

Hetero-atoms on spin exchange coupling pathways (ECPs): A computational investigation

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Table S1. Energy (Hartree), S^2 and magnetic exchange coupling Constant value of the Part-I (Set A) diradicals (B3LYP/6-311++G(d,p))

Hetero atoms	Triplet		BS		J (cm ⁻¹)
	E	S^2	E	S^2	
B	-1387.15301	2.047	-1387.15299	1.045	5.41
N	-1417.08824	2.048	-1417.08822	1.046	4.82
O	-1436.93952	2.048	-1436.93949	1.046	7.19
S	-1759.92569	2.047	-1759.92567	1.046	4.75

Table S2. Energy (Hartree), S^2 and magnetic exchange coupling Constant value of the Part-I (Set B) diradicals (B3LYP/6-311++G(d,p))

Hetero atoms	Triplet		BS		J (cm ⁻¹)
	E	S^2	E	S^2	
B	-1387.15677	2.047	-1387.15687	1.052	-20.66
N	-1417.08365	2.046	-1417.08373	1.050	-17.67
O	-1436.94495	2.046	-1436.94503	1.050	-17.58
S	-1759.92703	2.046	-1759.92711	1.050	-17.25

Table S3. Energy (Hartree), S2 and magnetic exchange coupling Constant value of the Part-I (Set A) diradicals (M06/6-311++G(d,p))

Systems	Triplet		BS		J (cm ⁻¹)	
	Meta	E	S ²	E		S ²
B		-1386.19841	2.05	-1386.19838	1.04	6.50
C		-1400.05965	2.05	-1400.05962	1.04	7.07
N		-1416.12156	2.05	-1416.12153	1.04	5.37
O		-1435.97563	2.05	-1435.97560	1.04	7.82
S		-1758.96197	2.05	-1758.96194	1.04	5.04

Table S4. Energy (Hartree), S2 and magnetic exchange coupling Constant value of the Part-I (Set B) diradicals (M06/6-311++G(d,p))

Systems	Triplet		BS		J (cm ⁻¹)	
	Para	E	S ²	E		S ²
B		-1386.20111	2.04	-1386.20120	1.05	-20.18
C		-1400.06053	2.04	-1400.06061	1.05	-17.88
N		-1416.11659	2.04	-1416.11667	1.05	-17.54
O		-1435.98086	2.04	-1435.98094	1.05	-17.21
S		-1758.96200	2.04	-1758.96208	1.05	-17.08

Table S5. Energy (Hartree), S2 and magnetic exchange coupling Constant value of the Part-I (Set A) diradicals (PBE0/6-311++G(d,p))

Systems	Triplet		BS		J (cm ⁻¹)	
	Meta	E	S ²	E		S ²
B		-1385.56150	2.06	-1385.56146	1.06	9.50
C		-1399.43018	2.06	-1399.43014	1.06	10.24
N		-1415.48226	2.06	-1415.48222	1.06	8.01
O		-1435.31701	2.06	-1435.31696	1.06	10.87
S		-1758.22810	2.06	-1758.22806	1.06	8.01

Table S6. Energy (Hartree), S^2 and magnetic exchange coupling Constant value of the Part-I (Set B) diradicals (PBE0/6-311++G(d,p))

Systems	Triplet		BS		J (cm ⁻¹)	
	Meta	E	S^2	E		S^2
B		-1385.56474	2.06	-1385.56487	1.07	-30.20
C		-1399.43129	2.06	-1399.43141	1.06	-25.89
N		-1415.47702	2.06	-1415.47714	1.06	-24.72
O		-1435.32210	2.06	-1435.32222	1.06	-24.79
S		-1758.22848	2.06	-1758.22859	1.06	-24.51

Table S7. Optimized B3LYP-level absolute energies (E , Hartree), $\langle S^2 \rangle$, and intramolecular exchange-coupling constants (J , cm⁻¹) using the 6-311+G(d,p) basis set for each diradical (Part-II diradicals).

Diradical		At B3LYP /6-311+G(d,p) level		
		Energy	$\langle S^2 \rangle$	J (cm ⁻¹)
B-ECP-I	Triplet	-1377.942554	2.0180	-3.95
	BS	-1377.942572	1.0189	
C-ECP-I	Triplet	-1391.803288	2.0202	-0.89
	BS	-1391.803292	1.0199	
N-ECP-I	Triplet	-1407.845631	2.0109	-1.77
	BS	-1407.845639	1.0112	
O-ECP-I	Triplet	-1427.710961	2.0114	- 1.09
	BS	-1427.710966	1.0115	
S-ECP-I	Triplet	-1750.687859	2.0118	-0.88
	BS	-1750.687863	1.0118	

Table S8. Optimized B3LYP-level absolute energies (E , Hartree), $\langle S^2 \rangle$, and intramolecular exchange-coupling constants (J , cm^{-1}) using the 6-311+G(d,p) basis set for each diradical (Part-II diradicals).

Diradical		At B3LYP /6-311+G(d,p) level		
		Energy	$\langle S^2 \rangle$	J (cm^{-1})
B-ECP-II	Triplet	-1864.417331	2.0237	-8.13
	BS	-1864.417368	1.0248	
C-ECP-II	Triplet	-1892.144268	2.0232	-1.76
	BS	-1892.144276	1.0225	
N-ECP-II	Triplet	-1924.231012	2.0224	-7.02
	BS	-1924.231044	1.0230	
O-ECP-II	Triplet	-1963.962023	2.0220	-7.24
	BS	-1963.962056	1.0216	
S-ECP-II	Triplet	-2609.915538	2.0237	-1.10
	BS	-2609.915543	1.0233	

Table S9. Optimized M06-level absolute energies (E , Hartree), $\langle S^2 \rangle$, and intramolecular exchange-coupling constants (J , cm^{-1}) using the 6-311+G(d,p) basis set for each diradical (Part-II diradicals).

Diradical		At UM06/6-311+G(d,p) level		
		Energy	$\langle S^2 \rangle$	J (cm^{-1})
B-ECP-I	Triplet	-1376.901258	2.0247	-12.53
	BS	-1376.901285	1.0259	
C-ECP-I	Triplet	-1390.75450	2.0279	-2.19
	BS	-1390.75451	1.0272	
N-ECP-I	Triplet	-1406.795107	2.0117	-1.97
	BS	-1406.795116	1.0122	
O-ECP-I	Triplet	-1426.661823	2.0122	-2.20
	BS	-1426.661833	1.0124	
S-ECP-I	Triplet	-1749.638275	2.0121	-1.98
	BS	-1749.638284	1.0123	

Table S10. Optimized M06-level absolute energies (E , Hartree), $\langle S^2 \rangle$, and intramolecular exchange-coupling constants (J , cm^{-1}) using the 6-311+G(d,p) basis set for each diradical (Part-II diradicals).

Diradical		At UM06/6-311+G(d,p) level		
		Energy(au)	$\langle S^2 \rangle$	J (cm^{-1})
B-ECP-II	Triplet	-1863.001596	2.0304	-15.91
	BS	-1863.001642	1.0319	
C-ECP-II	Triplet	-1890.709352	2.0293	-1.97
	BS	-1890.709361	1.0284	
N-ECP-II	Triplet	-1922.795310	2.0283	-7.91
	BS	-1922.795346	1.0293	
O-ECP-II	Triplet	-1962.531498	2.0277	-8.12
	BS	-1962.531535	1.0273	
S-ECP-II	Triplet	-2608.480737	2.0297	-3.51
	BS	-2608.480753	1.0292	

Table S11. Optimized UPBE0-level absolute energies (E , Hartree), $\langle S^2 \rangle$, and intramolecular exchange-coupling constants (J , cm^{-1}) using the 6-311+G(d,p) basis set for each diradical (Part-II diradicals).

Diradical		At UPBE0/6-311+G(d,p) level		
		Energy	$\langle S^2 \rangle$	J (cm^{-1})
B-ECP-I	Triplet	-1376.278158	2.0255	-6.81
	BS	-1376.278189	1.0270	
C-ECP-I	Triplet	-1390.134742	2.0292	-1.97
	BS	-1390.134751	1.0287	
N-ECP-I	Triplet	-1406.165548	2.0133	-3.30
	BS	-1406.165563	1.0140	
O-ECP-I	Triplet	-1426.014462	2.0142	-1.98
	BS	-1426.014471	1.0144	
S-ECP-I	Triplet	-1748.916022 -1748.916022	2.0147 2.014661	-1.76
	BS	-1748.916030 1748.9160303	1.0148 1.01483	

Table S12. Optimized UPBE0-level absolute energies (E , Hartree), $\langle S^2 \rangle$, and intramolecular exchange-coupling constants (J , cm^{-1}) using the 6-311+G(d,p) basis set for each diradical (Part-II diradicals).

Diradical		At UPBE0/6-311+G(d,p) level		
		Energy	$\langle S^2 \rangle$	J (cm^{-1})
B-ECP-II	Triplet	-1862.170077	2.0326	-11.03
	BS	-1862.170127	1.0345	
C-ECP-II	Triplet	-1889.888869	2.0316	-0.88
	BS	-1889.888873	1.0308	
N-ECP-II	Triplet	-1921.953406	2.0300	-9.23
	BS	-1921.953448	1.0312	
O-ECP-II	Triplet	-1961.651982	2.0297	-6.80
	BS	-1961.652013	1.0294	
S-ECP-II	Triplet	-2607.454643	2.0324	-1.10
	BS	-2607.454648	1.0319	

Table S13: Spin density on the individual atoms of radical and their average for ECP-I diradicals with 6-311++G(d,p) basis set for all the functionals

Diradicals	Atoms	B3LYP	M06	PBE0
B-ECP-I	N	0.402733	0.373103	0.391855
	O	0.519188	0.501323	0.518571
	Average	0.460961	0.437213	0.455213
	O	0.528377	0.501306	0.518559
	N	0.404025	0.373097	0.391847
	Average	0.466201	0.437202	0.455203
C-ECP-I	N	0.376425	0.357996	0.361871
	O	0.502589	0.493321	0.518528
	Average	0.439507	0.425659	0.4402
	O	0.50525	0.498023	0.515186
	N	0.382554	0.377398	0.376406
	Average	0.443902	0.437711	0.445796
N-ECP-I	N	0.407837	0.396628	0.428542
	O	0.502339	0.52912	0.535683
	Average	0.455088	0.462874	0.482113
	O	0.526997	0.517332	0.527229
	N	0.409977	0.39765	0.432984
	Average	0.468487	0.457491	0.480107
O-ECP-I	N	0.421357	0.391955	0.42539
	O	0.520522	0.524038	0.530275
	Average	0.47094	0.457997	0.477833
	O	0.514837	0.514775	0.524697
	N	0.427346	0.394003	0.431798
	Average	0.471092	0.454389	0.478248
S-ECP-I	N	0.417499	0.390125	0.435325
	O	0.52013	0.519622	0.527161
	Average	0.468815	0.454874	0.481243
	O	0.515611	0.511903	0.524696
	N	0.412381	0.3862	0.414275
	Average	0.463996	0.449052	0.469486

Table S14: Spin density on the individual atoms of radical and their average for ECP-II diradicals with 6-311+G(d,p) basis set for all the functionals

Diradicals	Atoms	B3LYP	M06	PBE0
B-ECP-II	N	0.346779	0.330173	0.348915
	O	0.483871	0.471829	0.494868
	Average	0.415325	0.401001	0.421892
	O	0.483873	0.471829	0.494879
	N	0.346778	0.330173	0.348903
	Average	0.415326	0.401001	0.421891
C-ECP-II	N	0.365583	0.331113	0.348788
	O	0.503955	0.478116	0.499928
	Average	0.434769	0.404615	0.424358
	O	0.503949	0.478115	0.499927
	N	0.36558	0.331112	0.348783
	Average	0.434765	0.404614	0.424355
N-ECP-II	N	0.34384	0.330685	0.349287
	O	0.490309	0.484031	0.505689
	Average	0.417075	0.407358	0.427488
	O	0.490335	0.48403	0.505687
	N	0.343867	0.330686	0.349288
	Average	0.417101	0.407358	0.427488
O-ECP-II	N	0.335833	0.32531	0.340756
	O	0.496051	0.489354	0.511391
	Average	0.415942	0.407332	0.426074
	O	0.496003	0.489353	0.51139
	N	0.335776	0.32531	0.340756
	Average	0.41589	0.407332	0.426073
S-ECP-II	N	0.325973	0.317104	0.330158
	O	0.495775	0.487557	0.511532
	Average	0.410874	0.402331	0.420845
	O	0.495775	0.487557	0.511532
	N	0.325973	0.317104	0.330158
	Average	0.410874	0.402331	0.420845

Optimized coordinates:

Part-I diradicals

B3LYP/6-311++G(d,p)

Boron(Set A)

C	-2.9459540000	3.7236140000	0.1950610000
C	-3.7947870000	2.6272930000	0.1193810000
C	-3.2728360000	1.3219510000	0.0490010000
C	-1.8851180000	1.1369940000	0.0224260000
C	-1.0369600000	2.2745430000	0.1161830000
C	-1.5545060000	3.5575960000	0.2022600000
H	-3.3677690000	4.7207240000	0.2586230000
H	-0.9057420000	4.4241790000	0.2690150000
C	0.4842250000	0.4494690000	-0.0577350000
C	1.7345140000	-0.1542610000	-0.1093420000
C	2.9043020000	0.6233670000	-0.0024410000
C	2.7860970000	2.0102280000	0.1429010000
C	1.5340970000	2.6341620000	0.1862070000
C	0.3895980000	1.8573810000	0.0911480000
H	1.8255910000	-1.2267110000	-0.2288750000
H	3.6870280000	2.6050050000	0.2208460000
H	1.4805410000	3.7122300000	0.2938560000
C	4.2436980000	-0.0153140000	-0.0461340000
N	4.2809340000	-1.3385410000	-0.2049410000
N	6.5184770000	0.1707790000	0.0324190000
C	6.7116830000	-1.1957950000	-0.1326000000
N	5.3059250000	0.7829270000	0.0767500000
N	5.5183110000	-1.8993690000	-0.2422540000
O	7.8101060000	-1.7204950000	-0.1747620000
C	7.6672890000	1.0607650000	0.1644500000
H	7.5995170000	1.5970680000	1.1126630000
H	8.5725970000	0.4614390000	0.1336190000

H	7.663380000	1.781481000	-0.655633000
C	5.537145000	-3.347547000	-0.421527000
H	5.066622000	-3.601153000	-1.373515000
H	6.570421000	-3.682124000	-0.412144000
H	4.978606000	-3.817155000	0.390067000
H	-4.868151000	2.767771000	0.124674000
C	-4.216421000	0.173699000	0.031640000
N	-5.367433000	0.352791000	-0.617930000
N	-4.726779000	-1.962360000	0.641631000
C	-5.969125000	-1.921948000	0.019378000
C	-7.481088000	-0.495735000	-1.312635000
H	-7.974491000	0.396874000	-0.925134000
H	-7.271550000	-0.355522000	-2.375344000
H	-8.109340000	-1.369837000	-1.167759000
C	-4.313926000	-3.156738000	1.371798000
H	-3.323050000	-3.455353000	1.028006000
H	-4.270872000	-2.937680000	2.441240000
H	-5.037269000	-3.944499000	1.181976000
N	-3.848390000	-0.923999000	0.690227000
N	-6.230030000	-0.700012000	-0.590138000
O	-6.748863000	-2.857333000	0.011987000
B	-0.963882000	-0.116640000	-0.170582000
H	-1.275270000	-1.228762000	-0.437923000

Carbon (Set A)

C	-2.987783000	3.738832000	-0.000344000
C	-3.784924000	2.598625000	-0.000280000
C	-3.225484000	1.306926000	-0.000220000
C	-1.827049000	1.196659000	-0.000208000
C	-1.028147000	2.362286000	-0.000233000

C	-1.5991480000	3.6329000000	-0.0003130000
H	-3.4574160000	4.7159720000	-0.0004100000
H	-0.9784930000	4.5220320000	-0.0003420000
C	0.4615220000	0.5691250000	-0.0000120000
C	1.6887910000	-0.0740270000	0.0001160000
C	2.8671000000	0.6900480000	0.0001380000
C	2.7835670000	2.0927830000	0.0000200000
C	1.5516160000	2.7374800000	-0.0001120000
C	0.3844480000	1.9721860000	-0.0001220000
H	1.7567000000	-1.1546990000	0.0002060000
H	3.6984490000	2.6701310000	0.0000350000
H	1.5106610000	3.8211970000	-0.0001950000
C	4.1921750000	0.0203120000	0.0002840000
N	4.2011640000	-1.3139870000	0.0004780000
N	6.4722860000	0.1629670000	0.0004430000
C	6.6357980000	-1.2167300000	0.0001230000
N	5.2729320000	0.8027350000	0.0002200000
N	5.4271020000	-1.9018780000	0.0005800000
O	7.7229140000	-1.7671440000	-0.0003490000
C	7.6404000000	1.0373640000	-0.0002450000
H	7.6160490000	1.6726920000	0.8871010000
H	8.5334050000	0.4190750000	0.0034500000
H	7.6198470000	1.6670390000	-0.8917760000
C	5.4144110000	-3.3607510000	0.0003000000
H	4.8937080000	-3.7175140000	-0.8904400000
H	6.4415100000	-3.7140720000	0.0025480000
H	4.8896250000	-3.7175010000	0.8886020000
H	-4.8618700000	2.6946760000	-0.0002810000
C	-4.1410450000	0.1342300000	-0.0001500000
N	-5.4528160000	0.3976900000	0.0005830000
N	-4.4751360000	-2.1267570000	-0.0007690000

C	-5.8578120000	-2.0040740000	0.0000400000
C	-7.7048850000	-0.3659850000	0.0015710000
H	-7.9453690000	0.2175460000	0.8921870000
H	-7.9457660000	0.2207030000	-0.8868340000
H	-8.2622030000	-1.2982140000	0.0001080000
C	-3.8593100000	-3.4493260000	-0.0013900000
H	-3.2360510000	-3.5583740000	-0.8910700000
H	-3.2364030000	-3.5594860000	0.8884120000
H	-4.6481300000	-4.1960550000	-0.0019800000
N	-3.6015380000	-1.0829650000	-0.0008520000
N	-6.2792520000	-0.6790730000	0.0005440000
O	-6.6206870000	-2.9534810000	0.0002510000
C	-0.9275670000	-0.0240950000	-0.0001090000
H	-1.1095800000	-0.6599540000	-0.8715440000
H	-1.1097380000	-0.6599550000	0.8712960000

Nitrogen (Set A)

C	3.1246850000	3.8024870000	-0.0000450000
C	3.8543410000	2.6104270000	-0.0001860000
C	3.2307800000	1.3553720000	-0.0003260000
C	1.8224020000	1.3516930000	-0.0003300000
C	1.0713350000	2.5607250000	-0.0001550000
C	1.7327540000	3.7886690000	-0.0000180000
H	3.6557430000	4.7469880000	0.0000530000
H	1.1729760000	4.7173580000	0.0001120000
C	-0.3595510000	0.7629670000	-0.0003030000
C	-1.5543690000	0.0506910000	-0.0003040000
C	-2.7512830000	0.7725990000	-0.0001190000
C	-2.7297760000	2.1846120000	0.0000470000
C	-1.5324710000	2.8845350000	0.0000400000
C	-0.3245780000	2.1794080000	-0.0001260000
H	-1.5724670000	-1.0310770000	-0.0004320000

H	-3.6700790000	2.7181060000	0.0001910000
H	-1.5400260000	3.9688490000	0.0001660000
C	-4.0486740000	0.0485580000	-0.0000740000
N	-3.9996410000	-1.2867290000	-0.0003710000
N	-6.3319060000	0.0984670000	0.0006250000
C	-6.4323300000	-1.2827160000	0.0001160000
N	-5.1588480000	0.7891800000	0.0003400000
N	-5.2037700000	-1.9225710000	-0.0005420000
O	-7.4961230000	-1.8772830000	0.0005040000
C	-7.5602270000	0.8876570000	0.0010350000
H	-8.1552450000	0.6635810000	-0.8861530000
H	-8.1572880000	0.6591430000	0.8856680000
H	-7.2637340000	1.9330800000	0.0039190000
C	-5.1784250000	-3.3821290000	-0.0004050000
H	-5.6805900000	-3.7704840000	0.8875470000
H	-5.6881790000	-3.7704560000	-0.8839570000
H	-4.1334280000	-3.6801140000	-0.0047610000
H	4.9356220000	2.6432370000	-0.0001780000
C	4.0324970000	0.1142250000	-0.0003820000
N	5.3637590000	0.2491400000	0.0001620000
N	4.1488470000	-2.1745050000	-0.0008980000
C	5.5362850000	-2.1814250000	0.0002700000
C	7.5312800000	-0.7264360000	0.0017240000
H	7.8257610000	-0.1599000000	-0.8833990000
H	7.8261850000	-0.1739380000	0.8956760000
H	7.9969530000	-1.7075970000	-0.0057600000
C	3.4124730000	-3.4331620000	-0.0009400000
H	2.7846200000	-3.4875470000	0.8909910000
H	2.7822390000	-3.4857510000	-0.8912610000
H	4.1287400000	-4.2497300000	-0.0026260000
N	3.3786970000	-1.0501490000	-0.0009770000

N	6.0816460000	-0.9014050000	-0.0000960000
O	6.2059540000	-3.1986310000	0.0011260000
N	0.9429770000	0.2911400000	-0.0004280000
H	1.2583300000	-0.6669720000	-0.0006590000

Oxygen (Set A):

C	3.1576620000	3.7902630000	-0.0001360000
C	3.8442440000	2.5742960000	-0.0000490000
C	3.1854620000	1.3339000000	0.0000550000
C	1.7855870000	1.3947060000	0.0000460000
C	1.0765870000	2.6153330000	-0.0000480000
C	1.7674980000	3.8269700000	-0.0001370000
H	3.7230130000	4.7147220000	-0.0002050000
H	1.2347460000	4.7708130000	-0.0002090000
C	-0.3482370000	0.8516340000	0.0000760000
C	-1.5094760000	0.1023020000	0.0001250000
C	-2.7214090000	0.8047430000	0.0000670000
C	-2.7243080000	2.2155590000	-0.0000420000
C	-1.5418560000	2.9428850000	-0.0000870000
C	-0.3254050000	2.2533690000	-0.0000250000
H	-1.4883930000	-0.9781550000	0.0002040000
H	-3.6751790000	2.7302720000	-0.0000850000
H	-1.5693750000	4.0264350000	-0.0001670000
C	-4.0053960000	0.0570690000	0.0001150000
N	-3.9291530000	-1.2758040000	0.0004620000
N	-6.2875720000	0.0641830000	-0.0000240000
C	-6.3604320000	-1.3195080000	0.0000660000
N	-5.1285260000	0.7774170000	-0.0002250000
N	-5.1193220000	-1.9356080000	0.0002390000
O	-7.4120990000	-1.9340060000	0.0002010000
C	-7.5315360000	0.8286360000	-0.0004870000

H	-8.1216040000	0.5919650000	-0.8876650000
H	-8.1240260000	0.5887690000	0.8841710000
H	-7.2562500000	1.8798200000	0.0017150000
C	-5.0643410000	-3.3947450000	0.0008540000
H	-5.5603210000	-3.7923760000	0.8880610000
H	-5.5644380000	-3.7930800000	-0.8836750000
H	-4.0135530000	-3.6714580000	-0.0013990000
O	0.9230190000	0.3281500000	0.0001190000
H	4.9255980000	2.5695150000	-0.0000500000
C	3.9745400000	0.0774300000	0.0001450000
N	5.3053310000	0.2157060000	-0.0000170000
N	4.0812290000	-2.1995310000	-0.0000210000
C	5.4692200000	-2.2149510000	-0.0000220000
C	7.4704010000	-0.7682040000	-0.0004280000
H	7.7683630000	-0.2105210000	-0.8903180000
H	7.7686160000	-0.2097400000	0.8888800000
H	7.9324390000	-1.7511800000	-0.0000790000
C	3.3343930000	-3.4535630000	-0.0001950000
H	2.7027710000	-3.4965180000	0.8888680000
H	2.7027530000	-3.4962690000	-0.8892570000
H	4.0432400000	-4.2765790000	-0.0003150000
N	3.3146980000	-1.0765230000	0.0000850000
N	6.0212160000	-0.9383040000	-0.0000940000
O	6.1349690000	-3.2348860000	-0.0004040000

Sulphur (Set A):

C	-2.8632900000	3.7214190000	-0.0000650000
C	-3.7288290000	2.6281110000	-0.0000430000
C	-3.2520640000	1.3116840000	-0.0000430000
C	-1.8550760000	1.1184860000	-0.0000720000

C	-0.9731180000	2.2279740000	-0.0000830000
C	-1.4894120000	3.5278530000	-0.0000800000
H	-3.2708600000	4.7254980000	-0.0000640000
H	-0.8168150000	4.3780200000	-0.0000880000
C	0.5725210000	0.4328710000	-0.0001110000
C	1.8269350000	-0.1709350000	-0.0001190000
C	2.9672190000	0.6356890000	-0.0000950000
C	2.8278370000	2.0384900000	-0.0000620000
C	1.5754050000	2.6294790000	-0.0000640000
C	0.4224700000	1.8316710000	-0.0000890000
H	1.9316240000	-1.2477390000	-0.0001410000
H	3.7183820000	2.6519430000	-0.0000410000
H	1.4933860000	3.7106300000	-0.0000450000
C	4.3178500000	0.0171520000	-0.0001050000
N	4.3741660000	-1.3169830000	-0.0007090000
N	6.5883670000	0.2504350000	0.0001990000
C	6.7980280000	-1.1190420000	-0.0001030000
N	5.3640260000	0.8451500000	0.0004630000
N	5.6239700000	-1.8553300000	-0.0004490000
O	7.9054860000	-1.6264070000	-0.0001580000
C	7.7508130000	1.1339980000	0.0009670000
H	8.3609670000	0.9564840000	0.8883470000
H	8.3642070000	0.9534180000	-0.8835050000
H	7.3734340000	2.1530150000	-0.0014050000
C	5.7144650000	-3.3125600000	-0.0013490000
H	6.2474730000	-3.6584920000	-0.8887610000
H	6.2520240000	-3.6590940000	0.8830260000
H	4.6963750000	-3.6924320000	0.0010530000
H	-4.7991900000	2.7829930000	-0.0000230000
C	-4.2199850000	0.1906040000	0.0000030000
N	-5.5214380000	0.5028460000	0.0000380000

N	-4.6209290000	-2.0583370000	0.0002250000
C	-5.9988710000	-1.8891270000	0.0000490000
C	-7.7950680000	-0.1945380000	0.0003510000
H	-8.0181140000	0.3969110000	0.8902680000
H	-8.0181940000	0.3976490000	-0.8890460000
H	-8.3797960000	-1.1098260000	0.0000130000
C	-4.0431810000	-3.3985280000	0.0005980000
H	-3.4231060000	-3.5245390000	-0.8888000000
H	-3.4233090000	-3.5241480000	0.8901950000
H	-4.8540570000	-4.1212030000	0.0006620000
N	-3.7219190000	-1.0397420000	0.0001410000
N	-6.3792230000	-0.5497430000	0.0000850000
O	-6.7921780000	-2.8126320000	0.0005740000
S	-0.9761200000	-0.4168350000	-0.0001150000

Boron (Set B):

C	-3.0008290000	-1.6072400000	0.0000020000
C	-3.5047550000	-0.3020230000	-0.0000120000
C	-2.6005710000	0.7788460000	-0.0000760000
C	-1.2308520000	0.5483200000	-0.0001090000
C	-0.7423930000	-0.7869280000	-0.0000690000
C	-1.6235400000	-1.8574260000	-0.0000170000
H	-3.6981690000	-2.4349750000	0.0000500000
H	-2.9898410000	1.7892930000	-0.0001010000
H	-1.2686160000	-2.8825020000	0.0000200000
C	1.2308510000	0.5483210000	-0.0000680000
C	2.6005710000	0.7788470000	-0.0000020000
C	3.5047550000	-0.3020210000	0.0000720000
C	3.0008290000	-1.6072390000	0.0000710000
C	1.6235410000	-1.8574260000	0.0000130000
C	0.7423930000	-0.7869270000	-0.0000500000

H	2.9898400000	1.7892940000	-0.0000190000
H	3.6981700000	-2.4349740000	0.0001310000
H	1.2686160000	-2.8825010000	0.0000360000
B	0.0000000000	1.5066300000	-0.0002020000
H	-0.0000010000	2.6958750000	-0.0000750000
C	4.9701920000	-0.0613670000	0.0001430000
N	5.3732770000	1.2104920000	0.0003230000
N	7.1010270000	-0.8803460000	0.0000880000
C	7.6611010000	0.3872960000	0.0000910000
C	-4.9701920000	-0.0613700000	0.0000360000
N	-5.7641530000	-1.1352100000	0.0001040000
N	-6.7200540000	1.4042670000	-0.0002440000
C	-7.6611010000	0.3872980000	-0.0000310000
N	5.7641520000	-1.1352100000	-0.0001040000
N	6.7200550000	1.4042670000	0.0000960000
N	-7.1010270000	-0.8803460000	-0.0001470000
N	-5.3732770000	1.2104920000	-0.0002230000
O	8.8626080000	0.5873050000	0.0000150000
O	-8.8626070000	0.5873070000	0.0001030000
C	7.9928570000	-2.0364760000	-0.0003600000
H	8.6284620000	-2.0244320000	-0.8875750000
H	8.6321940000	-2.0219790000	0.8840850000
H	7.3627910000	-2.9217920000	0.0021100000
C	7.1873150000	2.7877450000	0.0004630000
H	7.7923720000	2.9828090000	0.8876460000
H	7.7963380000	2.9817510000	-0.8841910000
H	6.3035410000	3.4199540000	-0.0018190000
C	-7.9928590000	-2.0364760000	0.0003000000
H	-8.6283500000	-2.0245250000	0.8875990000
H	-8.6323080000	-2.0218830000	-0.8840600000
H	-7.3627930000	-2.9217920000	-0.0023420000

C	-7.1873140000	2.7877440000	-0.0003320000
H	-7.7944590000	2.9821850000	-0.8862020000
H	-7.7942500000	2.9823760000	0.8856390000
H	-6.3035370000	3.4199540000	-0.0005050000

Carbon (Set B)

C	-3.0145500000	-1.6975230000	-0.0005690000
C	-3.4692340000	-0.3682160000	-0.0003950000
C	-2.5366310000	0.6822650000	-0.0001450000
C	-1.1828570000	0.3904900000	-0.0001430000
C	-0.7323150000	-0.9443400000	-0.0001940000
C	-1.6553890000	-1.9912160000	-0.0004440000
H	-3.7423700000	-2.4978320000	-0.0008260000
H	-2.8902510000	1.7056040000	-0.0000600000
H	-1.3268760000	-3.0246820000	-0.0004400000
C	1.1828570000	0.3904900000	0.0000800000
C	2.5366310000	0.6822650000	0.0000600000
C	3.4692340000	-0.3682160000	0.0003730000
C	3.0145510000	-1.6975220000	0.0006280000
C	1.6553900000	-1.9912160000	0.0005240000
C	0.7323150000	-0.9443400000	0.0002130000
H	2.8902510000	1.7056040000	-0.0000910000
H	3.7423700000	-2.4978320000	0.0009320000
H	1.3268760000	-3.0246820000	0.0005840000
C	4.9252490000	-0.0749470000	0.0004130000
N	5.2851810000	1.2109520000	0.0019740000
N	7.0840730000	-0.8193490000	-0.0012280000
C	7.6005090000	0.4661500000	-0.0001510000
C	-4.9252490000	-0.0749480000	-0.0004620000
N	-5.7566040000	-1.1197770000	0.0013080000
N	-6.6253370000	1.4500340000	-0.0014840000

