	-0.016350	-0.830224
C	-5.020101	-1.172345	-1.134926
C	-3.658426	-1.441874	-1.002959
H	3.315268	2.512268	-1.316393
H	5.535437	2.047945	-1.614544
H	6.737075	0.063151	-1.159198
H	5.861019	-1.944124	-0.271656
H	3.722484	-2.476565	0.311397
H	2.008882	-2.619825	1.698978

H	1.877532	-3.281033	0.055689
H	-0.532314	-2.421946	1.744825
H	0.153024	-4.036724	1.719323
H	-0.416393	-4.381544	-0.621320
H	-1.855274	-3.779104	0.217962
H	0.071326	-2.199114	-1.575600
H	-1.596573	-2.616244	-1.962902
H	-0.145864	2.289571	-1.489519
H	1.512495	2.734501	-1.877219
H	1.793146	3.804153	0.344512
H	0.350905	4.438002	-0.464934
H	0.474346	2.412525	1.847615
H	-0.206019	4.034476	1.860675
H	-1.956391	3.318599	0.219667
H	-2.054976	2.600262	1.838160
H	-3.785140	2.502101	0.424067
H	-5.933749	1.962965	-0.116584
H	-6.815122	-0.039265	-1.010038
H	-5.610427	-2.007912	-1.521440
H	-3.380518	-2.458465	-1.280850

Co(TC-4,4)(NO), PW91, *S* = 1

Co	0.013826	-0.010120	0.539462
N	-0.106080	-0.195001	2.240557
N	1.530050	-1.187006	0.401235
N	-1.217784	-1.016828	-0.613731
N	-1.559714	1.250599	0.417314
N	1.174602	1.101133	-0.555441
O	0.556374	-0.505697	3.182645
C	2.456572	0.718379	-0.631323
C	3.470451	1.529339	-1.208125
C	4.832561	1.315343	-1.396089
C	5.621272	0.210105	-1.062487
C	5.184514	-0.957953	-0.433752
C	3.911458	-1.320047	0.001459
C	2.665980	-0.638657	-0.057152
C	1.515099	-2.577333	0.876979
C	0.109205	-3.176590	1.002507
C	-0.630251	-3.437934	-0.320182
C	-0.730085	-2.224670	-1.262351
C	0.679946	2.343340	-1.133226
C	0.597331	3.490579	-0.108002
C	-0.131868	3.135920	1.197047
C	-1.548640	2.575782	1.026384
C	-2.701589	0.700357	-0.002032
C	-2.499172	-0.631347	-0.643647
C	-3.961473	1.346131	0.157540
C	-5.242924	0.996478	-0.259737
C	-5.686298	-0.124806	-0.966206
C	-4.891175	-1.188514	-1.399156
C	-3.523530	-1.407807	-1.249284
H	3.119909	2.499435	-1.561109
H	5.360560	2.143551	-1.876615
H	6.682785	0.270184	-1.308386
H	5.958312	-1.705766	-0.239670
H	3.871935	-2.291983	0.491771
H	2.017087	-2.638729	1.859059

H	2.099427	-3.205203	0.180104
H	-0.507802	-2.550143	1.658795
H	0.222345	-4.139632	1.526054
H	-0.125902	-4.249014	-0.873228
H	-1.643152	-3.800788	-0.083087
H	0.273574	-1.990400	-1.647301
H	-1.341291	-2.490414	-2.140986
H	-0.329511	2.125257	-1.508114
H	1.279452	2.659847	-2.002414
H	1.615045	3.833252	0.140098
H	0.089364	4.338287	-0.598540
H	0.471683	2.426407	1.780869
H	-0.205121	4.048829	1.809315
H	-2.137892	3.282057	0.410103
H	-2.039102	2.543670	2.018991
H	-3.915534	2.287479	0.705026
H	-6.019334	1.716680	0.014764
H	-6.753044	-0.180661	-1.189286
H	-5.420475	-1.986801	-1.927703
H	-3.179427	-2.353440	-1.669696

Co(TC-5,5)(NO), B3LYP, *S* = 0

Co	-0.002559	-0.052947	0.830008
N	1.773402	-0.810197	0.823802
N	0.935623	1.274100	-0.346650
N	-0.829254	-1.093569	-0.534036
N	-1.706287	0.838777	0.793698
N	-0.469016	-0.724490	2.349491
O	-1.310235	-1.415210	2.793680
C	5.120079	-0.307218	-0.795346
C	3.986918	-0.777889	-0.139090
C	2.703340	-0.214536	0.069204
C	-2.100501	-0.812302	-0.813495
C	-2.856663	-1.555813	-1.760902
C	2.091753	-2.016254	1.584618
C	4.379337	1.873456	-1.694131
C	5.332113	0.876150	-1.487042
C	-3.906666	0.917579	-0.192813
C	2.226448	1.049916	-0.556699
C	3.054755	1.940677	-1.299811
C	-2.617323	0.345422	-0.042589
C	-2.018313	1.887351	1.758834
C	0.245034	2.369077	-1.020881
C	-5.137594	-0.482010	-1.891598
C	-4.157084	-1.415888	-2.219000
C	-0.063294	-2.050086	-1.330202
C	-4.991486	0.558343	-0.981725
C	-1.753518	3.332927	1.297251
C	0.397568	-3.754740	0.591968
C	0.292864	3.716751	-0.280820
C	-0.114692	-3.502773	-0.833732
C	1.867906	-3.363544	0.866721
C	-0.263947	3.717266	1.149963
H	-4.452966	-2.164237	-2.950133
H	5.967930	-0.986911	-0.759544
H	4.119761	-1.762785	0.285902

