

The QUEST Database of Highly-Accurate Excitation Energies: Geometries

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Below are given the Cartesian coordinates of the compounds investigated in this study.
All structures are given in atomic units (bohrs).

S1 MAIN subset

S1.1 Acetaldehyde

CASRN: 75-07-0

Level of theory: CC3(Full)/*aug-cc-pVTZ*

C	-0.00234503	0.00000000	0.87125063
C	-1.75847785	0.00000000	-1.34973671
O	2.27947397	0.00000000	0.71968028
H	-0.92904537	0.00000000	2.73929404
H	-2.97955463	1.66046488	-1.25209463
H	-2.97955463	-1.66046488	-1.25209463
H	-0.70043433	0.00000000	-3.11066412

S1.2 Acetone

CASRN: 67-64-1

Level of theory: CC3(Full)/*aug-cc-pVTZ*

C	0.00000000	0.00000000	0.18807702
C	0.00000000	2.42007545	-1.31764698
C	0.00000000	-2.42007545	-1.31764698
O	0.00000000	0.00000000	2.48269094
H	0.00000000	4.03690733	-0.05185132
H	0.00000000	-4.03690733	-0.05185132
H	1.66061256	2.48420530	-2.53995285
H	-1.66061256	2.48420530	-2.53995285
H	1.66061256	-2.48420530	-2.53995285
H	-1.66061256	-2.48420530	-2.53995285

S1.3 Acetylene

CASRN: 74-86-2

Level of theory: CC3(Full)/*aug-cc-pVTZ*

Ground state

C	0.00000000	0.00000000	1.14048351
C	0.00000000	0.00000000	-1.14048351

H	0.00000000	0.00000000	3.14009043
H	0.00000000	0.00000000	-3.14009043

Trans excited state (1A_u state in the C_{2h} point group)

C	1.29567779	0.00000000	-0.01846047
C	-1.29567779	0.00000000	0.01846047
H	2.41938674	0.00000000	1.70881682
H	-2.41938674	0.00000000	-1.70881682

Cis excited state (1A_2 state in the C_{2v} point group)

C	0.00000000	1.26834508	-0.11726146
C	0.00000000	-1.26834508	-0.11726146
H	0.00000000	2.67282325	1.39629264
H	0.00000000	-2.67282325	1.39629264

S1.4 Acrolein

CASRN: 107-02-8

Level of theory: CC3(Full)/*aug*-cc-pVTZ

C	-1.11645072	-0.68348783	0.00000000
C	1.20647847	0.83714564	0.00000000
C	3.46831059	-0.28872636	0.00000000
O	-3.23666415	0.19187203	0.00000000
H	-0.80613858	-2.74747338	0.00000000
H	0.98699813	2.86613511	0.00000000
H	5.20930864	0.77443560	0.00000000
H	3.60951559	-2.33000749	0.00000000

S1.5 Aminobenzonitrile

CASRN: 873-74-5 (4-Aminobenzonitrile)

Level of theory: CC3(FC)/cc-pVTZ

C	0.00000000	0.00000000	-3.36820633
C	2.27829762	0.00000000	-2.01450309
C	-2.27829762	0.00000000	-2.01450309
C	0.00000000	0.00000000	1.93909521
C	2.27351166	0.00000000	0.59753796

C	-2.27351166	0.00000000	0.59753796
C	0.00000000	0.00000000	4.63257112
N	0.00000000	0.00000000	-5.94870080
N	0.00000000	0.00000000	6.83060124
H	4.04775542	0.00000000	-3.02611570
H	-4.04775542	0.00000000	-3.02611570
H	4.03704439	0.00000000	1.61551747
H	-4.03704439	0.00000000	1.61551747
H	-1.62177115	0.00000000	-6.91608217
H	1.62177115	0.00000000	-6.91608217

S1.6 Ammonia

CASRN: 7664-41-7

Level of theory: CC3(Full)/*aug*-cc-pVTZ

N	0.12804615	0.00000000	0.00000000
H	-0.59303935	0.88580079	-1.53425197
H	-0.59303935	-1.77160157	0.00000000
H	-0.59303935	0.88580079	1.53425197

S1.7 Aniline

CASRN: 62-53-3

Level of theory: CC3(FC)/cc-pVTZ – C_{2v} enforced

C	0.00000000	0.00000000	-1.78643569
C	2.27316118	0.00000000	-0.43457234
C	-2.27316118	0.00000000	-0.43457234
C	0.00000000	0.00000000	3.53007775
C	2.26327651	0.00000000	2.18912925
C	-2.26327651	0.00000000	2.18912925
N	0.00000000	0.00000000	-4.38230793
H	4.03982526	0.00000000	3.18807501
H	-4.03982526	0.00000000	3.18807501
H	0.00000000	0.00000000	5.56493193
H	4.04200589	0.00000000	-1.45016965
H	-4.04200589	0.00000000	-1.45016965
H	-1.62137595	0.00000000	-5.34754284
H	1.62137595	0.00000000	-5.34754284

S1.8 Azanaphthalene

CASRN: 255-53-8 (Pyrazino[2,3-*b*]pyrazine or 1,4,5,8-Tetraazanaphthalene)

Level of theory: CC3(Full)/cc-pVTZ

C	0.00000000	1.33735978	0.00000000
C	0.00000000	-1.33735978	0.00000000
C	4.26447087	1.34122299	0.00000000
C	-4.26447087	1.34122299	0.00000000
C	4.26447087	-1.34122299	0.00000000
C	-4.26447087	-1.34122299	0.00000000
N	2.18301381	2.68816340	0.00000000
N	-2.18301381	2.68816340	0.00000000
N	2.18301381	-2.68816340	0.00000000
N	-2.18301381	-2.68816340	0.00000000
H	6.03657953	2.35467535	0.00000000
H	-6.03657953	2.35467535	0.00000000
H	6.03657953	-2.35467535	0.00000000
H	-6.03657953	-2.35467535	0.00000000

S1.9 Azulene

CASRN: 275-51-4

Level of theory: CC3(FC)/cc-pVTZ

C	0.00000000	0.00000000	-5.08442654
C	2.16799436	0.00000000	-3.55850254
C	-2.16799436	0.00000000	-3.55850254
C	1.40560615	0.00000000	-1.02382432
C	-1.40560615	0.00000000	-1.02382432
C	0.00000000	0.00000000	4.72891515
C	2.38587647	0.00000000	3.61219185
C	-2.38587647	0.00000000	3.61219185
C	3.00158451	0.00000000	1.05184313
C	-3.00158451	0.00000000	1.05184313
H	0.00000000	0.00000000	-7.11850559
H	4.09656030	0.00000000	-4.20278074
H	-4.09656030	0.00000000	-4.20278074
H	0.00000000	0.00000000	6.77201689
H	3.96514987	0.00000000	4.90481753
H	-3.96514987	0.00000000	4.90481753
H	5.00047162	0.00000000	0.61482964
H	-5.00047162	0.00000000	0.61482964

S1.10 Benzene

CASRN: 71-43-2

Level of theory: CC3(Full)/*aug*-cc-pVTZ

C	0.00000000	2.63144965	0.00000000
C	-2.27890225	1.31572483	0.00000000
C	-2.27890225	-1.31572483	0.00000000
C	0.00000000	-2.63144965	0.00000000
C	2.27890225	-1.31572483	0.00000000
C	2.27890225	1.31572483	0.00000000
H	-4.04725813	2.33668557	0.00000000
H	-4.04725813	-2.33668557	0.00000000
H	0.00000000	-4.67337115	0.00000000
H	4.04725813	-2.33668557	0.00000000
H	4.04725813	2.33668557	0.00000000
H	0.00000000	4.67337115	0.00000000

S1.11 Benzonitrile

CASRN: 100-47-0

Level of theory: CC3(FC)/cc-pVTZ

C	0.00000000	0.00000000	-3.73018216
C	0.00000000	0.00000000	-1.02720486
C	2.28760421	0.00000000	0.28592358
C	-2.28760421	0.00000000	0.28592358
C	0.00000000	0.00000000	4.22270922
C	2.28059554	0.00000000	2.90986462
C	-2.28059554	0.00000000	2.90986462
N	0.00000000	0.00000000	-5.92640038
H	4.03930466	0.00000000	-0.75078588
H	-4.03930466	0.00000000	-0.75078588
H	4.04556576	0.00000000	3.92452034
H	-4.04556576	0.00000000	3.92452034
H	0.00000000	0.00000000	6.25892556

S1.12 Benzoquinone

CASRN: 106-51-4 (1,4-Benzoquinone)

Level of theory: CC3(Full)/*aug*-cc-pVTZ

C	2.71467427	0.00000000	0.00000000
C	-2.71467427	0.00000000	0.00000000
C	1.26645689	2.38719964	0.00000000
C	1.26645689	-2.38719964	0.00000000
C	-1.26645689	2.38719964	0.00000000
C	-1.26645689	-2.38719964	0.00000000
O	5.02607647	0.00000000	0.00000000
O	-5.02607647	0.00000000	0.00000000
H	2.37218673	4.10318853	0.00000000
H	2.37218673	-4.10318853	0.00000000
H	-2.37218673	4.10318853	0.00000000
H	-2.37218673	-4.10318853	0.00000000

S1.13 Benzothiadiazole

CASRN: 273-13-2 (2,1,3-Benzothiadiazole)

Level of theory: CC3(FC)/cc-pVTZ

S	0.00000000	0.00000000	4.12782363
N	0.00000000	2.37994968	2.16794907
N	0.00000000	-2.37994968	2.16794907
C	0.00000000	1.35464582	-0.15090868
C	0.00000000	-1.35464582	-0.15090868
C	0.00000000	2.70608821	-2.46599859
C	0.00000000	-2.70608821	-2.46599859
C	0.00000000	1.34964552	-4.66429754
C	0.00000000	-1.34964552	-4.66429754
H	0.00000000	4.74051264	-2.44976392
H	0.00000000	-4.74051264	-2.44976392
H	0.00000000	2.32640888	-6.45161040
H	0.00000000	-2.32640888	-6.45161040

S1.14 Benzoxadiazole

CASRN: 273-09-6 (2,1,3-Benzoxadiazole)

Level of theory: CC3(FC)/cc-pVTZ

O	0.00000000	0.00000000	4.23105351
N	0.00000000	2.15721782	2.80042430
N	0.00000000	-2.15721782	2.80042430
C	0.00000000	1.34474119	0.44505130

C	0.00000000	-1.34474119	0.44505130
C	0.00000000	2.73330026	-1.85469062
C	0.00000000	-2.73330026	-1.85469062
C	0.00000000	1.35965956	-4.03354365
C	0.00000000	-1.35965956	-4.03354365
H	0.00000000	4.76633138	-1.84544064
H	0.00000000	-4.76633138	-1.84544064
H	0.00000000	2.32124878	-5.82853313
H	0.00000000	-2.32124878	-5.82853313

S1.15 Beryllium

CASRN: 7440-41-7

Level of theory: N/A

Be	0.00000000	0.00000000	0.00000000
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S1.16 BF

CASRN: 13768-60-0 (Boron fluoride)

Level of theory: CC3(Full)/*aug-cc-pVTZ*

B	0.00000000	0.00000000	0.00000000
F	0.00000000	0.00000000	2.39729626

S1.17 BH

CASRN: 13766-26-2 (Boron hydride or borane)

Level of theory: CC3(Full)/*aug-cc-pVTZ*

Ground state

B	0.00000000	0.00000000	0.00000000
H	0.00000000	0.00000000	2.31089693

Excited state

B	0.00000000	0.00000000	0.00000000
H	0.00000000	0.00000000	2.27596436

S1.18 Borole

CASRN: 287-87-6

Level of theory: CC3(Full)/*aug-cc-pVTZ*

B	0.00000000	0.00000000	2.44991435
C	0.00000000	2.35991046	0.62561328
C	0.00000000	-2.35991046	0.62561328
C	0.00000000	1.42526648	-1.74135978
C	0.00000000	-1.42526648	-1.74135978
H	0.00000000	0.00000000	4.69246473
H	0.00000000	4.35732912	1.03002724
H	0.00000000	-4.35732912	1.03002724
H	0.00000000	2.51021632	-3.47247633
H	0.00000000	-2.51021632	-3.47247633

S1.19 Butadiene

CASRN: 106-99-0

Level of theory: CC3(Full)/*aug-cc-pVTZ*

C	1.14656244	0.00000000	0.75468820
C	-1.14656244	0.00000000	-0.75468820
C	3.48132647	0.00000000	-0.22482805
C	-3.48132647	0.00000000	0.22482805
H	0.90770978	0.00000000	2.78883925
H	-0.90770978	0.00000000	-2.78883925
H	3.77525814	0.00000000	-2.24895470
H	-3.77525814	0.00000000	2.24895470
H	5.13664967	0.00000000	0.96861890
H	-5.13664967	0.00000000	-0.96861890

S1.20 Carbon dimer

CASRN: 12070-15-4 (1,2-Ethynediyl)

Level of theory: CC3(Full)/*aug-cc-pVTZ*

C	0.00000000	0.00000000	1.17922927
C	0.00000000	0.00000000	-1.17922927

S1.21 Carbon dioxide

CASRN: 124-38-9

Level of theory: CC3(FC)/*aug-cc-pVTZ*

C	0.00000000	0.00000000	0.00000000
O	0.00000000	0.00000000	-2.20193016
O	0.00000000	0.00000000	2.20193016

S1.22 Carbonic acid

CASRN: 463-79-6

Level of theory: CC3(FC)/*aug-cc-pVTZ*

O	0.00000000	0.00000000	2.46279243
C	0.00000000	0.00000000	0.18750328
O	0.00000000	2.04786599	-1.29140793
O	0.00000000	-2.04786599	-1.29140793
H	0.00000000	3.47810449	-0.16385522
H	0.00000000	-3.47810449	-0.16385522

