Supplementary Information

Cationic Tetranuclear Macrocyclic $CaCo_3$ Complexes as Highly Active Catalysts for Alternating Copolymerization of Propylene Oxide and Carbon Dioxide

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1. General information

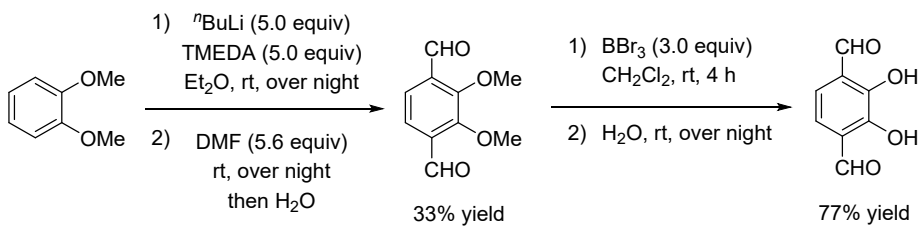
All the manipulations were carried out under the protection of argon using standard Schlenk or glovebox techniques when we treated air and moisture sensitive compound. Solvents, such as Et_2O and CH_2Cl_2, were dried and deoxygenated using a Grubbs column (Glass Counter Solvent Dispending System, Nikko Hansen & Co, Ltd.).[S1] MeOH and DMF were used as purchased. Carbon dioxide (>99.99 vol%) was purchased from NIPPON EKITAN Corporation. Propylene oxide was dried over calcium hydride and distilled under argon twice. NMR spectra were recorded on Bruker Avance III-400 spectrometers. All ^{1}H NMR chemical shifts are reported in ppm (δ) relative to tetramethylsilane at δ 0.00 or referenced to the chemical shifts of residual solvent resonances ($CDCl_3$: 7.26 ppm, acetonitrile-d_3: 1.94 ppm). All ^{13}C{^{1}H} NMR chemical shifts are reported in ppm (δ) relative to carbon resonances of $CDCl_3$. Polymer selectivity was determined from the ^{1}H NMR spectrum by comparing normalized integrals for poly(propylene carbonate) (PPC) (4.92 ppm, 1H) and propylene carbonate (PC) (4.77 ppm, 1H), poly(propylene oxide) (PPO) (3.46-3.64 ppm, 3H) resonances using phenanthrene as an internal standard. Carbonate Linkage of polymer was determined from the ^{1}H NMR spectrum by comparing normalized integrals for PPC and PPO resonances. GPC analyses were carried out at 40 °C by using a Shimadzu LC-20AD liquid chromatograph system and a RID 10A refractive index detector, equipped with a Shodex KF806L column which was calibrated versus commercially available polystyrene standards (SHOWA DENKO). The molecular weight and PDI were calibrated against standard polystyrene samples. ESI-MS spectrometric data was obtained using BRUKER microTOF-II spectrometer. FAB mass spectra were recorded on a JEOL JMS-700 spectrometer. Flash column chromatography was performed using silica gel 60 (0.040-0.063 nm, 230-400 mesh ASTM). The elemental analyses were recorded by using Perkin Elmer 2400 at the Faculty of Engineering Science, Osaka University.

General procedure for the alternating copolymerization

Before starting reaction, a 100 mL autoclave reactor was dried at 65 °C for 1 h under reduced pressure. In a typical experiment, macrocyclic complexes (0.0100 mmol), additives and epoxides (60.0 mmol) were added to the autoclave under an argon atomosphere. The reactor was then pressurized with CO_2 and heated by an oil-bath. After the reaction, the autoclave was cooled, and CO_2 pressure was releaced. The polymerization mixture was diluted with CH_2Cl_2, and phenanthrene was added as an internal standard. The yield of copolymer, cyclic carbonate, and carbonate linkage content were determined by the ^{1}H NMR analyses of the small portion of the mixture. The mixture was then passed through silica gel and dropped into MeOH to give white precipitation of copolymer. The molecular weight and molecular-weight distribution was determined by GPC analysis in THF using polystyrene standards as calibrates.

Synthesis of 2,3-dihydroxybenzene-1,4-dicarbaldehyde[S2]

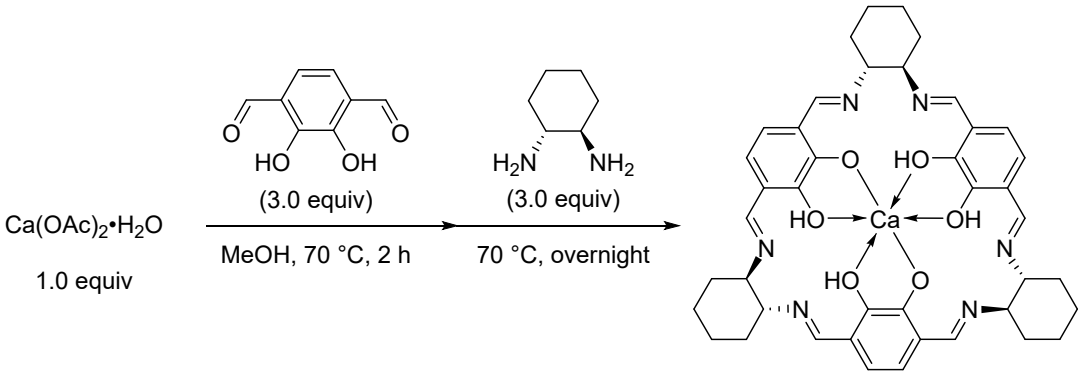
Scheme S1. Preparation of 2,3-dihydroxybenzene-1,4-dicarbaldehyde

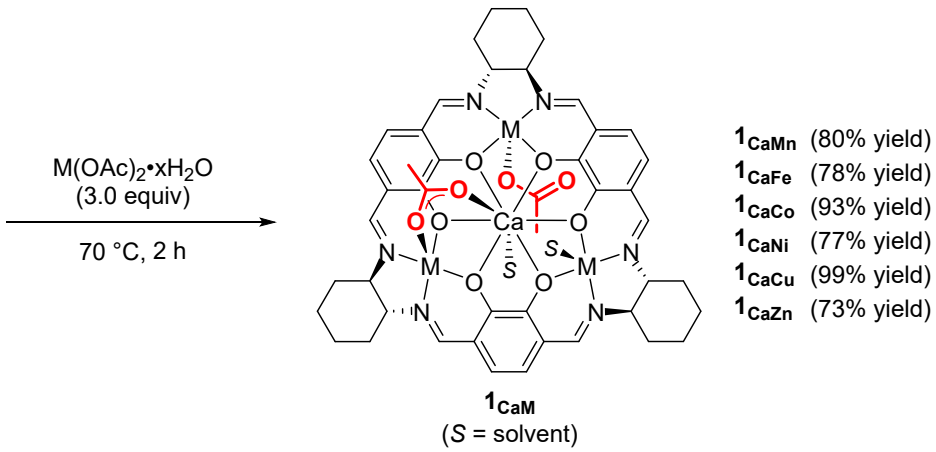


2,3-dihydroxybenzene-1,4-dicarbaldehyde was prepared from *o*-dimethoxybenzene (6.30 mL, 50.0 mmol) according to the literature to obtain the desired product. The product was recrystallized from $CHCl_3$/hexane to give yellow crystal (1.92 g, 11.6 mmol, 23% yield). ^{1}H NMR (400 MHz, $CDCl_3$, 30 °C): δ 10.85 (s, 2H, O*H*), 10.02 (s, 2H, C*H*O), 7.27 (s, 2H, *Ar*); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$, 30 °C): δ 196.5 (CHO), 150.9 (Ar), 123.3 (Ar), 122.4 (Ar).

2. Preparation of complexes $\mathbf{1}_{CaM}$

Scheme S2. Praparation of $\mathbf{1}_{Ca}$ and $\mathbf{1}_{CaM}$





A solution of 2,3dihydroxybenzene-1,4-dicarbaldehyde (3.0 equiv) in methanol were added to a solution of $Ca(OAc)_2 \cdot nH_2O$ (1.0 equiv) in methanol. After stirring at 70 °C for 2 hours, a solution of (*R*,*R*)-1,2-cyclohexanediamine (3.3 equiv) in methanol was added and the resulting mixture was

stirred for 18 h at 70 °C, and then a solution of $M(OAc)_2 \cdot mH_2O$ (3.0 equiv) in methanol was added. After stirring at 70 °C for 2 hours, solvent was removed.

1$_{CaCo}$: Reddish purple solid (93%yield) Calcd for $CaCo_3C_{46}H_{62}N_6O_{14}$ (**1$_{CaCo}$**•2MeOH•6H_2O): C, 46.72; H, 4.99; N, 6.39. Found: C, 46.68; H, 5.27; N, 6.60; MS (ESI^+) *m/z*: 471.54 ($[M-2OAc]^{2+}$); m.p.: >300 °C.

1$_{CaMn}$: Orange red solid (80%yield): Calcd for $CaMn_3C_{44}H_{58}N_6O_{12}$ (**1$_{CaMn}$**•2MeOH•4H_2O): C, 48.61; H, 5.44; N, 7.09. Found: C, 48.58; H, 5.76; N, 7.04; m.p.: >300 °C.

1$_{CaFe}$: Dark brown solid (78%yield): Calcd for $CaFe_3C_{48}H_{60}N_6O_{15}$ (**1$_{CaFe}$**•3AcOH•3H_2O): C, 48.54; H, 5.17; N, 6.53. Found: C, 48.26; H, 5.22; N, 6.62; m.p. >300 °C.

1$_{CaNi}$: Red brown solid (77%yield): Calcd for $CaNi_3C_{43}H_{50}N_6O_9$ (**1$_{CaNi}$**•MeOH•2H_2O): C, 49.99; H, 5.00; N, 7.17. Found: C, 50.20; H, 5.19; N, 7.14; m.p.: >300 °C.

1$_{CaCu}$: Red brown solid (>99%yield): Calcd for $CaCu_3C_{44}H_{60}N_6O_{13}$ (**1$_{CaCu}$**•MeOH•AcOH · 4H_2O): C, 46.47; H, 5.20; N, 6.78. Found: C, 47.36; H, 5.48; N, 6.97; MS (ESI^+) *m/z*: 478.53 ($[M-2OAc]^{2+}$); m.p.: >300 °C.

1$_{CaZn}$: Red solid (73%yield): Calcd for $CaCo_3C_{54}H_{72}N_6O_{22}$ (**1$_{CaZn}$**•4AcOH•4H_2O): C, 46.55; H, 5.21; N, 6.03. Found: C, 46.68; H, 5.32; N, 5.99; m.p.: >300 °C.

2$_{CaCo}$: Reddish purple solid (61%yield): Calcd for $CaCo_3C_{74}H_{70}N_6O_{18}$ (**2$_{CaCo}$**•2AcOH•4H_2O): C, 57.41; H, 4.56; N, 5.43. Found: C, 57.38; H, 4.54; N, 5.24; MS (ESI^+) *m/z*: 618.58 ($[M-2OAc]^{2+}$), 1296.17 ($[M-OAc]^+$); m.p.: >300 °C.

Preparation of complex $\mathbf{1}_{Ca}$

A solution of 2,3dihydroxybenzene-1,4-dicarbaldehyde (32.0 mg, 190 mmol) in methanol (5 mL) were added to a solution of $Ca(OAc)_2 \cdot nH_2O$ (11.0 mg, 0.064 mmol) in methanol (5 mL). After stirring at 70 °C for 2 hours, a solution of (*R*,*R*)-1,2-cyclohexanediamine (22.0 mg, 0.19 mmol) in methanol was added and the resulting mixture was stirred for 18 h at 70 °C, then, the resulting suspension was filtrated and all volatiles were removed and residual solid was washed with acetonitrile (1 ml × 2) to obtain red solid (51.3 mg, 0.064 mmol, quant. yield). Two singlet signals assignable to imine and aromatic were observed though the resulting solid was less soluble to non-protic solvents, such as CD_2Cl_2, CD_3CN, and DMSO. ^{1}H NMR spectrum using methanol-d_4 as solvent afforded broad signals. m.p.: >300 °C, ^{1}H NMR (400 MHz, acetonitrile-d_3, 30 °C) (well-resolved signals): δ 8.43 (s, 6H, N=CH), 6.87 (s, 6H, Ar). HRMS-FAB (*m/z*): $[M+H]^+$ calcd for $C_{42}H_{47}N_6O_6Ca$ ($[\mathbf{1}_{Ca}+H]^+$), 771.3183; found, 771.3186; Calcd for $CaCo_3C_{42}H_{60}N_6O_{13}$ ($\mathbf{1}_{Ca}\bullet 7H_2O$): C, 56.24; H, 6.74; N, 9.37. Found: C, 56.32; H, 6.23; N, 9.52.

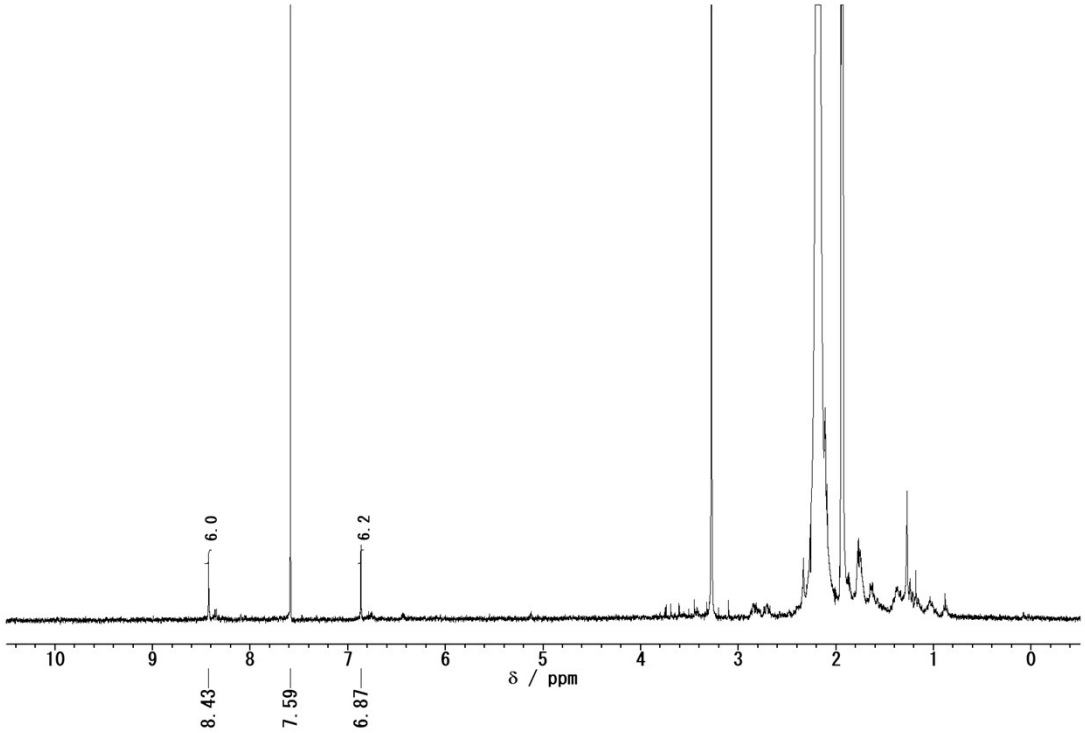
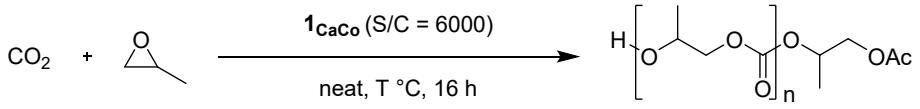


Figure S1. ^{1}H NMR spectrum of complex $\mathbf{1}_{Ca}$

3. Optimization of Reaction Conditions

Table S1. Optimization of reaction conditions for alternating copolymerization with $\mathbf{1}_{\mathbf{CaCo}}$.



x MPa 60 mmol

entry	pressure [MPa]	temperature [°C]	TON[a]	polymer selectivity [%][a]	carbonate linkage [%][a]
1	0.3	40	152	78	>99
2	0.5	40	224	90	>99
3	1.0	40	180	95	>99
4	2.0	40	164	93	>99
5	3.0	40	126	92	>99
6	0.5	50	236	73	>99
7	1.0	50	235	92	>99
8	1.0	60	167	65	>99
9	1.0	70	168	43	>99

[a] Determined by ^{1}H NMR analysis using phenanthrene as an internal standard.

4. X-Ray Crystallographic Analysis

The crystal of $\mathbf{1}_{\mathbf{CaZn}}$ was mounted on the CryoLoop (Hampton Research Corp.) with a layer of light mineral oil and placed in a nitrogen stream at 113(2) K. Measurement was made on Rigaku XtaLAB P200 system with graphite-monochromated Mo–Kα (0.71075 Å) radiation. The structures of complex $\mathbf{1}_{\mathbf{CaZn}}$ was solved by SHELXS-2013 in the CrystalClear program.[S3] The structure was refined on F^2 by full-matrix least-squares method, using SHELXL-2013.[S3] The ORTEP-3 program was used to draw the molecule.[S4]

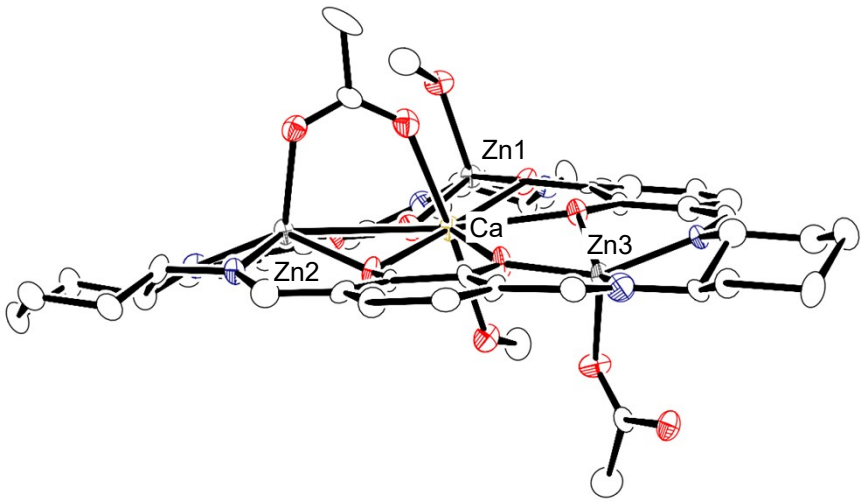
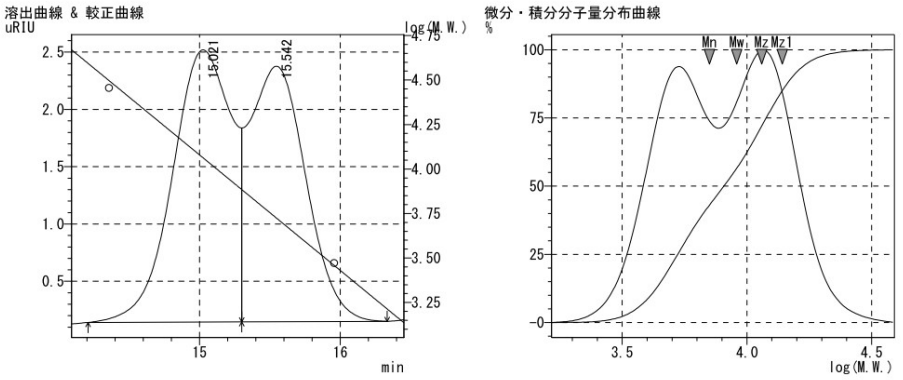


Figure S2. Preliminary crystal structure of $\mathbf{1}_{\mathbf{CaZn}}$. All hydrogen atoms and solvent molecules are omitted for clarity.

5. GPC Charts

==== Shimadzu LCsolution GPC Report ====

operator : Admin
sample name : MTS-5044
sample ID : MTS-5044
vial No : -1
Inj. Vol. : 20 uL
data file : MTS-5044.lcd
methot file : mashima-lab 20211208.lcm
batch file :
report file : Default.lcr
acquisition data : 2021/12/08 16:00:57
modified data : 2021/12/09 13:46:02



peak report

検出器A Ch1

Peak#	etention tim	area	height	area%	height%
1	15.021	69816	2375	53.063	51.577
2	15.542	61757	2230	46.937	48.423
合計		131573	4605	100.000	100.000

GPC計算結果

Peak#:1 (検出器A Ch1)
[ﾋﾟｰｸ情報]

	time(min)	tion amount(lecular weig		height
開始	14.208	11.367	39236	141
頂点	15.021	12.017	11634	2375
終了	15.300	12.240	7668	146

area : 69816
area% : 53.0628

[平均分子量]

NAMW(Mn)	11605
WAMW(Mw)	12512
ZAMW(Mz)	13652
Z+1 AMW(Mz1)	15074
Mw/Mn	1.07816
Mv/Mn	0.00000
Mz/Mw	1.09112

Peak#:2 (検出器A Ch1)
[ﾋﾟｰｸ情報]

	time(min)	tion amount(lecular weig		height
開始	15.300	12.240	7668	146
頂点	15.542	12.434	5340	2230
終了	16.333	13.067	1635	151

area : 61757
area% : 46.9372

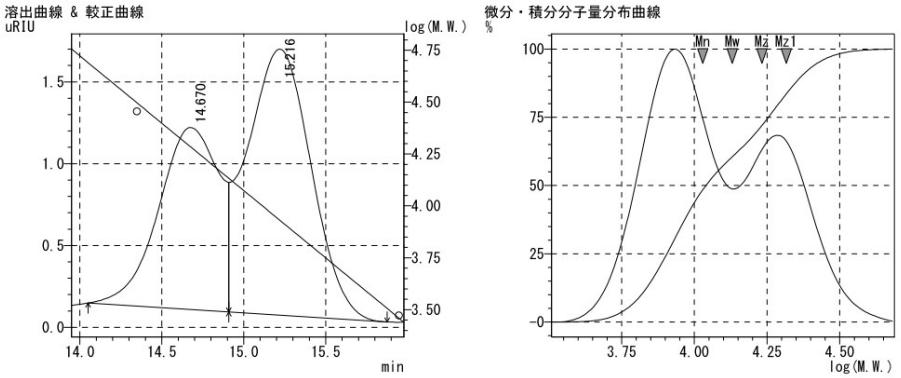
[平均分子量]

D:¥DATA¥matsushiro¥MTS-5044.lcd

Figure S3. GPC chart of a sample for Table 1, entry 1.

