

Supporting information

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Example of input files for small model system

Structure 1 with HBandHLYP functional, and a locally dense combination of the basis sets QZ4P, TZ2P and DZP:

\$AMSBIN/ams <<eor

System
atoms

Cd	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	3.73505939
S	1.11073907	0.00000000	2.25813240
C	-2.09897131	-1.72235683	-2.28248921
S	-0.51656264	-0.83728367	-2.19705366
C	3.28454244	-0.51367097	-1.26517557
O	2.68057970	0.15906085	-0.45925529
C	1.59430961	2.84431269	-0.88434308
O	0.72372314	2.49049666	-0.10925697
N	2.76878430	3.42724499	-0.43360860
H	0.40442242	0.79024465	4.37823633
H	-0.47590642	0.74121093	3.12758970
H	-2.97195791	-1.01680177	-2.34880530
H	-2.11276955	-2.12865122	-3.32176235
H	3.49494154	3.72107377	-1.09838042
H	1.44272158	3.00290627	-1.93161053
H	3.08794567	3.21210596	0.48934927
H	-0.07577403	-0.95556336	4.21051387
H	-2.26065455	-2.48636997	-1.55102325
N	4.51822804	-0.18726565	-1.99481889
H	4.81705331	-0.98529847	-2.51812291
H	4.98736921	0.46771644	-1.79258322
H	2.87731797	-1.39205508	-1.72070776

end
end

Task SinglePoint

Engine ADF

title Structure 1 t479 step10000 small spin-orbit ZORA

basis

PerAtomType
core None
type ZORA/QZ4P
Symbol Cd

end

PerAtomType
core None
type ZORA/QZ4P
Symbol S

end

PerAtomType
core None
type ZORA/DZP
Symbol N

end

PerAtomType
core None
type ZORA/QZ4P
Symbol O

end

PerAtomType
core None
type ZORA/TZ2P
Symbol C

end

PerAtomType
core None
type ZORA/DZP
Symbol H

end

end

numericalquality verygood

symmetry nosym

relativity

level spin-orbit
formalism ZORA

end

save TAPE10

xc

hybrid BHandHLYP

end

NUCLEARMODEL gaussian
QTENS

EndEngine
eor

Structure 2 with HBandHLYP functional, and a locally dense combination of the basis sets
QZ4P, TZ2P and DZP:
\$AMSBIN/ams <<eor

System

atoms

Cd	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	3.49761130
S	1.22646584	0.00000000	2.11753239
C	-1.69513494	-2.54621089	-1.85978151
S	-1.73368164	-0.70396016	-1.41262011
C	2.82771104	-0.40947822	-1.86639394
O	2.13400366	0.18329479	-1.12217105
H	0.23603535	0.97929655	4.00920782
H	-1.05096799	0.00843125	3.10922821
H	-2.51071232	-2.64862394	-2.57597377
H	-0.68912023	-2.78298723	-2.34507942
N	4.07608533	0.11180972	-2.44147699
H	4.48126913	-0.57907832	-3.04022552
H	4.23705717	1.03910932	-2.10353687
H	-1.82743937	-3.14500016	-0.98294233
H	0.25909266	-0.80342305	4.15509316
H	2.53538196	-1.39844982	-2.15166381

end
end

Task SinglePoint
Engine ADF

Title Structure 2 t480 step10000 small spin-orbit ZORA

basis

PerAtomType

core None

type ZORA/QZ4P

Symbol Cd

end

PerAtomType

```

core None
type ZORA/QZ4P
Symbol S
end
PerAtomType
core None
type ZORA/DZP
Symbol N
end
PerAtomType
core None
type ZORA/QZ4P
Symbol O
end
PerAtomType
core None
type ZORA/TZ2P
Symbol C
end
PerAtomType
core None
type ZORA/DZP
Symbol H
end
end

```

```

numericalquality verygood
symmetry nosym
relativity
level spin-orbit
formalism ZORA
end
save TAPE10
xc
hybrid BHandHLYP
end
NUCLEARMODEL gaussian
QTENS
EndEngine
eor

```

Structure 3 with HBandHLYP functional, and a locally dense combination of the basis sets QZ4P, TZ2P and DZP:
 \$AMSBIN/ams <<eor

System
atoms

Cd	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	3.67151254
S	1.23684272	0.00000000	2.21869338
C	-1.89620072	-2.61250042	-1.54030846
S	-1.74157906	-0.76565991	-1.44636652
C	2.66343291	-1.24703114	-1.80031321
O	2.07484453	-0.25583512	-1.39896508
C	1.49497467	2.59745234	-1.52507685
O	0.64559683	2.01395985	-0.87664292
N	2.83966797	2.64049675	-1.03628565
H	0.09731910	1.02153077	4.14891435
H	-1.04532577	-0.17473322	3.35914584
H	-2.81130704	-2.71098074	-2.16233969
H	-0.99620262	-3.06514294	-1.92080873
H	2.99067160	2.04792716	-0.24504663
H	3.72845971	-1.07102171	-2.04300625
H	-2.11091341	-3.07577590	-0.60000304
H	0.19040271	-0.72776936	4.43243210
H	3.46315351	3.24579796	-1.53113537
H	1.28202861	3.09817871	-2.44639495
N	2.03783025	-2.57598571	-1.85863174
H	1.10105702	-2.51886248	-1.51338853
H	2.69088369	-3.23580889	-2.23032323

end
end

Task SinglePoint

Engine ADF

Title Structure 3 t482 step10000 small spin-orbit ZORA

basis

PerAtomType

core None

type ZORA/QZ4P

Symbol Cd

end

PerAtomType

core None

type ZORA/QZ4P

Symbol S

end

PerAtomType

```
core None
type ZORA/DZP
Symbol N
end
PerAtomType
core None
type ZORA/QZ4P
Symbol O
end
PerAtomType
core None
type ZORA/TZ2P
Symbol C
end
PerAtomType
core None
type ZORA/DZP
Symbol H
end
end
```

```
numericalquality verygood
symmetry nosym
```

```
relativity
level spin-orbit
formalism ZORA
end
save TAPE10
xc
hybrid BHandHLYP
end
```

```
NUCLEARMODEL gaussian
QTENS
```

```
EndEngine
eor
```

Structure 4 with HBandHLYP functional, and a locally dense combination of the basis sets QZ4P, TZ2P and DZP:
\$AMSBIN/ams <<eor

```
System
atoms
```

Cd	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	3.73505939
S	1.11073907	0.00000000	2.25813240
C	-2.09897131	-1.72235683	-2.28248921
S	-0.51656264	-0.83728367	-2.19705366
C	3.28454244	-0.51367097	-1.26517557
O	2.68057970	0.15906085	-0.45925529
C	1.59430961	2.84431269	-0.88434308
O	0.72372314	2.49049666	-0.10925697
N	2.76878430	3.42724499	-0.43360860
H	0.40442242	0.79024465	4.37823633
H	-0.47590642	0.74121093	3.12758970
H	-2.97195791	-1.01680177	-2.34880530
H	-2.11276955	-2.12865122	-3.32176235
H	3.49494154	3.72107377	-1.09838042
H	1.44272158	3.00290627	-1.93161053
H	3.08794567	3.21210596	0.48934927
H	-0.07577403	-0.95556336	4.21051387
H	-2.26065455	-2.48636997	-1.55102325
N	4.51822804	-0.18726565	-1.99481889
H	4.81705331	-0.98529847	-2.51812291
H	4.98736921	0.46771644	-1.79258322
H	2.87731797	-1.39205508	-1.72070776

end
end

Task SinglePoint

Engine ADF

title t482 step10000 small spin-orbit ZORA

basis

PerAtomType

core None

type ZORA/QZ4P

Symbol Cd

end

PerAtomType

core None

type ZORA/QZ4P

Symbol S

end

PerAtomType

core None

type ZORA/DZP


```
Symbol N
end
PerAtomType
core None
type ZORA/QZ4P
Symbol O
end
PerAtomType
core None
type ZORA/TZ2P
Symbol C
end
PerAtomType
core None
type ZORA/DZP
Symbol H
end
end
```

numericalquality verygood

symmetry nosym

```
relativity
level spin-orbit
formalism ZORA
end
```

save TAPE10

```
xc
hybrid BHandHLYP
end
```

NUCLEARMODEL gaussian

QTENS

EndEngine

eor

Structure 5 with HBandHLYP functional, and a locally dense combination of the basis sets QZ4P, TZ2P and DZP:
\$AMSBIN/ams <<eor

System

atoms

Cd	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	3.35848764
S	1.24584318	0.00000000	2.07840457
C	-2.14890533	1.19956578	-2.39816173
S	-1.88770129	-0.19548680	-1.18756801
C	1.48648648	3.22053201	-0.35459524
O	1.13313722	2.08436175	-0.23748292
N	2.70991945	3.72675491	-0.72093352
C	1.30478510	-3.03074356	-1.40102809
O	1.41660471	-1.89707172	-0.91488280
N	1.29093174	-4.21087914	-0.67958243
H	-0.74581932	-0.83176383	3.26484918
H	0.77580078	-0.26288104	4.12856145
H	-1.20524794	1.27112646	-3.06514391
H	-3.00786219	0.94589464	-2.95217930
H	2.79097990	4.79275424	-0.79592951
H	1.18107346	-5.05170161	-1.20962841
H	1.30618484	-3.13364463	-2.46606771
H	3.44134762	3.24370836	-1.20226383
H	0.76917334	3.97886415	-0.11944793
H	-0.49763250	0.89736551	3.66179778
H	-2.33523043	2.16501988	-1.97616489
H	1.43204052	-4.21791105	0.31038668

end

end

Task SinglePoint

Engine ADF

title t483 step7000 small spin-orbit ZORA

basis

PerAtomType

core None

type ZORA/QZ4P

Symbol Cd

end

PerAtomType

core None

type ZORA/QZ4P

Symbol S

end

```
PerAtomType
  core None
  type ZORA/DZP
  Symbol N
end
PerAtomType
  core None
  type ZORA/QZ4P
  Symbol O
end
PerAtomType
  core None
  type ZORA/TZ2P
  Symbol C
end
PerAtomType
  core None
  type ZORA/DZP
  Symbol H
end
end
```

numericalquality verygood

symmetry nosym

```
relativity
  level spin-orbit
  formalism ZORA
end
```

save TAPE10

```
xc
  hybrid BHandHLYP
end
```

NUCLEARMODEL gaussian

QTENS

EndEngine

eor

Structure 6 with HBandHLYP functional, and a locally dense combination of the basis sets QZ4P, TZ2P and DZP:
\$AMSBIN/ams <<eor

```
System
atoms
Cd      0.00000000  0.00000000  0.00000000
C       0.00000000  0.00000000  3.23916863
S       1.35541681  0.00000000  1.98065071
C      -2.07637286  1.47793489 -2.21698264
S      -2.12631096  0.03767796 -1.10562796
C       2.17557528  2.35030478 -0.96804745
O       1.52194398  1.36123322 -1.27614987
N       3.51295548  2.43562213 -1.18415938
C      -1.34101343 -3.71920072 -0.79056241
O      -0.67898254 -2.68306429 -0.51602626
N      -1.76220419 -4.64340864  0.13658758
H      -0.85819448 -0.57393404  2.88085355
H       0.31392835 -0.64521130  4.07288899
H      -1.37434816  1.26084732 -3.09170112
H      -3.07055200  1.55135195 -2.59413938
H       4.04342311  3.12188200 -0.66883581
H      -2.49442767 -5.24123354 -0.30325489
H      -1.90496808  2.46342972 -1.83708746
H       1.79543329  3.27786978 -0.59386132
H       4.09902491  1.83046539 -1.72296169
H      -1.49050373 -4.10031870 -1.77914813
H      -0.27028772  0.93907388  3.67504105
H      -1.73116194 -4.59490310  1.13492799
end
end
```