S1.23 Carbon monoxide

CASRN: 630-08-0

Level of theory: CC3(Full)/*aug-cc-pVTZ*

C	0.00000000	0.00000000	-1.24942055
O	0.00000000	0.00000000	0.89266692

S1.24 Carbon trimer

CASRN: 12075-35-3 (1,2-Propadiene-1,3-diylidene)

Level of theory: CC3(Full)/*aug-cc-pVTZ*

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	2.45345613
C	0.00000000	0.00000000	-2.45345613

S1.25 Carbonyl fluoride

CASRN: 353-50-4

Level of theory: CC3(Full)/*aug-cc-pVTZ*

C	0.00000000	0.00000000	-0.30652633
O	0.00000000	0.00000000	-2.52469534
F	0.00000000	2.00254958	1.16003038
F	0.00000000	-2.00254958	1.16003038

S1.26 CCl₂

CASRN: 1605-72-7 (Dichlorocarbene)

Level of theory: CC3(Full)/*aug-cc-pVTZ*

C	0.00000000	0.00000000	-1.60920674
Cl	0.00000000	2.65360612	0.27602958
Cl	0.00000000	-2.65360612	0.27602958

S1.27 CCIF

CASRN: 1691-88-9 (Chlorofluorocarbene)

Level of theory: CC3(Full)/*aug-cc-pVTZ*

C	0.29776085	0.00000000	1.47969075
F	2.16980264	0.00000000	-0.10569879
Cl	-2.46756349	0.00000000	-0.32822320

S1.28 CF₂

CASRN: 2154-59-8 (Difluorocarbene)

Level of theory: CC3(Full)/*aug-cc-pVTZ*

C	0.00000000	0.00000000	-1.14170749
F	0.00000000	1.94810617	0.36114458
F	0.00000000	-1.94810617	0.36114458

S1.29 Chlorobenzene

CASRN: 108-90-7

Level of theory: CC3(FC)/cc-pVTZ

Cl	0.00000000	0.00000000	-4.09694569
C	0.00000000	0.00000000	-0.80648356
C	2.28704058	0.00000000	0.47978453
C	-2.28704058	0.00000000	0.47978453
C	0.00000000	0.00000000	4.42840669
C	2.27492426	0.00000000	3.10862132
C	-2.27492426	0.00000000	3.10862132
H	4.03299260	0.00000000	-0.56250521
H	-4.03299260	0.00000000	-0.56250521
H	4.04398612	0.00000000	4.11768561
H	-4.04398612	0.00000000	4.11768561
H	0.00000000	0.00000000	6.46409111

S1.30 Criegee's Intermediate

CASRN: 56077-92-0 (Formaldehyde oxide)

Level of theory: CC3(Full)/*aug*-cc-pVTZ

C	-2.14193693	0.46449461	0.00000000
O	-0.12214743	-0.85046436	0.00000000
O	2.09779397	0.38347786	0.00000000
H	-3.86593284	-0.61908241	0.00000000
H	-1.98533536	2.49983926	0.00000000

S1.31 Cyanoacetylene

CASRN: 1070-71-9

Level of theory: CC3(Full)/*aug*-cc-pVTZ

Ground state

C	0.00000000	0.00000000	-3.59120182
C	0.00000000	0.00000000	-1.30693904
C	0.00000000	0.00000000	1.28880240
N	0.00000000	0.00000000	3.48692211
H	0.00000000	0.00000000	-5.59619886

Lowest excited state

C	1.99411175	0.00000000	2.81781077
C	-0.07304269	0.00000000	1.33125774
C	-0.63630126	0.00000000	-1.14556678
N	-1.39755756	0.00000000	-3.26154643
H	1.90749857	0.00000000	4.87279180

S1.32 Cyanoformaldehyde

CASRN: 4471-47-0

Level of theory: CC3(Full)/*aug-cc-pVTZ*

C	-0.91561483	0.00000000	-1.22522833
C	-0.01092219	0.00000000	1.39523175
N	0.64170259	0.00000000	3.48820325
O	0.50833684	0.00000000	-3.00337867
H	-2.97202213	0.00000000	-1.42565674

S1.33 Cyanogen

CASRN: 460-19-5 (Ethanedinitrile)

Level of theory: CC3(Full)/*aug-cc-pVTZ*

Ground state

C	0.00000000	0.00000000	1.30401924
C	0.00000000	0.00000000	-1.30401924
N	0.00000000	0.00000000	3.49784121
N	0.00000000	0.00000000	-3.49784121

Excited state

C	0.00000000	0.00000000	1.22784115
C	0.00000000	0.00000000	-1.22784115
N	0.00000000	0.00000000	3.56462559
N	0.00000000	0.00000000	-3.56462559

S1.34 Cyclobutadiene

CASRN: 1120-53-2

Level of theory: CC3(Full)/*aug-cc-pVTZ*

C	-1.47868321	-1.27004715	0.00000000
C	1.47868321	-1.27004715	0.00000000
C	-1.47868321	1.27004715	0.00000000
C	1.47868321	1.27004715	0.00000000
H	-2.91448237	-2.70994518	0.00000000
H	2.91448237	-2.70994518	0.00000000
H	-2.91448237	2.70994518	0.00000000
H	2.91448237	2.70994518	0.00000000

S1.35 Cyclopentadiene

CASRN: 542-92-7

Level of theory: CC3(Full)/*aug-cc-pVTZ*

C	0.00000000	0.00000000	-2.33113051
C	0.00000000	2.22209092	-0.56871188
C	0.00000000	-2.22209092	-0.56871188
C	0.00000000	1.38514451	1.83772922
C	0.00000000	-1.38514451	1.83772922
H	1.66130504	0.00000000	-3.56414299
H	-1.66130504	0.00000000	-3.56414299
H	0.00000000	4.16550405	-1.18116624
H	0.00000000	-4.16550405	-1.18116624
H	0.00000000	2.54514584	3.51352303
H	0.00000000	-2.54514584	3.51352303

S1.36 Cyclopentadienethione

CASRN: 77825-99-1 (2,4-Cyclopentadiene-1-thione)

Level of theory: CC3(Full)/*aug-cc-pVTZ*

C	0.00000000	0.00000000	0.54718884
C	0.00000000	2.23394142	-1.11648863
C	0.00000000	-2.23394142	-1.11648863
C	0.00000000	1.40618242	-3.52381930
C	0.00000000	-1.40618242	-3.52381930
S	0.00000000	0.00000000	3.63323789
H	0.00000000	4.14572930	-0.42732005
H	0.00000000	-4.14572930	-0.42732005
H	0.00000000	2.55090221	-5.20908210
H	0.00000000	-2.55090221	-5.20908210

S1.37 Cyclopentadienone

CASRN: 13177-38-3 (2,4-Cyclopentadien-1-one)

Level of theory: CC3(Full)/*aug*-cc-pVTZ

C	0.00000000	0.00000000	1.45232781
C	0.00000000	2.26718523	-0.25413145
C	0.00000000	-2.26718523	-0.25413145
C	0.00000000	1.41557636	-2.63852689
C	0.00000000	-1.41557636	-2.63852689
O	0.00000000	0.00000000	3.74438847
H	0.00000000	4.18416912	0.42151096
H	0.00000000	-4.18416912	0.42151096
H	0.00000000	2.53760914	-4.33851399
H	0.00000000	-2.53760914	-4.33851399

S1.38 Cyclopropene

CASRN: 2781-85-3

Level of theory: CC3(Full)/*aug*-cc-pVTZ

C	0.00000000	0.00000000	-1.66820880
C	0.00000000	1.22523906	0.90681419
C	0.00000000	-1.22523906	0.90681419
H	1.72255446	0.00000000	-2.77881149
H	-1.72255446	0.00000000	-2.77881149
H	0.00000000	2.97844519	1.92076771
H	0.00000000	-2.97844519	1.92076771

S1.39 Cyclopropenethione

CASRN: 69903-36-2

Level of theory: CC3(Full)/*aug*-cc-pVTZ

C	0.00000000	1.26230744	-2.86571925
C	0.00000000	-1.26230744	-2.86571925
C	0.00000000	0.00000000	-0.49233236
S	0.00000000	0.00000000	2.57821680
H	0.00000000	2.97773331	-3.95114059
H	0.00000000	-2.97773331	-3.95114059

S1.40 Cyclopropenone

CASRN: 2961-80-0

Level of theory: CC3(Full)/*aug-cc-pVTZ*

C	0.00000000	1.27491826	-1.86930519
C	0.00000000	-1.27491826	-1.86930519
C	0.00000000	0.00000000	0.51814554
O	0.00000000	0.00000000	2.79326776
H	0.00000000	2.92791371	-3.05679837
H	0.00000000	-2.92791371	-3.05679837

S1.41 Diacetylene

CASRN: 460-12-8

Level of theory: CC3(Full)/*aug-cc-pVTZ*

C	0.00000000	0.00000000	1.29447700
C	0.00000000	0.00000000	-1.29447700
C	0.00000000	0.00000000	3.58448429
C	0.00000000	0.00000000	-3.58448429
H	0.00000000	0.00000000	5.58943003
H	0.00000000	0.00000000	-5.58943003

S1.42 Diazete

CASRN: 287-42-3 (1,3-Diazete)

Level of theory: CC3(Full)/*aug-cc-pVTZ*

C	1.04088890	1.37023206	0.00000000
C	-1.04088890	-1.37023206	0.00000000
N	1.80420222	-0.93584807	0.00000000
N	-1.80420222	0.93584807	0.00000000
H	2.06402011	3.13844681	0.00000000
H	-2.06402011	-3.13844681	0.00000000

S1.43 Diazirine

CASRN: 157-22-2 (3*H*-Diazirine)

Level of theory: CC3(Full)/*aug-cc-pVTZ*

C	0.00000000	0.00000000	-0.26696099
H	0.00000000	1.75890895	-1.28616478
H	0.00000000	-1.75890895	-1.28616479
N	1.16058100	0.00000000	2.27183007
N	-1.16058100	0.00000000	2.27183007

S1.44 Diazomethane

CASRN: 334-88-3

Level of theory: CC3(Full)/*aug*-cc-pVTZ

Ground state

C	0.00000000	0.00000000	-2.30830005
N	0.00000000	0.00000000	0.14457890
N	0.00000000	0.00000000	2.29923216
H	0.00000000	1.79875201	-3.24272317
H	0.00000000	-1.79875201	-3.24272317

Excited state

C	1.80206107	0.00000000	-1.03389466
N	-0.01743713	0.00000000	0.84742344
N	-2.25203764	0.00000000	0.54034983
H	3.74280590	0.00000000	-0.44375913
H	1.20115546	0.00000000	-2.98380249

S1.45 Difluorodiazirine

CASRN: 693-85-6 (Difluoro-3*H*-diazirine)

Level of theory: CC3(Full)/*aug*-cc-pVTZ

C	0.00000000	0.00000000	-0.15283028
F	0.00000000	2.06077297	-1.57706828
F	0.00000000	-2.06077297	-1.57706828
N	1.20382241	0.00000000	2.20566821
N	-1.20382241	0.00000000	2.20566821

S1.46 Dimethylaminobenzonitrile

CASRN: 1197-19-9 (4-(Dimethylamino)benzonitrile)

Level of theory: CCSD(T)(FC)/cc-pVTZ

Planar

C	0.00000000	0.00000000	-1.96083197
C	2.27891314	0.00000000	-0.58294740
C	-2.27891314	0.00000000	-0.58294740
C	0.00000000	0.00000000	3.37434994
C	2.26711046	0.00000000	2.02803761
C	-2.26711046	0.00000000	2.02803761
C	0.00000000	0.00000000	6.06798788
C	2.36485177	0.00000000	-5.90186899
C	-2.36485177	0.00000000	-5.90186899
N	0.00000000	0.00000000	-4.53733249
N	0.00000000	0.00000000	8.26382999
H	4.06469412	0.00000000	-1.55103579
H	-4.06469412	0.00000000	-1.55103579
H	4.03369195	0.00000000	3.04099978
H	-4.03369195	0.00000000	3.04099978
H	1.96836611	0.00000000	-7.91292844
H	-1.96836611	0.00000000	-7.91292844
H	3.49551175	-1.67111709	-5.47003452
H	3.49551175	1.67111709	-5.47003452
H	-3.49551175	1.67111709	-5.47003452
H	-3.49551175	-1.67111709	-5.47003452

Twisted

C	0.00000000	0.00000000	-1.92629020
C	2.27225178	0.00000000	-0.58317962
C	-2.27225178	0.00000000	-0.58317962
C	0.00000000	0.00000000	3.35560653
C	2.28330254	0.00000000	2.03752961
C	-2.28330254	0.00000000	2.03752961
C	0.00000000	0.00000000	6.05799119
C	0.00000000	2.39191725	-5.88267373
C	0.00000000	-2.39191725	-5.88267373
N	0.00000000	0.00000000	-4.58434634
N	0.00000000	0.00000000	8.25212738
H	4.02777860	0.00000000	-1.61674521
H	-4.02777860	0.00000000	-1.61674521
H	4.03804248	0.00000000	3.06961213
H	-4.03804248	0.00000000	3.06961213
H	0.00000000	2.05258096	-7.90903256
H	0.00000000	-2.05258096	-7.90903256
H	1.66857920	3.52919279	-5.43615170

H	-1.66857920	3.52919279	-5.43615170
H	-1.66857920	-3.52919279	-5.43615170
H	1.66857920	-3.52919279	-5.43615170

S1.47 Dimethylaniline

CASRN: 121-69-7 (*N,N*-Dimethylaniline)

