

Rational Investigation of the Role of the Epoxides as Substrates for CO₂ Capture in the Cycloaddition Reaction Catalysed by Ascorbic Acid

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Table S1. %V_{Bur} global and by quadrants, whether or not considering the hydrogens for the isolated epoxide.

	Substrate	%V _{Bur}				
		global	SW	NW	NE	SE
Without hydrogen atoms	<i>EPO-H</i>	32.1	24.5	24.5	39.8	39.8
	<i>EPO-CH₃</i>	36.9	24.5	24.5	58.5	40.1
	<i>EPO-(CH₃)₂</i>	41.9	24.5	24.5	59.4	59.4
	<i>EPO-cis(CH₃)₂</i>	46.5	55.1	25.1	40.2	65.6
	<i>EPO-trans(CH₃)₂</i>	46.8	54.7	25.0	58.4	49.2
	<i>EPO-tBu</i>	42.5	24.5	27.8	75.0	42.5
	<i>EPO-CH₂-nBu</i>	38.7	24.5	24.5	64.2	41.4
	<i>EPO-OH</i>	35.8	24.5	24.5	54.4	39.8
	<i>EPO-CH₂-OH</i>	38.3	24.5	24.5	63.2	40.8
	<i>EPO-Glyc</i>	41.7	29.8	24.5	40.1	72.6
	<i>EPO-Ph</i>	39.9	24.5	26.3	67.9	40.9
	<i>EPO-(Ph)₂</i>	48.1	24.5	27.3	68.4	72.1
	<i>EPO-cis(Ph)₂</i>	58.1	76.3	27.5	42.4	86.1
	<i>EPO-trans(Ph)₂</i>	59.0	74.6	30.7	68.2	62.3
	<i>EPO-CH₂Ph</i>	40.7	24.5	24.5	72.3	41.7
	<i>EPO-CF₃</i>	40.5	24.5	25.9	70.9	40.6
	<i>EPO-C(CF₃)₃</i>	49.2	24.5	36.0	89.0	47.1
	<i>EPO-CH₂F</i>	38.1	24.5	24.5	62.8	40.5
	<i>EPO-CH₂Cl</i>	39.2	24.5	24.5	66.2	41.6
	<i>EPO-CH₂Br</i>	39.6	24.5	24.5	67.4	41.9
	<i>EPO-Cyc</i>	50.9	24.8	60.0	78.6	40.2
With hydrogen atoms	Substrate	global	SW	NW	NE	SE
	<i>EPO-H</i>	34.6	26.6	26.6	42.6	42.6
	<i>EPO-CH₃</i>	39.3	26.6	26.6	60.9	42.9
	<i>EPO-(CH₃)₂</i>	44.3	26.6	26.6	61.9	61.9

<i>EPO-cis(CH₃)₂</i>	50.0	27.2	60.1	69.6	43.1
<i>EPO-trans(CH₃)₂</i>	50.4	59.4	27.1	60.8	54.3
<i>EPO-tBu</i>	45.4	26.7	31.2	78.4	45.3
<i>EPO-CH₂-nBu</i>	41.3	26.6	26.6	67.8	44.2
<i>EPO-OH</i>	37.7	26.7	26.6	54.9	42.6
<i>EPO-CH₂-OH</i>	40.6	26.6	26.6	65.5	43.6
<i>EPO-Glyc</i>	43.7	32.3	26.7	42.8	73.1
<i>EPO-Ph</i>	42.1	26.6	29.9	68.3	43.8
<i>EPO-(Ph)₂</i>	50.1	26.6	31.0	68.7	74.0
<i>EPO-cis(Ph)₂</i>	60.4	30.1	78.1	86.6	46.8
<i>EPO-trans(Ph)₂</i>	61.4	75.6	35.5	69.1	65.4
<i>EPO-CH₂Ph</i>	43.4	26.7	26.6	75.7	44.5
<i>EPO-CF₃</i>	42.3	26.6	28.0	71.1	43.4
<i>EPO-C(CF₃)₃</i>	50.8	26.6	37.8	89.1	49.8
<i>EPO-CH₂F</i>	40.4	26.6	26.6	65.0	43.2
<i>EPO-CH₂Cl</i>	41.5	26.6	26.6	68.3	44.3
<i>EPO-CH₂Br</i>	41.8	26.6	26.6	69.4	44.7
<i>EPO-Cyc</i>	54.0	27.0	64.9	81.1	43.0

Table S2. %V_{Bur} global and by quadrants, whether or not considering the hydrogens for TS-CD.