C	-7.6005090000	0.4661500000	0.0003470000
N	5.7566040000	-1.1197770000	-0.0014360000
N	6.6253370000	1.4500340000	0.0012940000
N	-7.0840730000	-0.8193490000	0.0011830000
N	-5.2851800000	1.2109520000	-0.0020110000
O	8.7947680000	0.7076660000	-0.0001620000
O	-8.7947670000	0.7076660000	0.0003780000
C	8.0144060000	-1.9446090000	-0.0032690000
H	8.6487760000	-1.9103960000	-0.8908110000
H	8.6533750000	-1.9095260000	0.8808810000
H	7.4145210000	-2.8506740000	-0.0013550000
C	7.0455680000	2.8481820000	0.0032250000
H	7.6438630000	3.0631280000	0.8904660000
H	7.6475560000	3.0642360000	-0.8811940000
H	6.1409190000	3.4502270000	0.0018000000
C	-8.0144060000	-1.9446090000	0.0032470000
H	-8.6485500000	-1.9105680000	0.8909590000
H	-8.6536000000	-1.9093540000	-0.8807320000
H	-7.4145220000	-2.8506740000	0.0010060000
C	-7.0455690000	2.8481810000	-0.0031470000
H	-7.6462070000	3.0624900000	-0.8889330000
H	-7.6452150000	3.0648770000	0.8827290000
H	-6.1409170000	3.4502240000	-0.0044710000
C	0.0000000000	1.3361040000	-0.0000610000
H	0.0000830000	1.9898200000	-0.8797550000
H	-0.0000830000	1.9898750000	0.8795930000

Nitrogen (Set B):

C	-3.0423020000	-1.7778420000	-0.0001450000
C	-3.4361810000	-0.4215980000	-0.0001530000
C	-2.4729000000	0.5911990000	-0.0000940000
C	-1.1321900000	0.2212280000	-0.0000730000

C	-0.7227190000	-1.1370390000	-0.0001050000
C	-1.7028350000	-2.1356900000	-0.0001240000
H	-3.8081470000	-2.5408760000	-0.0001740000
H	-2.7780060000	1.6294460000	-0.0000790000
H	-1.4227340000	-3.1831620000	-0.0001370000
C	1.1321900000	0.2212270000	-0.0000770000
C	2.4729000000	0.5911980000	-0.0001000000
C	3.4361810000	-0.4215990000	-0.0001810000
C	3.0423030000	-1.7778440000	-0.0001960000
C	1.7028350000	-2.1356920000	-0.0001640000
C	0.7227210000	-1.1370400000	-0.0001130000
H	2.7780110000	1.6294440000	-0.0000680000
H	3.8081490000	-2.5408770000	-0.0002420000
H	1.4227330000	-3.1831640000	-0.0001830000
C	4.8787540000	-0.0660520000	-0.0002240000
N	5.1841300000	1.2346440000	0.0001560000
N	7.0670670000	-0.7181610000	0.0000440000
C	7.5290890000	0.5874840000	-0.0001140000
C	-4.8787540000	-0.0660530000	-0.0002260000
N	-5.7533070000	-1.0738900000	0.0004480000
N	-6.5134000000	1.5296560000	-0.0001940000
C	-7.5290900000	0.5874780000	-0.0000810000
N	5.7533100000	-1.0738930000	-0.0002300000
N	6.5134010000	1.5296560000	0.0002820000
N	-7.0670680000	-0.7181600000	0.0002280000
N	-5.1841320000	1.2346480000	-0.0006340000
O	8.7121290000	0.8794150000	0.0003090000
O	-8.7121300000	0.8794140000	0.0002310000
C	8.0431630000	-1.8040090000	-0.0001430000
H	8.6763360000	-1.7445160000	-0.8872130000
H	8.6793650000	-1.7418850000	0.8845350000

H	7.4809700000	-2.7339450000	0.0021300000
C	6.8755150000	2.9437910000	0.0007030000
H	7.4664230000	3.1836400000	0.8865150000
H	7.4662350000	3.1842060000	-0.8850830000
H	5.9469150000	3.5082000000	0.0009850000
C	-8.0431590000	-1.8040130000	0.0012180000
H	-8.6757630000	-1.7444270000	0.8886940000
H	-8.6799280000	-1.7419860000	-0.8830520000
H	-7.4809640000	-2.7339470000	-0.0012940000
C	-6.8755210000	2.9437900000	-0.0008130000
H	-7.4634690000	3.1844040000	-0.8884180000
H	-7.4691970000	3.1834330000	0.8831700000
H	-5.9469290000	3.5082040000	0.0023900000
N	0.0000000000	1.0215060000	0.0000100000
H	0.0000140000	2.0276010000	-0.0003240000

Oxygen (Set B):

C	-3.0563750000	-1.8302000000	-0.0001000000
C	-3.4080210000	-0.4640420000	-0.0001360000
C	-2.4119430000	0.5211440000	-0.0001620000
C	-1.0991950000	0.0904490000	-0.0001500000
C	-0.7236730000	-1.2642770000	-0.0001220000
C	-1.7291630000	-2.2362570000	-0.0000960000
H	-3.8473500000	-2.5673380000	-0.0000790000
H	-2.6648940000	1.5718660000	-0.0001880000
H	-1.4826590000	-3.2916800000	-0.0000730000
C	1.0992130000	0.0904410000	-0.0001330000
C	2.4119630000	0.5211120000	-0.0001190000
C	3.4080300000	-0.4640930000	-0.0000950000
C	3.0563690000	-1.8302390000	-0.0000860000
C	1.7291450000	-2.2362770000	-0.0000970000

C	0.7236730000	-1.2642880000	-0.0001170000
H	2.6649520000	1.5718250000	-0.0001250000
H	3.8473220000	-2.5674000000	-0.0000670000
H	1.4826340000	-3.2916980000	-0.0000850000
C	4.8387310000	-0.0637120000	-0.0000590000
N	5.1005440000	1.2452780000	0.0002330000
N	7.0449300000	-0.6463610000	0.0000720000
C	7.4639560000	0.6742230000	0.0002310000
C	-4.8387180000	-0.0636600000	-0.0001490000
N	-5.7434940000	-1.0442320000	0.0001990000
N	-6.4187020000	1.5836420000	-0.0003290000
C	-7.4639400000	0.6742830000	0.0000810000
N	5.7434970000	-1.0442740000	-0.0002230000
N	6.4185790000	1.5836490000	0.0001930000
N	-7.0448330000	-0.6464290000	0.0001240000
N	-5.1005290000	1.2453170000	-0.0004460000
O	8.6366770000	1.0035330000	0.0003640000
O	-8.6367210000	1.0033810000	0.0002590000
C	8.0558090000	-1.6996560000	-0.0002680000
H	8.6868920000	-1.6191730000	-0.8871200000
H	8.6894660000	-1.6170550000	0.8845130000
H	7.5246440000	-2.6476050000	0.0015720000
C	6.7332520000	3.0092760000	0.0006770000
H	7.3134760000	3.2689430000	0.8878880000
H	7.3177150000	3.2684160000	-0.8838560000
H	5.7862950000	3.5421860000	-0.0016650000
C	-8.0557540000	-1.6996660000	0.0007710000
H	-8.6865870000	-1.6191440000	0.8877990000
H	-8.6896710000	-1.6170480000	-0.8838220000
H	-7.5246470000	-2.6476500000	-0.0012100000
C	-6.7333060000	3.0092970000	-0.0005550000

H	-7.3158030000	3.2685430000	-0.8863750000
H	-7.3154610000	3.2689010000	0.8853840000
H	-5.7863140000	3.5421440000	-0.0008480000
O	0.0000110000	0.9185470000	-0.0001610000

Sulphur (Set B):

C	-2.9829870000	-1.6730050000	-0.0000930000
C	-3.5027650000	-0.3630730000	-0.0001690000
C	-2.6292120000	0.7271750000	-0.0002040000
C	-1.2583140000	0.4918980000	-0.0001650000
C	-0.7247630000	-0.8147510000	-0.0000870000
C	-1.6164500000	-1.8968320000	-0.0000510000
H	-3.6709460000	-2.5072450000	-0.0000660000
H	-3.0269990000	1.7330250000	-0.0002600000
H	-1.2386000000	-2.9130190000	0.0000080000
C	1.2583140000	0.4918970000	-0.0001020000
C	2.6292120000	0.7271740000	-0.0000790000
C	3.5027650000	-0.3630740000	-0.0000030000
C	2.9829860000	-1.6730070000	0.0000500000
C	1.6164490000	-1.8968330000	0.0000240000
C	0.7247620000	-0.8147510000	-0.0000520000
H	3.0270000000	1.7330230000	-0.0001220000
H	3.6709450000	-2.5072450000	0.0001100000
H	1.2385990000	-2.9130200000	0.0000660000
C	4.9710950000	-0.1385820000	0.0000220000
N	5.3899260000	1.1290830000	0.0001950000
N	7.0900490000	-0.9846550000	0.0002070000
C	7.6663830000	0.2752820000	0.0001380000
C	-4.9710950000	-0.1385810000	-0.0002030000
N	-5.7497970000	-1.2217160000	-0.0000730000
N	-6.7391980000	1.3050310000	-0.0001750000

C	-7.6663840000	0.2752800000	0.0000240000
N	5.7497990000	-1.2217150000	-0.0000540000
N	6.7392000000	1.3050310000	0.0000650000
N	-7.0900500000	-0.9846540000	-0.0001710000
N	-5.3899290000	1.1290830000	-0.0002840000
O	8.8703450000	0.4598910000	0.0001950000
O	-8.8703450000	0.4598920000	0.0003880000
C	7.9659410000	-2.1526800000	-0.0000640000
H	8.6016300000	-2.1495320000	-0.8872790000
H	8.6054880000	-2.1467760000	0.8843090000
H	7.3239890000	-3.0293720000	0.0026080000
C	7.2248410000	2.6818810000	0.0004330000
H	7.8324660000	2.8689400000	0.8875690000
H	7.8365110000	2.8677960000	-0.8841160000
H	6.3498620000	3.3261580000	-0.0019080000
C	-7.9659380000	-2.1526820000	0.0003590000
H	-8.6013720000	-2.1495390000	0.8877580000
H	-8.6057380000	-2.1467780000	-0.8838300000
H	-7.3239850000	-3.0293720000	-0.0024960000
C	-7.2248440000	2.6818810000	-0.0000620000
H	-7.8347000000	2.8683580000	-0.8857650000
H	-7.8342870000	2.8683710000	0.8859250000
H	-6.3498630000	3.3261600000	-0.0002690000
S	0.0000000000	1.7316050000	-0.0001990000

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Boron (Set A):

C	-2.9328490000	3.7155010000	0.1936860000
C	-3.7836770000	2.6266360000	0.1246560000
C	-3.2691950000	1.3258250000	0.0568460000
C	-1.8888750000	1.1344660000	0.0272420000

C	-1.0404540000	2.2616360000	0.1138290000
C	-1.5483650000	3.5431730000	0.1970400000
H	-3.3507080000	4.7159590000	0.2557360000
H	-0.8903410000	4.4058650000	0.2594270000
C	0.4726570000	0.4436610000	-0.0490040000
C	1.7182610000	-0.1561170000	-0.0981600000
C	2.8796760000	0.6226170000	0.0003850000
C	2.7612570000	2.0045460000	0.1348300000
C	1.5141400000	2.6242270000	0.1760480000
C	0.3771300000	1.8448950000	0.0891650000
H	1.8118270000	-1.2320480000	-0.2113710000
H	3.6658400000	2.5994460000	0.2058260000
H	1.4531230000	3.7047660000	0.2764600000
C	4.2135340000	-0.0101880000	-0.0426190000
N	4.2510490000	-1.3324490000	-0.1625760000
N	6.4749820000	0.1832460000	-0.0001140000
C	6.6724040000	-1.1827250000	-0.1254030000
N	5.2705180000	0.7911080000	0.0416280000
N	5.4812610000	-1.8862180000	-0.2017780000
O	7.7635490000	-1.7025140000	-0.1632610000
C	7.6153460000	1.0734620000	0.0918660000
H	7.5638920000	1.6331110000	1.0293490000
H	8.5255820000	0.4783180000	0.0588850000
H	7.5957200000	1.7782630000	-0.7435790000
C	5.5008300000	-3.3295790000	-0.3357840000
H	4.9950140000	-3.6155730000	-1.2616490000
H	6.5361440000	-3.6636360000	-0.3548510000
H	4.9743420000	-3.7800870000	0.5095800000
H	-4.8592170000	2.7692440000	0.1335760000
C	-4.2032010000	0.1814660000	0.0416510000
N	-5.3765100000	0.3679770000	-0.5524490000
N	-4.6497800000	-1.9744400000	0.5769080000

C	-5.9118470000	-1.9343550000	0.0060440000
C	-7.4922840000	-0.4784830000	-1.1820180000
H	-7.9959290000	0.3722060000	-0.7164360000
H	-7.3325430000	-0.2590040000	-2.2412690000
H	-8.0938490000	-1.3786190000	-1.0737710000
C	-4.1766190000	-3.1902360000	1.2092950000
H	-3.1889960000	-3.4330820000	0.8098520000
H	-4.0950760000	-3.0401120000	2.2897420000
H	-4.8814940000	-3.9918850000	0.9982350000
N	-3.7967550000	-0.9297100000	0.6424610000
N	-6.2150430000	-0.6924810000	-0.5309670000
O	-6.6674850000	-2.8777340000	-0.0171880000
B	-0.9729920000	-0.1202930000	-0.1627970000
H	-1.2821310000	-1.2314880000	-0.4355380000

Carbon (Set A):

C	-2.9759240000	3.7268950000	0.0398620000
C	-3.7690260000	2.5901920000	0.0295130000
C	-3.2115920000	1.3053650000	0.0247330000
C	-1.8198270000	1.1938290000	0.0301720000
C	-1.0260280000	2.3541940000	0.0356500000
C	-1.5929800000	3.6203140000	0.0418640000
H	-3.4464420000	4.7051710000	0.0455600000
H	-0.9671280000	4.5085270000	0.0472560000
C	0.4528460000	0.5688030000	0.0167800000
C	1.6749120000	-0.0725620000	0.0054950000
C	2.8466040000	0.6892670000	0.0046630000
C	2.7661310000	2.0859620000	0.0161300000
C	1.5399180000	2.7293680000	0.0275610000
C	0.3789520000	1.9656530000	0.0276320000
H	1.7422840000	-1.1560980000	-0.0029440000
H	3.6856570000	2.6607490000	0.0155360000

H	1.4950810000	3.8150720000	0.0360870000
C	4.1642910000	0.0215740000	-0.0087010000
N	4.1699340000	-1.3074590000	-0.0237980000
N	6.4309940000	0.1605230000	-0.0174070000
C	6.5948110000	-1.2147850000	-0.0349040000
N	5.2417520000	0.7996090000	-0.0048620000
N	5.3866600000	-1.8923630000	-0.0365900000
O	7.6728360000	-1.7633600000	-0.0471580000
C	7.5930210000	1.0270000000	-0.0136750000
H	7.5733480000	1.6569440000	0.8794080000
H	8.4884410000	0.4088610000	-0.0179390000
H	7.5726540000	1.6672110000	-0.8995300000
C	5.3701850000	-3.3415520000	-0.0540180000
H	4.8403920000	-3.6884800000	-0.9450780000
H	6.3968300000	-3.7018170000	-0.0636870000
H	4.8495890000	-3.7100160000	0.8338070000
H	-4.8489330000	2.6839540000	0.0249490000
C	-4.1175030000	0.1362940000	0.0110140000
N	-5.4202780000	0.3888260000	-0.1087300000
N	-4.4365690000	-2.1110710000	0.1024530000
C	-5.8118340000	-2.0036950000	-0.0103160000
C	-7.6460740000	-0.3878080000	-0.2422460000
H	-7.9639210000	0.2374260000	0.5961400000
H	-7.8175310000	0.1555910000	-1.1749560000
H	-8.2013940000	-1.3234180000	-0.2443850000
C	-3.8194710000	-3.4169020000	0.2228580000
H	-3.1130110000	-3.5622740000	-0.5986940000
H	-3.2787970000	-3.4794590000	1.1711380000
H	-4.5986160000	-4.1755650000	0.1858690000
N	-3.5756280000	-1.0693930000	0.1201300000
N	-6.2331170000	-0.6866380000	-0.1126850000
O	-6.5628640000	-2.9511540000	-0.0192750000

C	-0.9270430000	-0.0181370000	0.0235860000
H	-1.1161710000	-0.6598190000	-0.8458420000
H	-1.1045810000	-0.6562870000	0.8972750000

Nitrogen (Set A):

C	3.0986850000	3.7832270000	0.0001960000
C	3.8293690000	2.5980250000	0.0000210000
C	3.2145740000	1.3460160000	-0.0001490000
C	1.8124490000	1.3327770000	-0.0001330000
C	1.0632520000	2.5328750000	0.0000450000
C	1.7130220000	3.7603920000	0.0002110000
H	3.6262420000	4.7313210000	0.0003230000
H	1.1419640000	4.6847660000	0.0003520000
C	-0.3586750000	0.7432910000	-0.0001630000
C	-1.5509590000	0.0367890000	-0.0002170000
C	-2.7394850000	0.7603810000	-0.0000760000
C	-2.7173080000	2.1661120000	0.0000960000
C	-1.5237620000	2.8602090000	0.0001470000
C	-0.3248250000	2.1520810000	0.0000240000
H	-1.5728670000	-1.0475910000	-0.0003540000
H	-3.6604630000	2.6996650000	0.0002030000
H	-1.5228140000	3.9467390000	0.0002830000
C	-4.0331670000	0.0446890000	-0.0000770000
N	-3.9889390000	-1.2853440000	-0.0003990000
N	-6.3021130000	0.1071310000	0.0004750000
C	-6.4113360000	-1.2691720000	0.0001600000
N	-5.1351750000	0.7883920000	0.0002100000
N	-5.1878110000	-1.9100660000	-0.0006060000
O	-7.4702930000	-1.8547880000	0.0002630000
C	-7.5231590000	0.8900920000	0.0007440000
H	-8.1218140000	0.6660950000	-0.8860250000
H	-8.1232500000	0.6629650000	0.8857070000

H	-7.2290930000	1.9380310000	0.0027730000
C	-5.1769350000	-3.3602070000	-0.0007280000
H	-5.6837290000	-3.7474070000	0.8871170000
H	-5.6910900000	-3.7469850000	-0.8844480000
H	-4.1337930000	-3.6709060000	-0.0050170000
H	4.9132600000	2.6331380000	0.0000200000
C	4.0184980000	0.1150220000	-0.0002860000
N	5.3440260000	0.2566500000	-0.0000770000
N	4.1434820000	-2.1594110000	-0.0005780000
C	5.5265630000	-2.1633780000	0.0001090000
C	7.5003180000	-0.7024740000	0.0008470000
H	7.7941660000	-0.1334860000	-0.8847540000
H	7.7952080000	-0.1461980000	0.8942610000
H	7.9744890000	-1.6816260000	-0.0060910000
C	3.4167350000	-3.4124490000	-0.0002940000
H	2.7868930000	-3.4704780000	0.8918910000
H	2.7841520000	-3.4689420000	-0.8906070000
H	4.1342800000	-4.2304420000	-0.0020230000
N	3.3719660000	-1.0469540000	-0.0006000000
N	6.0610780000	-0.8830630000	-0.0003820000
O	6.1964450000	-3.1698440000	0.0009170000
N	0.9390860000	0.2725790000	-0.0002520000
H	1.2567210000	-0.6867940000	-0.0004610000

Oxygen (Set A):

C	3.1440530000	3.7751930000	-0.0000730000
C	3.8264470000	2.5627250000	-0.0001450000
C	3.1710920000	1.3287340000	-0.0001790000
C	1.7766410000	1.3870080000	-0.0001100000
C	1.0737210000	2.6029600000	-0.0000400000
C	1.7599510000	3.8108800000	-0.0000230000
H	3.7108340000	4.7004580000	-0.0000570000

H	1.2222040000	4.7543720000	0.0000340000
C	-0.3401700000	0.8469790000	-0.0000160000
C	-1.4978250000	0.1006020000	0.0000320000
C	-2.7024310000	0.8015920000	0.0000950000
C	-2.7080160000	2.2063340000	0.0001080000
C	-1.5313300000	2.9314750000	0.0000700000
C	-0.3212590000	2.2427560000	0.0000110000
H	-1.4778380000	-0.9824190000	0.0000170000
H	-3.6632740000	2.7183320000	0.0001570000
H	-1.5548050000	4.0172340000	0.0000910000
C	-3.9803410000	0.0577610000	0.0001600000
N	-3.9029570000	-1.2698130000	0.0006200000
N	-6.2483120000	0.0672020000	0.0000680000
C	-6.3238120000	-1.3123340000	0.0004120000
N	-5.0984320000	0.7762740000	-0.0002520000
N	-5.0849620000	-1.9240150000	0.0004830000
O	-7.3681770000	-1.9224620000	0.0003960000
C	-7.4885420000	0.8196600000	-0.0005150000
H	-8.0809950000	0.5801740000	-0.8873530000
H	-8.0829680000	0.5779940000	0.8843740000
H	-7.2208970000	1.8746410000	0.0010240000
C	-5.0381250000	-3.3738340000	0.0010500000
H	-5.5370050000	-3.7724540000	0.8882030000
H	-5.5408490000	-3.7730920000	-0.8836030000
H	-3.9876220000	-3.6585530000	-0.0010610000
O	0.9215450000	0.3276650000	-0.0000940000
H	4.9105020000	2.5556330000	-0.0001900000
C	3.9537730000	0.0775410000	-0.0002880000
N	5.2795250000	0.2109140000	-0.0001300000
N	4.0486510000	-2.1865820000	-0.0003930000
C	5.4325020000	-2.2107150000	-0.0004490000
C	7.4251040000	-0.7755250000	0.0000980000

H	7.7281150000	-0.2172920000	-0.8895760000
H	7.7277190000	-0.2168430000	0.8896180000
H	7.8869340000	-1.7606950000	0.0004290000
C	3.3013560000	-3.4292040000	-0.0003680000
H	2.6670150000	-3.4704820000	0.8886710000
H	2.6669170000	-3.4704430000	-0.8893390000
H	4.0047210000	-4.2593970000	-0.0004260000
N	3.2906610000	-1.0690250000	-0.0003550000
N	5.9847510000	-0.9385700000	-0.0001470000
O	6.0893940000	-3.2258780000	-0.0002080000

Sulphur (Set A):

C	-2.8495700000	3.7101070000	0.0002020000
C	-3.7126450000	2.6209360000	0.0001590000
C	-3.2392670000	1.3108460000	0.0001200000
C	-1.8482930000	1.1136760000	0.0001250000
C	-0.9714050000	2.2176180000	0.0001630000
C	-1.4819430000	3.5136280000	0.0002030000
H	-3.2563380000	4.7160340000	0.0002320000
H	-0.8030200000	4.3618610000	0.0002330000
C	0.5629710000	0.4309750000	0.0000910000
C	1.8128450000	-0.1710920000	0.0000500000
C	2.9465700000	0.6330620000	0.0000490000
C	2.8102910000	2.0301200000	0.0001080000
C	1.5635040000	2.6197080000	0.0001580000
C	0.4166880000	1.8234550000	0.0001440000
H	1.9183470000	-1.2508280000	0.0000050000
H	3.7052680000	2.6416200000	0.0001050000
H	1.4778970000	3.7029190000	0.0001980000
C	4.2905400000	0.0179560000	-0.0000480000
N	4.3451210000	-1.3110790000	-0.0003310000
N	6.5466520000	0.2518540000	-0.0002460000

C	6.7583760000	-1.1131540000	-0.0003220000
N	5.3319080000	0.8435870000	0.0001360000
N	5.5862680000	-1.8444920000	-0.0002110000
O	7.8580900000	-1.6170820000	-0.0005020000
C	7.7058570000	1.1239510000	0.0000330000
H	8.3191830000	0.9450260000	0.8869890000
H	8.3214870000	0.9422300000	-0.8847180000
H	7.3346180000	2.1470980000	-0.0019980000
C	5.6833570000	-3.2918100000	-0.0006050000
H	6.2188880000	-3.6391960000	-0.8879620000
H	6.2238500000	-3.6390950000	0.8837320000
H	4.6662330000	-3.6792220000	0.0021770000
H	-4.7859410000	2.7751950000	0.0001530000
C	-4.2000810000	0.1941090000	0.0000680000
N	-5.4980590000	0.4974670000	0.0000250000
N	-4.5816870000	-2.0453160000	0.0000770000
C	-5.9565460000	-1.8897470000	-0.0000650000
C	-7.7499140000	-0.2117620000	0.0000250000
H	-7.9791130000	0.3802020000	0.8898310000
H	-7.9789580000	0.3809350000	-0.8893270000
H	-8.3326190000	-1.1305370000	-0.0003890000
C	-3.9923350000	-3.3699220000	0.0002330000
H	-3.3678050000	-3.4891240000	-0.8891960000
H	-3.3679750000	-3.4889960000	0.8897990000
H	-4.7924740000	-4.1073240000	0.0002080000
N	-3.6960330000	-1.0281520000	0.0001160000
N	-6.3410760000	-0.5552420000	-0.0000410000
O	-6.7380690000	-2.8117860000	0.0001060000
S	-0.9767110000	-0.4171380000	0.0000680000

Boron (Set B):

C	-2.9817090000	-1.5922140000	-0.0000120000
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C	-3.4864220000	-0.2937050000	-0.0000550000
C	-2.5920780000	0.7863280000	-0.0000660000
C	-1.2275360000	0.5607070000	-0.0000320000
C	-0.7382890000	-0.7657630000	-0.0000070000
C	-1.6098300000	-1.8373330000	0.0000080000
H	-3.6810230000	-2.4217370000	-0.0000040000
H	-2.9864740000	1.7979660000	-0.0000880000
H	-1.2453160000	-2.8613330000	0.0000300000
C	1.2275350000	0.5607070000	0.0000130000
C	2.5920780000	0.7863280000	0.0000220000
C	3.4864220000	-0.2937050000	0.0000070000
C	2.9817090000	-1.5922140000	-0.0000250000
C	1.6098310000	-1.8373320000	-0.0000300000
C	0.7382890000	-0.7657620000	-0.0000020000
H	2.9864730000	1.7979670000	0.0000400000
H	3.6810230000	-2.4217360000	-0.0000400000
H	1.2453160000	-2.8613320000	-0.0000520000
B	0.0000000000	1.5177950000	0.0000050000
H	-0.0000010000	2.7051180000	-0.0000310000
C	4.9455290000	-0.0599720000	0.0000320000
N	5.3512240000	1.2056660000	0.0004560000
N	7.0586490000	-0.8853660000	-0.0001010000
C	7.6252710000	0.3749460000	0.0001110000
C	-4.9455300000	-0.0599740000	-0.0000980000
N	-5.7307500000	-1.1335620000	0.0002540000
N	-6.6893150000	1.3909500000	-0.0004600000
C	-7.6252700000	0.3749480000	-0.0000740000
N	5.7307490000	-1.1335610000	-0.0003710000
N	6.6893160000	1.3909500000	0.0002790000
N	-7.0586490000	-0.8853660000	0.0000380000
N	-5.3512240000	1.2056650000	-0.0004960000
O	8.8192660000	0.5682680000	0.0001490000

O	-8.8192660000	0.5682700000	0.0001300000
C	7.9454880000	-2.0333230000	-0.0006400000
H	8.5844400000	-2.0229700000	-0.8874970000
H	8.5872950000	-2.0213910000	0.8840960000
H	7.3167230000	-2.9217520000	0.0011050000
C	7.1664400000	2.7609390000	0.0008030000
H	7.7754200000	2.9536370000	0.8878510000
H	7.7790280000	2.9528550000	-0.8838910000
H	6.2883420000	3.4040520000	-0.0011970000
C	-7.9454890000	-2.0333230000	0.0007160000
H	-8.5842640000	-2.0230060000	0.8877010000
H	-8.5874720000	-2.0213530000	-0.8838910000
H	-7.3167240000	-2.9217510000	-0.0011890000
C	-7.1664390000	2.7609380000	-0.0006920000
H	-7.7773830000	2.9530370000	-0.8865010000
H	-7.7770670000	2.9534550000	0.8852450000
H	-6.2883400000	3.4040520000	-0.0010000000

Carbon (Set B):

C	-2.9987120000	-1.6913390000	-0.0004070000
C	-3.4497830000	-0.3672970000	-0.0003710000
C	-2.5236920000	0.6797220000	-0.0002460000
C	-1.1749440000	0.3891190000	-0.0001570000
C	-0.7285470000	-0.9400730000	-0.0001430000
C	-1.6451980000	-1.9844380000	-0.0002950000
H	-3.7311000000	-2.4909600000	-0.0005570000
H	-2.8783670000	1.7057300000	-0.0002230000
H	-1.3116340000	-3.0185330000	-0.0003300000
C	1.1749440000	0.3891190000	0.0000400000
C	2.5236920000	0.6797220000	0.0001340000
C	3.4497830000	-0.3672970000	0.0002670000
C	2.9987120000	-1.6913390000	0.0003000000

C	1.6451980000	-1.9844380000	0.0001790000
C	0.7285470000	-0.9400730000	0.0000230000
H	2.8783670000	1.7057300000	0.0001110000
H	3.7311000000	-2.4909600000	0.0004570000
H	1.3116340000	-3.0185330000	0.0002110000
C	4.8986200000	-0.0755400000	0.0003660000
N	5.2551250000	1.2059740000	0.0026580000
N	7.0440320000	-0.8156830000	-0.0018850000
C	7.5606230000	0.4651690000	0.0000000000
C	-4.8986200000	-0.0755400000	-0.0004540000
N	-5.7265700000	-1.1163860000	0.0020810000
N	-6.5855080000	1.4430650000	-0.0022100000
C	-7.5606230000	0.4651690000	0.0002270000
N	5.7265700000	-1.1163860000	-0.0021490000
N	6.5855080000	1.4430660000	0.0020450000
N	-7.0440320000	-0.8156830000	0.0019520000
N	-5.2551250000	1.2059740000	-0.0027480000
O	8.7462730000	0.7060670000	0.0000590000
O	-8.7462730000	0.7060680000	0.0003420000
C	7.9749360000	-1.9281750000	-0.0044880000
H	8.6125720000	-1.8916370000	-0.8915980000
H	8.6160320000	-1.8926730000	0.8801320000
H	7.3810000000	-2.8402520000	-0.0039230000
C	7.0089450000	2.8303850000	0.0047240000
H	7.6103150000	3.0454440000	0.8918630000
H	7.6132770000	3.0477530000	-0.8797950000
H	6.1064720000	3.4388430000	0.0040760000
C	-7.9749360000	-1.9281750000	0.0047210000
H	-8.6123240000	-1.8917170000	0.8920130000
H	-8.6162780000	-1.8925920000	-0.8797160000
H	-7.3810010000	-2.8402520000	0.0039090000
C	-7.0089450000	2.8303850000	-0.0046880000

H	-7.6124430000	3.0448190000	-0.8905130000
H	-7.6111520000	3.0483820000	0.8811440000
H	-6.1064720000	3.4388390000	-0.0065660000
C	0.0000000000	1.3266900000	-0.0000610000
H	0.0000770000	1.9836900000	-0.8796460000
H	-0.0000770000	1.9836950000	0.8795200000

Nitrogen (Set B):