Level of theory: CCSD(T)(FC)/cc-pVTZ

C	0.00000000	0.00000000	4.89686867
C	2.25704297	0.00000000	3.55138467
C	-2.25704297	0.00000000	3.55138467
C	2.27412639	0.00000000	0.92841898
C	-2.27412639	0.00000000	0.92841898
C	0.00000000	0.00000000	-0.44595239
C	2.36139267	0.00000000	-4.39675011
C	-2.36139267	0.00000000	-4.39675011
N	0.00000000	0.00000000	-3.03916783
H	4.05922248	0.00000000	-0.04344476
H	-4.05922248	0.00000000	-0.04344476
H	4.03670718	0.00000000	4.54551891
H	-4.03670718	0.00000000	4.54551891
H	0.00000000	0.00000000	6.93154996
H	1.97020408	0.00000000	-6.40997108
H	-1.97020408	0.00000000	-6.40997108
H	3.49800498	-1.66955347	-3.96565000
H	3.49800498	1.66955347	-3.96565000
H	-3.49800498	1.66955347	-3.96565000
H	-3.49800498	-1.66955347	-3.96565000

S1.48 Dinitrogen

CASRN: 7727-37-9

Level of theory: CC3(Full)/*aug*-cc-pVTZ

N	0.00000000	0.00000000	1.04008632
N	0.00000000	0.00000000	-1.04008632

S1.49 Ethylene

CASRN: 74-85-1

Level of theory: CC3(Full)/*aug*-cc-pVTZ

C	0.00000000	1.26026583	0.00000000
C	0.00000000	-1.26026583	0.00000000
H	0.00000000	2.32345976	1.74287672
H	0.00000000	-2.32345976	1.74287672
H	0.00000000	2.32345976	-1.74287672
H	0.00000000	-2.32345976	-1.74287672

S1.50 Fluorobenzene

CASRN: 462-06-6

Level of theory: CC3(FC)/cc-pVTZ

F	0.00000000	0.00000000	-4.15873063
C	0.00000000	0.00000000	-1.61842149
C	2.29188824	0.00000000	-0.35805545
C	-2.29188824	0.00000000	-0.35805545
C	0.00000000	0.00000000	3.59063853
C	2.27621870	0.00000000	2.27153776
C	-2.27621870	0.00000000	2.27153776
H	4.02397454	0.00000000	-1.42355397
H	-4.02397454	0.00000000	-1.42355397
H	4.04329770	0.00000000	3.28356917
H	-4.04329770	0.00000000	3.28356917
H	0.00000000	0.00000000	5.62589878

S1.51 Formaldehyde

CASRN: 50-00-0

Level of theory: CC3(Full)/*aug*-cc-pVTZ

Ground state

C	0.00000000	0.00000000	-1.13947666
O	0.00000000	0.00000000	1.14402883
H	0.00000000	1.76627623	-2.23398653
H	0.00000000	-1.76627623	-2.23398653

Excited state

C	-0.09942705	0.00000000	1.27071070
O	0.01987299	0.00000000	-1.23280536
H	0.42778855	1.76729629	2.18470884
H	0.42778855	-1.76729629	2.18470884

S1.52 Formamide

CASRN: 75-12-7

Level of theory: CC3(Full)/*aug-cc-pVTZ*

C	0.00183118	0.00000000	0.79313299
O	2.26817156	0.00000000	0.43918824
N	-1.76886033	0.00000000	-1.06219243
H	-0.84133459	0.00000000	2.68872485
H	-1.21254414	0.00000000	-2.87596907
H	-3.61627502	0.00000000	-0.65031317

S1.53 Formylfluoride

CASRN: 1493-02-3 (Formyl fluoride)

Level of theory: CC3(Full)/*aug-cc-pVTZ*

C	0.00536098	0.00000000	0.75320959
O	2.17369813	0.00000000	0.22287752
H	-0.83846350	0.00000000	2.62640974
F	-1.84051320	0.00000000	-0.99373750

S1.54 Furan

CASRN: 110-00-9

Level of theory: CC3(Full)/*aug-cc-pVTZ*

C	0.00000000	2.06365826	-0.60051250
C	0.00000000	-2.06365826	-0.60051250
C	0.00000000	1.35348578	1.86336416
C	0.00000000	-1.35348578	1.86336416
O	0.00000000	0.00000000	-2.13945332
H	0.00000000	3.86337287	-1.53765695
H	0.00000000	-3.86337287	-1.53765695
H	0.00000000	2.59168789	3.47168051
H	0.00000000	-2.59168789	3.47168051

S1.55 Furofuran

CASRN: 251-24-1 (Furo[3,2-*b*]furan)

Level of theory: CC3(FC)/cc-pVTZ

C	0.06548932	1.28240874	0.00000000
C	-0.06548932	-1.28240874	0.00000000
C	-2.43794558	2.25427215	0.00000000
C	2.43794558	-2.25427215	0.00000000
C	-3.90023785	0.12403225	0.00000000
C	3.90023785	-0.12403225	0.00000000
O	2.50066120	2.07485533	0.00000000
O	-2.50066120	-2.07485533	0.00000000
H	-3.10620733	4.16541687	0.00000000
H	3.10620733	-4.16541687	0.00000000
H	-5.90761266	-0.13384378	0.00000000
H	5.90761266	0.13384378	0.00000000

S1.56 Glyoxal

CASRN: 107-22-2

Level of theory: CC3(Full)/*aug*-cc-pVTZ

C	1.21360282	0.75840215	0.00000000
C	-1.21360282	-0.75840215	0.00000000
O	3.25581408	-0.26453186	0.00000000
O	-3.25581408	0.26453186	0.00000000
H	0.96135276	2.81883243	0.00000000
H	-0.96135276	-2.81883243	0.00000000

S1.57 HCCl

CASRN: 2108-20-5 (Chlorocarbene)

Level of theory: CC3(Full)/*aug*-cc-pVTZ

H	-1.88068369	0.00000000	-0.14323924
Cl	2.28559426	0.00000000	-0.43261163
C	-0.40491057	0.00000000	1.32161964

S1.58 HCF

CASRN: 13453-52-6 (Fluorocarbene)

Level of theory: CC3(Full)/*aug-cc-pVTZ*

C	-0.13561085	0.00000000	1.20394474
F	1.85493976	0.00000000	-0.27610752
H	-1.71932891	0.00000000	-0.18206846

S1.59 HCN

CASRN: 74-90-8 (Hydrogen cyanide)

Level of theory: CC3(FC)/*aug-cc-pVTZ*

H	0.00000000	0.00000000	3.06256364
C	0.00000000	0.00000000	1.05824145
N	0.00000000	0.00000000	-1.12728289

S1.60 HCP

CASRN: 6829-52-3 (Phosphine, methylidyne-)

Level of theory: CC3(Full)/*aug-cc-pVTZ*

H	0.00000000	0.00000000	-4.03090449
C	0.00000000	0.00000000	-2.01691641
P	0.00000000	0.00000000	0.91401621

S1.61 Hexatriene

CASRN: 2235-12-3

Level of theory: CC3(Full)/*aug-cc-pVTZ*

C	1.14024826	0.56596845	0.00000000
C	-1.14024826	-0.56596845	0.00000000
C	3.51540649	-0.78907931	0.00000000
C	-3.51540649	0.78907931	0.00000000
C	5.78668151	0.33754155	0.00000000
C	-5.78668151	-0.33754155	0.00000000
H	1.23448067	2.61584039	0.00000000

H	-1.23448067	-2.61584039	0.00000000
H	3.40773630	-2.83459321	0.00000000
H	-3.40773630	2.83459321	0.00000000
H	5.95047109	2.37626316	0.00000000
H	-5.95047109	-2.37626316	0.00000000
H	7.51470672	-0.74809921	0.00000000
H	-7.51470672	0.74809921	0.00000000

S1.62 HNC

CASRN: 6914-07-4 (Hydrogen isocyanide)

Level of theory: CC3(FC)/*aug-cc-pVTZ*

H	0.00000000	0.00000000	2.79539858
N	0.00000000	0.00000000	0.91469554
C	0.00000000	0.00000000	-1.30215184

S1.63 HPO

CASRN: 13817-06-6 (Oxophosphine)

Level of theory: CC3(Full)/*aug-cc-pVTZ*

H	0.31668637	0.00000000	0.14072725
P	-0.80573521	0.00000000	2.65136926
O	1.43391190	0.00000000	4.38886277

S1.64 HPS

CASRN: 109306-51-6 (Thioxophosphine)

Level of theory: CC3(Full)/*aug-cc-pVTZ*

H	-2.56278959	0.00000000	2.36296006
P	0.09114182	0.00000000	1.82568543
S	0.07946992	0.00000000	-1.85778170

S1.65 HSiF

CASRN: 50561-30-3 (Fluorosilylene)

Level of theory: CC3(Full)/*aug-cc-pVTZ*

Si	-0.06438136	0.00000000	1.67253150
F	2.24990164	0.00000000	-0.33928119
H	-2.18552027	0.00000000	-0.28748154

S1.66 Hydrogen chloride

CASRN: 7647-01-0

Level of theory: CC3(Full)/*aug-cc-pVTZ*

Cl	0.00000000	0.00000000	-0.02489783
H	0.00000000	0.00000000	2.38483140

S1.67 Hydrogen peroxide

CASRN: 7722-84-1

Level of theory: CC3(FC)/*aug-cc-pVTZ*

O	-1.37083247	-0.11183297	-0.05928025
O	1.37083247	0.11183297	-0.05928025
H	-1.80587866	1.34729428	0.94082062
H	1.80587866	-1.34729428	0.94082062

S1.68 Hydrogen sulfide

CASRN: 7783-06-4

Level of theory: CC3(Full)/*aug-cc-pVTZ*

S	0.00000000	0.00000000	-0.50365086
H	0.00000000	1.81828105	1.25212288
H	0.00000000	-1.81828105	1.25212288

S1.69 Imidazole

CASRN: 288-32-4

Level of theory: CC3(Full)/*aug-cc-pVTZ*

C	0.41662795	2.06006259	0.00000000
C	-1.52618386	-1.62343163	0.00000000
C	1.04160471	-1.93007427	0.00000000
N	-1.90345764	0.94914956	0.00000000
N	2.24215443	0.38083431	0.00000000
H	0.65501634	4.07748278	0.00000000
H	-3.57500545	1.84103166	0.00000000
H	-3.06363894	-2.94559167	0.00000000
H	2.08673940	-3.67001102	0.00000000

S1.70 Isobutene

CASRN: 115-11-7

Level of theory: CC3(Full)/*aug-cc-pVTZ*

C	0.00000000	0.00000000	2.70790758
C	0.00000000	0.00000000	0.18431282
C	0.00000000	2.39894572	-1.32482735
C	0.00000000	-2.39894572	-1.32482735
H	0.00000000	1.74848405	3.76691310
H	0.00000000	-1.74848405	3.76691310
H	0.00000000	4.05897160	-0.10582007
H	0.00000000	-4.05897160	-0.10582007
H	1.66026992	2.48337908	-2.55086178
H	-1.66026992	2.48337908	-2.55086178
H	1.66026992	-2.48337908	-2.55086178
H	-1.66026992	-2.48337908	-2.55086178

S1.71 Ketene

CASRN: 463-51-4 (Ethenone)

Level of theory: CC3(Full)/*aug-cc-pVTZ*

Ground state

C	0.00000000	0.00000000	-2.44810151
C	0.00000000	0.00000000	0.03498545
O	0.00000000	0.00000000	2.23663914
H	0.00000000	1.77432079	-3.43705988
H	0.00000000	-1.77432079	-3.43705988

Excited state

C	2.04306304	0.00000000	-0.93056721
C	0.00400918	0.00000000	0.83531393
O	-2.23710378	0.00000000	0.46984584
H	1.63603518	0.00000000	-2.93687368
H	3.96212800	0.00000000	-0.26649149

S1.72 Maleimide

CASRN: 541-59-3 (*1H*-Pyrrole-2,5-dione)

Level of theory: CC3(Full)/*aug*-cc-pVTZ

C	0.00000000	2.17350401	0.25165554
C	0.00000000	-2.17350401	0.25165554
C	0.00000000	1.26218315	-2.42188951
C	0.00000000	-1.26218315	-2.42188951
N	0.00000000	0.00000000	1.72344743
O	0.00000000	4.32709218	1.01147397
O	0.00000000	-4.32709218	1.01147397
H	0.00000000	0.00000000	3.62206099
H	0.00000000	2.54941470	-3.99634348
H	0.00000000	-2.54941470	-3.99634348

S1.73 Methanimine

CASRN: 2053-29-4 (Formalimine)

Level of theory: CC3(Full)/*aug*-cc-pVTZ

C	0.10696646	0.00000000	1.11091130
N	0.10764012	0.00000000	-1.29677742
H	-1.59140953	0.00000000	2.27296652
H	1.90475160	0.00000000	2.09393982
H	-1.69956184	0.00000000	-1.96217482

S1.74 Methylene cyclopropene

CASRN: 4095-06-1

Level of theory: CC3(Full)/*aug*-cc-pVTZ

C	0.00000000	0.00000000	0.53512883
C	0.00000000	0.00000000	3.04739824

C	0.00000000	1.25042956	-1.88571561
C	0.00000000	-1.25042956	-1.88571561
H	0.00000000	2.96887531	-2.96270271
H	0.00000000	-2.96887531	-2.96270271
H	0.00000000	1.75335023	4.08608382
H	0.00000000	-1.75335023	4.08608382

S1.75 Naphthalene

CASRN: 91-20-3

Level of theory: CC3(Full)/cc-pVTZ

C	0.00000000	1.33999524	0.00000000
C	0.00000000	-1.33999524	0.00000000
C	2.33779858	2.63841577	0.00000000
C	-2.33779858	2.63841577	0.00000000
C	2.33779858	-2.63841577	0.00000000
C	-2.33779858	-2.63841577	0.00000000
C	4.57964958	1.33587048	0.00000000
C	-4.57964958	1.33587048	0.00000000
C	4.57964958	-1.33587048	0.00000000
C	-4.57964958	-1.33587048	0.00000000
H	2.32888235	4.67949410	0.00000000
H	-2.32888235	4.67949410	0.00000000
H	2.32888235	-4.67949410	0.00000000
H	-2.32888235	-4.67949410	0.00000000
H	6.34884007	2.34551705	0.00000000
H	-6.34884007	2.34551705	0.00000000
H	6.34884007	-2.34551705	0.00000000
H	-6.34884007	-2.34551705	0.00000000