==== Shimadzu LCsolution GPC Report ====

operator : Admin
sample name : MTS-5024_20211117
sample ID : MTS-5024_20211117
vial No : -1
Inj. Vol. : 20 uL
data file : MTS-5024_20211117.lcd
methot file : mashima-lab 20211117.lcm
batch file :
report file : Default.lcr
acquisition data : 2021/11/17 20:59:02
modified data : 2021/11/18 13:20:35



peak report

検出器A Ch1

Peak#	etention tim	area	height	area%	height%
1	14.670	28697	1112	39.471	40.628
2	15.216	44007	1625	60.529	59.372
合計		72704	2737	100.000	100.000

GPC計算結果

Peak#:1 (検出器A Ch1)
[ﾋﾟｰｸ情報]

	time(min)	tion amount(lecular weig	height
開始	14.050	11.240 48993	149
頂点	14.670	11.736 19401	1112
終了	14.908	11.927 13587	94

area : 28697
area% : 39.4714

[平均分子量]

NAMW(Mn)	19577
WAMW(Mw)	20732
ZAMW(Mz)	22108
Z+1 AMW(Mz1)	23709
Mw/Mn	1.05899
Mv/Mn	0.00000
Mz/Mw	1.06635

Peak#:2 (検出器A Ch1)
[ﾋﾟｰｸ情報]

	time(min)	tion amount(lecular weig	height
開始	14.908	11.927 13587	94
頂点	15.216	12.172 8584	1625
終了	15.875	12.700 3205	33

area : 44007
area% : 60.5286

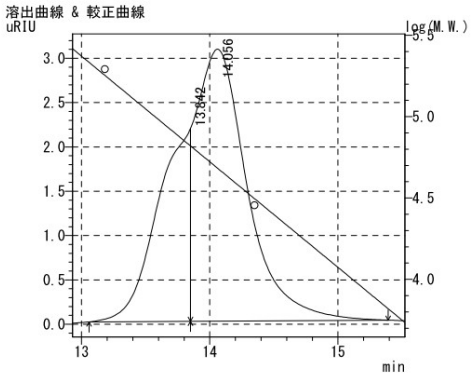
[平均分子量]

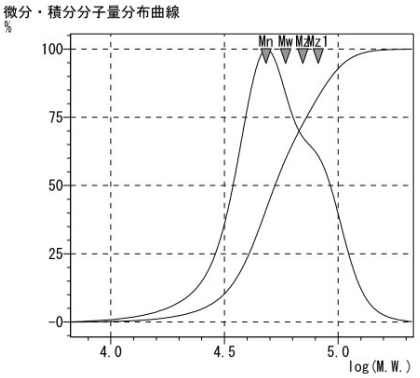
D:¥DATA¥matsushiro¥MTS-5024_20211117.lcd

Figure S4. GPC chart of a sample for Table 1, entry 7.

==== Shimadzu LCsolution GPC Report ====

operator : Admin
sample name : MTS-5027_20211117
sample ID : MTS-5027_20211117
vial No : -1
Inj. Vol. : 20 uL
data file : MTS-5027_20211117.lcd
methot file : mashima-lab 20211117.lcm
batch file :
report file : Default.lcr
acquisition data : 2021/11/17 23:50:49
modified data : 2021/11/18 13:25:05





peak report

検出器A Ch1

Peak#	etention tim	area	height	area%	height%
1	13.842	39269	2148	31.838	41.186
2	14.056	84070	3068	68.162	58.814
合計		123340	5216	100.000	100.000

GPC計算結果

Peak#:1 (検出器A Ch1)
[ﾋﾟｰｸ情報]

	time(min)	tion amount(lecular weig	height
開始	13.058	10.447 215620	26
頂点	13.842	11.073 66886	2148
終了	13.850	11.080 66058	33

area : 39269
area% : 31.8382

[平均分子量]

NAMW(Mn)	85657
WAMW(Mw)	89191
ZAMW(Mz)	93563
Z+1 AMW(Mz1)	98927
Mw/Mn	1.04126
Mv/Mn	0.00000
Mz/Mw	1.04902

Peak#:2 (検出器A Ch1)
[ﾋﾟｰｸ情報]

	time(min)	tion amount(lecular weig	height
開始	13.850	11.080 66058	33
頂点	14.056	11.245 48541	3068
終了	15.392	12.313 6598	46

area : 84070
area% : 68.1618

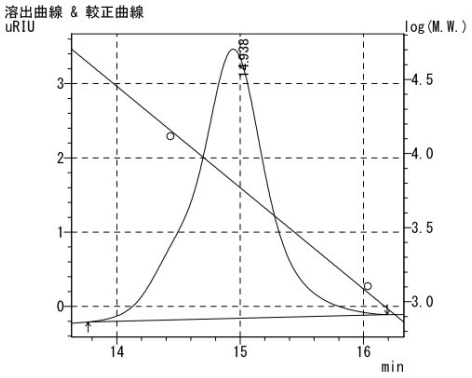
[平均分子量]

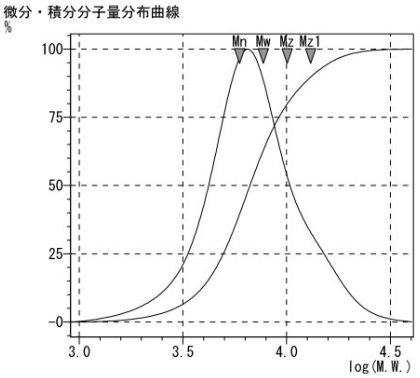
D:¥DATA¥matsushiro¥MTS-5027_20211117.lcd

Figure S5. GPC chart of a sample for Table 2, entry 2.

==== Shimadzu LCsolution GPC Report ====

operator : Admin
sample name : NAG18155B
sample ID : NAG18155B
vial No : -1
Inj. Vol. : 20 uL
data file : NAG18155B-2.lcd
methot file : mashima-lab 解析用20220712-2.lcm
batch file :
report file : Default.lcr
acquisition data : 2022/07/13 13:33:36
modified data : 2022/09/01 15:37:49





peak report

検出器A Ch1

Peak#	etention tim	area	height	area%	height%
1	14.938	150433	3624	100.000	100.000
合計		150433	3624	100.000	100.000

GPC計算結果

Peak#:1 (検出器A Ch1)
[ﾋﾟｰｸ情報]

	time(min)	tion amount(lecular weig		height
開始	13.767	11.013	41069	-208
頂点	14.938	11.951	6486	3624
終了	16.192	12.953	901	-110

area : 150433
area% : 100.0000

[平均分子量]

NAMW(Mn)	5941
WAMW(Mw)	7725
ZAMW(Mz)	10054
Z+1 AMW(Mz1)	13051
Mw/Mn	1.30021
Mv/Mn	0.00000
Mz/Mw	1.30156

検出器A Ch1
[平均分子量(ﾄｰﾀﾙ)]

NAMW(Mn)	5941
WAMW(Mw)	7725
ZAMW(Mz)	10054
Z+1 AMW(Mz1)	13051
Mw/Mn	1.30021
Mv/Mn	0.00000
Mz/Mw	1.30156

D:¥DATA¥nagae¥NAG18155B-2.lcd

Figure S6. GPC chart of a sample for Table 2, entry 3.

==== Shimadzu LCsolution GPC Report ====

operator : Admin
sample name : MTS-5070
sample ID : MTS-5070
vial No : -1
Inj. Vol. : 20 uL
data file : MTS-5070.lcd
methot file : mashima-lab 20220307.lcm
batch file :
report file : Default.lcr
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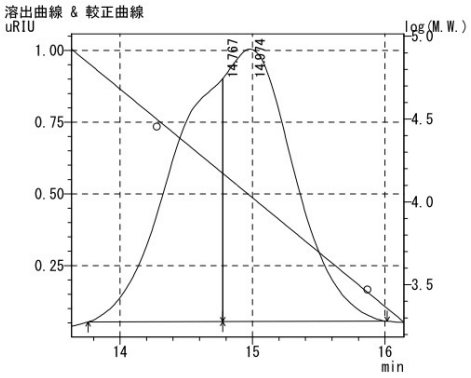
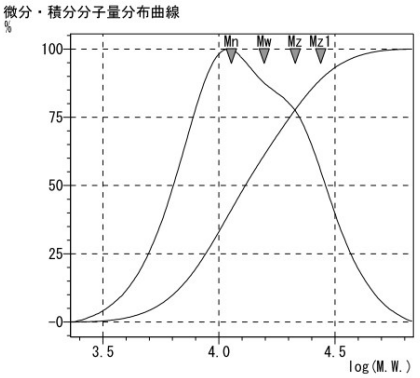
modified data : 2022/03/08 12:56:45





peak report

検出器A Ch1

Peak#	etention tim	area	height	area%	height%
1	14.767	24324	843	42.188	47.022
2	14.974	33331	950	57.812	52.978
合計		57655	1792	100.000	100.000

GPC計算結果

Peak#:1 (検出器A Ch1)
[ﾋﾟｰｸ情報]

	time(min)	tion amount(lecular weig		height
開始	13.758	11.007	69166	54
頂点	14.767	11.813	15069	843
終了	14.775	11.820	14880	55

area : 24324
area% : 42.1880

[平均分子量]

NAMW(Mn)	22056
WAMW(Mw)	24237
ZAMW(Mz)	27137
Z+1 AMW(Mz1)	30739
Mw/Mn	1.09890
Mv/Mn	0.00000
Mz/Mw	1.11964

Peak#:2 (検出器A Ch1)
[ﾋﾟｰｸ情報]

	time(min)	tion amount(lecular weig		height
開始	14.775	11.820	14880	55
頂点	14.974	11.979	11022	950
終了	16.017	12.813	2278	56

area : 33331
area% : 57.8120

[平均分子量]

D:¥DATA¥matsushiro¥MTS-5070.lcd

Figure S7. GPC chart of a sample for Table 2, entry 5.

==== Shimadzu LCsolution GPC Report ====

operator : Admin
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sample ID : MTS-5062
vial No : -1
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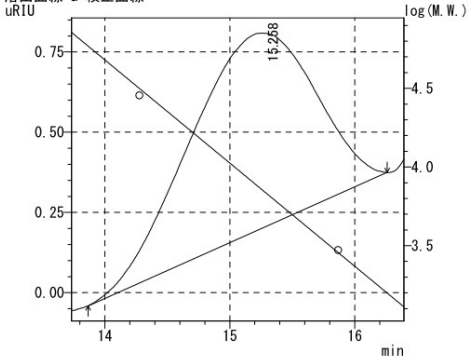
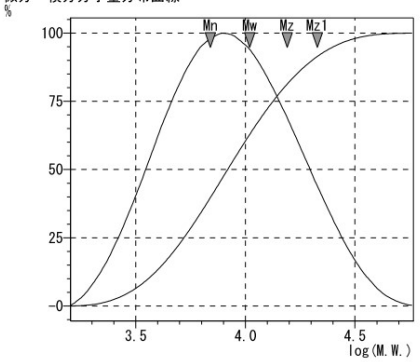
methot file : mashima-lab 20220307.lcm
batch file :
report file : Default.lcr
acquisition data : 2022/03/07 21:54:36
modified data : 2022/03/08 12:58:02

溶出曲線 & 較正曲線



微分・積分分子量分布曲線



peak report

検出器A Ch1

Peak#	etention tim	area	height	area%	height%
1	15.258	42823	608	100.000	100.000
合計		42823	608	100.000	100.000

GPC計算結果

Peak#:1 (検出器A Ch1)
[ﾋﾟｰｸ情報]

	time(min)	tion amount(lecular weig		height
開始	13.867	11.093	58721	-41
頂点	15.258	12.207	7169	608
終了	16.258	13.007	1581	375

area : 42823
area% : 100.0000

[平均分子量]

NAMW(Mn)	6924
WAMW(Mw)	10463
ZAMW(Mz)	15531
Z+1 AMW(Mz1)	21302
Mw/Mn	1.51107
Mv/Mn	0.00000
Mz/Mw	1.48438

検出器A Ch1
[平均分子量(ﾄｰﾀﾙ)]

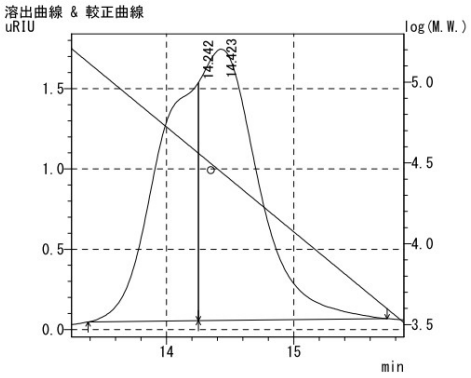
NAMW(Mn)	6924
WAMW(Mw)	10463
ZAMW(Mz)	15531
Z+1 AMW(Mz1)	21302
Mw/Mn	1.51107
Mv/Mn	0.00000
Mz/Mw	1.48438

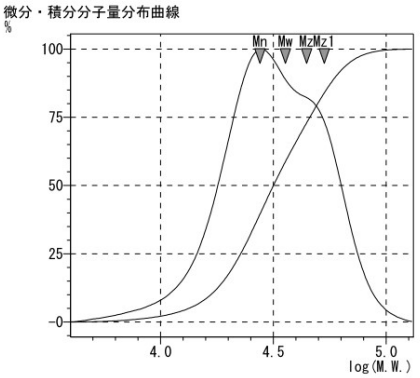
D:¥DATA¥matsushiro¥MTS-5062.lcd

Figure S8. GPC chart of a sample for Table 2, entry 7.

==== Shimadzu LCsolution GPC Report ====

operator : Admin
sample name : MTS-5029_20211117
sample ID : MTS-5029_20211117
vial No : -1
Inj. Vol. : 20 uL
data file : MTS-5029_20211117.lcd
methot file : mashima-lab 20211117.lcm
batch file :
report file : Default.lcr
acquisition data : 2021/11/17 23:09:26
modified data : 2021/11/18 13:27:48





peak report

検出器A Ch1

Peak#	etention tim	area	height	area%	height%
1	14.242	35455	1472	40.548	46.566
2	14.423	51984	1689	59.452	53.434
合計		87439	3161	100.000	100.000

GPC計算結果

Peak#:1 (検出器A Ch1)
[ﾋﾟｰｸ情報]

	time(min)	tion amount(lecular weig	height
開始	13.383	10.707 132671	48
頂点	14.242	11.393 36792	1472
終了	14.250	11.400 36336	55

area : 35455
area% : 40.5480

[平均分子量]

NAMW(Mn)	50075
WAMW(Mw)	52997
ZAMW(Mz)	56601
Z+1 AMW(Mz1)	60925
Mw/Mn	1.05836
Mv/Mn	0.00000
Mz/Mw	1.06800

Peak#:2 (検出器A Ch1)
[ﾋﾟｰｸ情報]

	time(min)	tion amount(lecular weig	height
開始	14.250	11.400 36336	55
頂点	14.423	11.539 28045	1689
終了	15.733	12.587 3960	68

area : 51984
area% : 59.4520

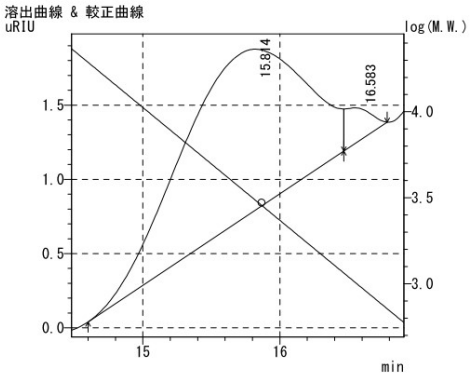
[平均分子量]

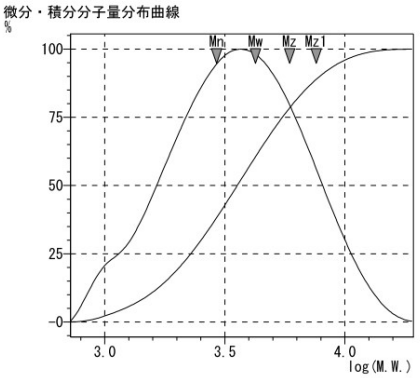
D:¥DATA¥matsushiro¥MTS-5029_20211117.lcd

Figure S9. GPC chart of a sample for Table 2, entry 8.

==== Shimadzu LCsolution GPC Report ====

operator : Admin
sample name : MTS-6003
sample ID : MTS-6003
vial No : -1
Inj. Vol. : 20 uL
data file : MTS-6003.lcd
methot file : mashima-lab 20220307.lcm
batch file :
report file : Default.lcr
acquisition data : 2022/03/07 19:43:21
modified data : 2022/03/08 12:57:13





peak report

検出器A Ch1

Peak#	etention tim	area	height	area%	height%
1	15.814	70361	1089	95.901	83.454
2	16.583	3007	216	4.099	16.546
合計		73369	1304	100.000	100.000

GPC計算結果

Peak#:1 (検出器A Ch1)
[ﾋﾟｰｸ情報]

	time(min)	tion amount(lecular weig	height
開始	14.600	11.680 19385	40
頂点	15.814	12.651 3094	1089
終了	16.467	13.173 1154	1190

area : 70361
area% : 95.9009

[平均分子量]

NAMW(Mn)	3198
WAMW(Mw)	4386
ZAMW(Mz)	5938
Z+1 AMW(Mz1)	7612
Mw/Mn	1.37147
Mv/Mn	0.00000
Mz/Mw	1.35370

Peak#:2 (検出器A Ch1)
[ﾋﾟｰｸ情報]

	time(min)	tion amount(lecular weig	height
開始	16.467	13.173 1154	1190
頂点	16.583	13.267 968	216
終了	16.783	13.427 715	1385

area : 3007
area% : 4.0991

[平均分子量]

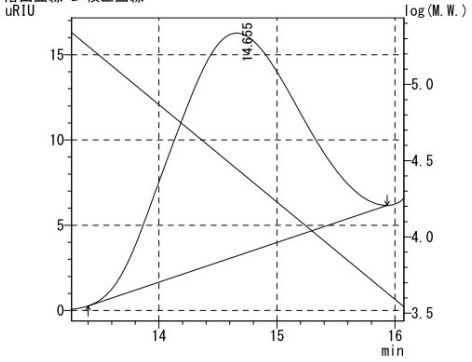
D:¥DATA¥matsushiro¥MTS-6003.lcd

Figure S10. GPC chart of a sample for Table 2, entry 9.

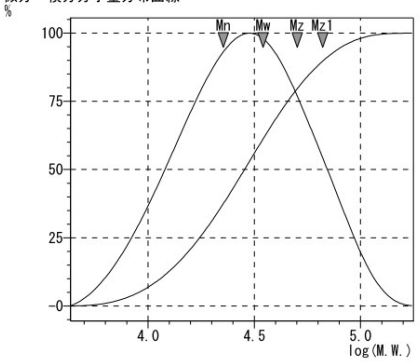
==== Shimadzu LCsolution GPC Report ====

operator : Admin
sample name : MTS-5023-2
sample ID : MTS-5023-2
vial No : -1
Inj. Vol. : 20 uL
data file : MTS-5023-2.lcd
methot file : mashima-lab method.lcm
batch file :
report file : Default.lcr
acquisition data : 2022/01/25 0:40:12
modified data : 2022/01/25 1:10:13

溶出曲線 & 較正曲線



微分・積分分子量分布曲線



peak report

検出器A Ch1

Peak#	etention tim	area	height	area%	height%
1	14.655	953778	13071	100.000	100.000
合計		953778	13071	100.000	100.000

GPC計算結果

Peak#:1 (検出器A Ch1)
[ﾋﾟｰｸ情報]

	time(min)	tion amount(lecular weig		height
開始	13.400	10.720	178090	270
頂点	14.655	11.724	28105	13071
終了	15.933	12.747	4291	6162

area : 953778
area% : 100.0000

[平均分子量]

NAMW(Mn)	22590
WAMW(Mw)	34811
ZAMW(Mz)	50389
Z+1 AMW(Mz1)	66369
Mw/Mn	1.54098
Mv/Mn	0.00000
Mz/Mw	1.44752

検出器A Ch1
[平均分子量(ﾄｰﾀﾙ)]

NAMW(Mn)	22590
WAMW(Mw)	34811
ZAMW(Mz)	50389
Z+1 AMW(Mz1)	66369
Mw/Mn	1.54098
Mv/Mn	0.00000
Mz/Mw	1.44752

D:¥DATA¥matsushiro¥MTS-5023-2.lcd

Figure S11. GPC chart of a sample for Table 2, entry 10.

6. DFT Calculations

The calculations were performed using the Gaussian 16[S5] program employing B3LYP functional, and using a standard double-ξ polarized basis set, namely the LANL2DZ set for calcium and cobalt.[S6] The solvent effects, in our case $\varepsilon = 12.42$ for ethylene oxide, were taken into account during some the calculations for organic molecules and complexes by means of the IEFPCM model.[S7] All stationary points were fully characterized *via* analytical frequency calculations as either true minima (all positive eigenvalues) or transition states (one imaginary eigenvalue). Zero-point vibrational energy corrections (ZPVE) were estimated by a frequency calculation at the same level of theory, to be considered for the calculation of the total energy values. The multiplicity of all $CaCo_3$ complexes were determined as quartet because structures of quartet complexes showed the lowest energies among the doublet and sextet ones in the preliminary calculations.