C	-3.0237210000	-1.7628500000	-0.0000240000
C	-3.4179260000	-0.4133900000	0.0001000000
C	-2.4640000000	0.5995880000	0.0002430000
C	-1.1270190000	0.2354980000	0.0002560000
C	-0.7190790000	-1.1150270000	0.0001250000
C	-1.6889780000	-2.1150600000	-0.0000060000
H	-3.7914930000	-2.5275540000	-0.0001340000
H	-2.7740160000	1.6392150000	0.0003510000
H	-1.3998500000	-3.1623390000	-0.0001070000
C	1.1270150000	0.2355080000	0.0002730000
C	2.4639990000	0.5995890000	0.0003060000
C	3.4179250000	-0.4133880000	0.0002110000
C	3.0237240000	-1.7628500000	0.0000890000
C	1.6889790000	-2.1150550000	0.0000570000
C	0.7190820000	-1.1150220000	0.0001350000
H	2.7740160000	1.6392160000	0.0004150000
H	3.7914940000	-2.5275540000	0.0000230000
H	1.3998460000	-3.1623330000	-0.0000360000
C	4.8549210000	-0.0651050000	0.0002350000
N	5.1630410000	1.2292810000	0.0001690000
N	7.0264300000	-0.7244480000	0.0000960000
C	7.4947830000	0.5743790000	0.0000020000

C	-4.8549230000	-0.0651150000	0.0000810000
N	-5.7210400000	-1.0732770000	0.0002900000
N	-6.4840540000	1.5156510000	-0.0000660000
C	-7.4947830000	0.5743730000	-0.0001090000
N	5.7210410000	-1.0732810000	0.0001240000
N	6.4840630000	1.5156510000	0.0000640000
N	-7.0264360000	-0.7244450000	-0.0001470000
N	-5.1630400000	1.2292840000	-0.0003010000
O	8.6707080000	0.8596750000	-0.0005200000
O	-8.6707050000	0.8596840000	-0.0003670000
C	7.9970830000	-1.8025260000	-0.0003400000
H	8.6331800000	-1.7445990000	-0.8874010000
H	8.6363060000	-1.7422480000	0.8842770000
H	7.4363730000	-2.7353520000	0.0018170000
C	6.8558420000	2.9175720000	-0.0002250000
H	7.4504810000	3.1563730000	0.8853690000
H	7.4501980000	3.1560950000	-0.8860860000
H	5.9315540000	3.4922980000	-0.0001680000
C	-7.9970830000	-1.8025280000	0.0001200000
H	-8.6330710000	-1.7448620000	0.8872820000
H	-8.6364160000	-1.7419990000	-0.8843950000
H	-7.4363710000	-2.7353510000	-0.0023670000
C	-6.8558430000	2.9175700000	-0.0005860000
H	-7.4479240000	3.1566700000	-0.8878380000
H	-7.4527580000	3.1557820000	0.8836110000
H	-5.9315620000	3.4923020000	0.0021450000
N	-0.0000010000	1.0345670000	0.0004200000
H	-0.0000260000	2.0415290000	0.0001320000

Oxygen (Set B):

C	-3.0406430000	-1.8230770000	-0.0000620000
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C	-3.3885980000	-0.4623300000	-0.0000870000
C	-2.3993740000	0.5197410000	-0.0000740000
C	-1.0906640000	0.0911260000	-0.0000380000
C	-0.7201890000	-1.2582060000	-0.0000100000
C	-1.7192920000	-2.2282090000	-0.0000220000
H	-3.8362300000	-2.5590390000	-0.0000740000
H	-2.6540620000	1.5726470000	-0.0000930000
H	-1.4670850000	-3.2845040000	-0.0000050000
C	1.0906670000	0.0911230000	0.0000100000
C	2.3993780000	0.5197350000	0.0000210000
C	3.3886000000	-0.4623390000	0.0000470000
C	3.0406420000	-1.8230850000	0.0000680000
C	1.7192890000	-2.2282140000	0.0000530000
C	0.7201890000	-1.2582080000	0.0000220000
H	2.6540720000	1.5726390000	0.0000010000
H	3.8362260000	-2.5590500000	0.0000900000
H	1.4670800000	-3.2845080000	0.0000660000
C	4.8126340000	-0.0638940000	0.0000370000
N	5.0719080000	1.2402820000	0.0002250000
N	7.0048380000	-0.6443380000	0.0000880000
C	7.4253240000	0.6718670000	0.0000870000
C	-4.8126300000	-0.0638790000	-0.0001240000
N	-5.7135160000	-1.0408840000	0.0000290000
N	-6.3804340000	1.5758620000	-0.0002160000
C	-7.4253190000	0.6718840000	0.0000220000
N	5.7135150000	-1.0408860000	-0.0001260000
N	6.3804110000	1.5758630000	0.0000250000
N	-7.0048190000	-0.6443510000	-0.0001040000
N	-5.0719080000	1.2402830000	-0.0002990000
O	8.5896390000	0.9991610000	0.0000640000
O	-8.5896480000	0.9991320000	0.0001760000

C	8.0156130000	-1.6848610000	-0.0001730000
H	8.6491980000	-1.6025320000	-0.8870830000
H	8.6517470000	-1.6002640000	0.8846610000
H	7.4909090000	-2.6384170000	0.0017440000
C	6.6998350000	2.9909380000	0.0002780000
H	7.2832170000	3.2512620000	0.8872290000
H	7.2866000000	3.2506460000	-0.8845840000
H	5.7547370000	3.5307340000	-0.0016590000
C	-8.0156070000	-1.6848590000	0.0002770000
H	-8.6490360000	-1.6025740000	0.8873030000
H	-8.6518970000	-1.6002020000	-0.8844390000
H	-7.4909170000	-2.6384240000	-0.0017890000
C	-6.6998410000	2.9909420000	-0.0002650000
H	-7.2850470000	3.2509030000	-0.8861020000
H	-7.2847750000	3.2510270000	0.8857160000
H	-5.7547340000	3.5307250000	-0.0004490000
O	0.0000030000	0.9128230000	-0.0000250000

Sulphur (Set B):

C	-2.9672190000	-1.6637380000	-0.0000080000
C	-3.4832760000	-0.3586050000	-0.0000810000
C	-2.6159130000	0.7277830000	-0.0001120000
C	-1.2493010000	0.4938630000	-0.0000780000
C	-0.7208670000	-0.8073110000	-0.0000270000
C	-1.6064050000	-1.8867650000	0.0000130000
H	-3.6591440000	-2.4980250000	0.0000190000
H	-3.0157720000	1.7359560000	-0.0001630000
H	-1.2232560000	-2.9035180000	0.0000570000
C	1.2493010000	0.4938630000	-0.0000410000
C	2.6159130000	0.7277830000	-0.0000260000
C	3.4832760000	-0.3586050000	-0.0000070000

C	2.9672190000	-1.6637380000	-0.0000070000
C	1.6064060000	-1.8867650000	-0.0000100000
C	0.7208670000	-0.8073110000	-0.0000230000
H	3.0157720000	1.7359560000	-0.0000330000
H	3.6591440000	-2.4980250000	0.0000050000
H	1.2232560000	-2.9035180000	0.0000000000
C	4.9448880000	-0.1368790000	0.0000220000
N	5.3631550000	1.1255040000	0.0004770000
N	7.0486580000	-0.9836080000	-0.0000740000
C	7.6284210000	0.2704660000	0.0001010000
C	-4.9448880000	-0.1368790000	-0.0001380000
N	-5.7180810000	-1.2175220000	0.0002300000
N	-6.7031160000	1.2967080000	-0.0004620000
C	-7.6284210000	0.2704660000	-0.0000700000
N	5.7180820000	-1.2175220000	-0.0003700000
N	6.7031170000	1.2967080000	0.0002970000
N	-7.0486580000	-0.9836080000	0.0000270000
N	-5.3631550000	1.1255040000	-0.0005170000
O	8.8241890000	0.4517690000	0.0002010000
O	-8.8241880000	0.4517700000	0.0002160000
C	7.9230570000	-2.1411400000	-0.0006080000
H	8.5617910000	-2.1377510000	-0.8876580000
H	8.5649660000	-2.1359470000	0.8840980000
H	7.2845130000	-3.0225580000	0.0013660000
C	7.1953180000	2.6612940000	0.0008770000
H	7.8062990000	2.8471450000	0.8879980000
H	7.8100130000	2.8463460000	-0.8838050000
H	6.3244410000	3.3141400000	-0.0011690000
C	-7.9230570000	-2.1411400000	0.0007700000
H	-8.5615870000	-2.1377550000	0.8879680000
H	-8.5651710000	-2.1359430000	-0.8837870000

H	-7.2845130000	-3.0225580000	-0.0013530000
C	-7.1953190000	2.6612930000	-0.0006440000
H	-7.8083720000	2.8465430000	-0.8864400000
H	-7.8079460000	2.8469460000	0.8853660000
H	-6.3244400000	3.3141400000	-0.0009990000
S	0.0000000000	1.7298340000	-0.0000920000

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Boron (Set A):

C	-2.9361600000	3.7091430000	0.1929400000
C	-3.7849760000	2.6167090000	0.1182540000
C	-3.2653380000	1.3154380000	0.0492240000
C	-1.8819960000	1.1287920000	0.0230250000
C	-1.0353430000	2.2601480000	0.1164230000
C	-1.5488330000	3.5417510000	0.2013100000
H	-3.3571530000	4.7077370000	0.2555650000
H	-0.8969380000	4.4073470000	0.2679430000
C	0.4821130000	0.4417890000	-0.0539070000
C	1.7297150000	-0.1595200000	-0.1048290000
C	2.8924230000	0.6199230000	0.0008910000
C	2.7741030000	2.0029950000	0.1435950000
C	1.5251250000	2.6235970000	0.1861890000
C	0.3855500000	1.8445390000	0.0926980000
H	1.8253290000	-1.2332430000	-0.2241130000
H	3.6780140000	2.5965690000	0.2197570000
H	1.4677390000	3.7026520000	0.2924040000
C	4.2269010000	-0.0129250000	-0.0432530000
N	4.2647920000	-1.3339080000	-0.1777590000
N	6.4858210000	0.1807850000	0.0108460000
C	6.6792690000	-1.1814870000	-0.1264560000
N	5.2837000000	0.7876160000	0.0545590000

N	5.4931650000	-1.8858340000	-0.2164650000
O	7.7749570000	-1.7033570000	-0.1639080000
C	7.6301020000	1.0620420000	0.1180930000
H	7.5866750000	1.5992870000	1.0681140000
H	8.5332610000	0.4584820000	0.0680290000
H	7.6110480000	1.7827790000	-0.7023900000
C	5.5214550000	-3.3264060000	-0.3642030000
H	5.0229840000	-3.6053710000	-1.2951540000
H	6.5598350000	-3.6487960000	-0.3817490000
H	4.9963410000	-3.7874110000	0.4752550000
H	-4.8599160000	2.7559370000	0.1231980000
C	-4.2031950000	0.1720640000	0.0318690000
N	-5.3723870000	0.3665620000	-0.5695750000
N	-4.6815820000	-1.9685880000	0.5915130000
C	-5.9356950000	-1.9156200000	0.0118880000
C	-7.4888390000	-0.4699010000	-1.2115730000
H	-7.9841190000	0.3971270000	-0.7699790000
H	-7.3195360000	-0.2820830000	-2.2746260000
H	-8.0979240000	-1.3612930000	-1.0815740000
C	-4.2469750000	-3.1795450000	1.2571240000
H	-3.2794450000	-3.4805860000	0.8515370000
H	-4.1435030000	-2.9937900000	2.3291540000
H	-4.9908240000	-3.9533090000	1.0825310000
N	-3.8112160000	-0.9394810000	0.6418800000
N	-6.2199510000	-0.6827510000	-0.5468740000
O	-6.7086530000	-2.8515820000	-0.0017110000
B	-0.9639400000	-0.1235370000	-0.1745850000
H	-1.2754290000	-1.2367960000	-0.4587360000

Carbon (Set A):

C	-2.9811270000	3.7271210000	-0.0000130000
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C	-3.7746340000	2.5882300000	0.0000260000
C	-3.2141640000	1.3025770000	0.0002920000
C	-1.8199900000	1.1929380000	0.0004530000
C	-1.0257900000	2.3557390000	0.0003410000
C	-1.5959450000	3.6230570000	0.0001480000
H	-3.4525860000	4.7044130000	-0.0001660000
H	-0.9745140000	4.5129500000	0.0001000000
C	0.4553360000	0.5671490000	0.0006530000
C	1.6793450000	-0.0758890000	0.0007540000
C	2.8523140000	0.6873250000	0.0005970000
C	2.7728090000	2.0859710000	0.0003920000
C	1.5451300000	2.7304880000	0.0003230000
C	0.3813670000	1.9664860000	0.0004430000
H	1.7501960000	-1.1579340000	0.0009040000
H	3.6919800000	2.6595240000	0.0002710000
H	1.5033240000	3.8152050000	0.0002490000
C	4.1710110000	0.0199920000	0.0006190000
N	4.1782290000	-1.3093480000	0.0014510000
N	6.4352320000	0.1628520000	-0.0001520000
C	6.5966420000	-1.2097730000	-0.0005220000
N	5.2476110000	0.7995870000	-0.0002550000
N	5.3940510000	-1.8910100000	0.0014270000
O	7.6799280000	-1.7590970000	-0.0020210000
C	7.5997820000	1.0237800000	-0.0025270000
H	7.5790770000	1.6635440000	0.8824530000
H	8.4888930000	0.3977440000	0.0056630000
H	7.5868470000	1.6500770000	-0.8973840000
C	5.3884170000	-3.3390440000	0.0009260000
H	4.8750230000	-3.7003270000	-0.8930450000
H	6.4190660000	-3.6857980000	0.0085540000
H	4.8613240000	-3.6997670000	0.8869730000

H	-4.8538030000	2.6792420000	-0.0001500000
C	-4.1216480000	0.1333100000	0.0003090000
N	-5.4291710000	0.3917950000	-0.0002450000
N	-4.4417850000	-2.1137350000	0.0008940000
C	-5.8178010000	-1.9966100000	-0.0005090000
C	-7.6604020000	-0.3828640000	-0.0017370000
H	-7.9077690000	0.2054740000	0.8845230000
H	-7.9090250000	0.1937000000	-0.8954680000
H	-8.2078550000	-1.3223690000	0.0045350000
C	-3.8322450000	-3.4272170000	0.0003470000
H	-3.2141450000	-3.5418960000	-0.8930930000
H	-3.2043270000	-3.5371060000	0.8874060000
H	-4.6243280000	-4.1723280000	0.0064020000
N	-3.5784700000	-1.0770750000	0.0009180000
N	-6.2426160000	-0.6803690000	-0.0000500000
O	-6.5744060000	-2.9460520000	-0.0016760000
C	-0.9268510000	-0.0207150000	0.0006130000
H	-1.1112110000	-0.6572630000	-0.8710580000
H	-1.1112660000	-0.6570590000	0.8724100000

Nitrogen (Set A):

C	3.1179170000	3.7893140000	0.0000960000
C	3.8433850000	2.5985660000	-0.0000390000
C	3.2187120000	1.3497560000	-0.0001440000
C	1.8146670000	1.3472140000	-0.0001130000
C	1.0685270000	2.5529270000	0.0000220000
C	1.7297100000	3.7774350000	0.0001290000
H	3.6510240000	4.7337060000	0.0001740000
H	1.1699670000	4.7073150000	0.0002360000
C	-0.3542780000	0.7599980000	-0.0001170000
C	-1.5458750000	0.0480230000	-0.0001590000

C	-2.7374460000	0.7693570000	-0.0000550000
C	-2.7200230000	2.1769090000	0.0000850000
C	-1.5268940000	2.8761800000	0.0001210000
C	-0.3221880000	2.1723780000	0.0000220000
H	-1.5672720000	-1.0352210000	-0.0002710000
H	-3.6643830000	2.7065200000	0.0001640000
H	-1.5338860000	3.9614910000	0.0002200000
C	-4.0284080000	0.0479490000	-0.0000920000
N	-3.9777990000	-1.2823130000	-0.0004730000
N	-6.2954200000	0.0993630000	0.0004530000
C	-6.3941070000	-1.2746940000	-0.0000860000
N	-5.1341790000	0.7862610000	0.0002950000
N	-5.1718330000	-1.9111600000	-0.0007110000
O	-7.4541200000	-1.8678890000	0.0001260000
C	-7.5195990000	0.8748940000	0.0008390000
H	-8.1144730000	0.6475370000	-0.8865200000
H	-8.1165180000	0.6430290000	0.8856100000
H	-7.2291760000	1.9230200000	0.0037520000
C	-5.1545610000	-3.3599310000	-0.0007350000
H	-5.6590370000	-3.7469560000	0.8873990000
H	-5.6667140000	-3.7466630000	-0.8845200000
H	-4.1101490000	-3.6634770000	-0.0051800000
H	4.9265270000	2.6258540000	-0.0000580000
C	4.0134080000	0.1123430000	-0.0002460000
N	5.3399290000	0.2435440000	-0.0000860000
N	4.1184740000	-2.1610360000	-0.0004720000
C	5.4988920000	-2.1719070000	0.0001960000
C	7.4862280000	-0.7396590000	0.0007780000
H	7.7870480000	-0.1763510000	-0.8850570000
H	7.7881220000	-0.1900350000	0.8949350000
H	7.9418540000	-1.7268840000	-0.0067100000

C	3.3897410000	-3.4115910000	-0.0001260000
H	2.7621310000	-3.4690060000	0.8925960000
H	2.7593590000	-3.4675520000	-0.8909510000
H	4.1099600000	-4.2263970000	-0.0018230000
N	3.3576700000	-1.0451500000	-0.0005040000
N	6.0460200000	-0.9007940000	-0.0004020000
O	6.1627700000	-3.1883670000	0.0009680000
N	0.9413020000	0.2916090000	-0.0001880000
H	1.2604340000	-0.6649150000	-0.0003590000

Oxygen (Set A):

C	3.1508540000	3.7759600000	-0.0002160000
C	3.8314840000	2.5605480000	-0.0002470000
C	3.1710200000	1.3268610000	-0.0002250000
C	1.7750740000	1.3896960000	-0.0001560000
C	1.0730760000	2.6089760000	-0.0001210000
C	1.7645830000	3.8164200000	-0.0001530000
H	3.7196840000	4.6993660000	-0.0002410000
H	1.2328340000	4.7619760000	-0.0001260000
C	-0.3423850000	0.8504670000	-0.0000450000
C	-1.5004460000	0.1010190000	0.0000160000
C	-2.7072830000	0.8022280000	0.0000740000
C	-2.7150750000	2.2085390000	0.0000690000
C	-1.5374350000	2.9360980000	0.0000060000
C	-0.3239650000	2.2486680000	-0.0000500000
H	-1.4815780000	-0.9810310000	0.0000180000
H	-3.6703760000	2.7184430000	0.0001150000
H	-1.5651730000	4.0206240000	0.0000040000
C	-3.9845650000	0.0565840000	0.0001410000
N	-3.9062440000	-1.2713220000	0.0003590000
N	-6.2507380000	0.0641210000	0.0002520000

C	-6.3213610000	-1.3124760000	0.0003420000
N	-5.1038090000	0.7739860000	-0.0000280000
N	-5.0861950000	-1.9245940000	0.0002260000
O	-7.3689530000	-1.9260380000	0.0003090000
C	-7.4909550000	0.8139230000	-0.0001030000
H	-8.0806070000	0.5733170000	-0.8874060000
H	-8.0828480000	0.5700560000	0.8847740000
H	-7.2228050000	1.8679590000	0.0020980000
C	-5.0389870000	-3.3730530000	0.0005810000
H	-5.5369880000	-3.7695690000	0.8880780000
H	-5.5415580000	-3.7699420000	-0.8841260000
H	-3.9885420000	-3.6549380000	-0.0019870000
O	0.9193510000	0.3310320000	-0.0001090000
H	4.9145380000	2.5488940000	-0.0002960000
C	3.9536890000	0.0746190000	-0.0002700000
N	5.2797190000	0.2104190000	-0.0001910000
N	4.0519520000	-2.1871700000	-0.0001710000
C	5.4328170000	-2.2049660000	-0.0002820000
C	7.4247640000	-0.7789060000	0.0000150000
H	7.7292430000	-0.2240980000	-0.8902430000
H	7.7289390000	-0.2234270000	0.8899530000
H	7.8774460000	-1.7676150000	0.0004430000
C	3.3147270000	-3.4341650000	0.0000090000
H	2.6829700000	-3.4806400000	0.8896120000
H	2.6827890000	-3.4807750000	-0.8894560000
H	4.0284500000	-4.2546450000	-0.0000020000
N	3.2929760000	-1.0734700000	-0.0002010000
N	5.9850800000	-0.9363750000	-0.0001350000
O	6.0941790000	-3.2231620000	0.0000120000

Sulphur (Set A):

C	-2.8623880000	3.7152610000	0.0001630000
C	-3.7223220000	2.6213810000	0.0001330000
C	-3.2413550000	1.3119560000	0.0000720000
C	-1.8484210000	1.1215970000	0.0000380000
C	-0.9735360000	2.2304700000	0.0000700000
C	-1.4913760000	3.5258990000	0.0001330000
H	-3.2733570000	4.7189410000	0.0002120000
H	-0.8191500000	4.3778350000	0.0001590000
C	0.5603570000	0.4395200000	-0.0000240000
C	1.8104210000	-0.1667600000	-0.0000570000
C	2.9468710000	0.6369920000	-0.0000370000
C	2.8144010000	2.0361660000	0.0000230000
C	1.5672710000	2.6294890000	0.0000620000
C	0.4165670000	1.8351920000	0.0000380000
H	1.9160360000	-1.2450800000	-0.0001030000
H	3.7104180000	2.6444190000	0.0000380000
H	1.4860760000	3.7118030000	0.0001080000
C	4.2895200000	0.0177050000	-0.0000840000
N	4.3407290000	-1.3117570000	-0.0003870000
N	6.5442400000	0.2457780000	-0.0001130000
C	6.7484840000	-1.1172910000	-0.0001760000
N	5.3334520000	0.8405660000	0.0001660000
N	5.5787410000	-1.8468380000	-0.0001960000
O	7.8508490000	-1.6261350000	-0.0002680000
C	7.7053550000	1.1129590000	0.0002870000
H	8.3155300000	0.9313140000	0.8877610000
H	8.3184390000	0.9278610000	-0.8844190000
H	7.3356480000	2.1358120000	-0.0022270000
C	5.6727430000	-3.2930000000	-0.0007080000
H	6.2067760000	-3.6391430000	-0.8883420000
H	6.2117330000	-3.6392060000	0.8838510000

H	4.6547050000	-3.6757710000	0.0020330000
H	-4.7954940000	2.7692390000	0.0001590000
C	-4.1966020000	0.1904110000	0.0000460000
N	-5.4955960000	0.4897960000	0.0000960000
N	-4.5683520000	-2.0476670000	0.0000410000
C	-5.9407480000	-1.8927080000	-0.0000470000
C	-7.7437180000	-0.2337550000	0.0002730000
H	-7.9778890000	0.3538480000	0.8906490000
H	-7.9779080000	0.3546600000	-0.8895550000
H	-8.3129960000	-1.1601730000	-0.0001270000
C	-3.9871540000	-3.3744620000	0.0001800000
H	-3.3661790000	-3.4982130000	-0.8897630000
H	-3.3662830000	-3.4980820000	0.8902150000
H	-4.7958760000	-4.1014550000	0.0001850000
N	-3.6869140000	-1.0299080000	0.0000500000
N	-6.3331920000	-0.5642870000	0.0000590000
O	-6.7221620000	-2.8213160000	0.0002310000
S	-0.9773560000	-0.4000580000	-0.0000530000

Boron (Set A):

C	-2.9878750000	-1.5952670000	-0.0000340000
C	-3.4917740000	-0.2942840000	-0.0000590000
C	-2.5955980000	0.7867910000	-0.0000580000
C	-1.2287890000	0.5590010000	-0.0000270000
C	-0.7395190000	-0.7700270000	0.0000030000
C	-1.6143230000	-1.8418300000	0.0000010000
H	-3.6875140000	-2.4232380000	-0.0000370000
H	-2.9905630000	1.7967650000	-0.0000780000
H	-1.2547080000	-2.8663300000	0.0000220000
C	1.2287880000	0.5590010000	0.0000250000
C	2.5955980000	0.7867910000	0.0000430000

C	3.4917740000	-0.2942840000	0.0000730000
C	2.9878750000	-1.5952670000	0.0000810000
C	1.6143240000	-1.8418300000	0.0000580000
C	0.7395190000	-0.7700270000	0.0000320000
H	2.9905630000	1.7967650000	0.0000350000
H	3.6875140000	-2.4232380000	0.0001050000
H	1.2547080000	-2.8663300000	0.0000640000
B	0.0000000000	1.5168320000	-0.0000110000
H	0.0000000000	2.7107510000	-0.0000320000
C	4.9512270000	-0.0596540000	0.0000920000
N	5.3563470000	1.2064770000	0.0002380000
N	7.0630250000	-0.8832930000	0.0001260000
C	7.6243630000	0.3759590000	0.0000720000
C	-4.9512270000	-0.0596550000	-0.0000850000
N	-5.7374930000	-1.1330010000	-0.0000200000
N	-6.6922370000	1.3914070000	-0.0002130000
C	-7.6243630000	0.3759590000	-0.0000410000
N	5.7374930000	-1.1330010000	-0.0000810000
N	6.6922370000	1.3914070000	0.0000200000
N	-7.0630250000	-0.8832930000	-0.0002240000
N	-5.3563470000	1.2064770000	-0.0002380000
O	8.8226190000	0.5708880000	0.0000070000
O	-8.8226190000	0.5708880000	0.0001250000
C	7.9507610000	-2.0287990000	-0.0002360000
H	8.5872890000	-2.0163870000	-0.8876910000
H	8.5910680000	-2.0137350000	0.8844080000
H	7.3218120000	-2.9161170000	0.0023470000
C	7.1689810000	2.7601040000	0.0002960000
H	7.7763590000	2.9509790000	0.8877170000
H	7.7804500000	2.9496940000	-0.8845440000
H	6.2900560000	3.4007290000	-0.0021170000

C	-7.9507610000	-2.0287990000	0.0001830000
H	-8.5871300000	-2.0164830000	0.8877540000
H	-8.5912260000	-2.0136400000	-0.8843450000
H	-7.3218120000	-2.9161170000	-0.0026070000
C	-7.1689820000	2.7601030000	-0.0001990000
H	-7.7785420000	2.9502940000	-0.8862470000
H	-7.7782710000	2.9503780000	0.8860190000
H	-6.2900540000	3.4007300000	-0.0003640000

Carbon (Set B):

C	-3.0043290000	-1.6921340000	-0.0007810000
C	-3.4548210000	-0.3659460000	-0.0005270000
C	-2.5276720000	0.6826500000	-0.0001290000
C	-1.1768100000	0.3907560000	-0.0000180000
C	-0.7296670000	-0.9406350000	-0.0001390000
C	-1.6491630000	-1.9859760000	-0.0005940000
H	-3.7368080000	-2.4903820000	-0.0011970000
H	-2.8849420000	1.7063890000	0.0001030000
H	-1.3189810000	-3.0199740000	-0.0007890000
C	1.1768100000	0.3907560000	-0.0002170000
C	2.5276710000	0.6826510000	-0.0001310000
C	3.4548210000	-0.3659450000	0.0003460000
C	3.0043290000	-1.6921330000	0.0007160000
C	1.6491630000	-1.9859760000	0.0005520000
C	0.7296670000	-0.9406340000	0.0000120000
H	2.8849420000	1.7063900000	-0.0004490000
H	3.7368080000	-2.4903810000	0.0011960000
H	1.3189820000	-3.0199740000	0.0008330000
C	4.9041970000	-0.0740670000	0.0004970000
N	5.2616450000	1.2073740000	0.0022940000
N	7.0468230000	-0.8157430000	-0.0014250000

C	7.5601200000	0.4632760000	0.0001700000
C	-4.9041970000	-0.0740670000	-0.0007130000
N	-5.7316120000	-1.1156260000	0.0015540000
N	-6.5902340000	1.4423430000	-0.0019470000
C	-7.5601200000	0.4632750000	-0.0002390000
N	5.7316110000	-1.1156250000	-0.0016740000
N	6.5902340000	1.4423440000	0.0017220000
N	-7.0468230000	-0.8157440000	0.0014270000
N	-5.2616450000	1.2073730000	-0.0024350000
O	8.7503630000	0.7040520000	-0.0000980000
O	-8.7503620000	0.7040530000	0.0007120000
C	7.9766940000	-1.9272640000	-0.0038820000
H	8.6119200000	-1.8899280000	-0.8915910000
H	8.6164310000	-1.8897550000	0.8805260000
H	7.3810800000	-2.8373000000	-0.0023700000
C	7.0152350000	2.8277000000	0.0038400000
H	7.6153200000	3.0403350000	0.8913340000
H	7.6190550000	3.0416830000	-0.8807460000
H	6.1129260000	3.4349760000	0.0024850000
C	-7.9766940000	-1.9272630000	0.0043050000
H	-8.6116430000	-1.8898410000	0.8922090000
H	-8.6167070000	-1.8898390000	-0.8799060000
H	-7.3810810000	-2.8373000000	0.0027020000
C	-7.0152350000	2.8277000000	-0.0035270000
H	-7.6176190000	3.0398520000	-0.8895550000
H	-7.6167580000	3.0421700000	0.8825270000
H	-6.1129240000	3.4349720000	-0.0047600000
C	0.0000000000	1.3298250000	-0.0001580000
H	-0.0001020000	1.9834100000	-0.8805640000
H	0.0001020000	1.9834880000	0.8801890000

Nitrogen (Set B):

C	-3.0324920000	-1.7733060000	-0.0000330000
C	-3.4216330000	-0.4204720000	0.0000920000
C	-2.4636000000	0.5905420000	0.0002290000
C	-1.1260450000	0.2198600000	0.0002360000
C	-0.7201520000	-1.1346680000	0.0001050000
C	-1.6971400000	-2.1315530000	-0.0000220000
H	-3.8030880000	-2.5338540000	-0.0001370000
H	-2.7724910000	1.6292300000	0.0003350000
H	-1.4159880000	-3.1797580000	-0.0001220000
C	1.1260400000	0.2198700000	0.0002500000
C	2.4635980000	0.5905460000	0.0002870000
C	3.4216320000	-0.4204670000	0.0001920000
C	3.0324950000	-1.7733020000	0.0000660000
C	1.6971420000	-2.1315460000	0.0000320000
C	0.7201540000	-1.1346640000	0.0001100000
H	2.7724840000	1.6292340000	0.0003990000
H	3.8030900000	-2.5338510000	0.0000000000
H	1.4159870000	-3.1797500000	-0.0000650000
C	4.8574970000	-0.0654580000	0.0002240000
N	5.1597240000	1.2308090000	0.0002080000
N	7.0301080000	-0.7138860000	0.0000580000
C	7.4879890000	0.5854790000	0.0000160000
C	-4.8574990000	-0.0654700000	0.0000790000
N	-5.7287390000	-1.0695200000	0.0003040000
N	-6.4773590000	1.5222540000	-0.0000960000
C	-7.4879900000	0.5854760000	-0.0000990000
N	5.7287380000	-1.0695220000	0.0000790000
N	6.4773700000	1.5222540000	0.0001240000
N	-7.0301160000	-0.7138820000	-0.0001000000
N	-5.1597210000	1.2308100000	-0.0003140000

O	8.6669380000	0.8775280000	-0.0004550000
O	-8.6669340000	0.8775420000	-0.0003250000
C	8.0059700000	-1.7853930000	-0.0004380000
H	8.6396370000	-1.7225670000	-0.8878050000
H	8.6430140000	-1.7200360000	0.8842860000
H	7.4489810000	-2.7195350000	0.0018770000
C	6.8431040000	2.9243640000	-0.0000790000
H	7.4356520000	3.1633480000	0.8857590000
H	7.4353910000	3.1631740000	-0.8861400000
H	5.9159170000	3.4928940000	0.0000020000
C	-8.0059720000	-1.7853920000	0.0002640000
H	-8.6394750000	-1.7228540000	0.8877750000
H	-8.6431820000	-1.7197610000	-0.8843150000
H	-7.4489810000	-2.7195320000	-0.0024400000
C	-6.8431000000	2.9243630000	-0.0007270000
H	-7.4328520000	3.1636900000	-0.8883640000
H	-7.4381820000	3.1628190000	0.8835260000
H	-5.9159210000	3.4928980000	0.0022450000
N	-0.0000020000	1.0151000000	0.0003990000
H	-0.0000290000	2.0198890000	0.0001040000

