

Supplementary information for
Mindless DFT Benchmarking

M. Korth and S. Grimme

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1 Benchmark set specifications for the 931 set

Number of entries:

83 (To combine the 931 and ORG sets, omit the 931 reactions 12 and 49.)

Type and size of systems:

8 atomic Artificial Molecules.

Elemental distribution:

Main group elements up to chlorine, excluding Nobel gases.

Table 1: Initial and final element distributions for the 931 benchmark set.

Element	Initial	Final	Factor
H	0.692	0.648	0.936416
Li	0.033	0.035	1.06061
Be	0.033	0.036	1.09091
B	0.033	0.047	1.42424
C	0.033	0.039	1.18182
N	0.033	0.038	1.15152
O	0.033	0.029	0.878788
F	0.033	0.032	0.969697
Na	0.011	0.011	1
Mg	0.011	0.012	1.09091
Al	0.011	0.020	1.81818
Si	0.011	0.014	1.27273
P	0.011	0.012	1.09091
S	0.011	0.017	1.54545
Cl	0.011	0.014	1.27273

Arrangement:

Optimized via PBE/TZVP from random cubic grid starting positions.

Complexity of electronic structure:

Uncharged, single-reference, 25% open-shell.

Reaction scheme:

Decomposition into simple hydrides (group 1-4) and diatomics (group 5-7).

2 Benchmark set specifications for the ORG set

Number of entries:

84

Type and size of systems:

8 atomic Artificial Molecules.

Elemental distribution:

Main group elements up to chlorine, excluding Nobel gases.

Table 2: Initial and final element distributions for the ORG benchmark set.

Element	Initial	Final	Factor
H	0.618	0.582	0.941748
LI	0.019	0.010	0.526316
BE	0.005	0.000	0
B	0.010	0.018	1.8
C	0.155	0.176	1.13548
N	0.039	0.043	1.10256
O	0.039	0.045	1.15385
F	0.010	0.013	1.3
NA	0.010	0.003	0.3
MG	0.010	0.012	1.2
AL	0.010	0.015	1.5
SI	0.019	0.024	1.26316
P	0.019	0.027	1.42105
S	0.019	0.019	1
CL	0.019	0.013	0.684211

Arrangement:

Optimized via PBE/TZVPP from random cubic grid starting positions.

Complexity of electronic structure:

Uncharged, single-reference, 25% open-shell.

Reaction scheme:

Decomposition into simple hydrides (group 1-4) and diatomics (group 5-7).

3 Cartesian coordinates for the 931 set

(Also available as Turbomole coord files. Please email to grimmes@uni-muenster.de or dgd@uni-muenster.de.)

```
1
$coord
0.12748830999475 1.37188618098161 2.05382962955034 h
-1.70801967682558 0.39523721065650 4.72176916180967 h
1.66632375266971 0.19182151519615 4.82988860754900 h
-0.00034348407427 0.01007689005110 3.61144648038371 c
0.00375066597250 0.06057412424942 -3.32337689248998 o
-1.46885124794772 -0.54992915376014 -2.41353660490869 h
1.41871881632529 -0.56807205457296 -2.33788464794116 h
-0.09110085664585 -1.92250831000094 2.86290049068928 h
$end

2
$coord
-0.71626222847232 -5.95383026930289 -0.23638164750456 h
1.26919421026635 -3.19048164927473 -2.23046783119902 h
-0.63534784014591 4.52901630532027 0.16364854942959 o
-1.59145514199056 4.61050200903037 -1.41409077196436 h
-0.07175149909361 -3.33039343770272 0.12190538313200 p
-2.39580316906628 -2.47244255067772 -0.98576721793796 h
0.99137332635997 2.51525615258826 -0.21406987198444 n
1.94790515197567 2.50508519623632 1.49781843235163 h
$end

3
$coord
-0.70323811401881 2.61190475071584 0.04288171937098 n
-1.40287137422028 -4.07241335529408 -0.40550478790857 li
-1.36959277939900 -0.19659431669047 0.49871573186497 b
-3.20931429189774 -1.01259742049451 -0.72840465539578 h
1.18433130168207 1.31057995223005 -0.54127941359250 c
2.06380122509587 -3.13017770152178 -1.32580114333568 h
2.98979046656737 -1.64470092925836 2.16380361364913 h
1.69337527431173 -1.48998973263805 0.29714804240689 b
```

\$end

4

\$coord

2.69821479177197 0.71633429411552 -3.77158678208130 h
2.68681915095241 -0.75317104901609 -3.76989879526099 h
0.12789969963203 -0.00316558128950 1.21870294831708 s
-1.48096138831601 1.90842238784991 1.81903732309916 h
-1.05852310882261 -2.44458363013088 -3.68699543262943 h
-0.48005545123437 0.00454247388078 -3.07112022328931 be
-1.58955526752126 -1.82251599405897 1.80237979067703 h
-1.03239648308043 2.45559863201154 -3.70174654311418 h

\$end

5

\$coord

0.02230465606155 -0.33962839876039 1.10932591603872 be
-1.21360886168175 4.50373164583967 7.70794943339668 h
-0.05664541191361 -0.85060279978635 3.91666352651566 n
0.31598732004163 -2.54265224943878 4.74094839420442 h
0.18259356850643 4.30972943549633 7.51922512977147 h
0.11957407373917 0.27768353668563 -2.29210207441258 cl
-0.49256332365162 0.45129473383037 5.25768408323379 h
-2.41043142867526 -1.63244527732603 -8.95062344706884 h

\$end

6

\$coord

-3.85775777230079 -2.54636520363678 0.70012197322897 h
5.69679653187578 0.08631809293378 1.26384863432362 h
-2.49337252539666 0.13053546334166 0.23388443378086 al
3.50314334431001 0.00473731301931 0.89665959149458 b
1.19501220670852 -0.05936607867841 -2.41366711199438 be
3.25650056300126 -0.09710499276812 -3.94045030387212 h
-1.50757150107794 0.13185490947010 -3.02729242228514 h
1.07207230570515 -0.04238056846380 0.77047150545094 n

\$end

7

\$coord

-0.33798305276378 5.10663584724628 4.03197046844269 h

0.28996328225119 5.77593662873667 2.94682790109626 h
0.04729323132243 -1.17187589997270 2.75102766874087 h
-1.99606800236420 1.05234741116991 -0.82832944474039 h
-0.12548579198827 -3.19251403504326 -1.47304056021616 h
0.25882820322135 7.24788152360254 -3.17245264958354 h
0.05975592396575 -0.74302325736864 -0.05318776919067 si
0.19841757522347 5.88513248534647 -2.77398339754058 h

\$end

8

\$coord

0.00403224242880 -2.71325219375153 0.19339436325300 h
-0.00195126870514 -0.52877152087334 2.43939153676670 li
0.00058855447832 -1.03764556164885 -1.25450508479272 c
-0.00023444725504 1.47791810847135 -0.98241857916835 c
0.00057719796665 -0.42585264874914 6.14241985846470 h
0.00427718833545 0.96840149827845 5.76160417369796 h
-0.00238410943280 -1.92697350674681 -3.12299896292838 h
0.00271067015200 2.49144450533670 0.88806436441324 h

\$end

9

\$coord

1.94809892923232 -7.24202538535160 -0.00732968641407 h
0.09742468233061 -5.00489253472472 -0.02947240048892 be
2.99323924566600 -6.02216339059516 0.05377372205010 h
0.73200978323659 2.74075031618098 -0.00813665515596 al
0.59842571640988 -1.53746030022577 0.02537849419613 b
1.78404635677781 -0.71376782513760 -1.84574886557611 h
1.75664914167646 -0.71412390364307 1.90942597580646 h
-1.87636583029805 0.13612712320511 0.00525226422349 f

\$end

10

\$coord

-1.15305167176393 -3.48348431895975 -1.08024217690948 h
-1.92527439798741 0.01077821431564 3.30898622166241 h
1.55440169745952 1.87640776359538 -4.82696168593521 h
-2.98928348733705 0.95033822436624 3.73251299032111 h
-0.60778348948952 -1.73418713026510 -1.17500463445129 o

0.85093087361155 -1.50749263802659 1.29170730822147 o
1.16472210228557 0.61204489219390 -4.26539067349048 h
-0.02240293820271 2.25748448501657 0.05606301035103 na
\$end

11

\$coord

-0.33135527032733 3.47793107456038 0.38136347736864 h
0.31155256316613 0.69734254453618 0.05237241647453 be
-0.34475963114148 3.19124371167325 -1.21174486921572 h
2.53533838579570 -0.50604338064675 0.25562945507928 h
-2.30297948700756 -0.31618769991551 -0.55957414057619 h
-2.28816461114031 -0.02414011161989 1.03367809066072 h
-0.45507103557610 -6.59659032871737 -0.16195801556256 h
0.40141865638558 -5.46111160543251 -0.20565266790485 h
\$end

12

\$coord

-1.78019161981989 -0.91679484618981 1.12255325677028 h
-2.62780540065272 5.88530570317760 0.21304417921595 h
-0.27591906699137 0.05780378716178 -1.74731876015312 h
-1.30229724222591 5.69383369252201 -0.26134349836343 h
-0.04140996587935 -1.03172319882900 -0.00004044876873 c
1.53774839790182 -0.25103046535633 1.09214476533736 h
0.35206729219050 -3.01206515002261 -0.46665234061812 h
4.58984616650984 4.83714462546855 0.04805439254159 h
\$end

13

\$coord

0.00809178797619 -6.25054485076530 -0.79693992537416 h
-1.62969642777338 0.37121447361059 -1.55507783746164 h
0.06227377803784 -6.64579318530156 0.56747446690839 h
2.09011980883986 1.05949062758960 -1.01654377815399 h
-0.61163539495464 -1.31932572471704 0.68310890801934 h
-0.66221047401713 2.60241594207992 1.39303792672764 h
0.54831575472096 -0.78003098471459 1.67617405710138 h
0.01815680827608 1.02210206406670 -0.08868884943988 b
\$end

14

\$coord

-0.26199016823899 -5.99935840688881 3.96792968089905 h
-0.02199693169545 -2.94805913092837 -0.82610905929445 be
-0.28135540059510 -5.33130607494707 5.22412185460510 h
-0.00939941392244 0.89390480783621 -0.19087203515899 p
1.71868022643785 0.52821572595386 1.89984411579346 h
-0.06560314225779 -5.43698903533727 -1.33790337866704 h
-0.26211485667158 8.20560698506470 2.05278762894283 h
-0.36210983329601 6.92354951087357 1.44469812533315 h

\$end

15

\$coord

0.09704031290997 -0.00928293767574 -2.24568257034887 li
-3.81756093690788 -0.05045343471429 1.12169762157118 li
-3.12507069105874 0.01260136079674 -2.15598320827589 h
-7.13771661091386 0.19281955186266 -0.71789573828484 h
2.42784917802150 -0.04639593125158 0.44563263902831 o
1.23408187360236 -0.15826427026775 1.93671718222285 h
3.89687344664380 0.91150925939955 1.02935196748200 h
-7.79259784149815 0.18900491230147 0.57199297165161 h

\$end

16

\$coord

0.18992942537483 2.63306827261349 1.33833554262577 h
2.71855245771844 -5.14701969275192 0.00734737921746 h
0.45627362532725 1.37091223425858 0.03071433932360 o
3.76445262217254 -5.49725124910915 0.90822917057115 h
-2.59581295893681 -1.51868469535531 2.12801018974709 h
-1.30636629385688 -1.33583430092819 -0.10969594258721 be
1.23500090694551 2.11535827358318 -1.45685670856425 h
-0.87436133693556 -2.40219890085676 -2.43180607856219 h

\$end

17

\$coord

5.29236128420488 1.52224132379181 0.05565360939441 h
-0.62892055330764 0.79371897111186 -2.00893844687133 h

-0.57170662012046 1.26594437151532 1.73908376450263 h
1.92346922713639 -0.49147081436252 0.01609598192540 li
5.85302694066670 0.21688052583122 -0.10547648088078 h
-3.92763994725937 0.50235271319016 -0.01957386173011 h
-1.14811096203612 -2.16793840738231 0.27630984617287 h
-1.68853659421703 0.11655858688409 -0.00446275135138 b

\$end

18

\$coord

0.18439495757737 6.83870253328203 -0.52279910393081 h
-0.31362601729072 6.80260623476698 0.81616305618392 h
0.50804005203411 0.50858117223355 -6.08300506557173 h
-0.67399433408600 1.84459330193290 0.10870817431384 s
0.95166550948854 -0.45029478914702 -7.03560807750401 h
-0.28729150586116 -2.23109480007481 0.14123525621096 cl
5.29564614488632 0.42038486058504 0.65152329120959 h
2.78704081768927 0.63485586887347 0.41920042335798 be

\$end

19

\$coord

0.02831499974082 5.37514011969795 4.73948638959115 h
-0.02574019698141 4.28703414411708 5.65528644011483 h
0.00861196189115 5.50615715233174 -1.16321890269566 h
-0.89210481070563 -0.36456164893942 2.11455812585410 h
-1.49784836149810 -1.00605877841697 -1.96922407318047 h
-0.00108500459995 2.33605632399014 -0.57646513565329 mg
2.38371009285497 -0.75824090364972 -0.44496950231990 h
0.00076178684613 -2.49012305100646 0.17844885389070 si

\$end

20

\$coord

-2.41466273544050 1.91783701009420 1.26068697616685 h
0.45797671930409 0.00005482701991 2.90754775248146 mg
0.61261721040306 0.00057019979760 -2.43776625432084 p
2.70722842684490 -0.01534117631604 -0.57997108070881 h
-2.38951351905650 -0.00065709541461 -0.13224453205303 b
2.18563735583238 0.00536743335513 5.60399972164665 h

-4.30629403297772 0.00128225800019 -1.34413501157734 h
-2.41447803593980 -1.92094185882559 1.25829345399721 h

\$end

21

\$coord

6.04623884801955 1.17365757085764 -0.71468549941972 h
2.36236419754328 0.35008533806004 0.29320909922949 li
-0.59224446611220 -1.35024206789481 -0.03358240720358 f
-0.37880448220255 2.26046724268597 2.00292851110541 h
6.22803791226715 -0.15858568692690 -0.22980794503915 h
0.03540671932803 2.35991105474673 -1.79372603979844 h
-3.48902535170876 1.85376257735427 -0.27415178651352 h
-1.26259209333331 1.44984691124683 -0.03506409361548 b

\$end

22

\$coord

2.91208581836471 1.45315561512981 2.35735757940025 h
-0.53566740891954 4.60257040239033 2.11699447586202 h
1.04809222262785 0.72616153588926 1.83823325027809 c
-0.98205380406720 2.63971079873818 1.65138471976942 c
0.10037303116082 1.75520873569124 -1.56974443088866 s
-0.28609561416312 -4.56438736106801 -0.12681064027069 f
0.22068517337893 -2.02102452661134 0.47360319765997 be
-2.93700873023273 2.10217916415903 2.03273950623779 h

\$end

23

\$coord

4.01304680398805 -0.26100376167932 0.56744199117350 h
0.92105315134355 -2.80459944645215 0.02809986705426 h
1.22980824368008 -0.12749473234162 0.06046531697122 p
1.53966572076368 0.38225245973526 -2.55329287360106 h
-4.42159099354263 -3.44885169632142 -0.23267228302870 h
-4.90941989433042 -4.76806240403944 -0.00265465114029 h
-2.03368621916157 0.86614836082101 -0.08239192349795 o
-2.65291410173802 1.06975625870296 1.64284401997101 h

\$end

24

\$coord
-0.07535123377606 -0.32607038716949 -2.38536041489167 li
-0.05551749967104 -3.44620129750874 2.00858171965399 h
0.03137425780758 2.98726258382034 0.41606120240546 li
0.00157318775964 -1.13521743532709 1.98763949046615 b
0.13967224331869 -1.96854952605760 -5.92240053432630 h
0.16957399557214 -3.18037948017550 -5.16049995976703 h
-0.04447913115788 2.97311946936080 -2.91044335766769 h
0.07662051046917 -0.52219679009096 4.22321834014123 h

\$end

25

\$coord
-1.64273700925300 1.79673865916004 0.01541226634279 b
-3.89094813292810 1.92863018008608 0.04830076329822 h
-0.65369335302787 2.82554608347229 -1.88314271320106 h
-0.60879477569549 2.95188934291749 1.81722925926190 h
0.09474225598373 -1.50492315301340 -0.08575331309145 s
0.11689010813028 -1.99941191538386 2.43966141425645 h
1.74905779310649 2.18710224293778 0.01262192248078 be
4.00373314136547 3.33995632730019 0.02764812227380 h

\$end

26

\$coord
-1.40877508969815 -1.85914095855077 -1.82119869713605 h
-1.59775202110782 -0.01305485438993 3.62576232497656 h
-0.18270422367632 3.84677837387915 8.71069894026992 h
-0.18172584541576 2.82595403083214 7.72161615603982 h
0.09194575536201 0.21527744252354 -1.92755856547270 s
0.03492311098501 -0.96428730093199 3.10414222592540 n
-1.46842921154681 1.41078999168190 -3.60031381746554 h
1.42925886923544 0.34028410028742 3.54497713072440 h

\$end

27

\$coord
-1.19983515349133 -6.22228508729437 -1.14796156958227 h
-0.84984371220542 -5.53286373575889 0.05055178483231 h
-0.07104836258965 -1.69113426631024 -2.26886503229971 h

-1.91421674170721 2.27729003582742 0.50659049235713 h
2.15225142973813 0.52965094696715 -2.16939482586356 h
0.57747632294932 -0.43217573851950 2.44251859669259 b
0.25545496780764 0.19708635124048 -2.01214201906469 n
-0.56569213484939 0.90212970766651 0.48880621281071 n
\$end

28

\$coord

-1.47142562690031 2.19452956422555 -2.79534245628537 h
-2.20758183492756 -0.45548408314447 2.41789324190131 h
0.46232947325357 3.71573017846088 5.33019171427497 h
0.57387907204434 4.67120630057148 6.37710259424684 h
0.04306855635495 0.92381760743604 -2.21085180865438 c
-0.05388569243167 -0.69736640811132 0.61369876860634 si
1.62534924788438 0.73752170473465 -3.51919187749469 h
2.00570394900429 -2.44051381132156 1.43419443402268 h
\$end

29

\$coord

1.73778930855323 -0.15852370712950 -1.46871356871394 h
1.00682362509810 -2.66553894491279 2.27965763469067 h
-0.05900041948801 -3.18450955196922 -3.24833868932617 h
-1.95455134895258 -1.42714983049330 -2.35553636232716 h
0.16546074559608 -1.81613029042416 -1.27512306820262 b
-0.12113923183807 -3.21877338910144 0.93807631581101 o
0.42696127685591 2.48703059790794 -0.58296223716438 h
-0.05357782632743 4.00669319725407 0.22083103708622 f
\$end

30

\$coord

-1.77580472151148 0.02654124047186 1.79335226798727 c
-1.33311979265773 -0.00810592175538 -2.19786907501022 mg
-3.23377504713984 0.06416878551219 3.27850967583889 h
-2.31299964822476 -0.07940878781180 -5.29302553542254 h
0.58194394687626 -0.02190092491500 3.12311526871297 f
2.77239663701313 -0.00005031436654 0.38191197972893 h
4.20854301671733 -0.13914375553381 -2.28029807299239 h

2.57751329090213 0.02812779184743 -1.46853853780091 o
\$end
31
\$coord
0.00314659620698 -0.54487488315762 1.63207308256719 n
-0.00716237039619 1.05603978029598 -0.74558231390042 be
-0.07307080847251 -2.46293756155461 1.67362155444101 h
-0.08272288685953 1.25145556611723 -3.43966603834137 h
0.07983340251571 0.13935211551129 3.42429117486725 h
0.04406115556772 3.47837447778204 -1.94048277436191 h
0.07518874490771 -2.52270519977815 -8.46188564563459 h
-0.02297621996682 -1.75397471069584 -7.26887579694885 h
\$end
32
\$coord
1.68483308323650 2.69954032516815 -0.51313858262308 h
-6.73756574067818 1.17253338822668 -2.23771057288868 h
-0.74796979361273 -0.43049690860003 0.54966915858718 f
-5.49924342627086 0.86326911586895 -1.61210390753660 h
1.54922887649441 0.56282267398165 0.25458174035091 b
2.05041200796431 -0.36314756329059 -5.00806817659504 h
3.33507015035852 -0.72918735259786 0.81555948729684 h
2.64808161469690 -1.56548919760883 -4.53532243511567 h
\$end
33
\$coord
-0.75192423910898 -4.11681825683214 1.29598427953707 h
0.54915794366557 3.07227869888601 4.51934623751367 h
-2.47876856552889 -0.28802714428817 -0.72155076124061 si
0.18854887811685 -0.17401685957008 4.21011644010357 li
-0.36397363485313 -2.23259095333385 1.04675273329689 n
0.47144889071907 4.22263104465117 1.43061985408151 li
2.65989129519731 -0.65714316496267 -0.81049758303256 al
-0.08915557544400 1.87825800304538 -1.09569009708456 o
\$end
34
\$coord

2.95719297736783 -5.09084053499262 1.06724879369931 h
0.93641369453824 -4.05674998799560 0.91963781083871 b
-0.84838887843472 -5.17531025831180 -0.46217179290426 f
0.39815116294534 -2.10390734819380 1.95379771844183 h
3.46253061030089 -0.06223783189308 -2.33567482590107 h
4.32109464728090 -1.09373150032674 -2.81003659293382 h
-0.14734154925030 4.07546277307114 0.06636692413580 cl
-0.00950843975915 6.06171738211794 -1.36213166865239 h
\$end

35

\$coord

0.62007773246552 -5.99473589687157 1.19136498729716 h
-0.21481123109817 -2.11496055532103 -4.07247940829187 h
0.71276178980556 -6.36555341886916 -0.18810785552110 h
-1.65014809913265 2.39957313403037 -1.68477643098069 h
-0.25336054202263 -2.64847657844395 -1.00815190676331 li
-0.07098928291565 0.19335892105405 1.16771891403562 f
1.97185413731447 2.03042082961031 -1.65417520601162 h
0.13783381122374 2.06721133688885 -0.72682281678149 c
\$end