Cartesian coordinates

$PhMe_2NH$

Energy: -230105.7577880

H	1.72006	-1.39336	-0.13122
C	2.23520	0.01849	1.26415
H	2.13118	1.09502	1.38579
H	1.73463	-0.50609	2.07618
H	3.28790	-0.25788	1.21495
C	2.24652	0.25356	-1.22797
H	1.75643	-0.11308	-2.12831
H	2.14385	1.33406	-1.15129
H	3.29904	-0.02654	-1.21809
C	0.10490	-0.16853	-0.01784
C	-0.39921	1.12809	0.04917
C	-0.72552	-1.28362	-0.06541
C	-1.78266	1.30410	0.06284
H	0.25822	1.98925	0.08979
C	-2.10823	-1.09159	-0.04967
H	-0.31195	-2.28690	-0.11369
C	-2.63560	0.19882	0.01284
H	-2.19041	2.30786	0.11200
H	-2.76640	-1.95274	-0.08722
H	-3.71058	0.34456	0.02284
N	1.57652	-0.38430	-0.03435

$PhMe_2N$

Energy: -229824.4398274

C	2.29321	-1.24514	0.06394
H	2.10887	-1.66991	1.06288
H	2.01590	-1.99939	-0.68026
H	3.36354	-1.06367	-0.03896
C	2.29334	1.24511	0.06399
H	2.01564	1.99954	-0.67983
H	2.10970	1.66950	1.06321
H	3.36360	1.06356	-0.03959
C	0.18570	0.00000	-0.07492
C	-0.55027	1.20907	-0.03494
C	-0.55018	-1.20898	-0.03493
C	-1.94255	1.19902	0.01716
H	-0.03815	2.16301	-0.04382
C	-1.94257	-1.19899	0.01723
H	-0.03818	-2.16298	-0.04392
C	-2.65792	-0.00005	0.04198
H	-2.47153	2.14815	0.04438
H	-2.47133	-2.14824	0.04444
H	-3.74242	0.00007	0.08564
N	1.57311	0.00002	-0.16160

Ethylene oxide

Energy: -96509.3187421

C	-0.66763	-0.48411	0.00000
C	0.00000	0.82378	0.00000
O	0.76741	-0.39087	0.00000
H	-1.11145	-0.86159	0.92071
H	-1.11145	-0.86159	-0.92071
H	0.04471	1.40607	0.92003
H	0.04471	1.40607	-0.92003

AcOH (dimer)

Energy: -287544.0304831

C	1.91245	0.05626	0.00006
O	1.24206	1.09258	0.00007
C	3.41611	0.06192	-0.00016
H	3.78724	1.08560	0.00000
H	3.78293	-0.47186	0.88112
H	3.78262	-0.47139	-0.88187
O	1.39227	-1.15690	0.00014
H	0.38612	-1.10936	0.00018
C	-1.91245	-0.05626	-0.00000
O	-1.24208	-1.09261	-0.00002
C	-3.41611	-0.06188	-0.00011
H	-3.78281	0.47176	0.88132
H	-3.78271	0.47159	-0.88167
H	-3.78726	-1.08555	-0.00003
O	-1.39225	1.15688	0.00007
H	-0.38611	1.10931	0.00016

CO_2

Energy: -118337.7952731

O	0.00000	0.00000	1.16911
C	0.00000	0.00000	0.00000
O	0.00000	0.00000	-1.16911

A1

Energy: -1992007.5553814

O	0.02115	2.45204	-0.06951
O	-2.21645	1.35369	-0.41383
O	-2.35039	-1.17823	-0.73653
O	-0.24744	-2.61133	-0.34325
O	2.02918	-1.48697	-0.07463
O	2.07886	1.02472	0.40441
O	3.93737	0.13146	-1.74268
O	6.18837	0.36996	-1.84814
O	-0.93449	-0.73361	2.08653
O	-2.30028	-2.52846	1.89300
N	-1.12573	4.96944	-0.31047
N	-3.47581	3.82732	-0.50930
N	-3.94144	-3.44480	-0.59998
N	-1.83016	-4.86405	0.03535
N	4.70303	-1.69784	0.68151
N	4.74757	0.87813	1.14780
C	-2.18838	5.87717	-0.76563
H	-2.14923	5.92911	-1.86111
C	-3.53633	5.28614	-0.33015
H	-3.69532	5.48969	0.73597
C	-4.54583	3.11519	-0.69657
H	-5.50284	3.63525	-0.79974
C	-4.58687	1.67361	-0.76728
C	-5.84853	1.01530	-0.94249
H	-6.74384	1.62295	-1.03986
C	-5.93477	-0.35171	-0.96362
H	-6.90143	-0.83678	-1.06787
C	-4.76623	-1.17218	-0.84424

C	-3.49758	-0.55674	-0.74966
C	-3.41749	0.88958	-0.64040
C	-4.90392	-2.61000	-0.84267
H	-5.90048	-3.00860	-1.05659
C	-4.14086	-4.89711	-0.71635
H	-3.97683	-5.18594	-1.76257
C	-3.10051	-5.58858	0.17213
H	-3.41576	-5.52287	1.22083
C	0.59752	-4.80505	0.21932
C	1.76500	-5.57249	0.53383
H	1.65845	-6.64187	0.69411
C	2.99104	-4.97325	0.65833
H	3.86501	-5.56533	0.91616
C	3.14964	-3.56146	0.47906
C	2.02695	-2.78128	0.12130
C	0.72891	-3.41773	-0.01616
C	4.44745	-2.96661	0.71661
H	5.26305	-3.65535	0.95861
C	6.05034	-1.15954	0.89472
H	6.45368	-0.91462	-0.09393
C	5.90846	0.15047	1.68220
H	5.71667	-0.06855	2.74094
C	4.64387	2.16344	1.25639
H	5.48094	2.72194	1.68710
C	3.48133	2.93826	0.87431
C	3.53828	4.36673	0.94338
H	4.47593	4.83604	1.22838
C	2.44301	5.13786	0.65122
H	2.50826	6.22153	0.69387
C	1.19229	4.53862	0.29420
C	1.10019	3.12934	0.23557
C	2.26869	2.31474	0.50628
C	0.07321	5.38711	-0.04394
H	0.27133	6.46224	-0.08930
C	5.03425	0.45179	-2.32118
C	4.87121	0.98339	-3.75684
H	4.21209	1.85804	-3.76242
H	4.39871	0.22146	-4.38656
H	5.83624	1.25560	-4.18964
C	-1.72968	-1.61154	2.54800
C	-2.01840	-1.53905	4.04954
H	-1.08132	-1.62325	4.60960
H	-2.70306	-2.32662	4.36876
H	-2.45067	-0.56291	4.29372
Ca	-0.13389	-0.10849	-0.09619
Co	3.45321	-0.29456	0.36346
Co	-2.10500	-3.00101	-0.27016
Co	-1.71527	3.16046	-0.24499
O	-0.02673	-0.00080	-2.61431
C	0.31123	-1.16345	-3.40741
H	-0.39146	-1.37268	-4.21077
H	0.63761	-2.02014	-2.82414
C	1.15217	0.03744	-3.46777
H	2.10099	0.06691	-2.93189
H	1.04502	0.70746	-4.31837
H	6.69934	-1.87191	1.41772
H	6.82398	0.74892	1.61769
H	-2.99882	-6.64790	-0.08994
H	-5.15881	-5.19139	-0.43708
H	-4.36386	5.73219	-0.89280
H	-2.05555	6.89066	-0.37111
O	-2.00692	3.36463	2.09171
C	-3.10063	2.75939	2.81592
C	-1.71644	2.36055	3.09713
H	-3.73255	2.10511	2.22034
H	-3.61972	3.43443	3.49285
H	-1.34840	1.40991	2.71649
H	-1.21997	2.75688	3.98051
C	-0.68936	-5.45938	0.19997
H	-0.68837	-6.54008	0.37295

A2

Energy: -1992009.3268344

O	-0.86651	-2.29007	0.02693
O	-2.43457	-0.32374	0.16663
O	-1.50039	2.04505	0.52558
O	1.06097	2.44774	0.39472
O	2.59640	0.44997	-0.00519
O	1.60242	-1.87969	-0.46783
O	3.39959	-1.69134	1.89766
O	1.35707	-0.84227	2.38654
O	-0.09255	0.83689	-1.93025
O	-0.54885	3.05604	-2.03913
N	-2.99685	-4.05995	0.15352
N	-4.63603	-2.01669	0.12505
N	-1.94916	4.76122	0.23856
N	0.61625	5.13486	-0.14989
N	5.15534	-0.54325	-0.33064
N	4.15316	-2.92483	-0.77064
C	-4.38063	-4.40562	0.50743
H	-4.46310	-4.41966	1.60180
C	-5.30071	-3.31505	-0.05919
H	-5.43750	-3.47838	-1.13537
C	-5.30684	-0.90635	0.20660
H	-6.39975	-0.96214	0.21261
C	-4.73111	0.41373	0.28174
C	-5.60170	1.55379	0.33113
H	-6.67569	1.38902	0.32754
C	-5.09718	2.82549	0.35660
H	-5.76795	3.68045	0.36357
C	-3.68324	3.06442	0.37047
C	-2.79258	1.96529	0.40618
C	-3.33018	0.61607	0.28428
C	-3.19480	4.42098	0.37245
H	-3.94190	5.21250	0.48990
C	-1.52608	6.16358	0.36324
H	-1.36485	6.38487	1.42641
C	-0.20586	6.32668	-0.39688
H	-0.41062	6.37812	-1.47365
C	2.79238	4.04904	-0.13659
C	4.19901	4.23086	-0.35568
H	4.57693	5.24064	-0.49169
C	5.05288	3.16131	-0.40762
H	6.11636	3.31674	-0.56891
C	4.56692	1.81810	-0.27962
C	3.18413	1.60681	-0.06752

C	2.29199	2.74653	0.08394
C	5.48710	0.71185	-0.38004
H	6.54587	0.96460	-0.49621
C	6.15757	-1.61296	-0.35147
H	6.34551	-1.92039	0.68458
C	5.57119	-2.79613	-1.13482
H	5.63499	-2.58559	-2.21031
C	3.52368	-4.05323	-0.88174
H	4.09107	-4.94127	-1.17829
C	2.11013	-4.23672	-0.64813
C	1.56063	-5.55996	-0.66568
H	2.23115	-6.39835	-0.83470
C	0.22261	-5.77765	-0.46905
H	-0.17640	-6.78819	-0.48240
C	-0.67834	-4.68610	-0.23897
C	-0.16745	-3.36843	-0.21355
C	1.24787	-3.13238	-0.45024
C	-2.07411	-4.96102	0.00877
H	-2.36000	-6.01467	0.08500
C	2.45700	-1.38990	2.68855
C	2.66988	-1.72753	4.16970
H	3.64641	-2.18261	4.34534
H	1.88689	-2.41430	4.50858
H	2.58105	-0.81813	4.77328
C	-0.33986	1.91416	-2.54776
C	-0.39512	1.82329	-4.07804
H	0.54566	1.41279	-4.45934
H	-0.57747	2.79704	-4.53655
H	-1.19019	1.13112	-4.37574
Ca	0.12431	0.06793	0.41485
Co	3.38320	-1.25078	-0.24857
Co	-0.45078	3.56913	0.11117
Co	-2.74506	-2.17531	0.03497
O	-1.32482	0.26068	2.85731
C	-0.72248	0.62355	4.11559
H	-1.27237	1.37198	4.68326
H	0.35792	0.72779	4.07663
C	-1.29749	-0.71179	3.92133
H	-0.62007	-1.54220	3.74546
H	-2.27200	-0.94702	4.34578
H	7.10593	-1.28107	-0.79024
H	6.12810	-3.71861	-0.93461
H	0.30853	7.24871	-0.10228
H	-2.28853	6.85372	-0.01590
H	-6.28561	-3.34140	0.42039
H	-4.66275	-5.39550	0.13158
O	-2.86139	-2.31721	-2.30874
C	-3.36967	-1.24703	-3.13648
C	-1.95106	-1.61873	-3.19658
H	-3.66176	-0.35278	-2.59178
H	-4.05104	-1.57135	-3.92006
H	-1.21772	-0.98457	-2.70315
H	-1.59786	-2.22695	-4.02679
C	1.91233	5.18988	-0.20046
H	2.38512	6.16549	-0.35189

A1-EO

Energy: -1895496.0483908

O	1.79912	1.91117	0.13373
O	-0.62827	2.49885	-0.20395
O	-2.34884	0.64074	-0.55498
O	-1.74056	-1.78788	0.05514
O	0.70477	-2.43318	0.38460
O	2.50782	-0.55415	0.45840
O	2.29252	-1.94737	-2.09790
O	0.62615	-0.41502	-1.95706
O	-1.57351	0.16101	2.31651
O	-3.69853	-0.47411	1.85613
N	2.52842	4.54015	-0.33910
N	0.00580	5.18369	-0.35657
N	-5.01142	-0.08807	-0.85545
N	-4.37591	-2.55774	-0.26992
N	2.67180	-4.30626	-0.21237
N	4.49307	-2.45335	0.07815
C	2.28209	5.94628	-0.69929
H	2.28823	6.02568	-1.79372
C	0.89938	6.33501	-0.16597
H	0.96520	6.54158	0.90983
C	-1.27093	5.33188	-0.55286
H	-1.66376	6.34854	-0.64361
C	-2.22279	4.25851	-0.66433
C	-3.59561	4.56578	-0.94255
H	-3.88285	5.60650	-1.06259
C	-4.52893	3.57072	-1.05296
H	-5.56738	3.81621	-1.25852
C	-4.16958	2.19235	-0.90321
C	-2.81911	1.84890	-0.65340
C	-1.83743	2.90965	-0.49701
C	-5.18600	1.17936	-1.06517
H	-6.16986	1.52379	-1.39916
C	-6.06735	-1.06511	-1.15876
H	-5.99452	-1.33545	-2.22014
C	-5.82035	-2.31297	-0.29977
H	-6.15290	-2.11985	0.72743
C	-2.47675	-4.07557	-0.18822
C	-2.05105	-5.43941	-0.30511
H	-2.80507	-6.21026	-0.44024
C	-0.72230	-5.76900	-0.28018
H	-0.41063	-6.80180	-0.41095
C	0.28782	-4.76581	-0.10258
C	-0.09947	-3.42433	0.11253
C	-1.50404	-3.06469	-0.00424
C	1.67599	-5.13821	-0.21255
H	1.88749	-6.20231	-0.35823
C	4.03676	-4.75983	-0.50856
H	4.18841	-4.68840	-1.59298
C	5.01454	-3.82095	0.20367
H	5.05791	-4.07920	1.26980
C	5.28200	-1.42599	0.12546
H	6.36198	-1.59730	0.17533
C	4.84403	-0.05228	0.10423
C	5.82363	0.98162	-0.04578
H	6.87059	0.69814	-0.11124
C	5.45897	2.29696	-0.12617

H	6.20976	3.07174	-0.25269
C	4.07743	2.67806	-0.07943
C	3.08606	1.68471	0.10268
C	3.47527	0.28744	0.23890
C	3.73626	4.06055	-0.27711
H	4.57170	4.75358	-0.41206
C	1.45701	-1.12794	-2.58828
C	1.44847	-0.99081	-4.11667
H	0.46830	-1.28803	-4.50511
H	2.22049	-1.60414	-4.58537
H	1.59829	0.05740	-4.39556
C	-2.77914	-0.06505	2.62609
C	-3.17650	0.20251	4.08314
H	-2.45416	-0.25947	4.76279
H	-4.17893	-0.16975	4.30324
H	-3.15266	1.28170	4.27309
Ca	-0.00022	0.02998	0.37791
Co	2.57587	-2.41040	0.03889
Co	-3.39214	-0.92163	-0.26029
Co	0.92927	3.53736	-0.18123
H	4.19764	-5.80159	-0.20819
H	6.02538	-3.91096	-0.21013
H	-6.37661	-3.17474	-0.68703
H	-7.06651	-0.65200	-0.98002
H	0.51880	7.23271	-0.66516
H	3.05951	6.60833	-0.30324
O	1.26430	0.66315	2.83153
C	0.69908	1.39433	3.93827
C	0.96719	-0.04318	4.05264
H	-0.32641	1.71393	3.78016
H	1.37782	2.10759	4.40254
H	0.12972	-0.73088	3.97601
H	1.84099	-0.38937	4.60156
C	-3.88041	-3.75789	-0.28092
H	-4.57011	-4.60401	-0.36280

A2-EO

Energy: -1895502.2646753

O	-1.17061	2.18525	0.05305
O	-2.43191	0.03922	-0.39251
O	-1.15391	-2.15453	-0.74555
O	1.35532	-2.22363	-0.20902
O	2.61985	-0.07803	0.23644
O	1.34916	2.14200	0.52118
O	2.88659	1.86070	-2.00161
O	0.94867	0.71092	-2.25034
O	-0.30947	-1.03730	2.07430
O	-0.45543	-3.29146	1.88678
N	-3.48449	3.66616	-0.39697
N	-4.83146	1.42518	-0.54711
N	-1.25203	-4.92795	-0.65399
N	1.29743	-4.97838	-0.02998
N	5.03664	1.25741	0.14404
N	3.75626	3.52311	0.46939
C	-4.87381	3.83652	-0.85265
H	-4.87330	3.88301	-1.94909
C	-5.67977	2.61574	-0.39300
H	-5.92495	2.72028	0.67108
C	-5.33646	0.24493	-0.74327
H	-6.41972	0.16010	-0.87169
C	-4.58386	-0.98510	-0.80018
C	-5.27941	-2.22304	-0.99846
H	-6.35973	-2.20098	-1.11153
C	-4.60507	-3.41492	-1.02414
H	-5.14848	-4.34780	-1.14703
C	-3.17967	-3.46525	-0.88889
C	-2.45350	-2.25761	-0.76975
C	-3.17828	-1.00351	-0.64840
C	-2.51076	-4.74554	-0.90840
H	-3.12597	-5.61690	-1.15401
C	-0.62426	-6.24945	-0.80506
H	-0.33543	-6.37683	-1.85634
C	0.63238	-6.28256	0.07452
H	0.34005	-6.43042	1.12156
C	3.31235	-3.61508	0.05596
C	4.74394	-3.60803	0.16210
H	5.26724	-4.55978	0.19764
C	5.44778	-2.43269	0.20680
H	6.53306	-2.44766	0.25952
C	4.77880	-1.16256	0.19347
C	3.36836	-1.13935	0.15088
C	2.63160	-2.38035	-0.01104
C	5.54286	0.06146	0.19737
H	6.63251	-0.04088	0.21503
C	5.88883	2.44638	0.01826
H	5.98141	2.68524	-1.04850
C	5.19789	3.60896	0.74252
H	5.35068	3.50509	1.82454
C	2.99081	4.56775	0.52892
H	3.45234	5.54537	0.70030
C	1.55401	4.54663	0.38010
C	0.84527	5.78648	0.27237
H	1.41038	6.71357	0.31574
C	-0.51279	5.81381	0.09980
H	-1.03525	6.76183	0.00637
C	-1.27159	4.60069	0.01486
C	-0.60479	3.36022	0.14394
C	0.83254	3.33024	0.36287
C	-2.68234	4.67982	-0.27634
H	-3.08948	5.68355	-0.43203
C	1.94434	1.36289	-2.68557
C	2.00300	1.57643	-4.20273
H	1.92391	0.61332	-4.71700
H	2.92386	2.07742	-4.50690
H	1.14544	2.18009	-4.51960
C	-0.49415	-2.20581	2.53457
C	-0.80052	-2.30089	4.03277
H	-0.00254	-1.81672	4.60496
H	-0.90578	-3.33677	4.36019
H	-1.72626	-1.75798	4.25218
Ca	0.12664	-0.03480	-0.09332
Co	3.18049	1.71936	0.19568
Co	0.03349	-3.56300	-0.26377
Co	-3.00148	1.83120	-0.22637
H	6.89462	2.27548	0.41918
H	5.61459	4.57346	0.43094

H	1.29459	-7.10617	-0.21652
H	-1.31365	-7.05924	-0.54075
H	-6.61610	2.52554	-0.95473
H	-5.31463	4.76473	-0.47256
O	-3.42630	1.86001	2.08407
C	-4.01657	0.75255	2.80057
C	-2.63830	1.16822	3.08642
H	-4.18976	-0.13598	2.19842
H	-4.82083	1.03280	3.47730
H	-1.81251	0.57245	2.70297
H	-2.43833	1.76537	3.97371
C	2.59055	-4.86439	0.03574
H	3.18862	-5.77806	0.10997