H	-6.094842	-0.572607	-2.392664
H	-4.072938	1.806380	0.400769
H	2.560280	2.853352	-1.601806
H	-2.334032	-2.401088	-2.186190
H	6.317900	1.036290	-1.909595
H	-5.858402	1.204458	-0.867208
H	4.723332	2.738123	-2.256487
H	-0.398884	-2.014792	-2.372453
H	0.970032	-1.706659	-1.336993
H	-1.143061	-3.872911	-0.898859
H	0.476216	-4.103533	-1.537285
H	0.285864	-4.827224	0.782398
H	-0.262734	-3.261755	1.309623
H	2.315474	-4.125952	1.514059
H	2.442594	-3.387824	-0.066170
H	1.474982	-1.999801	2.487071
H	3.127394	-1.969734	1.935998
H	-3.059160	1.794918	2.087683
H	-1.406180	1.702638	2.646778
H	-2.291184	3.532000	0.363397
H	-2.210718	3.980870	2.053258
H	0.346865	3.059909	1.777942
H	-0.121244	4.725716	1.551478
H	1.325446	4.078762	-0.244184
H	-0.268270	4.442541	-0.883290
H	0.633699	2.505215	-2.036764
H	-0.795669	2.064377	-1.132630

Co(TC-5,5)(NO) B3LYP, M_S = 0

Co	0.040959	-0.050878	0.770125
N	1.795385	-0.855296	0.786882
N	0.979722	1.242503	-0.358029
N	-0.900526	-1.178896	-0.553452
N	-1.669553	0.857285	0.729676
N	-0.365346	-0.670075	2.409949
O	-1.316136	-0.722315	3.111912
C	5.157743	-0.378147	-0.795122
C	4.022580	-0.838873	-0.145056
C	2.738616	-0.264258	0.053606
C	-2.162256	-0.855049	-0.812224
C	-2.979501	-1.603306	-1.704028
C	2.086130	-2.057525	1.565722
C	4.434973	1.804950	-1.706080
C	5.378788	0.808061	-1.488166
C	-3.886956	0.962543	-0.209052
C	2.277698	1.004405	-0.568848
C	3.104495	1.881224	-1.315925
C	-2.611120	0.355522	-0.068810
C	-1.962161	1.934647	1.672439
C	0.300833	2.330010	-1.062266
C	-5.220247	-0.451937	-1.818161
C	-4.286210	-1.435410	-2.133540
C	-0.197843	-2.208059	-1.310892
C	-5.006612	0.615178	-0.953733
C	-1.702407	3.371500	1.181020
C	0.301884	-3.769538	0.707286
C	0.366109	3.701658	-0.372699

C	-0.272759	-3.619026	-0.708923
C	1.797303	-3.405552	0.873494
C	-0.214734	3.763498	1.046171
H	-4.630589	-2.202060	-2.823379
H	6.001559	-1.062462	-0.758143
H	4.139664	-1.827350	0.276493
H	-6.194841	-0.523405	-2.287944
H	-4.009123	1.878152	0.353126
H	2.615444	2.792032	-1.630956
H	-2.500776	-2.485944	-2.105927
H	6.368060	0.961692	-1.904932
H	-5.844470	1.298770	-0.839946
H	4.783753	2.664126	-2.273397
H	-0.557406	-2.238557	-2.345698
H	0.848498	-1.900956	-1.365698
H	-1.315012	-3.954792	-0.697670
H	0.264415	-4.294400	-1.387466
H	0.163321	-4.814992	1.000827
H	-0.299316	-3.183404	1.407232
H	2.276121	-4.170777	1.494163
H	2.307965	-3.443443	-0.095584
H	1.477512	-2.000837	2.470714
H	3.127819	-2.039840	1.899478
H	-2.997414	1.852835	2.019199
H	-1.345660	1.771998	2.559640
H	-2.229747	3.550751	0.237254
H	-2.171522	4.031396	1.919273
H	0.387573	3.138990	1.715063
H	-0.086348	4.790199	1.403952
H	1.403175	4.050150	-0.334003
H	-0.175100	4.411735	-1.010984
H	0.693879	2.421120	-2.081132
H	-0.742087	2.033753	-1.164677

Co(TC-5,5)(NO), B3LYP, *S* = 1

Co	0.029551	-0.042312	0.830499
N	1.831336	-0.774721	0.866928
N	0.899512	1.214876	-0.378985
N	-0.839814	-1.157130	-0.573335
N	-1.720876	0.800510	0.785095
N	-0.449767	-0.811560	2.375083
O	-1.232419	-0.756500	3.245705
C	5.150508	-0.209728	-0.784452
C	4.050262	-0.689613	-0.088978
C	2.736431	-0.178539	0.090328
C	-2.107877	-0.879956	-0.831618
C	-2.885461	-1.639416	-1.753976
C	2.169752	-1.978466	1.622272
C	4.304785	1.878505	-1.801645
C	5.301994	0.943732	-1.546641
C	-3.913472	0.852806	-0.214833
C	2.203191	1.028270	-0.595839
C	2.977253	1.906839	-1.398717
C	-2.621756	0.288588	-0.055026
C	-2.062044	1.860093	1.726902
C	0.168113	2.269813	-1.078088
C	-5.166616	-0.571581	-1.879669