Oxygen (Set B):

C	-3.0474330000	-1.8283810000	-0.0000600000
C	-3.3927390000	-0.4653390000	-0.0000720000
C	-2.4006900000	0.5167430000	-0.0000610000
C	-1.0911480000	0.0841460000	-0.0000360000
C	-0.7211960000	-1.2679610000	-0.0000210000
C	-1.7248740000	-2.2367800000	-0.0000330000
H	-3.8440860000	-2.5618490000	-0.0000690000
H	-2.6555610000	1.5685980000	-0.0000710000
H	-1.4791590000	-3.2934150000	-0.0000240000

C	1.0911560000	0.0841420000	0.0000050000
C	2.4006980000	0.5167300000	0.0000250000
C	3.3927430000	-0.4653590000	0.0000520000
C	3.0474310000	-1.8283960000	0.0000530000
C	1.7248670000	-2.2367880000	0.0000290000
C	0.7211970000	-1.2679650000	0.0000060000
H	2.6555870000	1.5685820000	0.0000230000
H	3.8440750000	-2.5618740000	0.0000720000
H	1.4791500000	-3.2934230000	0.0000310000
C	4.8163390000	-0.0636330000	0.0000740000
N	5.0730510000	1.2413370000	0.0002230000
N	7.0079450000	-0.6390300000	0.0000670000
C	7.4210120000	0.6760530000	0.0000520000
C	-4.8163330000	-0.0636100000	-0.0000960000
N	-5.7197180000	-1.0387000000	0.0000600000
N	-6.3789350000	1.5783150000	-0.0002510000
C	-7.4210040000	0.6760840000	-0.0000620000
N	5.7197170000	-1.0387100000	-0.0000930000
N	6.3788830000	1.5783190000	0.0000330000
N	-7.0079050000	-0.6390590000	-0.0000930000
N	-5.0730480000	1.2413460000	-0.0002900000
O	8.5889500000	1.0073800000	0.0000720000
O	-8.5889690000	1.0073150000	0.0001330000
C	8.0205150000	-1.6760350000	-0.0002200000
H	8.6517900000	-1.5909620000	-0.8874010000
H	8.6545710000	-1.5884860000	0.8846980000
H	7.4966190000	-2.6291260000	0.0018640000
C	6.6955820000	2.9927210000	0.0003480000
H	7.2772120000	3.2519220000	0.8876650000
H	7.2812180000	3.2512170000	-0.8844960000
H	5.7491350000	3.5285300000	-0.0019280000

C	-8.0205040000	-1.6760300000	0.0003540000
H	-8.6516690000	-1.5909130000	0.8876110000
H	-8.6546710000	-1.5884820000	-0.8844840000
H	-7.4966420000	-2.6291400000	-0.0017700000
C	-6.6955900000	2.9927320000	-0.0003070000
H	-7.2793010000	3.2515410000	-0.8863510000
H	-7.2791270000	3.2516550000	0.8858190000
H	-5.7491220000	3.5285060000	-0.0004360000
O	0.0000050000	0.9055470000	-0.0000200000

Sulphur (Set B):

C	-2.9737090000	-1.6693520000	-0.0000370000
C	-3.4874250000	-0.3615500000	-0.0000740000
C	-2.6179930000	0.7257980000	-0.0000790000
C	-1.2499850000	0.4884860000	-0.0000470000
C	-0.7220050000	-0.8159300000	-0.0000060000
C	-1.6113110000	-1.8950770000	-0.0000010000
H	-3.6669030000	-2.5013730000	-0.0000340000
H	-3.0180420000	1.7324520000	-0.0001080000
H	-1.2328980000	-2.9122720000	0.0000290000
C	1.2499850000	0.4884860000	0.0000050000
C	2.6179930000	0.7257980000	0.0000230000
C	3.4874250000	-0.3615500000	0.0000680000
C	2.9737080000	-1.6693520000	0.0000890000
C	1.6113110000	-1.8950770000	0.0000650000
C	0.7220050000	-0.8159300000	0.0000230000
H	3.0180420000	1.7324520000	0.0000040000
H	3.6669030000	-2.5013730000	0.0001230000
H	1.2328980000	-2.9122720000	0.0000810000
C	4.9490360000	-0.1364870000	0.0000920000
N	5.3644380000	1.1270920000	0.0001990000

N	7.0527980000	-0.9776690000	0.0001740000
C	7.6247770000	0.2764860000	0.0000760000
C	-4.9490350000	-0.1364870000	-0.0001070000
N	-5.7250760000	-1.2153760000	-0.0000750000
N	-6.7017880000	1.3005280000	-0.0001700000
C	-7.6247770000	0.2764850000	-0.0000180000
N	5.7250770000	-1.2153750000	-0.0000280000
N	6.7017890000	1.3005280000	-0.0000050000
N	-7.0527990000	-0.9776680000	-0.0002530000
N	-5.3644380000	1.1270920000	-0.0002040000
O	8.8245660000	0.4614360000	0.0000220000
O	-8.8245660000	0.4614370000	0.0001650000
C	7.9298650000	-2.1315540000	-0.0001420000
H	8.5663480000	-2.1252580000	-0.8876610000
H	8.5703080000	-2.1224400000	0.8844530000
H	7.2925720000	-3.0128700000	0.0025940000
C	7.1906490000	2.6650190000	0.0002320000
H	7.7997170000	2.8505460000	0.8875970000
H	7.8037630000	2.8491880000	-0.8845850000
H	6.3176110000	3.3135970000	-0.0021790000
C	-7.9298640000	-2.1315540000	0.0001230000
H	-8.5662000000	-2.1253300000	0.8877500000
H	-8.5704550000	-2.1223700000	-0.8843630000
H	-7.2925720000	-3.0128700000	-0.0027890000
C	-7.1906500000	2.6650190000	-0.0000960000
H	-7.8019050000	2.8498510000	-0.8860800000
H	-7.8015800000	2.8498810000	0.8861070000
H	-6.3176100000	3.3135980000	-0.0002670000
S	0.0000000000	1.7149850000	-0.0000480000

Set-II diradicals

B3LYP/6-311+G(d,p)

B-ECP1

C	-1.3819130000	-1.3941330000	-0.0098490000
C	-1.5718470000	-0.1125380000	-0.5526360000
C	-2.8420830000	0.4710860000	-0.5632100000
C	-3.9138400000	-0.2037560000	0.0363020000
C	-3.7650490000	-1.4783090000	0.5910430000
C	-2.4989670000	-2.0673540000	0.5266060000
C	1.3820900000	-1.3940220000	0.0093550000
C	1.5718770000	-0.1125100000	0.5523620000
C	2.8420770000	0.4712150000	0.5632000000
C	3.9139580000	-0.2034890000	-0.0362530000
C	3.7653220000	-1.4779790000	-0.5911890000
C	2.4992660000	-2.0670970000	-0.5270580000
H	-0.7228200000	0.4136220000	-0.9627470000
H	-4.8700980000	0.3012240000	0.0434840000
H	-2.3475020000	-3.0686070000	0.9086430000
H	0.7227720000	0.4135390000	0.9624500000
H	4.8701860000	0.3015470000	-0.0432250000
H	2.3479060000	-3.0682850000	-0.9093050000
C	2.4074000000	2.3660310000	2.3146520000
C	-2.4079420000	2.3661430000	-2.3145930000
N	-3.1047240000	1.7633250000	-1.1088420000
O	-4.0496780000	2.4409260000	-0.5713510000
O	4.0497130000	2.4410260000	0.5720190000
N	3.1045440000	1.7633690000	1.1090650000
H	0.0001900000	-3.2987550000	-0.0005210000
C	4.9862640000	-2.1736880000	-1.2213470000
C	4.6469700000	-3.5773070000	-1.7551590000
H	5.5420240000	-4.0275330000	-2.1928490000
H	4.2981470000	-4.2433430000	-0.9611440000

H	3.881180000	-3.542991000	-2.534854000
C	6.104524000	-2.317371000	-0.162892000
H	6.977293000	-2.811617000	-0.600217000
H	6.429573000	-1.347960000	0.221304000
H	5.764147000	-2.917829000	0.685463000
C	5.503377000	-1.318500000	-2.401641000
H	4.733540000	-1.208692000	-3.170601000
H	5.797956000	-0.317379000	-2.079189000
H	6.376107000	-1.793549000	-2.860445000
C	-4.985829000	-2.174148000	1.221363000
C	-6.104426000	-2.317491000	0.163231000
H	-6.977118000	-2.811715000	0.600734000
H	-6.429490000	-1.347978000	-0.220697000
H	-5.764387000	-2.917832000	-0.685345000
C	-4.646442000	-3.577930000	1.754692000
H	-4.297879000	-4.243767000	0.960397000
H	-3.880427000	-3.543863000	2.534178000
H	-5.541387000	-4.028235000	2.192523000
C	-5.502519000	-1.319234000	2.402051000
H	-5.797128000	-0.318014000	2.079936000
H	-6.375138000	-1.794342000	2.861004000
H	-4.732429000	-1.209682000	3.170791000
B	0.000117000	-2.100915000	-0.000350000
C	-2.089001000	1.281442000	-3.357430000
H	-1.712273000	1.766775000	-4.261030000
H	-1.335038000	0.568727000	-3.027719000
H	-2.990626000	0.724950000	-3.624926000
C	-1.140395000	3.106241000	-1.848256000
H	-0.684202000	3.625178000	-2.695658000
H	-1.397547000	3.849677000	-1.090525000
H	-0.391044000	2.432743000	-1.430231000

C	-3.3800350000	3.3772320000	-2.9429980000
H	-2.9080420000	3.8045080000	-3.8310990000
H	-4.3116390000	2.8933000000	-3.2428100000
H	-3.6249230000	4.1808080000	-2.2511400000
C	1.1399750000	3.1061670000	1.8480370000
H	1.3973360000	3.8497690000	1.0905370000
H	0.3907840000	2.4327320000	1.4296310000
H	0.6834930000	3.6249110000	2.6954030000
C	3.3792940000	3.3770880000	2.9434340000
H	3.6245010000	4.1806530000	2.2516740000
H	2.9069530000	3.8043800000	3.8313390000
H	4.3107640000	2.8931290000	3.2436200000
C	2.0881540000	1.2812320000	3.3573150000
H	2.9896370000	0.7245230000	3.6248250000
H	1.7114330000	1.7665310000	4.2609350000
H	1.3340590000	0.5687240000	3.0274500000

B-ECP2

C	-1.3307900000	-2.7996590000	-0.5504920000
C	-1.8029070000	-1.5524400000	-0.1128640000
C	-2.9994750000	-1.0476070000	-0.6312550000
C	-3.6800460000	-1.7376430000	-1.6389490000
C	-3.2167010000	-2.9632000000	-2.1258010000
C	-2.0648710000	-3.4910700000	-1.5375710000
C	1.1718000000	-2.8329720000	0.6539910000
C	1.7027180000	-1.6518180000	0.1108420000
C	2.9514130000	-1.1970750000	0.5410220000
C	3.6379260000	-1.8665220000	1.5570140000
C	3.1189270000	-3.0204010000	2.1520930000
C	1.9053120000	-3.5024570000	1.6569300000
H	-1.2849880000	-1.0227430000	0.6767420000

H	-4.6001810000	-1.3005170000	-2.0014140000
H	-1.7089190000	-4.4690490000	-1.8347210000
H	1.1837930000	-1.1406160000	-0.6906560000
H	4.6049350000	-1.4746770000	1.8418500000
H	1.4981550000	-4.4296100000	2.0392360000
C	1.8029100000	1.5522850000	-0.1129640000
C	1.3308030000	2.7995340000	-0.5505210000
C	2.9994890000	1.0474800000	-0.6313650000
C	2.0649120000	3.4910160000	-1.5375310000
C	-1.1718270000	2.8328650000	0.6539420000
C	3.6800910000	1.7375980000	-1.6389900000
C	3.2167690000	2.9631940000	-2.1257550000
H	1.7089690000	4.4690160000	-1.8346200000
C	-1.7027430000	1.6516610000	0.1108990000
C	-1.9053480000	3.5024500000	1.6568100000
H	4.6002250000	1.3004830000	-2.0014710000
C	-2.9514460000	1.1969600000	0.5411110000
H	-1.1838120000	1.1403860000	-0.6905480000
C	-3.1189710000	3.0204480000	2.1520040000
H	-1.4981840000	4.4296340000	2.0390340000
C	-3.6379650000	1.8665120000	1.5570360000
H	-4.6049770000	1.4746950000	1.8418970000
N	-3.6322610000	0.1147070000	-0.0987720000
H	1.2849680000	1.0225390000	0.6765930000
O	-4.9117810000	0.1886550000	-0.1769950000
O	4.9117400000	-0.1889850000	-0.1773780000
N	3.6322390000	-0.1148920000	-0.0989870000
H	-0.1565380000	-4.7004760000	0.1625430000
C	3.9129200000	-3.7193680000	3.2699220000
C	3.1783960000	-4.9555790000	3.8201620000
H	3.7724990000	-5.4063370000	4.6195250000

H	2.2025190000	-4.6962730000	4.2399860000
H	3.0293760000	-5.7194490000	3.0522510000
C	4.1323800000	-2.7290450000	4.4371940000
H	4.6948290000	-3.2124290000	5.2416680000
H	4.6947410000	-1.8470730000	4.1223270000
H	3.1771840000	-2.3895380000	4.8474410000
C	5.2838290000	-4.1741970000	2.7173600000
H	5.1572650000	-4.8829360000	1.8943380000
H	5.8726550000	-3.3329950000	2.3449600000
H	5.8636820000	-4.6662110000	3.5042680000
C	-3.9992400000	-3.6820000000	-3.2392040000
C	-4.0281120000	-2.7839910000	-4.4981330000
H	-4.5831710000	-3.2770080000	-5.3020120000
H	-4.5095710000	-1.8236530000	-4.3000290000
H	-3.0150110000	-2.5838540000	-4.8583010000
C	-3.3613580000	-5.0299980000	-3.6219090000
H	-2.3393170000	-4.9086510000	-3.9910450000
H	-3.3411550000	-5.7257020000	-2.7785100000
H	-3.9463530000	-5.4968750000	-4.4187450000
C	-5.4468400000	-3.9491570000	-2.7654030000
H	-5.9760250000	-3.0243670000	-2.5253290000
H	-6.0113180000	-4.4621350000	-3.5500110000
H	-5.4558520000	-4.5805360000	-1.8726710000
C	-3.9129820000	3.7195390000	3.2697450000
C	-5.2838970000	4.1742680000	2.7171120000
H	-5.8727050000	3.3329980000	2.3448320000
H	-5.8637620000	4.6663870000	3.5039470000
H	-5.1573400000	4.8828880000	1.8939870000
C	-4.1324350000	2.7293680000	4.4371460000
H	-3.1772380000	2.3899320000	4.8474480000
H	-4.6948970000	3.2128550000	5.2415500000

H	-4.6947820000	1.8473440000	4.1224000000
C	-3.1784830000	4.9558340000	3.8198340000
H	-2.2025870000	4.6966030000	4.2396570000
H	-3.0295100000	5.7196280000	3.0518400000
H	-3.7725790000	5.4066590000	4.6191650000
C	3.9993260000	3.6820760000	-3.2390920000
C	4.0284090000	2.7840600000	-4.4980120000
H	4.5835090000	3.2771200000	-5.3018360000
H	4.5099320000	1.8237670000	-4.2998440000
H	3.0153640000	2.5838300000	-4.8582840000
C	5.4468540000	3.9494130000	-2.7651740000
H	5.9761500000	3.0246890000	-2.5250920000
H	6.0113220000	4.4624960000	-3.5497200000
H	5.4557140000	4.5807630000	-1.8724190000
C	3.3613170000	5.0299960000	-3.6218580000
H	2.3393620000	4.9085150000	-3.9911880000
H	3.3408540000	5.7256610000	-2.7784330000
H	3.9463880000	5.4969920000	-4.4185690000
H	0.1565240000	4.7003360000	0.1624650000
B	-0.1094960000	-3.5054080000	0.0957160000
B	0.1094840000	3.5052650000	0.0956600000

C-ECP1

C	0.9634160000	0.9356690000	-1.1169830000
C	1.9576360000	-0.0233690000	-1.2864430000
C	3.1173690000	0.0171310000	-0.4962150000
C	3.2537260000	1.0194600000	0.4696980000
C	2.2714700000	1.9981560000	0.6510680000
C	1.1307170000	1.9405480000	-0.1553980000
C	-1.5561030000	0.4177170000	-1.2199590000
C	-1.4840050000	-0.5199280000	-0.1935160000

C	-2.6589820000	-0.9842440000	0.4156110000
C	-3.8993390000	-0.5081440000	-0.0275680000
C	-3.9930250000	0.4369370000	-1.0510690000
C	-2.8053530000	0.8943030000	-1.6333750000
H	1.8051880000	-0.8061660000	-2.0145770000
H	4.1521770000	1.0073800000	1.0700290000
H	0.3446950000	2.6765810000	-0.0442830000
H	-0.5162610000	-0.8903000000	0.1046840000
H	-4.7812320000	-0.9008860000	0.4572690000
H	-2.8357570000	1.6276880000	-2.4294090000
C	-1.5229410000	-2.2447630000	2.4110630000
C	4.5345050000	-1.7252720000	-1.8420720000
N	4.1621320000	-0.9481910000	-0.5918100000
O	4.8811050000	-1.1350520000	0.4512830000
O	-3.7497790000	-2.6245750000	1.6219510000
N	-2.6678110000	-1.9607910000	1.4539210000
H	-0.4960200000	1.8766690000	-2.3690400000
C	-5.3818190000	0.9347680000	-1.4938610000
C	-5.2977210000	1.9850240000	-2.6163560000
H	-6.3056160000	2.3047370000	-2.8942070000
H	-4.7457290000	2.8751590000	-2.3014810000
H	-4.8209120000	1.5847140000	-3.5153020000
C	-6.1095850000	1.5761520000	-0.2898090000
H	-7.0983890000	1.9346280000	-0.5924380000
H	-6.2484320000	0.8647440000	0.5268650000
H	-5.5438000000	2.4275200000	0.0989960000
C	-6.2104050000	-0.2628350000	-2.0153930000
H	-5.7213460000	-0.7312880000	-2.8741660000
H	-6.3440000000	-1.0298160000	-1.2494080000
H	-7.2032620000	0.0728770000	-2.3309520000
C	2.4853010000	3.0927840000	1.7135110000

C	3.7715130000	3.8854280000	1.3833770000
H	3.9373040000	4.6657460000	2.1325810000
H	4.6535300000	3.2416460000	1.3711040000
H	3.6932690000	4.3663730000	0.4042510000
C	1.3114450000	4.0873760000	1.7732600000
H	1.1738270000	4.6128480000	0.8242130000
H	0.3705530000	3.5944670000	2.0326940000
H	1.5098910000	4.8411640000	2.5399980000
C	2.6326700000	2.4340450000	3.1049050000
H	3.4768960000	1.7421060000	3.1397090000
H	2.7944020000	3.1992210000	3.8704200000
H	1.7308180000	1.8747660000	3.3690620000
C	-0.3009760000	0.8840400000	-1.9507560000
H	-0.1340590000	0.2244670000	-2.8104700000
C	-2.1091680000	-3.0004810000	3.6132720000
H	-2.5384180000	-3.9563160000	3.3177960000
H	-1.3039460000	-3.1799020000	4.3300430000
H	-2.8905000000	-2.4183520000	4.1043320000
C	-0.4844950000	-3.1492780000	1.7186080000
H	0.0250580000	-2.6589810000	0.8892010000
H	0.2772590000	-3.4489100000	2.4432610000
H	-0.9682650000	-4.0522980000	1.3391710000
C	-0.9056670000	-0.9296110000	2.9186020000
H	-0.4239830000	-0.3431550000	2.1388630000
H	-1.6708370000	-0.3080100000	3.3904100000
H	-0.1492770000	-1.1647530000	3.6714010000
C	4.4638190000	-0.8191560000	-3.0833490000
H	3.4557920000	-0.4852420000	-3.3218290000
H	5.0913450000	0.0650010000	-2.9478700000
H	4.8435750000	-1.3735650000	-3.9451240000
C	3.6175290000	-2.9575630000	-1.9680150000

H	3.9489120000	-3.5773950000	-2.8056650000
H	3.6696950000	-3.5591020000	-1.0578120000
H	2.5739450000	-2.6936650000	-2.1431720000
C	5.9857410000	-2.1996520000	-1.6699550000
H	6.2821400000	-2.7358230000	-2.5748940000
H	6.6619420000	-1.3548480000	-1.5281500000
H	6.0933260000	-2.8632900000	-0.8140560000

C-ECP2

C	-2.8318280000	-1.1531960000	-1.3167010000
C	-2.3484510000	-0.0600510000	-0.6063270000
C	-3.1195730000	1.1054290000	-0.5224900000
C	-4.3765460000	1.1710860000	-1.1213050000
C	-4.8847290000	0.0803880000	-1.8351490000
C	-4.0934640000	-1.0699120000	-1.9230750000
C	-0.9741390000	-2.6852420000	-0.4075020000
C	0.3552850000	-2.3246840000	-0.6040290000
C	1.2918310000	-2.5563000000	0.4105860000
C	0.9072110000	-3.1713860000	1.6003330000
C	-0.4243090000	-3.5435030000	1.8184880000
C	-1.3497250000	-3.2851540000	0.8022650000
H	-1.3975480000	-0.1195890000	-0.0962140000
H	-4.9420740000	2.0847520000	-1.0023020000
H	-4.4546500000	-1.9339370000	-2.4667250000
H	0.6672390000	-1.8863340000	-1.5438060000
H	1.6738340000	-3.3554360000	2.3403440000
H	-2.3897210000	-3.5546880000	0.9342670000
C	2.3485710000	0.0601920000	-0.6061390000
C	2.8319540000	1.1532630000	-1.3166190000
C	3.1196400000	-1.1053210000	-0.5222760000
C	4.0935420000	1.0698620000	-1.9230820000

C	0.9742610000	2.6853550000	-0.4075040000
C	4.3765620000	-1.1710910000	-1.1211670000
C	4.8847520000	-0.0804710000	-1.8351340000
H	4.4547400000	1.9338300000	-2.4668150000
C	-0.3551570000	2.3248420000	-0.6041630000
C	1.3497550000	3.2852000000	0.8023230000
H	4.9420610000	-2.0847730000	-1.0021280000
C	-1.2917790000	2.5564310000	0.4103840000
H	-0.6670460000	1.8865420000	-1.5439860000
C	0.4242630000	3.5435170000	1.8184850000
H	2.3897460000	3.5547060000	0.9344210000
C	-0.9072480000	3.1714430000	1.6001950000
H	-1.6739310000	3.3554820000	2.3401480000
N	-2.6719980000	2.2319310000	0.2322120000
H	1.3977070000	0.1198030000	-0.0959590000
O	-3.5495430000	2.9833710000	0.7894470000
O	3.5495870000	-2.9830410000	0.7899790000
N	2.6720450000	-2.2317390000	0.2325540000
H	2.6948280000	3.2781980000	-1.5365720000
H	-2.6945540000	-3.2781080000	-1.5367980000
C	-0.8134450000	-4.2099540000	3.1508060000
C	-2.3150680000	-4.5415860000	3.2235210000
H	-2.5392670000	-5.0079280000	4.1865410000
H	-2.9359420000	-3.6453930000	3.1398670000
H	-2.6163900000	-5.2433900000	2.4409040000
C	-0.4737900000	-3.2550720000	4.3191910000
H	-0.7419040000	-3.7173660000	5.2741260000
H	0.5914000000	-3.0158930000	4.3519980000
H	-1.0264310000	-2.3156640000	4.2297750000
C	-0.0181270000	-5.5261020000	3.3160320000
H	-0.2432010000	-6.2228930000	2.5038530000

H	1.0602440000	-5.3530550000	3.3177210000
H	-0.2812010000	-6.0099330000	4.2617170000
C	-6.2744930000	0.1890770000	-2.4893910000
C	-6.2606470000	1.3359980000	-3.5272190000
H	-7.2426650000	1.4298770000	-4.0011510000
H	-6.0189580000	2.2964510000	-3.0667200000
H	-5.5223190000	1.1448390000	-4.3111770000
C	-6.6880470000	-1.1065640000	-3.2106330000
H	-5.9981040000	-1.3632200000	-4.0192780000
H	-6.7446440000	-1.9555990000	-2.5237150000
H	-7.6788240000	-0.9762850000	-3.6540100000
C	-7.3319380000	0.4935720000	-1.4027990000
H	-7.1253060000	1.4314620000	-0.8832330000
H	-8.3250550000	0.5737340000	-1.8554140000
H	-7.3624560000	-0.3030690000	-0.6543970000
C	0.8133000000	4.2099120000	3.1508590000
C	0.0179430000	5.5260370000	3.3160880000
H	-1.0604240000	5.3529670000	3.3177010000
H	0.2809470000	6.0098360000	4.2618090000
H	0.2430540000	6.2228650000	2.5039520000
C	0.4735900000	3.2549740000	4.3191820000
H	1.0262490000	2.3155770000	4.2297550000
H	0.7416470000	3.7172290000	5.2741520000
H	-0.5915980000	3.0157810000	4.3519220000
C	2.3149120000	4.5415700000	3.2236880000
H	2.9358070000	3.6453920000	3.1400300000
H	2.6162730000	5.2434200000	2.4411260000
H	2.5390390000	5.0078680000	4.1867460000
C	6.2744710000	-0.1892730000	-2.4894530000
C	6.2604640000	-1.3361820000	-3.5272960000
H	7.2424450000	-1.4301430000	-4.0012870000

H	6.0187150000	-2.2966170000	-3.0667910000
H	5.5221050000	-1.1449450000	-4.3112060000
C	7.3319500000	-0.4938770000	-1.4029270000
H	7.1252670000	-1.4317520000	-0.8833520000
H	8.3250320000	-0.5741280000	-1.8556030000
H	7.3625890000	0.3027540000	-0.6545180000
C	6.6881040000	1.1063380000	-3.2107000000
H	5.9981520000	1.3630600000	-4.0193170000
H	6.7447980000	1.9553620000	-2.5237760000
H	7.6788520000	0.9759820000	-3.6541180000
C	-2.0081410000	-2.4276340000	-1.4836660000
C	2.0083570000	2.4277630000	-1.4835790000
H	-1.5051160000	-2.3853960000	-2.4569540000
H	1.5054380000	2.3856300000	-2.4569260000

N-ECP1

C	-1.2088740000	-1.3324730000	-0.0094100000
C	-1.4365560000	0.0043130000	0.3300340000
C	-2.7220380000	0.5277180000	0.2032800000
C	-3.7758520000	-0.2531490000	-0.2656540000
C	-3.5711350000	-1.5997300000	-0.5937860000
C	-2.2828840000	-2.1189860000	-0.4616980000
C	1.3192960000	-1.3456480000	0.0282240000
C	1.5534340000	-0.1945320000	-0.7275230000
C	2.8556810000	0.2985050000	-0.8262220000
C	3.9213120000	-0.3618460000	-0.2166930000
C	3.7056930000	-1.5245360000	0.5338170000
C	2.3970370000	-1.9913750000	0.6581730000
H	-0.6284010000	0.6261350000	0.6839130000
H	-4.7439580000	0.2142610000	-0.3816460000
H	-2.0787850000	-3.1486770000	-0.7273910000

H	0.7500860000	0.2702340000	-1.2792430000
H	4.9145550000	0.0404450000	-0.3599010000
H	2.1822700000	-2.8747130000	1.2459580000
C	2.6953620000	2.8572160000	-1.3604890000
C	-3.0375780000	2.4704680000	1.9134340000
N	-2.9736480000	1.9163780000	0.5036980000
O	-3.6287060000	2.5736130000	-0.3831200000
O	4.1819410000	1.3395860000	-2.4071850000
N	3.1484500000	1.4393510000	-1.6536440000
N	0.0478240000	-1.9319310000	0.1301880000
H	0.0417630000	-2.9369650000	0.2022430000
C	4.9030240000	-2.2324590000	1.1949490000
C	4.4830250000	-3.4779660000	1.9963060000
H	5.3679900000	-3.9394760000	2.4424770000
H	3.7968320000	-3.2281360000	2.8104910000
H	4.0061810000	-4.2301930000	1.3617300000
C	5.6097820000	-1.2544290000	2.1621830000
H	6.4658270000	-1.7442130000	2.6365160000
H	5.9788430000	-0.3670430000	1.6436700000
H	4.9281420000	-0.9234070000	2.9508430000
C	5.8977540000	-2.6767580000	0.0971600000
H	5.4232630000	-3.3726690000	-0.6001390000
H	6.2692740000	-1.8286750000	-0.4815250000
H	6.7591300000	-3.1800350000	0.5474520000
C	-4.7535300000	-2.4422970000	-1.1078220000
C	-5.2777300000	-1.8289960000	-2.4273940000
H	-6.1225190000	-2.4130300000	-2.8054470000
H	-5.6154660000	-0.7995600000	-2.2907280000
H	-4.4969010000	-1.8251310000	-3.1926990000
C	-4.3611930000	-3.9060710000	-1.3795200000
H	-3.5936050000	-3.9874510000	-2.1539760000

H	-3.9961710000	-4.4049110000	-0.4771460000
H	-5.2373050000	-4.4589830000	-1.7288390000
C	-5.8863210000	-2.4377850000	-0.0551500000
H	-6.2535750000	-1.4286100000	0.1429630000
H	-6.7316100000	-3.0360960000	-0.4087100000
H	-5.5425340000	-2.8623540000	0.8922990000
C	1.4254160000	2.8996250000	-0.5058520000
H	0.5626940000	2.4786600000	-1.0242690000
H	1.5552620000	2.3826750000	0.4467040000
H	1.1964990000	3.9460950000	-0.2899780000
C	2.4430090000	3.5381120000	-2.7130650000
H	2.1758780000	4.5858500000	-2.5537340000
H	3.3344400000	3.4920940000	-3.3379730000
H	1.6214010000	3.0513220000	-3.2447140000
C	3.8497280000	3.5483000000	-0.6095620000
H	4.7663750000	3.5002240000	-1.1985970000
H	3.6019740000	4.5976310000	-0.4292300000
H	4.0286780000	3.0692690000	0.3571670000
C	-2.1375930000	1.6885580000	2.8755270000
H	-2.4019930000	0.6310520000	2.9223410000
H	-1.0822010000	1.7723820000	2.6094500000
H	-2.2593990000	2.1094750000	3.8767080000
C	-4.5049000000	2.3755980000	2.3730490000
H	-4.6169400000	2.8240500000	3.3637400000
H	-5.1536820000	2.9050280000	1.6737590000
H	-4.8297220000	1.3333230000	2.4336510000
C	-2.5874110000	3.9360270000	1.8425850000
H	-2.6713210000	4.3950770000	2.8310000000
H	-1.5459580000	4.0056870000	1.5178600000
H	-3.2053330000	4.4947720000	1.1404140000