B1

Energy: -1848532.9274194

O	2.16671	1.42903	-0.27014
O	-0.08154	2.55889	-0.09556
O	-2.16355	1.13674	-0.45520
O	-1.98397	-1.40885	-0.32727
O	0.29668	-2.54383	-0.23986
O	2.35682	-1.13133	-0.14598
O	-1.30653	0.02731	2.28238
O	-3.53494	-0.06669	1.90574
N	3.43175	3.89721	-0.35457
N	1.10074	5.05373	-0.12137
N	-4.92523	0.97791	-0.60148
N	-4.75501	-1.62652	-0.30603
N	1.78447	-4.82630	-0.24166
N	3.91693	-3.37062	0.04714
C	3.46817	5.35158	-0.57904
H	3.42233	5.53005	-1.66046
C	2.23483	5.96562	0.09481
H	2.40880	6.04591	1.17505
C	-0.12590	5.48170	-0.16755
H	-0.29811	6.56017	-0.11296
C	-1.29317	4.64383	-0.28584
C	-2.58790	5.24634	-0.41554
H	-2.66013	6.33004	-0.42763
C	-3.71614	4.47622	-0.52167
H	-4.69072	4.94740	-0.61484
C	-3.64529	3.04560	-0.51652
C	-2.38222	2.41986	-0.41168
C	-1.19319	3.23672	-0.25636
C	-4.85593	2.27104	-0.67315
H	-5.77253	2.83288	-0.87736
C	-6.17397	0.25886	-0.89685
H	-6.23295	0.10154	-1.98148
C	-6.12075	-1.09938	-0.18608
H	-6.33044	-0.95996	0.88111
C	-3.19949	-3.49977	-0.32963
C	-3.07802	-4.92547	-0.33003
H	-3.98535	-5.52292	-0.34819
C	-1.85340	-5.54127	-0.30398
H	-1.78183	-6.62487	-0.30631
C	-0.64755	-4.76898	-0.27215
C	-0.73523	-3.36358	-0.26956
C	-2.02584	-2.70954	-0.31021
C	0.63066	-5.42915	-0.27754
H	0.62230	-6.52032	-0.33716
C	3.03717	-5.58827	-0.38859
H	3.25643	-5.67639	-1.45934
C	4.15275	-4.80173	0.30243
H	4.10998	-4.96778	1.38544
C	4.90161	-2.51388	0.05759
H	5.91620	-2.90161	0.18116
C	4.76630	-1.09159	-0.06331
C	5.93990	-0.26695	-0.07255
H	6.91340	-0.74445	-0.01333
C	5.83908	1.09403	-0.15402
H	6.73438	1.70890	-0.16462
C	4.56229	1.74397	-0.22266
C	3.38483	0.96290	-0.21171
C	3.49202	-0.48453	-0.13919
C	4.51562	3.18200	-0.32725
H	5.47687	3.69793	-0.40074
C	-2.51829	0.00732	2.65471
C	-2.77227	0.09274	4.16234
H	-2.19169	-0.67508	4.68315
H	-3.83068	-0.02508	4.40091
H	-2.42861	1.06367	4.53574
Ca	0.02387	0.03240	0.22589
Co	2.08680	-2.97235	-0.15303
Co	-3.46684	-0.22155	-0.27913
Co	1.65767	3.23901	-0.21260
O	0.15636	0.11129	-2.35114
C	-0.21454	-0.94225	-3.26634
H	-0.89063	-0.63212	-4.05961
H	-0.43759	-1.89301	-2.79155
C	1.15925	-0.42670	-3.23984
H	1.93732	-1.00113	-2.74503
H	1.48892	0.26238	-4.01391
H	2.94499	-6.59675	0.02722
H	5.13872	-5.11735	-0.05458
H	-6.86514	-1.79044	-0.59753
H	-7.05572	0.83087	-0.58738
H	2.02946	6.96835	-0.29462
H	4.39231	5.79737	-0.19645
O	1.60154	0.18627	2.38270
C	1.31476	0.90769	3.60176
C	1.40089	-0.55592	3.60634
H	0.32960	1.36354	3.62385
H	2.14647	1.49876	3.97884
H	0.47569	-1.12394	3.63207
H	2.29528	-1.04404	3.98706
C	-4.51630	-2.90028	-0.33352
H	-5.36573	-3.58984	-0.34140

B1’

Energy: -1848528.2564962

O	2.32567	1.52662	-0.01606
O	0.01081	2.49332	-0.15154
O	-1.97154	0.92682	-0.46468
O	-1.67336	-1.57538	-0.12793
O	0.68297	-2.53759	-0.12121
O	2.65069	-0.99783	0.15745

O	-5.63468	-0.04582	2.19988
N	3.43923	4.06361	-0.15746
N	1.02499	5.06701	-0.15651
N	-4.69154	0.59023	-0.90311
N	-4.40580	-1.98239	-0.46740
N	2.34776	-4.74951	-0.15565
N	4.37440	-3.16448	0.30925
C	3.39975	5.51056	-0.42994
H	3.43836	5.65171	-1.51706
C	2.07580	6.06120	0.11286
H	2.15001	6.19110	1.19968
C	-0.21727	5.40937	-0.32284
H	-0.46136	6.47518	-0.33677
C	-1.31788	4.49065	-0.48424
C	-2.63200	5.00109	-0.73206
H	-2.77052	6.07611	-0.80036
C	-3.69981	4.15419	-0.88743
H	-4.68949	4.55670	-1.08377
C	-3.54367	2.73542	-0.79679
C	-2.26179	2.20194	-0.54433
C	-1.13544	3.09449	-0.38536
C	-4.68771	1.87690	-1.03880
H	-5.60287	2.37073	-1.37911
C	-5.85285	-0.22136	-1.30313
H	-5.77437	-0.41836	-2.38035
C	-5.80554	-1.54215	-0.52375
H	-6.10980	-1.33583	0.50737
C	-2.72003	-3.74166	-0.38778
C	-2.49464	-5.15238	-0.46728
H	-3.35249	-5.80999	-0.57570
C	-1.22923	-5.67776	-0.41169
H	-1.07854	-6.75166	-0.47095
C	-0.08380	-4.82762	-0.28641
C	-0.27575	-3.43135	-0.21061
C	-1.61335	-2.87937	-0.23425
C	1.23508	-5.41095	-0.27246
H	1.29112	-6.49740	-0.38292
C	3.65713	-5.41249	-0.27280
H	3.93999	-5.42364	-1.33275
C	4.67775	-4.58907	0.52141
H	4.56880	-4.80232	1.59191
C	5.29406	-2.25034	0.37434
H	6.33007	-2.56844	0.51913
C	5.06170	-0.82830	0.27988
C	6.18024	0.06566	0.30352
H	7.17887	-0.35219	0.38977
C	6.00517	1.42116	0.21422
H	6.86395	2.08573	0.22642
C	4.69690	1.99185	0.09696
C	3.57321	1.13736	0.08552
C	3.75798	-0.29609	0.17987
C	4.56303	3.42239	-0.04422
H	5.49177	3.99857	-0.07595
C	-4.44635	0.03536	2.57488
Ca	0.29382	-0.02301	0.02397
Co	2.51797	-2.86930	0.04597
Co	-3.23192	-0.49130	-0.30516
Co	1.70459	3.29511	-0.12027
O	0.57632	0.29506	2.46834
C	-0.48293	0.11023	3.45398
H	-1.46965	-0.06171	3.02353
H	-0.18807	-0.51412	4.29380
C	0.15909	1.41826	3.28170
H	0.90962	1.74945	3.99489
H	-0.35878	2.20219	2.73469
H	1.83866	7.03254	-0.33329
H	4.25559	6.02904	0.01444
H	-6.79451	0.30757	-1.12111
H	-6.45443	-2.29820	-0.98014
H	3.62039	-6.44713	0.08344
H	5.70294	-4.83362	0.22459
C	-4.17005	0.39788	4.04429
H	-3.50017	1.26166	4.10617
H	-5.09881	0.62025	4.57380
H	-3.66671	-0.43667	4.54527
O	-3.39848	-0.16401	1.86165
C	-4.07424	-3.23347	-0.49343
H	-4.86572	-3.97973	-0.61162
O	0.54838	-0.15390	-2.46842
C	-0.21164	-1.03414	-3.33320
C	-0.35578	0.42095	-3.44577
H	-0.98088	-1.60905	-2.82492
H	0.39149	-1.57283	-4.05904
H	-1.22876	0.90351	-3.01553
H	0.14258	0.94923	-4.25408

B1-EO

Energy: -1752021.8538810

O	-2.00583	-1.65943	-0.29111
O	0.35986	-2.47946	-0.30275
O	2.22810	-0.79534	-0.67880
O	1.75688	1.68187	-0.30212
O	-0.63733	2.50960	-0.22994
O	-2.50663	0.84694	-0.25084
O	1.40548	-0.14797	2.20349
O	3.56230	0.35111	1.74325
N	-2.94872	-4.26800	-0.46823
N	-0.48502	-5.11298	-0.30010
N	4.95468	-0.28924	-0.84235
N	4.47327	2.24911	-0.40309
N	-2.42583	4.60479	-0.50409
N	-4.37629	2.89207	-0.24554
C	-2.80303	-5.71534	-0.69988
H	-2.76541	-5.88340	-1.78334
C	-1.48293	-6.16726	-0.06467
H	-1.61472	-6.27611	1.01907
C	0.78348	-5.37602	-0.40222
H	1.09712	-6.42327	-0.38081
C	1.82617	-4.39036	-0.54176
C	3.18255	-4.81914	-0.71371
H	3.39358	-5.88421	-0.74249
C	4.19840	-3.90760	-0.83520
H	5.22329	-4.24661	-0.95809
C	3.94313	-2.49931	-0.80277
C	2.61298	-2.04221	-0.66205
C	1.54611	-3.00780	-0.49310

C	5.04582	-1.57628	-0.95895
H	6.02007	-2.01372	-1.19715
C	6.09897	0.59311	-1.11432
H	6.11176	0.82131	-2.18776
C	5.89333	1.89011	-0.32014
H	6.13038	1.71128	0.73520
C	2.69428	3.90833	-0.44344
C	2.39001	5.30502	-0.52902
H	3.21230	6.01236	-0.59167
C	1.09537	5.75293	-0.54197
H	0.88262	6.81500	-0.62157
C	-0.00300	4.83556	-0.45776
C	0.26531	3.45510	-0.34350
C	1.63340	2.97867	-0.35997
C	-1.35141	5.33640	-0.53373
H	-1.46650	6.41712	-0.65373
C	-3.75637	5.18724	-0.74738
H	-3.92900	5.19765	-1.83084
C	-4.79838	4.29103	-0.07082
H	-4.82449	4.50439	1.00508
C	-5.23574	1.91805	-0.26105
H	-6.29971	2.16738	-0.22641
C	-4.90238	0.51670	-0.30427
C	-5.96077	-0.44767	-0.35291
H	-6.98732	-0.09309	-0.36400
C	-5.69236	-1.78884	-0.38836
H	-6.50388	-2.50938	-0.43259
C	-4.34396	-2.27359	-0.37418
C	-3.27698	-1.34913	-0.31233
C	-3.56070	0.07314	-0.28399
C	-4.11424	-3.69457	-0.45961
H	-5.00191	-4.32715	-0.54489
C	2.62514	0.00487	2.51763
C	2.99421	-0.26875	3.97765
H	2.33804	0.30087	4.64296
H	4.03528	-0.01519	4.18468
H	2.83473	-1.32957	4.20025
Ca	-0.03850	-0.00195	0.25969
Co	-2.49153	2.71880	-0.30292
Co	3.36910	0.69425	-0.41434
Co	-1.27489	-3.38682	-0.33215
H	-3.82177	6.21681	-0.38011
H	-5.79897	4.46664	-0.47971
H	6.54283	2.69040	-0.69227
H	7.05090	0.11685	-0.85513
H	-1.15842	-7.13174	-0.46937
H	-3.65070	-6.27766	-0.29463
O	-1.52259	-0.13498	2.39336
C	-1.23209	-0.92418	3.57132
C	-1.24268	0.53978	3.64236
H	-0.27068	-1.42746	3.53793
H	-2.08068	-1.48949	3.94921
H	-0.28966	1.06027	3.66034
H	-2.09790	1.05498	4.07322
C	4.07642	3.48250	-0.44311
H	4.83171	4.27363	-0.47021

B1’-EO

Energy: -1752012.6512287

O	2.29241	1.54352	-0.21616
O	-0.04053	2.47198	-0.28254
O	-1.98757	0.87238	-0.63993
O	-1.64758	-1.62203	-0.30760
O	0.72515	-2.54327	-0.32789
O	2.66107	-0.97354	-0.04999
O	-5.61300	-0.16342	2.06085
N	3.36200	4.10264	-0.30960
N	0.93122	5.06417	-0.29013
N	-4.70510	0.49164	-1.06373
N	-4.37456	-2.07380	-0.62526
N	2.42317	-4.73121	-0.32433
N	4.41954	-3.11034	0.14705
C	3.29582	5.54992	-0.57451
H	3.32428	5.69678	-1.66118
C	1.96592	6.07467	-0.02005
H	2.04482	6.19921	1.06701
C	-0.31688	5.38459	-0.45602
H	-0.58036	6.44572	-0.46595
C	-1.40006	4.44685	-0.62552
C	-2.72149	4.93555	-0.87924
H	-2.87816	6.00826	-0.94495
C	-3.77333	4.07046	-1.04195
H	-4.76947	4.45613	-1.23970
C	-3.59265	2.65423	-0.95746
C	-2.30166	2.14104	-0.70691
C	-1.19454	3.05387	-0.52919
C	-4.72298	1.77828	-1.19843
H	-5.64767	2.25778	-1.53349
C	-5.85574	-0.33924	-1.45405
H	-5.78089	-0.53955	-2.53088
C	-5.78132	-1.65541	-0.66890
H	-6.07693	-1.44823	0.36485
C	-2.66004	-3.80474	-0.55672
C	-2.41232	-5.21192	-0.63003
H	-3.26036	-5.88376	-0.72848
C	-1.13851	-5.71672	-0.57752
H	-0.97093	-6.78856	-0.62805
C	-0.00626	-4.84710	-0.46424
C	-0.22036	-3.45359	-0.40110
C	-1.56654	-2.92338	-0.41559
C	1.32113	-5.41026	-0.44175
H	1.39388	-6.49673	-0.54196
C	3.74355	-5.37432	-0.42461
H	4.03623	-5.39001	-1.48181
C	4.74387	-4.52853	0.37210
H	4.62876	-4.73538	1.44319
C	5.32239	-2.18021	0.21801
H	6.36183	-2.47911	0.37785
C	5.06646	-0.76242	0.11471
C	6.16842	0.15086	0.15444
H	7.17303	-0.24933	0.25394
C	5.97038	1.50341	0.06514
H	6.81714	2.18286	0.09023
C	4.65400	2.05136	-0.06607
C	3.54609	1.17703	-0.09691

C	3.75570	-0.25244	-0.00578
C	4.49661	3.48052	-0.20102
H	5.41560	4.07219	-0.23073
C	-4.42379	-0.00175	2.40628
Ca	0.28681	-0.04303	-0.15320
Co	2.56193	-2.84706	-0.14116
Co	-3.22260	-0.56485	-0.47739
Co	1.64017	3.30320	-0.27026
O	0.59456	0.28297	2.27946
C	-0.46148	0.12105	3.27243
H	-1.45225	-0.04502	2.84843
H	-0.16956	-0.49891	4.11667
C	0.19659	1.41892	3.08380
H	0.95521	1.74685	3.79013
H	-0.31387	2.20411	2.53186
H	1.70983	7.04469	-0.45865
H	4.14588	6.08086	-0.13383
H	-6.80447	0.17546	-1.26781
H	-6.42367	-2.42347	-1.11442
H	3.71999	-6.40634	-0.05985
H	5.77544	-4.75875	0.08614
C	-4.14265	0.48564	3.83856
H	-3.49922	1.37128	3.82204
H	-5.07174	0.72131	4.36181
H	-3.60837	-0.29057	4.39801
O	-3.37881	-0.21073	1.69207
C	-4.02311	-3.31944	-0.65091
H	-4.80340	-4.07886	-0.75888

B2

Energy: -1848536.2128708

O	-2.08220	1.32706	-0.25259
O	-2.07164	-1.18994	-0.38540
O	0.14676	-2.41279	-0.70529
O	2.33176	-1.08560	-0.42436
O	2.30336	1.46923	-0.27581
O	0.10075	2.64483	-0.05558
O	0.41515	-0.79342	2.06865
O	1.47263	-2.78910	1.91583
N	-4.86267	1.34880	-0.43981
N	-4.84190	-1.27171	-0.38325
N	1.52760	-4.80155	-0.45591
N	3.73085	-3.45315	0.00389
N	3.65722	3.81409	0.04136
N	1.38466	5.03254	0.35683
C	-6.15610	0.73614	-0.78233
H	-6.22955	0.68667	-1.87587
C	-6.17808	-0.68391	-0.20260
H	-6.38269	-0.63523	0.87378
C	-4.66448	-2.55496	-0.47386
H	-5.54783	-3.19983	-0.49264
C	-3.38234	-3.21646	-0.54127
C	-3.33038	-4.64663	-0.61269
H	-4.26367	-5.20200	-0.63264
C	-2.13075	-5.30929	-0.63272
H	-2.10727	-6.39511	-0.65727
C	-0.88863	-4.59711	-0.61567
C	-0.90452	-3.18521	-0.62098
C	-2.17173	-2.48978	-0.51310
C	0.35560	-5.33277	-0.61395
H	0.28629	-6.41616	-0.75126
C	2.75432	-5.60536	-0.56567
H	3.04400	-5.65098	-1.62324
C	3.85449	-4.89903	0.23459
H	3.70055	-5.07966	1.30523
C	4.71530	-1.22702	-0.03884
C	5.92579	-0.48202	0.11553
H	6.85773	-1.02675	0.23729
C	5.92531	0.88909	0.12808
H	6.85318	1.43941	0.25134
C	4.70072	1.61842	0.00405
C	3.49527	0.91121	-0.16894
C	3.49656	-0.53322	-0.22323
C	4.71520	3.05752	0.05563
H	5.69422	3.54070	0.10495
C	3.77109	5.28116	-0.00224
H	3.77273	5.58918	-1.05461
C	2.54698	5.86788	0.70437
H	2.68755	5.82258	1.79080
C	0.17504	5.52059	0.38258
H	0.05647	6.58765	0.58840
C	-1.02895	4.76682	0.18348
C	-2.29587	5.43632	0.20423
H	-2.31534	6.51309	0.34257
C	-3.46091	4.73529	0.04785
H	-4.41469	5.25491	0.05268
C	-3.45968	3.31248	-0.11889
C	-2.22878	2.61985	-0.12395
C	-0.99260	3.36626	0.00295
C	-4.71912	2.63167	-0.32966
H	-5.60526	3.26628	-0.42143
C	0.90526	-1.86131	2.55760
C	0.78923	-2.02467	4.07387
H	1.28438	-1.18554	4.57341
H	1.23322	-2.96143	4.41426
H	-0.26539	-1.99492	4.36696
Ca	0.12089	0.04018	-0.15657
Co	1.86527	3.24180	0.00036
Co	1.91277	-2.93412	-0.25760
Co	-3.47991	0.05048	-0.27801
O	0.08124	0.35432	-2.65257
C	1.20384	0.75100	-3.47696
H	1.36291	0.11856	-4.34640
H	2.09051	1.03635	-2.91783
C	0.00356	1.59108	-3.40009
H	0.01727	2.48848	-2.78750
H	-0.71719	1.57450	-4.21356
H	4.70150	5.62709	0.45949
H	2.39058	6.91405	0.42142
H	4.84676	-5.27429	-0.03941
H	2.60220	-6.62990	-0.20893
H	-6.95803	-1.29085	-0.67471
H	-6.99837	1.32850	-0.40907
O	-3.73191	0.10824	2.05897
C	-3.64862	-1.06251	2.90260
C	-2.69836	0.04245	3.07452

H	-3.32653	-1.96677	2.39219
H	-4.47958	-1.17696	3.59494
H	-1.68232	-0.06862	2.70230
H	-2.84358	0.74460	3.89270
C	4.76283	-2.67064	0.04321
H	5.75159	-3.11753	0.18315

B2-EO

Energy: -1752021.6122334

O	-2.39946	0.54145	-0.38139
O	-1.50702	-1.81336	-0.50298
O	0.99900	-2.18651	-0.82578
O	2.57235	-0.18698	-0.51654
O	1.65585	2.18993	-0.39619
O	-0.81342	2.54411	-0.20566
O	0.66134	-0.65600	1.96016
O	2.39006	-2.10705	1.79668
N	-5.01012	-0.41673	-0.59993
N	-4.07206	-2.86228	-0.49038
N	3.13123	-3.94181	-0.57464
N	4.72291	-1.90422	-0.13318
N	2.10137	4.88089	-0.26703
N	-0.45604	5.24608	0.00205
C	-6.00779	-1.45375	-0.91371
H	-6.06464	-1.55125	-2.00496
C	-5.52777	-2.77584	-0.30334
H	-5.72623	-2.77333	0.77489
C	-3.45628	-4.00277	-0.55410
H	-4.05754	-4.91651	-0.55125
C	-2.02366	-4.17359	-0.62016
C	-1.47512	-5.49539	-0.67440
H	-2.15476	-6.34273	-0.67715
C	-0.11933	-5.69663	-0.70058
H	0.28274	-6.70574	-0.71426
C	0.79400	-4.59457	-0.70497
C	0.28406	-3.27756	-0.72233
C	-1.14491	-3.06858	-0.61056
C	2.21722	-4.85016	-0.71260
H	2.52916	-5.89141	-0.83819
C	4.56105	-4.26586	-0.68845
H	4.84345	-4.21476	-1.74769
C	5.34821	-3.21296	0.10117
H	5.27394	-3.43032	1.17341
C	4.86283	0.52502	-0.21538
C	5.73884	1.65512	-0.12147
H	6.80599	1.47641	-0.02465
C	5.25749	2.93673	-0.14359
H	5.93653	3.78125	-0.07480
C	3.84920	3.18917	-0.23795
C	2.96152	2.09551	-0.33469
C	3.47571	0.74094	-0.36451
C	3.36043	4.53686	-0.24942
H	4.10913	5.33350	-0.25297
C	1.69970	6.29114	-0.39652
H	1.60907	6.52493	-1.46400
C	0.34037	6.45203	0.28739
H	0.47854	6.51511	1.37317
C	-1.75534	5.29228	-0.01672
H	-2.23916	6.26427	0.10736
C	-2.62025	4.15045	-0.16878
C	-4.03688	4.33931	-0.22077
H	-4.43284	5.34889	-0.16765
C	-4.88295	3.26764	-0.34091
H	-5.95666	3.42412	-0.38929
C	-4.38398	1.92909	-0.40277
C	-2.98782	1.71059	-0.34134
C	-2.09685	2.84354	-0.23556
C	-5.32254	0.84043	-0.57246
H	-6.37141	1.11969	-0.70720
C	1.51382	-1.46821	2.44314
C	1.45357	-1.69394	3.95468
H	1.45929	-0.73226	4.47673
H	2.28608	-2.30667	4.30420
H	0.51258	-2.19328	4.21056
Ca	0.11436	0.10432	-0.23259
Co	0.61751	3.71646	-0.21096
Co	2.83695	-2.06011	-0.37607
Co	-3.26081	-1.14597	-0.40193
H	2.44445	6.96451	0.04013
H	-0.17106	7.35972	-0.04850
H	6.40720	-3.21722	-0.17991
H	4.77829	-5.27637	-0.32556
H	-6.04856	-3.62945	-0.75041
H	-7.00197	-1.18400	-0.54198
O	-3.53841	-1.24628	1.93221
C	-2.54323	-1.18992	2.98552
C	-3.54413	-0.12597	2.84458
H	-1.52027	-1.01581	2.65675
H	-2.68044	-1.94509	3.75672
H	-3.25522	0.82315	2.40056
H	-4.40181	-0.09551	3.51277
C	5.41529	-0.80841	-0.11860
H	6.49989	-0.87876	0.00563