C	-4.189503	-1.513472	-2.199449
C	-0.072503	-2.120873	-1.349744
C	-5.006347	0.482229	-0.990626
C	-1.805350	3.300226	1.243620
C	0.484203	-3.720236	0.640278
C	0.207159	3.642462	-0.386288
C	-0.060165	-3.552038	-0.787117
C	1.960081	-3.308694	0.867733
C	-0.320431	3.682077	1.055225
H	-4.493478	-2.277569	-2.910955
H	6.030933	-0.843775	-0.716481
H	4.234105	-1.634985	0.401258
H	-6.129336	-0.668732	-2.368853
H	-4.081983	1.751075	0.363263
H	2.436610	2.768673	-1.762989
H	-2.364364	-2.492523	-2.167688
H	6.276460	1.124065	-1.986570
H	-5.869427	1.134149	-0.878844
H	4.600597	2.721440	-2.421082
H	-0.424751	-2.150423	-2.387426
H	0.953318	-1.747757	-1.391616
H	-1.076307	-3.960025	-0.816393
H	0.539630	-4.165287	-1.472240
H	0.376549	-4.778800	0.898081
H	-0.158764	-3.180435	1.339836
H	2.450427	-4.082212	1.468903
H	2.498491	-3.282732	-0.086061
H	1.537428	-1.991528	2.511841
H	3.200381	-1.921527	1.986110
H	-3.107163	1.766900	2.040650
H	-1.471299	1.698875	2.633567
H	-2.364494	3.490935	0.320625
H	-2.242708	3.957470	2.003501
H	0.304271	3.043008	1.689087
H	-0.170333	4.701456	1.425106
H	1.233253	4.024171	-0.384375
H	-0.380436	4.336061	-1.001096
H	0.534159	2.371825	-2.105764
H	-0.866262	1.940626	-1.157915

Co(TC-5,5)(NO), B3LYP, M_S = 1

Co	0.004905	-0.003125	0.762292
N	1.915935	-0.839291	0.718533
N	1.017831	1.294590	-0.365686
N	-0.913166	-1.167011	-0.556772
N	-1.880887	0.811208	0.753670
N	-0.095041	-0.181887	2.568145
O	-0.756974	-0.788542	3.321860
C	5.230322	-0.229534	-0.913567
C	4.122134	-0.732437	-0.255568
C	2.818409	-0.205232	-0.013005
C	-2.198403	-0.920429	-0.823828
C	-2.953546	-1.730697	-1.706532
C	2.259057	-2.025481	1.491114
C	4.448034	1.968598	-1.726533
C	5.415308	0.987504	-1.568935
C	-4.043470	0.808933	-0.314808

C	2.314651	1.076917	−0.599702
C	3.118511	1.996651	−1.316688
C	−2.744536	0.267381	−0.092974
C	−2.259989	1.904785	1.642024
C	0.312485	2.400929	−1.009962
C	−5.250422	−0.716120	−1.917629
C	−4.262240	−1.656578	−2.170789
C	−0.163557	−2.174790	−1.304906
C	−5.114501	0.395235	−1.088199
C	−1.883747	3.314539	1.145394
C	0.415483	−3.707671	0.713555
C	0.314206	3.712037	−0.207088
C	−0.195616	−3.582670	−0.689785
C	1.923734	−3.376194	0.826254
C	−0.368433	3.634974	1.165795
H	−4.543261	−2.463683	−2.842608
H	6.088931	−0.896792	−0.917295
H	4.272825	−1.729202	0.137255
H	−6.205579	−0.851597	−2.412957
H	−4.229645	1.735689	0.210737
H	2.610332	2.912643	−1.584754
H	−2.416235	−2.589514	−2.084157
H	6.393561	1.177806	−1.996478
H	−5.982972	1.047003	−1.034267
H	4.767782	2.860860	−2.259330
H	−0.508570	−2.224180	−2.343622
H	0.870269	−1.829555	−1.345725
H	−1.229738	−3.940899	−0.651176
H	0.340262	−4.254220	−1.372720
H	0.257879	−4.739406	1.043520
H	−0.152794	−3.087914	1.414058
H	2.408259	−4.147603	1.434621
H	2.399321	−3.427625	−0.159817
H	1.700845	−1.970760	2.432198
H	3.316396	−2.018794	1.776235
H	−3.328819	1.873218	1.875584
H	−1.745725	1.742356	2.594583
H	−2.293622	3.471341	0.141556
H	−2.404854	4.023075	1.798065
H	0.155248	2.899397	1.784267
H	−0.217467	4.598110	1.663236
H	1.345749	4.050373	−0.065309
H	−0.184729	4.478315	−0.814177
H	0.714868	2.586798	−2.012028
H	−0.719757	2.076777	−1.155051

Co(TC-5,5)(NO), PW91, *S* = 0

Co	0.019521	−0.065155	0.816421
N	1.779307	−0.802465	0.798905
N	0.908259	1.260876	−0.346942
N	−0.809445	−1.149255	−0.522874
N	−1.691167	0.802506	0.753610
N	−0.344092	−0.569683	2.400345
O	−1.275463	−0.847340	3.087960
C	5.084310	−0.343428	−0.929107
C	3.964400	−0.810712	−0.242981
C	2.696776	−0.219381	0.009573