36

\$coord

-1.74092504557999 0.35009664206993 -5.03854833589210 h
0.00444677335320 1.27659158175932 -1.35828281025820 b
-0.00223189814922 0.41873106453095 -3.90472089389591 c
-0.00056523213028 0.16594058040432 2.98517732838636 mg
-0.00494929795068 -3.28108538127584 2.01826111866426 h
0.00288267467434 -3.13382930596068 -1.27803465321681 li
1.72210579562888 0.35604182878945 -5.05985031836863 h
-0.00354115306197 1.46441876685122 5.97415727562990 h
\$end

37

\$coord

-3.36273484853332 -2.43646019532701 -3.71089431436477 h
1.49644338489587 -2.80324260113508 0.67757339602255 li
-1.75271803587013 -3.22070119331307 1.30322649582779 h
-1.87176146279589 0.64041948578379 0.38855330131211 na

-3.56807886355130 -1.58230653951419 -4.83668254037202 h
4.09818405580124 1.86568925316147 0.82529631661361 h
3.31430029122774 1.34274944710122 -2.34819786823094 h
2.82477353777979 0.73196496970248 -0.39940535029971 c

\$end

38

\$coord

-2.99417157416676 -0.24800883786254 0.35433940970262 si
1.94064817947348 1.99241576117407 4.50517025713661 h
-5.71086042676708 0.31176305063299 -0.44041056932756 h
3.19475053414273 1.60374824855894 5.06516320739370 h
-0.26603901635197 0.64854118535262 -1.20780426414447 c
3.37416251890036 -0.22416892316431 -0.09426921121229 mg
-0.63390496147027 1.69699362907052 -2.97226931081874 h
6.42489710092151 -1.01565154280527 0.63522178826024 h

\$end

39

\$coord

-1.45174240776958 3.35752535029039 0.00277062191657 h
-0.66858369674959 1.43022889032226 0.00089572258648 c
2.11993461985521 -4.19574983403369 1.10474088884699 h
1.75243206827822 1.04672828927926 -0.00042150287532 o
0.94090884542745 -2.02410838960357 -0.00136196115305 be
-3.87286288832368 -0.73293730379486 0.00042081129225 h
2.12253349391059 -4.19871890700882 -1.09281819907328 h
-1.95594247360816 -0.70453297743373 -0.00049798892532 n

\$end

40

\$coord

-4.65665211885798 -1.48212879325257 -0.70997704208006 h
-3.14321994647081 0.11379085342678 0.86518740514686 p
1.95336823119113 -0.28581651358559 -4.73913017823926 h
0.03588967117627 -0.05884200621553 -0.86033416712916 b
-1.47695798617865 0.27688167945469 -4.91690508199168 h
-2.76250966651864 -1.61791733567994 2.90213597492268 h
0.18173345099172 0.00279128571273 -3.71383642318794 c
2.87097622974565 0.00597520049858 0.97689168215347 cl

```

$end
41
$coord
-2.70846692677360 2.44742811475899 0.15732851671039 be
1.84882156203891 3.53701207484806 0.17868765713647 li
-2.84391621821756 -1.44932184944915 -0.04938497811604 n
-4.64574882926696 0.01995155494764 -0.57045389749780 n
-0.19390245122439 -1.38875179190207 3.97980721313572 h
0.02271255562175 -0.66373807378105 1.49329573093466 be
-3.28824526549785 -3.37201393029862 -0.23878086432376 h
3.37886707977696 -0.44562740094410 -0.31604136877692 cl
$end
42
$coord
2.35636647687098 1.04361484721426 0.15402375022209 p
2.53684441966683 1.29463785267509 -2.55500041462886 h
3.12710601238396 5.34687842881422 -0.18569328092652 h
1.85894305011346 5.55905635055891 -0.84106284596235 h
1.95920392048122 -2.39345423977772 -0.06243418649055 f
-2.64668722551431 1.68217946449454 0.01209169238177 al
-0.47400861982959 -2.62584294784992 -0.04372192530989 h
-2.41603697383199 -2.20501105496741 -0.01349743419433 f
$end
43
$coord
1.66263371150049 2.53296591152818 2.10408513273508 h
1.27859554488340 1.62019465388601 0.03640961300060 b
-1.32855122394936 0.33601171358907 0.03205609866326 f
1.43143493345589 3.03414456936359 -1.75857302149692 h
0.48931346647615 -6.33065902725245 0.48748170985652 h
0.44028175680753 -2.43031637472750 -0.28315255606690 li
1.88162269984850 -6.00755693417356 0.42343976972645 h
2.83121038049828 -0.20890783174514 -0.30188467016412 h
$end
44
$coord
0.97821106581266 -0.00163499246931 3.84835062259540 s

```


-1.78421890500545 -0.00076746468338 2.18401051778825 c
2.61806890271435 -1.81646120437723 2.87235462039894 h
-3.32948812567255 -0.01337146328821 3.55145148798126 h
1.41928044081983 -0.00043350547513 -3.36627980095559 cl
2.59161282781913 1.87059700699704 2.93237529931041 h
-4.65400956298778 0.00185041526658 -2.98499067819710 h
-2.12948371700732 0.00126224292145 -1.36031145896115 al

\$end

45

\$coord

-0.01195395645319 7.66627495167116 -0.06400753734586 h
-0.23206078700356 1.64216702203625 3.25449543195088 h
0.00226612128025 6.63718512513253 -1.04536752996039 h
-0.08259742205052 2.68786821527123 2.26347499958949 h
-2.98741811900732 -0.88362605724578 -0.44875203466805 h
0.00943611385804 -0.61860857720713 -0.13950355794943 al
1.53421152412054 1.31981610528090 -1.89853112109521 h
1.52496525450848 -2.51067336187435 1.67294104193608 h

\$end

46

\$coord

0.08346162826039 4.27926630039688 2.63839053967416 h
-0.08237509933392 4.00472086462741 4.02934454010426 h
-2.07760635683434 0.86643914991591 -1.86234934572504 h
0.37643839693967 -2.05228663195457 -2.36537387721337 h
1.71041139434360 1.50419341609871 -1.77777780243471 h
-0.01670500316232 0.60389007147805 -5.05387711394349 h
0.00109080374756 -0.51645095996805 1.50689105297780 na
-0.00172523458900 0.23989524653054 -2.79497543936975 b

\$end

47

\$coord

-3.36566953997398 -1.79948803987353 2.79974501955584 h
0.53780931108893 0.11319420626285 3.88905161109275 h
3.71961896057475 1.33706124292680 2.26663908560301 h
1.48902865400176 1.10407707279091 1.95277717925490 b
0.21148447680174 -3.44181932898393 -0.65512760630628 na

```

-1.82959352802169 0.15961273618167 2.02807675714638 be
-0.08680034906606 2.30507748953673 -1.17261607143066 si
-2.90901837838872 1.35292566030622 -0.41704648841523 h
$end
48
$coord
3.49329401667588 0.05093650834553 -3.89196068662466 h
-1.53231074936105 0.05538310301514 -7.06555847694382 h
-2.70677572139427 0.01087367671180 -6.24483235054682 h
-1.39550383589121 -1.97920577201885 0.09470836073698 h
-1.44732236283306 1.96843230904985 0.13568205517805 h
2.03916887866039 0.04422818517375 -0.48881715515089 h
0.42261003860238 -0.02287777942301 -3.74499049697167 li
-0.04425327757714 0.00022277655622 1.40720317541008 p
$end
49
$coord
-1.99938162936995 2.25697163266825 0.78043027201591 h
-0.03536037855222 1.63803976375487 0.43050668855975 c
-0.17534651027370 -6.47520296343711 2.04427010382651 h
-0.76989077021092 -0.89865186727560 -2.16399491386847 h
0.97073443071534 1.62584641858441 2.24385356966057 h
0.89361984649099 3.03090915817603 -0.81771403722568 h
-0.09385119040163 -5.16792690315429 1.48102163839906 h
0.10051579040508 -0.87514726736166 -0.54796948274097 o
$end
50
$coord
-0.72393271825388 -0.00705165510195 0.20476698387878 o
-4.07888512765765 1.94441658588055 0.70875651491350 h
-3.97114871773911 -1.14514143562293 2.06859781641087 h
-3.36828282411032 0.00351376751307 0.43697051015724 c
-1.43643864654364 0.01339152403475 -5.32940853698766 h
-1.91669563744564 -0.01012119055875 -6.66760006516695 h
2.51386797350858 0.00177912437598 0.07615848732633 al
-4.26048193160585 -0.78010987788901 -1.27623097450497 h
$end

```

51

\$coord

1.93517893153927 2.42757630112549 3.35025158272502 h
-0.56873392880043 0.01510832065083 2.39826597033635 be
0.98717437591772 2.32669813588051 4.44869760765214 h
1.16486683497240 -2.31393417894944 4.51767231253434 h
-0.04224128039237 -0.01278957437037 -1.26371879329968 s
-2.33132605882055 -0.07689109565409 4.25155038442070 h
2.51397321982225 0.27267436449057 -1.27673643225117 h
2.15886403543441 -2.36436374709579 3.46530017246316 h

\$end

52

\$coord

0.40692994079217 -0.29670027728876 -5.81979419000397 h
-0.00176128404757 -2.28244353972760 0.16812860453852 cl
-0.37125606168687 -1.38780157586597 -6.29682662769042 h
-2.87704593199824 3.17515296363530 -0.75708898076153 h
2.24125015071873 3.10680966296554 -1.89732735584657 h
0.04520120096719 -2.37463059905791 2.62475062425500 h
-0.00115031386961 2.81048105784566 0.11747360708650 al
0.64766155362448 2.82541149123666 3.08820191809613 h

\$end

53

\$coord

-1.59396120792129 -0.81927674118141 2.72619704432465 h
-0.39013991980410 -1.32845286999041 1.28383089447585 n
-1.37171750813561 2.35899021861964 -4.29085671879305 h
0.42573682987586 1.46473552141603 0.47856935565089 f
-0.36545521512126 -0.71884676260626 -2.10309502366368 li
2.25962318673785 -3.57175436560957 -2.05572809154822 h
-1.73528004445937 1.38459959448081 -5.27222579079675 h
2.35417818192437 -3.55140671790783 -3.48960998838178 h

\$end

54

\$coord

0.99230919409336 -0.91353921811311 0.09789901170160 s
-2.58204066041019 -5.79002723598734 -1.06718835679297 h

-2.02120541052274 0.47089528984357 0.32715991078572 b
-4.15974631782290 -0.07187917807321 0.75110083167084 h
0.15947078038262 3.21182474361843 -2.26595386818440 h
-3.20605558492769 -7.06418953634756 -1.15755682960854 h
-0.06613215056120 2.51164344890782 -0.33426379622600 c
0.68906612285283 3.79459730749797 1.09957212028839 h
\$end

55

\$coord

-1.90585759067960 2.72911961524244 0.21932849133544 h
-0.27202206632346 1.51343790535905 0.56939138512156 c
-0.75933841741709 -1.23031671565783 -0.26082601768656 o
1.03464705410477 0.03708779959952 -1.52465732190097 b
1.14348586328932 -0.93038914353403 6.86580031974325 h
0.48630410347892 1.61771374001237 2.48949181633185 h
2.02219604238528 -1.93565797496896 7.35179955029021 h
2.45110722903281 -0.38428201334021 -3.21858685027737 h
\$end

56

\$coord

1.82111730049407 2.48518398767632 1.17333062790350 h
1.65822658511083 -0.66554379718041 -3.25597443704248 h
0.02454686750801 2.32692957494391 0.47699515578582 n
-0.30888520983430 3.89883881695724 -0.60209463520034 h
0.14675796868300 -3.89287413171472 0.85948286051089 be
-0.14384204719132 -0.41537230278871 -1.40835964488640 be
-1.20474156079731 2.34924345936651 1.97079459787462 h
-2.33289022210125 -1.88284192507232 -1.00688186501105 h
\$end

57

\$coord

-4.11665336520602 0.87610547333116 0.11679019982869 cl
3.05709369452609 3.30205023574150 2.11259227557436 h
1.86498867759038 -3.64508889446001 0.39631158081298 f
0.25064984366411 -2.85857602992898 -4.08387134191666 h
-0.39322121556018 -1.11880993970439 -0.11293213149315 mg
3.51532916623548 2.08272095748945 -0.10604195937765 s

-0.76653360372039 -1.94879754243696 -4.52983051046252 h
4.76098226454487 0.12674260470874 1.02067511437306 h
\$end
58
\$coord
-1.67572312695067 0.14233993266942 -0.12183436487694 li
-2.16147337411827 -0.86356145639868 4.03844398637773 h
-4.75747612902180 -1.68402150358418 -1.91216594071480 h
-5.49185578561900 -0.65922863653118 -1.24102872904760 h
1.38180529408727 -0.26651523644844 -0.20801438000320 f
-0.83087264435103 -0.88472484149364 3.48451188485001 h
-0.05074611710557 3.64085622742828 0.16954846031907 h
-1.21618922327144 4.49412026866533 0.22010684360164 h
\$end
59
\$coord
0.01153415487204 2.97259802888493 -0.16149195729933 b
-0.95560428705451 2.01645614577191 -2.09097652851849 h
-0.01353614233221 -1.37185731132522 0.19732256397735 na
2.22120397214820 2.17590254596608 0.06930483283982 h
0.02288425375586 5.25259923662241 -0.34634012263145 h
-0.61969636052021 -6.14786196962089 -1.24059912124107 h
-1.24400727711519 2.32996316856533 1.73171114186853 h
0.76024252354010 -6.22036257321142 -0.89155236950830 h
\$end
60
\$coord
-3.86439300556407 0.09243462755121 -1.90917228156690 h
-2.06807351195900 -1.30001132968555 0.77072786388071 li
0.66195848648359 3.01840520649779 -0.33486631992314 h
-0.23528208015714 1.38293630870563 0.17255520758336 n
-4.93163331584781 -0.91989989775480 -1.92266073519912 h
2.97737928779946 -0.77110740731716 1.03764558369389 h
2.20728980247972 -0.90221292814969 -1.98097411613314 h
1.47206644422058 -0.77615287023389 -0.18664316950322 n
\$end
61

\$coord
-3.88880938532608 5.28033200089979 -1.09552876050273 h
-0.24197630685614 -0.73401740200022 0.01378646232037 cl
-4.22586789523816 5.33327673615489 0.28450375354144 h
-0.08651666984221 1.70671338685962 0.19428899169109 h
6.81113869711578 1.49395309388477 -0.39387043262171 h
5.71268566904568 0.59025554456436 -0.36421832478461 h
2.67653530167946 5.29828433301298 0.42423063438859 h
1.51178798849999 6.11453954128303 0.46568739637700 h

\$end

62

\$coord
0.71823631526783 4.00476730984933 0.00745133769205 h
2.52207604873906 -0.09791314070825 1.95107009933353 h
2.52351833641988 -0.09835260183878 -1.95028762025050 h
1.29239008205517 -0.22220400663016 -0.00009451912110 b
-0.42103512485669 2.43926653995711 -0.00007811043282 n
-1.56415985429014 2.50673895130317 1.56324404352275 h
-1.55593250882859 2.51593563726429 -1.56903247828132 h
-0.56528578330936 -2.14046381586716 -0.00001836765694 f

\$end

63

\$coord
2.25956031341240 -4.18252541986373 1.62797931979558 h
-0.45936849058387 -2.14896163488868 0.95581474646987 be
-0.53945875912378 -6.14643288231360 -2.97986588297517 h
0.41320048863228 -6.26919812802497 -4.03004451569030 h
3.02324882749267 -3.01717795313046 1.21456276620341 h
-1.87479008622307 -4.14687023477978 1.65009700702088 h
2.51616262217205 1.37411250832978 -0.23113927430612 h
-0.05315032887573 1.30780305794166 -0.18225044429459 s

\$end

64

\$coord
-0.78804990647379 3.13689451248642 4.53736010122770 h
-1.15642217095629 3.38111960900411 3.18154965348594 h
-1.83342985347866 6.98825667597872 -1.55099953779912 h

3.26053141508255 3.67146878739929 -0.74482642333203 h
-1.29582506730113 1.09750095890955 -2.48909137767760 h
-0.03530181594328 -1.22174169349086 -0.05035258927107 na
-1.76903588230100 5.58996997806876 -1.85297358977236 h
4.38739599232181 4.00029855582023 0.06742404104011 h

\$end

65

\$coord

-6.45708017206544 0.19867948211193 3.85190192619349 h
-5.04545933320909 0.06561213120220 3.99267175347978 h
-0.38067776559091 3.23368007680902 -1.71605965486311 s
-2.63344209510897 3.14402954215817 -0.47258264014028 h
-0.30739238924429 -4.57967015065817 -1.71124573374756 mg
-0.34339375839780 -0.30999741674182 3.48149720602986 f
1.33843393035630 0.37891543287961 0.82640698152032 al
4.30468952904253 -0.11261702738958 0.75024132995562 h

\$end

66

\$coord

-0.82058389450931 -3.72650774414816 1.86997861058925 h
-0.93978614903082 -2.81382029908932 -0.00288559392464 c
1.23235571581173 0.12599575078131 -0.00247244263882 si
-0.24393360534399 -4.22237157532212 -1.36922662788409 h
-0.68152696098566 4.31669665097306 0.03496471967231 h
-2.94510614525660 -2.42979238529988 -0.40989225955783 h
-1.11072327509028 2.44289035253308 0.00006641960605 n
-3.01390265258231 2.13494223351254 -0.02347020020752 h

\$end

67

\$coord

3.85185379412993 1.16705022050213 2.57633499728986 h
-0.60013443356850 -0.06392943410908 1.95707888688622 o
-0.06814154161088 0.20373012762726 -1.43011588447084 mg
0.29641723726720 0.63122064918067 -4.59560276153594 h
5.22677600987027 1.56700652368006 2.54478406868652 h
-1.26761612462882 0.68221196907598 3.46978227309469 h
1.29005968455747 -3.73296686657213 0.35123819810177 h

```

1.77193707629400 -4.21370032337072 -0.91698089559327 h
$end
68
$coord
-1.01903363110276 -3.94822930544941 -0.25399030911989 h
-1.24523657618557 -3.77377796160484 1.19207667336636 h
-1.63289224960767 0.29227079436836 0.06930909382199 al
3.49721776831010 0.84367861519795 1.57614328453544 h
-1.38319266159902 -1.02921317331802 -2.83254722755203 h
3.35592242660716 -1.74455352868605 -0.17008547339555 h
3.29086891662147 1.03778820975916 -1.53985424714070 h
2.67797257859340 0.05690553333690 0.01244827082923 n
$end
69
$coord
0.00028898638888 -1.43879726102876 -1.26658970746177 n
-0.00133198380588 -4.64475678132568 1.83213111221720 h
-2.65390369622826 3.19080067055562 0.46940579660015 h
2.65295471651216 3.19312013139964 0.46571446186444 h
-0.00299293997758 -2.42336773965676 -2.91069627741822 h
0.00012464589807 -2.49580270696141 1.11599787447568 b
-0.00010722552527 1.80295181970247 0.11028344703561 al
0.00279150129796 -0.81526537458760 2.82217166284730 h
$end
70
$coord
5.89915865046152 2.89530719339448 0.20698375216101 h
1.69346322235402 -1.50109552727950 2.05044535684737 h
0.73680557479973 -1.04008225049489 0.04569196497530 b
-2.15986894643074 1.32116891036255 1.54649686742768 h
6.56403616430846 1.83607655819188 -0.44894775561191 h
-2.28390436514536 1.01820418446599 -1.64327096547156 h
1.53326581196517 -1.88723126591182 -1.90791792384197 h
-1.37801105374264 0.53778193217193 -0.02114712000905 n
$end
71
$coord

```


-0.12679985753160 -1.74442042634369 3.57334181761008 h
-0.00014294590430 -0.05893273729639 2.63851371219684 n
-0.00065264795039 -0.36810682309043 -0.40526724363233 h
-1.48825843824569 1.03609813478713 3.20320207066505 h
0.00001681381267 -0.45859601017489 -2.26326228216492 f
1.61802993935866 0.81607943916998 3.22856237813838 h
0.00207034339515 5.54920247808142 -1.61437858654620 h
-0.00271987975738 4.17377367556053 -1.99173827302127 h
\$end

72

\$coord

0.21510009065798 1.19704635343769 3.27748564036294 h
1.76706550359452 -0.23776397291384 -2.40251247339495 h
-0.04124146240801 3.00047225164568 0.19059925419756 be
0.20321503595190 2.60418628019591 3.65192050230201 h
-0.03346815983073 -1.93841287965910 0.57872788563647 f
0.04521080822320 0.07262583444532 -1.26111547930527 c
-0.16572325791460 5.53292651101200 0.44635255559167 h
-1.55884604253635 -0.25330714804406 -2.55767361049580 h
\$end

73

\$coord

2.38007670221717 1.45480055298954 3.47242129408292 h
-0.41194911268091 0.00065881384615 -2.68357509074833 al
0.95155666887403 -0.00251931531934 3.04623614086733 c
-0.74058903074188 0.39021098860154 4.20038265901833 h
0.34843410301530 -0.00186225260323 0.46302868410901 o
-5.09959886875063 -0.25561569941780 8.86157605537497 h
1.71659024070535 -1.85260292783290 3.62802314975085 h
-4.09893614763886 0.30515179900238 8.02286124360420 h
\$end

74

\$coord

-0.36250306369330 -2.89467025957634 -4.46227000024817 h
0.18513978653789 -2.85460776580358 0.26751695329003 na
-0.11620416112655 0.68925464307370 -1.72967720313826 o
0.00089018415251 2.57500981532408 0.67596821363630 si

-1.08141935882238 -5.99694802336109 4.13273259085238 h
-0.87568013229732 -4.66520876491607 4.61251544610444 h
-0.36328970988143 -4.30434200163238 -4.73860593862885 h
0.27991249235177 0.27877592735516 2.97394981919328 h

\$end

75

\$coord

-1.48204001548661 0.44270478181965 -0.00014214426612 c
-3.37217896167524 1.22820442009422 0.00091863614732 h
1.03987184027337 1.50749849247361 0.00038435512900 b
2.28794455315466 3.39358141623502 0.00070588827482 h
0.43667673279282 -1.83292918862106 -0.00103497853793 be
1.21842995307757 -4.67180581921998 0.00116751001273 h
2.77202105862692 -0.41882119376586 -0.00047870238674 h
-0.30342840954599 -4.58709829435408 0.00451175836317 h