Task SinglePoint

Engine ADF

title t483 step10000 small spin-orbit ZORA

```
basis
  PerAtomType
  core None
  type ZORA/QZ4P
  Symbol Cd
end
PerAtomType
  core None
```

type ZORA/QZ4P
Symbol S

end

PerAtomType

core None

type ZORA/DZP

Symbol N

end

PerAtomType

core None

type ZORA/QZ4P

Symbol O

end

PerAtomType

core None

type ZORA/TZ2P

Symbol C

end

PerAtomType

core None

type ZORA/DZP

Symbol H

end

end

numericalquality verygood

symmetry nosym

relativity

level spin-orbit

formalism ZORA

end

save TAPE10

xc

hybrid BHandHLYP

end

NUCLEARMODEL gaussian

QTENS

EndEngine

eor

Structure 7 with HBandHLYP functional, and a locally dense combination of the basis sets QZ4P, TZ2P and DZP:

\$AMSBIN/ams <<eor

System

atoms

Cd	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	3.34955344
O	0.55833902	0.00000000	2.26312380
C	2.07672960	-2.44358244	1.23467238
O	1.65952283	-1.69884646	0.38377056
N	3.18309703	-2.18404648	1.96929595
H	3.49989422	-2.92019562	2.60396080
C	1.52468111	1.90617629	-2.40766339
S	1.77809649	1.67365128	-0.52074584
H	2.46211159	1.61395503	-2.89955214
H	0.77058924	1.24274265	-2.74919716
C	-3.22581227	-0.92072477	0.45980042
S	-1.84185181	-1.31583435	-0.62565396
H	-3.99922366	-1.68823472	0.32337525
H	-3.02774382	-0.91518565	1.58887430
O	-1.30700075	2.22597952	-0.05745454
H	-1.29594222	2.38240339	-0.99324338
H	-1.47801036	3.07307612	0.22177087
H	-3.58008564	0.01861583	0.08962528
H	1.30701311	2.92528489	-2.65043552
H	3.83216698	-1.43145183	1.85834784
H	1.72263290	-3.42644221	1.46597782
N	0.82500049	-0.17328427	4.55381534
H	0.54134734	-0.19972491	5.53445334
H	1.82750192	-0.28372741	4.39380815
H	-1.04291543	0.22864058	3.41991613

end

end

Task SinglePoint

Engine ADF

title t682 step12000 small spin-orbit ZORA

basis

PerAtomType

core None

```
type ZORA/QZ4P
Symbol Cd
end
PerAtomType
core None
type ZORA/QZ4P
Symbol S
end
PerAtomType
core None
type ZORA/DZP
Symbol N
end
PerAtomType
core None
type ZORA/QZ4P
Symbol O
end
PerAtomType
core None
type ZORA/TZ2P
Symbol C
end
PerAtomType
core None
type ZORA/DZP
Symbol H
end
end
```

numericalquality verygood

symmetry nosym

```
relativity
level spin-orbit
formalism ZORA
end
```

save TAPE10

```
xc
hybrid BHandHLYP
end
```

NUCLEARMODEL gaussian

QTENS

EndEngine

eor

Example of input files for large model system

Structure 1 with HBandHLYP functional, and a locally dense combination of the basis sets QZ4P, TZ2P and DZP:

!/bin/bash

\$AMSBIN/ams <<eor

System

atoms

Cd	-14.32111401	13.66765794	-0.43349291
N	-12.48399891	18.62699857	0.65699996
C	-13.62059489	19.16674759	-0.04271364
C	-13.80051977	18.58008552	-1.43006547
O	-14.64829097	19.02660790	-2.19822306
C	-13.56014557	20.68509873	-0.06475369
O	-12.85146622	21.15191842	1.03377362
H	-11.67188576	19.05662253	0.28311641
H	-14.59469568	18.92788377	0.51065550
H	-14.55171434	21.16021390	-0.16184557
H	-13.07800274	20.96789327	-1.06116562
H	-11.97130630	21.44531289	0.75708105
N	-9.51499938	15.38599878	-2.10199982
C	-10.43855648	14.82335050	-1.12779342
C	-11.72811910	14.67037564	-2.03113000
O	-12.91969586	14.78242663	-1.65432692
C	-10.69219579	15.79291009	0.15243776
C	-11.55397331	14.94531049	1.16168956
C	-9.41216554	16.23619693	0.85746345
H	-9.71913919	16.41771096	-2.16141282
H	-10.13791330	13.78131674	-0.74802708
H	-11.31280513	16.70175837	-0.06567258
H	-11.02412048	14.66819232	2.06536260
H	-12.30861169	15.60198479	1.54133487
H	-11.88228798	14.03714903	0.71174716
H	-9.61705183	17.01082340	1.59673378
H	-8.72162153	15.52923882	1.30393022
H	-8.76218223	16.85752936	0.21540648

N	-11.55593165	14.41298217	-3.37539535
C	-12.71964153	14.12955614	-4.21086004
C	-12.26764664	13.31974804	-5.41580402
O	-13.02716445	12.49510501	-5.94675131
C	-13.38152731	15.42794487	-4.70444593
C	-14.84844050	15.41276894	-4.85018836
C	-15.37455576	14.69717638	-6.11196651
C	-15.80626435	13.25299100	-5.87268588
N	-17.05524406	13.16149010	-5.04893083
H	-10.67991751	14.46278187	-3.82674620
H	-13.44359375	13.42666077	-3.57467217
H	-12.93836248	15.70081520	-5.66175346
H	-13.05748058	16.22058865	-4.02442139
H	-15.05720917	16.49520189	-4.87252164
H	-15.34252430	15.03787468	-3.96414850
H	-14.72273799	14.55897935	-6.90120500
H	-16.25051726	15.23990333	-6.52234823
H	-15.11879677	12.60441459	-5.24525201
H	-16.05348511	12.67481325	-6.81973490
H	-17.94772706	13.49372346	-5.46559007
H	-17.23576610	12.15553401	-4.64097989
H	-16.96494205	13.82440223	-4.13250909
N	-18.88464755	10.74431720	-0.26213216
C	-17.70408083	11.45184994	-0.66120099
C	-18.27898230	12.28010030	-1.81430930
O	-18.06230272	11.98409837	-3.02165510
C	-16.42178004	10.73321282	-1.16247416
S	-14.95252678	11.80119548	-1.75809458
H	-19.25816081	10.10439362	-0.93467329
H	-17.43616761	12.14608215	0.17503439
H	-16.60970824	9.97190627	-1.97182142
H	-16.02972865	10.15874833	-0.26525289
N	-19.17211194	13.33194035	-1.49017334
C	-19.80133071	14.30100916	-2.49448916
C	-18.64476300	15.12717300	-3.10482336
O	-18.30114756	15.07314110	-4.28927265
C	-20.71064018	15.18980148	-1.67953408
C	-20.32233520	14.98733173	-0.26209365
C	-19.71006727	13.59620314	-0.16117096
H	-20.38355159	13.79063555	-3.39514594
H	-21.72491523	14.86372599	-1.79143434
H	-20.70515089	16.19642713	-1.99805424
H	-21.30596800	15.24252371	0.29413317
H	-19.51959634	15.74186192	0.08577649
H	-19.01907400	13.60146320	0.62357812
H	-20.49815963	12.84547658	0.20309873

N	-17.93779949	15.99432086	-2.27477806
C	-17.28420959	17.19123874	-2.86722083
H	-17.99999872	15.85499902	-1.24999965
H	-18.07021165	17.99066064	-2.79775393
H	-16.79822700	17.04663145	-3.89077009
C	-16.17302106	16.82403594	5.07776810
O	-17.39716972	16.83750911	4.95837344
N	-15.22797800	16.38201675	4.09385641
C	-15.63787245	15.69217919	2.92668803
C	-15.06399450	14.31451203	3.05325728
O	-13.82049657	14.25455781	2.95036990
C	-14.97261342	16.36428011	1.64082905
S	-15.58606036	15.55484081	0.17656827
H	-14.33277139	16.14876338	4.31954438
H	-16.77650293	15.75401011	2.83852298
H	-13.89000039	16.41504062	1.59380531
H	-15.28756055	17.43412640	1.57024379
N	-15.91638729	13.32655786	3.37218127
C	-15.67938971	11.87848578	3.67447486
C	-14.90194586	11.03944432	2.65212161
O	-15.48204614	10.34331474	1.84321586
C	-17.02204266	11.15450045	3.86241626
C	-18.11599860	12.21999928	3.58999957
C	-17.40967165	13.54371855	3.11329861
H	-15.04755986	11.83342357	4.55091239
H	-17.17429322	10.58704758	4.88873201
H	-17.13031707	10.19658147	3.18438585
H	-18.71202115	12.45408244	4.58257453
H	-18.77862487	11.91777272	2.78759860
H	-17.54066557	13.70462020	2.02223945
H	-17.74065786	14.27942214	3.80272381
N	-13.54134277	11.09319040	2.81915700
C	-12.48589794	10.25992418	2.24431618
C	-11.60233118	9.86334238	3.40520004
O	-10.78285667	8.98035347	3.13724331
C	-11.62369492	11.19928101	1.26866819
C	-11.05749193	10.31758433	-0.01761762
C	-10.33280131	11.71721283	1.89132601
C	-11.27890382	11.09742265	-1.27290995
H	-13.16889750	12.00856016	3.08072550
H	-12.89562370	9.45915765	1.67604772
H	-12.21046189	12.07800086	0.95532357
H	-11.67790558	9.43049985	0.01341227
H	-10.10294768	9.91840568	0.26969130
H	-10.42086489	12.03887068	2.88892285
H	-9.54935379	10.97472634	1.91968442

```
H      -9.91559932  12.53547105  1.32064601
H     -11.00153048  12.19009620 -1.20752525
H     -10.70255455  10.68371382 -2.14492996
H     -12.34743346  10.79601207 -1.48370698
O     -18.28996592   8.63845641  0.92329935
H     -17.37499860   8.67321536  1.31048048
H     -18.60977859   7.89362805  1.49509516
O     -18.79899863  16.52999894  2.57999977
H     -19.35629139  16.09839147  3.13856292
H     -18.63189009  17.47070330  2.67957610
H     -15.69339888  17.29769855  5.92989947
H     -16.47871866  17.50639587 -2.13752349
H     -13.13809898  17.79829860 -1.87710004
H     -11.74499924  10.39409925  4.35159987
H     -12.59252067  18.89839653  1.60058855
H     -8.56502956  15.29123512 -1.90253310
H     -18.74353802  10.31472546  0.66780293
H     -11.27659909  13.48069889 -5.87739980
end
end
```