C	-2.083223	-0.866745	-0.838177
C	-2.830961	-1.639411	-1.774056
C	2.114030	-1.969904	1.609540
C	4.336946	1.876824	-1.770454
C	5.282341	0.858690	-1.609288
C	-3.876853	0.900949	-0.288447
C	2.210511	1.048604	-0.585865
C	3.019723	1.954924	-1.329517
C	-2.596816	0.306158	-0.104094
C	-2.045136	1.847301	1.712235
C	0.214740	2.367418	-1.002750
C	-5.093569	-0.524197	-1.988945
C	-4.122553	-1.491315	-2.268450
C	-0.063172	-2.173405	-1.247937
C	-4.951941	0.541048	-1.097989
C	-1.778901	3.297143	1.267900
C	0.350189	-3.721459	0.792051
C	0.289353	3.706508	-0.250732
C	-0.173465	-3.581228	-0.644397
C	1.837983	-3.354089	0.990181
C	-0.286826	3.683836	1.170674
H	-4.419567	-2.261352	-2.986309
H	5.929807	-1.036991	-0.938660
H	4.082429	-1.815750	0.161086
H	-6.046029	-0.610561	-2.513810
H	-4.039059	1.812266	0.285943
H	2.522978	2.888496	-1.590390
H	-2.308581	-2.514778	-2.157370
H	6.261456	1.015512	-2.064770
H	-5.815396	1.208087	-1.020462
H	4.679390	2.752765	-2.328634
H	-0.387713	-2.196459	-2.301871
H	0.989410	-1.861612	-1.263559
H	-1.224780	-3.908786	-0.672555
H	0.387784	-4.268004	-1.302006
H	0.201523	-4.770014	1.092967
H	-0.275333	-3.124536	1.472677
H	2.299755	-4.085955	1.672194
H	2.380772	-3.449906	0.034072
H	1.525467	-1.879443	2.536889
H	3.173919	-1.913059	1.906257
H	-3.104209	1.736865	1.999684
H	-1.468483	1.666711	2.630633
H	-2.290561	3.499637	0.311889
H	-2.269791	3.939718	2.016416
H	0.309120	2.997232	1.793832
H	-0.143800	4.685348	1.604902
H	1.335321	4.048197	-0.200241
H	-0.256015	4.455359	-0.851041
H	0.596724	2.500964	-2.028855
H	-0.837252	2.069327	-1.101098

Co(TC-5,5)(NO), PW91, *S* = 1

Co	0.010184	-0.063628	0.852622
N	1.838232	-0.738886	0.891717
N	0.868288	1.215454	-0.365496
N	-0.796441	-1.130590	-0.575139

N	-1.738878	0.777333	0.790236
N	-0.432371	-0.751987	2.371705
O	-1.225627	-0.683243	3.257660
C	5.146486	-0.173952	-0.803217
C	4.061464	-0.645117	-0.072803
C	2.734648	-0.148160	0.089991
C	-2.082988	-0.893356	-0.843360
C	-2.825198	-1.678439	-1.772663
C	2.190397	-1.918961	1.671739
C	4.243048	1.867929	-1.901369
C	5.260456	0.955439	-1.620115
C	-3.926354	0.809096	-0.246756
C	2.175565	1.029834	-0.620120
C	2.916333	1.891980	-1.475137
C	-2.627771	0.256116	-0.070318
C	-2.107679	1.828640	1.730999
C	0.121712	2.265748	-1.051991
C	-5.123582	-0.638171	-1.943614
C	-4.128070	-1.571646	-2.247179
C	-0.002112	-2.094588	-1.323542
C	-5.000163	0.424294	-1.047495
C	-1.841324	3.267317	1.248821
C	0.527825	-3.673470	0.688644
C	0.186103	3.630412	-0.346109
C	-0.000384	-3.521118	-0.746866
C	2.000015	-3.256897	0.926067
C	-0.351170	3.646348	1.092532
H	-4.410169	-2.343730	-2.968657
H	6.047759	-0.787620	-0.719952
H	4.265822	-1.568640	0.466958
H	-6.081093	-0.748856	-2.454465
H	-4.114297	1.709754	0.336915
H	2.347474	2.734179	-1.866269
H	-2.273430	-2.527145	-2.176423
H	6.231118	1.135011	-2.084945
H	-5.881293	1.065531	-0.954186
H	4.518528	2.692165	-2.565228
H	-0.337349	-2.129865	-2.374751
H	1.028685	-1.711253	-1.346136
H	-1.024917	-3.925475	-0.783566
H	0.606122	-4.147451	-1.424450
H	0.415832	-4.734720	0.959861
H	-0.125768	-3.119438	1.378585
H	2.495701	-4.027852	1.537210
H	2.549195	-3.228808	-0.030007
H	1.536475	-1.921596	2.557076
H	3.223387	-1.839985	2.048481
H	-3.167525	1.728666	2.019275
H	-1.537085	1.659083	2.657213
H	-2.380393	3.450064	0.303668
H	-2.305118	3.931826	1.995347
H	0.264751	2.980444	1.719097
H	-0.195862	4.660671	1.491186
H	1.227562	3.989830	-0.336631
H	-0.388928	4.349037	-0.955381
H	0.462745	2.369512	-2.095648
H	-0.923231	1.935626	-1.104233