\$end

76

\$coord

-3.44483220101367 -3.14124555099641 -0.00092959562734 li
1.20656778232119 -2.04295696248262 0.00127771269603 si
-2.03709572571208 1.05474835326590 -0.00109586202356 be
1.39815375714662 1.41796263946641 -0.00460776175393 b
0.50363182722451 6.26606764331462 0.00521286001226 h
-0.02253268812267 4.06544953877442 0.00161329192112 b
-4.50952391447959 0.08592096800104 -0.00009636831782 h
-2.43983285435492 3.95468714132229 0.00759615488107 h

\$end

77

\$coord

-2.05092534705092 -2.85821724185418 -0.43916380028669 h
-1.12448562279156 -1.35218641483100 0.34573744924945 n
0.69095723073259 6.74892865974228 1.10712191537673 h
-2.50310189695742 0.84165370630087 -0.20560814764104 f
2.23460540153216 -3.16405607113934 0.16434085245844 h
1.46498555068601 -1.19896855201636 0.02371048083973 c
1.07636877556705 5.44145380715842 0.69789460226891 h
2.73401171767084 0.69585845859935 -0.17273111821479 o

\$end
 78
 \$coord
 -0.03816554953439 6.12373161754941 -0.05133663230413 h
 0.84040518223261 -2.95100662814600 1.84804660187065 h
 -0.36023033038304 2.13002748173692 -0.00046526469916 li
 1.76281603964398 -0.24403586848680 -0.65041819799066 h
 -1.91851122024604 -0.65995954235726 0.60881160585105 h
 0.08251780405201 -1.81709408703269 0.00020818313934 b
 1.32663868886386 5.71012537279983 0.05541838389202 h
 -0.37835563327459 -3.15297374543246 -1.80955168896749 h
 \$end
 79
 \$coord
 2.26696206602272 -0.00057851029398 -0.56938924118047 h
 0.00581022600692 3.91919585771846 0.19426356327227 f
 1.51297876287127 -1.79268567817127 -0.71637967824727 n
 -0.02589472016153 -2.50292759135503 1.37611572675243 b
 -2.21681642280113 0.03540167435705 -0.62143042426561 h
 -0.05079911136151 5.57174054317406 -0.42688192585228 h
 -1.49648910256963 -1.76662952366693 -0.74663181562675 n
 -0.06026392330075 -3.17101518451541 3.52656702266323 h
 \$end
 80
 \$coord
 -1.46506787564834 0.44303029549560 -0.97464085894006 o
 0.43846820311244 -0.02086263861251 2.08735770128583 al
 4.31514191733585 3.43355593780071 -4.42388490619625 h
 2.18758418719726 -1.74138687365477 -0.60072899992038 h
 -3.01240002449014 1.28347159991966 -1.46783503253202 h
 0.43157866890890 -1.11912140159959 -2.65731572112191 be
 3.73204044861703 2.27060162993979 -5.00529990262062 h
 0.43679383070484 -1.71396229612141 -5.14769905581414 h
 \$end
 81
 \$coord
 -1.64891928463071 -1.97866741878013 4.03898588161385 h

4.99107010468669 -2.84271397866521 0.38369909714870 h
 -1.62650437285439 -2.99194821008724 3.03418106572960 h
 -0.07957709722178 0.93577475919787 -0.16571155389203 f
 -1.57777806523551 -3.24988865283193 -2.71323292085040 h
 4.07485881480729 -1.82064332920804 0.01108070533159 h
 -2.11049245540294 -4.56884840670633 -2.73367931583665 h
 -0.60235128863052 -0.18494110955250 1.10232668358774 h
 \$end
 82
 \$coord
 2.76435342519076 -3.13813251262591 0.00002985895577 h
 0.52155022987703 -1.75994090139449 -0.00208236581421 be
 -0.03416951835365 1.26788557461665 -0.00152305613444 c
 0.00731379662025 3.33085805378507 -0.00326473921857 h
 -2.47019653187784 -0.06017517065184 0.00159139018755 b
 3.82774085323716 0.46233582689287 0.00258954999727 li
 -2.20051948666719 -2.51812267913030 0.00276936472454 h
 -4.68366978025000 0.41520242890067 0.00233754162164 h
 \$end
 83
 \$coord
 -5.94603101144352 0.01404553867337 -2.85560697186309 h
 -6.09081255431154 0.04098173242308 2.74095252531496 h
 -3.12341613369470 0.00364172224787 0.02002074071166 li
 1.46932769938073 -2.59814259667466 -0.49949556386008 h
 -4.66309333893101 0.00370870944802 -3.49832103153620 h
 -4.84423174849080 -0.16319536627780 3.42612300762247 h
 1.30503460364711 0.09453859457364 -0.06805877560487 p
 1.47458870944624 -0.22753426299908 2.63989326288212 h
 \$end

4 Cartesian coordinates for the ORG set

(Also available as Turbomole coord files. Please email to grimmes@uni-muenster.de or dgd@uni-muenster.de.)

```
1
$coord
-0.00037668565793 0.93489653793823 0.21221338410837 n
-1.65809653213930 0.29676053534736 -3.30898312111394 h
0.00014919588292 -0.43204566385713 2.18478961834637 c
-0.00129221246145 -2.52823940631734 2.14608359562426 h
1.67485203255879 0.27607167154175 -3.29576101124142 h
-0.00003340286225 -0.33133809485676 -2.22146903466325 c
0.00131287557090 0.48355106868070 4.04443534542094 h
-0.01292156898274 -2.42280194882142 -2.09760277568913 h
$end

2
$coord
-0.28788740197876 1.02323485098021 -0.81236496113015 c
-0.61906087476915 0.00986249383920 3.58558769683117 f
1.49269421862928 0.11016740774278 -2.27731298421748 c
3.37840567332844 -0.02896230910096 -3.06879601744187 h
-1.31626823034305 -0.53578830619558 -2.92853583480546 c
2.00971578858182 -0.76467228996720 2.08012797956945 li
-2.21435214412119 0.44799568313865 -4.51362743955818 h
-2.00284037274627 -2.46209160867956 -2.60515048292266 h
$end

3
$coord
-1.09050297143398 1.59829714493111 2.20521091893137 h
-0.00002741639952 0.00000628407315 1.44471287291907 c
0.83848667905537 1.74386984809465 -2.20517626963561 h
1.92927233979483 0.14533278196106 2.20542808063656 h
0.00004229023857 -0.00000755042867 -1.44471020513557 c
-0.83875925085626 -1.74374934010979 2.20513865657920 h
1.09062748409803 -1.59819237374670 -2.20526118688400 h
-1.92930151997264 -0.14554297101243 -2.20537198941074 h
```

\$end
4
\$coord
8.32297069486148 -0.95389611069961 -4.90837312867630 h
-4.39291404922907 -1.55944380073460 0.38431834898462 h
-7.24280797625592 -0.21135520351386 -1.27156899749403 h
-5.34393791345599 0.02054283571768 -0.52138059572361 c
7.57736714406270 -0.30492231099361 -3.88684736177106 h
3.31778986592035 0.46096491097549 0.06250987053543 c
1.52954957954226 -0.28650150340665 0.99632256895931 o
-4.39905178055194 1.83949309874025 -0.66406516565894 h

\$end
5
\$coord
-2.22454945370724 0.72584973074080 -0.91900736663085 h
-0.02039973500553 0.17992568619258 -0.90250702554818 b
-0.15634459469799 -1.33871648660197 1.18336171204891 h
0.66385898536995 -0.94341366536184 -2.78808275702007 h
0.51736855525951 0.49141756986114 5.82124645889285 h
1.55004923058376 1.58614876940725 -0.05744474566308 h
-0.47503039291712 -0.24436721315156 6.52473653227831 h
0.34344538744674 -2.20671482325840 -0.08495482512467 h

\$end
6
\$coord
-0.14683469680667 4.74561241573534 1.86511238067744 h
0.98107106872370 -4.97236149060751 -0.11982491469421 h
-2.78560985083742 2.98040612925621 -0.10812370436105 h
-2.49052396136902 -0.72000518364342 0.03938863059405 mg
-0.05730456130761 4.65323011274167 -2.04085733801221 h
0.75798287349526 -2.91966414621053 -0.09637399088869 c
-0.43933941304331 3.56477065598452 -0.06859596197026 b
2.15776580829238 0.24344956413836 0.04997676306783 al

\$end
7
\$coord
2.91768782575761 0.98072597263510 0.65282968103672 c

3.03632639914773 1.10964773601450 2.72656316167480 h
4.54086457828031 1.87365222803539 -0.29203911177506 h
2.43960073770899 -1.80536485522345 0.01620267573533 n
0.36667695633671 1.82157399480475 -0.55077874537674 c
-2.66106822197645 -0.12508287675675 0.28365918868630 s
0.06612293953963 3.31416907973706 -1.93009544857865 h
0.33306607903875 -0.89155858081820 -0.92051071191230 c

\$end

8

\$coord

3.64632575718662 -1.97865292550276 0.48165308718349 h
-2.29803352905272 0.00061100308208 0.37762448436796 n
-0.13721064805141 -1.77729994275015 -2.75121810736570 h
-0.02013894414941 -0.00031319035419 -1.72197202735514 c
2.54450745254547 0.00040873276150 0.37385330823230 b
-0.17873466074671 -0.00118631526308 1.32581670054233 c
3.63874718173199 1.98368985085623 0.48342216093897 h
-0.13585115823254 1.77725705505693 -2.75042065638559 h

\$end

9

\$coord

-1.78019161981989 -0.91679484618981 1.12255325677028 h
-2.62780540065272 5.88530570317760 0.21304417921595 h
-0.27591906699137 0.05780378716178 -1.74731876015312 h
-1.30229724222591 5.69383369252201 -0.26134349836343 h
-0.04140996587935 -1.03172319882900 -0.00004044876873 c
1.53774839790182 -0.25103046535633 1.09214476533736 h
0.35206729219050 -3.01206515002261 -0.46665234061812 h
4.58984616650984 4.83714462546855 0.04805439254159 h

\$end

10

\$coord

-0.00018298387303 -0.19303382805115 -3.80144872491252 c
-0.01462950636111 -2.22769863524622 -4.16194757765227 h
0.01359124661055 0.99440277686468 -5.49010702346759 h
0.00113094182469 -1.23054011411002 4.27881765916797 h
-0.00088084094624 0.93822910364389 -1.15574411108530 b

0.00157403378382 -0.84889503474217 0.74764543188375 o
-0.00381975252046 3.14392032816383 -0.64272580178723 h
-0.00060666041894 0.31699126312046 3.26615698595586 o
\$end

11

\$coord

0.00293495247069 -5.02452961239918 1.88098391779736 h
-0.00360363897704 -4.62171996539102 3.24856926819476 h
-1.83573206629406 0.36809307098851 -3.47221675164315 h
0.39341294622326 -2.10189669703244 -3.13788061141256 h
1.43636445884176 1.04411578695142 -3.57375343618133 h
-0.00371170955264 1.08440427116286 4.50582837657613 h
-0.00006250809271 -0.12376566352550 -2.62013397102193 c
0.00045937075405 0.44471190417677 1.31719573389787 mg
\$end

12

\$coord

0.03266832315194 1.85370633263182 -4.44762878769973 h
-2.18871599852983 -2.06058435294610 3.19483199472803 h
0.03552131888773 3.12989709558583 -0.06671811766525 h
2.39628666260680 -1.73274362987028 3.40331662171630 h
0.00043872918490 -0.39608509265834 -2.90131855133225 p
0.00105633478878 -0.27362465259435 2.96686306508824 si
-0.00718974026169 1.20881163670815 -0.03410187177343 n
-0.21876733408541 1.80765156022954 4.87592842628151 h
\$end

13

\$coord

0.00046201593478 2.49098437033490 2.06826419865268 c
-0.00890908312903 1.60413908600445 -1.09146892360157 s
-0.20074627675380 4.49623222432649 2.47664552315111 h
-1.70106662640281 -5.16752364509363 0.60339525881027 h
0.48135330585462 1.14915206047764 3.54393188427119 h
0.25125508194307 -0.94383617218738 -0.70643366818931 h
0.74096266194215 -6.02019219958188 -0.73287628835007 h
0.04448707074908 -4.67622786382686 0.30805177476806 o
\$end

14

\$coord

-1.53630890921451 0.21971297249672 -2.03461830020736 p
-0.36101596232857 1.97171221062379 6.96052369677481 h
2.01513519765739 1.01667494675388 -3.10376138526773 c
-0.02819335156565 0.39499432433892 4.17487600151308 mg
-2.05090219629110 -2.02538408978780 -3.51978308158412 h
0.10344265890830 -3.65314530653998 0.59920731667854 h
1.88005428637722 -0.48339801798857 -1.17025393381981 c
0.31736599191371 -1.58830389638894 0.73131779564397 c

\$end

15

\$coord

1.73406431582023 2.39710158606716 2.26478660739982 h
0.01070663724967 1.41092710826648 1.71786250301932 c
1.73420048588128 -2.39729578484466 2.26430867999696 h
0.01068201953867 -1.41097626916092 1.71777510407750 c
2.60899351675827 0.00002850734602 -1.89632550607734 h
-1.72331682163920 2.37392677548325 2.28191750471611 h
-0.09390185476341 0.00002967900719 -1.56647333276092 p
-1.72331270420993 -2.37408727704933 2.28163112600961 h

\$end

16

\$coord

-1.84586440586547 -1.40718704502629 -2.34524933527530 h
-1.62685114783595 -3.92730075584776 1.68769008185505 h
0.07889571273503 1.98561557758419 0.19002630123169 s
-2.09142375170607 1.77377331990434 1.55255654722137 h
-0.10075396455309 -1.32233674793677 -1.23331224901392 c
0.07030575932093 -3.25346738856406 0.73261674758072 c
1.52331625619372 -1.32896751960941 -2.52524340583734 h
1.89393953793700 -3.74758699108470 1.55179680238066 h

\$end

17

\$coord

0.04176426935260 0.10594991582953 2.30297315711537 s
0.56217942608609 0.27030781662592 -2.30423943458249 h

-4.34657800870625 -0.13558371469204 -2.91837764926081 h
-5.65257257495989 0.07868223578359 -2.38664139859532 h
2.09279728800714 -1.38613290126922 2.72306443144614 h
0.45144333375428 -0.11389125723886 -4.11220211660086 o
-1.46020478019768 -1.92088846989427 1.81345749942988 h
0.31012583808987 1.53108210082833 -4.91337887390006 h
\$end

18

\$coord

-1.99938162936995 2.25697163266825 0.78043027201591 h
-0.03536037855222 1.63803976375487 0.43050668855975 c
-0.17534651027370 -6.47520296343711 2.04427010382651 h
-0.76989077021092 -0.89865186727560 -2.16399491386847 h
0.97073443071534 1.62584641858441 2.24385356966057 h
0.89361984649099 3.03090915817603 -0.81771403722568 h
-0.09385119040163 -5.16792690315429 1.48102163839906 h
0.10051579040508 -0.87514726736166 -0.54796948274097 o

\$end

19

\$coord

-0.73255810095325 1.72711860188522 3.44150404779938 h
-1.90330637840336 0.00010467206565 -4.01557865870087 h
-0.00826534825749 0.00018832573532 2.52098092678406 c
-0.76537209673282 -1.71633924979945 3.43489100920538 h
2.05829481984639 0.00137199244810 -3.81406046332391 h
0.01782212504853 -0.00083179561919 -2.78632625679495 b
2.06081445098650 -0.02407425977934 2.90901595783564 h
-0.06801953154337 0.00155213850141 -0.17719088441436 c

\$end

20

\$coord

0.39797838409858 8.37151669774355 0.63103301237556 h
-0.15153881317286 4.22102731150718 -3.11512686071128 h
-0.10987878612050 0.94985187711083 -0.22455466220982 h
-0.21979025616706 3.01198385724261 -3.86383266190411 h
1.65275457259351 -0.92701578434268 1.10314101769305 h
0.34978527707444 -3.76333413679252 -4.60481540450991 h

```

-0.12378929454351 -0.54441820917096 0.84392758517316 o
0.04558385378360 -3.22253781793528 -3.32141673576155 h
$end
21
$coord
2.14001367847008 1.45747961660214 1.95745067417034 h
0.18280358623837 1.90233942842980 1.41293124225113 c
-1.38704673270641 -4.99623703675022 1.68668592230803 h
-1.04686319121259 2.77527625767917 2.81661215788769 h
1.66683888786350 -1.26921354026286 -2.65470044168581 h
0.77253572090105 1.50509886453959 -2.11569564578949 h
-0.00946215035356 -2.67673910377015 -0.11670574860333 mg
-0.25802313345016 2.67256257372762 -0.98987485205485 o
$end
22
$coord
-3.91442742381108 -2.15040422436691 -0.00066644093754 h
3.19346528644137 0.15308343214797 -0.00090006026657 o
-3.50781332901240 -0.14257180645663 -0.00201930889086 c
3.06688381582665 2.03931306453972 -0.00309595178520 h
0.97065622940806 -1.04563471743903 0.00138367659303 c
-0.68365049962538 2.51844289478657 0.00096996702196 h
-4.94332773378939 1.31968743010587 0.00569760786839 h
-1.00617777395833 0.57584870511758 0.00136411593264 n
$end
23
$coord
0.84479149405366 1.68118244632239 -0.04076406030592 c
-3.89562609816288 0.21169995710577 2.19784442650873 h
4.74819064181436 1.51702239734051 0.25058332266860 h
3.03244812066285 0.33998075937600 0.05792403361285 c
0.71514973496571 3.76218275511130 -0.11340957234553 h
-2.20841190739168 -0.13189345662968 -0.09316341948888 si
-1.44511931388659 -2.96415781117082 0.02377718349537 h
2.20950831331619 -3.33175101449460 0.00473869823176 li
$end
24

```

\$coord
-0.79851491692356 -0.14279008984495 -0.01302607926238 c
-2.86441340439091 -0.06650863248926 0.02779231138177 h
-0.66120086329792 3.67235556253838 -0.69481256937176 h
0.32581418138379 2.22975525855623 0.09516574730622 n
0.38409692667446 -2.39155104301674 -0.01497002583173 c
2.44156574951578 -2.55182194217939 -0.04550177440876 h
-0.70464441403443 -4.13376216745231 0.05072308929797 h
2.19947415505361 2.29483139662495 -0.32701288174822 h

\$end

25

\$coord
3.25297404660735 -0.46077203190090 2.24241476248932 h
-3.48295446104176 0.35625476574525 2.79593976565364 h
0.82578688592582 0.10410884721660 1.28343661166870 p
-1.55924325224742 -0.09011738380794 3.35223411722514 c
2.78617235156492 0.30713719634701 -2.85343470379334 h
-1.08091724711856 0.02623025588283 -3.39744289070143 f
1.01734370502767 -0.19828509153615 -1.91781600432100 c
-1.10101258957409 -0.45950665653523 5.31933027772623 h

\$end

26

\$coord
0.85202501048098 -3.85585444399665 -0.34846806091514 h
-0.39724748382575 -2.24102418101351 0.01010322837979 c
1.08827596326201 0.04648467730736 -0.04376090232003 n
-1.91736195512323 -2.24995574168147 -1.44395964769914 h
-2.24137655888418 1.96650331685914 -0.64777040303553 h
-1.31941554222831 -2.52968120500654 1.86957944024526 h
-0.44756736267562 2.08632467636571 0.09793472116736 n
0.45654657754673 3.73602064194547 -0.30256983619274 h

\$end

27

\$coord
2.57619447668160 -2.55585235034953 -0.89472895206882 h
-1.74859208624038 0.43242891836192 4.10661788140316 h
1.71483173899898 -0.07800397800847 -1.34925451005657 s

-2.34324703768340 0.14343105569542 -0.75241984859789 p
1.78163299782847 2.38704963179398 2.14469325698834 h
-0.83536399945509 -0.48400054262552 2.48217766458635 c
1.83242564806598 0.43909384297741 2.03073243665859 n
-0.66240542921937 -2.52394931945325 2.88784000919185 h

\$end

28

\$coord

2.09070434510653 0.25232888666419 -1.58459405827844 h
0.84955777250942 5.75746389527460 -0.44064908276806 h
1.32344645652663 -0.57668695936807 -0.01144960585251 n
2.08956315136947 0.27758405641927 1.53803175148443 h
-1.97331715580846 1.35114034220403 -0.76477984011162 h
-0.26423021351593 5.76146247512446 0.44278082061384 h
-2.17477549279704 -1.76897425576209 -0.76392939189525 h
-1.36788404004357 -0.26031993825677 0.12465812214605 n

\$end

29

\$coord

-0.00116569101527 -0.47122762198106 0.80318329225322 c
-0.00963222282192 1.54879256654977 2.69621990537819 c
0.00635681169261 -1.02572210098451 3.29140863484026 c
0.01785000404657 -2.49178633845224 4.73800692538996 h
0.03967167980718 4.36939386670147 -2.50944377871917 h
-0.00515454843808 -0.43606774126122 -6.35393429759484 h
-0.00109021390896 -0.25686585133398 -3.13911343617997 mg
0.02684953232120 4.13623574890629 -1.08047196066124 h

\$end

30

\$coord

1.32012317690951 -0.09228190778956 1.94524996709031 n
-1.14880879487824 -0.14075909263074 1.88542015978886 c
0.68084098982752 -2.19387521194244 -3.14801002425713 h
-2.69263078401442 -0.61691605368257 3.17255911223004 h
1.46859969211018 0.94428858672259 -4.05065345158790 h
-0.24183371473016 0.60975035068013 -0.41030272822235 c
0.04382316234075 -0.20120117775759 -3.06195311126341 c