Task SinglePoint

Engine ADF

Title Structure 1 t479 s12000 spin-orbit ZORA

```
basis
  PerAtomType
  core None
  type ZORA/QZ4P
  Symbol Cd
end
  PerAtomType
  core None
  type ZORA/QZ4P
  Symbol S
end
  PerAtomType
  core None
  type ZORA/QZ4P
  Symbol O
end
  PerAtomType
  core None
  type ZORA/QZ4P
```

```
Symbol N
end
PerAtomType
core None
type ZORA/TZ2P
Symbol C
end
PerAtomType
core None
type ZORA/DZP
Symbol H
end
end
```

numericalquality verygood

symmetry nosym

```
relativity
level spin-orbit
formalism ZORA
end
```

save TAPE10

```
xc
hybrid BHandHLYP
end
```

NUCLEARMODEL gaussian

QTENS

EndEngine

eor

Structure 2 with HBandHLYP functional, and a locally dense combination of the basis sets QZ4P, TZ2P and DZP:
\$AMSBIN/ams <<eor

```
System
atoms
Cd 76.626229937405724968 21.459777297672001595 78.044063048158719198
N 72.716777438463637395 19.188405530888982042 81.718238758524350374
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C 74.029798910614999841 19.689653725578398991 81.359738705929501634
C 74.543246719872058748 20.826972185478055621 82.339567950438691923
O 73.741463635217286310 21.695305020658427253 82.621037901244235968
C 73.970250184693455253 20.287454880022362858 79.994631300699111875
S 75.136747105022863025 21.718338747800689958 79.968315834674470466
N 75.771572481625057094 20.935205102885710460 82.924105375965055487
C 76.191022788372166019 21.978430057751960902 83.887484642750223429
C 76.564516547206807218 23.345262362484852758 83.319123854500304560
O 75.702589274271645081 23.995452699197123536 82.776642834349019040
C 77.363507036075830570 21.283032728415040680 84.725145841210149911
C 77.733721187211344272 20.063844387030044913 83.905559436930786887
C 76.926969331061954449 20.088964543007158170 82.582989226129683402
N 80.288040831170803813 17.724921642744138950 79.012817952710875602
C 79.099552556781432600 18.440266695882993275 78.478544366245941433
C 78.095286597304337306 17.468443042238448015 77.921884020539337712
O 78.155156719324466508 17.099953567862343107 76.731363279462371452
C 79.513046172383582189 19.435734297958571659 77.423578051965563418
S 77.984373835072062775 20.202567960370558353 76.604765521302667253
N 77.076755509885487072 17.069962615973775399 78.714287348593202864
C 76.042094578553133033 16.127983111837789210 78.245826156514553418
C 74.931290271473301345 16.952445221251039698 77.438510550359325180
O 73.780861917797977867 17.182684553258830817 77.781801405408785399
C 75.499308010690285187 15.532480514048861764 79.605513667954170387
C 75.845989176531517728 16.476997735851568905 80.698987785896221681
C 76.816689068214202507 17.516436537745146751 80.112896871486711348
N 75.467716331233035021 17.458748452562872444 76.259469530097689471
C 74.669502563943439100 17.726195061496586192 75.011734173606328113
C 75.398571970840748691 17.078255282555097949 73.892310568412298721
O 74.821777609119550334 16.697338612236841016 72.946373351904014726
C 74.499527846252519225 19.271369690648487705 74.766554200317386858
C 73.760790063484890311 19.862843536233356190 75.996578241715340596
C 73.806873045189234972 19.664642564494847932 73.430856024217632694
C 74.067639778038696363 21.358291874971001789 76.148745487344541516
N 80.769987809440166870 23.409996203102462431 78.224988026841828059
C 79.806599127437195307 23.150249764963593435 79.283274015590720296
C 78.580216331473906166 24.107345909983578736 78.949251478328974940
O 77.566629966053199041 23.614966068826163337 78.607663628334876194
C 80.254626646227720244 23.530336050218611632 80.671725635519294428
O 80.178948013813283069 22.457583133294278355 81.637591038313033209
N 77.696988026159402807 25.192996067219496581 74.810989255171747914
C 76.454367061753160328 24.852990191856335400 74.099809031156681272
C 75.293709683704548752 24.685791662995356432 75.155108485275647467
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C 76.484039681509557340 23.533888786277728400 73.311190964493391675
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C 77.919814465947268900 23.071982132928411602 72.900906558792058831

N 75.617471435702427129 25.065265837112601588 76.447543217910904900
C 74.581319244490686060 25.487096045984984016 77.388288162724364838
C 73.481868434259055789 26.309151954043556998 76.714380146153615669
O 72.406339264298352987 26.268542191326492485 77.219987456534965986
C 75.304538821259114911 26.373529196310837364 78.417097146484920245
C 74.418408926292457295 26.632772165678108678 79.600686778413646039
C 74.474704179355256883 25.631100321629855188 80.718389254226352136
C 73.315352000449877323 24.589380229243090525 80.516271605401328770
N 73.174668925180569090 23.703563508023975714 81.693732618045274307
H 72.116834217428177567 19.873184719384092034 82.075181531847562155
H 74.776894851103591577 18.835436511245141844 81.394571367028078157
H 72.974442732475267803 20.805812110723788777 79.867592998721818276
H 74.158201937868085452 19.592213279881239174 79.136284350959229528
H 75.411316435028112437 22.179733264930021619 84.601977178898934540
H 76.996593355798012226 20.942481620739030745 85.704686130947735023
H 78.238679438631237417 21.903745591583508201 84.902295140638699422
H 77.619241342421830154 19.207316858764247769 84.531137068132650825
H 78.824762544571711942 20.001050308554699342 83.624139641387188249
H 77.545352555148241436 20.588964846527563424 81.820103924153102071
H 76.684448610079073205 19.064605665608102214 82.232783182751475692
H 80.066606287705752720 16.980169686172061461 79.634604596459354298
H 80.885252524466736190 17.376274762676217733 78.225633236114546776
H 78.776227692233931066 18.963826921383372337 79.359164342746737475
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H 80.131125111186577215 20.270925621917623261 77.896945339311471912
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H 75.514418867529627732 19.702504531144956701 74.730544135407583894
H 74.049319341142847861 19.365984113230755526 76.856652052021473764
H 72.689134365793961479 19.678148702248812185 76.009835940899009188
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H 72.867199963721489553 19.147658830844481059 73.229524874229639408
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H 78.511014940735350365 23.954816758278184352 72.524936367240201207
H 76.594346205652030335 25.178908577535001001 76.739788082746997588
H 74.110219686542279760 24.566742194509551211 77.836511194735379604
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H 74.560710398587502823 27.761812296384842824 80.006385595629112117
H 74.328720851049837393 26.055886824334482554 81.754934243912245506
H 75.422814087865376109 25.058171021642706933 80.673433997466190704
H 73.589674610298061452 23.947610789979350443 79.656733282397951257
H 72.318254974321291684 25.017494015430742138 80.211663334650808110
H 72.775693744079646308 22.739530312676674129 81.460784668365334937
H 74.076701910954355412 23.385199244551976960 82.136862776302947964
H 72.538439256820538503 24.131676568276571260 82.401935064452402457
H 72.288566144157840654 18.521487285544058210 81.142312223867989474
H 77.476088080655770796 23.743896178698765453 83.644987579235589692
H 76.479288139020155768 17.156497683992469661 74.044189307820005297
H 81.007434174656992809 22.549938809664428874 77.756691548040436146
H 78.746087980069773948 25.188496065950872094 79.054087954008991801
H 78.296209752960123751 25.850830880042501292 74.328505703399116555
H 73.860789346429399416 26.833195942938186107 75.837489161787758007
end
end

Task SinglePoint

Engine ADF

Title Structure 2 t480 s10000 spin-orbit ZORA

basis
PerAtomType
core None
type ZORA/QZ4P
Symbol Cd
end

PerAtomType
core None
type ZORA/QZ4P
Symbol S
end

PerAtomType
core None
type ZORA/QZ4P
Symbol N
end

PerAtomType
core None
type ZORA/QZ4P
Symbol O
end

PerAtomType
core None
type ZORA/TZ2P
Symbol C
end

PerAtomType
core None
type ZORA/DZP
Symbol H
end
end

numericalquality verygood

symmetry nosym

relativity
level spin-orbit
formalism ZORA
end

save TAPE10

xc
hybrid BHandHLYP
end

NUCLEARMODEL gaussian

QTENS

EndEngine

eor

Structure 3 with HBandHLYP functional, and a locally dense combination of the basis sets QZ4P, TZ2P and DZP:
\$AMSBIN/ams <<eor

System

atoms

Cd 76.674584680018426752 21.555670155430945556 77.737340502027038269
N 72.716777438463637395 19.188405530888982042 81.718238758524350374
C 74.078421801967138549 19.582160117226933949 81.493894695009018392
C 74.498228260605102946 20.735399498096402482 82.382587837838769929
O 73.638663137607849762 21.463474263631297845 82.829461778839558406
C 74.107061920679527134 20.151337489775858813 79.954473993343682992
S 75.082569157820316263 21.771995971791305635 79.704843974641065074
N 75.782649051008419860 20.939464362320610036 82.811570457824601021
C 76.184459219591616375 21.955850910347141536 83.695634997786726217
C 76.635211026859124672 23.283651853195220127 83.196729552302585375
O 76.108483498549617252 23.877743401673956924 82.250551418621554944
C 77.386160257705881804 21.392945894481961489 84.537527978597509559
C 78.027989782572149124 20.369286449695270136 83.508342625789566682
C 76.850044169405464345 20.040338691580267039 82.459170314239486288
N 80.288040831170803813 17.724921642744138950 79.012817952710875602
C 79.227090125102080265 18.646866444658517281 78.502306693947005556
C 78.180891096846750088 17.669751473066398262 77.925272796543083587
O 78.308792286533389415 17.396703343210685233 76.736172354536336115
C 79.679278700727920182 19.636582898807809272 77.450628617012256427
S 78.289752010827385220 20.352735359216303834 76.450681580909517265
N 77.241971521993789906 17.088722544026428096 78.799923754470370341