Co(TC-6,6)(NO), B3LYP, *S* = 0

Co	0.007952000	0.025902000	0.751433000
N	-1.834729000	0.625812000	0.776633000
N	-0.830090000	-1.355278000	-0.459340000
N	1.792908000	-0.704401000	0.697316000
N	0.749611000	1.193452000	-0.572570000
C	-2.727395000	-0.067027000	0.059951000
C	-4.106351000	0.263352000	0.054163000
H	-4.369407000	1.099991000	0.684891000
C	-5.200075000	-0.282056000	-0.610072000
H	-6.146322000	0.198747000	-0.374438000
C	-5.267171000	-1.311650000	-1.537025000
H	-6.241122000	-1.549284000	-1.950171000
C	-4.180545000	-2.058947000	-1.988653000
H	-4.410979000	-2.812339000	-2.738046000
C	-2.846678000	-2.010590000	-1.623011000
H	-2.236020000	-2.740259000	-2.135153000
C	-2.127246000	-1.197424000	-0.698724000
C	-0.071877000	-2.404006000	-1.138594000
H	-0.319463000	-2.439275000	-2.207013000
H	0.975240000	-2.118127000	-1.083596000
C	-0.265912000	-3.813546000	-0.536618000
H	-1.304825000	-4.116209000	-0.694472000
H	0.347459000	-4.516686000	-1.114666000
C	0.049364000	-3.957299000	0.963444000
H	-0.529549000	-4.801739000	1.352411000
H	-0.332172000	-3.078215000	1.492576000
C	1.518472000	-4.214936000	1.336809000
H	1.562433000	-4.406748000	2.416360000
H	1.844844000	-5.145040000	0.855295000
C	2.540753000	-3.115707000	1.003540000
H	3.520825000	-3.455955000	1.355158000
H	2.639345000	-3.000446000	-0.077938000
C	2.224487000	-1.735466000	1.640594000
H	3.090366000	-1.375220000	2.209563000
H	1.422107000	-1.853053000	2.371220000
C	2.668491000	-0.065015000	-0.075821000
C	4.049613000	-0.384502000	-0.085804000
H	4.338651000	-1.142815000	0.629181000
C	5.101464000	0.087890000	-0.860283000
H	6.065584000	-0.353453000	-0.620352000
C	5.106584000	1.010326000	-1.899049000
H	6.055540000	1.205566000	-2.385770000
C	3.993913000	1.702185000	-2.373909000
H	4.183726000	2.368217000	-3.212055000
C	2.677796000	1.700201000	-1.940782000
H	2.037859000	2.371892000	-2.494799000
C	2.027253000	0.993755000	-0.890879000
C	-0.077031000	2.139595000	-1.325010000
H	0.118938000	2.034274000	-2.398912000
H	-1.109375000	1.839745000	-1.180141000
C	0.115451000	3.614769000	-0.919652000
H	1.147161000	3.901725000	-1.141982000
H	-0.519103000	4.226172000	-1.574407000
C	-0.168411000	3.959937000	0.552333000

H	0.376657000	4.880210000	0.789368000
H	0.274812000	3.194807000	1.193911000
C	-1.637130000	4.209272000	0.935950000
H	-2.011182000	5.058717000	0.350503000
H	-1.655810000	4.539919000	1.982053000
C	-2.637532000	3.051245000	0.782103000
H	-3.613720000	3.419567000	1.116776000
H	-2.770647000	2.797142000	-0.271844000
C	-2.285848000	1.765602000	1.582786000
H	-3.146322000	1.460040000	2.188801000
H	-1.498286000	1.996659000	2.298364000
N	0.411493000	0.653397000	2.305546000
O	1.140882000	1.430188000	2.800101000

Co(TC-6,6)(NO), B3LYP, M_S = 0

C	0.086265000	2.336065000	-1.291020000
C	0.325469000	3.761500000	-0.754301000
C	1.440693000	-4.285890000	1.220711000
C	2.105536000	1.041850000	-0.888832000
C	2.139936000	-1.812041000	1.526264000
C	2.449046000	-3.181101000	0.861772000
C	2.666437000	-0.094702000	-0.111343000
C	2.826591000	1.768594000	-1.875101000
C	4.035116000	-0.472011000	-0.100336000
C	4.150343000	1.719672000	-2.285274000
C	5.128373000	-0.021828000	-0.827400000
C	5.209908000	0.943261000	-1.824939000
C	-0.030355000	3.991858000	0.724934000
C	-0.040655000	-4.014133000	0.910470000
C	-0.177405000	-2.405882000	-1.145195000
C	-0.403877000	-3.821107000	-0.571462000
C	-1.508831000	4.277601000	1.040870000
C	-2.204522000	-1.142876000	-0.704749000
C	-2.251848000	1.837531000	1.547409000
C	-2.531930000	3.158402000	0.778071000
C	-2.768420000	0.018804000	0.027088000
C	-2.937752000	-1.944597000	-1.615416000
C	-4.139984000	0.393121000	0.020152000
C	-4.274159000	-1.948072000	-1.995667000
C	-5.242006000	-0.117342000	-0.647377000
C	-5.333150000	-1.158425000	-1.566823000
Co	-0.033921000	0.025671000	0.664011000
H	0.167227000	-4.527388000	-1.187787000
H	0.313608000	2.316182000	-2.364098000
H	0.331010000	3.145871000	1.316218000
H	0.540302000	4.858177000	1.076707000
H	0.874851000	-2.145686000	-1.093200000
H	1.321061000	-1.941376000	2.233467000
H	1.381765000	4.009152000	-0.895525000
H	1.527006000	-4.493823000	2.294591000
H	1.742907000	-5.209864000	0.712443000
H	2.240660000	2.512370000	-2.396898000
H	2.513364000	-3.058946000	-0.221304000
H	2.991620000	-1.484151000	2.132476000
H	3.441265000	-3.520578000	1.177871000
H	4.272335000	-1.271193000	0.588222000