-1.75223545531546 -0.04218689029195 -4.09597401158712 h

\$end

31

\$coord

-1.46489471141068 -2.86185828950007 1.80947941531296 h

-1.15083314766009 -0.90487091683009 1.20608290332742 c

-1.68848504835244 -0.51376098795925 -1.57633198009361 o

-3.26514516220765 0.89440598439179 1.24385147230198 c

0.77134853573010 0.36298063682006 -2.07352035914853 c

2.37858553997860 0.09578183593086 0.70383741691168 p

1.08279433685854 1.03588913308868 -3.99861988705928 h

-2.47799487029244 2.83693289373996 1.09652986261762 h

\$end

32

\$coord

2.10454958603972 -3.95768518357577 2.00274543057454 h

-0.86550939921346 -3.36473712722878 0.20723649532327 mg

-0.05151808470484 2.39064300172455 -0.39761372077914 c

-0.76779963874784 4.19056081030743 0.71315867935645 o

-3.63518533589252 -4.97990614912528 -0.31847342686604 h

3.62649272857443 -1.20804595050761 0.94643028157765 li

1.05766784904620 0.19660727821191 -3.41937980932732 h

0.77077498061056 0.26941127756837 -1.37297342182024 c

\$end

33

\$coord

0.10795630536661 -0.32988091101401 2.62185193650829 al

0.10920617652520 -0.16700070155666 -3.27664682418047 n

6.21565556918327 -0.84441826788338 -1.46509599495624 h

-0.84040443854379 -0.09989434718157 -4.94389540318811 h

-1.05544775636536 -0.19356161686096 -0.97989892659969 c

2.01984914124189 -0.23277144486267 -3.41418546566746 h

-3.12988674840584 -0.11911183201888 -1.20923606134299 h

6.28012796885184 0.55249831244073 -1.72716258584357 h

\$end

34

\$coord

-2.25205512569957 0.86945650383734 -0.05820770117550 o
8.16430861315821 2.88833823850110 0.76040446989293 h
2.45524041181445 1.03261594950970 -1.62865529023922 h
6.91314383889022 2.57846542990347 1.35926349824600 h
-0.46611489250724 -0.66657742327864 0.32514856208737 n
-0.90361699415373 -2.24268936777839 1.42513729585781 h
1.88403724363894 -0.56249933451019 -0.46834935426763 c
3.14413990463434 -2.09195204359814 0.07046101278946 h
\$end

35

\$coord

-2.69773127266126 -0.12363578722504 -1.05384395306551 p
-1.06749799502093 3.12272650132186 1.85508616466898 h
-1.12071350969175 1.28475328312678 1.81276134422298 o
-6.39655475676465 -2.64942429357960 3.67710026146454 h
-1.50271401711728 1.63071293093326 -2.78169108660751 h
1.37961723066531 -1.04085973477597 0.51822891826312 al
3.74975924686060 0.65822185857028 -0.81938109356671 f
2.04807299365660 -3.24196245428176 2.43100231675421 h
\$end

36

\$coord

0.03535838640082 0.69916086633070 -0.03498650342943 c
-0.02976511637196 0.06307718893132 2.44742493122940 f
0.02019488239168 -1.02162240072085 -1.85969481669867 c
-0.04621848887190 -3.03791827152511 -1.44759652820598 h
0.09845815710260 2.74574737258267 -0.29263534989280 h
-0.12358422196403 1.86149699500990 -9.68046812597501 h
0.07905046371095 -0.40599014728185 -3.82192785043180 h
-0.10867028151243 1.49028290157442 -8.30951781968319 h
\$end

37

\$coord

3.58494174454193 0.37795478156594 -3.02067031653600 h
3.00337606731656 1.56743777082462 -2.42235808472682 h
3.11701767968270 -3.00050788479854 0.87894857384115 h
1.17869351320226 -0.87276696611740 0.17142315445019 al

-4.81128366026367 -4.72475809239859 1.76680928729059 h
-0.22510268613830 2.05608262682776 0.73451809088081 o
-4.41706594975989 -3.49730771559093 1.15516735243866 h
-1.79270463697757 0.00022462034295 -0.92015399545844 o

\$end

38

\$coord

-0.46634162963943 -1.27345093620920 -3.78355571566262 h
-0.80271289951781 -2.78660804164197 6.14363726956220 h
1.78732374605297 1.52520459004917 1.56827915545735 h
0.04746092339750 -1.59179105489209 5.16483393380057 f
0.07172170051261 -2.15940600247966 -5.31358993225993 o
-0.31453270695431 -0.97540780119858 -6.66164892611960 h
-0.11080223591062 2.06531260991964 -0.29763794701991 p
1.16811038271578 4.32388149930336 -1.12630284478859 h

\$end

39

\$coord

1.61560193409019 -1.73764114898712 1.82354374639225 h
2.72492229089770 1.44471839384660 -1.02776670825618 h
-0.14587126185919 0.03413049543174 1.22610656087945 s
-0.41211162464882 3.30086176507977 -4.64068195602770 h
-0.51207746036692 -3.05215856563307 -5.47653497817039 h
0.57070390719673 -0.05043259929483 -2.98765972082430 li
-1.03573949665955 -3.36965035748722 -4.18056723352592 h
-1.66916402509468 2.67534753749874 -4.93357127576027 h

\$end

40

\$coord

1.76295474344681 4.50776784093272 0.00566186825806 h
-0.01135776725554 -5.26401133091797 0.00169652679594 h
3.05975170647839 -1.82893369475658 -0.00135447784455 h
-0.60565674183345 -3.27842957545889 0.00057140415503 c
-3.15770511200060 2.59221225224188 -0.00475633465468 h
-0.15749657573105 2.16601211834919 0.00007841500298 al
1.04339734349066 -1.33843997131513 -0.00098358348921 c
-2.65394533511408 -2.97174960712302 0.00156499461194 h


```

$end
41
$coord
-1.56701686485361 2.53438389883977 0.09752866462991 p
3.04843574439676 3.80429755119133 0.80677379096426 h
1.70250605734270 2.27252946494318 0.41890991775154 c
2.78435198798971 -0.03618895086034 0.11504763346244 o
-0.87331819611934 -3.99589087868207 0.81315296855915 o
-1.25438626503579 -3.75802918243387 2.59322097647775 h
-0.15680953330483 -1.39005575088229 -0.81263875590483 si
0.10696924212849 -2.27175964793716 -3.47867153833454 h
$end
42
$coord
-0.10710774470452 -1.70240258094640 2.55786811000513 h
-1.61024034430688 1.27706421493841 2.04415432986339 h
-0.00023831307417 0.08945864856379 1.48713752016264 c
-1.59127959333465 -1.06709237657745 -1.91251208576915 h
1.72534046297615 1.08898379021503 2.06638837376868 h
0.03286873055321 3.24322197074455 -3.02646213437848 h
1.53379352942862 -1.17707799883943 -1.90034397020048 h
0.00140074924109 -0.19636673602471 -1.26296431827613 n
$end
43
$coord
-0.67077417623082 -2.20966784412558 -2.06192185685392 c
0.06455999377404 -1.72843372459447 1.67618216017832 si
-0.25684992192110 0.20595978375471 -1.98468383977165 c
-0.15079074850925 2.53320030864669 0.28249303676216 p
-1.21617182926771 -3.74402591841021 -3.30747373497535 h
2.97163639273230 -1.90276507567056 1.66854975828510 h
6.29803450970714 -0.34697809702883 -2.14745332684328 h
5.83497249597791 0.18882245412935 -3.37925953070534 h
$end
44
$coord
-2.89243130021680 -1.28355433147654 -0.00715216501773 li

```

-3.02591636267048 4.49468496698354 -0.00295303323480 h
-6.08039977397854 -3.75875753932355 0.03040740863035 h
-2.13684167126672 2.60222307230932 -0.00378396584624 c
-4.91826157587870 -4.59629524540778 0.02295121404605 h
0.75255672295434 -3.25455460587585 -0.00072040073238 cl
1.56550024140330 0.30597878514422 0.00146563249582 h
0.98598083369851 3.01326515114950 0.00213118718878 s

\$end

45

\$coord

-0.27296127893390 2.14276778505967 1.89522339651511 h
-0.15700473852220 2.78990481784372 -2.72483289680770 h
0.04091076764262 0.36694469525553 2.24294451814396 o
-1.86425362369255 -1.99457155860664 -0.32845837047328 h
0.15049425334829 -0.66347377425390 -4.58391073854167 h
0.04434142158365 0.51818955049277 -2.64506038707637 b
1.37643985078492 -2.48160426709789 -0.05421958115347 h
-0.03001561397674 -0.93782989838002 -0.12052341273490 c

\$end

46

\$coord

0.00442598246759 0.64411381326393 0.28673214989760 si
-2.36884543053928 2.14205827003815 0.56470650275980 h
-0.00720535149239 -2.54055800211743 -0.39929617694318 c
-1.75853153041791 -3.59356890942524 -0.66969085412294 h
2.38875211653613 2.10341714638161 0.65773802916418 h
-0.52559234551512 7.64753313488148 -1.09735819823148 h
1.73734464980773 -3.62081817255934 -0.59507317876606 h
0.48940755009198 7.64758138176219 -2.09172093998214 h

\$end

47

\$coord

-0.28800675283539 0.39114416153504 -2.77873781722744 p
0.78847046602191 -1.24938415097677 -0.25062872238675 c
2.95945558207349 3.72706028697428 2.46398576705473 h
-0.31612019878447 -0.07528691423972 3.36939464703891 mg
0.82730891743923 -0.99471431235008 -4.88545357129357 h

2.00307909414870 -2.89875467641410 -0.58998702661679 h
 2.65684334080983 4.18923763058125 3.78158512851669 h
 -1.36736830806198 0.66153159131026 6.33492830857220 h
 \$end
 48
 \$coord
 -0.59822114493486 -1.56591917227520 0.17959027450340 c
 -1.93064700703389 4.74228362471822 -0.20717543083365 h
 -3.92714851987794 0.57495044368646 -0.12720124663547 h
 -1.86509331168320 0.63227908763930 0.00294042670200 c
 0.65547385667297 -3.63210409049885 1.19717954798518 c
 -0.59191980271428 3.12061290052043 -0.06455265777351 c
 0.64437570157945 -3.59066961782854 -1.32918455588385 c
 1.68685520142239 3.44551342333682 0.03159628697599 o
 \$end
 49
 \$coord
 -0.11315458050155 -3.65322641824342 -3.03643134988600 h
 -2.29352269544512 2.83353034933273 -1.19271398105693 h
 -2.53320684291660 -1.19039725408664 -2.89827195508202 h
 -0.15533701112246 2.49382512358546 0.26527321805484 s
 -0.76562326821521 -1.92480869575797 -2.09428213411666 c
 0.01955027583407 -1.90740353450235 1.53755226164078 si
 1.29311538252591 -0.12607170547160 -1.40907874005577 c
 3.05079016641613 0.26674683313875 -2.40661678278380 h
 \$end
 50
 \$coord
 -3.04188421817186 -1.60985113760046 -0.00107483126342 h
 -0.99326673253950 -1.32484672377972 0.00020701421361 c
 -1.36060648760787 2.91237106336859 1.94501701857634 h
 0.27725546295712 1.93642700516253 0.00039928573064 p
 -0.17160451163447 -5.25418561471496 -0.00130427516598 h
 0.55617053325707 -3.32099894236321 -0.00004882947276 c
 -1.34758291165663 2.90654951354331 -1.95814197502372 h
 2.61044144094507 -3.09841349275183 0.00134949774714 h
 \$end

51

\$coord

0.23588487570295 0.15274701459576 1.33178646997624 c
0.09221640931194 -0.02330976395997 -5.20979511051309 f
-1.44314208144069 -0.03836772401191 3.26185789737612 c
-3.48323889825061 -0.08308532164808 3.54440467604048 h
0.23432078167877 0.33639614857801 -0.71971060318961 h
-0.67957115823861 -0.20636422176057 -6.78450820226399 h
1.26913661091969 -0.07259607134777 3.91859597522095 b
2.96412253311397 -0.19193352852845 5.38731573812552 h

\$end

52

\$coord

0.02752053999154 -4.76563732275321 -1.45708985005728 h
0.00012171180059 -2.35192646953451 -0.00203052427501 p
0.00116838877381 4.29753384316251 -0.05340818630227 f
-0.02968646996273 0.15787226978107 1.58555244153495 h
-2.70209066173926 -2.16574988902821 -0.18580764534000 h
1.55172368125544 -1.10041591110316 -1.84234526488617 h
-0.01471233680280 2.69757584086032 0.81618048194476 h
1.14148317671067 -3.55224493008716 2.15255270458198 h

\$end

53

\$coord

1.04892143338286 -0.36004299724927 -1.99878017408452 n
-0.99525216961431 -0.57637182926189 -3.37680600889302 c
-0.00476698010872 1.29510545874265 0.92960240612007 si
-2.55412747812175 0.52203592271402 -2.32263478870616 h
2.69268239602788 -1.17050704543711 -2.61526324718305 h
0.31965187806044 -3.18035888987590 2.40501475440447 h
-0.97274294436250 -1.27573701708282 4.61587741526143 h
-0.14887748999183 -1.37528316725048 2.88056637057651 n

\$end

54

\$coord

0.90933325987576 -0.62714942680324 -2.11555700382965 p
-0.43966161130918 -0.25019468644194 3.35644178820515 cl

-1.69855557849048 0.32560436633707 -3.78432486446420 n
-3.21230317630044 -0.84977870873375 -3.64955685630349 h
2.62115125514245 1.84012527743926 1.18278266948144 h
0.80965862877223 1.38452048023574 0.64377196882639 n
-2.21629790788783 2.18151994370433 -3.72289335497080 h
2.68078880403811 1.13594765453282 -3.21568078076445 h
\$end

55

\$coord

-1.70455570974926 6.60753374139036 -0.29318406707174 h
-1.21410211133012 5.36078878772874 -0.77279938783583 h
-1.36855234303720 1.06754923508363 2.63803125178144 h
-1.32389670728020 -3.20364821792800 -2.07663089060842 h
1.70217372392860 -0.55363356412961 2.85590600050213 h
0.62810240336858 0.63605055638328 -0.97413657299081 o
-0.00154169691460 -0.19760088473051 1.74164677718889 c
-0.56337588520081 -1.58686095175938 -0.71257450303004 b

\$end

56

\$coord

-1.93857558984928 -0.09926667825766 3.17146988164303 h
-1.17051925921245 -2.38526918803144 -2.15538929601262 h
0.00003952339778 -0.00011454923391 2.43309902494784 c
1.05519907366633 -1.62835729252199 3.17416164775684 h
2.64971660675667 0.17820910036126 -2.15544852212123 h
-1.48125615236413 2.20636139591375 -2.15295989508994 h
0.88390991310859 1.73070182072704 3.16564639135290 h
0.00003784248152 -0.00003639721039 -1.14989980696024 si

\$end

57

\$coord

1.12613648229714 -4.21702954359659 -0.63659361110172 h
-1.28341846538794 -1.77572945198207 -6.23335054145195 h
-0.85698636026935 -2.77515867601590 -5.31188733279370 h
1.30798706217094 0.14015027816943 3.78162675392503 h
0.68837807697752 -3.40001818399188 0.53435494153977 h
-1.74098812924237 0.19517149592387 3.65519022568619 h

0.14088022068940 0.64606645593839 -1.38673814749445 na
 -0.17662036027211 -0.20890135385279 2.57912650261596 n
 \$end
 58
 \$coord
 -1.62174944695946 2.71955683597837 1.10833253921820 h
 0.00645547547169 -2.21454532324721 2.74420092449091 h
 -0.00060786716183 3.22878429437917 0.21089984662582 n
 1.57035339531966 2.73576863420011 1.20177339235997 h
 0.00094992286311 -1.20371426885834 -1.28357582174228 c
 -0.00067838439196 -2.65382900440909 0.72971056005983 c
 0.05307246207393 2.53255462267051 -1.59522923375024 h
 -0.00292069542611 -4.67318505222384 0.21022588485223 h
 \$end
 59
 \$coord
 -0.37810951746288 0.19809169290840 1.84721963992869 h
 0.10249399561148 -0.06468824138505 3.61720671179462 o
 -1.57610043923389 2.40077281529427 -2.97925774946098 h
 -1.48446187658961 0.00350899230400 4.53566049217842 h
 0.00543343899312 -1.38321780047171 -2.61685307429722 b
 -0.03317011735331 -3.60769190485178 -2.79805780724692 h
 0.01202287810847 1.22380506727067 -2.37334128710740 c
 1.64342251877819 2.28475574510663 -1.67283867861610 h
 \$end
 60
 \$coord
 0.91700177695209 -3.16704234998236 1.72797899078254 h
 -0.48522881141330 0.95672576770769 -2.66941413996431 h
 0.08765731965079 1.07679166717692 0.00001102967519 s
 -0.48576949437748 0.95871064028991 2.66892761025535 h
 -0.04359416072535 -2.52723408285503 0.00010991657040 c
 0.93224626714073 -3.16689883329787 -1.71917784134096 h
 -2.01367492612376 -3.16843358097072 -0.00916141875345 h
 -1.13351961578022 3.44866007210163 -0.00081384556152 h
 \$end
 61

\$coord
0.04471960262505 0.02109907600604 1.85377901992347 h
0.32330939116174 2.12142498776168 -2.37800602280582 h
-0.00517699869449 -1.82819607129395 2.23747188082531 o
0.07102743523584 3.64704833482360 -0.31853427473145 s
-0.00534596165855 -4.27263372638323 -1.84680139216181 c
0.00345185000628 -5.39315845740460 -3.52567149979577 h
-0.00014272700797 -3.07069635026854 0.10674173326493 c
-2.48331884255544 3.75950019862334 -0.59766744980866 h

\$end

62

\$coord
2.67190008096644 0.00219117621049 0.28823881852266 h
-0.34198060549435 0.00016668893752 -2.29327711083951 c
-0.37664679393691 0.00052377084915 2.49729306094515 c
0.25008117270930 1.70588653606242 -3.32501377796760 h
0.73461205961811 -0.00071047708820 0.28711331678804 n
0.29717357444128 -1.67507297514401 -3.34652380616926 h
-2.45646346787812 -0.00216908557454 2.09098903109770 h
-2.40753123322534 -0.02919053973095 -2.12849274310328 h

\$end

63

\$coord
1.85266963603471 -2.98471283318294 -2.33168914662324 h
-1.57747811753514 0.06430659387338 0.33623346076607 al
0.51195265170741 3.46705239911771 -0.22290214933091 cl
-4.42654076242959 0.34216561164531 1.26743942040746 h
6.45684820187202 -0.33790480203927 2.60248074234765 h
0.52796655298121 -3.78861261280208 -0.10093635472992 p
5.66744158746076 0.60138096891776 1.88340037148867 h
-1.55480565008803 -4.86793800523917 -1.48025491540144 h

\$end

64

\$coord
2.42089660620139 -0.21458591351468 -0.94944859152261 b
0.00535050420566 3.52269735305279 -2.01362695264389 h
0.00239266565276 1.68974723326998 -1.09040398178472 c

-4.63053324771551 -0.00425723962376 -1.17116739704302 h
4.63862301304638 0.00071655946585 -1.12086942213123 h
0.00636408587690 -1.36661443885083 -1.84276493767507 c
-0.00602867344677 -0.08987803089440 1.94549114369462 p
-2.41460626479122 -0.21502620950338 -0.96420803668193 b
\$end

65

\$coord

-0.10199508627374 -4.60778166213263 -2.93853176805357 h
0.57503335551100 -3.00482679180603 -1.80817601179976 c
-2.85373239530975 -2.42326846258624 -0.06773662728877 h
2.61320584830195 -2.63444169463284 -2.00641907730737 h
-0.03440776187008 2.25098778543192 -2.44048715858133 na
0.60653805492934 3.26836145005976 1.29547583764142 h
-0.88714635116134 -1.71124238111932 -0.13009213554710 c
0.15839530563601 0.42042772845078 3.08114741389832 al

\$end

66

\$coord

-3.47751545588141 1.35166790646925 -0.31732342793871 h
2.40264791164883 -1.57808232444454 -1.75947675695873 h
-1.56276254682374 0.96272974084611 -1.00314313918174 c
-1.15372529163111 1.93885747606640 -2.78109390365210 h
0.22338325502149 -2.05377112957503 0.13103292535564 si
5.03414807242290 2.52972723110569 -1.99133513015148 h
0.19214330023707 2.01211216397240 0.91835561925181 f
5.97071587123625 3.58724217592352 -2.15756207682301 h

\$end

67

\$coord

0.98996721610869 1.97072375939720 -0.06741158840101 c
0.37388629660940 -0.70280987889760 2.31073055662416 s
0.24737645415274 -4.37881911099947 -0.57708373345529 h
-0.71372569636719 -2.53858037091560 -0.46886228601996 c
-1.14763571098639 2.66168082286775 1.39598127045219 b
-2.97208983993360 3.69369751254224 2.18197368297610 h
0.09384122726444 0.14846162002964 -2.99120075103911 si

-2.76632660727667 -2.87611290233515 -0.34601105631952 h

\$end

68

\$coord

0.01376764970814 0.53845510232119 -3.07914788279580 c

-1.86492123592251 1.28306836491418 -3.62698650860521 h

1.28387623483903 2.18773344937935 -2.81546566261333 h

0.59436893012985 -1.68284894353946 3.33787433226521 h

0.72422771192283 -0.54035170213513 -4.70787715521774 h

-0.08941894678034 -1.24045260536690 -0.95126449199966 n

-2.31947361981938 0.60534785083115 3.00781693777590 h

0.08363363750929 0.28191945740432 1.72003226279438 s

\$end

69

\$coord

-0.46347083320614 -2.06835788845123 -0.02421936391248 n

0.13784940816059 0.65161817269702 2.32219940332384 al

0.46671986515141 -0.75153811532859 -2.05812134848464 c

-2.12733385076416 2.35779894985415 -1.74186481285661 h

-0.06953295949445 -3.95118055145190 0.03437936893636 h

0.71989010407202 2.95542250986307 -3.70735072908437 h

2.06280767255641 -1.51051589465232 -3.15272101808478 h

-0.28507089115544 1.71221973545437 -2.41117170125388 c

\$end

70

\$coord

-0.50385762549895 1.57486471501050 0.02348112640620 c

-2.56752336791988 1.65327916295140 0.07817697676765 h

0.84024390452029 -0.54087839387569 1.13815213049253 c

1.62714529086207 -1.53186434581679 2.76428964089846 h

0.46599638979233 3.35890964532507 -0.35403340364780 h

-6.31524441001733 -1.71860886611373 -0.24110169031441 h

0.66739718113428 -0.82663006885289 -1.21988466842154 n

-6.49293008222713 -2.59607119789812 0.86189523064485 h

\$end

71

\$coord

1.00020315654380 -2.73757196385126 0.01487357627141 c
1.26093462282436 -4.80298046678602 -0.08529902256372 h
2.71371208920189 -1.57219462670816 0.12183840924042 h
-0.13971740710965 4.30383147875507 1.57329103407385 h
-1.13242151197362 -1.61943543489404 0.01177513055282 n
-2.61693451936371 -2.87295882967404 -0.10611829730242 h
-0.61972997740624 1.98480058342019 -0.12298111940380 h
0.20281168477395 3.65935115631633 -0.10846124897765 o
\$end