C1-EO

Energy: -1752015.9396356

O	0.24922	2.52441	-0.28435
O	2.47892	1.41316	-0.02417
O	2.64289	-1.14992	0.08966
O	0.58268	-2.54321	-0.26253
O	-1.72826	-1.43454	-0.32871
O	-1.84673	1.08006	-0.57482
O	-4.16003	-0.04981	1.59515
O	-3.40788	0.56922	3.64259
N	1.41178	4.99469	-0.26412
N	3.73863	3.84974	-0.18683
N	4.20278	-3.39167	0.16926
N	2.11597	-4.81388	-0.42156
N	-4.42866	-1.66424	-0.93757
N	-4.53163	0.91862	-1.30442
C	2.50956	5.92823	0.03613
H	2.55445	6.05676	1.12393
C	3.80987	5.29547	-0.46247
H	3.89964	5.43330	-1.54656
C	4.82499	3.14012	-0.06307
H	5.78514	3.66183	-0.09083

C	4.87306	1.71363	0.07957
C	6.14321	1.06212	0.18757
H	7.04121	1.67223	0.20516
C	6.23150	-0.30151	0.25767
H	7.19986	-0.78624	0.33559
C	5.05596	-1.11744	0.21736
C	3.79014	-0.50638	0.13148
C	3.69240	0.93463	0.06712
C	5.18767	-2.55084	0.27380
H	6.19458	-2.94901	0.41960
C	4.41976	-4.83914	0.32784
H	4.26390	-5.08938	1.38373
C	3.38118	-5.56054	-0.53239
H	3.69604	-5.55158	-1.58262
C	-0.30558	-4.75452	-0.65396
C	-1.48339	-5.53062	-0.90448
H	-1.38334	-6.60358	-1.03708
C	-2.71031	-4.93174	-0.98845
H	-3.59582	-5.52693	-1.19157
C	-2.85999	-3.51719	-0.82214
C	-1.72541	-2.72744	-0.53427
C	-0.42140	-3.35771	-0.47154
C	-4.17439	-2.93374	-0.96532
H	-5.00590	-3.62777	-1.11596
C	-5.79666	-1.13760	-1.01482
H	-6.14171	-0.97229	0.01130
C	-5.73763	0.20335	-1.75541
H	-5.64572	0.02504	-2.83404
C	-4.44060	2.20802	-1.38862
H	-5.31284	2.77003	-1.73412
C	-3.25499	2.98083	-1.09560
C	-3.31179	4.40348	-1.22651
H	-4.25982	4.86298	-1.49066
C	-2.20105	5.18100	-1.02852
H	-2.26018	6.26082	-1.12533
C	-0.94275	4.58544	-0.70320
C	-0.85496	3.18537	-0.56692
C	-2.03145	2.36602	-0.74348
C	0.20865	5.42597	-0.49905
H	0.04472	6.50561	-0.53634
C	-4.31871	0.07637	2.80411
C	-5.58437	-0.33134	3.51790
H	-5.54778	-1.40937	3.70857
H	-6.44575	-0.13094	2.87849
H	-5.68896	0.18529	4.47243
Ca	0.33868	-0.02032	0.22179
Co	-3.16492	-0.26522	-0.70170
Co	2.38515	-2.97551	-0.08475
Co	1.96412	3.19918	-0.16809
O	0.04941	0.04766	2.49549
C	-1.11035	-0.26292	3.15943
H	-0.95786	-0.50817	4.23474
H	-1.65440	-1.14230	2.74134
C	-2.09769	0.91957	3.09990
H	-2.21902	1.24831	2.06701
H	-1.75486	1.75413	3.71627
H	-6.47741	-1.83757	-1.51102
H	-6.64453	0.79195	-1.58176
H	3.26120	-6.60217	-0.21759
H	5.43933	-5.12604	0.05139
H	4.68196	5.75286	0.01589
H	2.34133	6.90872	-0.42085
C	0.97204	-5.40350	-0.63270
H	0.97834	-6.47973	-0.82412

C2-EO

Energy: -1752017.2043935

O	-2.12306	1.03298	-0.40221
O	-1.90740	-1.49819	-0.19456
O	0.41125	-2.56605	-0.33440
O	2.45064	-1.12766	-0.12223
O	2.21608	1.42250	-0.26571
O	-0.04995	2.50414	-0.32306
O	0.38531	0.29694	2.34289
O	-1.08531	0.64319	4.02393
N	-4.86995	0.80716	-0.82924
N	-4.66398	-1.77855	-0.46485
N	1.96762	-4.80294	-0.59723
N	4.06378	-3.33768	-0.15184
N	3.44036	3.90837	-0.52853
N	1.08132	5.02317	-0.46011
C	-6.09879	0.05741	-1.13362
H	-6.12935	-0.13194	-2.21439
C	-6.03778	-1.27820	-0.37997
H	-6.24597	-1.10510	0.68144
C	-4.38988	-3.03879	-0.56658
H	-5.21640	-3.74983	-0.65815
C	-3.05174	-3.59705	-0.57192
C	-2.88931	-5.00650	-0.76461
H	-3.77947	-5.61752	-0.88561
C	-1.64991	-5.58766	-0.80070
H	-1.54651	-6.65853	-0.94810
C	-0.46621	-4.79352	-0.65217
C	-0.59456	-3.39956	-0.46135
C	-1.90649	-2.78811	-0.40149
C	0.82189	-5.41506	-0.72999
H	0.83702	-6.48998	-0.92839
C	3.23687	-5.52088	-0.80595
H	3.47422	-5.50039	-1.87634
C	4.32137	-4.78142	-0.01967
H	4.24910	-5.04099	1.04304
C	4.86699	-1.04361	-0.15738
C	6.02264	-0.20257	-0.19381
H	7.00576	-0.66285	-0.17307
C	5.89600	1.15978	-0.26619
H	6.78017	1.78902	-0.30628
C	4.60981	1.78350	-0.30428
C	3.44916	0.97838	-0.24129
C	3.58552	-0.45744	-0.16514
C	4.53627	3.21712	-0.45912
H	5.48853	3.74647	-0.54971
C	3.45888	5.34942	-0.83491
H	3.46203	5.46253	-1.92598
C	2.18439	5.97469	-0.25721
H	2.30661	6.12806	0.82218
C	-0.14798	5.41748	-0.60743

H	-0.34158	6.49243	-0.65854
C	-1.29417	4.54759	-0.69517
C	-2.58986	5.11060	-0.92727
H	-2.67811	6.18612	-1.04954
C	-3.70078	4.31077	-1.00272
H	-4.67595	4.75029	-1.19294
C	-3.61239	2.89285	-0.83358
C	-2.35135	2.30903	-0.58268
C	-1.17568	3.15064	-0.53096
C	-4.80916	2.08986	-0.99037
H	-5.71415	2.62561	-1.29337
C	0.10916	0.34688	3.54373
C	1.13227	0.08991	4.61785
H	0.69927	0.16919	5.61427
H	1.94794	0.81057	4.50935
H	1.55544	-0.90825	4.47438
Ca	0.11617	-0.03025	-0.04379
Co	1.67584	3.22255	-0.38659
Co	2.22554	-2.96028	-0.27576
Co	-3.43712	-0.34087	-0.27721
H	4.35566	5.83524	-0.43677
H	1.97429	6.94468	-0.71980
H	5.32340	-5.04546	-0.37255
H	3.16376	-6.56667	-0.49015
H	-6.76576	-1.99423	-0.77859
H	-6.99684	0.62270	-0.86108
O	-3.90144	-0.14759	1.77034
C	-2.92079	-0.40919	2.69138
C	-2.18692	0.88936	3.08518
H	-2.14335	-1.12016	2.33497
H	-3.31410	-0.85426	3.63340
H	-1.79359	1.38659	2.19918
H	-2.85018	1.56894	3.62370
C	5.03409	-2.47472	-0.11230
H	6.05769	-2.84995	-0.03961

D1-EO

Energy: -1870358.5633142

O	-0.68417	-2.18724	-0.61997
O	-2.63408	-0.61697	-0.40471
O	-2.23810	1.87114	-0.04859
O	0.09654	2.79380	-0.20775
O	2.10204	1.21744	-0.36542
O	1.68147	-1.24352	-0.76266
O	4.12402	-0.76931	1.51039
O	3.16159	-1.40060	3.46532
N	-2.39007	-4.35839	-0.83522
N	-4.41997	-2.72229	-0.70425
N	-3.27844	4.42013	0.23441
N	-0.89096	5.38912	-0.17918
N	4.80417	0.88810	-0.91922
N	4.34961	-1.62725	-1.45840
C	-3.67602	-5.03486	-0.60767
H	-3.77696	-5.20762	0.47041
C	-4.79080	-4.09666	-1.08261
H	-4.86614	-4.13937	-2.17626
C	-5.31815	-1.80113	-0.53091
H	-6.37153	-2.08831	-0.58887
C	-5.04337	-0.40507	-0.29073
C	-6.13890	0.50192	-0.12392
H	-7.15007	0.10631	-0.14640
C	-5.92635	1.84314	0.05350
H	-6.76734	2.51950	0.17462
C	-4.60053	2.38347	0.07788
C	-3.49914	1.51246	-0.06359
C	-3.72353	0.09543	-0.25701
C	-4.42078	3.80369	0.25705
H	-5.32419	4.39493	0.42901
C	-3.16870	5.85771	0.52906
H	-3.00471	5.97053	1.60778
C	-1.95795	6.40289	-0.23541
H	-2.22640	6.55675	-1.28794
C	1.45955	4.78527	-0.38716
C	2.78610	5.29585	-0.55751
H	2.93063	6.37164	-0.59013
C	3.85427	4.44971	-0.69248
H	4.85396	4.84931	-0.83613
C	3.68244	3.02950	-0.65660
C	2.39222	2.49270	-0.44976
C	1.25882	3.38810	-0.33739
C	4.83696	2.18097	-0.84389
H	5.80469	2.68274	-0.93222
C	6.02584	0.08070	-1.02669
H	6.30925	-0.22108	-0.01265
C	5.69077	-1.16504	-1.85447
H	5.66084	-0.90243	-2.91940
C	3.97827	-2.85554	-1.64146
H	4.71441	-3.56932	-2.02199
C	2.64442	-3.36554	-1.42135
C	2.38457	-4.75161	-1.66858
H	3.21245	-5.39232	-1.95793
C	1.12174	-5.26783	-1.54987
H	0.94037	-6.32240	-1.73562
C	0.01519	-4.43263	-1.19311
C	0.23915	-3.06094	-0.94005
C	1.58033	-2.52154	-1.03457
C	-1.29831	-5.01800	-1.07681
H	-1.36427	-6.10336	-1.19314
C	4.19364	-1.03679	2.70459
C	5.47842	-0.97000	3.49406
H	5.45728	-1.65234	4.34480
H	5.60395	0.04924	3.87551
H	6.32318	-1.19666	2.84225
Ca	-0.24745	0.26639	0.06143
Co	3.26098	-0.21274	-0.78948
Co	-1.57745	3.62554	-0.04448
Co	-2.53752	-2.47703	-0.63540
O	-0.07448	-0.06397	2.32819
C	1.10152	-0.06868	3.03646
H	0.96501	0.08982	4.13005
H	1.82645	0.71972	2.72343
C	1.83182	-1.41483	2.86017
H	1.92780	-1.64649	1.79895
H	1.30050	-2.22286	3.36761
H	6.85115	0.64568	-1.47311
H	6.44470	-1.94723	-1.71656

H	-1.62703	7.36098	0.17860
H	-4.08325	6.39721	0.26172
H	-5.75896	-4.38507	-0.66056
H	-3.72375	-6.00133	-1.11996
C	0.35960	5.71437	-0.30808
H	0.61127	6.77579	-0.38260
O	-0.75702	-4.10531	3.57403
C	-1.78490	-3.77566	3.12595
O	-2.81732	-3.45352	2.67885

D2-EO

Energy: -1870342.4605741

O	-1.79938	0.19458	-0.89346
O	-0.62826	-2.05077	-0.65207
O	1.90847	-2.13441	-0.41106
O	3.15951	-0.02228	0.05913
O	1.97774	2.24980	-0.19445
O	-0.48963	2.36741	-0.58705
O	-7.04760	0.10179	1.32223
O	-5.76864	-0.36234	3.13778
N	-4.17371	-1.07339	-1.60380
N	-3.00793	-3.38767	-1.19620
N	4.21656	-3.59369	-0.25947
N	5.47797	-1.42981	0.42465
N	2.13982	4.99495	-0.28829
N	-0.44200	5.09227	-0.55320
C	-4.96201	-2.23160	-2.05652
H	-4.79112	-2.36228	-3.13269
C	-4.46708	-3.47311	-1.30348
H	-4.86438	-3.45979	-0.28303
C	-2.25472	-4.43948	-1.21509
H	-2.71964	-5.41492	-1.38751
C	-0.81783	-4.43452	-1.02101
C	-0.10132	-5.67185	-1.09453
H	-0.66168	-6.58275	-1.28570
C	1.25698	-5.72642	-0.92597
H	1.78213	-6.67525	-0.97983
C	2.01065	-4.53325	-0.67691
C	1.33188	-3.29695	-0.61053
C	-0.10628	-3.24224	-0.76489
C	3.43296	-4.60501	-0.52081
H	3.89147	-5.59043	-0.63828
C	5.67955	-3.75951	-0.21936
H	6.06906	-3.64301	-1.23768
C	6.24530	-2.66028	0.68211
H	6.10049	-2.93385	1.73382
C	5.31969	0.99614	0.42821
C	6.04880	2.22218	0.54339
H	7.11600	2.17814	0.73826
C	5.42086	3.42995	0.40043
H	5.98517	4.35431	0.47919
C	4.01545	3.50404	0.14010
C	3.26515	2.30947	0.04012
C	3.93333	1.03624	0.18207
C	3.40521	4.78853	-0.05624
H	4.07062	5.65495	-0.02330
C	1.63732	6.34422	-0.60183
H	1.74425	6.50538	-1.68103
C	0.15881	6.39247	-0.21216
H	0.06695	6.53307	0.87131
C	-1.70310	4.99525	-0.85718
H	-2.28858	5.91541	-0.92780
C	-2.40297	3.75921	-1.09055
C	-3.78177	3.78111	-1.46800
H	-4.27551	4.73948	-1.59702
C	-4.46945	2.61076	-1.66993
H	-5.51363	2.63935	-1.96838
C	-3.84663	1.33791	-1.49162
C	-2.48875	1.28597	-1.10064
C	-1.76017	2.51758	-0.92095
C	-4.60757	0.13482	-1.77077
H	-5.61160	0.28160	-2.17978
C	-6.74247	0.29501	2.48590
C	-7.41953	1.29544	3.39445
H	-6.68372	1.99957	3.79318
H	-7.87253	0.77945	4.24630
H	-8.18740	1.83548	2.84116
Ca	0.61184	0.07063	-0.33269
Co	0.78899	3.67805	-0.39212
Co	3.69092	-1.79550	-0.03072
Co	-2.47198	-1.58984	-0.89404
H	2.20952	7.11833	-0.08003
H	-0.35762	7.21847	-0.71141
H	7.31564	-2.51101	0.50808
H	5.96187	-4.75254	0.14528
H	-4.79237	-4.39415	-1.80086
H	-6.03509	-2.07724	-1.89918
O	-3.00514	-1.72796	1.12916
C	-3.73385	-0.74725	1.75605
C	-4.99814	-1.35055	2.39326
H	-4.07614	0.06587	1.08228
H	-3.17980	-0.22923	2.57609
H	-5.63363	-1.79469	1.62466
H	-4.72809	-2.11125	3.13053
C	6.01633	-0.25726	0.57763
H	7.07427	-0.20387	0.84542
C	1.33559	-0.96389	4.19185
O	1.15802	-1.65303	5.11789
O	1.51713	-0.27226	3.26466

E1-EO

Energy: -1870377.5219692

O	-0.45404	-2.32976	-0.84289
O	-2.59407	-0.91118	-0.83288
O	-2.37308	1.60671	-0.44572
O	-0.10915	2.68817	-0.44846
O	1.99993	1.25583	-0.52118
O	1.82016	-1.20992	-0.99979
O	3.88923	-0.42738	1.60779
O	2.87004	-0.78605	3.59639
N	-1.91532	-4.62210	-0.32132
N	-4.11462	-3.19963	-0.40988
N	-3.58203	4.04141	0.09821
N	-1.26979	5.20081	-0.25255
N	4.77411	1.13086	-0.80422
N	4.55943	-1.43626	-1.27981

C	-3.12348	-5.36254	0.06898
H	-3.19413	-5.33346	1.16278
C	-4.33585	-4.64710	-0.53948
H	-4.40549	-4.89012	-1.60735
C	-5.09950	-2.36249	-0.33952
H	-6.12002	-2.75493	-0.30680
C	-4.95299	-0.92410	-0.28477
C	-6.10180	-0.11794	-0.01057
H	-7.06147	-0.60874	0.12384
C	-6.00370	1.24447	0.10081
H	-6.88379	1.84281	0.31719
C	-4.74058	1.90283	-0.03920
C	-3.59331	1.13208	-0.32736
C	-3.70362	-0.30028	-0.49717
C	-4.66603	3.32832	0.16407
H	-5.60218	3.83602	0.41146
C	-3.57877	5.47106	0.45145
H	-3.43067	5.55275	1.53536
C	-2.40702	6.13529	-0.27866
H	-2.67762	6.30894	-1.32750
C	1.12381	4.77009	-0.37813
C	2.42140	5.37237	-0.41303
H	2.49581	6.45470	-0.36417
C	3.55204	4.60530	-0.51496
H	4.53025	5.07587	-0.55122
C	3.47673	3.17756	-0.57469
C	2.21221	2.55165	-0.51226
C	1.01687	3.36362	-0.44251
C	4.70343	2.41905	-0.68828
H	5.63431	2.99263	-0.66975
C	6.05876	0.41556	-0.80124
H	6.29580	0.16894	0.23959
C	5.88264	-0.88059	-1.60312
H	5.90495	-0.65513	-2.67657
C	4.31511	-2.70904	-1.32817
H	5.14227	-3.38964	-1.54840
C	3.01533	-3.31125	-1.13022
C	2.89186	-4.73718	-1.08989
H	3.78859	-5.34156	-1.19151
C	1.67199	-5.33655	-0.90443
H	1.59928	-6.41882	-0.84604
C	0.47574	-4.56090	-0.77734
C	0.55897	-3.15581	-0.87643
C	1.85254	-2.52288	-1.00770
C	-0.78107	-5.22325	-0.50801
H	-0.75118	-6.31379	-0.42900
C	3.88998	-0.37357	2.82810
C	5.04657	0.11784	3.65843
H	5.65929	-0.74120	3.95254
H	4.69538	0.60730	4.56822
H	5.66049	0.79875	3.06884
Ca	-0.30750	0.11762	-0.53855
Co	3.30616	-0.07277	-0.83566
Co	-1.83875	3.39193	-0.26877
Co	-2.25841	-2.75134	-0.47951
O	-0.36701	-0.75283	1.82959
C	0.68065	-0.24655	2.66783
H	0.26899	0.13257	3.60488
H	1.14868	0.57175	2.11242
C	1.71175	-1.34332	2.93150
H	2.01444	-1.81085	1.99339
H	1.30810	-2.08781	3.61585
H	6.86805	1.02952	-1.21040
H	6.68637	-1.59221	-1.38631
H	-2.15120	7.09857	0.17450
H	-4.52843	5.95317	0.19737
H	-5.26669	-4.96120	-0.05513
H	-3.08167	-6.41042	-0.24760
C	-0.04116	5.61809	-0.29713
H	0.13951	6.69619	-0.28214
O	-1.20607	-1.74451	3.71417
C	-1.31377	-1.65307	2.49060
O	-2.10540	-2.19407	1.68809

E2-EO

Energy: -1870380.6057640

O	0.43310	2.51496	-0.36505
O	2.63930	1.31495	-0.22717
O	2.69863	-1.22605	-0.03637
O	0.58855	-2.54659	-0.36608
O	-1.63592	-1.34181	-0.70160
O	-1.66076	1.16742	-0.89248
O	-5.23630	0.10434	1.57018
O	-4.37905	0.35257	3.65041
N	1.70724	4.97189	-0.25802
N	4.00294	3.73403	-0.17714
N	4.18900	-3.55416	0.14564
N	2.04115	-4.91386	-0.44620
N	-4.30952	-1.46754	-1.42859
N	-4.29426	1.11939	-1.77629
C	2.83066	5.84342	0.11708
H	2.85671	5.91057	1.21154
C	4.12053	5.18676	-0.38834
H	4.22694	5.36784	-1.46508
C	5.05143	2.97944	-0.04693
H	6.03386	3.45855	-0.01993
C	5.03368	1.54061	0.04971
C	6.27187	0.84062	0.21638
H	7.18930	1.41734	0.28817
C	6.30806	-0.52627	0.28058
H	7.25424	-1.04490	0.40311
C	5.10729	-1.30130	0.18879
C	3.86862	-0.64020	0.04136
C	3.83165	0.80508	-0.04698
C	5.19233	-2.73890	0.26539
H	6.18419	-3.16261	0.44427
C	4.34004	-5.00413	0.34443
H	4.16374	-5.22045	1.40528
C	3.27999	-5.70888	-0.50809
H	3.61021	-5.73957	-1.55378
C	-0.36511	-4.73364	-0.77550
C	-1.56073	-5.46192	-1.07458
H	-1.50330	-6.54257	-1.16505
C	-2.75361	-4.81490	-1.25850
H	-3.65166	-5.37838	-1.49396
C	-2.84351	-3.39011	-1.15988