C 76.664701464296200584 15.724837053991420177 78.446910698305472920
C 75.577110784363611629 15.842469409279935633 77.430631034533845991
O 74.522564897407534090 15.218128409657238009 77.571586917477077350
C 76.077993496070646984 15.279190263755726420 79.822611384450311789
C 75.845989176531517728 16.476997735851568905 80.698987785896221681
C 76.909300447227749942 17.456704129857122609 80.195407401818428639
N 75.663685251324636738 16.839838969725942519 76.518744854208406991
C 74.686164375398874427 16.917022339108349627 75.485977290907655401
C 75.346402395706988386 17.360542280652669689 74.105422598782951127
O 74.707527161841923657 17.697130117008910588 73.196845617194853162
C 73.699784896265967404 17.985022334339568317 76.058274223189684449
C 72.373745447069794068 17.898512089249067003 75.217467384706921507
C 74.383202858699561943 19.360321720499843678 76.009146261581904014
C 71.591210673490238037 16.658990480654438215 75.544526334106109289

N 80.769987809440166870 23.409996203102462431 78.224988026841828059
C 79.765499826266449190 23.140404717240446786 79.240904571337750895
C 78.736895381537522098 24.119655450745661085 78.768331842309720514
O 77.767700710681367582 23.791537059038258661 78.102759799088346426
C 80.166799878737606377 23.543011340693663414 80.651443083829960301
O 80.816071294421092830 22.583820810235515353 81.335814059146457566
N 77.696988026159402807 25.192996067219496581 74.810989255171747914
C 76.263290126416563908 24.785196700869821740 74.568846215826994239
C 75.837414328167284339 24.296737467122110132 75.978573000840711416
O 75.828400054769247163 23.121820425846465241 76.297730394792367292
C 76.107255476553788753 23.645332298684568428 73.457309452990969589
C 74.669527471984409317 23.216795646429631006 73.237659988317332704
C 76.599577360946284443 24.246667629640242581 72.207162682306588408
N 75.420870418320788531 25.282029929194752782 76.929708984930158522
C 73.996036777016215069 25.162809316033019513 77.418228138785480041
C 73.235762486718527953 26.207885456240681776 76.515992947076256314
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C 73.905055912474026059 25.579203585167459067 78.865310660701680945
C 72.581845550922224675 25.134998534234522793 79.574253347495456978
C 72.547174283489027857 25.779111402302646638 80.999309516807031173
C 72.353462064691768774 24.787296995003551103 82.099640346977622585
N 73.569931852619561141 23.857939886474301971 82.148860220657738296
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H 75.428198237610757815 22.177093202932862681 84.549073980636691772
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H 78.852181736807580137 20.815317968991642772 83.059013665596623355
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H 77.484890451863776661 15.069572303870687691 78.115987284685928671
H 76.892151895670153294 14.676729153155269714 80.324355443107577912
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H 77.768049692515376137 17.595581954043804984 80.853746402240361135
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H 73.400202889872190326 17.683059637741678216 77.100724806771111730
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H 81.723699465866815217 23.567896292134150826 78.609837424599504629
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H 78.309914705485113018 24.446671210982604094 74.521448756824753445
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H 76.730037831978265217 22.786329896533967343 73.770008144080378543
H 74.563264236445675692 22.731995521813352923 72.230972328537092153
H 74.292348097299580445 22.488450121940484649 73.993693996945665958
H 73.958860955125501846 24.044171989775563247 73.317615986877342493
H 77.615070313266926405 24.593833918522022941 72.234832396180053138
H 76.406469740616032027 23.593321180715065566 71.337324513834417417
H 76.000076929002460702 25.184675464020791935 71.988257825343040963
H 76.063765027098710902 25.349797191805418350 77.770104407195503882
H 73.414415245797243870 24.165391980735957844 77.326563685520596891
H 73.975833097810962613 26.722294148035700800 78.872332393040153420
H 74.706502963792630112 25.234543262777290096 79.543842220751884042
H 72.454188730455854284 24.044210464919437698 79.552024930056973062
H 71.745998329744480770 25.540224212582447905 78.943807356166871614
H 71.739415774948170679 26.537733202312448810 81.011846570237679543
H 73.405972893100994270 26.462066090299860122 81.143788542897098637
H 71.373801807071984626 24.220375446699488720 82.045393020716019805
H 72.278689177299185076 25.266477345787180298 83.116301286457670017
H 73.480200160411641264 23.234572102012336359 81.332579706148578680
H 74.408939962156622983 24.381484752919501346 81.996614300090485017
H 73.694898748914937414 23.264869043757361311 83.016253647086230671
H 72.467416830201941025 18.753875118873487793 82.638047257777998311
H 77.476088080655770796 23.743896178698765453 83.644987579235589692
H 76.479288139020155768 17.156497683992469661 74.044189307820005297
H 80.891444872667278787 22.692430828881473559 77.562433861533875756
H 78.746087980069773948 25.188496065950872094 79.054087954008991801
H 77.952096213906344246 26.062894722873224396 74.342456144181824129
H 73.860789346429399416 26.833195942938186107 75.837489161787758007

end

end

Task SinglePoint

Engine ADF

title Structure 3 t481 s10000 spin-orbit ZORA

basis

PerAtomType

core None

type ZORA/QZ4P

Symbol Cd

end

PerAtomType

core None

type ZORA/QZ4P

Symbol S

end

PerAtomType

core None

type ZORA/QZ4P

Symbol N

end

PerAtomType

core None

type ZORA/QZ4P

Symbol O

end

PerAtomType

core None

type ZORA/TZ2P

Symbol C

end

PerAtomType

core None

type ZORA/DZP

Symbol H

end

end

numericalquality verygood

symmetry nosym

relativity

level spin-orbit

formalism ZORA
end

save TAPE10

xc
 hybrid BHandHLYP
end

NUCLEARMODEL gaussian

QTENS

EndEngine

eor

Structure 4 with HBandHLYP functional, and a locally dense combination of the basis sets
QZ4P, TZ2P and DZP:

\$AMSBIN/ams <<eor

System

atoms

Cd 76.757210076034567692 21.181233619427423776 77.851977272947678443
N 72.716777438463637395 19.188405530888982042 81.718238758524350374
C 73.925181248386863331 19.895668094415235316 81.309023719813751541
C 74.465921052078471121 20.878048427090323713 82.458423081726223813
O 73.725838017148447534 21.596957796441248689 83.094725000914266388
C 73.715075184261493746 20.663411665681326923 79.956245419933750895
S 75.062330706795108881 21.870922159478176638 79.579581643786497125
N 75.793130255219580249 21.056453008622948886 82.752983013880552221
C 76.311844445641938250 21.847663806596681724 83.879156427623314585
C 76.462118445733295857 23.278176123303740752 83.604644245094988264
O 75.560757949688451163 24.035315494809193382 83.346452608689105546
C 77.676736695031266322 21.242092864940115504 84.201265178694924884
C 77.884152440016137575 20.081785904599986026 83.187306485056481620
C 76.979321504095850059 20.451930665671380183 82.065663223030924200
N 80.288040831170803813 17.724921642744138950 79.012817952710875602
C 79.054542614411857926 18.106930491704122943 78.212660864019213136
C 78.222273490912073157 16.799118654140215767 77.891900408591197902
O 78.280225672708851903 16.227645214948189789 76.824019734656175729
C 79.317430936002367048 18.901512551065664525 76.940883689270094692
S 78.952992196743934983 20.678588998157263035 77.002969069505297739
N 77.597774021896171348 16.145379547811540277 78.952174721356456644
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C 75.852336136808062861 15.202292258356154164 77.401697575588855216
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N 80.769987809440166870 23.409996203102462431 78.224988026841828059
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O 77.389630930771048156 23.729636470337169385 78.578207305250032277
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O 75.658698252936531503 22.875109896023094080 76.473800862414591961
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C 78.800720100456473460 23.156713970916790402 73.179558311712753493
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H 77.623788301145836499 20.861174324888590803 85.236656848168166789
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H 76.138125365090232322 24.191235342936433739 73.846475107028751950
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H 77.697293803834853065 20.648398910445667553 73.777682269448987995
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H 79.826371786367104733 23.034343762302398773 73.580558927992854024
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H 72.301281539258042130 23.788349864956916946 82.552007724624132834
H 73.383318457278292613 23.622637918114413935 81.381495611397681955
H 73.911303001030105975 23.480672713856641565 82.880921565232796411
H 71.933490563664349793 19.782679503051426195 81.771459133312461631
H 77.476088080655770796 23.743896178698765453 83.644987579235589692
H 76.479288139020155768 17.156497683992469661 74.044189307820005297
H 80.760863376525051649 22.800512720520252685 77.399609206413813922
H 78.746087980069773948 25.188496065950872094 79.054087954008991801
H 77.858267367358578781 25.732244371804746663 73.979226161099063575
H 73.860789346429399416 26.833195942938186107 75.837489161787758007
end
end

Task SinglePoint

Engine ADF

Title Structure 4 t482 s10000 spin-orbit ZORA

basis
PerAtomType
core None
type ZORA/QZ4P
Symbol Cd
end
PerAtomType
core None
type ZORA/QZ4P
Symbol S
end
PerAtomType
core None
type ZORA/QZ4P
Symbol N
end
PerAtomType
core None
type ZORA/QZ4P
Symbol O
end
PerAtomType
core None
type ZORA/TZ2P
Symbol C
end