	Substrate	%V _{Bur}				
		global	SW	NW	NE	SE
Without hydrogen atoms	<i>EPO-H</i>	40.6	27.1	26.9	50.5	58.1
	<i>EPO-CH₃</i>	46.0	27.4	26.9	69.9	59.8
	<i>EPO-(CH₃)₂</i>	50.9	27.0	27.3	76.3	73.2
	<i>EPO-cis(CH₃)₂</i>	55.1	28.1	60.6	71.4	60.4
	<i>EPO-trans(CH₃)₂</i>	55.3	60.7	27.1	68.0	65.4
	<i>EPO-tBu</i>	51.1	27.3	27.3	89.7	60.3

With hydrogen atoms	<i>EPO-CH₂-nBu</i>	49.1	27.6	27.1	80.6	61.2
	<i>EPO-OH</i>	44.8	27.1	26.9	65.9	59.3
	<i>EPO-CH₂-OH</i>	47.5	27.5	27.0	75.7	59.9
	<i>EPO-Glyc</i>	46.5	27.4	26.7	71.4	60.5
	<i>EPO-Ph</i>	49.2	27.2	27.2	82.4	59.7
	<i>EPO-(Ph)₂</i>	57.2	27.4	28.8	86.1	86.7
	<i>EPO-cis(Ph)₂</i>	66.3	35.9	81.6	87.5	60.1
	<i>EPO-trans(Ph)₂</i>	67.7	80.3	32.6	79.9	77.8
	<i>EPO-CH₂Ph</i>	50.8	27.3	31.3	83.6	60.8
	<i>EPO-CF₃</i>	49.4	27.2	26.8	83.9	59.8
	<i>EPO-C(CF₃)₃</i>	56.6	27.6	40.7	95.7	62.3
	<i>EPO-CH₂F</i>	46.1	27.3	26.9	70.5	59.8
	<i>EPO-CH₂Cl</i>	46.2	27.3	26.9	70.8	59.9
	<i>EPO-CH₂Br</i>	46.3	27.3	26.9	71.0	60.0
	<i>EPO-Cyc</i>	59.4	27.6	64.7	86.0	59.3
	Substrate	global	SW	NW	NE	SE
	<i>EPO-H</i>	43.0	29.4	29.1	53.0	60.5
	<i>EPO-CH₃</i>	48.5	29.7	29.2	73.0	62.3
	<i>EPO-(CH₃)₂</i>	53.5	29.2	29.6	78.2	77.0
	<i>EPO-cis(CH₃)₂</i>	58.8	30.5	66.4	75.5	62.8
	<i>EPO-trans(CH₃)₂</i>	59.0	65.9	29.4	71.0	69.7
	<i>EPO-tBu</i>	54.0	29.5	32.6	91.0	62.7
	<i>EPO-CH₂-nBu</i>	51.8	29.9	31.1	82.5	63.6
	<i>EPO-OH</i>	46.6	29.4	29.1	66.0	61.8
	<i>EPO-CH₂-OH</i>	50.5	29.7	29.2	80.5	62.4
	<i>EPO-Glyc</i>	49.1	29.7	29.0	74.7	63.0
	<i>EPO-Ph</i>	51.2	29.5	29.7	83.5	62.3
	<i>EPO-(Ph)₂</i>	59.2	29.6	32.0	87.0	88.2
	<i>EPO-cis(Ph)₂</i>	68.2	39.9	81.6	88.7	62.7

<i>EPO-trans(Ph)₂</i>	69.8	80.3	37.0	80.7	81.4
<i>EPO-CH₂Ph</i>	53.2	29.6	34.4	85.5	63.2
<i>EPO-CF₃</i>	51.2	29.5	29.1	83.9	62.3
<i>EPO-C(CF₃)₃</i>	58.1	29.8	42.5	95.7	64.4
<i>EPO-CH₂F</i>	48.7	29.6	29.1	73.9	62.2
<i>EPO-CH₂Cl</i>	48.8	29.6	29.1	74.1	62.3
<i>EPO-CH₂Br</i>	48.8	29.6	29.1	74.2	62.4
<i>EPO-Cyc</i>	62.4	29.9	69.7	88.3	61.7

Table S3. Selected distances for the free epoxide **EPO-CH₃** and for **TS-CD** (in Å).

Nucleophile	Distances				%V _{Bur}	
	d(C-O) epoxide	d(C-C) epoxide	d(C⋯O) TS-CD	d(C⋯X) TS-CD	epoxide	TS-CD
I⁻	1.434	1.480	2.065	2.735	36.9	46.0
Br⁻	1.434	1.480	2.018	2.523	36.9	46.0
Cl⁻	1.434	1.480	1.917	2.451	36.9	46.2
F⁻	1.434	1.480	1.614	2.185	36.9	46.2

Table S4. %V_{Bur} global and by quadrants, whether or not considering the hydrogens for **TS-CD** for **EPO-CH₃**.

	Substrate	%V _{Bur}				
		global	SW	NW	NE	SE
<i>Without hydrogen atoms</i>	<i>I-</i>	46.0	27.4	26.9	69.9	59.8
	<i>Br-</i>	46.0	27.2	26.8	70.4	59.7
	<i>Cl-</i>	46.2	26.9	26.7	71.4	59.7
	<i>F-</i>	46.2	25.6	25.4	74.1	59.8
<i>With hydrogen atoms</i>	<i>I-</i>	48.5	29.7	29.2	73.0	62.3
	<i>Br-</i>	48.6	29.5	29.1	73.4	62.2
	<i>Cl-</i>	48.7	29.2	28.9	74.5	62.1
	<i>F-</i>	48.8	27.9	27.8	77.2	62.2

Table S5. Electronic parameters for intermediate **C** (H = HOMO, L = LUMO, η = chemical hardness, ϵ = electrophilicity, q = NPA charge).