N-ECP2

C	0.3139060000	2.9785510000	0.1296170000
C	-0.7805670000	2.1619350000	-0.1502130000
C	-1.9235810000	2.2720970000	0.6483600000
C	-1.9732240000	3.1882250000	1.7037010000
C	-0.8820750000	4.0110850000	1.9911780000
C	0.2617070000	3.8873360000	1.1950370000
C	2.3097000000	1.8687300000	-0.9116260000
C	2.1897350000	0.6737180000	-0.2002440000
C	3.1323530000	-0.3337730000	-0.4230130000
C	4.1779880000	-0.1705240000	-1.3260560000
C	4.3003640000	1.0192180000	-2.0560290000
C	3.3549900000	2.0201330000	-1.8422770000
H	-0.7593230000	1.5059920000	-1.0092220000
H	-2.8910400000	3.2464820000	2.2705340000
H	1.1376630000	4.4925230000	1.3889190000
H	1.4211310000	0.5519430000	0.5499820000
H	4.8887060000	-0.9777610000	-1.4308040000
H	3.4055380000	2.9507800000	-2.3934300000
C	0.7805430000	-2.1619300000	-0.1496780000
C	-0.3139660000	-2.9785220000	0.1300930000
C	1.9234320000	-2.2719700000	0.6490900000
C	-0.2619210000	-3.8871590000	1.1956470000
C	-2.3095690000	-1.8688640000	-0.9116990000
C	1.9729170000	-3.1879440000	1.7045720000
C	0.8817330000	-4.0107780000	1.9919900000
H	-1.1378990000	-4.4923330000	1.3894730000
C	-2.1897420000	-0.6737310000	-0.2004960000
C	-3.3546720000	-2.0204180000	-1.8425360000
H	2.8906430000	-3.2461100000	2.2715590000
C	-3.1323100000	0.3337250000	-0.4236260000

H	-1.4212840000	-0.5518250000	0.5498590000
C	-4.3000060000	-1.0195390000	-2.0566380000
H	-3.4051080000	-2.9511560000	-2.3935450000
C	-4.1777680000	0.1703270000	-1.3268460000
H	-4.8884650000	0.9775480000	-1.4318700000
N	-3.1081280000	1.5403500000	0.3507810000
H	0.7594290000	-1.5061090000	-1.0087840000
O	-4.2333750000	2.0121970000	0.7459590000
O	4.2332090000	-2.0120570000	0.7470290000
N	3.1080300000	-1.5402660000	0.3515920000
N	1.4491190000	2.9590110000	-0.7152540000
N	-1.4490490000	-2.9591230000	-0.7149480000
H	-1.8962220000	-3.8565600000	-0.8273900000
H	1.8963020000	3.8564340000	-0.8277800000
C	5.4555060000	1.1721410000	-3.0623470000
C	5.4334060000	2.5330310000	-3.7814210000
H	6.2697080000	2.5886700000	-4.4833540000
H	4.5132250000	2.6771900000	-4.3545260000
H	5.5375890000	3.3662430000	-3.0807620000
C	5.3522790000	0.0598960000	-4.1316640000
H	6.1683560000	0.1534520000	-4.8548480000
H	5.4120260000	-0.9362270000	-3.6882360000
H	4.4061750000	0.1285860000	-4.6758740000
C	6.8028990000	1.0421810000	-2.3141950000
H	6.9039900000	1.8214680000	-1.5537540000
H	6.8994200000	0.0757060000	-1.8152440000
H	7.6359760000	1.1421150000	-3.0168530000
C	-0.9683750000	4.9996290000	3.1685290000
C	-1.2008110000	4.2118960000	4.4791710000
H	-1.2688260000	4.9008580000	5.3266690000
H	-2.1254610000	3.6318770000	4.4445940000

H	-0.3766180000	3.5188890000	4.6699730000
C	0.3158070000	5.8333410000	3.3301230000
H	1.1886020000	5.2058380000	3.5309050000
H	0.5230600000	6.4393190000	2.4435370000
H	0.2028610000	6.5172910000	4.1754370000
C	-2.1490810000	5.9713390000	2.9375870000
H	-3.1019600000	5.4437420000	2.8603980000
H	-2.2235650000	6.6778200000	3.7699320000
H	-2.0090890000	6.5445850000	2.0168940000
C	-5.4549510000	-1.1726210000	-3.0631560000
C	-6.8024840000	-1.0426060000	-2.3152640000
H	-6.8990960000	-0.0760890000	-1.8164110000
H	-7.6354300000	-1.1425980000	-3.0180680000
H	-6.9037120000	-1.8218310000	-1.5547780000
C	-5.3515580000	-0.0604950000	-4.1325780000
H	-4.4053710000	-0.1292450000	-4.6766360000
H	-6.1675240000	-0.1541310000	-4.8558780000
H	-5.4113760000	0.9356760000	-3.6892680000
C	-5.4326800000	-2.5335960000	-3.7820720000
H	-4.5123870000	-2.6777950000	-4.3549860000
H	-5.5369750000	-3.3667320000	-3.0813400000
H	-6.2688470000	-2.5893360000	-4.4841570000
C	0.9678630000	-4.9991640000	3.1694870000
C	1.2001100000	-4.2112590000	4.4800580000
H	1.2680160000	-4.9001120000	5.3276530000
H	2.1247590000	-3.6312370000	4.4455370000
H	0.3758850000	-3.5182370000	4.6706590000
C	2.1486050000	-5.9709000000	2.9388390000
H	3.1014920000	-5.4433090000	2.8617170000
H	2.2229720000	-6.6772730000	3.7712870000
H	2.0087450000	-6.5442650000	2.0182000000

C	-0.3163410000	-5.8328570000	3.3310090000
H	-1.1891690000	-5.2053270000	3.5315670000
H	-0.5234590000	-6.4389690000	2.4444840000
H	-0.2035190000	-6.5166810000	4.1764430000

O-ECP1

C	-1.1097420000	-1.3567530000	0.1294580000
C	-1.3490110000	-0.1100410000	0.6951580000
C	-2.6058960000	0.4682520000	0.5107410000
C	-3.5855520000	-0.1838500000	-0.2382250000
C	-3.3488180000	-1.4447460000	-0.7990110000
C	-2.0914820000	-2.0240640000	-0.6005620000
C	1.2914250000	-1.3613000000	0.1535190000
C	1.4818350000	-0.4229480000	-0.8537160000
C	2.7548270000	0.1319230000	-1.0064770000
C	3.8099470000	-0.2748390000	-0.1896580000
C	3.6193590000	-1.2274570000	0.8187140000
C	2.3378960000	-1.7597870000	0.9847850000
H	-0.5698620000	0.4018010000	1.2408620000
H	-4.5292060000	0.3248940000	-0.3813940000
H	-1.8382490000	-2.9930290000	-1.0071680000
H	0.6748010000	-0.1652500000	-1.5233640000
H	4.7835210000	0.1570120000	-0.3764490000
H	2.1203430000	-2.5013480000	1.7406160000
C	2.4632890000	2.4611670000	-2.1642930000
C	-3.0723720000	2.0860180000	2.5024470000
N	-2.8960120000	1.7824120000	1.0256080000
O	-3.5034700000	2.5768550000	0.2213560000
O	4.1378360000	0.8724500000	-2.7005020000
N	3.0350620000	1.0573390000	-2.0715780000

C	4.8099240000	-1.6555980000	1.6958960000
C	4.4051040000	-2.6826380000	2.7688230000
H	5.2810030000	-2.9526370000	3.3648060000
H	3.6518270000	-2.2827250000	3.4535190000
H	4.0133190000	-3.6021010000	2.3256980000
C	5.3976600000	-0.4171390000	2.4112460000
H	6.2433790000	-0.7112160000	3.0403290000
H	5.7553920000	0.3310780000	1.7007140000
H	4.6482630000	0.0575510000	3.0510410000
C	5.8957310000	-2.2945920000	0.7988880000
H	5.5065710000	-3.1780700000	0.2855410000
H	6.2561110000	-1.5992780000	0.0376930000
H	6.7529560000	-2.6035700000	1.4050550000
C	-4.4581720000	-2.1396230000	-1.6095440000
C	-4.8493290000	-1.2481140000	-2.8109310000
H	-5.6427320000	-1.7274700000	-3.3922880000
H	-5.2136190000	-0.2694950000	-2.4913420000
H	-3.9935720000	-1.0868290000	-3.4721170000
C	-4.0139350000	-3.5103830000	-2.1513020000
H	-3.1574040000	-3.4241220000	-2.8254140000
H	-3.7497580000	-4.2021880000	-1.3468350000
H	-4.8331540000	-3.9615560000	-2.7172620000
C	-5.6948060000	-2.3547460000	-0.7059840000
H	-6.0895600000	-1.4100420000	-0.3255970000
H	-6.4929380000	-2.8467220000	-1.2703330000
H	-5.4475170000	-2.9856450000	0.1524350000
C	1.1030620000	2.5868250000	-1.4723810000
H	0.3338620000	1.9811960000	-1.9541310000
H	1.1503580000	2.3193660000	-0.4157260000
H	0.7824390000	3.6293060000	-1.5369770000
C	2.3270580000	2.7921760000	-3.6568270000

H	1.9786750000	3.8213460000	-3.7742310000
H	3.2849690000	2.6837260000	-4.1644470000
H	1.6038790000	2.1276440000	-4.1365880000
C	3.4804620000	3.4002690000	-1.4882000000
H	4.4591980000	3.3000730000	-1.9592670000
H	3.1495170000	4.4378450000	-1.5817870000
H	3.5779960000	3.1690410000	-0.4237360000
C	-2.1851500000	1.2002000000	3.3828420000
H	-2.3896460000	0.1376270000	3.2440550000
H	-1.1229930000	1.3804780000	3.2046950000
H	-2.3888820000	1.4450710000	4.4281480000
C	-4.5559240000	1.8422490000	2.8384840000
H	-4.7509660000	2.1054540000	3.8813490000
H	-5.1934960000	2.4541080000	2.1984120000
H	-4.8221390000	0.7910480000	2.6984110000
C	-2.7059090000	3.5620930000	2.7060660000
H	-2.8690970000	3.8381260000	3.7509030000
H	-1.6544850000	3.7371670000	2.4637830000
H	-3.3167380000	4.2035360000	2.0721370000
O	0.0875560000	-2.0224010000	0.3239320000

O-ECP2

C	-2.6312180000	-1.3147000000	-0.9061720000
C	-2.2770930000	-0.1765120000	-0.1877840000
C	-2.9501430000	1.0119530000	-0.4780330000
C	-3.9579750000	1.0680260000	-1.4414520000
C	-4.3028270000	-0.0754700000	-2.1668570000
C	-3.6198550000	-1.2646360000	-1.8879070000
C	-1.0023530000	-2.7336180000	0.1664990000
C	0.2554110000	-2.2688380000	-0.2033950000
C	1.3363870000	-2.5856890000	0.6212470000

C	1.1603980000	-3.3605390000	1.7752330000
C	-0.1034220000	-3.8186760000	2.1426820000
C	-1.1909370000	-3.4870400000	1.3173530000
H	-1.5333510000	-0.2166910000	0.5949250000
H	-4.4535470000	2.0143040000	-1.5953500000
H	-3.8476360000	-2.1836920000	-2.4127220000
H	0.3877080000	-1.7172350000	-1.1240700000
H	2.0412520000	-3.5933750000	2.3535940000
H	-2.1952210000	-3.8224650000	1.5424390000
C	2.2770950000	0.1764690000	-0.1877680000
C	2.6312500000	1.3146640000	-0.9061280000
C	2.9501640000	-1.0119900000	-0.4779980000
C	3.6199300000	1.2646130000	-1.8878210000
C	1.0023640000	2.7335860000	0.1665140000
C	3.9580340000	-1.0680520000	-1.4413780000
C	4.3029100000	0.0754510000	-2.1667620000
H	3.8477330000	2.1836760000	-2.4126150000
C	-0.2553900000	2.2687770000	-0.2033820000
C	1.1909250000	3.4870460000	1.3173470000
H	4.4536290000	-2.0143230000	-1.5952450000
C	-1.3363800000	2.5856530000	0.6212320000
H	-0.3876660000	1.7171440000	-1.1240410000
C	0.1033970000	3.8186830000	2.1426600000
H	2.1952010000	3.8225000000	1.5424190000
C	-1.1604130000	3.3605370000	1.7751980000
H	-2.0412800000	3.5933930000	2.3535330000
N	-2.6609390000	2.1988370000	0.2670890000
H	1.5333260000	0.2166490000	0.5949150000
O	-3.6374470000	2.9563000000	0.6083600000
O	3.6374500000	-2.9563420000	0.6084020000
N	2.6609480000	-2.1988820000	0.2671140000

C	-0.3375660000	-4.6683930000	3.4044390000
C	-0.9299810000	-6.0369130000	2.9943330000
H	-1.1010930000	-6.6537400000	3.8817060000
H	-1.8843390000	-5.9286300000	2.4740020000
H	-0.2462190000	-6.5758270000	2.3329490000
C	-1.3301950000	-3.9374030000	4.3382540000
H	-1.5036100000	-4.5299210000	5.2415350000
H	-0.9366770000	-2.9634050000	4.6419720000
H	-2.2974510000	-3.7729360000	3.8578770000
C	0.9643240000	-4.9210200000	4.1856800000
H	1.7004720000	-5.4637550000	3.5869910000
H	1.4216690000	-3.9889270000	4.5280980000
H	0.7473180000	-5.5262910000	5.0698270000
C	-5.3975570000	-0.0643310000	-3.2494190000
C	-6.0310680000	1.3279380000	-3.4223920000
H	-6.8004470000	1.2844110000	-4.1978290000
H	-6.5083670000	1.6760780000	-2.5027020000
H	-5.2948260000	2.0751930000	-3.7305520000
C	-4.7848820000	-0.4890900000	-4.6041030000
H	-3.9925730000	0.2005230000	-4.9082690000
H	-4.3571990000	-1.4933880000	-4.5614720000
H	-5.5539200000	-0.4867710000	-5.3825320000
C	-6.5149820000	-1.0586200000	-2.8560490000
H	-6.9658080000	-0.7802480000	-1.8996640000
H	-7.3024010000	-1.0596140000	-3.6157860000
H	-6.1381970000	-2.0798970000	-2.7645270000
C	0.3374960000	4.6684730000	3.4043740000
C	-0.9644490000	4.9212050000	4.1854870000
H	-1.4218420000	3.9891540000	4.5279560000
H	-0.7474990000	5.5265570000	5.0695910000
H	-1.7005350000	5.4638980000	3.5866850000

C	1.3300170000	3.9375060000	4.3383240000
H	2.2973190000	3.7729940000	3.8580530000
H	1.5033580000	4.5300680000	5.2415910000
H	0.9364510000	2.9635320000	4.6420540000
C	0.9300000000	6.0369370000	2.9942130000
H	1.8843870000	5.9285710000	2.4739530000
H	0.2463080000	6.5758350000	2.3327420000
H	1.1010780000	6.6538220000	3.8815520000
C	5.3976150000	0.0643150000	-3.2493480000
C	6.0312890000	-1.3278970000	-3.4222000000
H	6.8007460000	-1.2843180000	-4.1975550000
H	6.5085130000	-1.6759500000	-2.5024370000
H	5.2951660000	-2.0752430000	-3.7304210000
C	6.5149480000	1.0587770000	-2.8561980000
H	6.9659050000	0.7805820000	-1.8998220000
H	7.3022930000	1.0597710000	-3.6160110000
H	6.1380780000	2.0800310000	-2.7647680000
C	4.7847740000	0.4888470000	-4.6040420000
H	3.9925450000	-0.2009180000	-4.9080640000
H	4.3569450000	1.4930830000	-4.5614460000
H	5.5537500000	0.4865640000	-5.3825330000
O	-2.0921800000	-2.5613000000	-0.6750780000
O	2.0922060000	2.5612630000	-0.6750410000

S-ECP1

C	-1.2660990000	0.1331270000	1.5730100000
C	-1.3616850000	0.9014930000	0.4141850000
C	-2.5029670000	0.7862610000	-0.3781830000
C	-3.5307690000	-0.0867250000	-0.0150480000
C	-3.4568270000	-0.8492640000	1.1544800000
C	-2.3039480000	-0.7284420000	1.9408420000

C	1.5472960000	0.0332510000	1.5557210000
C	1.5696950000	-1.0081540000	0.6308050000
C	2.7084240000	-1.1856910000	-0.1560270000
C	3.8276720000	-0.3702490000	0.0299430000
C	3.8241200000	0.6664880000	0.9678990000
C	2.6580190000	0.8676490000	1.7164960000
H	-0.5494230000	1.5519180000	0.1232440000
H	-4.3805820000	-0.1643710000	-0.6800050000
H	-2.1864110000	-1.3160860000	2.8405620000
H	0.7314710000	-1.6840980000	0.5490860000
H	4.7028720000	-0.5790350000	-0.5701250000
H	2.5964350000	1.6715510000	2.4367840000
C	1.9500390000	-2.4105390000	-2.3416490000
C	-2.8100170000	3.0053330000	-1.7168590000
N	-2.6210580000	1.5018510000	-1.6228060000
O	-3.0715160000	0.8242500000	-2.6153720000
O	3.9341880000	-2.8805830000	-1.1315410000
N	2.8065470000	-2.2704410000	-1.0939440000
C	5.0790040000	1.5433730000	1.1381000000
C	4.8797270000	2.6546740000	2.1846680000
H	5.7949470000	3.2470100000	2.2664040000
H	4.0705720000	3.3362370000	1.9075310000
H	4.6623580000	2.2482780000	3.1761270000
C	5.4317440000	2.2110630000	-0.2112660000
H	6.3234600000	2.8356410000	-0.1011690000
H	5.6375710000	1.4733250000	-0.9898090000
H	4.6129860000	2.8474990000	-0.5588860000
C	6.2587320000	0.6527590000	1.5936810000
H	6.0391160000	0.1743070000	2.5519690000
H	6.4750900000	-0.1354220000	0.8693360000
H	7.1632090000	1.2570310000	1.7138770000

C	-4.6152750000	-1.7948110000	1.5231270000
C	-4.8045450000	-2.8372970000	0.3966120000
H	-5.6312440000	-3.5106940000	0.6422020000
H	-5.0307250000	-2.3660410000	-0.5622880000
H	-3.9020240000	-3.4410290000	0.2680200000
C	-4.3583290000	-2.5496930000	2.8399380000
H	-3.4691530000	-3.1832790000	2.7814090000
H	-4.2388570000	-1.8672000000	3.6858120000
H	-5.2097590000	-3.1992510000	3.0592720000
C	-5.9151870000	-0.9725250000	1.6849430000
H	-6.1818600000	-0.4477350000	0.7648440000
H	-6.7483690000	-1.6323090000	1.9453010000
H	-5.8113980000	-0.2276290000	2.4788890000
C	0.5759460000	-1.7521210000	-2.1909600000
H	-0.0359650000	-2.2397040000	-1.4303040000
H	0.6450270000	-0.6892840000	-1.9563460000
H	0.0462140000	-1.8450310000	-3.1417330000
C	1.7867840000	-3.9137970000	-2.6051690000
H	1.2218240000	-4.0633540000	-3.5285570000
H	2.7584400000	-4.3967940000	-2.7021730000
H	1.2423130000	-4.3931030000	-1.7873980000
C	2.7270330000	-1.7374390000	-3.4892640000
H	3.7178230000	-2.1828280000	-3.5887980000
H	2.1866770000	-1.8668150000	-4.4305190000
H	2.8399410000	-0.6649290000	-3.3078320000
C	-2.0981640000	3.7482980000	-0.5819330000
H	-2.4505910000	3.4401010000	0.4034570000
H	-1.0149350000	3.6186120000	-0.6247670000
H	-2.3052790000	4.8156760000	-0.6906530000
C	-4.3256940000	3.2723590000	-1.6503110000
H	-4.5230320000	4.3401050000	-1.7760260000

H	-4.8407450000	2.7262510000	-2.4421770000
H	-4.7359550000	2.9631420000	-0.6850460000
C	-2.2399260000	3.4472450000	-3.0713210000
H	-2.4017280000	4.5201300000	-3.2023950000
H	-1.1655360000	3.2524530000	-3.1221320000
H	-2.7254000000	2.9147920000	-3.8881660000
S	0.1538770000	0.2708130000	2.6673100000

S-ECP2

C	-2.9200130000	-1.0811550000	-1.3248530000
C	-2.4187890000	-0.0698940000	-0.5071510000
C	-3.1547120000	1.1071750000	-0.3756510000
C	-4.3771910000	1.2787470000	-1.0312120000
C	-4.8806560000	0.2739500000	-1.8577600000
C	-4.1346410000	-0.9060800000	-1.9916340000
C	-0.8996750000	-2.7411050000	-0.2490850000
C	0.4221200000	-2.3342920000	-0.4295380000
C	1.3245900000	-2.5063030000	0.6232570000
C	0.9140770000	-3.0971660000	1.8250980000
C	-0.4053930000	-3.5069230000	2.0123020000
C	-1.3083590000	-3.3176630000	0.9536820000
H	-1.4926830000	-0.2015530000	0.0336570000
H	-4.9078020000	2.2043070000	-0.8679280000
H	-4.5055750000	-1.7120460000	-2.6136740000
H	0.7381990000	-1.9187670000	-1.3762300000
H	1.6637290000	-3.2300750000	2.5904160000
H	-2.3400560000	-3.6302780000	1.0495270000
C	2.4187910000	0.0698760000	-0.5071310000
C	2.9200250000	1.0811230000	-1.3248450000
C	3.1547140000	-1.1071880000	-0.3755970000
C	4.1346620000	0.9060380000	-1.9916060000

C	0.8996740000	2.7410950000	-0.2491340000
C	4.3772040000	-1.2787700000	-1.0311380000
C	4.8806780000	-0.2739890000	-1.8576990000
H	4.5056040000	1.7119930000	-2.6136550000
C	-0.4221180000	2.3342760000	-0.4295890000
C	1.3083460000	3.3176830000	0.9536220000
H	4.9078140000	-2.2043260000	-0.8678280000
C	-1.3245980000	2.5063110000	0.6231930000
H	-0.7381880000	1.9187280000	-1.3762740000
C	0.4053710000	3.5069670000	2.0122300000
H	2.3400420000	3.6303030000	1.0494690000
C	-0.9140970000	3.0972030000	1.8250230000
H	-1.6637560000	3.2301290000	2.5903320000
N	-2.6991570000	2.1562230000	0.4837350000
H	1.4926770000	0.2015440000	0.0336600000
O	-3.5716730000	2.8218090000	1.1465170000
O	3.5716590000	-2.8217950000	1.1466050000
N	2.6991500000	-2.1562200000	0.4838030000
C	-0.8894860000	-4.1622510000	3.3183660000
C	-1.4166420000	-5.5830660000	3.0084150000
H	-1.7639630000	-6.0644250000	3.9275460000
H	-2.2529580000	-5.5637520000	2.3058180000
H	-0.6292670000	-6.2059270000	2.5753660000
C	-2.0289810000	-3.3126420000	3.9276410000
H	-2.3842710000	-3.7699620000	4.8558980000
H	-1.6832500000	-2.3013970000	4.1589790000
H	-2.8824750000	-3.2278210000	3.2512850000
C	0.2358670000	-4.2819330000	4.3618690000
H	1.0632990000	-4.8988510000	4.0016940000
H	0.6353010000	-3.3043280000	4.6449950000
H	-0.1561330000	-4.7525290000	5.2673350000

C	-6.2165190000	0.4170300000	-2.6101980000
C	-6.8849090000	1.7805150000	-2.3564060000
H	-7.8235270000	1.8346630000	-2.9141090000
H	-7.1202680000	1.9303340000	-1.2994800000
H	-6.2557760000	2.6107060000	-2.6886610000
C	-5.9681310000	0.2768360000	-4.1300790000
H	-5.2876950000	1.0542330000	-4.4882560000
H	-5.5340060000	-0.6922520000	-4.3864350000
H	-6.9115480000	0.3733810000	-4.6758300000
C	-7.1884000000	-0.6919670000	-2.1432260000
H	-7.3817480000	-0.6148350000	-1.0698580000
H	-8.1440040000	-0.6005260000	-2.6683540000
H	-6.7939750000	-1.6912180000	-2.3417330000
C	0.8894510000	4.1623270000	3.3182830000
C	-0.2359110000	4.2820320000	4.3617730000
H	-0.6353470000	3.3044330000	4.6449180000
H	0.1560800000	4.7526500000	5.2672310000
H	-1.0633410000	4.8989400000	4.0015760000
C	2.0289410000	3.3127330000	3.9275890000
H	2.8824410000	3.2278960000	3.2512420000
H	2.3842220000	3.7700770000	4.8558370000
H	1.6832090000	2.3014940000	4.1589480000
C	1.4166070000	5.5831350000	3.0083030000
H	2.2529300000	5.5638060000	2.3057140000
H	0.6292350000	6.2059850000	2.5752330000
H	1.7639190000	6.0645160000	3.9274260000
C	6.2165520000	-0.4170800000	-2.6101150000
C	6.8849450000	-1.7805560000	-2.3562820000
H	7.8235700000	-1.8347130000	-2.9139710000
H	7.1202900000	-1.9303490000	-1.2993490000
H	6.2558200000	-2.6107570000	-2.6885260000

C	7.1884210000	0.6919320000	-2.1431550000
H	7.3817560000	0.6148250000	-1.0697830000
H	8.1440330000	0.6004840000	-2.6682680000
H	6.7939940000	1.6911780000	-2.3416890000
C	5.9681840000	-0.2769220000	-4.1300030000
H	5.2877570000	-1.0543300000	-4.4881710000
H	5.5340570000	0.6921580000	-4.3863870000
H	6.9116080000	-0.3734740000	-4.6757390000
S	2.0550420000	2.6273130000	-1.6233620000
S	-2.0550310000	-2.6273530000	-1.6233260000

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B-ECP1

C	-1.3606600000	-1.4915160000	-0.0513190000
C	-1.4725980000	-0.2187040000	-0.6157570000
C	-2.7034240000	0.4330520000	-0.6602500000
C	-3.8153610000	-0.1744960000	-0.0745150000
C	-3.7426860000	-1.4431990000	0.4954430000
C	-2.5138190000	-2.0986660000	0.4687930000
C	1.3603600000	-1.4916190000	0.0518170000
C	1.4724660000	-0.2186900000	0.6159600000
C	2.7033460000	0.4329880000	0.6601350000
C	3.8151540000	-0.1747690000	0.0743770000
C	3.7423140000	-1.4435990000	-0.4952760000
C	2.5134060000	-2.0989720000	-0.4683060000
H	-0.5834210000	0.2531610000	-1.0142560000
H	-4.7470130000	0.3811390000	-0.0935830000
H	-2.4208310000	-3.1026890000	0.8724470000
H	0.5833760000	0.2533290000	1.0144620000
H	4.7468460000	0.3808100000	0.0931790000
H	2.4202940000	-3.1030790000	-0.8717230000

C	2.035860000	2.296794000	2.336385000
C	-2.035218000	2.296487000	-2.336573000
N	-2.879583000	1.718906000	-1.227326000
O	-3.833990000	2.426427000	-0.787942000
O	3.834138000	2.426259000	0.787162000
N	2.879717000	1.718964000	1.226882000
H	-0.000237000	-3.425291000	0.000504000
C	5.001173000	-2.058818000	-1.101141000
C	4.748604000	-3.452638000	-1.666870000
H	5.678692000	-3.849376000	-2.088520000
H	4.411077000	-4.153597000	-0.894906000
H	4.002655000	-3.438607000	-2.469494000
C	6.085908000	-2.171618000	-0.026247000
H	6.989743000	-2.626595000	-0.448711000
H	6.365918000	-1.195549000	0.382068000
H	5.746384000	-2.799282000	0.805669000
C	5.500249000	-1.166120000	-2.241096000
H	4.738290000	-1.070746000	-3.023154000
H	5.752076000	-0.158890000	-1.894807000
H	6.400220000	-1.599067000	-2.694198000
C	-5.001678000	-2.058194000	1.101257000
C	-6.086307000	-2.171015000	0.026259000
H	-6.990254000	-2.625798000	0.448693000
H	-6.366133000	-1.194971000	-0.382243000
H	-5.746777000	-2.798859000	-0.805519000
C	-4.749335000	-3.451967000	1.667204000
H	-4.411869000	-4.153087000	0.895360000
H	-4.003424000	-3.437926000	2.469864000
H	-5.679500000	-3.848514000	2.088865000
C	-5.500779000	-1.165284000	2.241034000
H	-5.752469000	-0.158078000	1.894576000

H	-6.4008410000	-1.5980740000	2.6941060000
H	-4.7388910000	-1.0698770000	3.0231570000
B	-0.0001840000	-2.2288660000	0.0004040000
C	-1.7073420000	1.2324350000	-3.3784240000
H	-1.2468060000	1.7220980000	-4.2425160000
H	-1.0125670000	0.4683070000	-3.0288870000
H	-2.6207390000	0.7346090000	-3.7205830000
C	-0.7817320000	2.9288400000	-1.7385780000
H	-0.2213730000	3.4468330000	-2.5245420000
H	-1.0651470000	3.6655120000	-0.9794400000
H	-0.1071380000	2.1999530000	-1.2788580000
C	-2.8637570000	3.3830110000	-3.0095830000
H	-2.2827720000	3.7909830000	-3.8428010000
H	-3.8005210000	2.9783940000	-3.4036570000
H	-3.1081600000	4.1923720000	-2.3204980000
C	0.7823630000	2.9295240000	1.7388120000
H	1.0657480000	3.6659510000	0.9794260000
H	0.1072890000	2.2008260000	1.2795030000
H	0.2225420000	3.4478750000	2.5249240000
C	2.8649410000	3.3830850000	3.0090950000
H	3.1093850000	4.1923400000	2.3198980000
H	2.2843390000	3.7912780000	3.8424730000
H	3.8016980000	2.9781930000	3.4029010000
C	1.7080280000	1.2328810000	3.3783880000
H	2.6213900000	0.7347440000	3.7201900000
H	1.2480140000	1.7227280000	4.2426530000
H	1.0128440000	0.4689890000	3.0291570000

B-ECP2

C	1.2337010000	-2.7893190000	0.6193630000
C	1.7319950000	-1.5811900000	0.1269190000

C	2.9559460000	-1.1072850000	0.5940470000
C	3.6372440000	-1.7844100000	1.6006470000
C	3.1397690000	-2.9632450000	2.1498930000
C	1.9589190000	-3.4655140000	1.6140410000
C	-1.2335720000	-2.7893060000	-0.6195870000
C	-1.7319100000	-1.5812680000	-0.1269600000
C	-2.9559190000	-1.1073820000	-0.5939490000
C	-3.6372490000	-1.7844370000	-1.6005750000
C	-3.1397410000	-2.9631780000	-2.1500000000
C	-1.9588170000	-3.4654270000	-1.6142970000
H	1.2122340000	-1.0625380000	-0.6753300000
H	4.5906280000	-1.3730770000	1.9160890000
H	1.5697640000	-4.4200620000	1.9571750000
H	-1.2121260000	-1.0627000000	0.6753260000
H	-4.5906830000	-1.3731410000	-1.9159100000
H	-1.5696050000	-4.4199030000	-1.9575600000
C	-1.7319850000	1.5811870000	0.1269620000
C	-1.2336950000	2.7893060000	0.6194350000
C	-2.9559380000	1.1072710000	0.5940740000
C	-1.9589190000	3.4654800000	1.6141230000
C	1.2335790000	2.7893180000	-0.6195140000
C	-3.6372400000	1.7843720000	1.6006860000
C	-3.1397700000	2.9631970000	2.1499590000
H	-1.5697660000	4.4200200000	1.9572800000
C	1.7319200000	1.5812700000	-0.1269160000
C	1.9588180000	3.4654610000	-1.6142130000
H	-4.5906250000	1.3730310000	1.9161160000
C	2.9559280000	1.1073950000	-0.5939200000
H	1.2121410000	1.0626830000	0.6753610000
C	3.1397410000	2.9632260000	-2.1499320000
H	1.5696040000	4.4199450000	-1.9574540000