C	-1.68871	-2.64540	-0.83444
C	-0.42777	-3.32932	-0.64038
C	-4.11634	-2.74936	-1.39478
H	-4.97468	-3.40747	-1.55525
C	-5.65282	-0.88499	-1.57472
H	-6.04664	-0.71322	-0.56742
C	-5.50213	0.45768	-2.29806
H	-5.35864	0.28706	-3.37229
C	-4.16743	2.41048	-1.78906
H	-5.01342	3.01087	-2.13443
C	-2.97812	3.13395	-1.40725
C	-2.98073	4.56368	-1.48116
H	-3.89449	5.06725	-1.78268
C	-1.85665	5.28914	-1.18712
H	-1.87210	6.37328	-1.24919
C	-0.63912	4.64042	-0.80582
C	-0.60999	3.23245	-0.70703
C	-1.80040	2.46634	-1.00670
C	0.52635	5.44252	-0.51764
H	0.38835	6.52702	-0.51902
C	-5.37171	0.07782	2.78085
C	-6.65143	-0.25172	3.50566
H	-6.49072	-1.09656	4.18124
H	-7.43159	-0.49451	2.78519
H	-6.96213	0.60091	4.11641
Ca	0.43267	-0.00584	0.09706
Co	-2.98732	-0.12800	-1.18813
Co	2.38127	-3.06702	-0.16659
Co	2.20026	3.13676	-0.24467
O	-1.02301	-0.21594	2.22751
C	-2.27647	-0.56417	2.81386
H	-2.11256	-1.12053	3.73986
H	-2.79178	-1.19508	2.08665
C	-3.08767	0.69810	3.09877
H	-3.21922	1.28709	2.18887
H	-2.59351	1.29459	3.86571
H	-6.32801	-1.55522	-2.11710
H	-6.39263	1.08074	-2.16539
H	3.11766	-6.73708	-0.16899
H	5.34795	-5.34615	0.08699
H	4.99954	5.59881	0.11782
H	2.71395	6.85431	-0.28723
C	0.88105	-5.45235	-0.66957
H	0.83385	-6.53429	-0.81974
O	-0.17987	0.20641	4.32202
C	0.04331	0.17694	3.11403
O	1.07092	0.43056	2.42812

E1'-EO

Energy: -1870383.0126958

O	-1.86397	-0.84110	-1.16802
O	-1.64360	1.64603	-0.94697
O	0.63857	2.67508	-0.38817
O	2.72974	1.27019	-0.48378
O	2.49319	-1.25930	-0.55111
O	0.23574	-2.31752	-1.13197
O	-4.88931	-0.44270	2.14249
O	-3.32210	-0.28581	3.76054
N	-4.59256	-0.62437	-1.26075
N	-4.34050	1.95997	-1.28071
N	2.14863	4.94359	0.17110
N	4.30993	3.48894	0.01455
N	3.56521	-3.75339	0.02077
N	1.29919	-4.85081	-0.70403
C	-5.87005	0.08988	-1.09263
H	-6.08109	0.13701	-0.01870
C	-5.68892	1.49989	-1.65577
H	-5.74459	1.47502	-2.75052
C	-4.08764	3.22226	-1.10652
H	-4.91407	3.93194	-1.19256
C	-2.78774	3.77155	-0.81179
C	-2.65223	5.17772	-0.59217
H	-3.53772	5.80366	-0.64710
C	-1.42940	5.72942	-0.31259
H	-1.33843	6.79833	-0.14361
C	-0.25285	4.92085	-0.23234
C	-0.35681	3.52712	-0.44537
C	-1.64537	2.94915	-0.74705
C	1.00395	5.54990	0.10033
H	0.96971	6.61998	0.32122
C	3.36398	5.63572	0.63217
H	3.41446	5.54101	1.72377
C	4.57325	4.93559	0.00067
H	4.67888	5.25394	-1.04371
C	5.08421	1.18375	0.08331
C	6.19889	0.32614	0.35501
H	7.16188	0.77694	0.57631
C	6.05554	-1.03694	0.36077
H	6.90439	-1.67378	0.59277
C	4.79323	-1.65132	0.08220
C	3.68888	-0.83350	-0.24146
C	3.83324	0.60643	-0.22075
C	4.66679	-3.08866	0.18191
H	5.57410	-3.64107	0.44310
C	3.49624	-5.20078	0.26746
H	3.19357	-5.34781	1.31111
C	2.42850	-5.79116	-0.66142
H	2.83687	-5.88343	-1.67576
C	0.09293	-5.24524	-0.95936
H	-0.09484	-6.31677	-1.07379
C	-1.04911	-4.36779	-1.09975
C	-2.35685	-4.94128	-1.20005
H	-2.45103	-6.02337	-1.18493
C	-3.47407	-4.15556	-1.29456
H	-4.46075	-4.60463	-1.35690
C	-3.36596	-2.72730	-1.28711
C	-2.08677	-2.13311	-1.21297
C	-0.90143	-2.96411	-1.14958
C	-4.55634	-1.92735	-1.28569
H	-5.50774	-2.46567	-1.28289
C	-4.49293	0.04680	3.18459
C	-5.21810	1.09805	3.98679
H	-5.25843	0.81420	5.04126
H	-6.22563	1.23016	3.59364
H	-4.67523	2.04645	3.92172
Ca	0.42810	0.13181	-0.58460

Co	1.86648	-3.04095	-0.46871
Co	2.46083	3.10175	-0.18109
Co	-3.10933	0.53957	-1.19064
O	-0.32065	-2.29512	3.22123
C	-1.17404	-1.30597	3.80065
H	-0.70447	-0.32014	3.76617
H	-1.31319	-1.60424	4.84325
C	-2.51453	-1.27075	3.07622
H	-3.01349	-2.24380	3.11819
H	-2.38360	-0.98306	2.03190
H	4.46583	-5.68799	0.11681
H	2.11687	-6.78629	-0.32591
H	5.49770	5.18513	0.53178
H	3.34387	6.70098	0.38002
H	-6.46212	2.18094	-1.28581
H	-6.69189	-0.43340	-1.59269
C	5.26287	2.61467	0.13208
H	6.28296	2.97839	0.28182
C	0.36087	-1.95297	2.06150
O	1.07708	-2.88306	1.62434
O	0.18871	-0.79152	1.60355

F1-EO

Energy: -1895499.4318341

O	-0.04023	2.58607	-0.11242
O	2.25678	1.66750	0.45820
O	2.58262	-0.87252	0.76649
O	0.53589	-2.45912	0.36247
O	-1.81781	-1.49047	-0.00311
O	-2.02884	1.00874	-0.46226
O	-4.42363	-0.12854	1.61580
O	-3.69659	0.52496	3.66346
O	1.01896	-0.39189	-1.91868
O	2.47433	-2.12941	-1.89786
N	0.99325	5.15254	-0.21931
N	3.38500	4.16500	0.05725
N	4.30106	-3.02399	0.47688
N	2.28218	-4.57581	-0.10265
N	-4.42582	-1.89824	-0.85112
N	-4.63122	0.64470	-1.38166
C	2.01270	6.17079	0.07008
H	1.99138	6.37521	1.14785
C	3.37591	5.58958	-0.31604
H	3.51017	5.65959	-1.40282
C	4.50390	3.52487	0.22592
H	5.43532	4.09583	0.17343
C	4.63205	2.10791	0.43629
C	5.94447	1.53655	0.49793
H	6.80463	2.19817	0.45110
C	6.11360	0.18129	0.57991
H	7.11211	-0.24667	0.59646
C	4.98933	-0.70311	0.62038
C	3.67794	-0.17318	0.64962
C	3.50043	1.26368	0.51834
C	5.22185	-2.12715	0.63548
H	6.25529	-2.45727	0.77990
C	4.60363	-4.45633	0.59353
H	4.48018	-4.75158	1.64345
C	3.59379	-5.21494	-0.27174
H	3.87937	-5.12675	-1.32738
C	-0.14287	-4.69549	-0.25023
C	-1.24385	-5.54931	-0.58003
H	-1.05238	-6.60689	-0.73957
C	-2.50841	-5.04653	-0.72328
H	-3.33372	-5.70015	-0.99143
C	-2.76564	-3.64721	-0.55917
C	-1.71117	-2.78329	-0.18208
C	-0.37278	-3.32234	0.00079
C	-4.09401	-3.15098	-0.81954
H	-4.86859	-3.89806	-1.01650
C	-5.80803	-1.45741	-1.06195
H	-6.24452	-1.25185	-0.07835
C	-5.75891	-0.16080	-1.87866
H	-5.57279	-0.39842	-2.93369
C	-4.59765	1.92930	-1.55215
H	-5.46615	2.41535	-2.00637
C	-3.48347	2.78585	-1.22489
C	-3.60480	4.19252	-1.46540
H	-4.55156	4.57666	-1.83441
C	-2.55471	5.04072	-1.24348
H	-2.65964	6.10610	-1.42723
C	-1.29394	4.54491	-0.77890
C	-1.13941	3.16214	-0.52764
C	-2.26278	2.26544	-0.73715
C	-0.21435	5.47487	-0.57148
H	-0.44297	6.53393	-0.72008
C	-4.57224	-0.03134	2.82866
C	-5.78915	-0.55366	3.55440
H	-5.63337	-1.61340	3.78394
H	-6.66474	-0.47137	2.90865
H	-5.95363	-0.02034	4.49150
C	1.81583	-1.20843	-2.46692
C	2.01142	-1.05411	-3.97986
H	1.03889	-1.04507	-4.48208
H	2.62900	-1.85352	-4.39340
H	2.48892	-0.09031	-4.18865
Ca	0.25726	0.04273	0.35141
Co	-3.26018	-0.42006	-0.59006
Co	2.42369	-2.69930	0.23910
Co	1.64919	3.39573	0.05913
O	-0.16751	0.36616	2.62369
C	-1.31691	-0.07632	3.22383
H	-1.19900	-0.31706	4.30673
H	-1.74132	-1.00244	2.76923
C	-2.42095	0.99472	3.12260
H	-2.56026	1.28550	2.08118
H	-2.17098	1.87239	3.72434
H	-6.41026	-2.22227	-1.56477
H	-6.70541	0.38663	-1.81323
H	3.56716	-6.27904	-0.01111
H	5.63366	-4.68051	0.29418
H	4.19145	6.13893	0.16600
H	1.81396	7.10755	-0.46163
C	1.18682	-5.25408	-0.24593
H	1.26273	-6.33133	-0.42327

F2-EO

Energy: -1895500.1338226

O	2.02472	-1.32514	0.00912
O	2.17349	1.22643	-0.12783
O	0.03299	2.61930	-0.25221
O	-2.19972	1.56771	0.27415
O	-2.37582	-0.98202	0.38077
O	-0.24271	-2.46264	0.38489
O	-1.79741	-2.51034	-2.14273
O	-0.59175	-0.59356	-2.18548
O	-0.06833	0.34097	2.52426
O	1.34754	-0.14812	4.21729
N	4.71653	-1.55212	-0.69872
N	4.91505	1.05282	-0.60660
N	-1.18052	5.08344	-0.66243
N	-3.46333	4.01688	0.00071
N	-3.94096	-3.23432	-0.10353
N	-1.79944	-4.72626	0.02302
C	6.01396	-1.03382	-1.15764
H	5.99228	-0.95794	-2.25271
C	6.20360	0.36125	-0.54903
H	6.45580	0.25937	0.51204
C	4.82119	2.32571	-0.81581
H	5.73358	2.89064	-1.03132
C	3.58521	3.07946	-0.79041
C	3.62464	4.47427	-1.10787
H	4.58578	4.92514	-1.33967
C	2.48625	5.23489	-1.12522
H	2.53384	6.29279	-1.36721
C	1.21028	4.65144	-0.83526
C	1.13738	3.27545	-0.51990
C	2.34688	2.47458	-0.47100
C	0.03406	5.47783	-0.90580
H	0.18664	6.51862	-1.20534
C	-2.33468	5.96911	-0.88699
H	-2.63346	5.88447	-1.93942
C	-3.48075	5.48602	0.00942
H	-3.30976	5.82435	1.03909
C	-4.59853	1.87340	0.16739
C	-5.87198	1.21802	0.12731
H	-6.77082	1.82647	0.08440
C	-5.95758	-0.14813	0.10901
H	-6.92670	-0.63486	0.04271
C	-4.78261	-0.96574	0.14927
C	-3.51389	-0.35403	0.27380
C	-3.42169	1.09485	0.24696
C	-4.92353	-2.39474	-0.00348
H	-5.94579	-2.77703	-0.08314
C	-4.17967	-4.64963	-0.41735
H	-4.14708	-4.76100	-1.50815
C	-3.04989	-5.47211	0.21077
H	-3.23197	-5.58027	1.28784
C	-0.65460	-5.32828	-0.05480
H	-0.63843	-6.42268	-0.05596
C	0.61934	-4.65890	-0.15444
C	1.78816	-5.42910	-0.45215
H	1.68621	-6.50358	-0.57810
C	3.00916	-4.82648	-0.60193
H	3.88607	-5.41934	-0.84788
C	3.15824	-3.40977	-0.46224
C	2.02904	-2.62514	-0.13063
C	0.73730	-3.26432	0.04710
C	4.44418	-2.81684	-0.75694
H	5.22818	-3.50653	-1.08655
C	-1.18384	-1.57381	-2.73145
C	-1.15659	-1.61452	-4.26252
H	-1.61600	-2.52473	-4.65199
H	-0.12331	-1.54568	-4.61713
H	-1.69060	-0.74484	-4.66081
C	0.22936	0.35490	3.71749
C	-0.66288	0.96192	4.76952
H	-0.67493	2.04833	4.63521
H	-0.31642	0.72844	5.77597
H	-1.68391	0.60059	4.62637
Ca	-0.09318	0.05480	0.07249
Co	-2.07777	-2.83044	0.03518
Co	-1.69955	3.32938	-0.14844
Co	3.51655	-0.15304	-0.16279
H	-5.16108	-4.98757	-0.06572
H	-2.99694	-6.47468	-0.22865
H	-4.44409	5.88366	-0.32755
H	-2.08699	7.01644	-0.68426
H	6.99800	0.91745	-1.06078
H	6.83882	-1.69966	-0.87923
O	4.17741	-0.16606	1.84792
C	3.32230	0.36416	2.78001
C	2.33615	-0.70728	3.28737
H	2.70391	1.20434	2.39507
H	3.85019	0.76939	3.67357
H	1.81720	-1.16334	2.44551
H	2.84926	-1.47527	3.87027
C	-4.54917	3.31187	0.10399
H	-5.50667	3.83915	0.13980

G1-EO

Energy: -2013832.7717485

O	-1.49009	2.47852	0.11673
O	1.04149	2.56142	0.21503
O	2.40042	0.38109	0.04335
O	1.10376	-1.84020	-0.44097
O	-1.46425	-1.90381	-0.41558
O	-2.73395	0.26145	-0.26229
O	3.60986	-2.15612	2.68377
O	1.99165	-2.08978	4.27540
O	0.35629	0.51918	-2.33391
O	2.35389	-0.46217	-2.76860
N	-1.60450	5.22945	0.42745
N	0.98504	5.32543	0.16854
N	4.74927	-0.80834	-0.80506
N	3.44102	-2.99372	-1.39964
N	-3.77210	-3.30591	-0.74341
N	-5.08893	-1.07229	-0.71097
C	-1.03317	6.54347	0.75831
H	-0.90702	6.59281	1.84703
C	0.33449	6.64335	0.07670
H	0.19860	6.88470	-0.98506

C	2.27566	5.20529	0.06277
H	2.87241	6.11929	-0.00541
C	2.99591	3.96243	-0.00970
C	4.41417	3.99350	-0.21173
H	4.91528	4.95653	-0.24769
C	5.12097	2.83463	-0.38674
H	6.19196	2.86817	-0.56658
C	4.47147	1.55956	-0.36057
C	3.08658	1.48285	-0.08362
C	2.33169	2.71638	0.05683
C	5.25022	0.37003	-0.61112
H	6.33739	0.49001	-0.64843
C	5.60847	-1.98821	-0.96545
H	5.79543	-2.41566	0.02766
C	4.84778	-3.00435	-1.82276
H	4.88503	-2.69467	-2.87454
C	1.28421	-4.10869	-1.25262
C	0.57464	-5.32006	-1.52936
H	1.14048	-6.18997	-1.85149
C	-0.78826	-5.39093	-1.41214
H	-1.31394	-6.31632	-1.62844
C	-1.54707	-4.23681	-1.03457
C	-0.87406	-3.03461	-0.73501
C	0.57264	-2.97456	-0.79466
C	-2.98110	-4.31473	-0.96892
H	-3.43150	-5.29951	-1.11774
C	-5.22457	-3.49066	-0.60410
H	-5.44910	-3.61479	0.46166
C	-5.90593	-2.22463	-1.12772
H	-5.93777	-2.24574	-2.22373
C	-5.61927	0.11412	-0.59627
H	-6.69904	0.20926	-0.73964
C	-4.90041	1.32188	-0.31900
C	-5.61875	2.55816	-0.21284
H	-6.70016	2.54207	-0.31090
C	-4.95902	3.73537	0.00282
H	-5.51154	4.66709	0.08257
C	-3.53078	3.77495	0.12238
C	-2.79040	2.57570	0.02890
C	-3.49192	1.32160	-0.18877
C	-2.88697	5.04453	0.34503
H	-3.54275	5.91205	0.45853
C	3.25414	-2.23046	3.84860
C	4.18746	-2.50206	5.00699
H	4.18760	-1.64772	5.69063
H	5.19757	-2.67403	4.63605
H	3.84421	-3.37294	5.57244
C	1.31685	0.19112	-3.09095
C	1.21910	0.65246	-4.54992
H	0.23166	0.41125	-4.95475
H	1.99298	0.19864	-5.17185
H	1.32635	1.74243	-4.59152
Ca	-0.12690	0.28401	0.04721
Co	-3.26354	-1.51004	-0.50696
Co	2.89032	-1.27264	-0.77032
Co	-0.26383	3.90091	0.24801
O	-0.33023	0.02292	2.34710
C	0.67040	-0.25155	3.24223
H	0.44063	0.06753	4.28636
H	1.64568	0.23810	3.00482
C	0.95508	-1.76498	3.29868
H	1.25566	-2.13081	2.31568
H	0.06780	-2.30661	3.63636
H	-5.57196	-4.38120	-1.13831
H	-6.93271	-2.14483	-0.75550
H	5.29180	-4.00294	-1.74225
H	6.57389	-1.73111	-1.41570
H	0.94667	7.42922	0.53140
H	-1.69201	7.36266	0.45084
C	2.70492	-4.05569	-1.50353
H	3.17353	-4.98248	-1.84831
C	-3.30275	-3.15476	3.06957
O	-4.27724	-2.53881	2.86918
O	-2.33511	-3.77828	3.27292

G2-EO

Energy: -2013829.2247763

O	1.47925	-1.19964	-0.53518
O	1.58638	1.34129	-0.61559
O	-0.52103	2.76135	-0.29775
O	-2.61740	1.66464	0.50851
O	-2.76148	-0.88955	0.53683
O	-0.68510	-2.35142	0.17098
O	-2.65181	-2.42806	-2.07334
O	-1.48185	-0.51375	-2.37564
O	7.84278	0.07244	1.14614
O	6.64651	-0.09859	3.06581
N	4.09253	-1.39501	-1.46293
N	4.29063	1.21134	-1.32786
N	-1.70900	5.21690	-0.22925
N	-3.85685	4.09570	0.69971
N	-4.39308	-3.14214	0.31011
N	-2.25408	-4.63011	0.05960
C	5.29201	-0.85391	-2.12338
H	5.08544	-0.77050	-3.19828
C	5.57705	0.53763	-1.54444
H	6.07948	0.43667	-0.57615
C	4.16711	2.49353	-1.45601
H	5.03780	3.07247	-1.77930
C	2.95497	3.24661	-1.20683
C	2.98092	4.66593	-1.37755
H	3.91618	5.13382	-1.67298
C	1.86466	5.43503	-1.17396
H	1.90507	6.51253	-1.30315
C	0.62530	4.83061	-0.79117
C	0.56505	3.43161	-0.62907
C	1.74671	2.61840	-0.81964
C	-0.54097	5.65051	-0.60720
H	-0.43147	6.71782	-0.81607
C	-2.87117	6.12064	-0.18794
H	-3.33107	6.13039	-1.18339
C	-3.86578	5.56061	0.83160
H	-3.54101	5.81618	1.84733
C	-4.97782	1.95141	0.93425
C	-6.23456	1.28771	1.12029
H	-7.12149	1.88824	1.29959