Substrate	H	L	η	ϵ	q(O)	q(C)
I-	-0.056	-0.003	0.054	0.008	-0.744	-0.544
Br-	-0.056	0.018	0.074	0.003	-0.745	-0.684
Cl-	-0.055	0.053	0.108	0.000	-0.746	-0.363
F-	-0.053	0.072	0.125	0.000	-0.748	0.032

Table S6. Selected distances for the free epoxide **EPO-CH₃** and for **TS-CD** (in Å) with nucleophiles with the counteraction.

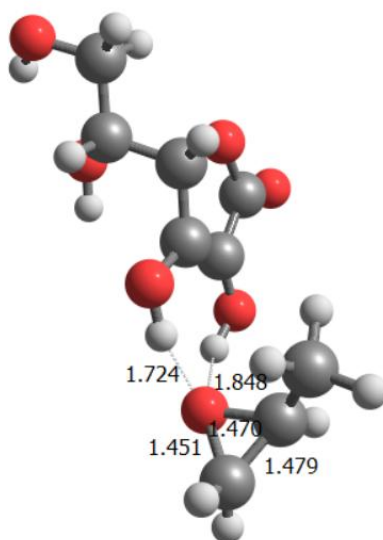
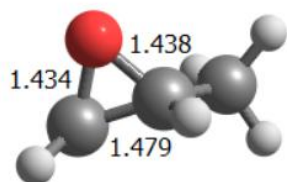
Nucleophile	Distances				%V _{Bur}	
	d(C-O) epoxide	d(C-C) epoxide	d(C...O) TS-CD	d(C...X) TS-CD	epoxide	TS-CD
KI	1.434	1.480	2.059	2.739	36.9	46.4
TBAI	1.434	1.480	-	-	36.9	-

Table S7. %V_{Bur} global and by quadrants, whether or not considering the hydrogens for **TS-CD** with nucleophiles with the counteraction.

Without hydrogen atoms	Substrate	%V _{Bur}				
		global	SW	NW	NE	SE
	KI	46.4	28.4	26.9	68.5	61.7
	TBAI	-	-	-	-	-
With hydrogen atoms	Substrate	global	SW	NW	NE	SE
	KI	48.9	30.7	29.2	71.5	64.1
	TBAI	-	-	-	-	-

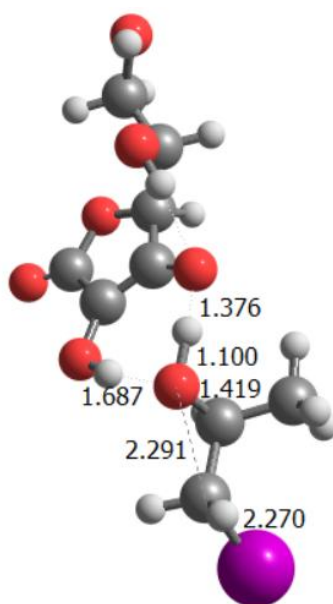
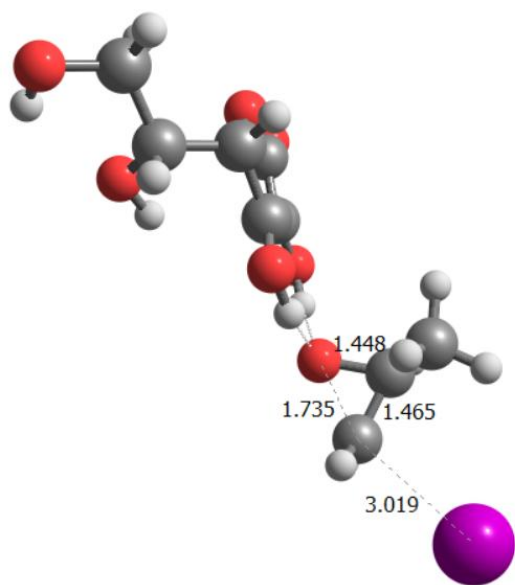
Table S8. Electronic parameters for intermediate **C** (H = HOMO, L = LUMO, η = chemical hardness, ϵ = electrophilicity, q = NPA charge) with nucleophiles with the counteraction.