H	4.396127000	2.419657000	-3.080177000
H	6.062025000	-0.522667000	-0.583441000
H	6.180156000	1.106803000	-2.280540000
H	-0.239764000	4.460855000	-1.384229000
H	-0.398629000	-3.149569000	1.478708000
H	-0.434326000	-2.409954000	-2.211563000
H	-0.610400000	-4.867754000	1.292783000
H	-0.966334000	2.077403000	-1.206010000
H	-1.450477000	1.999091000	2.265857000
H	-1.456362000	-4.088007000	-0.701019000
H	-1.576144000	4.555780000	2.100102000
H	-1.821860000	5.167264000	0.479869000
H	-2.353461000	-2.707933000	-2.107809000
H	-2.608275000	2.950324000	-0.291373000
H	-3.128232000	1.559426000	2.143315000
H	-3.516410000	3.539518000	1.071436000
H	-4.371104000	1.247866000	0.639626000
H	-4.524171000	-2.704914000	-2.734895000
H	-6.174102000	0.397654000	-0.429095000
H	-6.310630000	-1.365216000	-1.988180000
N	0.276999000	0.542024000	2.364746000
N	0.834317000	1.295759000	-0.588122000
N	1.749820000	-0.737165000	0.609696000
N	-0.904188000	-1.339300000	-0.452320000
N	-1.852713000	0.697738000	0.715788000
O	1.189588000	0.533700000	3.120201000

Co(TC-6,6)(NO), B3LYP, *S* = 1

Co	-0.009112000	0.010132000	0.696425000
N	-1.870358000	0.630446000	0.755602000
N	-0.834203000	-1.277030000	-0.558286000
N	1.824137000	-0.681031000	0.677614000
N	0.840864000	1.315016000	-0.577556000
C	-2.751459000	-0.030521000	0.006132000
C	-4.135799000	0.287357000	0.009688000
H	-4.409375000	1.074149000	0.698523000
C	-5.210692000	-0.211067000	-0.711756000
H	-6.164471000	0.249105000	-0.466157000
C	-5.253132000	-1.184459000	-1.704477000
H	-6.218065000	-1.396471000	-2.151492000
C	-4.160571000	-1.903374000	-2.175913000
H	-4.375363000	-2.612530000	-2.971445000
C	-2.829449000	-1.874309000	-1.783587000
H	-2.207274000	-2.569690000	-2.328858000
C	-2.134347000	-1.112139000	-0.808703000
C	-0.060050000	-2.295413000	-1.267987000
H	-0.288595000	-2.280506000	-2.340830000
H	0.984449000	-2.009448000	-1.180673000
C	-0.264745000	-3.727214000	-0.728348000
H	-1.305633000	-4.016025000	-0.899350000
H	0.344622000	-4.409022000	-1.335218000
C	0.051941000	-3.933181000	0.764128000
H	-0.538166000	-4.782831000	1.123471000
H	-0.313334000	-3.068752000	1.327999000
C	1.519082000	-4.222971000	1.120697000
H	1.562890000	-4.467978000	2.189344000

H	1.835585000	-5.131425000	0.593260000
C	2.549202000	-3.116077000	0.841076000
H	3.527332000	-3.483850000	1.169867000
H	2.646884000	-2.943995000	-0.233016000
C	2.247639000	-1.769567000	1.555855000
H	3.119053000	-1.455263000	2.143115000
H	1.453131000	-1.927541000	2.287939000
C	2.716899000	-0.010228000	-0.053149000
C	4.092431000	-0.358652000	-0.056850000
H	4.347401000	-1.173594000	0.606050000
C	5.182633000	0.135993000	-0.763077000
H	6.124071000	-0.353415000	-0.525664000
C	5.252961000	1.130933000	-1.728669000
H	6.224200000	1.333053000	-2.166409000
C	4.176229000	1.888881000	-2.184700000
H	4.411894000	2.615857000	-2.958220000
C	2.846807000	1.881860000	-1.797602000
H	2.243524000	2.613273000	-2.317306000
C	2.126142000	1.113294000	-0.838550000
C	0.069714000	2.335185000	-1.282238000
H	0.316422000	2.346190000	-2.351506000
H	-0.974684000	2.035739000	-1.219492000
C	0.241272000	3.760167000	-0.715965000
H	1.286759000	4.055532000	-0.845381000
H	-0.349146000	4.446194000	-1.337260000
C	-0.131254000	3.950824000	0.765990000
H	0.419277000	4.821349000	1.139092000
H	0.243363000	3.101215000	1.343809000
C	-1.616858000	4.202463000	1.080775000
H	-1.949645000	5.085021000	0.519933000
H	-1.690563000	4.479576000	2.140010000
C	-2.615150000	3.061030000	0.818649000
H	-3.609520000	3.421453000	1.104148000
H	-2.678129000	2.843474000	-0.249773000
C	-2.306813000	1.748884000	1.593766000
H	-3.174645000	1.451396000	2.194236000
H	-1.506962000	1.942790000	2.309362000
N	0.206890000	0.457943000	2.443580000
O	0.265203000	-0.213774000	3.408329000