S1.76 Nitroaniline

CASRN: 100-01-6 (4-Nitroaniline)

Level of theory: CC3(FC)/cc-pVTZ

C	0.00000000	0.00000000	-4.05915738
C	2.28068352	0.00000000	-2.70811066
C	-2.28068352	0.00000000	-2.70811066
C	0.00000000	0.00000000	1.19144079
C	2.28308329	0.00000000	-0.09681843

C	-2.28308329	0.00000000	-0.09681843
N	0.00000000	0.00000000	3.94052757
N	0.00000000	0.00000000	-6.63741535
O	2.04948184	0.00000000	5.01410797
O	-2.04948184	0.00000000	5.01410797
H	4.04799128	0.00000000	-3.72195018
H	-4.04799128	0.00000000	-3.72195018
H	4.02032559	0.00000000	0.95557275
H	-4.02032559	0.00000000	0.95557275
H	-1.62132329	0.00000000	-7.60488781
H	1.62132329	0.00000000	-7.60488781

S1.77 Nitrobenzene

CASRN: 98-95-3

Level of theory: CC3(FC)/cc-pVTZ

C	0.00000000	0.00000000	-0.33719774
C	2.29667056	0.00000000	0.92138137
C	-2.29667056	0.00000000	0.92138137
C	0.00000000	0.00000000	4.85826496
C	2.28247086	0.00000000	3.54756893
C	-2.28247086	0.00000000	3.54756893
N	0.00000000	0.00000000	-3.11429157
O	-2.05476165	0.00000000	-4.18095202
O	2.05476165	0.00000000	-4.18095202
H	4.02347357	0.00000000	-0.14769848
H	-4.02347357	0.00000000	-0.14769848
H	4.04624818	0.00000000	4.56388578
H	-4.04624818	0.00000000	4.56388578
H	0.00000000	0.00000000	6.89454456

S1.78 Nitrodimethylaniline

CASRN: 100-23-2 (*N,N*-Dimethyl-4-nitroaniline)

Level of theory: CCSD(T)(FC)/cc-pVTZ

C	0.00000000	0.00000000	-2.70893747
C	2.28286889	0.00000000	-1.33300281
C	-2.28286889	0.00000000	-1.33300281
C	0.00000000	0.00000000	2.57206374

C	2.27821428	0.00000000	1.27798588
C	-2.27821428	0.00000000	1.27798588
C	2.36504204	0.00000000	-6.64945038
C	-2.36504204	0.00000000	-6.64945038
N	0.00000000	0.00000000	-5.28314977
N	0.00000000	0.00000000	5.31851989
O	2.04957627	0.00000000	6.39360902
O	-2.04957627	0.00000000	6.39360902
H	4.06683325	0.00000000	-2.30372191
H	-4.06683325	0.00000000	-2.30372191
H	4.01906768	0.00000000	2.32551175
H	-4.01906768	0.00000000	2.32551175
H	1.96723800	0.00000000	-8.66013185
H	-1.96723800	0.00000000	-8.66013185
H	3.49498309	-1.67118066	-6.21739275
H	3.49498309	1.67118066	-6.21739275
H	-3.49498309	1.67118066	-6.21739275
H	-3.49498309	-1.67118066	-6.21739275

S1.79 Nitropyridine *N*-oxide

CASRN: 1124-33-0 (4-Nitropyridine *N*-oxide)

Level of theory: CCSD(T)(FC)/cc-pVTZ

C	0.00000000	0.00000000	-1.21738204
C	2.26825255	0.00000000	0.09038008
C	-2.26825255	0.00000000	0.09038008
C	2.22988276	0.00000000	2.68605086
C	-2.22988276	0.00000000	2.68605086
N	0.00000000	0.00000000	-3.96704616
N	0.00000000	0.00000000	4.00601244
O	0.00000000	0.00000000	6.38961931
O	-2.05398155	0.00000000	-5.02438491
O	2.05398155	0.00000000	-5.02438491
H	4.03491913	0.00000000	-0.90939267
H	-4.03491913	0.00000000	-0.90939267
H	3.88274506	0.00000000	3.86446617
H	-3.88274506	0.00000000	3.86446617

S1.80 Nitrosomethane

Level of theory: CC3(Full)/*aug*-cc-pVTZ

CASRN: 865-40-7

Ground state

C	-1.78426612	0.00000000	-1.07224050
N	-0.00541753	0.00000000	1.08060391
O	2.18814985	0.00000000	0.43452135
H	-0.77343975	0.00000000	-2.86415606
H	-2.97471478	1.66801808	-0.86424584
H	-2.97471478	-1.66801808	-0.86424584

Excited state

C	1.86306273	0.00000000	-1.06035094
N	0.00638693	0.00000000	1.02546010
O	-2.26923072	0.00000000	0.47699489
H	3.72600129	0.00000000	-0.21094854
H	1.58491147	1.68964774	-2.20977225
H	1.58491147	-1.68964774	-2.20977225

S1.81 Nitrous acid

CASRN: 7782-77-6

Level of theory: CC3(FC)/*aug-cc-pVTZ*

H	-3.27788005	0.93588010	0.00000000
N	0.29308547	0.93895729	0.00000000
O	-2.05678600	-0.42335161	0.00000000
O	2.00673459	-0.45764664	0.00000000

S1.82 Nitrous oxide

CASRN: 10024-97-2

Level of theory: CC3(FC)/*aug-cc-pVTZ*

N	0.00000000	0.00000000	0.13652607
N	0.00000000	0.00000000	2.27480281
O	0.00000000	0.00000000	-2.11104702

S1.83 Nitroxyl

CASRN: 14332-28-6

Level of theory: CC3(Full)/*aug*-cc-pVTZ

O	0.21099695	0.00000000	2.15462460
N	-0.44776863	0.00000000	-0.03589263
H	1.18163475	0.00000000	-1.17386890

S1.84 Octatetraene

CASRN: 1482-91-3

Level of theory: CC3(Full)/cc-pVTZ

C	1.19649232	0.64794934	0.00000000
C	-1.19649232	-0.64794934	0.00000000
C	3.45745137	-0.52964709	0.00000000
C	-3.45745137	0.52964709	0.00000000
C	5.85705040	0.77625595	0.00000000
C	-5.85705040	-0.77625595	0.00000000
C	8.10525884	-0.39700663	0.00000000
C	-8.10525884	0.39700663	0.00000000
H	1.14813002	2.69304901	0.00000000
H	-1.14813002	-2.69304901	0.00000000
H	3.50962357	-2.57436634	0.00000000
H	-3.50962357	2.57436634	0.00000000
H	5.78969253	2.81832245	0.00000000
H	-5.78969253	-2.81832245	0.00000000
H	8.22516217	-2.43500100	0.00000000
H	-8.22516217	2.43500100	0.00000000
H	9.85247043	0.65022932	0.00000000
H	-9.85247043	-0.65022932	0.00000000

S1.85 Oxalyl fluoride

CASRN: 359-40-0

Level of theory: CC3(Full)/*aug*-cc-pVTZ

C	-1.39903565	0.34476183	0.00000000
C	1.39903565	-0.34476183	0.00000000
O	-2.24825627	2.40855549	0.00000000

O	2.24825627	-2.40855549	0.00000000
F	-2.78737061	-1.74488227	0.00000000
F	2.78737061	1.74488227	0.00000000

S1.86 Pentalene

CASRN: 250-25-9

Level of theory: CC3(FC)/cc-pVTZ

C	-0.07378347	1.37547375	0.00000000
C	0.07378347	-1.37547375	0.00000000
C	2.30364735	2.30974227	0.00000000
C	-2.30364735	-2.30974227	0.00000000
C	4.08788978	0.11767244	0.00000000
C	-4.08788978	-0.11767244	0.00000000
C	2.75907835	-2.07144063	0.00000000
C	-2.75907835	2.07144063	0.00000000
H	2.88453811	4.25947081	0.00000000
H	-2.88453811	-4.25947081	0.00000000
H	6.11180520	0.29622071	0.00000000
H	-6.11180520	-0.29622071	0.00000000
H	3.52044397	-3.95397547	0.00000000
H	-3.52044397	3.95397547	0.00000000

Level of theory: CC3(FC)/cc-pVTZ [D_{2h} constrained]

C	0.00000000	-1.32183553	0.00000000
C	4.12643396	0.00000000	0.00000000
C	0.00000000	1.32183553	0.00000000
C	-4.12643396	0.00000000	0.00000000
C	2.55477535	-2.15447186	0.00000000
C	-2.55477535	-2.15447186	0.00000000
C	2.55477535	2.15447186	0.00000000
C	-2.55477535	2.15447186	0.00000000
H	6.15419256	0.00000000	0.00000000
H	-6.15419256	0.00000000	0.00000000
H	3.20834414	-4.08294363	0.00000000
H	-3.20834414	-4.08294363	0.00000000
H	3.20834414	4.08294363	0.00000000
H	-3.20834414	4.08294363	0.00000000

S1.87 Phenol

CASRN: 108-95-2

Level of theory: CC3(FC)/cc-pVTZ

C	-3.53896151	-0.00090430	0.00000000
C	-2.20193059	-2.26940360	0.00000000
C	0.42215955	-2.27848829	0.00000000
C	1.72887083	0.00401463	0.00000000
C	0.41326561	2.28038150	0.00000000
C	-2.21662249	2.26943538	0.00000000
O	4.30714712	-0.10549070	0.00000000
H	-5.57402535	-0.00548883	0.00000000
H	-3.20490358	-4.04260115	0.00000000
H	1.47915023	-4.01756951	0.00000000
H	1.43787439	4.04468538	0.00000000
H	-3.22333595	4.04049312	0.00000000
H	4.94381975	1.59474054	0.00000000

S1.88 Phenolate

CASRN: 3229-70-7

Level of theory: CC3(FC)/cc-pVTZ

C	0.00000000	0.00000000	-1.94817868
C	2.27737723	0.00000000	-0.45104645
C	-2.27737723	0.00000000	-0.45104645
C	0.00000000	0.00000000	3.54287236
C	2.25856599	0.00000000	2.16672471
C	-2.25856599	0.00000000	2.16672471
O	0.00000000	0.00000000	-4.33677175
H	4.04811102	0.00000000	-1.47084405
H	-4.04811102	0.00000000	-1.47084405
H	4.04319440	0.00000000	3.17158878
H	-4.04319440	0.00000000	3.17158878
H	0.00000000	0.00000000	5.58190673

S1.89 Phenyl-pyrrole

CASRN: 635-90-5 (*N*-Phenylpyrrole)

Level of theory: CCSD(T)(FC)/cc-pVTZ

Planar

C	0.00000000	0.00000000	0.78511855
C	2.26951425	0.00000000	2.12513335
C	-2.26951425	0.00000000	2.12513335
C	0.00000000	0.00000000	6.08505036
C	2.26188550	0.00000000	4.74952804
C	-2.26188550	0.00000000	4.74952804
C	2.11189435	0.00000000	-3.40622062
C	-2.11189435	0.00000000	-3.40622062
C	1.34457992	0.00000000	-5.87759851
C	-1.34457992	0.00000000	-5.87759851
N	0.00000000	0.00000000	-1.87596109
H	4.04529764	0.00000000	1.13844406
H	-4.04529764	0.00000000	1.13844406
H	4.03918748	0.00000000	5.74456463
H	-4.03918748	0.00000000	5.74456463
H	0.00000000	0.00000000	8.12006610
H	3.97993856	0.00000000	-2.63372956
H	-3.97993856	0.00000000	-2.63372956
H	2.56993408	0.00000000	-7.49221560
H	-2.56993408	0.00000000	-7.49221560

Twisted

C	0.00000000	0.00000000	0.80351712
C	2.28073444	0.00000000	2.10816686
C	-2.28073444	0.00000000	2.10816686
C	0.00000000	0.00000000	6.05091031
C	2.27731959	0.00000000	4.73583348
C	-2.27731959	0.00000000	4.73583348
C	0.00000000	2.11496090	-3.38187966
C	0.00000000	-2.11496090	-3.38187966
C	0.00000000	1.34265418	-5.86240596
C	0.00000000	-1.34265418	-5.86240596
N	0.00000000	0.00000000	-1.87814812
H	4.02558097	0.00000000	1.05801658
H	-4.02558097	0.00000000	1.05801658
H	4.04316226	0.00000000	5.75023395
H	-4.04316226	0.00000000	5.75023395
H	0.00000000	0.00000000	8.08702673
H	0.00000000	3.96297102	-2.54995976
H	0.00000000	-3.96297102	-2.54995976
H	0.00000000	2.56243264	-7.48144109
H	0.00000000	-2.56243264	-7.48144109

S1.90 Phthalazine

CASRN: 253-52-1

Level of theory: CC3(FC)/cc-pVTZ

C	0.00000000	1.32459443	-0.07132677
C	0.00000000	-1.32459443	-0.07132677
C	0.00000000	2.65486490	-2.37693013
C	0.00000000	-2.65486490	-2.37693013
C	0.00000000	1.33510515	-4.61541123
C	0.00000000	-1.33510515	-4.61541123
C	0.00000000	2.49806192	2.33813333
C	0.00000000	-2.49806192	2.33813333
N	0.00000000	1.29575320	4.50170701
N	0.00000000	-1.29575320	4.50170701
H	0.00000000	4.69409431	-2.36246981
H	0.00000000	-4.69409431	-2.36246981
H	0.00000000	2.33538579	-6.38945264
H	0.00000000	-2.33538579	-6.38945264
H	0.00000000	4.53863166	2.46976178
H	0.00000000	-4.53863166	2.46976178

S1.91 Propynal

CASRN: 624-67-9

Level of theory: CC3(Full)/*aug*-cc-pVTZ

C	-0.78051115	0.00000000	-1.38900384
C	-0.17873562	0.00000000	1.27825868
C	0.23763714	0.00000000	3.52644798
O	0.80143996	0.00000000	-3.04628328
H	-2.80713069	0.00000000	-1.82768750
H	0.64026209	0.00000000	5.48853193