Substrate	H	L	η	ϵ	q(O)	q(C)
KI	-0.193	-0.084	0.109	0.088	-0.835	-0.569
TBAI	-0.173	-0.077	0.096	0.082	-0.776	-0.568



EPO-CH₃

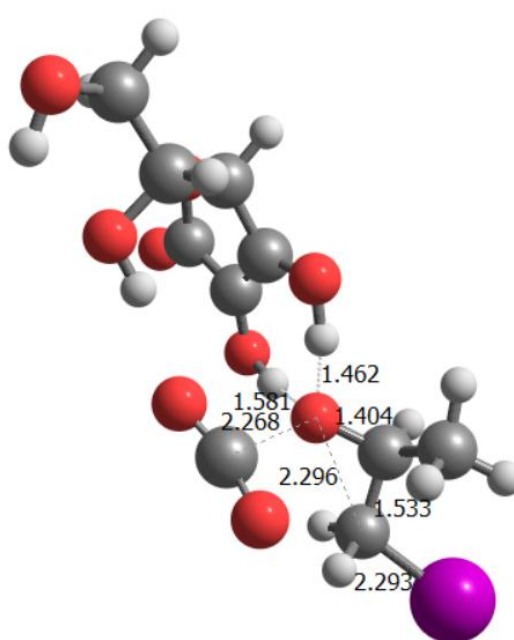
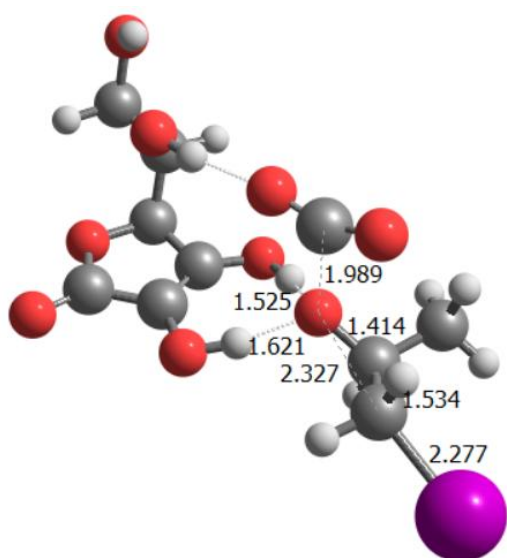
A



[352.6i]

TS-AB

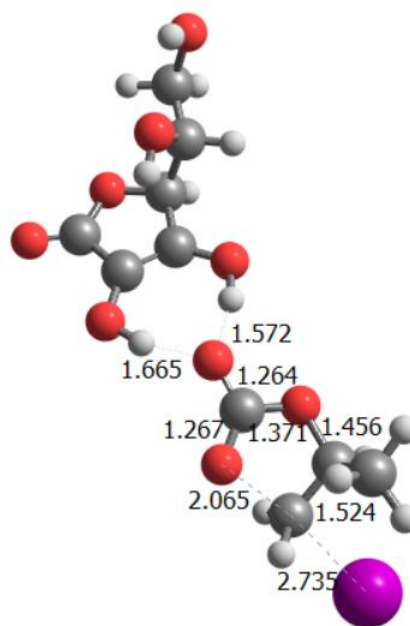
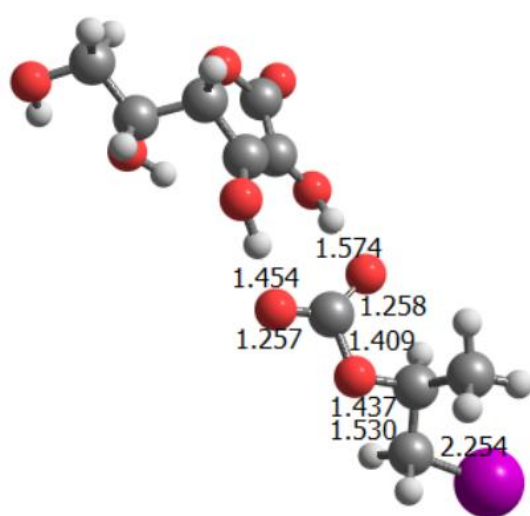
B



[7.2i]