72

\$coord

0.02125875203811 2.51289614302014 -1.29963401145924 si
-0.01208618900339 -5.52622059761912 -0.68117898114197 cl
0.04610573147420 5.65497934581317 -1.04059099700976 o
-2.30300633839144 1.53435417156410 -2.57190152918854 h
2.42953385860087 1.81542126263490 -2.56632305725535 h
-0.04065077053603 -3.52983013841631 0.77140053578080 h
-1.45368501268202 6.44855596176982 -0.34412725394297 h
0.01332648869521 0.80526781983327 2.31429465625850 cl
\$end

73

\$coord

-2.86583567473583 -0.37831903569787 4.35367091204284 h
-3.63239376009399 1.25194209079115 -0.71504578057899 h
-1.57636227012830 0.07473280180056 2.82873301422392 c
-2.07699170149529 0.14702144582132 0.10483250709970 c
3.71374207936290 1.74069673092123 2.25971067305388 h
0.25122771186990 0.24730990725913 -3.77166777484423 f
1.54513385434141 -0.00759978888846 1.69510184882331 si
-0.12337633934013 -0.81455350381796 -1.42649276087442 c
\$end

74

\$coord

-2.50395497538676 -1.09004091049724 0.54545103197623 al
-1.41862465764472 2.21231389974634 -2.82570379750143 li
-4.26567079833156 1.06386156697562 -1.13479273326406 h
0.81997129751109 1.63949731046543 0.43777902343164 c

-0.72513936836578 -1.74227783399295 -2.35449666460991 h
 2.14734056745554 -2.17010647189731 -0.20163449087699 al
 1.48580454783283 5.92215567028096 1.01903534677570 h
 1.09481360323860 3.96586840734102 0.62963039390796 c
 \$end
 75
 \$coord
 2.28712577453646 0.18548975428092 3.02056537968679 h
 1.88159990406748 -4.38462181607157 -1.96298807963652 h
 0.03308310975221 1.15027262475463 1.56586620071594 si
 -0.11837163883701 4.47360993157204 -1.14778457652030 si
 -0.06273499233637 -4.59044352567720 -0.48091344125078 cl
 2.79339864376387 4.41875121659169 -0.92327670764264 h
 -2.29889799888415 0.26497389184072 2.93622962332839 h
 -0.08019576585104 4.27014056531384 2.19508655411357 h
 \$end
 76
 \$coord
 -1.77148915921006 0.12431092125235 -2.75077101085197 h
 0.00102785199074 -0.00210704160130 1.38146772837174 c
 0.00031292552002 0.00458687176594 -1.69706392009949 c
 0.16777058384376 2.28628381793595 0.35373751973303 c
 -0.17000339495092 -2.28963181626305 0.34981047730623 c
 1.13770950616022 -3.87260990693278 0.43381043256813 h
 1.77143891060396 -0.11964408212861 -2.75128474153941 h
 -1.12702962638319 3.87828831421965 0.44534252870123 h
 \$end
 77
 \$coord
 0.00330414460453 -1.20720460549069 -3.41957712202339 c
 -1.67562444208705 -0.57015254314633 -4.49098423711268 h
 1.68457926347219 -0.50613748004266 -4.43910934302009 h
 -1.55283016892027 3.16779522321472 -0.75576388851464 h
 0.03142821571351 -3.28384538082176 -3.47220485333991 h
 -0.00584969480962 -0.71287739233687 2.50266149968937 si
 -0.02464793904698 -0.31107152158751 -0.77776807466974 c
 0.12157702041968 2.46633998005960 -0.41325774981071 o

```

$end
78
$coord
-3.59963230621185 0.00908611636603 -3.24698805768810 h
-2.17506195169209 1.81357973647134 2.43009004672209 h
-0.36030452076683 -0.00113121053269 -3.73580573095390 mg
-0.23143338621219 0.01061091153943 3.02728580777837 p
2.51237508265700 0.01438005292699 -5.33089834911349 h
-1.91416042198246 -2.08054105046905 2.59286855230099 h
1.13462582108675 -0.00647419190417 0.02996990052795 o
2.96883707299451 0.04748229172531 0.16084202296203 h
$end
79
$coord
-0.77865270603263 3.72977035954853 9.88350972449518 h
-0.10879046091055 0.95721690455499 6.76879281573079 h
0.50051603110062 2.57916029280758 -0.36999241968188 h
0.06599212555090 2.83255306198361 10.59732417746354 h
-0.02532252337551 -1.88313146781959 -2.72326143317905 cl
0.04057966799452 -0.31013761817321 4.67174041840828 cl
2.52036985630182 2.40111477906380 -3.70615401442140 h
-0.08903899069248 2.10366600091118 -2.98438029511323 p
$end
80
$coord
-1.82051803387013 1.70135126172640 1.47108091208516 h
6.09743915158931 1.45046732337797 2.50777010036391 h
-1.00572473066944 3.29601059384825 0.56463198537631 n
-1.87834706087909 5.01128127662287 1.13394710746045 h
-0.06815832818393 -2.68634188945588 -0.06319991785962 cl
-1.04221334353035 -4.72411408521441 0.91193240516276 h
0.71179930852038 3.15558830310212 -0.94417542035145 n
5.12532268949001 1.39575011539317 1.47229589291955 h
$end
81
$coord
-3.36778918903728 -0.72635950113871 -0.32214712234446 h

```

-1.46872229486795 -1.47374043134026 -0.03290811557783 c
-7.01493523045851 2.73001752170841 -0.09848475302677 h
-1.33235661783152 -3.51300436119603 0.23232342879645 h
0.99608534812816 3.24499902573559 -0.35688976808895 h
1.15861759657534 0.45245449905409 0.00424104383801 si
-7.82761320876984 3.77187593261691 0.42333752367353 h
3.76453202523302 -0.55333323347919 0.39582753046798 h

\$end

82

\$coord

1.30643430645376 2.51887232706270 0.49327229181289 o
-1.39415459884698 2.60264321962737 0.12162657952614 c
-0.13304497548434 -2.57663047009965 0.18472256697397 s
-2.52123020174644 2.14519146092705 1.79638531453491 h
0.15747787168530 0.61169284806332 -1.03321014427910 c
-2.09105966009954 4.16234122190844 -1.04539548884123 h
0.63262594106338 0.71222391258665 -3.04260052383155 h
2.21145526645911 -3.34032087389754 -0.55156733226173 h

\$end

83

\$coord

0.00028329345942 -1.12567082538548 1.43403549368556 c
-1.77778776938908 -2.13501903599647 0.91883032880431 h
-0.00015096262513 0.86529446909208 2.57827201011797 o
-1.52359811678394 1.34152052087054 -3.41053320998904 h
1.77853589334551 -2.13661993170640 0.92297212977012 h
-0.06271238973474 -0.82478593970951 -5.10591630317728 h
1.57868849446863 1.26789613393489 -3.48574464080939 h
0.00042417587091 0.15587101272371 -3.44362702145753 n

\$end

84

\$coord

-1.09656185276242 -0.38479592618970 0.76304157506663 c
1.23750739240012 -1.00863354182606 -0.04121841413698 c
2.79450261970638 2.16594326848439 0.90124569796213 h
3.35069754439576 0.62395093644130 0.06400409594519 o
-4.69120550675854 0.59918346164706 2.21847990703709 h

1.84807612597234 -2.95520512436763 -0.34578534739006 h
-3.41339037872323 0.43004797911660 0.60214630782374 c
-2.05423117833371 0.25653152859639 -2.84226424250540 li
\$end

5 Decomposition energies for the 931 set

No Ref CCSD(T)/cc-pV(TQ)Z CCSD/cc-pVQZ CCSD(T)/cc-pVDZ /cc-pVTZ /cc-pVQZ CCSD(T)/cc-pV(DT)Z

1	128.981	128.921	128.976	110.122	122.608	126.585	127.224
2	10.1995	9.82792	15.4248	-4.07305	4.01615	7.53477	7.99794
3	-64.5198	-66.2892	-85.5845	-81.4918	-70.9377	-68.0006	-67.3879
4	64.2156	62.8851	62.8716	61.3162	61.5287	62.3444	62.1194
5	103.341	103.269	101.431	92.2781	98.1735	101.006	100.751
6	94.8625	92.8063	82.7507	70.7528	87.7004	90.8247	92.8486
7	-83.7923	-82.7383	-81.8052	-78.3415	-80.5524	-82.0044	-81.3767
8	-87.8609	-88.6287	-92.7047	-92.0761	-89.3406	-88.7607	-88.8941
9	101.855	99.9777	91.9807	88.0511	98.1918	99.1034	101.716
10	73.4314	73.0608	69.495	60.3006	67.841	70.857	71.2286
11	-69.9266	-70.7725	-74.7205	-75.6138	-72.5754	-71.4369	-71.4306
12	-108.999	-108.999	-108.719	-103.535	-108.046	-108.641	-109.606
13	6.29251	5.8623	3.5078	2.43968	4.63202	5.35964	5.55187
14	-7.72743	-7.29796	-2.93809	-8.38064	-6.50257	-7.24381	-5.36337
15	212.84	211.643	210.976	203.784	208.511	210.373	210.584
16	167.785	167.117	167.192	154.259	163.374	165.625	166.901
17	70.6529	69.7324	67.3023	66.659	68.8457	69.366	69.6167
18	93.7936	93.9028	90.7904	87.3905	91.6597	92.6367	93.5413
19	-2.14101	-2.50876	-4.53714	-3.27039	-1.71843	-2.37272	-1.17002
20	79.8097	77.4036	76.1209	69.7079	75.9669	76.6977	78.4094
21	315.129	313.435	310.794	301.883	309.424	311.893	312.319
22	145.384	144.415	137.352	121.094	138.731	142.229	143.707
23	82.0241	78.6155	79.0926	44.7119	66.6561	74.5436	73.9281
24	33.4068	32.6725	31.167	30.9736	32.7968	32.6664	33.3364
25	166.621	164.884	159.323	155.949	161.61	163.433	164.121
26	-34.7981	-34.5691	-29.6481	-41.0404	-38.0949	-35.972	-36.0101
27	-53.9231	-53.5264	-55.5766	-62.3531	-56.3851	-54.6836	-54.0658
28	-64.2575	-64.3706	-67.5082	-66.7879	-64.8426	-64.4632	-64.4815
29	228.294	227.4	224.486	201.718	218.603	224.048	224.646
30	141.522	141.02	141.429	120.964	133.432	138.182	137.985
31	-5.2389	-5.8472	-9.31914	-24.3567	-11.4692	-8.0407	-6.6334
32	199.354	199.064	199.927	187.822	197.031	198.29	199.312
33	346.765	341.465	327.77	303.586	333.898	338.303	344.099
34	246.838	246.475	248.831	238.748	244.524	245.72	246.073

35 -9.71568 -10.2604 -7.43142 -6.45352 -9.55585 -9.87122 -10.7051
36 -4.9177 -5.77143 -9.63905 -8.85686 -6.25095 -5.97622 -5.56435
37 -34.4301 -34.8201 -35.6612 -36.0644 -34.2626 -34.5983 -33.8446
38 -199.36 -199.428 -209.03 -205.424 -199.424 -199.432 -198.197
39 41.6549 40.9683 33.0217 16.6327 33.7689 38.1676 39.387
40 25.5228 24.0911 23.9908 21.2429 20.3746 22.6168 20.5899
41 144.978 145.756 135.559 138.093 145.288 144.718 148.786
42 273.134 271.547 271.41 249.57 263.368 268.23 269.2
43 316.083 314.476 312.078 303.357 310.441 312.982 313.194
44 31.849 26.9448 19.1359 -2.57283 14.3392 22.6139 19.1064
45 3.75113 3.5232 2.78056 2.0403 2.82258 3.25392 3.14253
46 65.5461 65.4422 62.9942 62.074 64.5455 65.061 65.3936
47 36.6235 36.3795 27.9887 31.1652 36.8679 36.2745 39.028
48 49.5159 47.3052 50.2241 45.8558 46.0005 46.8546 46.3419
49 67.8673 67.9944 67.5544 54.3327 62.85 66.0136 66.0033
50 96.3261 94.1288 91.0199 77.1458 89.5913 92.5036 93.2726
51 93.5031 93.3396 91.4429 85.7217 89.9866 91.8161 92.1352
52 62.6219 62.0519 61.772 63.8908 61.5214 61.7984 61.1949
53 88.2948 87.4639 83.132 70.0358 80.8473 84.8275 85.6362
54 -12.6939 -13.7427 -20.5563 -20.6227 -17.1771 -15.1047 -15.9754
55 47.9831 47.0958 40.9241 30.2789 42.3243 45.3081 45.7567
56 16.9482 17.857 14.1657 11.387 18.8959 17.8012 21.9587
57 433.664 433.118 432.951 413.038 420.556 428.211 424.195
58 248.457 246.488 244.387 231.515 239.068 243.787 242.222
59 65.2968 65.1537 62.7956 62.0607 64.3508 64.8122 65.1277
60 13.2213 12.641 10.0244 -1.28579 8.11558 10.8268 11.9712
61 49.8152 49.7566 50.6918 52.705 49.2586 49.518 48.6418
62 282.122 281.738 281.035 259.292 275.738 279.178 281.797
63 96.9399 96.8113 95.7761 91.1106 93.9485 95.4967 95.4666
64 2.20915 2.16117 1.61473 1.10252 1.58883 1.9369 1.801
65 331.099 328.39 325.201 301.745 317.119 324.464 321.748
66 -45.3574 -45.7393 -50.8793 -69.8072 -49.6511 -47.4048 -43.2135
67 185.358 184.382 180.792 156.904 173.979 180.509 180.226
68 7.87624 7.13069 4.79089 0.472904 6.16216 6.28959 9.03757
69 133.716 131.512 124.894 107.336 124.689 128.987 130.362
70 103.749 103.212 100.712 89.7773 98.8035 101.454 102.289
71 201.248 201.549 201.753 176.967 193.011 198.159 199.502

72 62.5938 62.5111 60.0665 48.5757 57.5077 60.5019 60.71
 73 95.3155 93.1307 90.2756 76.033 88.6604 91.5805 92.3426
 74 148.937 147.329 140.24 121.493 142.006 145.347 148.137
 75 -37.5031 -38.6058 -45.3226 -46.4901 -41.0511 -39.4988 -39.2498
 76 17.3911 16.5904 3.75551 9.84 17.0608 16.4636 19.7624
 77 32.5568 32.7334 28.7219 13.4653 24.6791 29.6114 28.5534
 78 65.4965 64.7742 62.4476 61.6505 64.0015 64.4499 64.8301
 79 91.6377 91.439 85.1424 57.9163 80.0728 87.0064 88.5183
 80 225.237 222.906 219.892 207.426 220.017 221.642 224.237
 81 139.537 139.547 140.751 128.991 135.557 138.059 137.98
 82 37.22 35.9534 29.5329 27.4782 33.82 35.1521 35.8855
 83 86.8257 85.6765 86.6499 77.2269 81.9826 84.1939 84.2125

No Ref LDA/TZVPP LDA/QZVP PBE-D/TZVPP PBE-D/QZVP B97-d/TZVPP B97-d/QZVP

1 128.981 133.195 134.953 115.812 117.605 108.649 110.161
 2 10.1995 58.364 59.2052 23.8131 25.1467 1.99101 3.23081
 3 -64.5198 -17.1106 -15.3669 -25.3822 -24.0235 -48.9578 -47.5105
 4 64.2156 99.4915 101.096 68.0654 69.4628 46.5227 48.2784
 5 103.341 122.054 127.474 103.931 109.521 81.2833 86.6558
 6 94.8625 136.54 141.608 109.643 114.072 81.858 86.7775
 7 -83.7923 -84.3867 -85.1376 -75.6211 -76.479 -75.7058 -76.5812
 8 -87.8609 -90.7108 -89.1097 -81.2685 -79.9862 -77.3389 -76.0182
 9 101.855 153.438 154.928 126.107 127.112 89.3767 91.2232
 10 73.4314 78.2878 80.7603 65.2623 67.355 57.8346 59.7802
 11 -69.9266 -28.1159 -23.9961 -48.6441 -44.8153 -72.6479 -68.8606
 12 -108.999 -111.379 -111.439 -103.74 -103.732 -113.709 -113.796
 13 6.29251 26.6903 26.6458 15.1354 15.0845 5.7621 5.63465
 14 -7.72743 3.08565 2.46006 0.778368 0.354506 -7.36948 -7.03431
 15 212.84 236.278 241.014 217.376 221.577 190.404 194.456
 16 167.785 185.786 190.288 154.745 158.682 139.568 143.426
 17 70.6529 85.3288 85.9881 80.1272 80.5239 72.9567 73.3018
 18 93.7936 107.016 109.698 89.3409 91.7002 74.492 76.8806
 19 -2.14101 2.07466 4.12375 0.375556 2.17333 -4.21034 -2.70771
 20 79.8097 112.928 117.061 92.4915 96.2763 66.8245 70.3334
 21 315.129 334.623 337.115 317.423 319.514 307.405 309.652
 22 145.384 137.303 144.92 126.615 134.027 116.801 125.042
 23 82.0241 114.281 120.061 81.9758 87.8695 61.8204 67.7598

24 33.4068 37.5676 38.4242 41.8642 42.411 40.8897 41.2635
25 166.621 211.219 213.809 173.5 175.939 138.053 140.452
26 -34.7981 -8.20892 -7.47503 -27.6649 -26.7747 -41.1686 -40.5279
27 -53.9231 -26.2485 -26.0125 -45.1593 -44.8161 -54.6738 -54.4309
28 -64.2575 -67.7742 -67.3945 -63.2813 -62.9453 -61.1805 -60.8381
29 228.294 278.151 279.662 235.17 237.112 212.558 214.385
30 141.522 134.708 141.271 119.364 125.663 116.328 122.567
31 -5.2389 47.4418 51.1415 15.8299 19.5024 -10.4186 -6.8915
32 199.354 204.32 204.446 192.127 192.471 191.939 192.547
33 346.765 358.222 364.807 338.016 343.353 320.932 326.272
34 246.838 249.919 249.989 235.008 235.513 235.112 235.842
35 -9.71568 -2.68531 -0.648416 2.45386 4.2006 8.66228 10.628
36 -4.9177 -7.40507 -5.71023 -2.62139 -1.20097 -2.22879 -0.938611
37 -34.4301 -51.433 -49.7626 -29.583 -28.15 -24.2535 -22.5335
38 -199.36 -213.958 -210.809 -193.148 -190.476 -187.185 -184.687
39 41.6549 95.8729 103.524 54.0954 61.514 24.876 32.5273
40 25.5228 46.359 45.2883 37.2346 36.6874 25.9827 25.8294
41 144.978 197.012 205.907 160.748 168.76 124.755 133.981
42 273.134 318.142 318.452 278.159 278.537 259.712 260.635
43 316.083 334.165 336.703 315.67 317.784 305.296 307.621
44 31.849 36.3474 41.515 21.2385 26.5739 11.1375 16.8533
45 3.75113 9.38583 9.51132 5.07033 5.15515 2.08481 2.21481
46 65.5461 76.1146 76.7267 69.8258 70.2529 63.6656 64.1023
47 36.6235 54.8732 55.8011 49.8321 50.2516 34.4644 34.9466
48 49.5159 82.2903 84.0142 70.2155 71.7116 61.1938 62.6587
49 67.8673 75.441 76.5437 57.86 59.0035 50.819 51.8784
50 96.3261 95.8831 98.0642 84.756 86.5002 80.9754 82.8559
51 93.5031 121.513 123.176 94.2475 95.811 74.535 76.5558
52 62.6219 71.5361 71.1991 60.5145 60.1922 54.84 54.6867
53 88.2948 113.543 117.493 99.3885 102.824 89.8184 93.3136
54 -12.6939 -0.240094 -0.904336 -9.07693 -9.67954 -19.3279 -19.7813
55 47.9831 57.301 58.2689 44.7598 45.6493 37.7692 38.7737
56 16.9482 71.7509 72.4468 34.6305 34.8036 3.40942 4.76528
57 433.664 407.596 426.287 386.824 404.587 381.576 399.146
58 248.457 247.771 252.438 244.636 248.793 244.05 248.387
59 65.2968 75.587 76.1256 69.6902 70.048 63.6704 64.0507
60 13.2213 47.0163 48.2344 25.9195 27.0126 12.0928 13.129

61 49.8152 51.9679 51.945 47.3811 47.4457 46.0244 46.0351
 62 282.122 334.183 334.527 284.742 285.454 261.236 262.017
 63 96.9399 115.636 117.236 94.5455 96.0776 79.6813 81.4468
 64 2.20915 5.58936 5.63102 3.70739 3.74976 2.52269 2.63345
 65 331.099 331.781 333.631 316.91 318.795 304.528 306.984
 66 -45.3574 -24.2483 -22.3393 -37.5838 -35.7988 -46.7869 -45.2986
 67 185.358 181.569 191.607 162.541 171.864 155.627 164.604
 68 7.87624 57.1047 56.6968 27.356 26.8874 5.74304 5.43055
 69 133.716 172.395 174.671 139.187 141.375 118.002 120.254
 70 103.749 143.554 143.702 113.836 114.179 96.5926 96.9878
 71 201.248 242.962 244.739 204.201 206.589 188.723 190.819
 72 62.5938 76.4882 78.2482 62.3101 64.3079 56.8097 59.1964
 73 95.3155 93.8305 96.1183 83.3931 85.2325 80.111 82.0663
 74 148.937 132.71 139.706 133.546 139.285 136.395 141.702
 75 -37.5031 -19.4049 -17.7142 -28.32 -26.8573 -39.6133 -38.1608
 76 17.3911 40.1105 40.7125 36.3748 36.4057 18.9558 19.0292
 77 32.5568 72.6812 73.529 41.9752 43.3049 31.4473 33.0729
 78 65.4965 79.7304 80.207 73.6934 73.9232 66.3356 66.5412
 79 91.6377 153.877 155.494 107.949 110.086 83.1093 85.2114
 80 225.237 240.052 245.737 212.757 217.449 195.157 199.947
 81 139.537 144.273 145.059 132.884 134.011 131.315 132.364
 82 37.22 49.6321 51.7931 43.7971 45.5158 32.9163 34.6547
 83 86.8257 106.472 107.72 98.4585 99.5107 89.1248 90.201