S1.92 Pyranone

CASRN: 108-97-4 (4*H*-Pyran-4-one)

Level of theory: CC3(FC)/cc-pVTZ

C	0.00000000	0.00000000	-2.03875103
C	2.29857501	0.00000000	-0.50612872

C	-2.29857501	0.00000000	-0.50612872
C	2.18356567	0.00000000	2.02781371
C	-2.18356567	0.00000000	2.02781371
O	0.00000000	0.00000000	3.36810442
O	0.00000000	0.00000000	-4.35224344
H	3.80117763	0.00000000	3.26042029
H	-3.80117763	0.00000000	3.26042029
H	4.10758504	0.00000000	-1.43183287
H	-4.10758504	0.00000000	-1.43183287

S1.93 Pyrazine

CASRN: 290-37-9

Level of theory: CC3(Full)/*aug-cc-pVTZ*

C	0.00000000	2.13188686	1.31510863
C	0.00000000	-2.13188686	1.31510863
C	0.00000000	2.13188686	-1.31510863
C	0.00000000	-2.13188686	-1.31510863
N	0.00000000	0.00000000	2.66620111
N	0.00000000	0.00000000	-2.66620111
H	0.00000000	3.88751412	2.35234226
H	0.00000000	-3.88751412	2.35234226
H	0.00000000	3.88751412	-2.35234226
H	0.00000000	-3.88751412	-2.35234226

S1.94 Pyridazine

CASRN: 289-80-5

Level of theory: CC3(Full)/*aug-cc-pVTZ*

C	0.00000000	1.30150855	-2.31552865
C	0.00000000	-1.30150855	-2.31552865
C	0.00000000	2.49271907	0.03513416
C	0.00000000	-2.49271907	0.03513416
N	0.00000000	1.26228251	2.23104685
N	0.00000000	-1.26228251	2.23104685
H	0.00000000	4.52804172	0.19299731
H	0.00000000	-4.52804172	0.19299731
H	0.00000000	2.39011496	-4.03967703
H	0.00000000	-2.39011496	-4.03967703

S1.95 Pyridine

CASRN: 110-86-1

Level of theory: CC3(Full)/*aug*-cc-pVTZ

C	0.00000000	0.00000000	-2.66451139
C	0.00000000	2.25494985	-1.32069889
C	0.00000000	-2.25494985	-1.32069889
C	0.00000000	2.15398594	1.30669632
C	0.00000000	-2.15398594	1.30669632
N	0.00000000	0.00000000	2.62778932
H	0.00000000	0.00000000	-4.70641516
H	0.00000000	4.05768507	-2.27625442
H	0.00000000	-4.05768507	-2.27625442
H	0.00000000	3.88059079	2.40341581
H	0.00000000	-3.88059079	2.40341581

S1.96 Pyridinium

CASRN: 16969-45-2

Level of theory: CC3(FC)/cc-pVTZ

C	0.00000000	0.00000000	-2.66667191
C	2.28175579	0.00000000	-1.35203950
C	-2.28175579	0.00000000	-1.35203950
C	2.23916852	0.00000000	1.25404098
C	-2.23916852	0.00000000	1.25404098
N	0.00000000	0.00000000	2.46287949
H	0.00000000	0.00000000	-4.70272202
H	4.06725168	0.00000000	-2.32197291
H	-4.06725168	0.00000000	-2.32197291
H	3.90684584	0.00000000	2.41825457
H	-3.90684584	0.00000000	2.41825457
H	0.00000000	0.00000000	4.37535718

S1.97 Pyrimidine

CASRN: 289-95-2

Level of theory: CC3(Full)/*aug*-cc-pVTZ

C	0.00000000	0.00000000	2.41518350
C	0.00000000	0.00000000	-2.60410885
C	0.00000000	2.23272561	-1.22869402
C	0.00000000	-2.23272561	-1.22869402
N	0.00000000	2.26214196	1.29619742
N	0.00000000	-2.26214196	1.29619742
H	0.00000000	0.00000000	4.45780256
H	0.00000000	0.00000000	-4.64120942
H	0.00000000	4.05149341	-2.16351748
H	0.00000000	-4.05149341	-2.16351748

S1.98 Pyrrole

CASRN: 109-97-7

Level of theory: CC3(Full)/*aug*-cc-pVTZ

C	0.00000000	2.11924634	0.62676569
C	0.00000000	-2.11924634	0.62676569
C	0.00000000	1.34568862	-1.85506908
C	0.00000000	-1.34568862	-1.85506908
N	0.00000000	0.00000000	2.10934391
H	0.00000000	0.00000000	4.00257355
H	0.00000000	3.97648410	1.44830201
H	0.00000000	-3.97648410	1.44830201
H	0.00000000	2.56726559	-3.47837232
H	0.00000000	-2.56726559	-3.47837232

S1.99 Pyrrolopyrrole

CASRN: 250-87-3 (Pyrrolo[3,2-*b*]pyrrole)

Level of theory: CC3(FC)/cc-pVTZ

C	0.01987029	1.31191436	0.00000000
C	-0.01987029	-1.31191436	0.00000000
C	-2.50055820	2.23026347	0.00000000
C	2.50055820	-2.23026347	0.00000000
C	-3.99867844	0.09474099	0.00000000
C	3.99867844	-0.09474099	0.00000000
N	2.50780926	2.04699311	0.00000000
N	-2.50780926	-2.04699311	0.00000000
H	-3.17172573	4.14262242	0.00000000

H	3.17172573	-4.14262242	0.00000000
H	-6.02037705	-0.05658473	0.00000000
H	6.02037705	0.05658473	0.00000000
H	3.16071224	3.82066088	0.00000000
H	-3.16071224	-3.82066088	0.00000000

S1.100 Quinoxaline

CASRN: 91-19-0

Level of theory: CC3(FC)/cc-pVTZ

C	0.00000000	1.33833541	0.04624026
C	0.00000000	-1.33833541	0.04624026
C	0.00000000	2.65319151	-2.27752466
C	0.00000000	-2.65319151	-2.27752466
C	0.00000000	1.33717941	-4.51073479
C	0.00000000	-1.33717941	-4.51073479
C	0.00000000	1.33936683	4.32768896
C	0.00000000	-1.33936683	4.32768896
N	0.00000000	2.68409862	2.24219152
N	0.00000000	-2.68409862	2.24219152
H	0.00000000	4.68915946	-2.22328575
H	0.00000000	-4.68915946	-2.22328575
H	0.00000000	2.33972888	-6.28367426
H	0.00000000	-2.33972888	-6.28367426
H	0.00000000	2.35369837	6.10018213
H	0.00000000	-2.35369837	6.10018213

S1.101 SiCl₂

CASRN: 13569-32-9 (Dichlorosilylene)

Level of theory: CC3(Full)/*aug*-cc-pVTZ

Si	0.00000000	0.00000000	-1.78528322
Cl	0.00000000	3.04414528	0.71619419
Cl	0.00000000	-3.04414528	0.71619419

S1.102 Silylidene

CASRN: 65632-07-7

Level of theory: CC3(Full)/*aug-cc-pVTZ*

C	0.00000000	0.00000000	-2.09539928
Si	0.00000000	0.00000000	1.14992930
H	0.00000000	1.70929524	-3.22894481
H	0.00000000	-1.70929524	-3.22894481

S1.103 Streptocyanine-C1

CASRN:

Level of theory: CC3(Full)/*aug-cc-pVTZ*, Charge: +1

C	0.00000000	0.00000000	0.80488833
N	0.00000000	2.19423463	-0.33580561
N	0.00000000	-2.19423463	-0.33580561
H	0.00000000	0.00000000	2.84436959
H	0.00000000	2.36978315	-2.23371976
H	0.00000000	-2.36978315	-2.23371976
H	0.00000000	3.79412648	0.69399206
H	0.00000000	-3.79412648	0.69399206

S1.104 Streptocyanine-C3

CASRN:

Level of theory: CC3(Full)/*aug-cc-pVTZ*, Charge: +1

C	0.00000000	0.00000000	0.65419136
C	0.00000000	2.24294899	-0.68901318
C	0.00000000	-2.24294899	-0.68901318
N	0.00000000	4.52279187	0.30876781
N	0.00000000	-4.52279187	0.30876781
H	0.00000000	0.00000000	2.69658250
H	0.00000000	2.18484165	-2.73430592
H	0.00000000	-2.18484165	-2.73430592
H	0.00000000	6.07453303	-0.78935070
H	0.00000000	-6.07453303	-0.78935070
H	0.00000000	4.78699964	2.19452692
H	0.00000000	-4.78699964	2.19452692

S1.105 Streptocyanine-C5

CASRN:

Level of theory: CC3(Full)/cc-pVTZ, Charge: +1

C	0.00000000	0.00000000	0.46857445
C	0.00000000	2.33439812	-0.72581892
C	0.00000000	-2.33439812	-0.72581892
C	0.00000000	4.51630408	0.70773577
C	0.00000000	-4.51630408	0.70773577
N	0.00000000	6.84533147	-0.19544059
N	0.00000000	-6.84533147	-0.19544059
H	0.00000000	0.00000000	2.51676448
H	0.00000000	2.44956750	-2.76140399
H	0.00000000	-2.44956750	-2.76140399
H	0.00000000	4.36770843	2.74488884
H	0.00000000	-4.36770843	2.74488884
H	0.00000000	8.34616080	0.96591148
H	0.00000000	-8.34616080	0.96591148
H	0.00000000	7.18140877	-2.06656349
H	0.00000000	-7.18140877	-2.06656349

S1.106 Tetrathiafulvalene

CASRN: 31366-25-3

Level of theory: CC3(FC)/cc-pVTZ

C	-1.27140171	0.00000000	0.00000000
C	1.27140171	0.00000000	0.00000000
C	-5.98994256	1.26331812	0.00000000
C	-5.98994256	-1.26331812	0.00000000
C	5.98994256	-1.26331812	0.00000000
C	5.98994256	1.26331812	0.00000000
S	-3.07078317	2.82030107	0.00000000
S	-3.07078317	-2.82030107	0.00000000
S	3.07078317	-2.82030107	0.00000000
S	3.07078317	2.82030107	0.00000000
H	-7.66536437	2.41057807	0.00000000
H	-7.66536437	-2.41057807	0.00000000
H	7.66536437	-2.41057807	0.00000000
H	7.66536437	2.41057807	0.00000000

S1.107 Tetrazine

CASRN: 290-96-0 (*s*-Tetrazine)

Level of theory: CC3(Full)/*aug*-cc-pVTZ

C	0.00000000	0.00000000	2.38208164
C	0.00000000	0.00000000	-2.38208164
N	2.25673244	0.00000000	1.24973261
N	-2.25673244	0.00000000	1.24973261
N	2.25673244	0.00000000	-1.24973261
N	-2.25673244	0.00000000	-1.24973261
H	0.00000000	0.00000000	4.41850901
H	0.00000000	0.00000000	-4.41850901

S1.108 Thienothiophene

CASRN: 251-41-2 (Thieno[3,2-*b*]thiophene)

Level of theory: CC3(FC)/cc-pVTZ

C	0.41618901	1.24091123	0.00000000
C	-0.41618901	-1.24091123	0.00000000
C	-1.56128826	3.05660382	0.00000000
C	1.56128826	-3.05660382	0.00000000
C	-3.86882315	1.90421786	0.00000000
C	3.86882315	-1.90421786	0.00000000
S	3.68518133	1.37661050	0.00000000
S	-3.68518133	-1.37661050	0.00000000
H	-1.30761309	5.07161572	0.00000000
H	1.30761309	-5.07161572	0.00000000
H	-5.68944011	2.79705270	0.00000000
H	5.68944011	-2.79705270	0.00000000

S1.109 Thioacetone [CC3(full)/*aug*-cc-pVTZ]

C	0.00000000	0.00000000	0.68476030
C	0.00000000	2.38541696	2.20685096
C	0.00000000	-2.38541696	2.20685096
S	0.00000000	0.00000000	-2.39920303
H	0.00000000	4.04609254	1.00090614
H	0.00000000	-4.04609254	1.00090614

H	1.65894780	2.42602225	3.43712000
H	-1.65894780	2.42602225	3.43712000
H	1.65894780	-2.42602225	3.43712000
H	-1.65894780	-2.42602225	3.43712000

S1.110 Thioacetone

CASRN: 4756-05-2 (2-Propanethione)

Level of theory: CC3(Full)/*aug-cc-pVTZ*

C	0.00000000	0.00000000	0.68476030
C	0.00000000	2.38541696	2.20685096
C	0.00000000	-2.38541696	2.20685096
S	0.00000000	0.00000000	-2.39920303
H	0.00000000	4.04609254	1.00090614
H	0.00000000	-4.04609254	1.00090614
H	1.65894780	2.42602225	3.43712000
H	-1.65894780	2.42602225	3.43712000
H	1.65894780	-2.42602225	3.43712000
H	-1.65894780	-2.42602225	3.43712000

S1.111 Thioacrolein

CASRN: 53439-64-8 (2-Propenethial)

Level of theory: CC3(Full)/*aug-cc-pVTZ*

C	4.27693176	0.00000000	-0.88320133
C	1.76449030	0.00000000	-1.23998444
C	0.00891877	0.00000000	0.85393278
S	-3.06510749	0.00000000	0.58558716
H	5.57642075	0.00000000	-2.45571463
H	5.06950243	0.00000000	1.00139499
H	0.96616458	0.00000000	-3.11935314
H	0.87110201	0.00000000	2.71756937

S1.112 Thioformaldehyde

CASRN: 865-36-1 (Methanethial)

Level of theory: CC3(Full)/*aug-cc-pVTZ*

Ground state

C	0.00000000	0.00000000	-2.08677304
S	0.00000000	0.00000000	0.97251194
H	0.00000000	1.73657773	-3.17013507
H	0.00000000	-1.73657773	-3.17013507