```
PerAtomType
  core None
  type ZORA/DZP
  Symbol H
end
end
```

```
numericalquality verygood
```

```
symmetry nosym
```

```
relativity
  level spin-orbit
  formalism ZORA
end
```

```
save TAPE10
```

```
xc
  hybrid BHandHLYP
end
```

```
NUCLEARMODEL gaussian
```

```
QTENS
```

```
EndEngine
```

```
eor
```

Structure 5 with HBandHLYP functional, and a locally dense combination of the basis sets QZ4P, TZ2P and DZP:
\$AMSBIN/ams <<eor

```
System
atoms
```

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Cd 76.079906896664084570 21.042204981683163112 78.207338812709693343
N 72.716777438463637395 19.188405530888982042 81.718238758524350374
C 73.931873966522658748 20.034718623615734856 81.542074965992597413
C 74.339016488413037109 20.802490188362401824 82.765026756633915284
O 73.494803732561933884 21.333869064674715332 83.470006748962262577
C 73.703833428255208560 21.251678061426964916 80.571622030276742521
S 73.729356100642377214 21.058576585203311993 78.796009926542978974
N 75.655852349225355624 21.323301938165261760 82.890436035739824661
C 76.192668032791715405 21.856873239598787251 84.138577336444910770
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C 76.417911928546146783 23.366876626810267226 83.827353594592892705
O 75.549580116541946495 24.189520164301658411 83.858224302907544256
C 77.543209913658174059 21.217047680229374151 84.318262746622878012
C 78.074283115630365160 20.917783346452036852 82.908874571289828737
C 76.755449051351448020 20.804432364533880673 82.075179462537846575
N 80.288040831170803813 17.724921642744138950 79.012817952710875602
C 79.104705088987827821 18.564281453156109336 78.931188999780474091
C 78.070729274393642072 17.813820908933212905 78.139508671285852870
O 78.096107239461559857 17.588841775043157156 76.933514648034488914
C 79.318895790730678641 19.895735051452721365 78.157443612398608934
S 78.249687893837517549 21.334043140937392735 78.675131468282884839
N 77.122978834870806963 17.176981184190143637 78.913033551099601937
C 75.848703282317970320 16.731352714097216250 78.325481328597390984
C 75.345781510083554622 17.684050816582018939 77.263375463503606966
O 75.489573482410619931 18.852722732171621089 77.470700556782759350
C 74.878175671207443997 16.650628951591368576 79.553201622387518910
C 75.845989176531517728 16.476997735851568905 80.698987785896221681
C 76.915901738986804048 17.436793684250584846 80.410317671449973886
N 74.750912447370538416 17.046841176013582952 76.201608880497346377
C 74.470474941580732775 17.625355651822694369 74.837325640475981459
C 75.494697498520238810 17.367091762617882011 73.777117180254577988
O 75.222142434356712215 17.348240853417749463 72.603974637514227197
C 74.246616707498006349 19.168954322306692717 74.797347612659720539
C 73.181685768490822852 19.626636466926711933 73.667574197305441430
C 75.529735382666459031 20.001109573229683747 74.672636913984732132
C 71.754961718778503155 19.975966680715345092 74.172092553884809263
N 80.769987809440166870 23.409996203102462431 78.224988026841828059
C 80.879820564141468253 24.554555897934374542 79.065318075893188166
C 79.482900338494445691 24.626025490681204388 79.693687832232271262
O 79.203355284438359263 24.136114389605932473 80.761525626565145330
C 81.123829818880366815 25.781400661362177118 78.201670014908188477
O 80.487043889321796541 25.562431656616453779 76.912964386086613899
N 77.696988026159402807 25.192996067219496581 74.810989255171747914
C 77.093111033819468503 23.857702006832823827 74.746737616177895802
C 76.084105500718834492 23.841063510825936334 75.980270038287088141
O 75.801009014944042974 22.752988387084201349 76.499886816898410302
C 77.900449072052509791 22.579139064008312943 74.798680616354474182
C 78.203789271338251865 22.239905095996423512 73.333245606526588745
C 79.265520332277134230 22.794204637672123681 75.533284300956154311
N 75.507195615286207158 25.055360716779052410 76.305927868676235448
C 74.434489002685467085 25.142588987407215484 77.254341131666578235
C 73.611212909544590843 26.345945894532945886 76.760608770633169229
O 72.795755452812329622 26.770487821001445639 77.513602692024164753
C 74.802772258766765390 25.501572628139260956 78.696895203109690442
C 73.532739947952407533 25.664486357939701122 79.602869248740859121
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H 74.735839951965246541 19.354855995045056716 81.119794751752436923
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H 73.572139950064737945 20.623442073005321618 73.274254872513552073
H 75.380980083698787553 21.093434356028353704 74.999399937212587020
H 76.351932770475471557 19.564531795156280936 75.312647991456813656
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H 71.363419858270077611 20.791246786020924020 73.554453772019982694
H 71.039136277802583663 19.184897342011641541 74.074417144485181552
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H 80.723617179915649444 26.719280208663640508 78.664312033534940838
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H 76.430229406975001893 23.896785570834019552 73.890785384522189361
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H 77.344225977976975628 22.366917322628250275 72.637619595745775314
H 79.019684322889659711 22.828653223177031606 72.866240591847954988
H 78.286659426685474727 21.180508902043573727 73.190913668595314334
H 79.944359539859618735 21.974562261372671657 75.458138140802986982
H 79.822690289365084482 23.590286364050371049 75.070854171738972127

H 79.111530730874747519 23.036950182218774330 76.608863733290476716
H 76.137004688582550216 25.880266961814509585 76.165028404426408315
H 73.791332878111845162 24.178572294415477728 77.160730905421900161
H 75.352538695414210679 26.492630767696724092 78.704504627760243807
H 75.478835727457379789 24.693797003465299156 79.006878447067705906
H 72.803007564342266278 24.864622077934622979 79.252710062252546663
H 73.121274371623570687 26.601877328987292515 79.607405814540712186
H 74.666420491145046867 26.127718395809370833 81.483205699587031745
H 74.782994659351672340 24.450753345873220468 80.958062682659658549
H 72.071260268358244616 24.360058138180995968 81.253261701058804078
H 72.403491029620283825 25.800045523190046737 82.231982098542289350
H 73.674490067921013292 23.190457531700559457 82.849849480243179300
H 73.829353785910953434 24.656305809153977293 83.678919826411259919
H 72.335815645173539679 23.736876472951951911 83.611274236186901021
H 72.201917098250405047 18.966519794029451873 80.849130948383233886
H 77.476088080655770796 23.743896178698765453 83.644987579235589692
H 76.479288139020155768 17.156497683992469661 74.044189307820005297
H 81.139702140313019640 22.527678190129666547 78.554658568207315739
H 78.746087980069773948 25.188496065950872094 79.054087954008991801
H 78.554720437384446541 25.214060458358925843 75.354883380940378856
H 73.860789346429399416 26.833195942938186107 75.837489161787758007
end
end

Task SinglePoint

Engine ADF

Title Structure 5 t483 s7000 spin-orbit ZORA

basis

PerAtomType

core None

type ZORA/QZ4P

Symbol Cd

end

PerAtomType

core None

type ZORA/QZ4P

Symbol S

end

PerAtomType

core None

type ZORA/QZ4P

Symbol N

end

```
PerAtomType
  core None
  type ZORA/QZ4P
  Symbol O
end
```

```
PerAtomType
  core None
  type ZORA/TZ2P
  Symbol C
end
```

```
PerAtomType
  core None
  type ZORA/DZP
  Symbol H
end
end
```

```
numericalquality verygood
```

```
symmetry nosym
```

```
relativity
  level spin-orbit
  formalism ZORA
end
```

```
save TAPE10
```

```
xc
  hybrid BHandHLYP
end
```

```
NUCLEARMODEL gaussian
```

```
QTENS
```

```
EndEngine
```

```
eor
```

Structure 6 with HBandHLYP functional, and a locally dense combination of the basis sets QZ4P, TZ2P and DZP:
\$AMSBIN/ams <<eor

```
System
```

atoms

Cd 75.794611835709702063 20.022972961872181230 77.497902243595632399
N 72.716777438463637395 19.188405530888982042 81.718238758524350374
C 73.856721389687507440 19.899756857912365149 81.162491987158574602
C 74.306426502235083831 21.027828313636049984 82.144615921176779239
O 73.506265533364128828 21.645994465914871085 82.869129782109396842
C 73.608291845229260275 20.671778110122808414 79.798178345953857615
S 73.542400029275057705 19.666841343591368485 78.246797525057999678
N 75.638523717126929569 21.420043784101142847 82.286625666183951466
C 76.154275832199544993 21.827697233349134365 83.581366788482569063
C 76.420600962594775751 23.353673196132305634 83.614311884599445079
O 75.498645086336452437 24.164781275161384855 83.732181272551571283
C 77.532983647142259542 21.194374333935755317 83.781142593621808601
C 77.921704103622033699 20.746849858820265666 82.320140123922470821
C 76.682243284352963997 20.878720264458429767 81.366089705168292312
N 80.288040831170803813 17.724921642744138950 79.012817952710875602
C 79.021923763420190312 18.402133323063853965 78.647599304080500815
C 78.143795802875388290 17.377696827155098447 78.039641519554976412
O 78.255493012158851229 16.918724299740425465 76.918989611438092879
C 79.132545682562380307 19.539418138122297108 77.684985747849111704
S 77.988018659699918089 20.952149934955279775 77.763661191480082380
N 77.082524558406504411 16.959822333497236002 78.849388588170441494
C 76.084513173649853002 16.051099171115591702 78.296932083515272893
C 75.677437262884595270 16.723803517858012668 76.953910183278921409
O 76.032798521240323453 17.823396206826902954 76.547661712700460157
C 75.093576954066691087 15.837111784630103273 79.520433457071135308
C 75.845989176531517728 16.476997735851568905 80.698987785896221681
C 77.258325877071726495 16.830385467084902018 80.274920996278197549
N 74.945501443524051410 15.868821690064756069 76.195065501754555726
C 74.637697026881255624 15.948610013415526865 74.778422862544815075
C 75.860534711026687660 16.220346016850136550 73.919573515250860396
O 76.065566361202215262 15.533949857008014561 72.964416199853729950
C 73.689891537392099963 17.154986219044069173 74.470777005009679783
C 72.812613020872603897 16.704995968939382323 73.305393868001218038
C 74.471367415612718332 18.502737962974560304 73.995569171556269339
C 71.415693201259770717 16.314850560984393013 73.903151865020134892
N 80.769987809440166870 23.409996203102462431 78.224988026841828059
C 80.001044259145601245 23.203354069486849198 79.448271129966542503
C 78.750388780158274926 24.105986313881555105 79.512316533502612970
O 77.797207961397987219 23.773841304880363623 80.199043647582357153
C 80.796598740879360889 23.616143492360947675 80.721570736000600732
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N 77.696988026159402807 25.192996067219496581 74.810989255171747914
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C 76.128268911225092097 23.611138548416306548 75.689726203802649707
O 75.803881606353570533 22.462172346397590417 76.092073388224278574

C 77.909947515809989227 22.606602579707939071 74.188482590371847891
C 78.085581512306191598 22.682164797215424556 72.711740515624995851
C 79.291006736312283465 22.643331281012578415 75.032266924901108496
N 75.512188714428646108 24.776695299320472543 76.080995517974358222
C 74.534698661680167220 24.982968676196637858 77.113454783915031499
C 73.944118345130831926 26.417718392523635629 76.845590482254294784
O 73.488068922300726626 26.992185101234721145 77.822577167262039666
C 75.097156117222453986 24.903610283090308997 78.598391120079000416
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C 72.459545108107832334 25.005195349375899383 81.445522337290327641
N 73.154673843560871660 24.102349038897376232 82.461797920668345796
H 72.197609145887227555 19.778110255291647235 82.323138570446005247
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H 72.641763742560740980 21.185134582786528057 79.908753239110140498
H 75.396585884924732568 21.595274709986810535 84.349345929202954153
H 77.515251629678218137 20.275448154320109495 84.425789555948838938
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H 73.471483061796647007 23.207635875130108616 82.039694889263557798
H 74.040556075492446553 24.487095141437560386 82.762386628116090037
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H 72.079452861565968647 18.829773721760123095 80.981300441728052419
H 77.476088080655770796 23.743896178698765453 83.644987579235589692
H 76.479288139020155768 17.156497683992469661 74.044189307820005297
H 81.168774133430673601 24.332937550739284660 78.209489740283430592
H 78.746087980069773948 25.188496065950872094 79.054087954008991801
H 78.420164040808586492 25.039104153808768416 75.475895769706923488
H 73.860789346429399416 26.833195942938186107 75.837489161787758007
end
end

Task SinglePoint

Engine ADF

Title Structure 6 t483 s10000 spin-orbit ZORA

basis

PerAtomType

core None