No Ref TPSS-D/TZVPP TPSS-D/QZVP PBEh/TZVPP PBEh/QZVP B3-LYP-D/TZVP B3-LYP-D/QZVP

1 128.981 104.577 106.087 120.58 121.855 117.352 118.83
 2 10.1995 15.2395 16.7903 31.2373 32.2924 18.1409 19.2094
 3 -64.5198 -36.023 -35.5951 -53.8575 -52.5976 -63.9161 -62.2361
 4 64.2156 60.8565 62.6431 66.5791 68.4417 55.5837 57.7391
 5 103.341 80.0224 86.4678 108.318 114.329 94.0083 99.68
 6 94.8625 96.5309 101.524 99.4908 104.301 86.1731 91.241
 7 -83.7923 -78.7113 -79.6555 -77.5736 -78.5236 -79.4286 -80.4104
 8 -87.8609 -77.8938 -77.1179 -93.5255 -92.2621 -83.0836 -81.6911
 9 101.855 98.9039 100.977 114.57 115.842 95.8558 97.5649
 10 73.4314 64.3085 66.2884 61.4998 63.3171 65.24 67.1642
 11 -69.9266 -58.7056 -54.9349 -56.5329 -52.5389 -68.0667 -63.5031
 12 -108.999 -112.152 -112.19 -104.119 -104.17 -109.933 -110.053

13 6.29251 9.17828 9.20268 11.6927 11.6752 6.6355 6.58082
14 -7.72743 -2.62993 -2.49029 -63.9493 4.49542 -3.6991 -4.041
15 212.84 205.281 208.765 210.933 214.616 213.359 217.701
16 167.785 142.601 146.778 158.546 162.579 153.128 157.492
17 70.6529 78.6301 78.8562 73.0902 73.5295 74.7552 75.3055
18 93.7936 83.7283 86.7144 86.6826 89.6821 79.5256 82.0613
19 -2.14101 -3.42124 -1.63227 -3.35762 -1.51849 -5.96789 -4.19352
20 79.8097 84.2443 88.0675 92.175 95.9907 71.8873 75.6745
21 315.129 315.936 317.895 312.427 314.568 316.325 318.874
22 145.384 123.839 132.41 123.329 131.644 117.179 125.259
23 82.0241 76.5823 82.5916 86.5306 92.0816 76.3802 82.0928
24 33.4068 43.2826 43.6078 33.16 33.6879 40.1059 40.6963
25 166.621 157.505 160.39 170.296 173.322 146.654 149.722
26 -34.7981 -37.1097 -36.1663 -21.9027 -21.3436 -30.6548 -30.1474
27 -53.9231 -56.3036 -56.0107 -46.6446 -46.4362 -53.0596 -52.854
28 -64.2575 -65.2905 -65.0547 -68.6829 -68.3932 -65.8937 -65.6319
29 228.294 212.489 214.228 236.263 237.806 225.089 226.918
30 141.522 118.644 125.001 125.383 131.452 127.909 134.268
31 -5.2389 0.266741 4.43679 13.2029 17.1243 1.57258 5.56369
32 199.354 189.189 189.591 196.157 196.69 195.603 196.255
33 346.765 323.704 329.271 319.261 323.753 331.303 336.701
34 246.838 228.717 229.164 242.622 243.243 239.659 240.472
35 -9.71568 9.26721 10.7651 -5.30823 -3.51665 7.38717 9.37774
36 -4.9177 -2.10031 -1.01179 -10.9599 -9.52489 -6.97479 -5.38664
37 -34.4301 -16.417 -15.1109 -38.6936 -37.2855 -25.4631 -24.0447
38 -199.36 -196.76 -194.49 -209.686 -207.232 -203.956 -201.548
39 41.6549 42.9878 51.0567 46.4906 54.3208 33.8656 42.0904
40 25.5228 32.8071 32.2349 36.7316 36.4209 25.6687 25.1971
41 144.978 145.44 155.773 148.076 157.505 130.244 139.584
42 273.134 257.517 258.944 280.437 280.76 274.826 275.459
43 316.083 314.402 316.354 312.863 315.005 315.126 317.713
44 31.849 15.2598 20.5586 16.7706 21.9412 10.2506 15.5321
45 3.75113 4.82641 4.901 4.12002 4.21617 2.74062 2.86678
46 65.5461 69.3309 69.7474 65.9775 66.4883 64.5644 65.0979
47 36.6235 38.3685 38.8707 38.8145 39.3505 30.2685 31.0092
48 49.5159 70.0915 71.6672 61.3836 63.204 66.7865 68.4213
49 67.8673 53.4844 54.3917 60.5619 61.3634 58.629 59.603

50 96.3261 77.0183 78.8568 79.3179 80.8113 86.4336 88.3057
 51 93.5031 87.1114 89.126 92.4179 94.4633 82.379 84.5137
 52 62.6219 56.8118 56.7295 61.2359 61.1185 57.029 56.7831
 53 88.2948 98.2817 101.616 90.3 93.5049 99.4207 102.984
 54 -12.6939 -14.9016 -15.7661 -16.6989 -17.2525 -25.0333 -25.6686
 55 47.9831 41.7977 42.4065 37.1504 38.0087 35.8234 36.8324
 56 16.9482 10.4404 12.0824 29.5869 30.3937 7.79356 8.97018
 57 433.664 382.617 401.558 397.529 415.908 395.562 413.37
 58 248.457 243.786 247.698 237.803 242.118 251.416 256.037
 59 65.2968 69.2914 69.6375 65.9483 66.389 64.5797 65.0583
 60 13.2213 17.5975 18.7139 23.214 24.1382 18.9235 19.971
 61 49.8152 43.4488 43.3513 48.6327 48.6846 46.8771 46.9895
 62 282.122 267.522 268.44 294.049 294.664 277.464 278.274
 63 96.9399 87.2607 89.155 93.9041 95.8791 85.9082 87.853
 64 2.20915 3.26843 3.30989 2.3975 2.46542 2.12915 2.21314
 65 331.099 301.138 303.33 318.388 319.807 315.049 317.208
 66 -45.3574 -55.9 -54.4379 -43.4123 -42.156 -46.174 -44.6638
 67 185.358 156.711 166.081 161.873 171.028 165.396 174.63
 68 7.87624 5.90148 5.86938 23.1004 22.2155 12.8868 12.3047
 69 133.716 127.971 130.167 137.682 139.794 125.038 127.322
 70 103.749 99.7874 100.322 114.941 115.258 104.634 104.965
 71 201.248 182.271 184.669 213.326 215.032 201.515 203.435
 72 62.5938 62.0159 64.1888 61.2207 63.3116 60.1728 62.4372
 73 95.3155 75.9287 77.8402 78.6994 80.2872 85.3976 87.3768
 74 148.937 130.59 135.878 121.061 126.414 136.481 142.187
 75 -37.5031 -35.1582 -33.8469 -37.1977 -35.5995 -41.9425 -40.1684
 76 17.3911 19.0732 19.0544 19.4532 19.589 10.3006 10.576
 77 32.5568 34.1459 35.4345 38.4395 39.6424 34.6095 35.9814
 78 65.4965 72.1715 72.1857 68.1188 68.3665 68.0237 68.4303
 79 91.6377 81.5022 83.759 108.906 110.536 90.8615 92.7219
 80 225.237 196.963 202.35 209.516 214.359 207.256 212.706
 81 139.537 124.52 125.48 138.006 138.914 135.59 136.657
 82 37.22 39.5129 41.0417 35.3137 37.2454 32.2438 34.3632
 83 86.8257 99.0633 99.9362 93.8786 95.0422 95.0648 96.3035

No Ref BMK/TZVPP BMK/QZVP M05/TZVPP M05/QZVP M052X/TZVPP M052X/QZVP
 1 128.981 122.562 123.329 120.718 121.453 127.262 129.093

2 10.1995 26.5144 24.9352 13.0058 12.4036 15.0432 16.0509
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4 64.2156 55.9377 58.7533 45.9566 48.366 61.7453 63.8486
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6 94.8625 96.8981 101.333 73.9107 80.364 101.887 108.126
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9 101.855 106.093 107.452 96.4464 100.539 122.555 127.149
10 73.4314 66.7323 68.2906 57.4558 58.7237 67.9526 70.7659
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15 212.84 196.821 200.663 199.395 203.439 200.473 206.024
16 167.785 158.522 162.873 151.696 155.855 165.292 171.117
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18 93.7936 91.3798 94.7603 82.5815 87.5857 92.0075 95.3353
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20 79.8097 84.1394 88.4522 70.5196 72.4289 75.0186 79.2642
21 315.129 313.147 315.67 313.605 313.849 320.927 324.82
22 145.384 142.211 149.633 140.58 151.779 146.625 155.767
23 82.0241 81.3308 84.3996 71.1907 75.3147 78.7474 83.6554
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25 166.621 167.147 171.657 151.014 155.496 159.355 162.187
26 -34.7981 -32.8775 -33.2999 -32.0599 -32.3859 -31.904 -30.8805
27 -53.9231 -50.4136 -50.8325 -54.0648 -53.8123 -50.2461 -49.1125
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29 228.294 232.829 233.128 232.176 232.982 238.833 241.106
30 141.522 135.64 140.573 133.273 138.686 147.842 155.167
31 -5.2389 2.89919 5.51593 -9.08888 -4.68715 5.12387 10.1995
32 199.354 200.058 200.191 206.53 207.841 211.373 211.716
33 346.765 332.188 336.99 320.535 325.594 376.378 383.589
34 246.838 242.629 242.666 253.017 253.668 257.954 257.849
35 -9.71568 -10.0891 -8.64605 5.67323 7.78966 4.12334 6.33199
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44 31.849 13.483 18.4284 15.2027 21.3516 27.6524 31.0058
45 3.75113 1.82937 2.01727 3.02652 3.41993 4.13641 4.1853
46 65.5461 65.5257 66.2527 57.7057 57.034 61.2975 62.3664
47 36.6235 34.9234 37.021 29.4347 31.1728 39.5039 40.6761
48 49.5159 50.8202 52.2268 50.9903 51.3485 47.8843 49.8728
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50 96.3261 89.9736 91.9754 88.4431 91.3603 111.476 114.25
51 93.5031 88.0463 90.4628 78.4018 82.4839 92.5639 94.9101
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57 433.664 405.863 423.348 411.011 426.534 421.881 442.272
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72 62.5938 65.2388 66.3712 60.8449 64.5141 73.9549 75.8212
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76 17.3911 10.2809 12.5133 12.187 14.3563 17.4533 18.7881
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 79 91.6377 110.204 109.356 110.818 111.871 105.066 108.29
 80 225.237 215.318 221.037 203.647 209.962 237.515 245.604
 81 139.537 135.279 135.627 148.792 150.21 147.742 148.335
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 83 86.8257 88.2548 88.7777 83.8835 83.9933 85.7018 86.7535

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 4 64.2156 61.2125 62.7472 54.2191 56.9322 60.4933 63.1576
 5 103.341 97.7664 103.281 93.1375 97.2013 103.348 109.735
 6 94.8625 96.0547 100.765 73.9282 80.8827 104.561 110.516
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44 31.849 14.8385 19.499 13.4936 17.9121 28.6481 31.8981
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46 65.5461 64.7409 65.2578 63.5666 63.2092 64.0696 64.9939
47 36.6235 38.3242 38.9969 20.9688 23.3642 37.971 39.1296
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 13 6.29251 10.3504 10.3315 5.82925 6.13077 5.92
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 16 167.785 157.752 161.661 154.504 161.039 164.32

17 70.6529 72.584 73.0185 72.6123 73.2474 72.65
18 93.7936 87.5008 90.498 80.4371 85.9736 87.60
19 -2.14101 -1.91144 0.132915 -6.1169 -3.77454 -4.15
20 79.8097 85.473 89.308 70.7631 74.9178 76.71
21 315.129 316.44 318.395 316.383 319.493 321.45
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24 33.4068 31.7647 32.2932 35.8699 36.6292 35.30
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27 -53.9231 -50.0496 -49.5859 -57.3095 -56.2078 -56.29
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29 228.294 234.278 235.47 225.485 228.776 231.94
30 141.522 127.173 133.034 130.266 137.641 141.24
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32 199.354 200.191 200.52 198.741 199.655 202.32
33 346.765 329.171 333.705 334.013 341.677 342.14
34 246.838 246.197 246.26 245.275 245.831 249.75
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54 -12.6939 -11.4925 -12.0054 -21.0275 -20.7661 -20.30
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 4 64.2156 62.95 51.18 57.4733 59.0379 62.2772
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6 94.8625 110.24 94.07 80.2857 99.2687 75.0118
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 17 70.6529 78.69 75.31 66.2299 69.9178 71.4284
 18 93.7936 85.85 78.99 81.0706 83.4741 81.371
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 21 315.129 316.29 312.14 312.212 307.113 305.028
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 23 82.0241 82.38 72.12 89.1875 82.1043 85.1485
 24 33.4068 41.55 41.72 29.5058 30.7268 27.8831
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 34 246.838 232.28 230.87 250.361 238.26 235.361
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 37 -34.4301 -25.22 -22.95 -35.9095 -39.2011 -38.7893
 38 -199.36 -188.01 -187.23 -221.99 -203.674 -225.46
 39 41.6549 56.91 42.58 35.4134 48.3242 25.6154
 40 25.5228 34.11 21.78 26.9906 30.4324 23.914
 41 144.978 159.72 136.93 127.445 145.028 123.903
 42 273.134 273.95 265.31 281.048 270.519 251.121

43 316.083 314.24 310.67 314.157 307.932 305.518
44 31.849 24.05 14.21 9.72213 17.3711 13.3422
45 3.75113 3.60 2.19 2.30465 2.22997 4.70483
46 65.5461 69.33 63.54 59.5213 63.6288 69.0071
47 36.6235 47.03 35.32 15.9498 36.347 23.1127
48 49.5159 68.41 63.58 58.6953 53.8821 65.4878
49 67.8673 56.70 54.60 62.5442 57.8939 51.9639
50 96.3261 86.97 90.58 82.3322 80.6943 60.6429
51 93.5031 89.54 78.37 83.5614 85.6669 85.6716
52 62.6219 56.50 52.02 58.5212 55.4659 64.5435
53 88.2948 99.40 101.23 94.6591 86.2463 86.6245
54 -12.6939 -13.80 -21.71 -34.7408 -19.1766 -22.8574
55 47.9831 44.08 41.48 28.1542 38.4895 28.6451
56 16.9482 26.53 5.22 4.28492 19.3202 -4.40284
57 433.664 400.39 396.02 426.316 407.177 420.763
58 248.457 245.93 251.72 248.817 236.041 237.739
59 65.2968 69.18 63.62 59.5754 63.7426 68.5206
60 13.2213 23.51 17.10 16.8335 18.1969 14.8751
61 49.8152 43.28 43.02 49.0892 43.9329 49.2568
62 282.122 278.88 262.93 289.374 283.179 273.665
63 96.9399 90.36 82.40 88.2096 88.7282 87.12
64 2.20915 1.86 1.62 1.26219 0.424664 3.3654
65 331.099 314.10 309.88 318.615 312.804 298.484
66 -45.3574 -36.98 -41.59 -52.2909 -44.0911 -70.3342
67 185.358 169.23 168.98 173.87 166.148 169.094
68 7.87624 21.37 9.24 7.08285 12.9512 2.92374
69 133.716 137.11 123.46 125.545 133.595 125.384
70 103.749 109.14 99.88 106.828 108.887 101.019
71 201.248 200.23 189.49 213.333 204.513 198.132
72 62.5938 62.69 59.31 62.3906 59.5282 48.791
73 95.3155 86.28 89.81 82.0563 81.0175 59.4848
74 148.937 142.03 146.22 125.96 127.285 116.863
75 -37.5031 -29.38 -34.65 -50.1723 -36.8175 -46.0623
76 17.3911 31.93 20.51 -11.0336 17.694 -3.47253
77 32.5568 39.65 34.58 34.2237 35.5315 27.8732
78 65.4965 71.80 68.36 61.3933 65.0935 66.5708
79 91.6377 102.42 85.23 93.36 100.187 90.2069

80 225.237 213.77 209.87 209.563 209.219 189.589
81 139.537 129.55 128.66 142.94 132.954 131.707
82 37.22 43.40 37.80 23.9213 35.4711 25.8027
83 86.8257 95.03 90.12 90.8688 85.9626 89.5825

6 Decomposition energies for the ORG set

No Ref CCSD(T)/cc-pV(TQ)Z CCSD/cc-pVQZ CCSD(T)/cc-pVDZ /cc-pVTZ /cc-pVQZ CCSD(T)/cc-pV(DT)Z

1 -120.44 -120.083 -124.402 -124.142 -122.787 -120.975 -122.376
2 -169.048 -170.564 -181.511 -182.409 -176.961 -172.573 -175.771
3 -18.3432 -18.3273 -18.9315 -17.8242 -18.4714 -18.3687 -18.7186
4 -117.717 -117.589 -115.428 -108.429 -115.704 -116.463 -119.358
5 6.35849 5.93245 3.58395 2.51217 4.71014 5.43158 5.63245
6 -54.4616 -56.4472 -68.3699 -66.0207 -58.4632 -57.2245 -56.3425
7 -394.886 -395.092 -413.534 -404.303 -400.475 -396.799 -399.95
8 -200.179 -200.522 -213.756 -207.355 -202.911 -201.276 -201.703
9 -108.999 -108.999 -108.719 -103.535 -108.046 -108.641 -109.606
10 37.6627 37.3231 33.6899 17.1901 31.9784 35.104 37.0385
11 -7.84241 -8.13081 -9.77896 -11.6352 -8.99844 -8.49849 -8.16884
12 17.4039 15.0767 16.435 -16.5054 7.112 12.3452 14.6596
13 44.6214 43.5658 44.5612 23.2009 34.8937 40.4621 39.223
14 -341.816 -344.539 -359.443 -364.146 -350.921 -346.488 -348.02
15 -87.749 -89.3025 -91.808 -99.6596 -92.7399 -90.4599 -90.7337
16 -131.461 -131.569 -131.456 -133.127 -133.614 -132.202 -133.99
17 181.605 181.009 183.114 161.348 172.757 177.917 177.561
18 67.8673 67.9944 67.5544 54.3327 62.85 66.0136 66.0033
19 -98.8525 -99.3983 -102.574 -101.419 -100.303 -99.6615 -100.136
20 20.4527 20.3963 20.7149 7.85788 15.0579 18.4224 17.8842
21 -10.5301 -10.7461 -12.6376 -20.7573 -13.978 -11.9276 -11.7914
22 -171.697 -171.159 -174.962 -185.645 -177.435 -173.434 -174.591
23 -207.901 -208.167 -217.35 -213.589 -208.494 -208.229 -207.813
24 -107.287 -107.459 -112.609 -121.489 -112.961 -109.374 -110.113
25 -100.917 -104.994 -112.532 -139.202 -117.338 -108.545 -111.983
26 -124.796 -123.993 -125.559 -138.31 -130.265 -126.449 -126.583
27 -125.96 -128.405 -136.062 -164.709 -140.553 -132.833 -132.327
28 -8.47506 -8.13506 -8.73482 -20.3462 -12.3128 -9.78589 -8.9629
29 -187.013 -187.218 -192.093 -189.815 -188.426 -187.496 -188.675
30 -362.354 -362.223 -371.488 -365.623 -364.921 -362.926 -365.449
31 -359.841 -359.849 -373.166 -373.526 -364.291 -361.141 -362.416
32 45.4665 42.9663 31.6346 30.763 38.9735 41.5579 40.7631
33 -146.899 -147.434 -151.211 -156.398 -148.91 -148.105 -146.756
34 -67.9433 -67.6982 -78.0251 -87.6527 -76.1936 -70.6529 -72.3879

35 275.154 271.945 271.314 224.357 254.427 266.08 264.362
 36 -25.4577 -25.6123 -27.7129 -33.4226 -28.4526 -26.4269 -27.69
 37 52.5672 51.2227 44.9634 26.1867 44.463 48.8579 49.9694
 38 241.368 240.419 248.608 210.571 229.556 236.626 236.664
 39 45.1749 44.1978 42.6644 40.3215 41.5284 42.9676 42.5576
 40 -59.449 -59.8087 -62.7662 -62.6245 -60.4869 -59.9783 -60.2077
 41 192.865 188.953 177.59 123.867 171.51 182.801 185.521
 42 -125.57 -125.205 -126.729 -132.414 -128.843 -126.712 -126.896
 43 -311.385 -312.556 -326.895 -322.392 -312.843 -312.752 -310.714
 44 62.623 61.4122 55.4733 60.8673 57.8517 59.8614 57.2767
 45 60.0493 59.6987 56.5475 40.6322 52.8163 57.1151 57.2429
 46 -64.1 -64.2059 -67.3094 -66.702 -64.7203 -64.3086 -64.3498
 47 -62.1802 -63.9518 -68.1599 -74.4213 -67.8 -65.1902 -66.0181
 48 -570.616 -570.863 -594.927 -573.447 -574.213 -571.427 -576.795
 49 -192.107 -193.943 -205.793 -208.47 -196.714 -195.206 -193.46
 50 -95.9995 -97.764 -98.9623 -104.817 -101.462 -98.8533 -100.87
 51 -37.9086 -39.2233 -45.3283 -58.1095 -46.5425 -41.6642 -43.2732
 52 107.648 102.952 106.64 73.3088 90.5877 99.1235 96.2317
 53 -81.9379 -82.11 -86.8596 -98.9365 -85.483 -83.4145 -81.2025
 54 39.5101 36.4577 33.34 -9.21771 21.7785 30.976 32.772
 55 49.1758 48.294 42.0136 32.0469 43.6422 46.5034 46.9902
 56 -6.34873 -6.63782 -7.80392 -10.0371 -7.45611 -6.95514 -6.69809
 57 47.4697 47.4902 42.2116 25.5606 39.4242 44.4796 44.8615
 58 -266.696 -265.947 -270.577 -275.761 -269.144 -267.052 -266.988
 59 25.3882 24.6663 19.0133 -3.49064 15.0954 21.2679 21.4183
 60 -114.797 -120.706 -125.001 -137.355 -128.714 -123.047 -126.186
 61 -86.2672 -87.8526 -92.1085 -103.373 -94.248 -90.0634 -91.443
 62 -192.415 -191.706 -195.081 -197.625 -194.866 -192.766 -193.882
 63 179.059 178.29 178.013 162.726 171.892 175.476 175.465
 64 -173.89 -177.232 -200.964 -201.489 -184.261 -179.816 -178.676
 65 -55.0056 -55.3343 -59.5883 -55.8546 -54.4287 -55.024 -54.3858
 66 -68.0568 -67.3193 -69.624 -73.657 -67.6562 -67.6974 -65.7775
 67 -259.774 -261.619 -281.599 -280.645 -265.804 -263.384 -261.726
 68 -116.996 -121.87 -128.69 -154.648 -134.956 -125.886 -129.204
 69 -119.366 -121.068 -131.687 -134.68 -123.709 -122.126 -120.732
 70 -225.208 -225.076 -232.187 -229.756 -227.585 -225.802 -227.299
 71 59.1866 59.5654 56.5167 34.8644 50.4349 56.2724 56.2857