B+CO₂

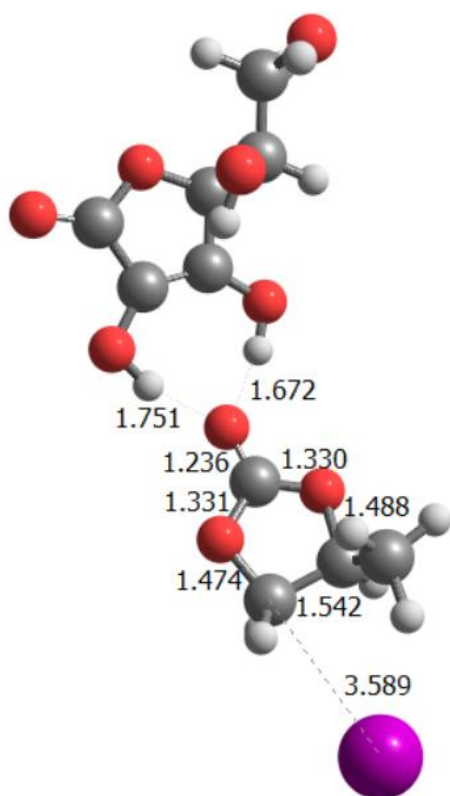
TS-BC



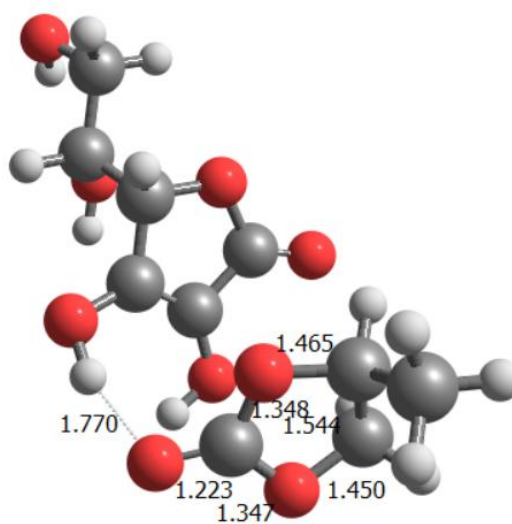
[270.6i]

C

TS-CD

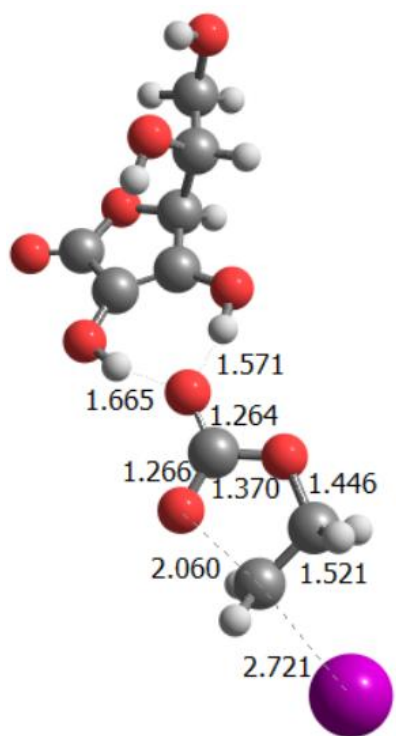


D

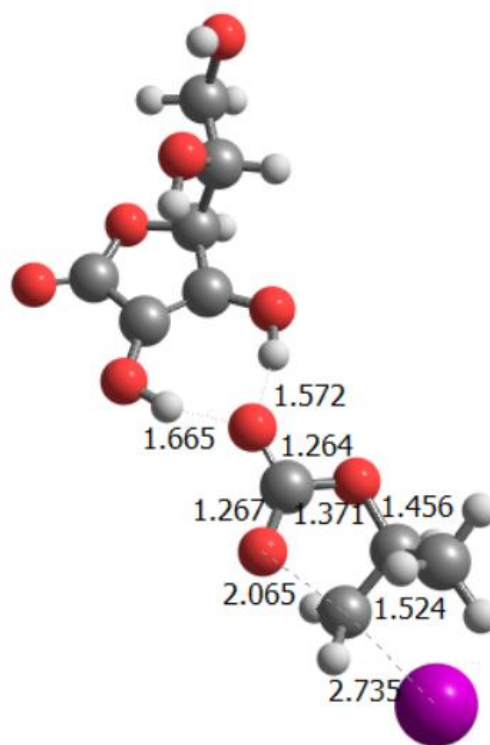


E

Figure S1. Intermediates and transition states of the cycloaddition of carbon dioxide (CO_2) to epoxide **EPO-CH₃** (selected distances in Å, and imaginary frequencies for the transition states included within brackets).



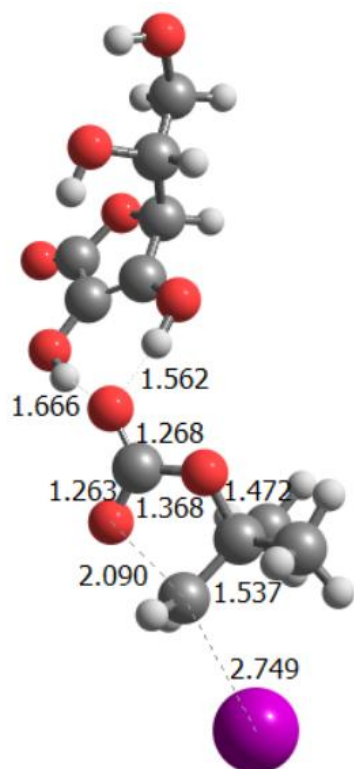
[273.8i]