Co(TC-6,6)(NO), B3LYP, M_S = 1

Co	-0.003586000	0.029557000	0.677578000
N	-1.948567000	0.712627000	0.677846000
N	-0.888606000	-1.275438000	-0.547934000
N	1.951202000	-0.712769000	0.676388000
N	0.948299000	1.335093000	-0.494033000
C	-2.804361000	0.045981000	-0.083626000
C	-4.185520000	0.388146000	-0.151875000
H	-4.466990000	1.209792000	0.492484000
C	-5.241307000	-0.108885000	-0.896490000
H	-6.192473000	0.382941000	-0.708582000
C	-5.267307000	-1.118266000	-1.856733000
H	-6.218522000	-1.324403000	-2.334961000
C	-4.176266000	-1.877544000	-2.254072000
H	-4.375697000	-2.615721000	-3.026869000
C	-2.858521000	-1.861290000	-1.809460000

H	-2.238663000	-2.599642000	-2.297695000
C	-2.177849000	-1.080674000	-0.843116000
C	-0.111274000	-2.308660000	-1.233866000
H	-0.327989000	-2.310745000	-2.309120000
H	0.932364000	-2.020581000	-1.137122000
C	-0.315151000	-3.731235000	-0.672993000
H	-1.368078000	-4.003056000	-0.790447000
H	0.252413000	-4.428496000	-1.302617000
C	0.076848000	-3.930405000	0.802416000
H	-0.513488000	-4.761394000	1.202795000
H	-0.234678000	-3.052742000	1.377161000
C	1.554462000	-4.257849000	1.079425000
H	1.648075000	-4.512833000	2.142632000
H	1.819334000	-5.170243000	0.530485000
C	2.598226000	-3.174987000	0.755732000
H	3.583531000	-3.576976000	1.015326000
H	2.633295000	-2.983294000	-0.319269000
C	2.377824000	-1.833626000	1.511038000
H	3.283596000	-1.568544000	2.069502000
H	1.606722000	-1.984127000	2.269760000
C	2.834138000	-0.027523000	-0.032776000
C	4.216321000	-0.380370000	-0.075634000
H	4.471547000	-1.231173000	0.541188000
C	5.296668000	0.135058000	-0.768949000
H	6.237014000	-0.375376000	-0.575114000
C	5.362033000	1.183096000	-1.686489000
H	6.328636000	1.397236000	-2.128930000
C	4.291157000	1.971467000	-2.078838000
H	4.520246000	2.741899000	-2.811113000
C	2.960457000	1.953133000	-1.671471000
H	2.365488000	2.724716000	-2.139154000
C	2.243240000	1.137722000	-0.762372000
C	0.196803000	2.398158000	-1.162070000
H	0.456587000	2.450473000	-2.226475000
H	-0.851170000	2.107925000	-1.123834000
C	0.375260000	3.794326000	-0.530670000
H	1.432201000	4.068226000	-0.594740000
H	-0.166646000	4.520457000	-1.150413000
C	-0.073122000	3.929961000	0.936035000
H	0.499711000	4.744335000	1.392249000
H	0.219410000	3.029401000	1.484782000
C	-1.560750000	4.246016000	1.172442000
H	-1.810159000	5.172288000	0.639801000
H	-1.690900000	4.472289000	2.238331000
C	-2.591515000	3.170972000	0.786146000
H	-3.586437000	3.568626000	1.013645000
H	-2.582464000	2.999256000	-0.292713000
C	-2.401865000	1.815672000	1.523856000
H	-3.325140000	1.541553000	2.047505000
H	-1.652004000	1.946510000	2.307089000
N	-0.030316000	0.030366000	2.497281000
O	-0.565966000	-0.607017000	3.321178000

Co(TC-6,6)(NO), PW91, *S* = 0

Co	-0.023196000	0.037839000	0.707532000
N	-1.845378000	0.626545000	0.735541000

N	-0.822119000	-1.353371000	-0.445148000
N	1.762306000	-0.675031000	0.626625000
N	0.724015000	1.251660000	-0.575572000
C	-2.732589000	-0.047247000	-0.016170000
C	-4.100434000	0.339603000	-0.090607000
H	-4.352256000	1.222718000	0.494324000
C	-5.182998000	-0.196180000	-0.784561000
H	-6.128126000	0.328700000	-0.619191000
C	-5.236702000	-1.269504000	-1.674885000
H	-6.203902000	-1.493725000	-2.127377000
C	-4.157934000	-2.077503000	-2.043157000
H	-4.385492000	-2.866389000	-2.765784000
C	-2.832885000	-2.056126000	-1.616988000
H	-2.223287000	-2.842878000	-2.057593000
C	-2.130659000	-1.203827000	-0.717205000
C	-0.067623000	-2.426863000	-1.092919000
H	-0.322547000	-2.480859000	-2.165969000
H	0.987360000	-2.140694000	-1.046073000
C	-0.275787000	-3.816489000	-0.452887000
H	-1.330743000	-4.104351000	-0.578248000
H	0.313482000	-4.551009000	-1.029445000
C	0.079559000	-3.917333000	1.040079000
H	-0.500659000	-4.742812000	1.481443000
H	-0.273138000	-3.006016000	1.550630000
C	1.559776000	-4.174460000	1.363766000
H	1.649214000	-4.338476000	2.451603000
H	1.868707000	-5.122202000	0.890403000
C	2.557155000	-3.075439000	0.961172000
H	3.561295000	-3.389547000	1.288921000
H	2.618744000	-2.987927000	-0.132832000
C	2.230285000	-1.688662000	1.576347000
H	3.104324000	-1.294402000	2.123049000
H	1.445916000	-1.811722000	2.333999000
C	2.639322000	-0.031075000	-0.158296000
C	4.020090000	-0.374619000	-0.193752000
H	4.311676000	-1.152396000	0.511059000
C	5.064116000	0.094126000	-0.987471000
H	6.031845000	-0.371459000	-0.779813000
C	5.060071000	1.044766000	-2.010083000
H	6.006518000	1.231778000	-2.519424000
C	3.951463000	1.783292000	-2.435903000
H	4.139199000	2.479627000	-3.258362000
C	2.642310000	1.796423000	-1.965222000
H	1.997626000	2.511428000	-2.473828000
C	2.003380000	1.050080000	-0.933020000
C	-0.081224000	2.272131000	-1.247411000
H	0.105442000	2.244353000	-2.335466000
H	-1.129839000	1.990977000	-1.117268000
C	0.171336000	3.698457000	-0.720628000
H	1.222068000	3.957915000	-0.922924000
H	-0.439320000	4.398273000	-1.318171000
C	-0.103903000	3.913142000	0.777557000
H	0.482964000	4.783599000	1.111520000
H	0.295027000	3.058773000	1.345349000
C	-1.566569000	4.183238000	1.165251000
H	-1.904129000	5.099381000	0.650160000
H	-1.595231000	4.418959000	2.243072000