C	-6.32219	-0.07595	1.04353
H	-7.28503	-0.56729	1.15236
C	-5.16578	-0.88688	0.80200
C	-3.89976	-0.27014	0.69250
C	-3.81486	1.17775	0.71808
C	-5.33711	-2.31203	0.62374
H	-6.35640	-2.69582	0.72773
C	-4.67912	-4.55117	0.00850
H	-4.82617	-4.63724	-1.07496
C	-3.46106	-5.38360	0.42589
H	-3.46826	-5.51948	1.51498
C	-1.12563	-5.22572	-0.17155
H	-1.10309	-6.31992	-0.17180
C	0.12062	-4.54959	-0.44194
C	1.25585	-5.31013	-0.87169
H	1.15362	-6.38726	-0.97120
C	2.44385	-4.69705	-1.17302
H	3.29187	-5.28565	-1.51266
C	2.59345	-3.27621	-1.07127
C	1.49663	-2.50051	-0.63012
C	0.24905	-3.15293	-0.27822
C	3.82147	-2.66232	-1.52259
H	4.55709	-3.33207	-1.97993
C	-2.16558	-1.50302	-2.78447
C	-2.41972	-1.57137	-4.29236
H	-3.01798	-2.44297	-4.56308
H	-1.46317	-1.60855	-4.82409
H	-2.93307	-0.66166	-4.62080
C	7.74392	-0.26728	2.31367
C	8.84844	-0.92795	3.10588
H	8.53099	-1.92578	3.42339
H	9.06271	-0.35059	4.00962
H	9.74606	-1.00658	2.49313
Ca	-0.61073	0.14752	-0.26144
Co	-2.53712	-2.73769	0.12647
Co	-2.16799	3.43804	0.17540
Co	2.94498	-0.01515	-0.77788
H	-5.58932	-4.90054	0.50881
H	-3.47997	-6.37463	-0.04127
H	-4.86793	5.97409	0.67659
H	-2.57527	7.14418	0.06436
H	6.22938	1.11282	-2.21250
H	6.15678	-1.51513	-1.99562
O	3.44116	0.02807	1.25770
C	4.55243	-0.56577	1.79403
C	5.47162	0.49211	2.43382
H	5.17210	-1.12464	1.05756
H	4.32121	-1.30855	2.59531
H	5.79562	1.21947	1.68647
H	4.95030	1.00935	3.24333
C	-4.91823	3.38336	0.96078
H	-5.84028	3.91118	1.21902
C	-1.58564	-1.33777	3.46679
O	-2.18353	-2.33900	3.55414
O	-0.98518	-0.33589	3.40578

H1-EO

Energy: -2013856.3347730

O	0.14858	2.54935	-0.45276
O	2.39186	1.73509	0.39227
O	2.76000	-0.76447	0.86475
O	0.87919	-2.42273	0.17074
O	-1.40211	-1.56544	-0.63355
O	-1.72944	0.89195	-1.02625
O	-6.32992	-1.02894	1.57157
O	-5.68588	0.52643	3.08940
O	1.67532	-0.47117	-2.06618
O	3.18385	-2.12590	-1.71998
N	1.03622	5.17077	-0.33089
N	3.43444	4.28676	0.18928
N	4.57689	-2.85149	0.94944
N	2.71589	-4.50605	0.14005
N	-3.93970	-2.08602	-1.45181
N	-4.25211	0.43502	-1.96247
C	1.97614	6.22727	0.07446
H	1.83542	6.41180	1.14669
C	3.39696	5.71263	-0.17632
H	3.63531	5.79830	-1.24395
C	4.55076	3.70094	0.50789
H	5.45177	4.31658	0.57935
C	4.71485	2.29196	0.75120
C	6.02344	1.78048	1.03206
H	6.85314	2.47813	1.10085
C	6.23244	0.43601	1.18510
H	7.23292	0.05563	1.37160
C	5.15255	-0.49825	1.08616
C	3.83556	-0.02439	0.88771
C	3.62493	1.39595	0.67233
C	5.43035	-1.91101	1.20419
H	6.43966	-2.19057	1.52149
C	4.90086	-4.26626	1.17571
H	4.62770	-4.52225	2.20739
C	4.05828	-5.09920	0.20361
H	4.49813	-5.04281	-0.79963
C	0.33785	-4.72360	-0.32735
C	-0.70518	-5.63313	-0.69754
H	-0.47572	-6.69431	-0.73999
C	-1.96384	-5.18961	-1.00329
H	-2.74537	-5.89202	-1.27748
C	-2.26639	-3.78879	-0.99462
C	-1.26079	-2.86871	-0.63013
C	0.05040	-3.34296	-0.23030
C	-3.58163	-3.33503	-1.34460
H	-4.33918	-4.10246	-1.52388
C	-5.34242	-1.71475	-1.69838
H	-5.82387	-1.55803	-0.72706
C	-5.33827	-0.40803	-2.49259
H	-5.12507	-0.61263	-3.54865
C	-4.29841	1.73124	-2.08639
H	-5.19858	2.17402	-2.52038
C	-3.24629	2.63647	-1.71801
C	-3.43462	4.04622	-1.88823
H	-4.38647	4.40335	-2.27001
C	-2.43626	4.92877	-1.57793

H	-2.58950	5.99615	-1.70802
C	-1.17245	4.47502	-1.07944
C	-0.95486	3.09029	-0.89815
C	-2.01540	2.15640	-1.22163
C	-0.15737	5.44765	-0.76034
H	-0.43063	6.49897	-0.88540
C	-6.57178	-0.32661	2.53604
C	-7.89092	-0.28272	3.26636
H	-7.74248	-0.53068	4.32114
H	-8.58578	-0.98886	2.81317
H	-8.30706	0.72805	3.22348
C	2.60241	-1.25254	-2.43040
C	3.07126	-1.11759	-3.88346
H	2.21628	-1.22033	-4.55938
H	3.82785	-1.86183	-4.13837
H	3.48563	-0.11593	-4.04162
Ca	0.52095	0.03982	0.00631
Co	-2.83523	-0.57823	-1.25532
Co	2.75722	-2.61141	0.39694
Co	1.75344	3.43948	-0.04127
O	-2.15481	-0.39653	2.54482
C	-3.42466	-0.39200	3.19042
H	-3.32088	-0.13286	4.24741
H	-3.81893	-1.40807	3.09732
C	-4.36510	0.59515	2.50029
H	-4.42678	0.38195	1.43168
H	-4.02198	1.61667	2.66434
H	-5.87827	-2.50446	-2.23591
H	-6.30595	0.10038	-2.42896
H	4.02726	-6.15165	0.50737
H	5.97055	-4.46540	1.04594
H	4.13368	6.29444	0.38750
H	1.79117	7.16322	-0.46324
C	1.67102	-5.23308	-0.10734
H	1.80018	-6.31581	-0.19885
C	-1.26732	0.64981	2.88372
O	-0.19419	0.58830	2.21827
O	-1.61470	1.46458	3.74790

H1'-EO

Energy: -2013864.9567907

O	2.05488	0.54208	-1.00859
O	1.45433	-1.82938	-0.38333
O	-0.92737	-2.40188	0.38310
O	-2.72472	-0.56609	0.31128
O	-2.07848	1.83140	-0.15993
O	0.26643	2.38100	-1.03045
O	5.06900	-0.41217	2.02916
O	3.65576	-0.09209	3.76176
O	-1.22710	-0.96474	-2.38867
O	-2.79827	-2.52886	-1.91756
N	4.69976	-0.19125	-1.34928
N	3.97783	-2.69000	-1.12168
N	-2.91193	-4.33311	0.58797
N	-4.73669	-2.45122	0.47478
N	-2.66534	4.51259	0.13461
N	-0.28769	5.09543	-0.80607
C	5.83123	-1.12680	-1.24815
H	6.14164	-1.14926	-0.19720
C	5.33402	-2.51337	-1.66792
H	5.27095	-2.56970	-2.76199
C	3.48416	-3.87160	-0.89883
H	4.13224	-4.73839	-1.05688
C	2.13363	-4.14686	-0.47958
C	1.71431	-5.50854	-0.32670
H	2.43944	-6.29975	-0.49421
C	0.41976	-5.81221	0.00130
H	0.10809	-6.84908	0.09268
C	-0.55321	-4.78433	0.21518
C	-0.15940	-3.42781	0.13847
C	1.20205	-3.10919	-0.25340
C	-1.91357	-5.15740	0.53205
H	-2.09716	-6.21727	0.73401
C	-4.24740	-4.76902	1.02134
H	-4.29317	-4.70163	2.11591
C	-5.28033	-3.81316	0.40994
H	-5.43090	-4.06731	-0.64653
C	-5.06628	-0.04258	0.59804
C	-6.01302	1.02449	0.75680
H	-7.05340	0.77241	0.94360
C	-5.62448	2.33709	0.68525
H	-6.35201	3.13086	0.83150
C	-4.26315	2.69621	0.40559
C	-3.32051	1.66746	0.19565
C	-3.71052	0.28133	0.37874
C	-3.87191	4.08420	0.35904
H	-4.65580	4.82215	0.55540
C	-2.32563	5.93863	0.21801
H	-1.94221	6.13679	1.22652
C	-1.22558	6.22771	-0.81207
H	-1.67337	6.29850	-1.81163
C	0.94287	5.23005	-1.18918
H	1.30584	6.23092	-1.44247
C	1.89397	4.14776	-1.30636
C	3.26700	4.45258	-1.57152
H	3.55481	5.49385	-1.68745
C	4.20911	3.46285	-1.66740
H	5.24821	3.70981	-1.86530
C	3.85160	2.08764	-1.48603
C	2.50296	1.75444	-1.23221
C	1.49367	2.79617	-1.18926
C	4.88392	1.08249	-1.52413
H	5.90409	1.43635	-1.69781
C	4.66476	-0.72410	3.13517
C	5.20453	-1.85667	3.97244
H	5.42528	-1.51023	4.98524
H	6.10420	-2.26027	3.50892
H	4.44961	-2.64524	4.05183
C	-2.08777	-1.83921	-2.70666
C	-2.28268	-2.08435	-4.20686
H	-2.55839	-1.14677	-4.70068
H	-3.05171	-2.83471	-4.39911
H	-1.33756	-2.41422	-4.65119
Ca	-0.36972	-0.01066	-0.34007
Co	-1.14583	3.45370	-0.33474
Co	-2.83261	-2.44456	0.29212

Co	3.05441	-1.04200	-0.96137
O	1.12962	2.49493	3.25214
C	1.78116	1.37362	3.84834
H	1.10755	0.51492	3.90008
H	2.05091	1.68436	4.86176
C	3.03079	1.00612	3.05708
H	3.72871	1.84775	3.00608
H	2.76987	0.69763	2.04391
H	-3.19922	6.57900	0.05063
H	-0.71984	7.17559	-0.59672
H	-6.24500	-3.89582	0.92375
H	-4.44946	-5.80724	0.73482
H	6.01450	-3.29907	-1.32251
H	6.67979	-0.80622	-1.86223
C	-5.50599	-1.41684	0.63890
H	-6.57664	-1.58480	0.79179
C	0.30652	2.24592	2.15354
O	-0.20913	3.29388	1.69663
O	0.18606	1.05357	1.77628

$TS_{AF}1$

Energy: -1991989.7902181

O	-0.31178	-2.44212	0.09796
O	-2.41086	-1.09745	0.48477
O	-2.26645	1.44212	0.76141
O	0.00949	2.62933	0.36935
O	2.15023	1.24694	0.04751
O	1.92084	-1.26831	-0.29932
O	4.47576	-0.52807	1.56298
O	3.77649	-0.62468	3.71763
O	-0.80239	0.79316	-2.00458
O	-1.95376	2.74017	-1.89595
N	-1.74210	-4.81214	0.33497
N	-3.94475	-3.40950	0.56699
N	-3.58613	3.86511	0.55857
N	-1.32611	5.03213	-0.06993
N	4.78367	1.15196	-0.84487
N	4.53146	-1.41966	-1.24539
C	-2.89889	-5.59562	0.79392
H	-2.85380	-5.66056	1.88835
C	-4.17275	-4.84977	0.37626
H	-4.36115	-5.02127	-0.69042
C	-4.92914	-2.57879	0.73053
H	-5.94077	-2.98595	0.82011
C	-4.80860	-1.14160	0.78714
C	-5.99144	-0.34384	0.92709
H	-6.95108	-0.84594	1.01287
C	-5.92431	1.02435	0.92752
H	-6.83201	1.61659	1.00495
C	-4.66862	1.70558	0.82031
C	-3.47549	0.95097	0.76084
C	-3.55622	-0.49691	0.67598
C	-4.64099	3.14853	0.79656
H	-5.58816	3.66169	0.99002
C	-3.62404	5.33148	0.66066
H	-3.43914	5.61017	1.70607
C	-2.50600	5.89394	-0.22265
H	-2.81762	5.85563	-1.27386
C	1.07610	4.69658	-0.28187
C	2.30817	5.32589	-0.65005
H	2.31177	6.39719	-0.83149
C	3.45593	4.59517	-0.80318
H	4.38010	5.08118	-1.10352
C	3.46121	3.17755	-0.60062
C	2.27531	2.53145	-0.18136
C	1.05822	3.30855	-0.01029
C	4.67533	2.44245	-0.86984
H	5.55974	3.03395	-1.12553
C	6.05814	0.46251	-1.06439
H	6.47132	0.22210	-0.07932
C	5.75757	-0.84129	-1.81577
H	5.57264	-0.61995	-2.87477
C	4.28873	-2.69005	-1.30543
H	5.05183	-3.34779	-1.73269
C	3.05843	-3.32370	-0.88443
C	2.94522	-4.74841	-0.97068
H	3.81322	-5.32030	-1.28655
C	1.77384	-5.38752	-0.65900
H	1.70922	-6.47063	-0.71281
C	0.60900	-4.64860	-0.27564
C	0.68306	-3.23822	-0.20017
C	1.94313	-2.56799	-0.46059
C	-0.60115	-5.36423	0.06011
H	-0.52841	-6.45531	0.09732
C	4.66215	-0.53201	2.80963
C	6.11236	-0.41557	3.29376
H	6.51821	0.55561	2.99046
H	6.72516	-1.18669	2.81668
H	6.18422	-0.51056	4.37875
C	-1.41759	1.77927	-2.51747
C	-1.54566	1.78342	-4.04361
H	-0.60280	1.47794	-4.50562
H	-1.84325	2.76433	-4.41911
H	-2.30591	1.05251	-4.34305
Ca	-0.18546	0.12242	0.24106
Co	3.39930	-0.09252	-0.46087
Co	-1.80345	3.21521	0.26746
Co	-2.12120	-2.94669	0.29533
O	0.13516	-0.10474	2.63587
C	1.19478	0.60208	3.24580
H	1.01041	0.90425	4.28460
H	1.60228	1.43703	2.66402
C	1.82895	-0.69428	3.04588
H	2.19450	-0.94702	2.06556
H	1.62651	-1.48068	3.75743
H	6.77360	1.08403	-1.61474
H	6.60109	-1.53770	-1.75464
H	-2.28740	6.93720	0.03220
H	-4.60035	5.73418	0.36829
H	-5.04113	-5.20436	0.94236
H	-2.88671	-6.61418	0.39046
O	-2.57727	-3.08455	-2.03309
C	-2.38079	-2.03257	-3.01142
C	-1.60789	-3.27739	-3.08699
H	-1.90708	-1.12993	-2.63134
H	-3.22685	-1.89312	-3.68137

H	-0.57239	-3.28430	-2.75737
H	-1.88014	-4.04110	-3.81233
C	-0.12841	5.49195	-0.25637
H	-0.00782	6.56182	-0.45270

$TS_{AF}2$

Energy: -1991986.6214020

O	-2.54584	-0.06523	-0.19803
O	-1.16944	-2.18931	0.02665
O	1.38551	-2.05982	-0.08115
O	2.52665	0.20924	0.03277
O	1.12407	2.34604	-0.04995
O	-1.41391	2.20451	0.01025
O	-0.29524	1.84748	-3.46130
O	-0.10933	-0.19874	-2.52281
O	0.15897	0.22676	2.26615
O	-1.10578	0.40111	4.12770
N	-4.86782	-1.54970	-0.51916
N	-3.46925	-3.73969	-0.11701
N	3.81719	-3.34546	0.26121
N	4.95692	-1.00482	0.59993
N	1.00502	5.10300	-0.03066
N	-1.60654	4.95839	0.03489
C	-5.59190	-2.79126	-0.83105
H	-5.50867	-2.97544	-1.90980
C	-4.92250	-3.93982	-0.06302
H	-5.22144	-3.89270	0.99052
C	-2.63391	-4.73037	-0.07103
H	-3.03421	-5.74891	-0.07173
C	-1.19355	-4.60545	-0.01138
C	-0.38905	-5.78996	0.04178
H	-0.88592	-6.75623	0.03506
C	0.97710	-5.71848	0.11768
H	1.57042	-6.62643	0.18111
C	1.65422	-4.45505	0.10907
C	0.89349	-3.26909	0.00285
C	-0.55819	-3.34321	0.00512
C	3.09319	-4.42207	0.21742
H	3.60122	-5.38969	0.26980
C	5.28559	-3.39529	0.26593
H	5.62429	-3.37797	-0.77680
C	5.80246	-2.14565	0.99014
H	5.70819	-2.28502	2.07448
C	4.58054	1.40115	0.48098
C	5.18820	2.69321	0.60935
H	6.25502	2.74814	0.80718
C	4.45019	3.84050	0.48784
H	4.92845	4.81170	0.57736
C	3.03658	3.78947	0.25530
C	2.40428	2.53228	0.13590
C	3.19595	1.31587	0.21220
C	2.29326	5.01802	0.11852
H	2.87356	5.94501	0.12853
C	0.33484	6.38786	-0.28320
H	0.27449	6.53171	-1.36912
C	-1.08088	6.30643	0.30181
H	-1.03586	6.44679	1.38914
C	-2.88115	4.73148	-0.08405
H	-3.56167	5.58726	-0.05885
C	-3.48423	3.43070	-0.23142
C	-4.90193	3.32247	-0.41405
H	-5.49173	4.23337	-0.46414
C	-5.50862	2.09889	-0.52792
H	-6.58352	2.03486	-0.67278
C	-4.75377	0.88333	-0.45611
C	-3.35551	0.95622	-0.27447
C	-2.71081	2.25148	-0.16373
C	-5.42932	-0.38633	-0.62662
H	-6.49211	-0.34068	-0.88419
C	-0.31872	0.59934	-3.50555
C	-0.61327	-0.08314	-4.85011
H	-0.81533	0.65042	-5.63354
H	-1.47343	-0.75364	-4.75028
H	0.23948	-0.70230	-5.15006
C	-0.02211	0.53369	3.47450
C	1.17150	1.09696	4.24729
H	1.88682	0.28880	4.43784
H	0.86660	1.52716	5.20292
H	1.68471	1.84957	3.64223
Ca	-0.01188	0.07176	-0.13753
Co	-0.22416	3.65484	-0.01955
Co	3.19632	-1.55466	0.11296
Co	-3.04472	-1.88849	-0.05875
H	0.89232	7.22810	0.14453
H	-1.72728	7.08479	-0.11767
H	6.85828	-1.96516	0.76005
H	5.66231	-4.30930	0.73841
H	-5.21956	-4.91327	-0.46975
H	-6.65568	-2.71659	-0.57890
O	-3.51545	-1.84838	2.10883
C	-2.40403	-1.93190	2.97331
C	-2.58636	-0.48486	3.00735
H	-1.47526	-2.28228	2.51254
H	-2.59824	-2.46466	3.91456
H	-2.26939	0.07939	2.14976
H	-3.34454	-0.07407	3.65879
C	5.38317	0.21773	0.69156
H	6.42481	0.38340	0.98256
O	3.80958	-1.64835	-2.14266
C	3.93234	-0.48968	-2.99891
C	2.86999	-1.47346	-3.23592
H	4.82185	-0.48934	-3.62504
H	3.68459	0.45403	-2.52090
H	2.99182	-2.20111	-4.03572
H	1.85153	-1.23742	-2.93363

$TS_{AF}1$-EO

Energy: -1895474.6753932

O	-0.29545	-2.45539	0.41873
O	-2.48241	-1.04715	0.56444
O	-2.41652	1.51918	0.43560
O	-0.24494	2.65364	-0.14411
O	1.95482	1.31427	-0.21783
O	1.90491	-1.23472	-0.10699
O	4.36155	-0.07075	1.61932
O	3.61754	-0.28610	3.75199

O	-0.85134	-0.60840	-2.07217
O	-2.01775	-2.54864	-1.98787
N	-1.79319	-4.76936	0.16181
N	-3.99210	-3.35661	0.19494
N	-3.75212	3.88987	0.32893
N	-1.56347	5.04530	-0.43738
N	4.64114	1.24424	-0.96151
N	4.51408	-1.36021	-1.07905
C	-2.99808	-5.55924	0.44475
H	-3.09313	-5.66781	1.53276
C	-4.20139	-4.78132	-0.09745
H	-4.24829	-4.89653	-1.18728
C	-4.99537	-2.55474	0.36761
H	-6.00556	-2.97526	0.36425
C	-4.89784	-1.12099	0.51147
C	-6.10107	-0.34962	0.56601
H	-7.05284	-0.87366	0.57118
C	-6.06952	1.01970	0.59003
H	-6.99127	1.59287	0.62415
C	-4.82219	1.71924	0.53607
C	-3.61820	0.98651	0.51185
C	-3.64601	-0.46133	0.54146
C	-4.81384	3.15679	0.49284
H	-5.77670	3.66157	0.60560
C	-3.82594	5.35807	0.37278
H	-3.61217	5.67890	1.39930
C	-2.75315	5.90330	-0.57164
H	-3.10640	5.84477	-1.60820
C	0.82403	4.71988	-0.78432
C	2.05135	5.35256	-1.16690
H	2.04310	6.41437	-1.39445
C	3.20823	4.62993	-1.25819
H	4.13222	5.11316	-1.56299
C	3.23687	3.22825	-0.96505
C	2.05431	2.57627	-0.54787
C	0.81822	3.33768	-0.48069
C	4.48592	2.51805	-1.12397
H	5.35557	3.11735	-1.40924
C	5.95349	0.59796	-1.05859
H	6.33519	0.49603	-0.03759
C	5.74212	-0.79488	-1.66196
H	5.60231	-0.70904	-2.74715
C	4.28595	-2.63523	-1.10881
H	5.06618	-3.29306	-1.50376
C	3.05719	-3.27656	-0.70438
C	2.94957	-4.69743	-0.84303
H	3.82289	-5.25632	-1.16741
C	1.76673	-5.34180	-0.59653
H	1.69154	-6.41845	-0.72160
C	0.60081	-4.61455	-0.19965
C	0.68349	-3.21736	0.00465
C	1.93649	-2.53555	-0.26610
C	-0.63760	-5.33017	-0.00488
H	-0.58179	-6.42309	-0.00971
C	4.52159	-0.17010	2.86591
C	5.96680	-0.14703	3.37899
H	6.01241	-0.27433	4.46208
H	6.43563	0.80462	3.10720
H	6.54185	-0.94204	2.89350
C	-1.45924	-1.58957	-2.59651
C	-1.51485	-1.61150	-4.12751
H	-1.95947	-0.68109	-4.49526
H	-2.08923	-2.46091	-4.50159
H	-0.49695	-1.66010	-4.52904
Ca	-0.27820	0.06584	0.17086
Co	3.30901	-0.01341	-0.45238
Co	-1.99027	3.27907	0.07433
Co	-2.13859	-2.88551	0.19864
O	0.02987	0.36807	2.55355
C	1.13402	1.07465	3.07768
H	0.96521	1.52592	4.06361
H	1.60518	1.79297	2.39710
C	1.66931	-0.28020	3.06389
H	2.01738	-0.69153	2.13185
H	1.40783	-0.94496	3.87338
H	6.65973	1.18856	-1.65280
H	6.60932	-1.43910	-1.48022
H	-2.52148	6.94956	-0.34607
H	-4.82199	5.72056	0.09805
H	-5.13990	-5.15326	0.32869
H	-2.94161	-6.56143	0.00503
C	-0.38105	5.49259	-0.76064
H	-0.29425	6.54172	-1.05603