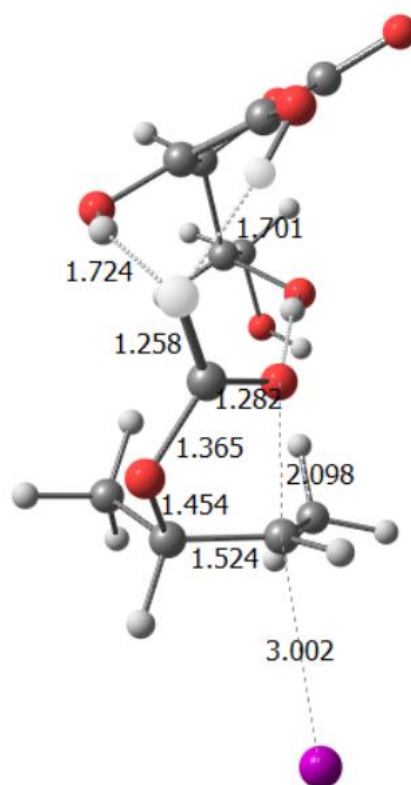
[270.6i]

EPO-H

EPO-CH₃



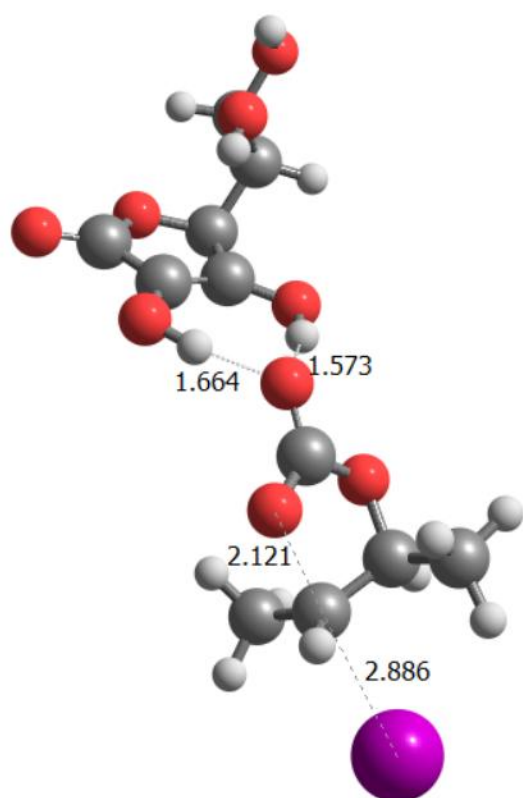
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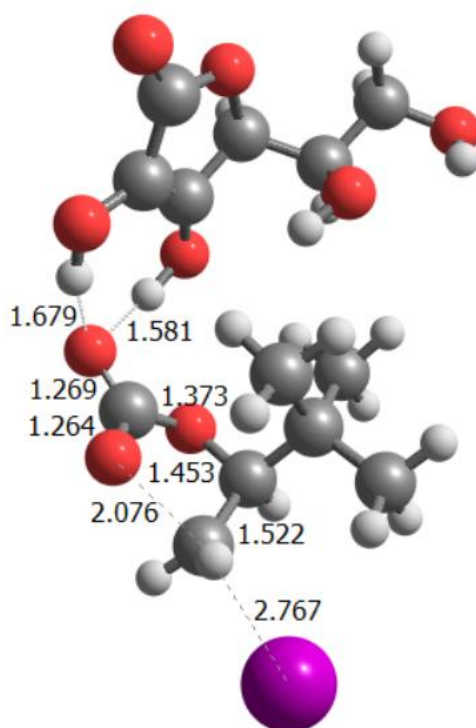
[225.9i]

EPO-(CH₃)₂

EPO-*cis*-(CH₃)₂



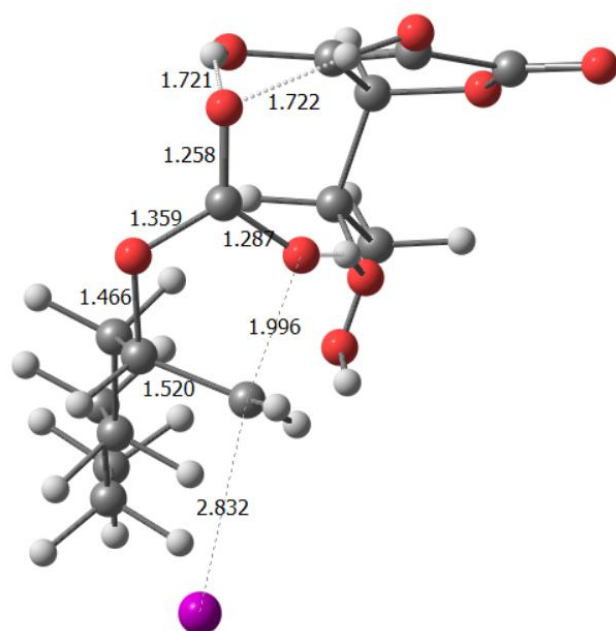
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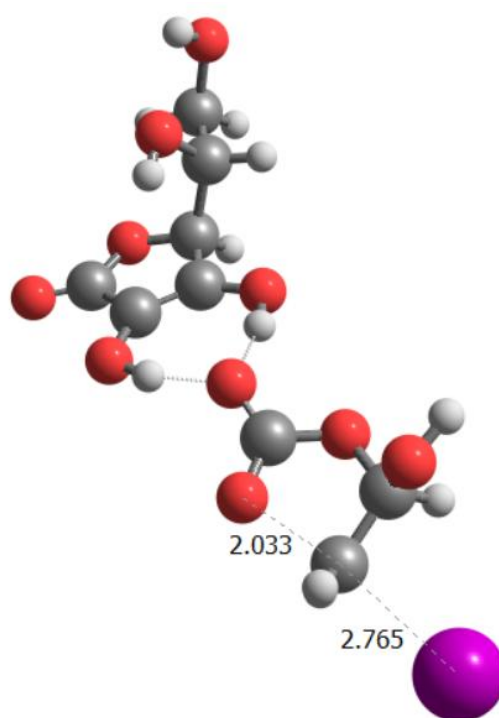
[261.1i]