C	3.6372540000	1.7844750000	-1.6005340000
H	4.5906880000	1.3731860000	-1.9158810000
N	3.6182690000	0.0000930000	0.0001230000
H	-1.2122190000	1.0625530000	-0.6752950000
O	4.8873810000	0.0001470000	0.0001960000
O	-4.8873710000	-0.0001480000	0.0001960000
N	-3.6182590000	-0.0000940000	0.0001230000
H	0.0002050000	-4.6820730000	-0.0004100000
C	-3.9248260000	-3.6680850000	-3.2507970000
C	-3.1953520000	-4.8990010000	-3.7802760000
H	-3.7854270000	-5.3552500000	-4.5824790000
H	-2.2137500000	-4.6431950000	-4.1954090000
H	-3.0543060000	-5.6601210000	-3.0048130000
C	-4.1411430000	-2.7053050000	-4.4215580000
H	-4.6897430000	-3.2088010000	-5.2262350000
H	-4.7190450000	-1.8227420000	-4.1297990000
H	-3.1829480000	-2.3612970000	-4.8274550000
C	-5.2808960000	-4.1137270000	-2.6964200000
H	-5.1498110000	-4.8089400000	-1.8594310000
H	-5.8756770000	-3.2676750000	-2.3381250000
H	-5.8591890000	-4.6236910000	-3.4761670000
C	3.9247860000	-3.6682190000	3.2506910000
C	4.1409420000	-2.7055340000	4.4215610000
H	4.6894710000	-3.2090820000	5.2262550000
H	4.7188420000	-1.8229200000	4.1299460000
H	3.1826900000	-2.3615970000	4.8273840000
C	3.1953120000	-4.8992170000	3.7799790000
H	2.2136670000	-4.6434950000	4.1950600000
H	3.0543610000	-5.6602590000	3.0044220000
H	3.7853350000	-5.3555320000	4.5821830000
C	5.2809300000	-4.1137550000	2.6964080000

H	5.8757200000	-3.2676500000	2.3382560000
H	5.8591630000	-4.6237740000	3.4761630000
H	5.1499530000	-4.8088910000	1.8593390000
C	3.9248200000	3.6681580000	-3.2507170000
C	5.2808870000	4.1138000000	-2.6963320000
H	5.8756750000	3.2677460000	-2.3380540000
H	5.8591750000	4.6237830000	-3.4760700000
H	5.1497970000	4.8089960000	-1.8593310000
C	4.1411440000	2.7054000000	-4.4214950000
H	3.1829510000	2.3613930000	-4.8273980000
H	4.6897400000	3.2089150000	-5.2261630000
H	4.7190520000	1.8228360000	-4.1297520000
C	3.1953370000	4.8990770000	-3.7801740000
H	2.2137350000	4.6432730000	-4.1953070000
H	3.0542890000	5.6601850000	-3.0046990000
H	3.7854060000	5.3553420000	-4.5823730000
C	-3.9247950000	3.6681470000	3.2507680000
C	-4.1409440000	2.7054400000	4.4216210000
H	-4.6894780000	3.2089700000	5.2263230000
H	-4.7188380000	1.8228280000	4.1299900000
H	-3.1826900000	2.3615030000	4.8274390000
C	-5.2809410000	4.1136820000	2.6964900000
H	-5.8757240000	3.2675790000	2.3383230000
H	-5.8591790000	4.6236820000	3.4762530000
H	-5.1499690000	4.8088340000	1.8594340000
C	-3.1953310000	4.8991410000	3.7800770000
H	-2.2136850000	4.6434200000	4.1951590000
H	-3.0543810000	5.6601960000	3.0045320000
H	-3.7853600000	5.3554410000	4.5822860000
H	-0.0002110000	4.6820720000	-0.0003260000
B	0.0000860000	-3.4847030000	-0.0001650000

B -0.0000740000 3.4847020000 -0.0000680000

C-ECP1

C 1.8925610000 0.7253960000 -1.1805370000

C 1.4496260000 -0.3695720000 -0.4520090000

C 2.3418150000 -1.1320890000 0.2942570000

C 3.7042410000 -0.8038340000 0.2819640000

C 4.1679340000 0.2811490000 -0.4466760000

C 3.2431320000 1.0450110000 -1.1696480000

C -0.4784300000 1.4876490000 -1.4094920000

C -1.3811120000 0.5389810000 -1.8507060000

C -2.5913170000 0.3545880000 -1.1737210000

C -2.9064390000 1.1801250000 -0.0978660000

C -2.0155280000 2.1575060000 0.3496930000

C -0.8000500000 2.2893480000 -0.3114630000

H 0.4003960000 -0.6130460000 -0.4809740000

H 4.3691320000 -1.4257010000 0.8663320000

H 3.5778850000 1.9088770000 -1.7406280000

H -1.1511700000 -0.1051670000 -2.6941750000

H -3.8663530000 1.0826500000 0.3924420000

H -0.0620490000 3.0113450000 0.0263070000

C -4.4453890000 -1.4195830000 -0.7919120000

C 0.4893290000 -2.5876950000 1.3806160000

N 1.9303280000 -2.2404600000 1.0662130000

O 2.8262290000 -3.0075890000 1.5250190000

O -3.3444490000 -1.0128870000 -2.8547580000

N -3.4461450000 -0.6723650000 -1.6390430000

H 1.2593110000 2.5799460000 -2.0391680000

C -2.3990260000 3.0101640000 1.5558060000

C -1.3305950000 4.0442460000 1.8963930000

H -1.6559740000 4.6352330000 2.7594850000

H	-1.1570120000	4.7388800000	1.0669100000
H	-0.3763760000	3.5749680000	2.1603600000
C	-2.5813040000	2.0983080000	2.7732800000
H	-1.6595150000	1.5427930000	2.9835670000
H	-2.8319280000	2.6921930000	3.6603980000
H	-3.3860510000	1.3700130000	2.6245900000
C	-3.7053340000	3.7559710000	1.2709660000
H	-3.9822650000	4.3755420000	2.1321380000
H	-3.5969450000	4.4124000000	0.4003310000
H	-4.5387600000	3.0738350000	1.0739130000
C	5.6443650000	0.6666890000	-0.4786090000
C	6.5064020000	-0.2590730000	0.3733430000
H	7.5532990000	0.0584910000	0.3124980000
H	6.2137150000	-0.2332300000	1.4288160000
H	6.4551370000	-1.2974890000	0.0282700000
C	6.1526770000	0.5941670000	-1.9215030000
H	6.0404850000	-0.4197950000	-2.3218460000
H	5.6110060000	1.2775530000	-2.5832580000
H	7.2155480000	0.8611950000	-1.9629360000
C	5.8122190000	2.0930950000	0.0521780000
H	5.4498770000	2.1687590000	1.0837850000
H	6.8710000000	2.3784800000	0.0413740000
H	5.2649550000	2.8249250000	-0.5504440000
C	0.9055060000	1.5424840000	-1.9908820000
H	0.8887440000	1.1709130000	-3.0243020000
C	-4.6653760000	-2.7743720000	-1.4521950000
H	-3.7270920000	-3.3354690000	-1.5149710000
H	-5.3736460000	-3.3454070000	-0.8433770000
H	-5.0672830000	-2.6735470000	-2.4606940000
C	-3.9062670000	-1.6669570000	0.6135380000
H	-3.8271260000	-0.7704760000	1.2299070000

H	-4.5808490000	-2.3604840000	1.1260580000
H	-2.9153650000	-2.1317870000	0.5669250000
C	-5.7585160000	-0.6440920000	-0.7803810000
H	-5.6666420000	0.3340250000	-0.2995470000
H	-6.1088890000	-0.4890620000	-1.8057750000
H	-6.5212800000	-1.2153680000	-0.2398050000
C	-0.2396640000	-1.3872840000	1.9859460000
H	0.3318170000	-0.9874260000	2.8305940000
H	-0.4325780000	-0.5693120000	1.2877130000
H	-1.2105230000	-1.7224900000	2.3691150000
C	0.5174520000	-3.6944920000	2.4259480000
H	-0.5167930000	-3.9398100000	2.6884760000
H	1.0078300000	-4.5942070000	2.0503420000
H	1.0427840000	-3.3772480000	3.3301710000
C	-0.1972540000	-3.1320030000	0.1269730000
H	-1.1540050000	-3.5867050000	0.4097300000
H	-0.4040890000	-2.3745880000	-0.6345880000
H	0.4201580000	-3.9145930000	-0.3261340000

C-ECP2

C	-2.8091560000	-1.1023340000	-1.3479040000
C	-2.3075130000	-0.0382530000	-0.6173860000
C	-3.0655680000	1.1260680000	-0.4953150000
C	-4.3245300000	1.2188560000	-1.0707730000
C	-4.8471210000	0.1577200000	-1.8078970000
C	-4.0709090000	-0.9909730000	-1.9369040000
C	-1.0090330000	-2.6467320000	-0.4601670000
C	0.3209680000	-2.3010010000	-0.6226740000
C	1.2208930000	-2.5299550000	0.4190160000
C	0.7973230000	-3.1239910000	1.5986730000
C	-0.5407240000	-3.4708000000	1.7840410000
C	-1.4290650000	-3.2179490000	0.7425810000

H	-1.3483140000	-0.1199690000	-0.1147620000
H	-4.8817440000	2.1372860000	-0.9183260000
H	-4.4448610000	-1.8404820000	-2.5015760000
H	0.6606580000	-1.8697160000	-1.5607060000
H	1.5448820000	-3.3062150000	2.3636190000
H	-2.4822110000	-3.4649580000	0.8461490000
C	2.3075220000	0.0382590000	-0.6173580000
C	2.8091720000	1.1023330000	-1.3478800000
C	3.0655740000	-1.1260630000	-0.4952750000
C	4.0709290000	0.9909650000	-1.9368720000
C	1.0090410000	2.6467360000	-0.4601700000
C	4.3245390000	-1.2188590000	-1.0707250000
C	4.8471360000	-0.1577290000	-1.8078520000
H	4.4448860000	1.8404680000	-2.5015470000
C	-0.3209590000	2.3010080000	-0.6226920000
C	1.4290600000	3.2179510000	0.7425840000
H	4.8817500000	-2.1372880000	-0.9182670000
C	-1.2208950000	2.5299630000	0.4189880000
H	-0.6606390000	1.8697240000	-1.5607280000
C	0.5407070000	3.4708030000	1.7840340000
H	2.4822050000	3.4649570000	0.8461650000
C	-0.7973390000	3.1239960000	1.5986500000
H	-1.5449070000	3.3062220000	2.3635860000
N	-2.6009910000	2.2225380000	0.2796790000
H	1.3483210000	0.1199790000	-0.1147390000
O	-3.4498970000	2.9504520000	0.8771060000
O	3.4498900000	-2.9504280000	0.8771760000
N	2.6009890000	-2.2225260000	0.2797270000
H	2.7043280000	3.2137540000	-1.6335730000
H	-2.7043030000	-3.2137560000	-1.6335930000
C	-0.9708670000	-4.1010830000	3.1054660000

C	-2.4662090000	-4.3987870000	3.1473030000
H	-2.7217250000	-4.8457710000	4.1142190000
H	-3.0679320000	-3.4897930000	3.0355970000
H	-2.7638070000	-5.1095920000	2.3681050000
C	-0.6451490000	-3.1420650000	4.2543460000
H	-0.9529560000	-3.5817400000	5.2104850000
H	0.4254860000	-2.9239280000	4.3177970000
H	-1.1757030000	-2.1909690000	4.1306900000
C	-0.2159180000	-5.4183010000	3.3073130000
H	-0.4333490000	-6.1207900000	2.4947520000
H	0.8679590000	-5.2712780000	3.3410660000
H	-0.5198430000	-5.8856350000	4.2515530000
C	-6.2285370000	0.2995890000	-2.4400300000
C	-6.2069360000	1.4639630000	-3.4354010000
H	-7.1904030000	1.5778370000	-3.9069830000
H	-5.9574670000	2.4128660000	-2.9502740000
H	-5.4686780000	1.2870870000	-4.2261160000
C	-6.6586110000	-0.9572300000	-3.1893740000
H	-5.9796190000	-1.1941880000	-4.0162910000
H	-6.7161780000	-1.8286300000	-2.5271470000
H	-7.6551150000	-0.8032370000	-3.6175070000
C	-7.2641190000	0.5793690000	-1.3474290000
H	-7.0494240000	1.5026980000	-0.8011240000
H	-8.2619150000	0.6783290000	-1.7912400000
H	-7.2940900000	-0.2400120000	-0.6203860000
C	0.9708350000	4.1010870000	3.1054630000
C	0.2158850000	5.4183080000	3.3072960000
H	-0.8679920000	5.2712860000	3.3410360000
H	0.5197990000	5.8856450000	4.2515380000
H	0.4333270000	6.1207930000	2.4947350000
C	0.6451030000	3.1420740000	4.2543430000

H	1.1756560000	2.1909770000	4.1306950000
H	0.9529020000	3.5817510000	5.2104830000
H	-0.4255330000	2.9239400000	4.3177850000
C	2.4661770000	4.3987890000	3.1473160000
H	3.0679000000	3.4897940000	3.0356130000
H	2.7637850000	5.1095970000	2.3681250000
H	2.7216830000	4.8457680000	4.1142380000
C	6.2285580000	-0.2996040000	-2.4399720000
C	6.2069650000	-1.4639870000	-3.4353350000
H	7.1904360000	-1.5778650000	-3.9069070000
H	5.9574910000	-2.4128850000	-2.9502020000
H	5.4687150000	-1.2871160000	-4.2260580000
C	7.2641300000	-0.5793770000	-1.3473600000
H	7.0494270000	-1.5027010000	-0.8010480000
H	8.2619290000	-0.6783440000	-1.7911610000
H	7.2940960000	0.2400100000	-0.6203240000
C	6.6586400000	0.9572080000	-3.1893220000
H	5.9796540000	1.1941610000	-4.0162460000
H	6.7162040000	1.8286130000	-2.5271010000
H	7.6551470000	0.8032100000	-3.6174470000
C	-2.0079030000	-2.3701290000	-1.5462430000
C	2.0079240000	2.3701300000	-1.5462320000
H	-1.4869890000	-2.3069320000	-2.5119900000
H	1.4870230000	2.3069330000	-2.5119860000

N-ECP1

C	-1.1983450000	-1.4213800000	-0.0589510000
C	-1.3357180000	-0.0716350000	0.2483060000
C	-2.5870030000	0.5201140000	0.1653320000
C	-3.7047070000	-0.2107600000	-0.2075600000
C	-3.5928240000	-1.5747720000	-0.4830660000

C	-2.3343770000	-2.1604880000	-0.4074890000
C	1.2969310000	-1.4614400000	-0.1026580000
C	1.4926250000	-0.3007830000	-0.8421480000
C	2.7599010000	0.2620380000	-0.8987590000
C	3.8440040000	-0.3563460000	-0.2910150000
C	3.6729990000	-1.5453070000	0.4184430000
C	2.3900210000	-2.0724650000	0.5198730000
H	-0.4752880000	0.5220260000	0.5278510000
H	-4.6517560000	0.3131070000	-0.2939370000
H	-2.2003420000	-3.2117240000	-0.6461090000
H	0.6772510000	0.1350430000	-1.4056150000
H	4.8190870000	0.1078810000	-0.3989760000
H	2.2073080000	-2.9772540000	1.0920590000
C	2.4427060000	2.8008610000	-1.2274630000
C	-2.6982000000	2.4980860000	1.8027970000
N	-2.7328150000	1.9265130000	0.4108240000
O	-3.4225460000	2.5718470000	-0.4387130000
O	4.0466720000	1.4945990000	-2.3465950000
N	2.9865100000	1.4578370000	-1.6492810000
N	0.0385860000	-2.0593770000	-0.0088030000
H	0.0233040000	-3.0605450000	0.1165160000
C	4.8862140000	-2.2114290000	1.0616660000
C	4.5197030000	-3.4720510000	1.8377540000
H	5.4253240000	-3.9060730000	2.2753370000
H	3.8264810000	-3.2601170000	2.6600680000
H	4.0703440000	-4.2349410000	1.1918380000
C	5.5537170000	-1.2350680000	2.0341670000
H	6.4250070000	-1.7070190000	2.5039130000
H	5.8986930000	-0.3259680000	1.5323500000
H	4.8583680000	-0.9388270000	2.8280000000
C	5.8797890000	-2.5996450000	-0.0376790000

H	5.4230010000	-3.3016220000	-0.7445890000
H	6.2209160000	-1.7297390000	-0.6069630000
H	6.7617700000	-3.0822890000	0.4005220000
C	-4.8362000000	-2.3585040000	-0.8946310000
C	-5.3746760000	-1.7830030000	-2.2077220000
H	-6.2663910000	-2.3366500000	-2.5251790000
H	-5.6504190000	-0.7285360000	-2.1103870000
H	-4.6239030000	-1.8597140000	-3.0022810000
C	-4.5495460000	-3.8416360000	-1.1074240000
H	-3.8244540000	-4.0081940000	-1.9120110000
H	-4.1736030000	-4.3205200000	-0.1958070000
H	-5.4749650000	-4.3545940000	-1.3911830000
C	-5.9042130000	-2.2344210000	0.1957320000
H	-6.2025350000	-1.1949580000	0.3636470000
H	-6.8019090000	-2.7957340000	-0.0896510000
H	-5.5389710000	-2.6376320000	1.1473230000
C	1.0895990000	2.7017350000	-0.5414050000
H	0.3078440000	2.3033840000	-1.1969210000
H	1.1313340000	2.0998250000	0.3725790000
H	0.7846790000	3.7144680000	-0.2552150000
C	2.3189650000	3.6520230000	-2.4805970000
H	1.9745150000	4.6548530000	-2.2078580000
H	3.2794430000	3.7359520000	-2.9922800000
H	1.5931610000	3.2151690000	-3.1743840000
C	3.4644700000	3.3932910000	-0.2609460000
H	4.4451070000	3.4644510000	-0.7394710000
H	3.1522300000	4.3961990000	0.0495260000
H	3.5563630000	2.7702880000	0.6365190000
C	-1.6540400000	1.8122860000	2.6665640000
H	-1.8444030000	0.7418380000	2.7830670000
H	-0.6437700000	1.9501580000	2.2662270000

H	-1.6805520000	2.2665080000	3.6626410000
C	-4.0879500000	2.2945620000	2.3985570000
H	-4.1411060000	2.7444700000	3.3958740000
H	-4.8449410000	2.7639780000	1.7631590000
H	-4.3193180000	1.2273070000	2.4927310000
C	-2.3698030000	3.9762880000	1.6795000000
H	-2.3520170000	4.4285740000	2.6765920000
H	-1.3846540000	4.1131660000	1.2197240000
H	-3.1094430000	4.4967200000	1.0689530000

N-ECP2

C	0.1159500000	2.9989630000	0.0969970000
C	-0.9022810000	2.0818060000	-0.1196590000
C	-2.0333670000	2.1336740000	0.6936680000
C	-2.1412570000	3.0869470000	1.7036940000
C	-1.1248510000	4.0095880000	1.9250690000
C	0.0052330000	3.9491110000	1.1131410000
C	2.1504580000	1.9899020000	-0.9180940000
C	2.0946900000	0.8153530000	-0.1770800000
C	3.1049760000	-0.1260090000	-0.3539250000
C	4.1485420000	0.0782570000	-1.2405940000
C	4.2005450000	1.2443030000	-2.0055440000
C	3.1919500000	2.1810460000	-1.8366700000
H	-0.8344180000	1.3877420000	-0.9510460000
H	-3.0526940000	3.0917770000	2.2903550000
H	0.8312890000	4.6390240000	1.2575980000
H	1.3215850000	0.6652860000	0.5703320000
H	4.9157660000	-0.6850480000	-1.3069210000
H	3.1870120000	3.1013390000	-2.4137740000
C	0.9022700000	-2.0817110000	-0.1190650000
C	-0.1159760000	-2.9988740000	0.0974910000
C	2.0332080000	-2.1334730000	0.6944750000

C	-0.0054240000	-3.9489180000	1.1137520000
C	-2.1502890000	-1.9899780000	-0.9181750000
C	2.1409290000	-3.0866340000	1.7046250000
C	1.1245030000	-4.0092750000	1.9259060000
H	-0.8314860000	-4.6388410000	1.2581230000
C	-2.0946700000	-0.8152780000	-0.1773870000
C	-3.1916130000	-2.1813160000	-1.8369030000
H	3.0522680000	-3.0913930000	2.2914400000
C	-3.1049380000	0.1260360000	-0.3546020000
H	-1.3217030000	-0.6650410000	0.5701350000
C	-4.2001910000	-1.2446220000	-2.0061420000
H	-3.1865750000	-3.1017220000	-2.4138250000
C	-4.1483410000	-0.0784210000	-1.2414190000
H	-4.9155610000	0.6848620000	-1.3080420000
N	-3.1536120000	1.3032510000	0.4533000000
H	0.8345460000	-1.3877330000	-0.9505350000
O	-4.2857870000	1.6581590000	0.8998400000
O	4.2855790000	-1.6578880000	0.9010390000
N	3.1534890000	-1.3030690000	0.4542120000
N	1.2322730000	3.0275750000	-0.7579830000
N	-1.2321310000	-3.0276160000	-0.7576990000
H	-1.6235450000	-3.9477980000	-0.9038110000
H	1.6237240000	3.9477320000	-0.9041540000
C	5.3455800000	1.4408160000	-2.9936260000
C	5.2506830000	2.7684440000	-3.7385560000
H	6.0923160000	2.8581630000	-4.4338940000
H	4.3287230000	2.8426950000	-4.3265360000
H	5.2960810000	3.6242990000	-3.0552870000
C	5.3178230000	0.3117200000	-4.0280510000
H	6.1302770000	0.4421560000	-4.7529580000
H	5.4392510000	-0.6719450000	-3.5641920000

H	4.3689420000	0.3094100000	-4.5767190000
C	6.6769900000	1.4113100000	-2.2376590000
H	6.7160540000	2.2076430000	-1.4858130000
H	6.8373770000	0.4588330000	-1.7234760000
H	7.5099200000	1.5597830000	-2.9352130000
C	-1.2778880000	5.0363510000	3.0425580000
C	-1.4471180000	4.3090820000	4.3794970000
H	-1.5481510000	5.0362800000	5.1939100000
H	-2.3364080000	3.6715900000	4.3895360000
H	-0.5776420000	3.6769220000	4.5929780000
C	-0.0677400000	5.9583410000	3.1533470000
H	0.8509540000	5.4035770000	3.3760240000
H	0.0898490000	6.5377540000	2.2364430000
H	-0.2258350000	6.6726840000	3.9686580000
C	-2.5125780000	5.9001160000	2.7692490000
H	-3.4293140000	5.3042910000	2.7269650000
H	-2.6343580000	6.6472060000	3.5627220000
H	-2.4137590000	6.4304170000	1.8151260000
C	-5.3450470000	-1.4413570000	-2.9943840000
C	-6.6765810000	-1.4118940000	-2.2386300000
H	-6.8371370000	-0.4593720000	-1.7245810000
H	-7.5093860000	-1.5605240000	-2.9362990000
H	-6.7156880000	-2.2081450000	-1.4867000000
C	-5.3172380000	-0.3123770000	-4.0289330000
H	-4.3682800000	-0.3100490000	-4.5774660000
H	-6.1295790000	-0.4429600000	-4.7539400000
H	-5.4388120000	0.6713300000	-3.5651990000
C	-5.2499080000	-2.7690640000	-3.7391470000
H	-4.3278600000	-2.8432890000	-4.3269940000
H	-5.2953110000	-3.6248450000	-3.0557860000
H	-6.0914360000	-2.8589520000	-4.4345910000

C	1.2773810000	-5.0359530000	3.0434960000
C	1.4460490000	-4.3086040000	4.3804620000
H	1.5469210000	-5.0357580000	5.1949360000
H	2.3352360000	-3.6709750000	4.3907840000
H	0.5764020000	-3.6765740000	4.5936300000
C	2.5123290000	-5.8994790000	2.7706030000
H	3.4289470000	-5.3034540000	2.7285280000
H	2.6340480000	-6.6464830000	3.5641670000
H	2.4138930000	-6.4298720000	1.8164910000
C	0.0673810000	-5.9581770000	3.1539420000
H	-0.8515170000	-5.4035690000	3.3761680000
H	-0.0897230000	-6.5377650000	2.2370660000
H	0.2253010000	-6.6723640000	3.9694240000

O-ECP1

C	-1.1403400000	-1.4702480000	-0.0254820000
C	-1.2117150000	-0.1763380000	0.4590590000
C	-2.4304950000	0.4886160000	0.3973080000
C	-3.5571760000	-0.1385230000	-0.1148710000
C	-3.4967250000	-1.4595900000	-0.5621910000
C	-2.2696850000	-2.1143290000	-0.5172630000
C	1.2269710000	-1.5381310000	-0.1408110000
C	1.3947410000	-0.4799140000	-1.0158720000
C	2.6389070000	0.1330120000	-1.0777710000
C	3.7115650000	-0.3567990000	-0.3445950000
C	3.5544900000	-1.4534810000	0.5031940000
C	2.2896280000	-2.0275410000	0.6078180000
H	-0.3268380000	0.3264650000	0.8264290000
H	-4.4762360000	0.4371000000	-0.1675030000
H	-2.1469110000	-3.1315770000	-0.8717000000
H	0.5783000000	-0.1389680000	-1.6420360000

H	4.6704320000	0.1400230000	-0.4593690000
H	2.0933510000	-2.8694210000	1.2620100000
C	2.2097450000	2.6018920000	-1.6979290000
C	-2.4217230000	2.3222900000	2.2096570000
N	-2.5246150000	1.8665450000	0.7788060000
O	-3.2045850000	2.6120940000	0.0080110000
O	3.8954170000	1.2540730000	-2.6446610000
N	2.8419740000	1.2535480000	-1.9374160000
C	4.7536330000	-1.9714320000	1.2919050000
C	4.3971130000	-3.1660730000	2.1701590000
H	5.2893450000	-3.5017870000	2.7096410000
H	3.6365870000	-2.9115130000	2.9170400000
H	4.0312540000	-4.0134000000	1.5794650000
C	5.2891550000	-0.8581500000	2.1965140000
H	6.1437750000	-1.2228840000	2.7786220000
H	5.6254670000	0.0111070000	1.6231540000
H	4.5179490000	-0.5215550000	2.8990510000
C	5.8483090000	-2.4071110000	0.3131760000
H	5.4876910000	-3.2048740000	-0.3458680000
H	6.1877890000	-1.5805550000	-0.3185480000
H	6.7168900000	-2.7866090000	0.8645230000
C	-4.7591740000	-2.1281050000	-1.0985330000
C	-5.2619730000	-1.3521080000	-2.3193910000
H	-6.1667780000	-1.8240670000	-2.7208050000
H	-5.5068940000	-0.3138160000	-2.0756140000
H	-4.5049360000	-1.3400860000	-3.1115290000
C	-4.5150020000	-3.5732230000	-1.5202640000
H	-3.7807720000	-3.6438930000	-2.3304850000
H	-4.1679310000	-4.1900980000	-0.6835350000
H	-5.4505950000	-4.0095800000	-1.8863510000
C	-5.8358230000	-2.1262780000	-0.0095230000

H	-6.1073150000	-1.1118570000	0.2985720000
H	-6.7447630000	-2.6171480000	-0.3772260000
H	-5.4924660000	-2.6682270000	0.8792110000
C	0.9874390000	2.5252050000	-0.7965320000
H	0.1603900000	1.9618060000	-1.2385780000
H	1.2271360000	2.0953070000	0.1829230000
H	0.6259300000	3.5460460000	-0.6316140000
C	1.8266600000	3.1664010000	-3.0560310000
H	1.4352380000	4.1823670000	-2.9399080000
H	2.6959220000	3.1971560000	-3.7169790000
H	1.0523810000	2.5504170000	-3.5259270000
C	3.2760970000	3.4629670000	-1.0268220000
H	4.1629150000	3.5372490000	-1.6604090000
H	2.8844160000	4.4697090000	-0.8473050000
H	3.5696510000	3.0316070000	-0.0620900000
C	-1.3749110000	1.5400060000	2.9832750000
H	-1.5925790000	0.4692400000	3.0223850000
H	-0.3720850000	1.6847560000	2.5667260000
H	-1.3613620000	1.9137620000	4.0123680000
C	-3.7983770000	2.1168100000	2.8340000000
H	-3.8013880000	2.4759310000	3.8687480000
H	-4.5568210000	2.6686890000	2.2709380000
H	-4.0684150000	1.0545530000	2.8403200000
C	-2.0450830000	3.7945060000	2.1902490000
H	-1.9770660000	4.1643900000	3.2186030000
H	-1.0717830000	3.9365090000	1.7067580000
H	-2.7866230000	4.3855660000	1.6505700000
O	0.0252590000	-2.1917270000	-0.0194760000
O-ECP2			
C	-2.6214210000	-1.2640790000	-0.9291580000
C	-2.2442200000	-0.1475920000	-0.1983660000

C	-2.9095730000	1.0464370000	-0.4556150000
C	-3.9255460000	1.1339760000	-1.3990380000
C	-4.2857580000	0.0140040000	-2.1422250000
C	-3.6157070000	-1.1818200000	-1.8956760000
C	-1.0440820000	-2.7017240000	0.1311380000
C	0.2189220000	-2.2457670000	-0.2089300000
C	1.2756660000	-2.5778660000	0.6312870000
C	1.0704370000	-3.3549920000	1.7725550000
C	-0.2002540000	-3.7947240000	2.1133820000
C	-1.2644390000	-3.4498460000	1.2726680000
H	-1.4865080000	-0.2103230000	0.5760430000
H	-4.4139330000	2.0924140000	-1.5241830000
H	-3.8603940000	-2.0922300000	-2.4346060000
H	0.3701950000	-1.6877800000	-1.1276690000
H	1.9416320000	-3.6021510000	2.3661980000
H	-2.2805670000	-3.7744240000	1.4756010000
C	2.2442210000	0.1475780000	-0.1983390000
C	2.6214340000	1.2640530000	-0.9291430000
C	2.9095790000	-1.0464550000	-0.4555560000
C	3.6157360000	1.1817780000	-1.8956430000
C	1.0440790000	2.7017210000	0.1311010000
C	3.9255680000	-1.1340100000	-1.3989600000
C	4.2857920000	-0.0140500000	-2.1421600000
H	3.8604330000	2.0921790000	-2.4345840000
C	-0.2189200000	2.2457530000	-0.2089730000
C	1.2644180000	3.4498760000	1.2726130000
H	4.4139580000	-2.0924490000	-1.5240810000
C	-1.2756760000	2.5778700000	0.6312220000
H	-0.3701790000	1.6877410000	-1.1276990000
C	0.2002200000	3.7947750000	2.1133030000
H	2.2805420000	3.7744590000	1.4755540000

C	-1.0704640000	3.3550260000	1.7724720000
H	-1.9416690000	3.6021990000	2.3660960000
N	-2.6042040000	2.2105310000	0.3061790000
H	1.4864950000	0.2103220000	0.5760560000
O	-3.5585330000	2.9570690000	0.6779120000
O	3.5585220000	-2.9570660000	0.6780170000
N	2.6041990000	-2.2105360000	0.3062540000
C	-0.4686960000	-4.6381470000	3.3553010000
C	-1.0714570000	-5.9809250000	2.9321630000
H	-1.2616490000	-6.6028170000	3.8147360000
H	-2.0205690000	-5.8572580000	2.4012890000
H	-0.3858250000	-6.5258070000	2.2736090000
C	-1.4513890000	-3.8988760000	4.2679480000
H	-1.6450560000	-4.4900850000	5.1706740000
H	-1.0432540000	-2.9300080000	4.5774420000
H	-2.4131990000	-3.7169830000	3.7779370000
C	0.8034200000	-4.9159390000	4.1490500000
H	1.5415350000	-5.4684380000	3.5573190000
H	1.2709910000	-3.9917490000	4.5066370000
H	0.5605610000	-5.5245820000	5.0267600000
C	-5.3825620000	0.0537420000	-3.2022530000
C	-5.9957540000	1.4427660000	-3.3472630000
H	-6.7754500000	1.4177590000	-4.1161990000
H	-6.4608230000	1.7845550000	-2.4160940000
H	-5.2529270000	2.1872010000	-3.6550850000
C	-4.7959910000	-0.3519190000	-4.5572000000
H	-3.9910450000	0.3301470000	-4.8538770000
H	-4.3879310000	-1.3674520000	-4.5434470000
H	-5.5735020000	-0.3160580000	-5.3293940000
C	-6.4973300000	-0.9212680000	-2.8126260000
H	-6.9297410000	-0.6508710000	-1.8427610000