```
type ZORA/QZ4P
Symbol Cd
end
PerAtomType
core None
type ZORA/QZ4P
Symbol S
end
PerAtomType
core None
type ZORA/QZ4P
Symbol N
end
PerAtomType
core None
type ZORA/QZ4P
Symbol O
end
PerAtomType
core None
type ZORA/TZ2P
Symbol C
end
PerAtomType
core None
type ZORA/DZP
Symbol H
end
end
```

numericalquality verygood

symmetry nosym

```
relativity
level spin-orbit
formalism ZORA
end
```

save TAPE10

```
xc
hybrid BHandHLYP
end
```

NUCLEARMODEL gaussian

QTENS

EndEngine

eor

Structure 7 with HBandHLYP functional, and a locally dense combination of the basis sets QZ4P, TZ2P and DZP:

\$AMSBIN/ams <<eor

System

atoms

Cd -14.267989241917430121 14.019596770861495472 -0.122904062020070939
N -12.483998912078915211 18.626998573046584795 0.656999962964864959
C -13.665633728531826563 17.725786563290963471 0.422672859221957353
C -13.453313438023659643 17.140849135165669992 -1.024899147506411756
O -13.749722343870805830 15.981483068461077579 -1.270019292029838542
C -15.031634278405283212 18.424669080172041191 0.255741917783260775
O -15.835288263941224685 17.424029126953914925 -0.508842994220669920
H -12.162637832438633723 19.092932775615619079 -0.162127566615344165
H -13.596665185674837062 16.838897340835394800 1.000694314382262862
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Task SinglePoint

Engine ADF

title Structure 7 t682 s12000 spin-orbit ZORA

basis

PerAtomType

core None

type ZORA/QZ4P

Symbol Cd

end

PerAtomType

core None

type ZORA/QZ4P

Symbol S

end

PerAtomType

core None

type ZORA/QZ4P

Symbol N

end

PerAtomType

core None

type ZORA/QZ4P

Symbol O

end

PerAtomType

core None

type ZORA/TZ2P

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Symbol C
end
PerAtomType
core None
type ZORA/DZP
Symbol H
end
end

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numericalquality verygood
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symmetry nosym
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relativity
level spin-orbit
formalism ZORA
end

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save TAPE10
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xc
hybrid BHandHLYP
end

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NUCLEARMODEL gaussian
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QTENS
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EndEngine
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eor
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111Cd Vzz and η for the small model

Structure 1	Nr atoms 24		
Functional		111Cd Vzz [au]	asym. parameter eta
B3LYP	Spin-orbit	-3,09602	0,36663
B3LYP	Spin-orbit w all QZ4P	-3,09728	0,36356
B3LYP	Scalar	-3,05336	0,36663
BHandH	Spin-orbit	-3,65915	0,36744
BHandH	Spin-orbit w all QZ4P	-3,66510	0,31757
BHandH	Scalar	-3,60802	0,36663
BHandHLYP	Spin-orbit	-3,68404	0,31966
BHandHLYP	Spin-orbit w all QZ4P	-3,69005	0,31141

BHandHLYP	Scalar	-3,63310	0,31880
KMLYP	Spin-orbit	-3,79538	0,31388
KMLYP	Spin-orbit w all QZ4P	-3,80187	0,30487
KMLYP	Scalar	-3,74305	0,31324
mPW1K	Spin-orbit	-3,63468	0,31388
mPW1K	Spin-orbit w all QZ4P	-3,63870	0,31210
mPW1K	Scalar	-3,74305	0,31324
PBE0	Spin-orbit	-3,07048	0,65837
PBE0	Spin-orbit w all QZ4P	-3,27558	0,34251
PBE0	Scalar	-3,02581	0,66893
PBE0	No-relativity	-3,03246	0,66251
Structure 2	Nr atoms 17		
B3LYP	Spin-orbit	-3,32989	0,40922
B3LYP	Spin-orbit w all QZ4P	-3,37258	0,40263
B3LYP	Scalar	-3,32989	0,40922
BHandH	Spin-orbit	-3,94717	0,25825
BHandH	Spin-orbit w all QZ4P	-3,95108	0,35882
BHandH	Scalar	-3,89872	0,36447
BHandHLYP	Spin-orbit	-3,97118	0,35859
BHandHLYP	Spin-orbit w all QZ4P	-3,97533	0,35929
BHandHLYP	Scalar	-3,92297	0,36481
KMLYP	Spin-orbit	-4,08879	0,35060
KMLYP	Spin-orbit w all QZ4P	-4,09299	0,35136
KMLYP	Scalar	-4,03903	0,35664
mPW1K	Spin-orbit	-3,92435	0,36193
mPW1K	Spin-orbit w all QZ4P	-3,92711	0,36324
mPW1K	Scalar	-3,87628	0,36804
PBE0	Spin-orbit	-3,54784	0,38640
PBE0	Spin-orbit w all QZ4P	-3,55517	0,38744
PBE0	Scalar	-3,49991	0,39685
PBE0	No-relativity	-3,50441	0,39310
Structure 3	Nr atoms 23		
B3LYP	Spin-orbit	-2,62332	0,58730
B3LYP	Spin-orbit w all QZ4P	-2,66091	0,57950
B3LYP	Scalar	-2,62332	0,58730
BHandH	Spin-orbit	-3,12056	0,53382
BHandH	Spin-orbit w all QZ4P	-3,11678	0,53361
BHandH	Scalar	-3,07422	0,54118
BHandHLYP	Spin-orbit	-3,13956	0,53608
BHandHLYP	Spin-orbit w all QZ4P	-3,13590	0,53580
BHandHLYP	Scalar	-3,09353	0,54328
KMLYP	Spin-orbit	-3,22894	0,52607
KMLYP	Spin-orbit w all QZ4P	-3,22448	0,52598
KMLYP	Scalar	-3,18104	0,53335
mPW1K	Spin-orbit	-3,09372	0,53469

mPW1K	Spin-orbit w all QZ4P	-3,08841	0,53557
mPW1K	Scalar	-3,04807	0,54184
PBE0	Spin-orbit	-2,80678	0,55956
PBE0	Spin-orbit w all QZ4P	-2,79766	0,55979
PBE0	Scalar	-2,75564	0,57153
PBE0	No-relativity	-2,76421	0,56785
Structure 4	Nr atoms 23		
B3LYP	Spin-orbit	-3,09602	0,36663
B3LYP	Spin-orbit w all QZ4P	-3,09728	0,36356
B3LYP	Scalar	-3,05336	0,36663
BHandH	Spin-orbit	-3,65915	0,32614
BHandH	Spin-orbit w all QZ4P	-3,66510	0,31757
BHandH	Scalar	-3,60802	0,32525
BHandHLYP	Spin-orbit	-3,68404	0,31966
BHandHLYP	Spin-orbit w all QZ4P	-3,69005	0,31141
BHandHLYP	Scalar	-3,63310	0,31880
KMLYP	Spin-orbit	-3,79538	0,31388
KMLYP	Spin-orbit w all QZ4P	-3,80187	0,30487
KMLYP	Scalar	-3,74305	0,31324
mPW1K	Spin-orbit	-3,63468	0,31915
mPW1K	Spin-orbit w all QZ4P	-3,63870	0,31210
mPW1K	Scalar	-3,58417	0,31827
PBE0	Spin-orbit	-3,17135	0,31024
PBE0	Spin-orbit w all QZ4P	-3,27558	0,34251
PBE0	Scalar	-3,12111	0,31918
PBE0	No-relativity	-3,12119	0,31858
Structure 5	Nr atoms 23		
B3LYP	Spin-orbit	-3,68468	0,16109
B3LYP	Spin-orbit w all QZ4P	-3,73353	0,16134
B3LYP	Scalar	-3,68468	0,16109
BHandH	Spin-orbit	-4,30333	0,13349
BHandH	Spin-orbit w all QZ4P	-4,28481	0,13662
BHandH	Scalar	-4,23748	0,13481
BHandHLYP	Spin-orbit	-4,33608	0,12714
BHandHLYP	Spin-orbit w all QZ4P	-4,31626	0,13039
BHandHLYP	Scalar	-4,27064	0,12838
KMLYP	Spin-orbit	-4,44219	0,12444
KMLYP	Spin-orbit w all QZ4P	-4,42118	0,12780
KMLYP	Scalar	-4,37463	0,12257
mPW1K	Spin-orbit	-4,26992	0,13020
mPW1K	Spin-orbit w all QZ4P	-4,25178	0,13326
mPW1K	Scalar	-4,20546	0,13149
PBE0	Spin-orbit	-3,90735	0,14938
PBE0	Spin-orbit w all QZ4P	-3,89509	0,15168
PBE0	Scalar	-3,84146	0,15168

PBE0	No-relativity	-3,84752	0,15104
Structure 6	Nr atoms 23		
B3LYP	Spin-orbit	-3,36226	0,15552
B3LYP	Spin-orbit w all QZ4P	-3,41557	0,15250
B3LYP	Scalar	-3,36226	0,15552
BHandH	Spin-orbit	-3,94989	0,13943
BHandH	Spin-orbit w all QZ4P	-3,96838	0,14192
BHandH	Scalar	-3,89610	0,14400