EPO-*trans*(CH₃)₂

EPO-*t*Bu



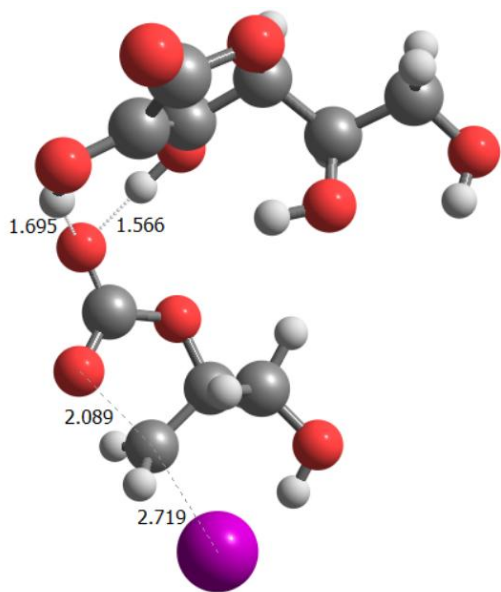
[271.2i]



[299.0i]

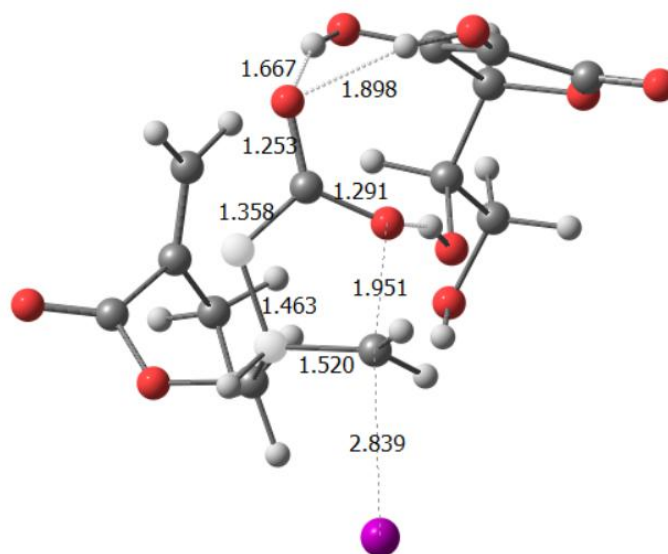
EPO-CH₂-*n*Bu

EPO-OH



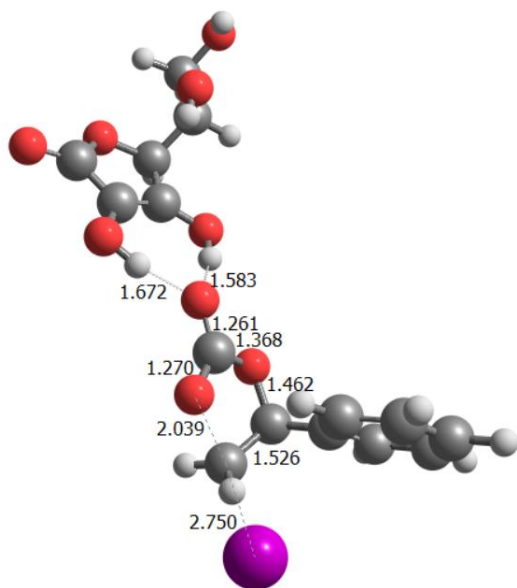
[266.2i]

EPO-CH₂-OH



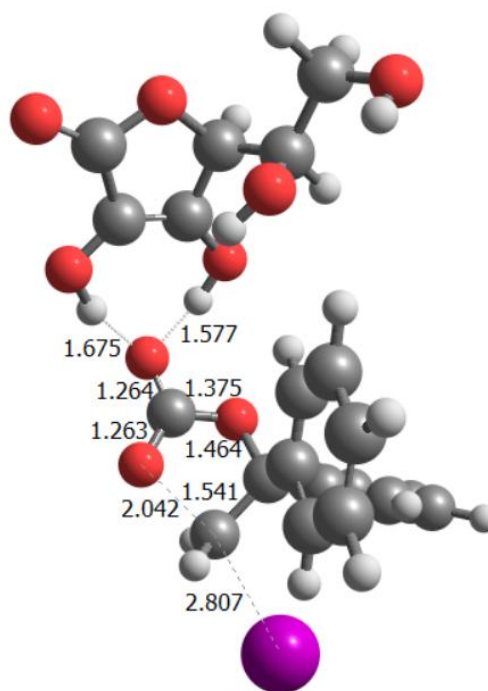
[284.8i]