H	-7.2978940000	-0.8958430000	-3.5612650000
H	-6.1371290000	-1.9526010000	-2.7441300000
C	0.4686460000	4.6382280000	3.3552030000
C	-0.8034600000	4.9159260000	4.1490040000
H	-1.2709160000	3.9917050000	4.5066600000
H	-0.5606190000	5.5246360000	5.0266720000
H	-1.5416620000	5.4683190000	3.5572820000
C	1.4514350000	3.8990390000	4.2678120000
H	2.4132290000	3.7171970000	3.7777500000
H	1.6451150000	4.4902790000	5.1705150000
H	1.0433780000	2.9301510000	4.5773480000
C	1.0712840000	5.9810510000	2.9320320000
H	2.0203890000	5.8574570000	2.4011290000
H	0.3855870000	6.5258700000	2.2734950000
H	1.2614540000	6.6029680000	3.8145930000
C	5.3826120000	-0.0538060000	-3.2021710000
C	5.9958150000	-1.4428300000	-3.3471400000
H	6.7755240000	-1.4178340000	-4.1160630000
H	6.4608700000	-1.7845960000	-2.4159560000
H	5.2529980000	-2.1872750000	-3.6549600000
C	6.4973680000	0.9212200000	-2.8125510000
H	6.9297690000	0.6508480000	-1.8426750000
H	7.2979420000	0.8957830000	-3.5611800000
H	6.1371610000	1.9525530000	-2.7440840000
C	4.7960570000	0.3518200000	-4.5571350000
H	3.9911180000	-0.3302570000	-4.8538060000
H	4.3879910000	1.3673510000	-4.5434110000
H	5.5735780000	0.3159450000	-5.3293180000
O	-2.1039130000	-2.5103120000	-0.7256240000
O	2.1039230000	2.5102890000	-0.7256400000

S-ECP1

C	-1.310360000	-1.668460000	0.151777000
C	-1.198164000	-0.379556000	0.650341000
C	-2.290816000	0.472581000	0.559453000
C	-3.491670000	0.028206000	0.020729000
C	-3.634674000	-1.281962000	-0.431703000
C	-2.520421000	-2.116883000	-0.375294000
C	1.451866000	-1.731286000	-0.110049000
C	1.408557000	-0.732443000	-1.071925000
C	2.517626000	0.084704000	-1.237352000
C	3.688034000	-0.157836000	-0.528572000
C	3.760483000	-1.188087000	0.406768000
C	2.614337000	-1.952386000	0.625784000
H	-0.254483000	-0.021542000	1.044294000
H	-4.305374000	0.743786000	-0.049228000
H	-2.568133000	-3.128800000	-0.764125000
H	0.524824000	-0.584075000	-1.683137000
H	4.540233000	0.484325000	-0.731977000
H	2.607310000	-2.736344000	1.375766000
C	1.707363000	2.424777000	-1.945831000
C	-2.071448000	2.285397000	2.373132000
N	-2.184313000	1.852513000	0.935687000
O	-2.728944000	2.683716000	0.144826000
O	3.498987000	1.262276000	-2.949326000
N	2.494498000	1.159512000	-2.179733000
C	5.063377000	-1.425931000	1.165165000
C	4.951157000	-2.569108000	2.168380000
H	5.912776000	-2.704604000	2.675071000
H	4.198679000	-2.366785000	2.939322000
H	4.699982000	-3.517711000	1.680585000
C	5.451368000	-0.158020000	1.930566000

H	6.3822550000	-0.3224460000	2.4861050000
H	5.6100060000	0.6944210000	1.2628120000
H	4.6709340000	0.1169650000	2.6494550000
C	6.1660470000	-1.7787450000	0.1622470000
H	5.9099430000	-2.6874360000	-0.3941430000
H	6.3324550000	-0.9786070000	-0.5655030000
H	7.1121620000	-1.9562290000	0.6874680000
C	-4.9768950000	-1.7396760000	-0.9959300000
C	-5.3256400000	-0.8950930000	-2.2245430000
H	-6.2872570000	-1.2163000000	-2.6419970000
H	-5.4046120000	0.1696300000	-1.9839200000
H	-4.5625680000	-1.0064400000	-3.0030950000
C	-4.9616160000	-3.2068760000	-1.4128660000
H	-4.2369260000	-3.3995830000	-2.2118860000
H	-4.7320410000	-3.8688400000	-0.5700850000
H	-5.9497090000	-3.4879520000	-1.7930820000
C	-6.0589000000	-1.5611930000	0.0733860000
H	-6.1649770000	-0.5160410000	0.3809410000
H	-7.0293960000	-1.8948960000	-0.3123370000
H	-5.8262080000	-2.1531190000	0.9660290000
C	0.5094260000	2.1952080000	-1.0410740000
H	-0.2240090000	1.5095280000	-1.4765040000
H	0.8019280000	1.8164820000	-0.0548870000
H	-0.0039490000	3.1508160000	-0.8881890000
C	1.2469610000	2.9295230000	-3.3030080000
H	0.7086840000	3.8747580000	-3.1789940000
H	2.0981540000	3.0927230000	-3.9671550000
H	0.5710320000	2.2079010000	-3.7737940000
C	2.6631490000	3.4159730000	-1.2882470000
H	3.5371540000	3.5857050000	-1.9222080000
H	2.1547990000	4.3723610000	-1.1257280000

H	3.0020320000	3.0407890000	-0.3150370000
C	-1.0927840000	1.4199340000	3.1476020000
H	-1.3944780000	0.3698510000	3.1832080000
H	-0.0812200000	1.4870330000	2.7322230000
H	-1.0522880000	1.7868290000	4.1784950000
C	-3.4682640000	2.1760160000	2.9768440000
H	-3.4632220000	2.5432990000	4.0087150000
H	-4.1784920000	2.7745430000	2.3979870000
H	-3.8117180000	1.1354000000	2.9878820000
C	-1.5892630000	3.7262080000	2.3764230000
H	-1.4900330000	4.0694230000	3.4113450000
H	-0.6109060000	3.8056380000	1.8899880000
H	-2.2868750000	4.3811210000	1.8525010000
S	0.0599290000	-2.8129760000	0.1767460000

S-ECP2

C	-2.9306130000	-1.0036170000	-1.3950170000
C	-2.3866230000	-0.0085100000	-0.5942740000
C	-3.1134820000	1.1591190000	-0.4001940000
C	-4.3657980000	1.3391840000	-0.9824960000
C	-4.9060540000	0.3546210000	-1.7997110000
C	-4.1726110000	-0.8192410000	-1.9925190000
C	-0.9672050000	-2.6446390000	-0.3531230000
C	0.3722430000	-2.3228940000	-0.5194310000
C	1.2261180000	-2.4552590000	0.5713910000
C	0.7510040000	-2.9139020000	1.7984580000
C	-0.5930410000	-3.2187310000	1.9755570000
C	-1.4447820000	-3.0817700000	0.8756980000
H	-1.4262110000	-0.1472090000	-0.1076860000
H	-4.8892440000	2.2634870000	-0.7715320000
H	-4.5762290000	-1.6191970000	-2.6083000000
H	0.7389200000	-1.9881990000	-1.4843220000

H	1.4730760000	-3.0191440000	2.5993610000
H	-2.5022990000	-3.3160120000	0.9614580000
C	2.3866230000	0.0084950000	-0.5942590000
C	2.9306210000	1.0035850000	-1.3950170000
C	3.1134830000	-1.1591270000	-0.4001400000
C	4.1726290000	0.8192000000	-1.9924970000
C	0.9672040000	2.6446280000	-0.3531790000
C	4.3658080000	-1.3392010000	-0.9824210000
C	4.9060730000	-0.3546550000	-1.7996500000
H	4.5762530000	1.6191440000	-2.6082900000
C	-0.3722430000	2.3228800000	-0.5194890000
C	1.4447720000	3.0817840000	0.8756370000
H	4.8892550000	-2.2634960000	-0.7714280000
C	-1.2261260000	2.4552720000	0.5713240000
H	-0.7389140000	1.9881640000	-1.4843740000
C	0.5930250000	3.2187670000	1.9754880000
H	2.5022890000	3.3160280000	0.9613990000
C	-0.7510200000	2.9139410000	1.7983840000
H	-1.4730980000	3.0192020000	2.5992800000
N	-2.6137220000	2.1819130000	0.4509470000
H	1.4262030000	0.1472050000	-0.1076890000
O	-3.4320890000	2.8614100000	1.1399130000
O	3.4320760000	-2.8613830000	1.1400090000
N	2.6137150000	-2.1819020000	0.4510190000
C	-1.1620740000	-3.6844140000	3.3122280000
C	-1.7991560000	-5.0662950000	3.1405280000
H	-2.2097620000	-5.4123220000	4.0963140000
H	-2.6161270000	-5.0565200000	2.4120120000
H	-1.0572070000	-5.7990830000	2.8038860000
C	-2.2235030000	-2.6834400000	3.7790610000
H	-2.6354330000	-2.9949000000	4.7461390000

H	-1.7907400000	-1.6836540000	3.8997410000
H	-3.0562260000	-2.6045690000	3.0731350000
C	-0.0918940000	-3.7834210000	4.3940070000
H	0.6898930000	-4.5053570000	4.1334650000
H	0.3830310000	-2.8153790000	4.5891320000
H	-0.5513680000	-4.1188180000	5.3301330000
C	-6.2646910000	0.5096250000	-2.4763050000
C	-6.9086900000	1.8594750000	-2.1758460000
H	-7.8709370000	1.9274120000	-2.6946690000
H	-7.1017820000	1.9928570000	-1.1057320000
H	-6.2874510000	2.6936340000	-2.5207290000
C	-6.0936880000	0.3924730000	-3.9936280000
H	-5.4218230000	1.1715360000	-4.3713660000
H	-5.6826980000	-0.5774350000	-4.2904630000
H	-7.0633690000	0.5087150000	-4.4919180000
C	-7.2078580000	-0.5896710000	-1.9785580000
H	-7.3390710000	-0.5271670000	-0.8924280000
H	-8.1932130000	-0.4814010000	-2.4471630000
H	-6.8358670000	-1.5916550000	-2.2149100000
C	1.1620460000	3.6844800000	3.3121530000
C	0.0918460000	3.7835520000	4.3939070000
H	-0.3831170000	2.8155320000	4.5890450000
H	0.5513120000	4.1189570000	5.3300340000
H	-0.6899100000	4.5055090000	4.1333290000
C	2.2234380000	2.6834930000	3.7790430000
H	3.0561790000	2.6045790000	3.0731440000
H	2.6353490000	2.9949710000	4.7461240000
H	1.7906470000	1.6837210000	3.8997410000
C	1.7991680000	5.0663370000	3.1404170000
H	2.6161510000	5.0565150000	2.4119150000
H	1.0572450000	5.7991350000	2.8037370000

H	2.2097680000	5.4123860000	4.0961980000
C	6.2647210000	-0.5096700000	-2.4762180000
C	6.9087180000	-1.8595120000	-2.1757160000
H	7.8709740000	-1.9274590000	-2.6945220000
H	7.1017920000	-1.9928680000	-1.1055970000
H	6.2874880000	-2.6936800000	-2.5205910000
C	7.2078770000	0.5896390000	-1.9784800000
H	7.3390710000	0.5271610000	-0.8923470000
H	8.1932410000	0.4813600000	-2.4470660000
H	6.8358880000	1.5916170000	-2.2148620000
C	6.0937430000	-0.3925530000	-3.9935460000
H	5.4218870000	-1.1716270000	-4.3712780000
H	5.6827540000	0.5773460000	-4.2904100000
H	7.0634330000	-0.5088030000	-4.4918180000
S	2.0768490000	2.5306300000	-1.7522030000
S	-2.0768420000	-2.5306730000	-1.7521580000

PBE0/6-311+G(d,p)

B-ECP1

C	-1.3721890000	-1.4262650000	-0.0236590000
C	-1.5290140000	-0.1530140000	-0.5845300000
C	-2.7836820000	0.4566340000	-0.6123270000
C	-3.8685230000	-0.1866170000	-0.0098240000
C	-3.7488160000	-1.4525370000	0.5619590000
C	-2.4998520000	-2.0698160000	0.5142720000
C	1.3722740000	-1.4262250000	0.0234340000
C	1.5290300000	-0.1530110000	0.5844080000
C	2.7836790000	0.4566670000	0.6123310000

C	3.8685770000	-0.1865100000	0.0098520000
C	3.7489410000	-1.4523910000	-0.5620330000
C	2.4999890000	-2.0697050000	-0.5144740000
H	-0.6619290000	0.3443920000	-0.9970150000
H	-4.8161690000	0.3383570000	-0.0164530000
H	-2.3719200000	-3.0698150000	0.9132530000
H	0.6619060000	0.3443480000	0.9968730000
H	4.8162100000	0.3384860000	0.0165820000
H	2.3721080000	-3.0696760000	-0.9135420000
C	2.2500540000	2.3171810000	2.3313990000
C	-2.2502510000	2.3173200000	-2.3312850000
N	-3.0197050000	1.7331810000	-1.1799530000
O	-3.9974820000	2.4001470000	-0.7246770000
O	3.9973330000	2.4002680000	0.7248480000
N	3.0196160000	1.7331780000	1.1800720000
H	0.0000750000	-3.3486080000	-0.0002280000
C	4.9809390000	-2.1068020000	-1.1896270000
C	4.6749670000	-3.4979570000	-1.7465670000
H	5.5825800000	-3.9219450000	-2.1865170000
H	4.3348230000	-4.1849810000	-0.9655520000
H	3.9128980000	-3.4640130000	-2.5311620000
C	6.0846570000	-2.2432270000	-0.1300530000
H	6.9722640000	-2.7109680000	-0.5685470000
H	6.3843750000	-1.2723000000	0.2730260000
H	5.7492410000	-2.8652410000	0.7053910000
C	5.4855470000	-1.2245940000	-2.3415510000
H	4.7186260000	-1.1151890000	-3.1143440000
H	5.7578610000	-0.2236750000	-1.9964630000
H	6.3716670000	-1.6742510000	-2.8019160000
C	-4.9807550000	-2.1070280000	1.1895860000
C	-6.0845230000	-2.2434440000	0.1300630000

H	-6.9720910000	-2.7112380000	0.5685810000
H	-6.3842960000	-1.2725090000	-0.2729560000
H	-5.7491280000	-2.8654060000	-0.7054270000
C	-4.6746980000	-3.4981980000	1.7464420000
H	-4.3345590000	-4.1851680000	0.9653780000
H	-3.9125970000	-3.4642590000	2.5310060000
H	-5.5822740000	-3.9222480000	2.1864110000
C	-5.4853370000	-1.2248970000	2.3415810000
H	-5.7577000000	-0.2239690000	1.9965580000
H	-6.3714190000	-1.6746080000	2.8019650000
H	-4.7183810000	-1.1155070000	3.1143420000
B	0.0000540000	-2.1461210000	-0.0001640000
C	-1.9394300000	1.2406520000	-3.3724150000
H	-1.4972940000	1.7205520000	-4.2496300000
H	-1.2397380000	0.4822500000	-3.0224310000
H	-2.8571200000	0.7374160000	-3.6891950000
C	-0.9813760000	2.9974280000	-1.8087510000
H	-0.4781620000	3.5134660000	-2.6316510000
H	-1.2405360000	3.7392540000	-1.0487920000
H	-0.2680470000	2.2943290000	-1.3752700000
C	-3.1442690000	3.3724620000	-2.9798220000
H	-2.6165140000	3.7864550000	-3.8431440000
H	-4.0853960000	2.9356850000	-3.3211280000
H	-3.3792010000	4.1796720000	-2.2867930000
C	0.9811650000	2.9972190000	1.8088160000
H	1.2403260000	3.7391550000	1.0489650000
H	0.2679640000	2.2940840000	1.3751780000
H	0.4778060000	3.5131080000	2.6317210000
C	3.1439510000	3.3723390000	2.9800830000
H	3.3788980000	4.1796040000	2.2871250000
H	2.6160940000	3.7862460000	3.8433840000

H	4.0850710000	2.9355950000	3.3214480000
C	1.9392280000	1.2404140000	3.3724230000
H	2.8569140000	0.7371510000	3.6891710000
H	1.4970780000	1.7202320000	4.2496750000
H	1.2395400000	0.4820410000	3.0223630000

B-ECP2

C	-1.2424850000	-2.7938120000	-0.6119950000
C	-1.7441630000	-1.5842520000	-0.1180780000
C	-2.9685710000	-1.1104120000	-0.5874260000
C	-3.6501340000	-1.7888640000	-1.5957100000
C	-3.1524380000	-2.9707040000	-2.1427420000
C	-1.9692910000	-3.4728910000	-1.6066850000
C	1.2430620000	-2.7936740000	0.6118530000
C	1.7445130000	-1.5839380000	0.1181420000
C	2.9688030000	-1.1099040000	0.5876290000
C	3.6504350000	-1.7883580000	1.5958650000
C	3.1529360000	-2.9703740000	2.1427010000
C	1.9699410000	-3.4727450000	1.6064920000
H	-1.2257180000	-1.0640680000	0.6805580000
H	-4.6015080000	-1.3778640000	-1.9121780000
H	-1.5826770000	-4.4257420000	-1.9508030000
H	1.2260000000	-1.0637520000	-0.6804480000
H	4.6016950000	-1.3772000000	1.9124680000
H	1.5835220000	-4.4257370000	1.9504450000
C	1.7441800000	1.5842470000	-0.1181010000
C	1.2424970000	2.7937950000	-0.6120380000
C	2.9685850000	1.1103980000	-0.5874480000
C	1.9692940000	3.4728540000	-1.6067480000
C	-1.2430510000	2.7936870000	0.6118100000
C	3.6501390000	1.7888300000	-1.5957510000
C	3.1524370000	2.9706570000	-2.1428040000

H	1.5826770000	4.4256990000	-1.9508810000
C	-1.7444970000	1.5839390000	0.1181220000
C	-1.9699390000	3.4727800000	1.6064270000
H	4.6015110000	1.3778250000	-1.9122180000
C	-2.9687900000	1.1099140000	0.5876110000
H	-1.2259760000	1.0637350000	-0.6804520000
C	-3.1529380000	2.9704200000	2.1426380000
H	-1.5835230000	4.4257790000	1.9503620000
C	-3.6504300000	1.7883910000	1.5958260000
H	-4.6016930000	1.3772400000	1.9124290000
N	-3.6295600000	-0.0003690000	0.0002140000
H	1.2257420000	1.0640790000	0.6805510000
O	-4.9001100000	-0.0006110000	0.0003990000
O	4.9001260000	0.0006050000	0.0003930000
N	3.6295760000	0.0003660000	0.0002110000
H	0.0005440000	-4.6886720000	-0.0003990000
C	3.9381180000	-3.6757220000	3.2481750000
C	3.2244220000	-4.9321890000	3.7497440000
H	3.8125630000	-5.3888020000	4.5512200000
H	2.2338930000	-4.7030230000	4.1548210000
H	3.1093380000	-5.6809100000	2.9601550000
C	4.1157640000	-2.7160490000	4.4343050000
H	4.6739100000	-3.2089150000	5.2370360000
H	4.6668070000	-1.8155010000	4.1501150000
H	3.1463000000	-2.4047840000	4.8349780000
C	5.3175220000	-4.0822370000	2.7081530000
H	5.2180030000	-4.7729440000	1.8654800000
H	5.8909850000	-3.2169670000	2.3653750000
H	5.8976450000	-4.5807000000	3.4918310000
C	-3.9376170000	-3.6761310000	-3.2481700000
C	-4.1160340000	-2.7163380000	-4.4340720000

H	-4.6742510000	-3.2093070000	-5.2366910000
H	-4.6673530000	-1.8160550000	-4.1495840000
H	-3.1468330000	-2.4046220000	-4.8350300000
C	-3.2235520000	-4.9322070000	-3.7502040000
H	-2.2331650000	-4.7025650000	-4.1553600000
H	-3.1080760000	-5.6811260000	-2.9608610000
H	-3.8116510000	-5.3888060000	-4.5517210000
C	-5.3166940000	-4.0833080000	-2.7077940000
H	-5.8903540000	-3.2183170000	-2.3646360000
H	-5.8968810000	-4.5818200000	-3.4913950000
H	-5.2166390000	-4.7741490000	-1.8652960000
C	-3.9381300000	3.6757940000	3.2480880000
C	-5.3175250000	4.0823040000	2.7080400000
H	-5.8909860000	3.2170290000	2.3652710000
H	-5.8976570000	4.5807830000	3.4917020000
H	-5.2179920000	4.7729950000	1.8653570000
C	-4.1157960000	2.7161450000	4.4342360000
H	-3.1463390000	2.4048820000	4.8349260000
H	-4.6739470000	3.2090300000	5.2369510000
H	-4.6668420000	1.8155950000	4.1500570000
C	-3.2244350000	4.9322680000	3.7496420000
H	-2.2339110000	4.7031060000	4.1547340000
H	-3.1093420000	5.6809750000	2.9600410000
H	-3.8125830000	5.3888970000	4.5511050000
C	3.9376070000	3.6760630000	-3.2482520000
C	4.1160110000	2.7162490000	-4.4341390000
H	4.6742200000	3.2092020000	-5.2367720000
H	4.6673330000	1.8159710000	-4.1496410000
H	3.1468060000	2.4045260000	-4.8350820000
C	5.3166890000	4.0832490000	-2.7078970000
H	5.8903510000	3.2182640000	-2.3647270000

H	5.8968700000	4.5817450000	-3.4915130000
H	5.2166430000	4.7741060000	-1.8654110000
C	3.2235370000	4.9321310000	-3.7503020000
H	2.2331460000	4.7024820000	-4.1554450000
H	3.1080680000	5.6810630000	-2.9609710000
H	3.8116300000	5.3887150000	-4.5518310000
H	-0.0005470000	4.6886700000	-0.0005150000
B	0.0003910000	-3.4858970000	-0.0002060000
B	-0.0003710000	3.4858940000	-0.0002480000
C-ECP1			
C	0.9209640000	0.8187270000	-1.2791900000
C	1.9348340000	-0.1265850000	-1.3464070000
C	3.0806950000	0.0132520000	-0.5507240000
C	3.1796890000	1.1059120000	0.3123010000
C	2.1751030000	2.0697920000	0.3878960000
C	1.0490370000	1.9113910000	-0.4179360000
C	-1.5589320000	0.2539590000	-1.2941020000
C	-1.4311500000	-0.5103710000	-0.1428590000
C	-2.5706820000	-0.9078500000	0.5647850000
C	-3.8330100000	-0.5429110000	0.0900810000
C	-3.9803290000	0.2256950000	-1.0619380000
C	-2.8282940000	0.6225580000	-1.7418700000
H	1.8049630000	-0.9745840000	-2.0038530000
H	4.0715710000	1.1749750000	0.9215200000
H	0.2414490000	2.6338630000	-0.3815250000
H	-0.4399100000	-0.7918680000	0.1791380000
H	-4.6913180000	-0.8780080000	0.6578180000
H	-2.9035520000	1.2267250000	-2.6392480000
C	-1.3113970000	-1.8650930000	2.6179200000
C	4.4385700000	-1.9156720000	-1.6252990000
N	4.1462950000	-0.9183810000	-0.5385480000

O	4.9400460000	-0.8834960000	0.4489030000
O	-3.5940350000	-2.2616030000	2.1081940000
N	-2.5226530000	-1.6919410000	1.7419690000
H	-0.5533220000	1.5869630000	-2.6228070000
C	-5.3868260000	0.6086150000	-1.5279430000
C	-5.3680530000	1.4518770000	-2.8037580000
H	-6.3945100000	1.6959370000	-3.0933110000
H	-4.8328980000	2.3958800000	-2.6611680000
H	-4.9083030000	0.9163360000	-3.6401590000
C	-6.0847240000	1.4199390000	-0.4258470000
H	-7.0959160000	1.6963260000	-0.7431090000
H	-6.1687920000	0.8512220000	0.5037330000
H	-5.5322260000	2.3392610000	-0.2085760000
C	-6.1916800000	-0.6696350000	-1.8069430000
H	-5.7170860000	-1.2648890000	-2.5929310000
H	-6.2752730000	-1.2975980000	-0.9164820000
H	-7.2047840000	-0.4147240000	-2.1359910000
C	2.3477190000	3.2547350000	1.3407940000
C	3.6121980000	4.0368420000	0.9548760000
H	3.7477600000	4.8895780000	1.6283920000
H	4.5086490000	3.4146670000	1.0174060000
H	3.5382250000	4.4186630000	-0.0679200000
C	1.1570520000	4.2134650000	1.2944260000
H	1.0195270000	4.6448080000	0.2980830000
H	0.2250780000	3.7214880000	1.5893210000
H	1.3279830000	5.0399730000	1.9905480000
C	2.4902510000	2.7330940000	2.7786710000
H	3.3513610000	2.0685600000	2.8867320000
H	2.6227600000	3.5707160000	3.4716270000
H	1.5970990000	2.1784480000	3.0824640000
C	-0.3347510000	0.6517210000	-2.0956620000

H	-0.1629720000	-0.1005420000	-2.8754550000
C	-1.7895930000	-2.4711680000	3.9352290000
H	-2.2392700000	-3.4527280000	3.7865150000
H	-0.9246180000	-2.5723150000	4.5963890000
H	-2.5298950000	-1.8321850000	4.4202990000
C	-0.3318600000	-2.8451260000	1.9627730000
H	0.1063500000	-2.4675930000	1.0383940000
H	0.4876710000	-3.0531240000	2.6567440000
H	-0.8392460000	-3.7879440000	1.7417580000
C	-0.6690980000	-0.5087750000	2.9198610000
H	-0.2534080000	-0.0113360000	2.0441960000
H	-1.4018800000	0.1613530000	3.3780270000
H	0.1459210000	-0.6582200000	3.6335160000
C	4.4054390000	-1.2370010000	-2.9965820000
H	3.4265710000	-0.8444890000	-3.2696430000
H	5.1210020000	-0.4108560000	-3.0268850000
H	4.6981550000	-1.9655280000	-3.7577950000
C	3.4611180000	-3.0921620000	-1.5270240000
H	3.7552940000	-3.8669610000	-2.2409270000
H	3.4974770000	-3.5243260000	-0.5235770000
H	2.4275150000	-2.8186760000	-1.7421780000
C	5.8516500000	-2.4434990000	-1.3885210000
H	6.0925090000	-3.1440360000	-2.1928210000
H	6.5839050000	-1.6340700000	-1.3964480000
H	5.9331670000	-2.9604550000	-0.4325780000
C-ECP2			
C	-2.8164980000	-1.1265280000	-1.3333010000
C	-2.3260670000	-0.0465270000	-0.6143600000
C	-3.0941060000	1.1144240000	-0.5092500000
C	-4.3537050000	1.1892440000	-1.0916060000
C	-4.8662560000	0.1113310000	-1.8140010000

C	-4.0795520000	-1.0348490000	-1.9264090000
C	-0.9833090000	-2.6532500000	-0.4330080000
C	0.3466810000	-2.3005890000	-0.6134830000
C	1.2657160000	-2.5362720000	0.4113580000
C	0.8648580000	-3.1456790000	1.5936610000
C	-0.4687270000	-3.5053040000	1.7949580000
C	-1.3779480000	-3.2442820000	0.7709630000
H	-1.3694690000	-0.1155960000	-0.1108390000
H	-4.9188240000	2.1028420000	-0.9526430000
H	-4.4484010000	-1.8916400000	-2.4799170000
H	0.6743480000	-1.8646770000	-1.5510730000
H	1.6234040000	-3.3348100000	2.3436730000
H	-2.4231950000	-3.5055260000	0.8929590000
C	2.3260930000	0.0465520000	-0.6143080000
C	2.8165310000	1.1265380000	-1.3332670000
C	3.0941210000	-1.1144050000	-0.5091860000
C	4.0795820000	1.0348360000	-1.9263810000
C	0.9833330000	2.6532690000	-0.4330080000
C	4.3537150000	-1.1892480000	-1.0915450000
C	4.8662740000	-0.1113500000	-1.8139600000
H	4.4484360000	1.8916150000	-2.4799030000
C	-0.3466550000	2.3006160000	-0.6135150000
C	1.3779470000	3.2442920000	0.7709750000
H	4.9188270000	-2.1028490000	-0.9525700000
C	-1.2657110000	2.5362970000	0.4113060000
H	-0.6743030000	1.8647100000	-1.5511150000
C	0.4687050000	3.5053120000	1.7949520000
H	2.4231930000	3.5055300000	0.8929960000
C	-0.8648770000	3.1456940000	1.5936220000
H	-1.6234400000	3.3348250000	2.3436190000
N	-2.6419540000	2.2240470000	0.2516560000

H	1.3694990000	0.1156360000	-0.1107830000
O	-3.5014620000	2.9626360000	0.8232650000
O	3.5014620000	-2.9625740000	0.8233940000
N	2.6419590000	-2.2240110000	0.2517420000
H	2.6835370000	3.2421450000	-1.5853400000
H	-2.6834780000	-3.2421320000	-1.5853880000
C	-0.8758490000	-4.1599990000	3.1157370000
C	-2.3712610000	-4.4759640000	3.1694500000
H	-2.6114740000	-4.9373910000	4.1318330000
H	-2.9826830000	-3.5732960000	3.0749830000
H	-2.6678120000	-5.1785700000	2.3845320000
C	-0.5422360000	-3.2092840000	4.2754940000
H	-0.8235510000	-3.6666780000	5.2298300000
H	0.5255470000	-2.9789560000	4.3170600000
H	-1.0865170000	-2.2652490000	4.1762580000
C	-0.0967440000	-5.4723470000	3.2910610000
H	-0.3196260000	-6.1704530000	2.4785760000
H	0.9835810000	-5.3059190000	3.3017450000
H	-0.3722530000	-5.9503960000	4.2369650000
C	-6.2527210000	0.2290580000	-2.4490560000
C	-6.2454220000	1.3836110000	-3.4628400000
H	-7.2324310000	1.4861620000	-3.9261590000
H	-5.9972650000	2.3368640000	-2.9888290000
H	-5.5136780000	1.2025550000	-4.2561490000
C	-6.6689630000	-1.0485860000	-3.1792950000
H	-5.9856070000	-1.2923240000	-3.9986240000
H	-6.7183510000	-1.9072600000	-2.5025070000
H	-7.6646770000	-0.9123920000	-3.6115300000
C	-7.2908310000	0.5178340000	-1.3543650000
H	-7.0752180000	1.4480610000	-0.8227620000
H	-8.2885990000	0.6078960000	-1.7965040000