$TS_{AF}2$-EO

Energy: -1895477.9721146

O	1.99581	-1.37136	0.00423
O	2.20699	1.16986	-0.12334
O	0.09848	2.64373	-0.19638
O	-2.17245	1.64369	0.22931
O	-2.40498	-0.91583	0.35029
O	-0.30173	-2.45782	0.38551
O	-1.82646	-2.42858	-2.16134
O	-0.57191	-0.54289	-2.11682
O	-0.04281	0.26999	2.55269
O	1.19769	-0.26469	4.36071
N	4.67910	-1.66351	-0.70043
N	4.94225	0.93394	-0.60919
N	-1.04701	5.10487	-0.60047
N	-3.35158	4.08974	0.00880
N	-4.01290	-3.12922	-0.16798
N	-1.91085	-4.67444	-0.01008
C	5.98728	-1.17914	-1.16993
H	5.95858	-1.10807	-2.26478
C	6.21835	0.21347	-0.57150
H	6.50108	0.11331	0.48238
C	4.87593	2.21154	-0.80367
H	5.80088	2.75626	-1.01554
C	3.66044	2.99494	-0.76567
C	3.73860	4.39272	-1.06906
H	4.71120	4.81722	-1.30181
C	2.62401	5.18471	-1.07369
H	2.69856	6.24242	-1.30830
C	1.33435	4.63282	-0.77925
C	1.22168	3.25696	-0.46856
C	2.40941	2.41956	-0.44565

C	0.18018	5.47696	-0.84409
H	0.34969	6.51595	-1.13969
C	-2.16999	6.03173	-0.82315
H	-2.45148	5.98634	-1.88214
C	-3.33880	5.55961	0.04394
H	-3.17869	5.87363	1.08227
C	-4.56173	1.98717	0.12180
C	-5.84895	1.36418	0.06481
H	-6.73386	1.99203	0.01905
C	-5.96078	-0.00068	0.03388
H	-6.93918	-0.46630	-0.04680
C	-4.80598	-0.84317	0.08253
C	-3.52359	-0.26043	0.22520
C	-3.40584	1.18359	0.20052
C	-4.97725	-2.26830	-0.07640
H	-6.00686	-2.62714	-0.16850
C	-4.28127	-4.53831	-0.48553
H	-4.23356	-4.65105	-1.57561
C	-3.18269	-5.38763	0.16143
H	-3.38267	-5.48685	1.23608
C	-0.78189	-5.30680	-0.07211
H	-0.79431	-6.40116	-0.07129
C	0.51031	-4.67017	-0.15829
C	1.66092	-5.46914	-0.44946
H	1.53271	-6.54069	-0.57563
C	2.89738	-4.89837	-0.59343
H	3.76076	-5.51237	-0.83437
C	3.07818	-3.48461	-0.45649
C	1.96741	-2.67311	-0.12921
C	0.65959	-3.27926	0.04841
C	4.37645	-2.92293	-0.74832
H	5.14769	-3.63087	-1.06764
C	-1.19511	-1.47556	-2.70602
C	-1.17271	-1.44353	-4.23790
H	-1.77122	-2.24710	-4.67066
H	-0.13961	-1.53516	-4.59019
H	-1.54735	-0.47814	-4.59336
C	0.13150	0.13057	3.79570
C	-1.04622	0.46254	4.71159
H	-1.37175	1.49209	4.53171
H	-0.78471	0.34047	5.76390
H	-1.89053	-0.19068	4.46810
Ca	-0.10200	0.06103	0.17444
Co	-2.14207	-2.77155	0.00107
Co	-1.61567	3.37290	-0.10819
Co	3.50281	-0.23901	-0.20480
H	-5.27627	-4.85162	-0.14986
H	-3.14874	-6.39264	-0.27408
H	-4.28905	5.98014	-0.30127
H	-1.89193	7.06388	-0.58536
H	7.01132	0.75087	-1.10400
H	6.79567	-1.86517	-0.89399
O	4.15182	-0.28307	1.90437
C	3.45598	0.59423	2.76425
C	2.73242	-0.63770	3.05219
H	2.88507	1.38412	2.26643
H	4.06144	1.00451	3.58361
H	2.02455	-0.99120	2.32476
H	3.16519	-1.33895	3.75120
C	-4.46488	3.42171	0.08218
H	-5.40214	3.98314	0.11391

$TS_{BC}1$

Energy: -1848511.2864062

O	0.14329	2.53636	-0.01079
O	2.43114	1.48446	0.17458
O	2.66553	-1.05258	0.34587
O	0.63755	-2.50663	-0.06457
O	-1.70523	-1.47627	-0.12247
O	-1.91831	1.05002	-0.28254
O	-4.20706	-0.23686	1.64815
O	-3.61177	0.45280	3.72346
N	1.27198	5.06611	-0.09953
N	3.64023	3.96949	-0.06541
N	4.31097	-3.27885	0.35639
N	2.24940	-4.76170	-0.24855
N	-4.39354	-1.78008	-0.78400
N	-4.57508	0.81247	-1.09578
C	2.35803	6.02427	0.15642
H	2.43296	6.16954	1.24110
C	3.65949	5.41050	-0.37117
H	3.70474	5.52586	-1.46116
C	4.73965	3.28776	0.04740
H	5.68919	3.82663	-0.00989
C	4.82116	1.85670	0.21200
C	6.10989	1.23834	0.29563
H	6.99269	1.87053	0.27985
C	6.23637	-0.12261	0.38052
H	7.22028	-0.57896	0.43539
C	5.08401	-0.97211	0.38506
C	3.79829	-0.39161	0.33415
C	3.66470	1.04746	0.24319
C	5.26496	-2.40307	0.44054
H	6.28974	-2.76444	0.56055
C	4.56097	-4.72052	0.50381
H	4.40925	-4.98460	1.55764
C	3.53948	-5.46321	-0.36469
H	3.85471	-5.42670	-1.41473
C	-0.17493	-4.74601	-0.49068
C	-1.32578	-5.55134	-0.76336
H	-1.19318	-6.61934	-0.90844
C	-2.57161	-4.98945	-0.85721
H	-3.43460	-5.60930	-1.08228
C	-2.76695	-3.58482	-0.67151
C	-1.65939	-2.76795	-0.35306
C	-0.33700	-3.35653	-0.29295
C	-4.09703	-3.03809	-0.83873
H	-4.89942	-3.75525	-1.03471
C	-5.77432	-1.29387	-0.87833
H	-6.13342	-1.15746	0.14646
C	-5.74472	0.06515	-1.58794
H	-5.62470	-0.08475	-2.66840
C	-4.51808	2.10280	-1.17668
H	-5.39346	2.64131	-1.55148
C	-3.36008	2.91046	-0.85491
C	-3.44635	4.32986	-1.01041

H	-4.40088	4.76537	-1.29112
C	-2.35171	5.13207	-0.82099
H	-2.43300	6.20837	-0.94105
C	-1.07976	4.57235	-0.48171
C	-0.96497	3.17491	-0.30882
C	-2.12996	2.33195	-0.47421
C	0.05220	5.45187	-0.31812
H	-0.14717	6.52501	-0.38163
C	-4.44822	0.06767	2.84924
C	-5.90732	-0.03925	3.30758
H	-6.26465	-1.06361	3.16001
H	-6.53338	0.61460	2.69152
H	-6.02062	0.23577	4.35769
Ca	0.35337	0.00248	0.24452
Co	-3.20150	-0.34086	-0.43293
Co	2.46471	-2.90855	0.10962
Co	1.87519	3.27041	0.00919
O	0.04357	-0.01686	2.63292
C	-0.99113	-0.75867	3.25499
H	-0.78280	-1.05210	4.28974
H	-1.38408	-1.60135	2.67628
C	-1.63316	0.53096	3.05139
H	-2.02917	0.76836	2.07937
H	-1.45586	1.32021	3.76589
H	-6.42541	-2.00282	-1.40148
H	-6.67563	0.61771	-1.42169
H	3.45607	-6.51348	-0.06713
H	5.58670	-4.98514	0.22685
H	4.53520	5.90386	0.06299
H	2.16007	6.99591	-0.30792
O	0.69173	-0.00763	-2.25006
C	0.01753	-0.83511	-3.22763
C	-0.12302	0.62464	-3.26633
H	-0.79127	-1.44039	-2.82739
H	0.68465	-1.32969	-3.92867
H	-1.03376	1.08385	-2.89203
H	0.44154	1.19917	-3.99590
C	1.12413	-5.37199	-0.46652
H	1.15114	-6.44649	-0.66773

$TS_{BC}2$

Energy: -1848512.6152328

O	-2.08408	1.16084	-0.26009
O	-2.01567	-1.37063	-0.03963
O	0.24871	-2.54102	-0.12175
O	2.37083	-1.19664	0.04203
O	2.28850	1.35412	-0.13105
O	0.07689	2.54234	-0.17832
O	0.25857	0.33808	2.47811
O	-1.06256	0.80603	4.24593
N	-4.82810	1.07487	-0.76658
N	-4.76968	-1.51815	-0.40011
N	1.70169	-4.89723	-0.29032
N	3.88267	-3.51823	0.11099
N	3.60647	3.74576	-0.38874
N	1.31548	4.96642	-0.29596
C	-6.08350	0.39116	-1.11779
H	-6.08263	0.20818	-2.19978
C	-6.12126	-0.94859	-0.37118
H	-6.37653	-0.77213	0.67948
C	-4.55824	-2.79415	-0.45121
H	-5.41888	-3.46301	-0.54350
C	-3.25340	-3.42103	-0.39941
C	-3.15854	-4.84107	-0.54406
H	-4.07344	-5.41267	-0.67166
C	-1.94592	-5.47961	-0.52710
H	-1.89196	-6.55861	-0.63821
C	-0.72857	-4.74114	-0.37736
C	-0.79092	-3.33821	-0.23572
C	-2.07283	-2.66645	-0.21874
C	0.52936	-5.44544	-0.40613
H	0.47876	-6.52769	-0.55263
C	2.93757	-5.68153	-0.45778
H	3.18018	-5.71159	-1.52723
C	4.05933	-4.96644	0.30313
H	3.96977	-5.17779	1.37569
C	4.78936	-1.25979	0.03085
C	5.99030	-0.47950	-0.02099
H	6.94581	-0.99444	0.01213
C	5.94540	0.88467	-0.11881
H	6.86339	1.46259	-0.16732
C	4.69271	1.57865	-0.16685
C	3.49063	0.83960	-0.09633
C	3.54051	-0.60504	0.00142
C	4.67758	3.00426	-0.33034
H	5.64861	3.49596	-0.43160
C	3.69996	5.18573	-0.68709
H	3.70714	5.30966	-1.77654
C	2.46359	5.86521	-0.09486
H	2.59953	6.00262	0.98436
C	0.11025	5.43517	-0.43450
H	-0.02007	6.51952	-0.47175
C	-1.08148	4.63318	-0.52999
C	-2.34436	5.26384	-0.75827
H	-2.37916	6.34356	-0.86789
C	-3.49081	4.51784	-0.85057
H	-4.44288	5.00439	-1.04274
C	-3.46987	3.09628	-0.69984
C	-2.24050	2.44775	-0.43986
C	-1.02835	3.23295	-0.37899
C	-4.70104	2.35728	-0.88869
H	-5.57482	2.94376	-1.18809
C	0.05610	0.54111	3.71064
C	1.26368	0.46471	4.64128
H	0.98462	0.65996	5.67761
H	2.01771	1.19096	4.32170
H	1.71841	-0.52844	4.56681
Ca	0.11971	-0.00681	0.15149
Co	1.81801	3.15534	-0.23153
Co	2.05216	-3.04768	-0.05188
Co	-3.46481	-0.14666	-0.21987
H	4.62104	5.62037	-0.28531
H	2.29210	6.84684	-0.54820
H	5.04545	-5.30314	-0.03330
H	2.81450	-6.71050	-0.10481
H	-6.86315	-1.62639	-0.80795

H	-6.95961	1.00229	-0.87555
O	-4.00963	0.09306	1.89630
C	-3.16901	-0.55928	2.82287
C	-2.64336	0.79435	2.95611
H	-2.48831	-1.30297	2.39589
H	-3.68710	-0.96427	3.70225
H	-2.01473	1.17539	2.17234
H	-3.17399	1.49335	3.58635
C	4.88836	-2.69772	0.11948
H	5.89537	-3.11445	0.20393
O	0.19764	0.00804	-2.36812
C	0.05900	-1.10597	-3.28149
C	1.31289	-0.34680	-3.21836
H	-0.63589	-0.92843	-4.09815
H	-0.00278	-2.07814	-2.80040
H	1.53744	0.38601	-3.98897
H	2.16612	-0.76535	-2.69148

$TS_{BC}1$-EO

Energy: -1751996.0816843

O	-0.40384	-2.52366	-0.18336
O	-2.57297	-1.24845	-0.06178
O	-2.55710	1.29699	0.06723
O	-0.39248	2.54308	-0.25066
O	1.83160	1.27836	-0.29615
O	1.79619	-1.25425	-0.44456
O	4.13950	-0.23705	1.51436
O	3.52070	0.37847	3.60567
N	-1.76608	-4.93402	-0.17227
N	-4.02018	-3.61371	-0.16250
N	-3.97205	3.67528	0.13763
N	-1.76320	4.95171	-0.42429
N	4.54617	1.30883	-0.93050
N	4.47074	-1.29191	-1.22693
C	-2.93700	-5.77423	0.12144
H	-3.01565	-5.87783	1.21063
C	-4.17897	-5.05590	-0.41816
H	-4.24489	-5.20203	-1.50337
C	-5.04718	-2.82622	-0.06031
H	-6.04550	-3.27139	-0.08585
C	-4.98639	-1.38898	0.05809
C	-6.20614	-0.64636	0.15877
H	-7.14593	-1.19007	0.18136
C	-6.19822	0.72213	0.21777
H	-7.13153	1.27255	0.28901
C	-4.96955	1.45564	0.17941
C	-3.74949	0.75083	0.10023
C	-3.75774	-0.69462	0.03420
C	-5.00725	2.89786	0.23109
H	-5.99010	3.35819	0.36364
C	-4.07835	5.13403	0.29878
H	-3.91980	5.36918	1.35840
C	-2.97420	5.78204	-0.54348
H	-3.27643	5.79452	-1.59799
C	0.64758	4.68863	-0.66141
C	1.87573	5.37249	-0.92779
H	1.85374	6.44889	-1.06996
C	3.05745	4.68531	-1.01964
H	3.98062	5.21326	-1.24039
C	3.10720	3.26784	-0.83584
C	1.91992	2.56834	-0.52697
C	0.66586	3.28897	-0.47168
C	4.37713	2.58981	-0.99256
H	5.24816	3.22289	-1.18540
C	5.87195	0.68722	-1.02198
H	6.22194	0.52378	0.00215
C	5.70801	-0.66706	-1.72261
H	5.60320	-0.51175	-2.80388
C	4.28773	-2.57166	-1.29215
H	5.10804	-3.19904	-1.65314
C	3.05469	-3.25598	-0.96712
C	3.00327	-4.68082	-1.08806
H	3.91347	-5.21264	-1.34974
C	1.83635	-5.36980	-0.88562
H	1.81470	-6.45190	-0.97499
C	0.62156	-4.68124	-0.57189
C	0.64094	-3.27507	-0.44481
C	1.88352	-2.55107	-0.61295
C	-0.58900	-5.44178	-0.37859
H	-0.49244	-6.53066	-0.40235
C	4.36822	0.02943	2.72665
C	5.82570	-0.06305	3.19406
H	5.90324	-0.00057	4.28108
H	6.39838	0.76021	2.75196
H	6.27455	-0.99715	2.84388
Ca	-0.35850	0.01189	0.05770
Co	3.21078	-0.00278	-0.58843
Co	-2.17103	3.12526	-0.10744
Co	-2.19423	-3.08607	-0.13688
O	-0.08433	-0.22703	2.42240
C	1.54213	0.39175	2.92443
H	1.30352	1.07563	3.72479
H	1.92293	0.77214	1.99250
C	1.00014	-0.95759	2.96736
H	1.46079	-1.69367	2.30074
H	0.80931	-1.38485	3.95823
H	6.58868	1.32503	-1.55076
H	6.58087	-1.30664	-1.55329
H	-2.78973	6.81375	-0.22703
H	-5.06731	5.50362	0.00846
H	-5.09358	-5.44921	0.03717
H	-2.83839	-6.77456	-0.31285
C	-0.57988	5.44508	-0.63158
H	-0.49409	6.51891	-0.81865

$TS_{BC}2$-EO

Energy: -1751998.0579250

O	2.04919	-1.11104	-0.41242
O	1.97952	1.41458	-0.13377
O	-0.29310	2.57596	-0.22246
O	-2.41224	1.22258	-0.06506
O	-2.31269	-1.32767	-0.26980
O	-0.10203	-2.50233	-0.33430
O	-0.25576	-0.33306	2.42449
O	1.10056	-0.86521	4.14644
N	4.79598	-1.01429	-0.91887

N	4.73114	1.57110	-0.53121	C	-0.12099	-5.39788	-0.59922
N	-1.75825	4.91279	-0.54274	H	0.01569	-6.48122	-0.64080
N	-3.93752	3.53784	-0.14005	C	1.06565	-4.58799	-0.69549
N	-3.62109	-3.72705	-0.55826	C	2.33003	-5.21155	-0.93035
N	-1.32755	-4.93603	-0.45517	H	2.36967	-6.29054	-1.04497
C	6.04923	-0.32476	-1.26638	C	3.47260	-4.45934	-1.02246
H	6.04520	-0.13089	-2.34646	H	4.42656	-4.93997	-1.21986
C	6.08452	1.00750	-0.50666	C	3.44475	-3.03934	-0.86402
H	6.34029	0.82158	0.54218	C	2.21306	-2.39781	-0.59794
C	4.51173	2.84439	-0.60090	C	1.00634	-3.18859	-0.53861
H	5.36755	3.51739	-0.70628	C	4.67321	-2.29547	-1.05158
C	3.20276	3.46224	-0.55933	H	5.54756	-2.87693	-1.35877
C	3.10111	4.87587	-0.75201	C	-0.02828	-0.58013	3.64519
H	4.01310	5.44718	-0.89994	C	-1.21560	-0.53468	4.60266
C	1.88485	5.50640	-0.76116	H	-0.91433	-0.76555	5.62529
H	1.82347	6.57981	-0.91484	H	-1.97716	-1.24918	4.27456
C	0.67264	4.76606	-0.58499	H	-1.67057	0.46062	4.57206
C	0.74160	3.37035	-0.38142	Ca	-0.15139	0.04251	0.11581
C	2.02749	2.70651	-0.34935	Co	-1.83804	-3.12700	-0.38386
C	-0.58715	5.46233	-0.65900	Co	-2.10010	3.07091	-0.23163
H	-0.53888	6.53797	-0.84857	Co	3.43020	0.19617	-0.35015
C	-2.99390	5.68350	-0.76406	H	-4.62875	-5.60529	-0.45649
H	-3.21556	5.67197	-1.83839	H	-2.29270	-6.82219	-0.70819
C	-4.12585	4.98994	0.00082	H	-5.10760	5.30919	-0.36410
H	-4.05629	5.23807	1.06704	H	-2.88293	6.72556	-0.44727
C	-4.82866	1.27487	-0.18754	H	6.82381	1.69187	-0.93753
C	-6.02449	0.49039	-0.27111	H	6.92683	-0.93680	-1.03233
H	-6.98201	1.00267	-0.27495	O	3.99169	-0.07121	1.75499
C	-5.97195	-0.87399	-0.35453	C	3.15126	0.55618	2.69846
H	-6.88549	-1.45653	-0.42558	C	2.65639	-0.80927	2.83014
C	-4.71515	-1.56170	-0.36313	H	2.44937	1.28846	2.28651
C	-3.51806	-0.81764	-0.26036	H	3.67330	0.96547	3.57349
C	-3.57579	0.62634	-0.16012	H	2.02527	-1.20077	2.05334
C	-4.69399	-2.98711	-0.52293	H	3.21199	-1.50132	3.44631
H	-5.66204	-3.48048	-0.64282	C	-4.93885	2.71308	-0.13426
C	-3.70792	-5.16776	-0.85552	H	-5.94997	3.12586	-0.08835
H	-3.71048	-5.29364	-1.94475				
C	-2.47131	-5.84080	-0.25718				
H	-2.61056	-5.97685	0.82176				

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