BHandHLYP	Spin-orbit	-3,97811	0,14372
BHandHLYP	Spin-orbit w all QZ4P	-3,99716	0,14609
BHandHLYP	Scalar	-3,92438	0,12838
KMLYP	Spin-orbit	-4,08247	0,14033
KMLYP	Spin-orbit w all QZ4P	-4,10289	0,14285
KMLYP	Scalar	-4,02763	0,14470
mPW1K	Spin-orbit	-3,92452	0,14433
mPW1K	Spin-orbit w all QZ4P	-3,93963	0,14718
mPW1K	Scalar	-3,87132	0,14882
PBE0	Spin-orbit	-3,57389	0,14903
PBE0	Spin-orbit w all QZ4P	-3,58289	0,14979
PBE0	Scalar	-3,51969	0,15700
PBE0	No-relativity	-3,52520	0,15402
Structure 7	Nr atoms 26		
B3LYP	Spin-orbit	-2,93039	0,37057
B3LYP	Spin-orbit w all QZ4P	-2,97619	0,36027
B3LYP	Scalar	-2,93039	0,37057
BHandH	Spin-orbit	-3,43653	0,32994
BHandH	Spin-orbit w all QZ4P	-3,43632	0,32901
BHandH	Scalar	-3,38265	0,33802
BHandHLYP	Spin-orbit	-3,46321	0,32549
BHandHLYP	Spin-orbit w all QZ4P	-3,46256	0,32468
BHandHLYP	Scalar	-3,40959	0,33341
KMLYP	Spin-orbit	-3,54780	0,32128
KMLYP	Spin-orbit w all QZ4P	-3,54725	0,32062
KMLYP	Scalar	-3,49280	0,32904
mPW1K	Spin-orbit	-3,40735	0,32864
mPW1K	Spin-orbit w all QZ4P	-3,40480	0,32833
mPW1K	Scalar	-3,35443	0,33659
PBE0	Spin-orbit	-3,10772	0,34885
PBE0	Spin-orbit w all QZ4P	-3,10895	0,34842
PBE0	Scalar	-3,05145	0,35949
PBE0	No-relativity	-3,05845	0,35768

111Cd Vzz and η for the large model

Structure 1	Nr atoms 138		
Functional		111Cd Vzz [au]	asym. parameter eta
B3LYP	Spin-orbit	-2,505110	0,889560
B3LYP	Spin-orbit w all QZ4P	-2,525730	0,890310
B3LYP	Scalar	-2,468160	0,897120
BHandH	Spin-orbit	-2,687520	0,750100
BHandH	Scalar	-2,648980	0,756730
BHandHLYP	Spin-orbit	-2,764600	0,781800
BHandHLYP	Scalar	-2,724730	0,788290
KMLYP	Spin-orbit	-2,750540	0,743250
KMLYP	Scalar	-2,711640	0,749500
mPW1K	Spin-orbit	-2,693200	0,798850
mPW1K	Spin-orbit w all QZ4P	-2,742020	0,802510
PBE0	Spin-orbit	-2,569300	0,863800
PBE0	Spin-orbit w all QZ4P	-2,592370	0,865040
PBE0	Scalar	-2,531760	0,870840
Structure 2	Nr atoms 125		
B3LYP	Spin-orbit	-2,984280	0,272490
B3LYP	Spin-orbit w all QZ4P	-3,005000	0,274490
B3LYP	Scalar	-2,944600	0,279110
BHandH	Spin-orbit	-3,411280	0,232070
BHandH	Scalar	-3,366110	0,237740
BHandHLYP	Spin-orbit	-3,494190	0,243970
BHandHLYP	Scalar	-3,447820	0,249580
KMLYP	Spin-orbit	-3,540250	0,235770
KMLYP	Scalar	-3,494000	0,241340
PBE0	Scalar	-3,054270	0,264920
Structure 3	Nr atoms 125		
B3LYP	Spin-orbit	-2,398669	0,650520
B3LYP	Spin-orbit w all QZ4P	-2,410710	0,645570
B3LYP	Scalar	-2,360770	0,661500
BHandH	Spin-orbit	-2,875140	0,547760
BHandH	Scalar	-2,831000	0,556260
BHandHLYP	Spin-orbit	-2,910340	0,553960
BHandHLYP	Spin-orbit w all QZ4P	-2,941810	0,544240
BHandHLYP	Scalar	-2,865910	0,562610
KMLYP	Spin-orbit	-2,990230	0,535370
KMLYP	Spin-orbit w all QZ4P	-3,020070	0,527510
KMLYP	Scalar	-2,945250	0,543280
mPW1K	Spin-orbit	-2,810630	0,580680

PBE0	Spin-orbit	-2,512850	0,627720
PBE0	Spin-orbit w all QZ4P	-2,525690	0,622580
PBE0	Scalar	-2,473380	0,637980
Structure 4	Nr atoms 125		
B3LYP	Spin-orbit	-2,749590	0,336040
B3LYP	Spin-orbit w all QZ4P	-2,759700	0,339070
B3LYP	Scalar	-2,709340	0,337550
BHandH	Spin-orbit	-3,078900	0,267560
BHandH	Scalar	-3,035370	0,269970
BHandHLYP	Spin-orbit	-3,141750	0,271940
BHandHLYP	Scalar	-3,097280	0,274390
KMLYP	Spin-orbit	-3,173860	0,263240
KMLYP	Scalar	-3,129270	0,265880
mPW1K	Spin-orbit	-3,085540	0,273950
PBE0	Spin-orbit	-2,854190	0,312130
PBE0	Spin-orbit w all QZ4P	-2,525690	0,315000
PBE0	Scalar	-2,812940	0,313780
Structure 5	Nr atoms 125		
B3LYP	Spin-orbit	-3,656520	0,225490
B3LYP	Spin-orbit w all QZ4P	-3,669930	0,225850
B3LYP	Scalar	-3,590690	0,228120
BHandH	Spin-orbit	-4,168950	0,194160
BHandH	Spin-orbit w all QZ4P	-4,189230	0,194870
BHandH	Scalar	-4,091980	0,195480
BHandHLYP	Spin-orbit	-4,229460	0,186900
BHandHLYP	Spin-orbit w all QZ4P	-4,249430	0,187720
BHandHLYP	Scalar	-4,152300	0,188130
KMLYP	Spin-orbit	-4,310340	0,183200
KMLYP	Spin-orbit w all QZ4P	-4,331330	0,184170
KMLYP	Scalar	-4,230710	0,184180
mPW1K	Spin-orbit	-3,731780	0,184960
mPW1K	Spin-orbit w all QZ4P	-3,748520	0,190840
PBE0	Spin-orbit	-3,791590	0,214470
PBE0	Spin-orbit w all QZ4P	-3,805740	0,214950
PBE0	Scalar	-3,723130	0,216820
Structure 6	Nr atoms 125		
B3LYP	Spin-orbit	-3,252900	0,201710
B3LYP	Spin-orbit w all QZ4P	-3,261930	0,339070
B3LYP	Scalar	-3,200890	0,208890
BHandH	Spin-orbit	-3,741160	0,171310
BHandH	Spin-orbit w all QZ4P	-3,771510	0,185000
BHandH	Scalar	-3,682240	0,177820
BHandHLYP	Spin-orbit	-3,807110	0,179420
BHandHLYP	Spin-orbit w all QZ4P	-3,839940	0,193190
BHandHLYP	Scalar	-3,747450	0,185900

KMLYP	Spin-orbit	-3,881600	0,174140
KMLYP	Scalar	-3,821020	0,180450
mPW1K	Spin-orbit	-4,139860	0,191670
mPW1K	Spin-orbit w all QZ4P	-4,158160	0,192480
PBE0	Spin-orbit	-3,393200	0,195500
PBE0	Spin-orbit w all QZ4P	-3,402420	0,200930
PBE0	Scalar	-3,339320	0,202300
Structure 7	Nr atoms 138		
B3LYP	Spin-orbit	-2,528770	0,459480
B3LYP	Spin-orbit w all QZ4P	-2,546130	0,460960
B3LYP	Scalar	-2,484560	0,468840
BHandH	Spin-orbit	-2,922770	0,410340
BHandH	Scalar	-2,870520	0,420550
BHandHLYP	Spin-orbit	-2,963790	0,414560
BHandHLYP	Scalar	-2,911600	0,424500
KMLYP	Spin-orbit	-3,014220	0,408000
KMLYP	Scalar	-2,960310	0,418230
mPW1K	Spin-orbit	-2,869720	0,426850
PBE0	Spin-orbit	-2,621230	0,446420
PBE0	Spin-orbit w all QZ4P	-2,640890	0,447230
PBE0	Scalar	-2,575510	0,455910

Bond length and angle for the small model system

Structure 1

Structure 1									
Row	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	
1	1	Cd							

2	2	C	1			3,2064793		
3	3	O	1	2		2,1672835	15,3289906	
4	4	N	2	1	3	1,3794743	121,8789239	-83,7792292
5	5	H	4	2	1	0,9867109	123,1720537	-161,1560498
6	6	C	1	3	2	3,6817359	131,8642562	-80,7531041
7	7	S	6	1	3	1,9115585	34,6996933	14,0779504
8	8	H	6	1	3	1,1269195	140,8770898	6,4019724
9	9	H	6	1	3	1,1352179	92,8540340	127,1271956
10	10	C	1	3	2	4,1380376	114,3006659	117,7110955
11	11	C	10	1	3	1,4977725	59,7802861	-127,5608993
12	12	O	1	10	11	3,4706767	34,0504332	-34,4162617
13	13	C	10	1	3	1,5961587	54,4946806	19,1500152
14	14	S	13	10	1	1,7820126	109,0994992	39,9300362
15	15	H	10	1	3	1,1437113	106,2988870	121,4970478
16	16	H	13	10	1	1,0848220	118,0707624	-85,4826216
17	17	H	13	10	1	1,1174726	109,6666139	156,3600097
18	18	N	11	10	1	1,3432570	116,9644654	-109,9759479
19	19	H	10	1	3	1,0700000	144,6205565	-54,1580633
20	20	H	18	11	10	1,0000000	118,3239554	20,7693529
21	21	H	18	11	10	1,0000000	131,1800599	-174,9035860
22	22	H	6	1	3	1,0700000	92,1996524	-127,4083559
23	23	H	4	2	1	1,0000000	119,6204424	22,6857323
24	24	H	2	1	3	1,0700000	113,8877863	124,0504647

Structure 2

Structure	2							