Excited state

C	0.00000000	0.00000000	-2.20256705
S	0.00000000	0.00000000	1.02717172
H	0.00000000	1.76634191	-3.21909384
H	0.00000000	-1.76634191	-3.21909384

S1.113 Thioformaldehyde-S-oxide

CASRN: 40100-16-1 (Methanethial, S-oxide)

Level of theory: CC3(Full)/*aug*-cc-pVTZ

C	-2.60499135	0.77983525	0.00000000
O	2.33211975	0.83760351	0.00000000
S	0.03093612	-0.78961636	0.00000000
H	-4.30439246	-0.34582852	0.00000000
H	-2.67226676	2.81674398	0.00000000

S1.114 Thiophene

CASRN: 110-02-1

Level of theory: CC3(Full)/*aug*-cc-pVTZ

C	0.00000000	2.33342542	-0.09858421
C	0.00000000	-2.33342542	-0.09858421
C	0.00000000	1.34371718	-2.48297725
C	0.00000000	-1.34371718	-2.48297725
S	0.00000000	0.00000000	2.17250692
H	0.00000000	4.29028016	0.44577296
H	0.00000000	-4.29028016	0.44577296
H	0.00000000	2.48760051	-4.16768392
H	0.00000000	-2.48760051	-4.16768392

S1.115 Thiopropynal

CASRN: 83797-21-1 (2-Propynethial)

Level of theory: CC3(Full)/*aug-cc-pVTZ*

C	-0.00382924	0.00000000	-1.25249909
C	-2.27832423	0.00000000	0.15152736
C	-4.26309583	0.00000000	1.29548793
S	2.81920288	0.00000000	-0.00828974
H	-0.23056990	0.00000000	-3.28862183
H	-5.97712967	0.00000000	2.33206931

S1.116 Triazapentalene

CASRN: 431877-36-0 (1,3a,6a-Triazapentalene)

Level of theory: CC3(FC)/cc-pVTZ

C	-2.50499953	2.11638523	0.00000000
C	-3.96445816	-0.07303868	0.00000000
C	-2.35355924	-2.15265577	0.00000000
C	3.83593935	-0.03073106	0.00000000
C	2.43560744	2.16757403	0.00000000
N	0.04006152	-1.21957559	0.00000000
N	-0.04182459	1.35780418	0.00000000
N	2.39603035	-2.14324663	0.00000000
H	-3.00087038	4.07607227	0.00000000
H	-5.98766760	-0.14484657	0.00000000
H	-2.68330099	-4.14581320	0.00000000
H	5.85502782	-0.19299220	0.00000000
H	2.92994089	4.12450552	0.00000000

S1.117 Triazine

CASRN: 290-88-3 (*s*-Triazine)

Level of theory: CC3(Full)/*aug-cc-pVTZ*

C	0.00000000	-2.11414732	-1.22060353
C	0.00000000	0.00000000	2.44120705
C	0.00000000	2.11414732	-1.22060353
N	0.00000000	-2.24624733	1.29687150
N	0.00000000	2.24624733	1.29687150

N	0.00000000	0.00000000	-2.59374300
H	0.00000000	3.88296710	-2.24183210
H	0.00000000	-3.88296710	-2.24183210
H	0.00000000	0.00000000	4.48366420

S1.118 Water

CASRN: 7732-18-5

Level of theory: CC3(Full)/*aug*-cc-pVTZ

O	0.00000000	0.00000000	-0.13209669
H	0.00000000	1.43152878	0.97970006
H	0.00000000	-1.43152878	0.97970006

S2 RAD subset

S2.1 AlCH₂

CASRN: 76392-50-2

Level of theory: RO-CCSD(T)(Full)/*aug-cc-pVTZ*

Al	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	3.71178683
H	1.67494363	0.00000000	4.90780205
H	-1.67494363	0.00000000	4.90780205

S2.2 Allyl

CASRN: 1981-80-2

Level of theory: U-CCSD(T)(Full)/*aug-cc-pVTZ*

C	0.00000000	0.00000000	0.84490222
C	0.00000000	2.30981224	0.37283352
C	0.00000000	-2.30981224	-0.37283352
H	0.00000000	0.00000000	2.88986557
H	0.00000000	4.06036949	0.67000051
H	0.00000000	-4.06036949	0.67000051
H	0.00000000	2.41059890	-2.41263791

S2.3 BeF

CASRN: 13597-96-1

Level of theory: U-CCSD(T)(FC)/*aug-cc-pVTZ* [Only F's 1s frozen]

Be	0.00000000	0.00000000	-1.77936990
F	0.00000000	0.00000000	0.79083149

S2.4 BeH

CASRN: 13597-97-2

Level of theory: U-CCSD(T)(Full)/*aug-cc-pVTZ*

Be	0.00000000	0.00000000	0.25103976
H	0.00000000	0.00000000	-2.24485003

S2.5 BH₂

CASRN: 14452-64-3

Level of theory: U-CCSD(T)(Full)/*aug-cc-pVTZ*

B	0.00000000	0.00000000	0.14984923
H	0.00000000	2.01119016	-0.81846345
H	0.00000000	-2.01119016	-0.81846345

S2.6 BO₂

CASRN: 13840-88-5

Level of theory: U-CCSD(T)(Full)/*aug-cc-pVTZ*

B	0.00000000	0.00000000	0.00000000
O	0.00000000	0.00000000	2.39114228
O	0.00000000	0.00000000	-2.39114228

S2.7 CH

CASRN: 3315-37-5

Level of theory: U-CCSD(T)(Full)/*aug-cc-pVTZ*

C	0.00000000	0.00000000	-0.16245872
H	0.00000000	0.00000000	1.93436816

S2.8 CH₂N

CASRN: 15845-29-1

Level of theory: U-CCSD(T)(Full)/*aug-cc-pVTZ*

N	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	2.35340256
H	1.76354344	0.00000000	3.42267385
H	-1.76354344	0.00000000	3.42267385

S2.9 CH₂O⁺

CASRN: 54288-05-0

Level of theory: U-CCSD(T)(Full)/*aug-cc-pVTZ*, Charge: +1

O	0.00000000	0.00000000	1.25868043
C	0.00000000	0.00000000	-0.99972181
H	0.00000000	1.82487639	-2.03556007
H	0.00000000	-1.82487639	-2.03556007

S2.10 CH₃

CASRN: 2229-07-4

Level of theory: U-CCSD(T)(Full)/*aug-cc-pVTZ*

C	0.00000000	0.00000000	0.00000000
H	0.00000000	0.00000000	2.03379507
H	0.00000000	1.76131924	-1.01689753
H	0.00000000	-1.76131924	-1.01689753

S2.11 ClO₂

CASRN: 10049-04-4

Level of theory: U-CCSD(T)(Full)/*aug-cc-pVTZ*

Cl	0.00000000	0.00000000	0.70662178
O	0.00000000	2.40622607	-0.77242528
O	0.00000000	-2.40622607	-0.77242528

S2.12 CN

CASRN: 2074-87-5

Level of theory: U-CCSD(T)(Full)/*aug-cc-pVTZ*

C	0.00000000	0.00000000	-1.18953886
N	0.00000000	0.00000000	1.01938091

S2.13 CNO

CASRN: 1015843-63-6

Level of theory: U-CCSD(T)(Full)/*aug-cc-pVTZ*

C	0.00000000	0.00000000	-2.50680714
N	0.00000000	0.00000000	-0.22402176
O	0.00000000	0.00000000	2.07682752

S2.14 CO⁺

CASRN: 12144-04-6

Level of theory: U-CCSD(T)(Full)/*aug-cc-pVTZ*, Charge: +1

C	0.00000000	0.00000000	-1.20324172
O	0.00000000	0.00000000	0.90271821

S2.15 CON

CASRN: 162615-05-6

Level of theory: U-CCSDT(Full)/*cc-pVTZ*

C	0.00000000	0.00000000	-2.44062558
O	0.00000000	0.00000000	-0.20455596
N	0.00000000	0.00000000	2.32515818

S2.16 Ethynyl

CASRN: 2122-48-7

Level of theory: U-CCSDT(Full)/*aug-cc-pVTZ*

C	0.00000000	0.00000000	-1.01441459
C	0.00000000	0.00000000	1.26723128
H	0.00000000	0.00000000	-3.01024506

S2.17 F₂BO

CASRN: 38150-67-3

Level of theory: U-CCSDT(Full)/*aug-cc-pVTZ*

O	0.00000000	0.00000000	2.65260017
B	0.00000000	0.00000000	0.07681654
F	0.00000000	2.16433924	-1.13888019
F	0.00000000	-2.16433924	-1.13888019

S2.18 F₂BS

CASRN: 1643772-15-9

Level of theory: U-CCSDT(Full)/*aug-cc-pVTZ*

S	0.00000000	0.00000000	2.64960984
B	0.00000000	0.00000000	-0.74406239
F	0.00000000	2.14169276	-2.01390354
F	0.00000000	-2.14169276	-2.01390354

S2.19 HBCl

CASRN: 158305-23-8

Level of theory: U-CCSDT(Full)/*aug-cc-pVTZ*

H	-1.78942324	3.56349057	0.00000000
B	0.08133759	2.34034266	0.00000000
Cl	0.08133759	-0.89795250	0.00000000

S2.20 H₂BO

CASRN: 60448-21-7

Level of theory: U-CCSDT(Full)/*aug-cc-pVTZ*

O	0.00000000	0.00000000	1.17360276
B	0.00000000	0.00000000	-1.27133435
H	0.00000000	1.98370787	-2.36904602
H	0.00000000	-1.98370787	-2.36904602

S2.21 HCO

CASRN: 2597-44-6

Level of theory: U-CCSDT(Full)/*aug-cc-pVTZ*

H	0.00000000	-2.55038496	1.39798104
C	0.00000000	-1.17300976	-0.19046167
O	0.00000000	1.04073447	0.05480615

S2.22 HOC

CASRN: 2597-44-6

Level of theory: U-CCSDT(Full)/*aug-cc-pVTZ*

H	0.00000000	1.82002973	1.50851586
O	0.00000000	0.96467865	-0.12887834
C	0.00000000	-1.43868535	0.04508983

S2.23 H₂PO

CASRN: 97516-21-7

Level of theory: U-CCSD(T)(Full)/*aug-cc-pVTZ*

P	0.00000000	0.87766783	-0.10010856
O	0.00000000	-1.95912323	0.05701315
H	2.08101554	2.05955113	1.08591181
H	-2.08101554	2.05955113	1.08591181

S2.24 H₂PS

CASRN: 121022-96-6

Level of theory: U-CCSD(T)(Full)/*aug-cc-pVTZ*

P	0.00000000	1.81994516	-0.10769248
S	0.00000000	-1.93707861	0.02086846
H	2.03762554	2.75934101	1.32385757
H	-2.03762554	2.75934101	1.32385757

S2.25 N₂⁺

CASRN: 13966-04-6

Level of theory: U-CCSD(T)(Full)/*aug-cc-pVTZ*, Charge: +1

N	0.00000000	0.00000000	-1.05634935
N	0.00000000	0.00000000	1.05634935

S2.26 NCO

CASRN: 22400-26-6

Level of theory: U-CCSD(T)(Full)/*aug-cc-pVTZ*

N	0.00000000	0.00000000	-2.39343558
C	0.00000000	0.00000000	-0.07238136
O	0.00000000	0.00000000	2.14968523

S2.27 NH₂

CASRN: 13770-40-6

Level of theory: U-CCSD(T)(Full)/*aug-cc-pVTZ*

N	0.00000000	0.00000000	0.15111603
H	0.00000000	1.51574744	-1.04982949
H	0.00000000	-1.51574744	-1.04982949

S2.28 Nitromethyl

CASRN: 16787-85-2

Level of theory: U-CCSD(T)(Full)/*aug-cc-pVTZ*

C	0.00000000	0.00000000	-2.58417104
N	0.00000000	0.00000000	0.08692471
O	0.00000000	-2.06715629	1.15098225
O	0.00000000	2.06715629	1.15098225
H	0.00000000	1.81656349	-3.48616378
H	0.00000000	-1.81656349	-3.48616378

S2.29 NO

CASRN: 10102-43-9

Level of theory: U-CCSD(T)(Full)/*aug-cc-pVTZ*

N	0.00000000	0.00000000	-1.15775086
O	0.00000000	0.00000000	1.01357658

S2.30 NO₂

CASRN: 10102-44-0

Level of theory: U-CCSD(T)(Full)/*aug-cc-pVTZ*

N	0.00000000	0.00000000	0.60658130
O	0.00000000	2.08052421	-0.26537991
O	0.00000000	-2.08052421	-0.26537991

S2.31 OH

CASRN: 3352-57-6

Level of theory: U-CCSD(T)(Full)/*aug-cc-pVTZ*

O	0.00000000	0.00000000	-0.10864763
H	0.00000000	0.00000000	1.72431679

S2.32 PH₂

CASRN: 13765-43-0

Level of theory: U-CCSD(T)(Full)/*aug-cc-pVTZ*

P	0.00000000	0.00000000	0.11427641
H	0.00000000	1.91899987	-1.75604411
H	0.00000000	-1.91899987	-1.75604411

S2.33 Vinyl

CASRN: 2669-89-8

Level of theory: U-CCSD(T)(Full)/*aug-cc-pVTZ*

C	0.00000000	1.16769663	-0.04303146
C	0.00000000	-1.29945364	0.15810072
H	0.00000000	2.38429609	1.59801822
H	0.00000000	2.08759130	-1.87998309
H	0.00000000	-2.90307925	-1.08814513