H	-7.3155020000	-0.2904540000	-0.6174180000
C	0.8758000000	4.1599980000	3.1157430000
C	0.0966950000	5.4723470000	3.2910580000
H	-0.9836310000	5.3059220000	3.3017190000
H	0.3721850000	5.9503900000	4.2369700000
H	0.3195950000	6.1704570000	2.4785810000
C	0.5421600000	3.2092780000	4.2754870000
H	1.0864400000	2.2652410000	4.1762580000
H	0.8234570000	3.6666650000	5.2298320000
H	-0.5256240000	2.9789530000	4.3170300000
C	2.3712120000	4.4759590000	3.1694900000
H	2.9826330000	3.5732900000	3.0750290000
H	2.6677820000	5.1785700000	2.3845830000
H	2.6114050000	4.9373780000	4.1318810000
C	6.2527360000	-0.2291000000	-2.4490170000
C	6.2454230000	-1.3836620000	-3.4627890000
H	7.2324300000	-1.4862300000	-3.9261080000
H	5.9972560000	-2.3369080000	-2.9887690000
H	5.5136800000	-1.2026070000	-4.2560990000
C	7.2908450000	-0.5178760000	-1.3543250000
H	7.0752210000	-1.4480940000	-0.8227100000
H	8.2886110000	-0.6079560000	-1.7964640000
H	7.3155280000	0.2904210000	-0.6173870000
C	6.6689900000	1.0485330000	-3.1792700000
H	5.9856320000	1.2922720000	-3.9985970000
H	6.7183950000	1.9072120000	-2.5024910000
H	7.6647000000	0.9123210000	-3.6115110000
C	-1.9983320000	-2.3908670000	-1.5143800000
C	1.9983810000	2.3908860000	-1.5143560000
H	-1.4844020000	-2.3343680000	-2.4820060000
H	1.4844760000	2.3343990000	-2.4819970000

N-ECP1

C	-1.2071290000	-1.3457860000	-0.0192700000
C	-1.4111300000	-0.0036580000	0.2980600000
C	-2.6892060000	0.5326970000	0.1845380000
C	-3.7580760000	-0.2410680000	-0.2500780000
C	-3.5749150000	-1.5922710000	-0.5530810000
C	-2.2959160000	-2.1259290000	-0.4335070000
C	1.3010960000	-1.3665540000	0.0014180000
C	1.5252230000	-0.2092510000	-0.7412460000
C	2.8196780000	0.2944290000	-0.8343200000
C	3.8895700000	-0.3643180000	-0.2396560000
C	3.6831200000	-1.5356350000	0.4922970000
C	2.3822130000	-2.0119530000	0.6171990000
H	-0.5868690000	0.6148690000	0.6231690000
H	-4.7227140000	0.2392660000	-0.3596750000
H	-2.1119240000	-3.1653140000	-0.6829680000
H	0.7165640000	0.2533100000	-1.2902400000
H	4.8806660000	0.0493820000	-0.3800920000
H	2.1781160000	-2.9057340000	1.1963360000
C	2.6204620000	2.8328470000	-1.3054670000
C	-2.9021230000	2.4904510000	1.8492010000
N	-2.9229640000	1.9198320000	0.4597990000
O	-3.6496650000	2.5408880000	-0.3779850000
O	4.1404290000	1.3902470000	-2.3591300000
N	3.0999060000	1.4471280000	-1.6325170000
N	0.0391660000	-1.9516690000	0.1011460000
H	0.0300210000	-2.9541050000	0.1898460000
C	4.8797780000	-2.2404600000	1.1335780000
C	4.4715700000	-3.4887650000	1.9170470000
H	5.3617930000	-3.9516330000	2.3530230000
H	3.7886990000	-3.2502960000	2.7386080000

H	3.9945280000	-4.2356990000	1.2749300000
C	5.5821620000	-1.2750490000	2.1001760000
H	6.4453100000	-1.7655500000	2.5623940000
H	5.9419330000	-0.3791870000	1.5878220000
H	4.9033770000	-0.9570590000	2.8974620000
C	5.8616350000	-2.6618310000	0.0297780000
H	5.3860540000	-3.3539330000	-0.6715550000
H	6.2207190000	-1.8030020000	-0.5427620000
H	6.7313760000	-3.1628700000	0.4680100000
C	-4.7681530000	-2.4236760000	-1.0276010000
C	-5.3016370000	-1.8297480000	-2.3401220000
H	-6.1614870000	-2.4086640000	-2.6933620000
H	-5.6222940000	-0.7924540000	-2.2147320000
H	-4.5327680000	-1.8499930000	-3.1180880000
C	-4.3989270000	-3.8869490000	-1.2762290000
H	-3.6452300000	-3.9909240000	-2.0628360000
H	-4.0245460000	-4.3727870000	-0.3695650000
H	-5.2878460000	-4.4359980000	-1.6007110000
C	-5.8742970000	-2.3826560000	0.0373360000
H	-6.2208260000	-1.3628810000	0.2232540000
H	-6.7357210000	-2.9732450000	-0.2918520000
H	-5.5199700000	-2.7961990000	0.9864840000
C	1.3362890000	2.8322970000	-0.4872390000
H	0.4889890000	2.4217090000	-1.0408450000
H	1.4503440000	2.2846910000	0.4515670000
H	1.0930630000	3.8700610000	-0.2427590000
C	2.3967040000	3.5547350000	-2.6309540000
H	2.1172390000	4.5945940000	-2.4410420000
H	3.3056610000	3.5364230000	-3.2334940000
H	1.5924220000	3.0798590000	-3.1998510000
C	3.7388780000	3.5067030000	-0.5048650000

H	4.6701400000	3.4913730000	-1.0745480000
H	3.4726570000	4.5458490000	-0.2916850000
H	3.9000410000	2.9919550000	0.4474650000
C	-1.8828870000	1.7956160000	2.7424840000
H	-2.0713910000	0.7237820000	2.8318440000
H	-0.8598820000	1.9454480000	2.3882490000
H	-1.9525810000	2.2335310000	3.7420520000
C	-4.3091990000	2.3103290000	2.4258210000
H	-4.3697770000	2.7658710000	3.4183000000
H	-5.0446280000	2.7883920000	1.7749320000
H	-4.5586350000	1.2491430000	2.5210570000
C	-2.5590230000	3.9712340000	1.7214370000
H	-2.5870720000	4.4396650000	2.7091180000
H	-1.5556190000	4.1009780000	1.3055200000
H	-3.2713630000	4.4765860000	1.0687270000

N-ECP2

C	0.3229260000	2.9599680000	0.1171900000
C	-0.7682060000	2.1401400000	-0.1493890000
C	-1.9046840000	2.2594000000	0.6506840000
C	-1.9511730000	3.1809390000	1.6957290000
C	-0.8607770000	4.0022670000	1.9708920000
C	0.2759350000	3.8744990000	1.1730100000
C	2.2977150000	1.8499600000	-0.9175330000
C	2.1693310000	0.6605650000	-0.2051420000
C	3.1144470000	-0.3426450000	-0.4133040000
C	4.1667400000	-0.1845920000	-1.3032290000
C	4.2922150000	0.9978920000	-2.0365130000
C	3.3475360000	1.9966990000	-1.8378320000
H	-0.7513780000	1.4761790000	-1.0048160000
H	-2.8698240000	3.2452140000	2.2645530000
H	1.1529090000	4.4838090000	1.3594110000

H	1.3930070000	0.5421610000	0.5407990000
H	4.8812480000	-0.9927360000	-1.3946260000
H	3.4050420000	2.9259390000	-2.3942220000
C	0.7682310000	-2.1401740000	-0.1489350000
C	-0.3229480000	-2.9599580000	0.1175850000
C	1.9045690000	-2.2593080000	0.6513540000
C	-0.2761420000	-3.8743210000	1.1735590000
C	-2.2975550000	-1.8501080000	-0.9176520000
C	1.9508760000	-3.1806800000	1.6965550000
C	0.8604300000	-4.0019610000	1.9716600000
H	-1.1531470000	-4.4836030000	1.3599050000
C	-2.1692960000	-0.6606080000	-0.2054140000
C	-3.3472120000	-1.9969810000	-1.8381160000
H	2.8694290000	-3.2448660000	2.2655460000
C	-3.1143740000	0.3425730000	-0.4138890000
H	-1.3931030000	-0.5420930000	0.5406460000
C	-4.2918560000	-0.9982030000	-2.0371100000
H	-3.4046190000	-2.9263020000	-2.3943810000
C	-4.1665100000	0.1843880000	-1.3039760000
H	-4.8810030000	0.9925190000	-1.3956190000
N	-3.0874740000	1.5372500000	0.3627290000
H	0.7515520000	-1.4763490000	-1.0044700000
O	-4.1978910000	2.0069340000	0.7594010000
O	4.1977590000	-2.0068340000	0.7604210000
N	3.0874110000	-1.5372060000	0.3634880000
N	1.4455630000	2.9374270000	-0.7298990000
N	-1.4454380000	-2.9375480000	-0.7297040000
H	-1.8965720000	-3.8317370000	-0.8421150000
H	1.8967160000	3.8316000000	-0.8423690000
C	5.4481140000	1.1456980000	-3.0266660000
C	5.4294030000	2.4943780000	-3.7471090000

H	6.2716750000	2.5473720000	-4.4432320000
H	4.5124590000	2.6337050000	-4.3282100000
H	5.5277030000	3.3308910000	-3.0481680000
C	5.3540770000	0.0336230000	-4.0819920000
H	6.1778290000	0.1220630000	-4.7981740000
H	5.4090230000	-0.9597470000	-3.6295940000
H	4.4122150000	0.0991600000	-4.6351010000
C	6.7786310000	1.0203380000	-2.2690490000
H	6.8715580000	1.8036350000	-1.5108130000
H	6.8690940000	0.0552120000	-1.7643310000
H	7.6188820000	1.1165910000	-2.9647500000
C	-0.9411250000	4.9932230000	3.1329580000
C	-1.1745400000	4.2193250000	4.4394010000
H	-1.2394500000	4.9147530000	5.2827870000
H	-2.1026260000	3.6429020000	4.4077380000
H	-0.3527910000	3.5233680000	4.6334850000
C	0.3390860000	5.8162870000	3.2841610000
H	1.2094530000	5.1846910000	3.4875270000
H	0.5461200000	6.4156620000	2.3920020000
H	0.2308830000	6.5068760000	4.1256570000
C	-2.1114810000	5.9594080000	2.8955050000
H	-3.0658200000	5.4319400000	2.8217380000
H	-2.1845310000	6.6722110000	3.7235430000
H	-1.9695060000	6.5253070000	1.9698510000
C	-5.4475810000	-1.1461560000	-3.0274430000
C	-6.7782290000	-1.0207140000	-2.2700690000
H	-6.8687830000	-0.0555290000	-1.7654810000
H	-7.6183610000	-1.1170530000	-2.9659030000
H	-6.8712830000	-1.8039220000	-1.5117560000
C	-5.3533810000	-0.0342190000	-4.0828990000
H	-4.4114250000	-0.0998180000	-4.6358410000

H	-6.1770110000	-0.1227650000	-4.7992080000
H	-5.4084160000	0.9592100000	-3.6306430000
C	-5.4287260000	-2.4949320000	-3.7477050000
H	-4.5116800000	-2.6343190000	-4.3286290000
H	-5.5271320000	-3.3313550000	-3.0486710000
H	-6.2708780000	-2.5480320000	-4.4439650000
C	0.9405750000	-4.9927320000	3.1338990000
C	1.1737540000	-4.2186250000	4.4402600000
H	1.2385160000	-4.9139210000	5.2837670000
H	2.1018430000	-3.6422040000	4.4086720000
H	0.3519670000	-3.5226420000	4.6340880000
C	2.1109760000	-5.9589520000	2.8968100000
H	3.0653290000	-5.4314960000	2.8231410000
H	2.1838690000	-6.6716280000	3.7249710000
H	1.9691740000	-6.5249920000	1.9712150000
C	-0.3396610000	-5.8157760000	3.2850060000
H	-1.2100650000	-5.1841500000	3.4881160000
H	-0.5465360000	-6.4152950000	2.3929080000
H	-0.2316040000	-6.5062270000	4.1266340000

O-ECP1

C	-1.0937130000	-1.3913000000	0.0965400000
C	-1.2887640000	-0.1443200000	0.6712840000
C	-2.5324530000	0.4626310000	0.5210980000
C	-3.5437090000	-0.1602000000	-0.2028530000
C	-3.3510930000	-1.4213620000	-0.7698720000
C	-2.1079420000	-2.0310540000	-0.6070910000
C	1.2780040000	-1.4044040000	0.0900300000
C	1.4465670000	-0.4391360000	-0.8907640000
C	2.7041640000	0.1436520000	-1.0326340000
C	3.7681290000	-0.2678340000	-0.2355010000
C	3.5995310000	-1.2505730000	0.7411310000

C	2.3324850000	-1.8084740000	0.9017120000
H	-0.4811510000	0.3480550000	1.1963290000
H	-4.4789950000	0.3741480000	-0.3208750000
H	-1.8892270000	-3.0050090000	-1.0265270000
H	0.6282710000	-0.1807030000	-1.5484910000
H	4.7339600000	0.1887470000	-0.4144750000
H	2.1334550000	-2.5746650000	1.6402680000
C	2.3266650000	2.4664650000	-2.1108480000
C	-2.8995610000	2.0495410000	2.5184290000
N	-2.7802170000	1.7713110000	1.0464800000
O	-3.4127710000	2.5673560000	0.2838980000
O	4.0923670000	1.0123110000	-2.6348050000
N	2.9646410000	1.1049820000	-2.0572650000
C	4.7960190000	-1.6799160000	1.5910680000
C	4.4182680000	-2.7396940000	2.6271670000
H	5.3030220000	-3.0112170000	3.2106730000
H	3.6608770000	-2.3740540000	3.3276730000
H	4.0415490000	-3.6530130000	2.1567730000
C	5.3606630000	-0.4596270000	2.3334460000
H	6.2186550000	-0.7557180000	2.9460170000
H	5.6963810000	0.3171580000	1.6416200000
H	4.6067640000	-0.0198530000	2.9936840000
C	5.8783490000	-2.2651390000	0.6713160000
H	5.5006010000	-3.1389860000	0.1322940000
H	6.2183700000	-1.5372820000	-0.0699750000
H	6.7465020000	-2.5767990000	1.2615700000
C	-4.4905740000	-2.0817360000	-1.5470670000
C	-4.8890580000	-1.1804320000	-2.7251600000
H	-5.7126010000	-1.6363290000	-3.2843700000
H	-5.2170010000	-0.1931980000	-2.3899970000
H	-4.0481260000	-1.0390590000	-3.4105460000

C	-4.0949850000	-3.4514430000	-2.1003690000
H	-3.2535850000	-3.3815220000	-2.7965170000
H	-3.8268660000	-4.1521220000	-1.3037080000
H	-4.9394580000	-3.8812350000	-2.6470330000
C	-5.6975140000	-2.2669000000	-0.6147560000
H	-6.0547720000	-1.3124680000	-0.2191280000
H	-6.5249460000	-2.7345030000	-1.1586050000
H	-5.4416840000	-2.9084940000	0.2339880000
C	0.9082880000	2.4789230000	-1.5572800000
H	0.2251170000	1.8688060000	-2.1527820000
H	0.8622230000	2.1484880000	-0.5176640000
H	0.5389300000	3.5072040000	-1.5942490000
C	2.3137830000	2.8960550000	-3.5747570000
H	1.9112880000	3.9095230000	-3.6530590000
H	3.3216620000	2.8811040000	-3.9901480000
H	1.6837930000	2.2278420000	-4.1686390000
C	3.2160120000	3.3984220000	-1.2826300000
H	4.2380080000	3.3823060000	-1.6674860000
H	2.8365080000	4.4227420000	-1.3351330000
H	3.2303070000	3.0925980000	-0.2318730000
C	-1.9656380000	1.1783070000	3.3482680000
H	-2.1555740000	0.1122150000	3.2074770000
H	-0.9143740000	1.3827850000	3.1297730000
H	-2.1331440000	1.4110290000	4.4034240000
C	-4.3545320000	1.7714360000	2.9063730000
H	-4.5144380000	2.0135560000	3.9608050000
H	-5.0272570000	2.3824900000	2.3004010000
H	-4.6044090000	0.7166080000	2.7569110000
C	-2.5594700000	3.5216730000	2.7269550000
H	-2.6882700000	3.7792570000	3.7817420000
H	-1.5217220000	3.7230350000	2.4462010000

H	-3.2095770000	4.1572170000	2.1252490000
O	0.0882070000	-2.0741780000	0.2464680000
O-ECP2			
C	-2.6303340000	-1.2621010000	-0.9351390000
C	-2.2548870000	-0.1440470000	-0.2022850000
C	-2.9241030000	1.0505670000	-0.4552890000
C	-3.9466420000	1.1358380000	-1.3945380000
C	-4.3091410000	0.0130050000	-2.1357730000
C	-3.6325540000	-1.1831790000	-1.8962180000
C	-1.0392970000	-2.6930530000	0.1192740000
C	0.2290050000	-2.2434460000	-0.2200120000
C	1.2834150000	-2.5755000000	0.6266600000
C	1.0727950000	-3.3466540000	1.7722620000
C	-0.2019820000	-3.7844830000	2.1097360000
C	-1.2638530000	-3.4402210000	1.2635900000
H	-1.4957590000	-0.2049010000	0.5672120000
H	-4.4397970000	2.0901250000	-1.5186150000
H	-3.8776190000	-2.0897900000	-2.4379500000
H	0.3896600000	-1.6921150000	-1.1384820000
H	1.9392260000	-3.5940340000	2.3700410000
H	-2.2786460000	-3.7632100000	1.4667990000
C	2.2548930000	0.1440380000	-0.2022570000
C	2.6303490000	1.2620790000	-0.9351260000
C	2.9241120000	-1.0505800000	-0.4552300000
C	3.6325820000	1.1831380000	-1.8961910000
C	1.0392980000	2.6930530000	0.1192360000
C	3.9466640000	-1.1358690000	-1.3944640000
C	4.3091710000	-0.0130500000	-2.1357150000
H	3.8776540000	2.0897400000	-2.4379370000
C	-0.2289990000	2.2434370000	-0.2200560000
C	1.2638370000	3.4402480000	1.2635390000

H	4.4398200000	-2.0901580000	-1.5185160000
C	-1.2834210000	2.5755080000	0.6265930000
H	-0.3896400000	1.6920840000	-1.1385160000
C	0.2019540000	3.7845280000	2.1096610000
H	2.2786270000	3.7632430000	1.4667540000
C	-1.0728180000	3.3466900000	1.7721800000
H	-1.9392570000	3.5940830000	2.3699410000
N	-2.6134430000	2.2129160000	0.3038720000
H	1.4957540000	0.2049070000	0.5672300000
O	-3.5643980000	2.9651940000	0.6772740000
O	3.5643920000	-2.9651870000	0.6773780000
N	2.6134420000	-2.2129150000	0.3039490000
C	-0.4741170000	-4.6251680000	3.3570710000
C	-1.0787600000	-5.9726710000	2.9341990000
H	-1.2788970000	-6.5881470000	3.8172910000
H	-2.0212460000	-5.8449000000	2.3951500000
H	-0.3914640000	-6.5221330000	2.2842070000
C	-1.4663510000	-3.8809230000	4.2633310000
H	-1.6739750000	-4.4735180000	5.1602540000
H	-1.0593380000	-2.9158150000	4.5796440000
H	-2.4184950000	-3.6945760000	3.7592960000
C	0.8003230000	-4.8980740000	4.1567380000
H	1.5385290000	-5.4527960000	3.5699760000
H	1.2659560000	-3.9727920000	4.5091340000
H	0.5562880000	-5.5010570000	5.0362740000
C	-5.4135900000	0.0531100000	-3.1926680000
C	-6.0380110000	1.4432650000	-3.3212150000
H	-6.8200300000	1.4212940000	-4.0859060000
H	-6.4996030000	1.7714440000	-2.3851930000
H	-5.3016400000	2.1939280000	-3.6238500000
C	-4.8258960000	-0.3409120000	-4.5558950000

H	-4.0349930000	0.3530870000	-4.8559050000
H	-4.4011960000	-1.3482250000	-4.5407550000
H	-5.6073070000	-0.3189100000	-5.3226250000
C	-6.5199550000	-0.9399190000	-2.8059070000
H	-6.9547100000	-0.6814940000	-1.8358370000
H	-7.3192850000	-0.9217650000	-3.5539690000
H	-6.1436620000	-1.9644990000	-2.7431960000
C	0.4740710000	4.6252440000	3.3569810000
C	-0.8003810000	4.8981700000	4.1566210000
H	-1.2660220000	3.9728970000	4.5090310000
H	-0.5563600000	5.5011720000	5.0361470000
H	-1.5385780000	5.4528800000	3.5698350000
C	1.4662900000	3.8810210000	4.2632730000
H	2.4184410000	3.6946600000	3.7592570000
H	1.6739010000	4.4736380000	5.1601850000
H	1.0592710000	2.9159210000	4.5796050000
C	1.0787210000	5.9727360000	2.9340840000
H	2.0212130000	5.8449510000	2.3950510000
H	0.3914330000	6.5221840000	2.2840690000
H	1.2788460000	6.5882330000	3.8171640000
C	5.4136300000	-0.0531750000	-3.1925990000
C	6.0380590000	-1.4433310000	-3.3211080000
H	6.8200840000	-1.4213740000	-4.0857920000
H	6.4996440000	-1.7714850000	-2.3850740000
H	5.3016940000	-2.1940040000	-3.6237320000
C	6.5199870000	0.9398690000	-2.8058580000
H	6.9547400000	0.6814700000	-1.8357800000
H	7.3193210000	0.9217010000	-3.5539150000
H	6.1436900000	1.9644480000	-2.7431730000
C	4.8259420000	0.3408100000	-4.5558400000
H	4.0350440000	-0.3532010000	-4.8558360000

H	4.4012370000	1.3481210000	-4.5407280000
H	5.6073580000	0.3187920000	-5.3225660000
O	-2.0977320000	-2.5063740000	-0.7432140000
O	2.0977460000	2.5063560000	-0.7432310000
S-ECP1			
C	-1.3826970000	-0.2607120000	-1.5319160000
C	-1.2310070000	-0.6647030000	-0.2112260000
C	-2.3149360000	-0.5503480000	0.6534050000
C	-3.5272550000	-0.0346330000	0.2068520000
C	-3.6962050000	0.3565840000	-1.1218810000
C	-2.6054800000	0.2395560000	-1.9829480000
C	1.3808810000	-0.1269160000	-1.7157660000
C	1.5350930000	1.0672160000	-1.0202990000
C	2.6905500000	1.2616750000	-0.2690350000
C	3.7010940000	0.3006330000	-0.2792340000
C	3.5691380000	-0.8873930000	-0.9956070000
C	2.3815420000	-1.0972080000	-1.7004330000
H	-0.2761120000	-1.0295570000	0.1437840000
H	-4.3271780000	0.0690110000	0.9305360000
H	-2.6831360000	0.5591500000	-3.0152130000
H	0.7768680000	1.8348810000	-1.0895250000
H	4.6017940000	0.5216110000	0.2814230000
H	2.2176550000	-2.0136700000	-2.2533640000
C	2.0819690000	2.9482280000	1.5958820000
C	-2.0483190000	-2.3053430000	2.5227250000
N	-2.1906770000	-0.8898750000	2.0389110000
O	-2.7190500000	-0.0773690000	2.8613910000
O	4.1286420000	2.8940440000	0.4444990000
N	2.9293730000	2.4755450000	0.4444930000
C	4.7054000000	-1.9116690000	-0.9776010000
C	4.3814360000	-3.1492490000	-1.8153150000

H	5.2245050000	-3.8452610000	-1.7771970000
H	3.5002250000	-3.6781940000	-1.4392080000
H	4.2101960000	-2.8962170000	-2.8659900000
C	4.9652710000	-2.3601560000	0.4682770000
H	5.7800170000	-3.0911700000	0.4952920000
H	5.2482170000	-1.5208850000	1.1089230000
H	4.0744810000	-2.8278020000	0.8989500000
C	5.9755300000	-1.2607370000	-1.5465030000
H	5.8191180000	-0.9373150000	-2.5798250000
H	6.2797450000	-0.3862550000	-0.9656600000
H	6.8034820000	-1.9772990000	-1.5341800000
C	-5.0454880000	0.9151550000	-1.5774030000
C	-5.3690090000	2.1787990000	-0.7661640000
H	-6.3377950000	2.5856400000	-1.0742810000
H	-5.4170690000	1.9727260000	0.3062290000
H	-4.6091910000	2.9497220000	-0.9250620000
C	-5.0508900000	1.2806030000	-3.0625430000
H	-4.3181010000	2.0595360000	-3.2945020000
H	-4.8458300000	0.4131840000	-3.6975520000
H	-6.0369740000	1.6653850000	-3.3388050000
C	-6.1359580000	-0.1397840000	-1.3362580000
H	-6.2139360000	-0.4088090000	-0.2795200000
H	-7.1098360000	0.2453590000	-1.6558060000
H	-5.9284110000	-1.0530780000	-1.9020780000
C	0.6095500000	2.5953930000	1.4340870000
H	0.1597330000	3.0977160000	0.5740300000
H	0.4372290000	1.5209630000	1.3479010000
H	0.0791700000	2.9389250000	2.3259870000
C	2.2424960000	4.4632030000	1.6749450000
H	1.6810890000	4.8416480000	2.5332860000
H	3.2915530000	4.7372420000	1.7871390000

H	1.8546430000	4.9411680000	0.7709530000
C	2.6424270000	2.2793410000	2.8542010000
H	3.7007170000	2.5233990000	2.9711820000
H	2.1008420000	2.6304220000	3.7369130000
H	2.5347160000	1.1916860000	2.8000020000
C	-1.2380180000	-3.1645840000	1.5608630000
H	-1.6860740000	-3.2126460000	0.5661910000
H	-0.2073830000	-2.8130820000	1.4678710000
H	-1.2036490000	-4.1814420000	1.9614590000
C	-3.4640680000	-2.8715560000	2.6623440000
H	-3.4242040000	-3.8861190000	3.0688870000
H	-4.0535970000	-2.2468020000	3.3370790000
H	-3.9653120000	-2.9124240000	1.6905050000
C	-1.3547490000	-2.2488700000	3.8801190000
H	-1.2813640000	-3.2581680000	4.2938570000
H	-0.3442690000	-1.8415930000	3.7829790000
H	-1.9147930000	-1.6211830000	4.5736540000
S	-0.0643240000	-0.4005400000	-2.7199750000

S-ECP2

C	-2.9107330000	-1.0375000000	-1.3446040000
C	-2.3920910000	-0.0416500000	-0.5242310000
C	-3.1213020000	1.1309270000	-0.3627870000
C	-4.3535870000	1.3142120000	-0.9879190000
C	-4.8717850000	0.3250670000	-1.8173550000
C	-4.1337980000	-0.8509720000	-1.9846740000
C	-0.9318290000	-2.6937070000	-0.2920080000
C	0.3952400000	-2.3087450000	-0.4544480000
C	1.2738810000	-2.4855850000	0.6128050000
C	0.8365570000	-3.0565430000	1.8096010000
C	-0.4893880000	-3.4398060000	1.9782620000
C	-1.3694750000	-3.2491710000	0.9066030000

H	-1.4543960000	-0.1849440000	-0.0020970000
H	-4.8807570000	2.2393620000	-0.7988060000
H	-4.5192640000	-1.6482870000	-2.6119710000
H	0.7334910000	-1.9042560000	-1.4004350000
H	1.5731910000	-3.1952270000	2.5895070000
H	-2.4096010000	-3.5439980000	0.9881120000
C	2.3920940000	0.0416320000	-0.5242110000
C	2.9107450000	1.0374670000	-1.3445960000
C	3.1213060000	-1.1309400000	-0.3627330000
C	4.1338190000	0.8509290000	-1.9846460000
C	0.9318290000	2.6936960000	-0.2920550000
C	4.3535990000	-1.3142350000	-0.9878460000
C	4.8718060000	-0.3251060000	-1.8172950000
H	4.5192910000	1.6482330000	-2.6119540000
C	-0.3952370000	2.3087280000	-0.4544980000
C	1.3694640000	3.2491890000	0.9065460000
H	4.8807690000	-2.2393800000	-0.7987080000
C	-1.2738880000	2.4855920000	0.6127420000
H	-0.7334780000	1.9042170000	-1.4004790000
C	0.4893670000	3.4398490000	1.9781930000
H	2.4095890000	3.5440220000	0.9880580000
C	-0.8365760000	3.0565790000	1.8095290000
H	-1.5732170000	3.1952810000	2.5894250000
N	-2.6482060000	2.1612290000	0.4950170000
H	1.4543920000	0.1849350000	-0.0020920000
O	-3.4925890000	2.8250620000	1.1701790000
O	3.4925760000	-2.8250470000	1.1702680000
N	2.6482010000	-2.1612260000	0.4950850000
C	-1.0024950000	-4.0661950000	3.2751090000
C	-1.5432290000	-5.4723960000	2.9737790000
H	-1.9164590000	-5.9362640000	3.8926290000

H	-2.3661150000	-5.4468230000	2.2543490000
H	-0.7576380000	-6.1133510000	2.5628270000
C	-2.1315850000	-3.1953780000	3.8465440000
H	-2.5135140000	-3.6356840000	4.7733660000
H	-1.7727680000	-2.1866530000	4.0719750000
H	-2.9700940000	-3.1049540000	3.1509350000
C	0.0968370000	-4.1875410000	4.3311440000
H	0.9202970000	-4.8232350000	3.9922830000
H	0.5065540000	-3.2111370000	4.6070460000
H	-0.3178480000	-4.6394740000	5.2368680000
C	-6.2123080000	0.4800660000	-2.5370440000
C	-6.8712250000	1.8287310000	-2.2433550000
H	-7.8214800000	1.8934220000	-2.7813230000
H	-7.0853330000	1.9552960000	-1.1779370000
H	-6.2482640000	2.6663060000	-2.5714860000
C	-5.9898080000	0.3708470000	-4.0529660000
H	-5.3170690000	1.1576890000	-4.4069140000
H	-5.5560990000	-0.5925900000	-4.3339050000
H	-6.9432760000	0.4740760000	-4.5811970000
C	-7.1659910000	-0.6334340000	-2.0777060000
H	-7.3396360000	-0.5782260000	-0.9989760000
H	-8.1314790000	-0.5337640000	-2.5844190000
H	-6.7718520000	-1.6278310000	-2.3039430000
C	1.0024600000	4.0662710000	3.2750290000
C	-0.0968820000	4.1876400000	4.3310510000
H	-0.5065990000	3.2112410000	4.6069730000
H	0.3177930000	4.6395970000	5.2367670000
H	-0.9203410000	4.8233230000	3.9921670000
C	2.1315480000	3.1954720000	3.8464960000
H	2.9700630000	3.1050330000	3.1508970000
H	2.5134660000	3.6358020000	4.7733100000

H	1.7727320000	2.1867510000	4.0719490000
C	1.5431920000	5.4724670000	2.9736690000
H	2.3660840000	5.4468780000	2.2542470000
H	0.7576030000	6.1134090000	2.5626950000
H	1.9164120000	5.9363580000	3.8925120000
C	6.2123390000	-0.4801160000	-2.5369620000
C	6.8712570000	-1.8287710000	-2.2432350000
H	7.8215190000	-1.8934710000	-2.7811880000
H	7.0853500000	-1.9553120000	-1.1778100000
H	6.2483040000	-2.6663560000	-2.5713560000
C	7.1660120000	0.6333990000	-2.0776370000
H	7.3396430000	0.5782140000	-0.9989040000
H	8.1315070000	0.5337210000	-2.5843360000
H	6.7718720000	1.6277890000	-2.3039020000
C	5.9898580000	-0.3709310000	-4.0528900000
H	5.3171260000	-1.1577830000	-4.4068300000
H	5.5561480000	0.5924970000	-4.3338550000
H	6.9433330000	-0.4741670000	-4.5811060000
S	2.0566200000	2.5646130000	-1.6701330000
S	-2.0566070000	-2.5646540000	-1.6700980000