Row	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral
1	1	Cd						
2	2	C	1			3,4976113		
3	3	S	2	1		1,8463034	41,6272545	
4	4	C	1	3	2	3,5798687	133,3833572	-78,1394747
5	5	S	4	1	3	1,8961347	36,4924950	145,9981143
6	6	C	1	5	4	3,4127772	104,3094700	65,4282678
7	7	O	1	6	5	2,4180233	12,5914643	-137,0176964
8	8	H	2	1	5	1,1298077	116,9245862	-125,6508479
9	9	H	2	1	5	1,1204670	69,7189098	-22,5592137
10	10	H	4	1	5	1,0902230	139,6695033	7,1831264
11	11	H	4	1	5	1,1417717	87,1967451	127,1774061
12	12	N	6	1	5	1,4700000	151,0504608	127,0308682
13	13	H	12	6	1	1,0000000	109,4712027	-174,6670800
14	14	H	12	6	1	1,0000000	109,4712028	5,3329199

15	15	H	4	1	5	1,0700000	91,7681347	-122,9295451
16	16	H	2	1	5	1,0700000	127,9133490	85,7742074
17	17	H	6	1	5	1,0700000	91,7382190	-48,0311140

Structure 3

Structure	3							
Row	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral
2	2	C	1			3,6715125		
3	3	S	1	2		2,5401536	29,1381134	
4	4	C	1	3	2	3,5767703	129,3665565	-70,8692073
5	5	S	1	4	3	2,3898345	28,2391694	-152,5712930
6	6	C	1	5	4	3,4482009	97,5297810	65,4431728
7	7	O	1	6	5	2,5154591	15,3641382	-113,6964350
8	8	C	7	6	1	2,9143443	151,2498190	-161,7004680
9	9	O	1	7	6	2,2893956	69,1399050	-169,9173864
10	10	N	8	7	6	1,4314223	80,0812885	-69,5855575
11	11	H	2	1	9	1,1317723	114,9494112	12,3317954
12	12	H	2	1	9	1,1049030	73,5780104	117,2634591
13	13	H	4	1	9	1,1108739	137,9538485	-44,8493899
14	14	H	4	1	9	1,0768762	90,9228966	89,1674803
15	15	H	10	8	7	1,0000000	113,2174295	-50,4420528
16	16	H	6	1	9	1,1064182	143,1786833	45,8133397
17	17	H	4	1	9	1,0700000	92,5321834	-163,5389941
18	18	H	2	1	9	1,0700000	135,3277261	-147,5647840
19	19	H	10	8	7	1,0000000	115,7810614	129,5579472
20	20	H	8	7	6	1,0700000	122,3454333	47,1777851
21	21	N	6	1	9	1,4700000	91,0850720	-155,0479431
22	22	H	21	6	1	1,0000000	109,4712022	9,0914075
23	23	H	21	6	1	1,0000000	109,4712028	-170,9085924

Structure 4

Structure	4							
Row	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral
1	1	Cd						
2	2	C	1			3,7350594		
3	3	S	2	1		1,8479866	36,9453954	

4	4	C	1	3	2	3,5471045	146,9915082	-63,0415671
5	5	S	4	1	3	1,8151228	38,4702600	-132,6317750
6	6	C	1	5	4	3,5570699	79,8222178	150,9124636
7	7	O	1	6	5	2,7242840	16,2398866	-153,9260360
8	8	C	7	6	1	2,9276714	126,7175914	-94,7031595
9	9	O	1	7	6	2,5958208	70,2788245	-136,2337348
10	10	N	8	7	6	1,3864929	91,3823028	-90,9305927
11	11	H	2	1	5	1,0962302	125,9243837	-175,4294074
12	12	H	2	1	5	1,0700000	55,4080087	-115,6243201
13	13	H	4	1	5	1,1244160	101,1097109	-111,4058248
14	14	H	4	1	5	1,1159544	141,5696749	9,6757952
15	15	H	10	8	7	1,0274051	120,5708303	95,4496042
16	16	H	8	7	6	1,0700000	109,3065444	23,0759313
17	17	H	10	8	7	1,0000000	118,6820021	-58,2636857
18	18	H	2	1	5	1,0700000	116,3817585	27,1385953
19	19	H	4	1	5	1,0700000	89,7842544	136,4217722
20	20	N	6	1	5	1,4700000	156,8416087	85,0754826
21	21	H	20	6	1	1,0000000	109,4712026	-136,9218564
22	22	H	20	6	1	0,8306589	121,8857948	60,4644215
23	23	H	6	1	5	1,0700000	85,3278797	-38,2733263

Structure 5

Structure	5							
Row	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral
1	1	Cd						
2	2	C	1			3,3584876		
3	3	S	2	1		1,7862637	44,2233814	
4	4	C	1	3	2	3,4362671	156,9424626	63,0394512
5	5	S	4	1	3	1,8654588	36,7238391	-117,7078438
6	6	C	1	5	4	3,5647169	112,1934993	11,8329972
7	7	O	1	6	5	2,3843158	3,7351025	141,6352163
8	8	N	6	1	5	1,3737735	136,9537578	-125,3417670
9	9	C	1	5	4	3,5847943	91,4762690	-117,1978483
10	10	O	1	9	5	2,5382397	12,6073012	-150,0139349
11	11	N	9	1	5	1,3832555	120,9182747	-102,1488042
12	12	H	2	1	5	1,1210913	85,2088234	42,2059427
13	13	H	2	1	5	1,1242718	133,2319459	155,3686193
14	14	H	4	1	5	1,1577890	85,0620041	-129,0037571
15	15	H	4	1	5	1,0531341	142,4770854	-8,4653966
16	16	H	8	6	1	1,0717041	116,9073834	175,0433829
17	17	H	11	9	1	1,0000000	116,2319336	147,7640621

18	18	H	9	1	5	1,0700000	118,0859323	51,6326223
19	19	H	8	6	1	1,0000000	126,9945849	16,2962736
20	20	H	6	1	5	1,0700000	109,8086918	53,7737889
21	21	H	2	1	5	1,0700000	106,4672609	-66,9018840
22	22	H	4	1	5	1,0700000	98,5478624	123,2335225
23	23	H	11	9	1	1,0000000	121,3933650	-35,3565268

Structure 6

Structure	6							
Row	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral
1	1	Cd						
2	2	C	1			3,2391686		
3	3	S	2	1		1,8496005	47,1229894	
4	4	C	1	3	2	3,3779621	152,7187992	72,6581906
5	5	S	4	1	3	1,8198745	43,0983436	-120,8282338
6	6	C	1	5	4	3,3457699	115,6160280	-2,9670864
7	7	O	1	6	5	2,4078679	15,9560581	64,0881540
8	8	N	6	1	5	1,3574127	136,9591460	-141,7955849
9	9	C	5	4	1	3,8509864	144,7291155	-88,5869292
10	10	O	1	5	4	2,8153391	73,5298844	-141,7729445
11	11	N	9	5	4	1,3751978	130,4160915	-164,0270275
12	12	H	2	1	5	1,0928347	70,8600476	34,7885543
13	13	H	2	1	5	1,0999719	139,2835370	116,9604625
14	14	H	4	1	5	1,1424089	92,3870810	-116,4103282
15	15	H	4	1	5	1,0658468	146,6915833	13,2459485
16	16	H	8	6	1	1,0089137	118,6497986	-122,4642673
17	17	H	11	9	5	1,0425964	108,4231743	104,1646795
18	18	H	4	1	5	1,0700000	94,0992718	132,9425188
19	19	H	6	1	5	1,0700000	106,0670838	70,6473576
20	20	H	8	6	1	1,0000000	128,6944073	49,6309715
21	21	H	9	5	4	1,0700000	104,0874010	-31,5649105
22	22	H	2	1	5	1,0700000	114,0389390	-72,9277595
23	23	H	11	9	5	1,0000000	129,1216605	-51,4142045

Structure 7

Structure	7							
Row	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral
1	1	Cd						
2	2	C	1			3,3495534		

3	3	O	1	2		2,3309809	13,8587813	
4	4	C	3	2	1	3,0552115	121,7736775	-109,8134140
5	5	O	1	3	2	2,4056964	71,3300184	-131,8064483
6	6	N	4	3	2	1,3531739	94,0248159	-80,0800670
7	7	H	6	4	3	1,0222893	116,8910734	123,3595505
8	8	C	1	3	2	3,4285571	125,1189854	137,1794531
9	9	S	8	1	3	1,9180055	45,6129459	1,2783649
10	10	H	8	1	3	1,0982366	123,1051870	82,9741415
11	11	H	8	1	3	1,0608695	64,0419398	177,3208275
12	12	C	1	3	2	3,3860029	95,5293844	-15,8543002
13	13	S	12	1	3	1,8026839	41,0995492	-136,3351883
14	14	H	12	1	3	1,0981114	147,5836129	-112,9413814
15	15	H	12	1	3	1,1463288	88,1562404	1,3341690
16	16	O	1	3	2	2,5819638	98,2131087	60,5821143
17	17	H	16	1	3	0,9488369	99,1010097	162,5190779
18	18	H	16	1	3	0,9081761	153,2044464	31,3807695
19	19	H	12	1	3	1,0700000	91,7040673	114,4840463
20	20	H	8	1	3	1,0700000	126,7549238	-83,4083152
21	21	H	6	4	3	1,0000000	127,9373263	-68,7488900
22	22	H	4	3	2	1,0700000	119,8304936	34,8169139
23	23	N	2	1	3	1,4700000	145,0073669	-11,8620517
24	24	H	23	2	1	1,0211803	129,3356481	-173,8815919
25	25	H	23	2	1	1,0211803	115,8072519	6,1184069
27	27	H	2	1	3	1,0700000	93,7704638	167,6345526