72 301.652 299.695 297.357 263.21 287.588 295.132 295.633
 73 -312.657 -313.98 -333.915 -337.1 -320.576 -316 -317.121
 74 -72.233 -74.5627 -84.5471 -78.4243 -73.4 -74.2782 -72.5156
 75 -77.7889 -77.6095 -83.2449 -75.9088 -75.442 -77.4843 -74.3344
 76 -240.681 -240.78 -249.332 -243.634 -242.184 -241.061 -242.393
 77 -164.123 -163.994 -174.771 -174.182 -165.902 -164.859 -163.541
 78 180.391 177.293 180.659 154.767 169.318 174.473 174.533
 79 127.82 126.599 130.718 120.653 121.433 124.555 122.539
 80 -79.3552 -78.8042 -80.221 -86.916 -84.219 -81.0994 -81.8652
 81 -64.248 -64.3474 -67.4327 -66.737 -64.8008 -64.4301 -64.4516
 82 -42.483 -43.1146 -47.6943 -59.8271 -50.2433 -45.6423 -47.5267
 83 52.2871 52.7059 50.4595 33.5159 45.2536 49.9139 49.6597
 84 -136.63 -138.352 -151.323 -161.572 -144.823 -140.63 -140.274

No Ref LDA/TZVPP LDA/QZVP PBE-D/TZVPP PBE-D/QZVP B97-d/TZVPP B97-d/QZVP

1 -120.44 -103.869 -103.56 -111.579 -110.984 -114.652 -113.855
 2 -169.048 -189.794 -185.452 -162.864 -158.544 -147.211 -142.468
 3 -18.3432 -17.5151 -17.6001 -18.0411 -18.0539 -18.7383 -18.7134
 4 -117.717 -180.899 -179.676 -143.341 -141.969 -121.487 -119.66
 5 6.35849 26.7431 26.6883 15.1599 15.1085 5.79844 5.673
 6 -54.4616 -45.6415 -42.4317 -46.9739 -44.1663 -57.9078 -55.3566
 7 -394.886 -373.659 -373.142 -378.257 -377.224 -387.532 -386.023
 8 -200.179 -178.31 -177.705 -181.329 -180.517 -190.75 -189.678
 9 -108.999 -111.379 -111.439 -103.74 -103.732 -113.709 -113.796
 10 37.6627 56.6587 57.9454 35.0443 36.2042 20.0457 21.2855
 11 -7.84241 -7.79975 -6.72313 -7.29753 -6.34783 -7.95522 -7.01858
 12 17.4039 47.7929 51.7401 22.8215 26.9527 7.53969 11.8098
 13 44.6214 52.1156 54.4215 31.3767 34.0271 20.7308 23.2318
 14 -341.816 -371.162 -365.635 -344.912 -339.338 -336.282 -330.461
 15 -87.749 -75.151 -74.4101 -81.4917 -80.4236 -90.2575 -88.9007
 16 -131.461 -132.006 -132.212 -130.865 -130.739 -133.25 -132.884
 17 181.605 198.025 199.185 164.499 165.832 149.282 150.27
 18 67.8673 75.441 76.5437 57.86 59.0035 50.819 51.8784
 19 -98.8525 -92.3454 -92.1843 -90.7638 -90.5724 -90.5295 -90.3059
 20 20.4527 24.3951 26.1193 13.5702 15.3804 -3.62098 -2.15717
 21 -10.5301 6.4955 9.76269 -7.71298 -4.48522 -13.9849 -10.7274
 22 -171.697 -141.254 -140.286 -159.713 -158.304 -165.681 -164.039

23 -207.901 -222.637 -221.327 -194.902 -193.912 -184.402 -183.304
24 -107.287 -82.7379 -81.9476 -96.7303 -95.5784 -101.675 -100.443
25 -100.917 -86.1753 -80.7624 -97.7506 -91.7894 -99.2748 -92.7482
26 -124.796 -62.4957 -61.8221 -95.0443 -93.9136 -115.706 -114.602
27 -125.96 -70.2925 -66.7164 -111.225 -107.485 -144.145 -140.321
28 -8.47506 22.8425 23.5599 1.0795 1.9089 -11.4987 -10.8054
29 -187.013 -211.184 -209.719 -190.672 -189.278 -177.148 -175.665
30 -362.354 -359.714 -358.93 -344.074 -342.889 -337.646 -336.183
31 -359.841 -364.045 -362.332 -359.951 -358.01 -359.27 -356.92
32 45.4665 30.6647 35.8292 42.5118 47.2619 51.459 56.2746
33 -146.899 -117.27 -117.323 -122.567 -122.602 -130.937 -130.555
34 -67.9433 -23.1141 -21.7636 -49.4701 -47.7756 -61.9485 -60.2018
35 275.154 282.161 288.478 252.028 258.205 224.785 231.047
36 -25.4577 -33.8093 -33.2536 -30.5576 -29.5814 -20.3582 -19.1018
37 52.5672 53.6957 57.04 42.5908 45.5918 35.3705 38.2319
38 241.368 251.006 253.926 223.248 227.019 213.982 217.495
39 45.1749 70.1865 71.6802 60.7336 61.9 48.6199 49.7805
40 -59.449 -67.9733 -67.5553 -60.9762 -60.5352 -56.768 -56.2349
41 192.865 195.542 202.858 164.786 171.738 148.306 155.465
42 -125.57 -84.7103 -83.9748 -108.133 -107.192 -131.816 -131.079
43 -311.385 -323.125 -322.238 -296.581 -295.738 -291.664 -290.695
44 62.623 60.3023 61.9179 60.0028 61.277 59.5856 61.1679
45 60.0493 77.8845 79.1885 55.1126 56.5003 43.8863 45.208
46 -64.1 -67.8879 -67.4802 -63.2844 -62.9359 -61.1277 -60.7767
47 -62.1802 -66.8085 -62.9515 -64.2916 -60.4955 -64.4362 -60.5138
48 -570.616 -622.268 -620.436 -568.747 -566.483 -530.392 -527.598
49 -192.107 -184.634 -183.897 -185.298 -184.696 -197.388 -196.808
50 -95.9995 -95.4645 -94.4612 -96.2279 -94.8006 -96.6748 -94.9501
51 -37.9086 -51.164 -49.3601 -44.6945 -42.3535 -36.3766 -34.0863
52 107.648 142.765 149.89 108.293 116.175 92.9836 100.75
53 -81.9379 -62.192 -60.9079 -72.963 -71.6931 -78.6039 -77.4505
54 39.5101 111.231 116.075 53.9079 59.0323 19.6771 24.8245
55 49.1758 59.2862 60.1856 46.1258 46.9443 38.639 39.5855
56 -6.34873 -6.59768 -6.23841 -6.80927 -6.44912 -7.98889 -7.5925
57 47.4697 76.599 79.8245 56.1228 59.0821 43.8871 46.9061
58 -266.696 -258.518 -257.509 -255.704 -254.568 -250.04 -248.926
59 25.3882 31.203 33.7357 17.0915 19.712 12.5924 14.869

60 -114.797 -83.7919 -76.9677 -109.147 -102.442 -127.359 -120.626
 61 -86.2672 -88.9367 -87.9115 -101.824 -100.805 -99.5564 -98.5351
 62 -192.415 -175.887 -175.624 -183.339 -182.793 -184.936 -184.303
 63 179.059 192.278 191.247 178.339 177.558 165.813 165.456
 64 -173.89 -144.671 -143.728 -151.506 -150.366 -176.715 -175.362
 65 -55.0056 -61.7342 -61.5542 -51.2496 -51.1983 -47.504 -47.2094
 66 -68.0568 -70.5011 -70.6496 -65.7041 -65.9509 -61.1471 -61.3659
 67 -259.774 -261.928 -260.798 -254.345 -253.511 -265.824 -264.942
 68 -116.996 -76.189 -68.7717 -108.766 -101.239 -129.343 -121.783
 69 -119.366 -95.7004 -95.2548 -104.495 -104.069 -112.283 -111.548
 70 -225.208 -220.024 -219.548 -214.91 -214.136 -212.709 -211.719
 71 59.1866 79.6203 82.0241 52.811 55.5199 42.1017 44.5873
 72 301.652 294.029 298.347 270.309 274.573 263.415 267.77
 73 -312.657 -323.233 -320.036 -305.628 -302.174 -295.871 -292.118
 74 -72.233 -74.3517 -73.7094 -60.3529 -60.1438 -61.3196 -60.9339
 75 -77.7889 -64.2415 -65.7592 -64.5132 -66.3577 -72.1674 -74.2696
 76 -240.681 -249.454 -248.812 -235.065 -234.304 -227.284 -226.363
 77 -164.123 -165.999 -165.309 -165.19 -164.819 -164.72 -164.495
 78 180.391 199.105 204.76 164.047 169.631 148.123 153.642
 79 127.82 142.513 143.037 125.597 126.596 116.699 117.835
 80 -79.3552 -29.4294 -28.8839 -59.3013 -58.2682 -74.6462 -73.7035
 81 -64.248 -68.112 -67.717 -63.4052 -63.0533 -61.198 -60.8443
 82 -42.483 -30.8896 -30.3004 -51.0357 -50.0725 -61.5922 -60.3307
 83 52.2871 74.4158 75.927 50.8357 52.6691 41.2286 43.1022
 84 -136.63 -147.133 -143.587 -140.005 -136.853 -132.496 -129.185

No Ref TPSS-D/TZVPP TPSS-D/QZVP PBEh/TZVPP PBEh/QZVP B3-LYP-D/TZVP B3-LYP-D/QZVP

1 -120.44 -111.082 -110.673 -118.471 -117.997 -117.253 -116.7
 2 -169.048 -150.83 -147.57 -185.163 -180.877 -167.735 -163.083
 3 -18.3432 -17.638 -17.7535 -19.0141 -19.0185 -19.2445 -19.2693
 4 -117.717 -126.588 -125.84 -145.462 -144.29 -127.045 -125.733
 5 6.35849 9.24224 9.26945 11.7091 11.6887 6.6793 6.62307
 6 -54.4616 -54.9356 -52.1818 -61.322 -58.4859 -65.9505 -63.1077
 7 -394.886 -374.863 -374.616 -402.754 -401.901 -408.363 -407.505
 8 -200.179 -180.594 -180.342 -199.868 -199.093 -205.217 -204.309
 9 -108.999 -112.152 -112.19 -104.119 -104.17 -109.933 -110.053
 10 37.6627 29.6043 30.3954 27.773 28.5476 27.9162 29.0034

11 -7.84241 -7.63086 -6.69736 -10.2693 -9.33668 -9.12254 -8.1943
12 17.4039 18.0769 22.2793 29.5072 33.441 19.0011 23.0223
13 44.6214 20.5658 22.7619 36.6216 38.667 30.6375 32.9348
14 -341.816 -327.925 -323.354 -364.801 -359.526 -358.614 -353.247
15 -87.749 -78.7398 -77.9811 -84.3126 -83.2139 -92.3473 -91.2626
16 -131.461 -128.079 -128.395 -132.668 -132.662 -134.649 -134.603
17 181.605 147.655 148.829 171.882 172.78 164.615 165.596
18 67.8673 53.4844 54.3917 60.5619 61.3634 58.629 59.603
19 -98.8525 -92.0112 -92.0641 -98.9834 -98.7804 -95.9404 -95.7235
20 20.4527 -6.32868 -4.82639 17.638 18.8858 8.81918 10.2167
21 -10.5301 -9.24079 -6.10159 -13.2902 -10.1284 -12.1115 -8.88438
22 -171.697 -164.135 -163.188 -166.834 -165.781 -166.349 -165.131
23 -207.901 -189.224 -189.088 -215.84 -215.191 -201.952 -201.051
24 -107.287 -102.814 -102.021 -102.274 -101.332 -103.716 -102.629
25 -100.917 -96.0098 -90.3256 -105.009 -98.7893 -106.604 -100.263
26 -124.796 -107.632 -106.471 -94.088 -93.3361 -108.474 -107.687
27 -125.96 -122.532 -118.874 -116.077 -112.781 -137.49 -134.164
28 -8.47506 -9.61832 -8.7484 3.90466 4.42233 -5.16 -4.57995
29 -187.013 -179.8 -179.055 -199.869 -198.578 -189.993 -188.586
30 -362.354 -334.892 -334.542 -358.417 -357.398 -356.503 -355.424
31 -359.841 -345.055 -344.018 -381.723 -379.89 -374.552 -372.609
32 45.4665 54.0718 58.2982 21.6627 26.4427 39.7922 44.9309
33 -146.899 -137.823 -137.854 -132.956 -133.312 -134.358 -134.398
34 -67.9433 -59.7283 -58.1573 -62.7033 -61.1748 -66.1349 -64.4285
35 275.154 237.035 243.676 263.16 268.888 250.794 256.927
36 -25.4577 -25.1587 -24.5557 -33.536 -32.5333 -26.5723 -25.3915
37 52.5672 42.158 45.1729 35.6175 38.3958 38.5455 41.5001
38 241.368 206.18 209.447 242.718 245.478 231.377 234.423
39 45.1749 58.9172 59.9855 49.6224 51.0702 56.2248 57.3972
40 -59.449 -58.0003 -57.7863 -66.1845 -65.791 -61.2666 -60.8078
41 192.865 157.839 164.602 163.532 169.906 156.014 162.886
42 -125.57 -117.633 -116.883 -107.891 -107.302 -118.589 -118.009
43 -311.385 -295.049 -294.949 -317.789 -317.259 -314.157 -313.537
44 62.623 63.9919 65.1209 47.7024 49.0702 58.2586 59.6052
45 60.0493 45.7201 46.6944 54.067 55.1175 49.7663 51.0253
46 -64.1 -65.2166 -64.9795 -68.5792 -68.2751 -65.815 -65.5392
47 -62.1802 -59.6613 -56.0675 -71.8848 -68.0913 -68.2195 -64.4409

48 -570.616 -543.763 -543.402 -610.882 -608.801 -576.478 -574.171
49 -192.107 -196.3 -196.173 -201.026 -200.708 -208.596 -208.311
50 -95.9995 -90.3579 -89.2434 -99.8569 -98.3849 -98.041 -96.5185
51 -37.9086 -48.5801 -47.211 -48.6041 -46.6523 -47.0071 -44.8055
52 107.648 101.022 109.03 117.178 124.771 104.6 112.345
53 -81.9379 -82.1316 -81.0417 -78.9306 -77.9453 -80.1951 -79.0959
54 39.5101 37.3651 42.65 60.1707 64.7394 38.0072 42.8185
55 49.1758 42.9852 43.5445 38.0822 38.8744 37.1518 38.0906
56 -6.34873 -7.74392 -7.45064 -7.8374 -7.51701 -8.4156 -8.06802
57 47.4697 47.9667 50.9179 51.0266 53.9852 48.4793 51.4864
58 -266.696 -257.741 -257.117 -269.632 -268.782 -259.055 -258.084
59 25.3882 1.86572 3.84131 11.6476 13.6093 13.6755 15.9319
60 -114.797 -121.314 -114.536 -116.024 -109.322 -126.591 -119.898
61 -86.2672 -105.51 -104.843 -110.251 -109.308 -101.327 -100.231
62 -192.415 -183.349 -183.237 -189.487 -189.11 -187.544 -187.14
63 179.059 173.243 172.916 183.728 183.058 172.614 171.925
64 -173.89 -156.915 -156.668 -173.421 -172.122 -202.637 -201.514
65 -55.0056 -49.0238 -49.0623 -61.8924 -61.9151 -54.3236 -54.1957
66 -68.0568 -69.436 -69.8099 -72.8615 -73.2925 -66.267 -66.4657
67 -259.774 -265.933 -265.933 -278.959 -278.527 -285.232 -284.671
68 -116.996 -118.756 -111.294 -114.913 -107.705 -127.548 -120.18
69 -119.366 -115.801 -115.521 -119.277 -119.157 -119.541 -118.99
70 -225.208 -210.072 -209.78 -226.747 -226.077 -225.919 -225.169
71 59.1866 39.1847 41.5427 53.5387 55.5043 51.2449 53.5455
72 301.652 259.908 264.232 279.411 283.217 275.374 279.476
73 -312.657 -304.7 -302.168 -331.263 -328.001 -324.081 -320.622
74 -72.233 -60.5365 -60.3924 -80.9195 -80.8587 -72.2751 -71.9815
75 -77.7889 -85.217 -87.095 -74.329 -76.5141 -80.9078 -83.1086
76 -240.681 -227.943 -227.849 -248.519 -247.797 -243.553 -242.758
77 -164.123 -176.683 -176.999 -183.465 -183.509 -175.095 -174.945
78 180.391 160.687 166.483 171.738 177.138 167.041 172.67
79 127.82 122.18 123.281 133.481 134.507 125.581 126.669
80 -79.3552 -75.6706 -74.4998 -60.5499 -59.8333 -69.4368 -68.6978
81 -64.248 -65.319 -65.0715 -68.7059 -68.4039 -65.8691 -65.5931
82 -42.483 -49.7336 -49.2918 -55.1209 -54.3033 -61.9523 -61.0288
83 52.2871 40.2902 42.0586 50.0338 51.3979 48.616 50.2074
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3 -18.3432 -19.637 -19.5645 -19.8741 -19.5212 -18.5737 -18.7733
4 -117.717 -127.373 -127.935 -127.282 -124.884 -130.138 -129.351
5 6.35849 6.88905 7.05085 5.82938 5.58252 5.30149 5.46514
6 -54.4616 -60.3028 -57.1245 -64.9274 -62.377 -59.5351 -56.1496
7 -394.886 -395.669 -394.957 -386.219 -382.213 -410.851 -411.364
8 -200.179 -195.235 -194.65 -190.413 -187.555 -206.926 -206.528
9 -108.999 -110.681 -110.934 -108.115 -108.5 -109.357 -109.041
10 37.6627 33.2728 33.5603 17.0531 18.7174 32.4258 34.4995
11 -7.84241 -10.2946 -9.36069 -9.68621 -9.16232 -8.40071 -7.35521
12 17.4039 32.3763 33.5464 15.6336 18.8065 25.5771 28.8678
13 44.6214 32.4539 33.8964 32.2754 34.5484 40.3665 42.2516
14 -341.816 -354.343 -348.447 -340.625 -333.849 -357.286 -354.455
15 -87.749 -83.8118 -83.3798 -84.3174 -82.55 -88.8045 -89.3187
16 -131.461 -136.809 -137.083 -136.666 -135.135 -132.819 -133.647
17 181.605 170.451 171.163 167.06 167.44 176.865 178.025
18 67.8673 63.9503 64.267 60.6395 61.8471 68.0707 69.0976
19 -98.8525 -98.0687 -97.7119 -100.671 -99.9417 -101.367 -101.259
20 20.4527 13.6155 14.0637 14.2043 14.9948 18.9599 20.9776
21 -10.5301 -15.0436 -12.2922 -17.8063 -14.2379 -9.17385 -5.78037
22 -171.697 -163.253 -164.145 -168.757 -166.781 -166.533 -165.407
23 -207.901 -219.425 -217.914 -218.569 -216.439 -207.375 -206.728
24 -107.287 -105.683 -105.419 -110.407 -108.836 -103.497 -102.94
25 -100.917 -101.635 -97.8582 -103.486 -97.0694 -103.913 -99.1073
26 -124.796 -106.509 -107.632 -111.055 -110.378 -110.1 -108.881
27 -125.96 -116.106 -114.667 -134.44 -130.893 -130.984 -128.133
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32 45.4665 33.3894 39.2239 37.0853 41.6538 34.5371 40.1543
33 -146.899 -137.646 -138.889 -138.356 -137.743 -127.115 -126.504
34 -67.9433 -68.0914 -67.5957 -66.2805 -63.8964 -69.6554 -68.3344
35 275.154 277.9 281.32 261.281 265.945 289.166 296.084