S3 CHROM subset

S3.1 Anthracene

CASRN: 120-12-7

Level of theory: CCSD(T)(FC)/cc-pVTZ

C	0.00000000	2.63580732	0.00000000
C	0.00000000	-2.63580732	0.00000000
C	-2.29791519	1.34956852	0.00000000
C	2.29791519	1.34956852	0.00000000
C	-2.29791519	-1.34956852	0.00000000
C	2.29791519	-1.34956852	0.00000000
C	-4.65745777	2.64726588	0.00000000
C	4.65745777	2.64726588	0.00000000
C	-4.65745777	-2.64726588	0.00000000
C	4.65745777	-2.64726588	0.00000000
C	-6.88218555	1.34593157	0.00000000
C	6.88218555	1.34593157	0.00000000
C	-6.88218555	-1.34593157	0.00000000
C	6.88218555	-1.34593157	0.00000000
H	0.00000000	4.67946059	0.00000000
H	0.00000000	-4.67946059	0.00000000
H	-4.64776022	4.68790486	0.00000000
H	4.64776022	4.68790486	0.00000000
H	-4.64776022	-4.68790486	0.00000000
H	4.64776022	-4.68790486	0.00000000
H	-8.65488616	2.34873329	0.00000000
H	8.65488616	2.34873329	0.00000000
H	-8.65488616	-2.34873329	0.00000000
H	8.65488616	-2.34873329	0.00000000

S3.2 Anthraquinone

CASRN: 84-65-1 (9,10-Anthraquinone)

Level of theory: CCSD(T)(FC)/cc-pVTZ

C	0.00000000	2.77266798	0.00000000
C	0.00000000	-2.77266798	0.00000000
C	-2.39604276	1.31893403	0.00000000
C	2.39604276	1.31893403	0.00000000
C	-2.39604276	-1.31893403	0.00000000

C	2.39604276	-1.31893403	0.00000000
C	-4.67770721	2.63091924	0.00000000
C	4.67770721	2.63091924	0.00000000
C	-4.67770721	-2.63091924	0.00000000
C	4.67770721	-2.63091924	0.00000000
C	-6.94595480	1.31915183	0.00000000
C	6.94595480	1.31915183	0.00000000
C	-6.94595480	-1.31915183	0.00000000
C	6.94595480	-1.31915183	0.00000000
O	0.00000000	5.07701524	0.00000000
O	0.00000000	-5.07701524	0.00000000
H	-4.62532501	4.66594073	0.00000000
H	4.62532501	4.66594073	0.00000000
H	-4.62532501	-4.66594073	0.00000000
H	4.62532501	-4.66594073	0.00000000
H	-8.70925236	2.33764025	0.00000000
H	8.70925236	2.33764025	0.00000000
H	-8.70925236	-2.33764025	0.00000000
H	8.70925236	-2.33764025	0.00000000

S3.3 Aza-BODIPY

CASRN: 934737-29-8

(Boron, difluoro[*N*-(2*H*-pyrrol-2-ylidene- κ *N*)-1*H*-pyrrol-2-aminato- κ *N*¹]-, (*T*-4))

Level of theory: CCSD(T)(FC)/cc-pVTZ

B	0.00000000	0.00000000	2.31704487
C	0.00000000	2.14450306	-2.14127722
C	0.00000000	-2.14450306	-2.14127722
C	0.00000000	4.63460750	-3.14651377
C	0.00000000	-4.63460750	-3.14651377
C	0.00000000	6.26996103	-1.12023173
C	0.00000000	-6.26996103	-1.12023173
C	0.00000000	4.75475012	1.08608078
C	0.00000000	-4.75475012	1.08608078
N	0.00000000	0.00000000	-3.41527163
N	0.00000000	2.31056089	0.47890837
N	0.00000000	-2.31056089	0.47890837
F	-2.14709422	0.00000000	3.76825470
F	2.14709422	0.00000000	3.76825470
H	0.00000000	5.07027917	-5.12686203
H	0.00000000	-5.07027917	-5.12686203

H	0.00000000	8.29623621	-1.15574338
H	0.00000000	-8.29623621	-1.15574338
H	0.00000000	5.33784503	3.03195696
H	0.00000000	-5.33784503	3.03195696

S3.4 Azobenzene

CASRN: 103-33-3

Level of theory: CCSD(T)(FC)/cc-pVTZ

N	0.70983759	0.94706332	0.00000000
N	-0.70983759	-0.94706332	0.00000000
C	3.32897155	0.35325415	0.00000000
C	-3.32897155	-0.35325415	0.00000000
C	4.95331207	2.41934773	0.00000000
C	-4.95331207	-2.41934773	0.00000000
C	4.29774859	-2.10116089	0.00000000
C	-4.29774859	2.10116089	0.00000000
C	7.55507717	2.05070219	0.00000000
C	-7.55507717	-2.05070219	0.00000000
C	6.89206075	-2.45941610	0.00000000
C	-6.89206075	2.45941610	0.00000000
C	8.52712206	-0.38973890	0.00000000
C	-8.52712206	0.38973890	0.00000000
H	4.14639892	4.28913452	0.00000000
H	-4.14639892	-4.28913452	0.00000000
H	3.00966091	-3.67317406	0.00000000
H	-3.00966091	3.67317406	0.00000000
H	8.81009192	3.65424541	0.00000000
H	-8.81009192	-3.65424541	0.00000000
H	7.65006326	-4.35029611	0.00000000
H	-7.65006326	4.35029611	0.00000000
H	10.54199682	-0.68600884	0.00000000
H	-10.54199682	0.68600884	0.00000000

S3.5 Bimane (*anti*)

CASRN: 77483-78-4 (1*H*,5*H*-Pyrazolo[1,2-*a*]pyrazole-1,5-dione)

Level of theory: CCSD(T)(FC)/cc-pVTZ

N	0.85541246	-0.97258019	-0.45355119
---	------------	-------------	-------------

N	-0.85541246	0.97258019	-0.45355119
C	3.32393035	-0.05259411	0.02808385
C	-3.32393035	0.05259411	0.02808385
C	2.94286963	2.69259588	0.18980355
C	-2.94286963	-2.69259588	0.18980355
C	0.44568700	3.18647777	-0.02731571
C	-0.44568700	-3.18647777	-0.02731571
O	5.17687487	-1.37077294	0.22137296
O	-5.17687487	1.37077294	0.22137296
H	4.43821129	4.02646675	0.46706643
H	-4.43821129	-4.02646675	0.46706643
H	-0.58057370	4.93386979	0.05227865
H	0.58057370	-4.93386979	0.05227865

S3.6 Bimane (*syn*)

CASRN: 79769-56-5 (1*H*,7*H*-Pyrazolo[1,2-*a*]pyrazole-1,7-dione)

Level of theory: CCSD(T)(FC)/cc-pVTZ

N	-2.28025963	-0.50360071	0.00000000
N	0.32822281	-0.58012028	0.00000000
C	1.24260594	-0.02312835	2.47750977
C	1.24260594	-0.02312835	-2.47750977
C	-1.07959410	0.33452863	3.96056188
C	-1.07959410	0.33452863	-3.96056188
C	-3.08345811	0.12284995	2.39997958
C	-3.08345811	0.12284995	-2.39997958
O	3.43458105	0.08666999	3.06946175
O	3.43458105	0.08666999	-3.06946175
H	-1.10355332	0.69492689	5.95117927
H	-1.10355332	0.69492689	-5.95117927
H	-5.07134531	0.28781393	2.77255340
H	-5.07134531	0.28781393	-2.77255340

S3.7 BODIPY

CASRN: 138026-71-8

(Boron, difluoro[2-[(2*H*-pyrrol-2-ylidene- κ *N*)methyl]-1*H*-pyrrolato- κ *N*]-, (*T*-4)-)

Level of theory: CCSD(T)(FC)/cc-pVTZ

C	0.00000000	0.00000000	-3.45756235
---	------------	------------	-------------

C	0.00000000	2.28455780	-2.18740413
C	0.00000000	-2.28455780	-2.18740413
C	0.00000000	4.79788592	-3.09298460
C	0.00000000	-4.79788592	-3.09298460
C	0.00000000	6.36180283	-0.99687598
C	0.00000000	-6.36180283	-0.99687598
C	0.00000000	4.76869637	1.13918303
C	0.00000000	-4.76869637	1.13918303
B	0.00000000	0.00000000	2.22139632
F	2.14645956	0.00000000	3.68028136
F	-2.14645956	0.00000000	3.68028136
N	0.00000000	2.34821228	0.42497916
N	0.00000000	-2.34821228	0.42497916
H	0.00000000	5.33956943	-5.04999407
H	0.00000000	-5.33956943	-5.04999407
H	0.00000000	8.38849882	-0.96278552
H	0.00000000	-8.38849882	-0.96278552
H	0.00000000	5.26355675	3.10891537
H	0.00000000	-5.26355675	3.10891537
H	0.00000000	0.00000000	-5.49610864

S3.8 Coumarin

CASRN: 91-64-5

Level of theory: CCSD(T)(FC)/cc-pVTZ

C	-4.94880904	-1.94740654	0.00000000
C	-2.47093848	-2.79532569	0.00000000
C	-0.51937217	-1.03691944	0.00000000
C	-1.01215298	1.55096378	0.00000000
C	-3.52597295	2.36676114	0.00000000
C	-5.48705921	0.63898323	0.00000000
C	1.12079288	3.23364340	0.00000000
C	3.48627701	2.30671360	0.00000000
C	3.97501526	-0.40562242	0.00000000
O	1.88373948	-1.96225124	0.00000000
O	6.03004743	-1.37035420	0.00000000
H	-6.46892150	-3.30170531	0.00000000
H	-2.01507343	-4.77869214	0.00000000
H	-3.90920136	4.37002329	0.00000000
H	-7.41766766	1.28158133	0.00000000
H	0.79237605	5.24728088	0.00000000
H	5.13342919	3.49535270	0.00000000

S3.9 Cyclazine

CASRN: 519-61-9 (Cycl[3.3.3]azine)

Level of theory: CCSD(T)(FC)/cc-pVTZ

C	0.00000000	-2.29619838	1.32571075
C	0.00000000	-4.57380843	-2.64068953
C	0.00000000	0.00000000	-2.65142150
C	0.00000000	4.57380843	-2.64068953
C	0.00000000	2.29619838	1.32571075
C	0.00000000	0.00000000	5.28137906
C	0.00000000	-4.57334297	-0.03501138
C	0.00000000	2.31699223	-3.94312550
C	0.00000000	2.25635074	3.97813688
C	0.00000000	-2.25635074	3.97813688
C	0.00000000	-2.31699223	-3.94312550
C	0.00000000	4.57334297	-0.03501138
N	0.00000000	0.00000000	0.00000000
H	0.00000000	6.33829394	-3.65941571
H	0.00000000	0.00000000	7.31883143
H	0.00000000	-6.33829394	-3.65941571
H	0.00000000	-6.29930356	1.03947702
H	0.00000000	2.24943827	-5.97509542
H	0.00000000	4.04986529	4.93561840
H	0.00000000	-4.04986529	4.93561840
H	0.00000000	-2.24943827	-5.97509542
H	0.00000000	6.29930356	1.03947702

S3.10 Diketopyrrolopyrrole

CASRN: 114482-12-1

Level of theory: CC3(FC)/cc-pVTZ

C	-0.78095706	1.10654573	0.00000000
C	0.78095706	-1.10654573	0.00000000
C	0.75770683	3.16221974	0.00000000
C	-0.75770683	-3.16221974	0.00000000
C	-3.42805036	0.33490251	0.00000000
C	3.42805036	-0.33490251	0.00000000
N	-3.23354900	-2.34444494	0.00000000
N	3.23354900	2.34444494	0.00000000
O	-5.40649570	1.49154645	0.00000000
O	5.40649570	-1.49154645	0.00000000

H	-4.76571395	-3.46112039	0.00000000
H	4.76571395	3.46112039	0.00000000
H	0.30840723	5.14301221	0.00000000
H	-0.30840723	-5.14301221	0.00000000

S3.11 Heptazine

CASRN: 204-34-2 (1,3,4,6,7,9,9b-Heptaazaphenalene)

Level of theory: CCSD(T)(FC)/cc-pVTZ

C	0.00000000	-2.28707566	1.32044375
C	0.00000000	-4.25961422	-2.45928942
C	0.00000000	0.00000000	-2.64088750
C	0.00000000	4.25961422	-2.45928942
C	0.00000000	2.28707566	1.32044375
C	0.00000000	0.00000000	4.91857884
N	0.00000000	0.00000000	0.00000000
N	0.00000000	-4.45372767	0.04447145
N	0.00000000	2.18835043	-3.87927703
N	0.00000000	2.26537724	3.83480558
N	0.00000000	-2.26537724	3.83480558
N	0.00000000	-2.18835043	-3.87927703
N	0.00000000	4.45372767	0.04447145
H	0.00000000	6.02612802	-3.47918663
H	0.00000000	0.00000000	6.95837327
H	0.00000000	-6.02612802	-3.47918663

S3.12 Indacene

CASRN: 267-21-0 (*s*-Indacene)

Level of theory: CCSD(T)(FC)/cc-pVTZ

C	-0.12187409	2.72754035	0.00000000
C	0.12187409	-2.72754035	0.00000000
C	-2.28967444	1.35454483	0.00000000
C	2.22799027	1.39213818	0.00000000
C	2.28967444	-1.35454483	0.00000000
C	-2.22799027	-1.39213818	0.00000000
C	-4.93933710	2.10101453	0.00000000
C	4.68186957	2.22844636	0.00000000
C	4.93933710	-2.10101453	0.00000000

C	-4.68186957	-2.22844636	0.00000000
C	6.36303738	0.04329761	0.00000000
C	-6.36303738	-0.04329761	0.00000000
H	-0.14271993	4.76943913	0.00000000
H	0.14271993	-4.76943913	0.00000000
H	-5.61765687	4.01700812	0.00000000
H	5.61765687	-4.01700812	0.00000000
H	5.28839356	4.17123105	0.00000000
H	-5.28839356	-4.17123105	0.00000000
H	8.39157765	0.14300626	0.00000000
H	-8.39157765	-0.14300626	0.00000000

Level of theory: CCSD(T)(FC)/cc-pVTZ [D_{2h} constrained]