C	-2.596091000	3.073773000	0.892149000
H	-3.577019000	3.443472000	1.233744000
H	-2.711437000	2.907417000	-0.189077000
C	-2.305300000	1.720689000	1.597325000
H	-3.208346000	1.381184000	2.131908000
H	-1.536557000	1.861128000	2.368674000
N	0.299214000	0.504041000	2.319471000
O	1.228955000	0.774032000	3.012787000

Co(TC-6,6)(NO), PW91, *S* = 1

Co	-0.009848000	0.038968000	0.764066000
N	-1.912972000	0.522660000	0.817005000
N	-0.748709000	-1.295912000	-0.493257000
N	1.832881000	-0.606513000	0.695650000
N	0.701928000	1.244653000	-0.618295000
C	-2.748168000	-0.159674000	0.024798000
C	-4.149567000	0.102240000	-0.004821000
H	-4.474237000	0.874394000	0.691338000
C	-5.181941000	-0.437853000	-0.763540000
H	-6.169104000	-0.019952000	-0.547227000
C	-5.145751000	-1.414796000	-1.763480000
H	-6.091951000	-1.667956000	-2.244432000
C	-4.008396000	-2.093742000	-2.202249000
H	-4.171907000	-2.817941000	-3.005308000
C	-2.686633000	-2.004956000	-1.769232000
H	-2.011182000	-2.679032000	-2.293930000
C	-2.057883000	-1.197829000	-0.781295000
C	0.073861000	-2.305821000	-1.155446000
H	-0.136854000	-2.343578000	-2.238507000
H	1.113807000	-1.979571000	-1.058121000
C	-0.107245000	-3.712056000	-0.543770000
H	-1.145149000	-4.032545000	-0.722221000
H	0.534059000	-4.417718000	-1.099789000
C	0.183950000	-3.810539000	0.965043000
H	-0.424186000	-4.626136000	1.386403000
H	-0.176928000	-2.891177000	1.456119000
C	1.645654000	-4.079965000	1.352565000
H	1.685460000	-4.251433000	2.442200000
H	1.968235000	-5.027303000	0.887183000
C	2.670205000	-2.988828000	1.002983000
H	3.657442000	-3.327135000	1.357708000
H	2.769556000	-2.883617000	-0.087339000
C	2.359033000	-1.602688000	1.630239000
H	3.260069000	-1.203139000	2.125850000
H	1.620405000	-1.724511000	2.434551000
C	2.667834000	0.048306000	-0.127497000
C	4.053958000	-0.265567000	-0.198348000
H	4.374352000	-1.045896000	0.490679000
C	5.082342000	0.226715000	-1.000320000
H	6.057990000	-0.229160000	-0.808484000
C	5.056484000	1.189700000	-2.009333000
H	5.996492000	1.400644000	-2.521441000
C	3.931040000	1.911389000	-2.418632000
H	4.099125000	2.625923000	-3.229721000
C	2.624548000	1.881949000	-1.943489000

H	1.959768000	2.587803000	-2.440269000
C	1.992888000	1.102745000	-0.929863000
C	-0.154399000	2.210896000	-1.298384000
H	0.048095000	2.206468000	-2.384602000
H	-1.186146000	1.860117000	-1.179563000
C	-0.016140000	3.652122000	-0.764240000
H	1.017718000	3.983777000	-0.947415000
H	-0.662007000	4.307973000	-1.374633000
C	-0.330413000	3.853299000	0.730318000
H	0.216179000	4.746850000	1.071979000
H	0.090649000	3.015292000	1.305587000
C	-1.807019000	4.068807000	1.104537000
H	-2.188683000	4.942082000	0.546955000
H	-1.845511000	4.356268000	2.169512000
C	-2.784942000	2.900342000	0.892961000
H	-3.783071000	3.240798000	1.213940000
H	-2.885914000	2.669221000	-0.177958000
C	-2.425245000	1.598659000	1.664172000
H	-3.297106000	1.240177000	2.238192000
H	-1.642934000	1.813707000	2.406272000
N	0.316078000	0.662614000	2.335337000
O	1.042076000	0.564314000	3.273697000