36 -25.4577 -28.0433 -27.3021 -23.2933 -20.8719 -18.7164 -18.8551
37 52.5672 40.2413 42.9375 35.3652 38.9649 46.2133 49.3693
38 241.368 243.407 243.12 243.047 244.558 248.713 250.84
39 45.1749 38.3707 40.0425 39.0822 40.5187 44.1808 46.2678
40 -59.449 -64.232 -63.6365 -66.404 -65.169 -60.7844 -60.9376
41 192.865 185.58 190.671 171.04 179.1 192.927 199.233
42 -125.57 -118.372 -119.086 -126.107 -125.807 -122.085 -121.063
43 -311.385 -310.964 -309.644 -299.709 -295.532 -310.416 -311.471
44 62.623 42.3319 43.6944 50.8104 51.5885 52.7839 54.2002
45 60.0493 57.1044 57.8674 50.0665 51.5365 59.381 60.9903
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47 -62.1802 -65.3104 -63.0659 -75.4498 -72.0725 -71.062 -68.1245
48 -570.616 -604.756 -600.414 -569.046 -562.622 -598.822 -599.342
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50 -95.9995 -97.2818 -96.8243 -110.525 -108.566 -101.504 -102.131
51 -37.9086 -43.7646 -41.4735 -29.1917 -25.5157 -35.1459 -34.6758
52 107.648 106.937 111.655 108.984 114.686 104.334 110.285
53 -81.9379 -76.7532 -76.4232 -79.881 -78.4943 -73.0455 -71.5938
54 39.5101 59.8118 60.5615 35.977 38.3893 44.5444 49.4669
55 49.1758 45.082 45.9053 44.3816 45.9571 46.6967 47.6661
56 -6.34873 -7.11579 -6.84825 -8.93434 -8.39268 -6.19521 -5.91733
57 47.4697 46.6248 49.1498 43.0577 44.1683 49.1179 53.5328
58 -266.696 -269.7 -269.699 -267.99 -267.208 -267.511 -266.182
59 25.3882 14.8319 16.3767 10.5907 12.7546 22.1906 24.7463
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61 -86.2672 -107.213 -103.873 -102.691 -100.499 -98.3201 -98.3034
62 -192.415 -186.511 -187.293 -191.421 -190.272 -189.945 -189.913
63 179.059 186.188 183.768 178.096 177.263 185.561 183.495
64 -173.89 -185.29 -181.84 -141.381 -137.428 -188.35 -187.799
65 -55.0056 -60.047 -59.7409 -64.0071 -63.3112 -52.9714 -53.0456
66 -68.0568 -65.8484 -65.968 -59.2317 -57.5566 -48.2591 -48.2042
67 -259.774 -263.3 -261.494 -266.586 -261.873 -268.081 -267.894
68 -116.996 -127.684 -121.282 -124.435 -117.353 -127.253 -120.315
69 -119.366 -119.575 -119.62 -124.101 -122.355 -99.6435 -99.3072
70 -225.208 -228.438 -227.836 -212.898 -210.459 -228.201 -228.541
71 59.1866 56.7949 57.1314 49.9276 51.7839 58.0445 60.3799
72 301.652 285.24 287.784 287.791 291.831 302.997 305.99

73 -312.657 -316.865 -313.254 -303.323 -296.113 -314.859 -313.237
 74 -72.233 -79.0737 -77.8685 -79.3988 -77.8501 -66.6811 -66.3078
 75 -77.7889 -89.6169 -89.3197 -71.7956 -71.9742 -62.3585 -64.1807
 76 -240.681 -250.098 -248.357 -232.261 -229.854 -246.847 -247.228
 77 -164.123 -174.563 -173.844 -175.852 -172.859 -159.326 -158.5
 78 180.391 181.132 184.872 164.676 168.902 178.859 184.316
 79 127.82 129.206 128.38 129.982 129.862 126.836 126.111
 80 -79.3552 -76.2694 -77.1112 -66.214 -66.404 -73.5293 -72.9736
 81 -64.248 -67.5854 -67.3564 -67.1089 -66.0172 -64.9346 -64.6893
 82 -42.483 -52.1998 -50.8234 -50.3869 -47.6223 -47.5644 -47.6916
 83 52.2871 56.347 55.882 51.7009 52.4904 52.1246 54.1952
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 4 -117.717 -131.515 -130.437 -125.768 -124.356 -121.748 -121.772
 5 6.35849 9.13421 9.08821 6.52705 5.98948 6.05666 6.22775
 6 -54.4616 -59.3799 -56.4682 -67.8511 -65.0162 -56.6214 -53.7882
 7 -394.886 -396.333 -394.868 -393.828 -391.953 -391.478 -392.534
 8 -200.179 -193.335 -192.351 -197.691 -196.467 -191.077 -191.731
 9 -108.999 -107.708 -107.795 - - - -
 10 37.6627 27.8531 29.1817 28.2346 29.4168 36.6653 37.4452
 11 -7.84241 -9.96453 -9.13031 -9.09182 -8.06649 -6.59435 -5.82608
 12 17.4039 18.5304 22.1791 18.328 22.4014 23.7625 27.1526
 13 44.6214 31.3644 33.5134 36.3622 37.3121 37.6116 39.3408
 14 -341.816 -349.947 -345.005 -347.142 -341.101 -334.351 -332.44
 15 -87.749 -85.5789 -84.6107 -85.5734 -84.0761 -80.9326 -81.2784
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 17 181.605 167.085 167.889 175.079 174.431 173.823 174.907
 18 67.8673 60.2691 61.3308 65.6371 66.131 67.771 68.2947
 19 -98.8525 -95.5215 -95.306 -97.9718 -97.8449 -97.3762 -97.767
 20 20.4527 12.1863 13.4226 18.0016 17.6842 15.523 17.399
 21 -10.5301 -15.2237 -12.1766 -9.38063 -6.28989 -8.39309 -5.37061
 22 -171.697 -169.012 -167.4 -163.099 -162.519 -162.204 -161.722
 23 -207.901 -209.144 -208.167 -221.332 -218.709 -199.045 -199.189

24 -107.287 -104.566 -103.28 -106.41 -105.673 -102.282 -101.987
 25 -100.917 -103.79 -97.9516 -103.885 -98.0087 -100.941 -96.5264
 26 -124.796 -110.868 -109.485 -110.239 -110.311 -114.75 -113.403
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 35 275.154 261.821 267.197 - - -
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 37 52.5672 39.8799 42.8058 37.7333 40.917 45.7135 48.446
 38 241.368 232.585 235.16 244.985 245.754 241.749 243.958
 39 45.1749 44.4324 45.7155 40.8969 43.246 45.7233 47.6192
 40 -59.449 -62.4574 -62.0109 -65.2222 -64.2531 -58.3036 -58.5812
 41 192.865 171.077 177.391 166.342 174.475 188.254 193.644
 42 -125.57 -120.576 -119.832 -122.553 -122.828 -122.047 -121.094
 43 -311.385 -306.022 -305.146 -316.672 -312.721 -301.376 -302.133
 44 62.623 49.889 50.9335 51.7086 52.7172 58.3643 58.6143
 45 60.0493 53.1534 54.4419 56.9009 57.2275 61.0273 61.7018
 46 -64.1 -66.106 -65.6779 -70.1145 -69.0648 -64.7736 -64.5047
 47 -62.1802 -70.7151 -67.1258 -69.606 -65.1845 -63.9877 -61.4167
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 52 107.648 103.496 110.293 115.37 120.45 100.44 106.822
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 54 39.5101 40.275 44.9826 46.8739 49.5262 42.8503 47.6234
 55 49.1758 45.135 46.0514 44.1179 45.386 50.2021 50.1552
 56 -6.34873 -7.93729 -7.62759 -9.88967 -9.42121 -6.19798 -5.97785
 57 47.4697 42.7905 45.8839 48.5618 51.2818 46.222 49.8442
 58 -266.696 -265.361 -264.284 -261.129 -261.396 -265.314 -264.587
 59 25.3882 14.8738 16.9296 13.752 14.8837 21.0636 22.5814
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 62 -192.415 -190.377 -189.607 -187.851 -187.459 -186.309 -186.541
 63 179.059 177.426 176.319 173.037 172.082 182.492 181.085
 64 -173.89 -160.556 -159.338 -174.37 -171.621 -159.052 -159.952
 65 -55.0056 -58.2283 -58.0462 -61.3114 -60.6509 -49.9682 -50.4043
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 69 -119.366 -116.208 -115.488 -125.652 -123.784 -103.58 -104.116
 70 -225.208 -221.651 -220.649 -218.102 -216.859 -218.083 -218.781
 71 59.1866 50.0946 52.3125 56.774 57.5312 55.6855 57.4193
 72 301.652 279.998 283.088 282.423 285.699 294.351 296.89
 73 -312.657 -314.161 -310.576 -321.687 -316.446 -305.56 -304.713
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 77 -164.123 -173.906 -173.071 -179.157 -177.196 -159.899 -160.067
 78 180.391 168.351 173.267 179.544 183.547 178.246 183.335
 79 127.82 126.777 127.136 131.207 130.657 126.36 126.036
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 82 -42.483 -52.3199 -51.1585 -46.5971 -45.3862 -39.0178 -39.6577
 83 52.2871 47.6647 49.1367 57.2023 57.4448 51.1277 52.4678
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No Ref MPW1B95/TZVPP MPW1B95/QZVP B2-PLYP-D/TZVPP B2-PLYP-D/QZVP B2GP-PLYP-D/QZVP

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 4 -117.717 -136.795 -135.796 -124.025 -124.245 -125.36
 5 6.35849 10.3898 10.3675 5.88222 6.1816 5.98
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 7 -394.886 -393.78 -392.351 -405.655 -404.466 -407.41
 8 -200.179 -191.422 -190.47 -204.274 -203.401 -205.81
 9 -108.999 -107.136 -107.229 -108.107 -108.469 -107.86
 10 37.6627 26.9454 28.1655 26.068 28.6363 28.91
 11 -7.84241 -10.2749 -9.43221 -9.04311 -8.03156 -8.26

12 17.4039 21.064 24.6516 13.8371 18.165 20.13
13 44.6214 33.0368 35.0391 32.2835 35.4425 38.33
14 -341.816 -350.596 -345.678 -354.309 -350.457 -353.32
15 -87.749 -82.7381 -81.7706 -92.9275 -92.2218 -91.75
16 -131.461 -136.053 -135.915 -135.487 -135.53 -135.44
17 181.605 169.417 170.138 168.267 170.399 174.82
18 67.8673 61.0321 61.9891 60.1365 61.9852 64.19
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21 -10.5301 -15.1364 -12.1063 -15.212 -11.1205 -10.97
22 -171.697 -168.545 -167.04 -174.75 -172.441 -173.82
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25 -100.917 -102.67 -96.8779 -108.562 -102.543 -103.17
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33 -146.899 -137.544 -137.287 -143.339 -142.248 -145.10
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35 275.154 265.075 270.308 257.589 264.991 271.89
36 -25.4577 -25.9384 -24.9307 -26.6108 -25.4598 -25.73
37 52.5672 38.2885 41.1659 42.2175 45.8951 45.91
38 241.368 235.764 238.126 232.242 235.929 242.43
39 45.1749 44.4549 45.8534 48.2734 50.5639 49.46
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41 192.865 173.355 179.519 165.602 173.878 178.10
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44 62.623 48.5496 49.5733 57.8363 59.7443 58.90
45 60.0493 54.9009 56.1017 50.8088 53.283 55.07
46 -64.1 -67.0241 -66.5799 -65.7236 -65.4326 -66.64
47 -62.1802 -71.6693 -68.0587 -69.5384 -66.1874 -67.22
48 -570.616 -584.819 -582.646 -576.346 -575.257 -585.00

49 -192.107 -191.158 -190.462 -203.345 -202.172 -203.00
50 -95.9995 -98.4972 -97.2089 -101.278 -100.296 -100.97
51 -37.9086 -36.0072 -34.2865 -43.5469 -40.9767 -40.32
52 107.648 107.744 114.426 100.874 108.371 112.00
53 -81.9379 -79.0238 -77.796 -83.9009 -81.9518 -83.21
54 39.5101 46.0673 50.5902 31.443 37.9329 41.07
55 49.1758 45.3652 46.2297 40.2258 41.9916 42.33
56 -6.34873 -7.71528 -7.41217 -7.79054 -7.43085 -7.35
57 47.4697 43.2491 46.3642 45.774 50.9413 51.79
58 -266.696 -267.818 -266.798 -267.89 -266.674 -270.83
59 25.3882 14.7458 16.6678 14.3939 17.8322 18.18
60 -114.797 -123.057 -116.478 -129.089 -121.96 -122.19
61 -86.2672 -101.25 -100.568 -98.2244 -96.7644 -96.53
62 -192.415 -190.041 -189.315 -193.567 -192.644 -194.34
63 179.059 180.255 179.076 174.108 173.63 176.72
64 -173.89 -152.514 -151.211 -190.431 -188.49 -188.15
65 -55.0056 -59.0959 -58.9192 -55.7857 -55.1763 -56.90
66 -68.0568 -65.503 -65.4197 -67.3946 -67.05 -68.07
67 -259.774 -264.796 -263.765 -277.295 -275.582 -278.13
68 -116.996 -122.295 -115.066 -130.149 -121.659 -121.47
69 -119.366 -115.281 -114.68 -121.898 -120.122 -122.40
70 -225.208 -221.697 -220.744 -227.869 -227.055 -229.37
71 59.1866 51.096 53.1289 50.0893 53.8079 55.57
72 301.652 281.892 284.791 285.922 290.416 296.42
73 -312.657 -315.164 -311.644 -320.125 -316.554 -320.82
74 -72.233 -71.9309 -71.5605 -73.4247 -72.7349 -76.27
75 -77.7889 -71.9083 -73.6797 -80.5303 -82.0173 -83.31
76 -240.681 -240.422 -239.666 -242.152 -241.805 -244.47
77 -164.123 -175.386 -174.614 -173.489 -172.146 -174.69
78 180.391 170.051 174.892 166.135 172.712 176.68
79 127.82 129.155 129.41 125.085 125.702 128.77
80 -79.3552 -68.9602 -68.4396 -78.5023 -76.7939 -77.17
81 -64.248 -67.1768 -66.7512 -65.7899 -65.5168 -66.74
82 -42.483 -49.2614 -48.1694 -57.1893 -55.6005 -53.43
83 52.2871 48.1897 49.5328 46.8658 49.6629 51.00
84 -136.63 -148.889 -146.288 -144.862 -141.496 -144.76

No Ref BP86/QZVP B-LYP/QZVP BH-LYP/QZVP B3PW91/QZVP M06-L/QZVP

1 -120.44 -110.92 -112.56 -124.162 -118.482 -127.801
2 -169.048 -154.72 -144.85 -186.936 -174.225 -183.199
3 -18.3432 -18.11 -18.99 -20.43 -19.3864 -21.869
4 -117.717 -135.28 -119.35 -127.513 -136.763 -145.263
5 6.35849 12.29 6.91 2.73827 8.61107 10.3763
6 -54.4616 -45.91 -53.22 -80.9052 -58.6217 -69.4893
7 -394.886 -378.64 -388.68 -436.728 -399.543 -407.664
8 -200.179 -181.96 -190.75 -226.127 -198.281 -202.965
9 -108.999 -112.21 -109.64 -108.756 -108.308 -
10 37.6627 35.42 32.84 23.3639 27.1303 10.7208
11 -7.84241 -6.69 -7.15 -11.8238 -10.0475 -11.105
12 17.4039 24.49 13.17 31.7491 25.5035 17.9954
13 44.6214 31.00 25.65 38.7317 33.2542 23.7415
14 -341.816 -335.41 -336.05 -377.352 -353.704 -358.586
15 -87.749 -82.44 -91.70 -95.0202 -86.4021 -87.9199
16 -131.461 -130.21 -133.89 -136.027 -134.268 -145.241
17 181.605 159.49 153.80 173.715 164.194 165.167
18 67.8673 56.70 54.60 62.5442 57.8939 51.9639
19 -98.8525 -89.81 -88.64 -103.74 -96.5529 -102.867
20 20.4527 3.83 4.10 15.8226 10.4975 9.27422
21 -10.5301 -4.44 -9.22 -14.7546 -13.5193 -18.6915
22 -171.697 -157.53 -160.94 -170.486 -167.264 -187.647
23 -207.901 -188.87 -184.36 -226.272 -209.938 -236.954
24 -107.287 -96.12 -99.74 -108.872 -102.385 -117.05
25 -100.917 -92.31 -96.89 -106.604 -99.519 -106.745
26 -124.796 -98.37 -113.04 -105.242 -102.284 -113.711
27 -125.96 -114.76 -136.93 -138.825 -123.306 -130.914
28 -8.47506 -1.87 -9.91 -1.56789 -1.37566 -4.65612
29 -187.013 -185.67 -179.72 -199.484 -193.955 -195.799
30 -362.354 -340.31 -341.46 -371.029 -353.431 -361.899
31 -359.841 -354.43 -354.77 -394.594 -374.955 -388.469
32 45.4665 50.96 57.09 19.6396 31.175 30.3688
33 -146.899 -123.29 -127.94 -146.573 -135.308 -162.835
34 -67.9433 -51.59 -57.19 -79.0182 -63.0423 -69.3822
35 275.154 247.66 241.61 271.773 257.517 -
36 -25.4577 -27.56 -22.30 -27.6372 -29.8222 -42.5973

37 52.5672 44.48 45.19 34.362 37.968 35.8059
38 241.368 221.93 213.92 255.917 234.98 229.835
39 45.1749 57.92 55.99 44.7897 42.7012 43.6706
40 -59.449 -58.84 -56.12 -66.8608 -63.6186 -71.1234
41 192.865 169.40 160.17 161.038 167.263 147.246
42 -125.57 -112.37 -121.36 -116.943 -115.351 -124.838
43 -311.385 -293.68 -293.02 -338.344 -311.445 -
44 62.623 60.06 62.29 46.3961 45.5332 47.9092
45 60.0493 54.31 48.56 49.7346 51.8637 39.5058
46 -64.1 -62.47 -60.58 -71.7127 -66.6595 -73.443
47 -62.1802 -60.35 -61.54 -72.8658 -69.4583 -70.9494
48 -570.616 -554.95 -531.60 -620.887 -587.433 -597.531
49 -192.107 -186.61 -196.74 -228.895 -200.207 -222.563
50 -95.9995 -94.16 -94.97 -99.54 -98.9463 -105.782
51 -37.9086 -41.88 -40.60 -51.0704 -43.8626 -59.1626
52 107.648 110.32 97.11 123.611 113.2 125.725
53 -81.9379 -71.92 -75.10 -85.3678 -78.5644 -92.1739
54 39.5101 51.08 29.09 51.8331 50.0922 47.3535
55 49.1758 44.95 42.58 29.1094 38.7179 29.5435
56 -6.34873 -6.61 -7.70 -9.47408 -7.83757 -11.5108
57 47.4697 55.53 48.39 45.7718 47.4448 52.5995
58 -266.696 -251.77 -246.86 -270.657 -266.179 -274.528
59 25.3882 18.47 18.76 8.78226 13.0158 -3.46481
60 -114.797 -107.67 -119.42 -127.712 -115.918 -115.33
61 -86.2672 -100.05 -95.09 -109.922 -107.123 -114.146
62 -192.415 -181.92 -183.49 -192.983 -189.74 -201.463
63 179.059 172.58 162.02 178.329 175.046 177.302
64 -173.89 -159.06 -186.29 -229.8 -174.992 -165.723
65 -55.0056 -48.38 -47.70 -67.7087 -59.9894 -69.3647
66 -68.0568 -64.90 -60.74 -73.5027 -71.7321 -92.4469
67 -259.774 -254.50 -263.23 -314.846 -274.142 -307.859
68 -116.996 -106.36 -120.23 -126.274 -114.6 -114.224
69 -119.366 -103.38 -108.62 -136.894 -118.485 -148.956
70 -225.208 -214.43 -215.30 -239.209 -224.003 -225.623
71 59.1866 52.60 49.29 53.8861 50.9971 42.1302
72 301.652 271.82 267.13 289.095 276.892 274.84
73 -312.657 -298.27 -296.58 -350.305 -318.766 -344.241

74 -72.233 -58.23 -58.66 -97.6818 -78.4642 -91.3872
75 -77.7889 -69.60 -76.10 -95.8846 -78.3408 -95.3538
76 -240.681 -231.98 -229.82 -258.866 -242.734 -245.015
77 -164.123 -162.14 -159.24 -196.923 -178.266 -211.877
78 180.391 165.55 159.01 183.265 167.767 176.629
79 127.82 121.57 114.69 136.874 125.449 138.777
80 -79.3552 -64.80 -73.42 -67.8921 -69.0073 -64.3914
81 -64.248 -62.51 -60.57 -71.8036 -66.6919 -73.7347
82 -42.483 -52.73 -61.04 -66.0091 -56.9329 -64.4082
83 52.2871 49.81 47.03 49.978 47.348 45.4291
84 -136.63 -132.98 -125.41 -166.385 -150.868 -172.987

7 Atomisation reference energies for the 931 set

No Ref

1 654.67
2 511.98
3 685.24
4 451.343
5 508.332
6 586.088
7 448.528
8 592.61
9 494.439
10 457.555
11 387.23
12 530.566
13 506.685
14 422.293
15 446.953
16 511.2
17 519.632
18 441.043
19 429.95
20 485.927
21 570.955
22 749.977
23 488.335

24 430.972
25 564.691
26 477.445
27 565.582
28 572.985
29 584.064
30 567.018
31 479.13
32 564.48
33 620.411
34 563.134
35 493.206
36 532.547
37 452.086
38 479.23
39 654.51
40 638.847
41 521.241
42 502.36
43 571.432
44 567.703
45 436.758
46 501.588
47 508.79
48 415.554
49 624.113
50 633.103
51 465.986
52 439.229
53 454.948
54 637.906
55 676.316
56 474.171
57 533.109
58 475.473
59 501.338
60 519.167

61 438.065
62 665.422
63 467.705
64 376.105
65 501.676
66 674.121
67 477.705
68 496.502
69 621.567
70 611.823
71 562.838
72 564.721
73 632.597
74 505.656
75 593.655
76 564.64
77 630.425
78 514.475
79 629.736
80 534.686
81 472.426
82 616.965
83 434.209

8 Atomisation reference energies for the ORG set

No Ref

1 731.22
2 707.177
3 713.541
4 678.14
5 506.751
6 529.177
7 737.858
8 753.497
9 530.566
10 676.27
11 518.89

12 562.646
13 609.531
14 653.425
15 691.973
16 663.195
17 531.204
18 624.113
19 695.177
20 453.586
21 526.581
22 710.705
23 628.698
24 737.797
25 649.801
26 641.78
27 582.647
28 548.884
29 633.356
30 757.082
31 707.86
32 649.984
33 565.933
34 615.764
35 544.073
36 683.567
37 495.802
38 532.419
39 406.462
40 667.196
41 747.866
42 581.837
43 632.333
44 536.916
45 682.349
46 573.143
47 499.605
48 892.147

49 685.05
50 687.848
51 739.487
52 460.446
53 674.418
54 555.989
55 676.913
56 630.894
57 457.187
58 658.093
59 665.019
60 524.708
61 690.906
62 695.233
63 501.412
64 773.194
65 607.289
66 567.626
67 713.363
68 583.165
69 726.519
70 678.837
71 679.329
72 596.187
73 738.964
74 597.759
75 478.619
76 784.841
77 707.114
78 479.186
79 455.943
80 492.593
81 572.995
82 712.798
83 675.879
84 764.089