C	0.00000000	2.70634052	0.00000000
C	0.00000000	-2.70634052	0.00000000
C	-2.25358383	1.35345832	0.00000000
C	2.25358383	1.35345832	0.00000000
C	-2.25358383	-1.35345832	0.00000000
C	2.25358383	-1.35345832	0.00000000
C	-4.81816884	2.15020878	0.00000000
C	4.81816884	2.15020878	0.00000000
C	-4.81816884	-2.15020878	0.00000000
C	4.81816884	-2.15020878	0.00000000
C	-6.36913809	0.00000000	0.00000000
C	6.36913809	0.00000000	0.00000000
H	0.00000000	4.74974165	0.00000000
H	0.00000000	-4.74974165	0.00000000
H	-5.45578565	4.08294742	0.00000000
H	5.45578565	4.08294742	0.00000000
H	-5.45578565	-4.08294742	0.00000000
H	5.45578565	-4.08294742	0.00000000
H	-8.39912836	0.00000000	0.00000000
H	8.39912836	0.00000000	0.00000000

S3.13 Naphthalimide

CASRN: 81-83-4 (1,8-Naphthalimide)

Level of theory: CCSD(T)(FC)/cc-pVTZ

C	0.00000000	0.00000000	0.88414254
C	0.00000000	0.00000000	3.55510034
C	2.35632602	0.00000000	-3.21426958

C	-2.35632602	0.00000000	-3.21426958
C	2.32275215	0.00000000	-0.42671489
C	-2.32275215	0.00000000	-0.42671489
C	4.57007817	0.00000000	0.87369931
C	-4.57007817	0.00000000	0.87369931
C	4.58083177	0.00000000	3.53384218
C	-4.58083177	0.00000000	3.53384218
C	2.33984212	0.00000000	4.84532412
C	-2.33984212	0.00000000	4.84532412
N	0.00000000	0.00000000	-4.35793673
O	4.27090495	0.00000000	-4.47823176
O	-4.27090495	0.00000000	-4.47823176
H	0.00000000	0.00000000	-6.26502060
H	6.30814973	0.00000000	-0.18744497
H	-6.30814973	0.00000000	-0.18744497
H	6.35338009	0.00000000	4.53440153
H	-6.35338009	0.00000000	4.53440153
H	2.33715237	0.00000000	6.88533156
H	-2.33715237	0.00000000	6.88533156

S3.14 Naphthoquinone

CASRN: 130-15-4 (1,4-Naphthoquinone)

Level of theory: CCSD(T)(FC)/cc-pVTZ

C	0.00000000	1.31868219	5.07583353
C	0.00000000	-1.31868219	5.07583353
C	0.00000000	2.63328396	2.80719633
C	0.00000000	-2.63328396	2.80719633
C	0.00000000	1.31896773	0.52975242
C	0.00000000	-1.31896773	0.52975242
C	0.00000000	2.74649968	-1.88121997
C	0.00000000	-2.74649968	-1.88121997
C	0.00000000	1.26627836	-4.24808471
C	0.00000000	-1.26627836	-4.24808471
O	0.00000000	5.05039066	-1.94176133
O	0.00000000	-5.05039066	-1.94176133
H	0.00000000	2.33629038	6.83936996
H	0.00000000	-2.33629038	6.83936996
H	0.00000000	4.66861735	2.75798976
H	0.00000000	-4.66861735	2.75798976
H	0.00000000	2.35501749	-5.96917497
H	0.00000000	-2.35501749	-5.96917497

S3.15 Phenazine

CASRN: 92-82-0

Level of theory: CCSD(T)(FC)/cc-pVTZ

N	0.00000000	2.68425897	0.00000000
N	0.00000000	-2.68425897	0.00000000
C	-2.14725285	1.35123660	0.00000000
C	2.14725285	1.35123660	0.00000000
C	-2.14725285	-1.35123660	0.00000000
C	2.14725285	-1.35123660	0.00000000
C	-4.49864069	2.66174043	0.00000000
C	4.49864069	2.66174043	0.00000000
C	-4.49864069	-2.66174043	0.00000000
C	4.49864069	-2.66174043	0.00000000
C	-6.71414814	1.34756473	0.00000000
C	6.71414814	1.34756473	0.00000000
C	-6.71414814	-1.34756473	0.00000000
C	6.71414814	-1.34756473	0.00000000
H	-4.44549427	4.69771133	0.00000000
H	4.44549427	4.69771133	0.00000000
H	-4.44549427	-4.69771133	0.00000000
H	4.44549427	-4.69771133	0.00000000
H	-8.49075377	2.34322156	0.00000000
H	8.49075377	2.34322156	0.00000000
H	-8.49075377	-2.34322156	0.00000000
H	8.49075377	-2.34322156	0.00000000

S3.16 Phthalimide

CASRN: 85-41-6

Level of theory: CCSD(T)(FC)/cc-pVTZ

C	0.00000000	2.20210348	2.25054900
C	0.00000000	-2.20210348	2.25054900
C	0.00000000	1.31050301	-0.41254468
C	0.00000000	-1.31050301	-0.41254468
C	0.00000000	2.68001925	-2.63336829
C	0.00000000	-2.68001925	-2.63336829
C	0.00000000	1.32018039	-4.89183006
C	0.00000000	-1.32018039	-4.89183006
N	0.00000000	0.00000000	3.69708218
O	0.00000000	4.33361053	3.05657131

O	0.00000000	-4.33361053	3.05657131
H	0.00000000	0.00000000	5.59565443
H	0.00000000	4.71538263	-2.60774609
H	0.00000000	-4.71538263	-2.60774609
H	0.00000000	2.31561890	-6.66791824
H	0.00000000	-2.31561890	-6.66791824

S3.17 Tolan

CASRN: 501-65-5 (Diphenylacetylene)

Level of theory: CCSD(T)(FC)/cc-pVTZ

C	-1.14632202	0.00000000	0.00000000
C	1.14632202	0.00000000	0.00000000
C	-3.83802475	0.00000000	0.00000000
C	3.83802475	0.00000000	0.00000000
C	-5.17616712	-2.27953873	0.00000000
C	-5.17616712	2.27953873	0.00000000
C	5.17616712	2.27953873	0.00000000
C	5.17616712	-2.27953873	0.00000000
C	-7.79943938	-2.27513115	0.00000000
C	-7.79943938	2.27513115	0.00000000
C	7.79943938	2.27513115	0.00000000
C	7.79943938	-2.27513115	0.00000000
C	-9.12002539	0.00000000	0.00000000
C	9.12002539	0.00000000	0.00000000
H	-4.14659821	-4.03713330	0.00000000
H	-4.14659821	4.03713330	0.00000000
H	4.14659821	4.03713330	0.00000000
H	4.14659821	-4.03713330	0.00000000
H	-8.81141954	-4.04290254	0.00000000
H	-8.81141954	4.04290254	0.00000000
H	8.81141954	4.04290254	0.00000000
H	8.81141954	-4.04290254	0.00000000
H	-11.15613663	0.00000000	0.00000000
H	11.15613663	0.00000000	0.00000000

S4 DNA subset

All five structures optimized within the C_s point group.

S4.1 Adenine

CASRN: 73-24-5

Level of theory: CCSD(T)(FC)/cc-pVTZ

C	4.34389426	-1.33930557	0.00000000
C	0.36503408	-0.97970268	0.00000000
C	-2.26915710	-1.24309632	0.00000000
C	-2.53876831	3.08920859	0.00000000
C	1.28293141	1.47400078	0.00000000
N	3.85894777	1.21215063	0.00000000
N	2.30159967	-2.73392473	0.00000000
N	-3.39157056	-3.52556500	0.00000000
N	-3.70537008	0.83433013	0.00000000
N	-0.07572621	3.60295597	0.00000000
H	6.24332770	-2.05381037	0.00000000
H	-5.28043911	-3.62079788	0.00000000
H	-2.33811893	-5.09589359	0.00000000
H	-3.78399739	4.70401819	0.00000000
H	5.12506600	2.62279018	0.00000000

S4.2 Cytosine

CASRN: 71-30-7

Level of theory: CCSD(T)(FC)/cc-pVTZ

C	0.13153616	-3.29434651	0.00000000
C	-2.16958868	-2.18889562	0.00000000
C	-2.18164163	0.52447245	0.00000000
C	2.19656249	0.81672316	0.00000000
N	2.23905741	-1.84899578	0.00000000
N	-0.14418728	1.93350477	0.00000000
N	-4.43045933	1.73167720	0.00000000
O	4.19248155	1.94651979	0.00000000
H	0.39918927	-5.31187887	0.00000000
H	-3.87818863	-3.28205605	0.00000000
H	3.97074213	-2.62813711	0.00000000

H	-6.06514617	0.78792181	0.00000000
H	-4.42374473	3.62537996	0.00000000

S4.3 Guanine

CASRN: 73-40-5

Level of theory: CCSD(T)(FC)/cc-pVTZ

C	5.04300746	1.12824617	0.00000000
C	1.57302763	-0.86835769	0.00000000
C	-0.40267804	-2.71708442	0.00000000
C	-3.19825976	1.07461599	0.00000000
C	0.92432676	1.66261664	0.00000000
N	3.16411910	2.93199554	0.00000000
N	4.16277548	-1.17626497	0.00000000
N	-2.78865487	-1.47177709	0.00000000
N	-1.39530616	2.75841554	0.00000000
N	-5.64049214	1.85006150	0.00000000
O	-0.33087398	-5.00601936	0.00000000
H	7.00588603	1.63926873	0.00000000
H	3.36597239	4.81669742	0.00000000
H	-4.26765198	-2.66994812	0.00000000
H	-5.96845324	3.71127812	0.00000000
H	-7.08863631	0.64037160	0.00000000

S4.4 Thymine

CASRN: 65-71-4

Level of theory: CCSD(T)(FC)/cc-pVTZ

C	-0.44648789	-2.87628686	0.00000000
C	-2.23106132	-1.07024906	0.00000000
C	-1.41814085	1.56526269	0.00000000
C	3.05578216	0.08300879	0.00000000
C	-5.00077150	-1.59149697	0.00000000
N	2.09834527	-2.33675187	0.00000000
N	1.19471324	1.90812636	0.00000000
O	-2.83684958	3.37116543	0.00000000
O	5.29613084	0.55170816	0.00000000
H	-0.91267841	-4.85754222	0.00000000
H	1.81222071	3.70986453	0.00000000

H	3.39365323	-3.72203743	0.00000000
H	-5.89402250	-0.75236289	1.65133872
H	-5.89402250	-0.75236289	-1.65133872
H	-5.36530215	-3.61421405	0.00000000

S4.5 Uracil

CASRN: 66-22-8

Level of theory: CCSD(T)(FC)/cc-pVTZ

C	0.01392074	-3.27902539	0.00000000
C	-2.26233984	-2.15421823	0.00000000
C	-2.42555647	0.58974159	0.00000000
C	2.29689984	0.69433245	0.00000000
N	2.21975844	-1.91565223	0.00000000
N	-0.06699876	1.78681963	0.00000000
O	-4.35746300	1.82310986	0.00000000
O	4.25135556	1.88203352	0.00000000
H	0.23773570	-5.30086095	0.00000000
H	-3.98274137	-3.22402227	0.00000000
H	-0.08859089	3.69140237	0.00000000
H	3.90983514	-2.77633676	0.00000000

S5 TM subset

S5.1 CuCl

CASRN: 7758-89-6

Level of theory: CC3(FC)/*aug-cc-pVTZ*

Cu	0.00000000	0.00000000	0.00000000
Cl	0.00000000	0.00000000	3.92055750

S5.2 CuF

CASRN: 13478-41-6

Level of theory: CC3(FC)/*aug-cc-pVTZ*

Cu	0.00000000	0.00000000	0.00000000
F	0.00000000	0.00000000	3.32142119

S5.3 CuH

CASRN: 13517-00-5

Level of theory: CC3(FC)/*aug-cc-pVTZ*

Cu	0.00000000	0.00000000	0.00000000
H	0.00000000	0.00000000	2.79612230

S5.4 ScF

CASRN: 14017-33-5

Level of theory: CC3(FC)/*aug-cc-pVTZ*

Sc	0.00000000	0.00000000	0.00000000
F	0.00000000	0.00000000	3.37830510

S5.5 ScH

CASRN: 33486-02-1

Level of theory: CC3(FC)/*aug-cc-pVTZ*

Sc	0.00000000	0.00000000	0.00000000
H	0.00000000	0.00000000	3.39341243

S5.6 ScO

CASRN: 12059-91-5

Level of theory: U-CCSD(T)(FC)/*aug-cc-pVTZ*

Sc	0.00000000	0.00000000	-0.44577894
O	0.00000000	0.00000000	1.25292306

S5.7 ScS

CASRN: 12294-10-9

Level of theory: U-CCSD(T)(FC)/*aug-cc-pVTZ*

Sc	0.00000000	0.00000000	-0.90101143
S	0.00000000	0.00000000	1.26691157

S5.8 TiN

CASRN: 25583-20-4

Level of theory: U-CCSD(T)(FC)/*aug-cc-pVTZ*

Ti	0.00000000	0.00000000	-0.68309383
N	0.00000000	0.00000000	2.33898264

S5.9 ZnH

CASRN: 13981-87-8

Level of theory: U-CCSD(T)(FC)/*aug-cc-pVTZ*

Zn	0.00000000	0.00000000	-0.04701678
H	0.00000000	0.00000000	2.98240506

S5.10 ZnO

CASRN: 1314-13-2

Level of theory: CC3(FC)/*aug-cc-pVTZ*

Zn	0.00000000	0.00000000	0.00000000
O	0.00000000	0.00000000	3.21175040

S5.11 ZnS

CASRN: 1314-98-3

Level of theory: CC3(FC)/*aug-cc-pVTZ*

Zn	0.00000000	0.00000000	0.00000000
S	0.00000000	0.00000000	3.90705603