EPO-Glyc



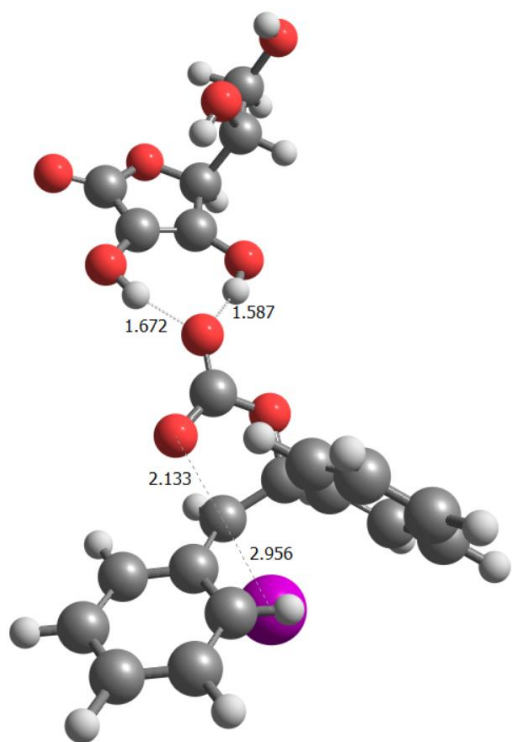
[283.5i]

EPO-Ph



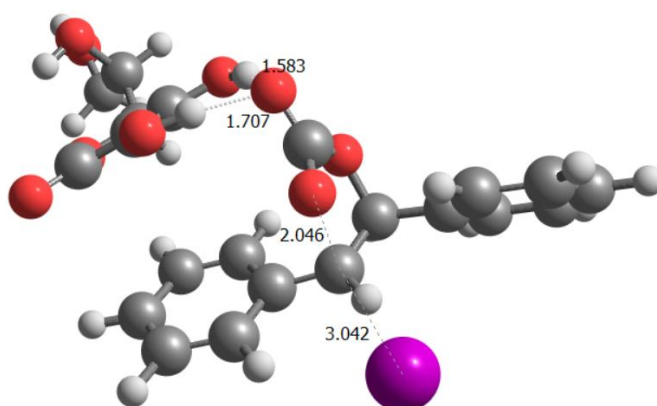
[268.1i]

EPO-(Ph)₂



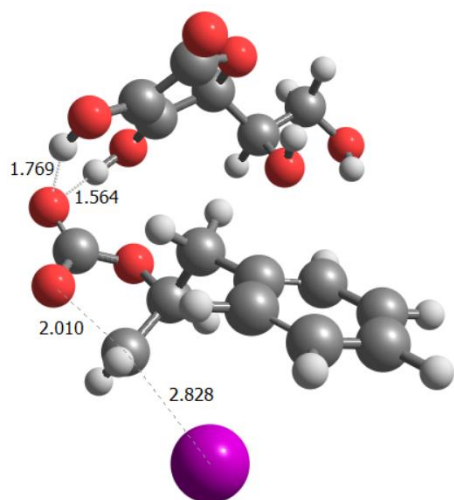
[164.7i]

EPO-*cis*(Ph)₂



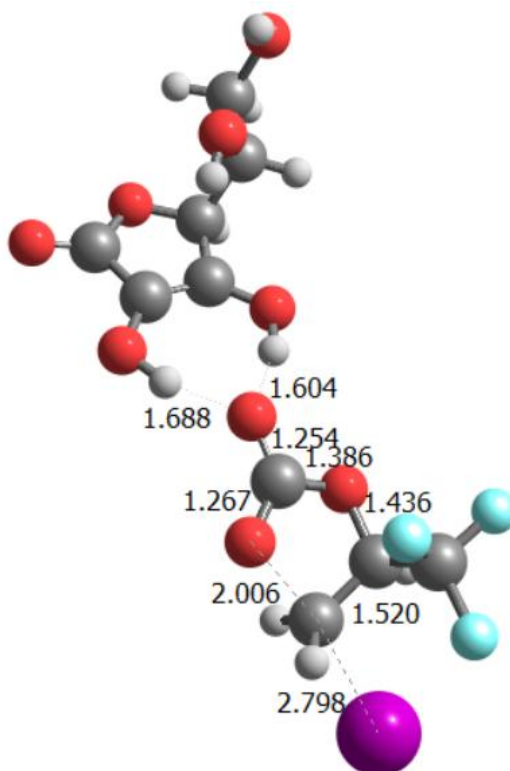
[180.7i]

EPO-*trans*(Ph)₂



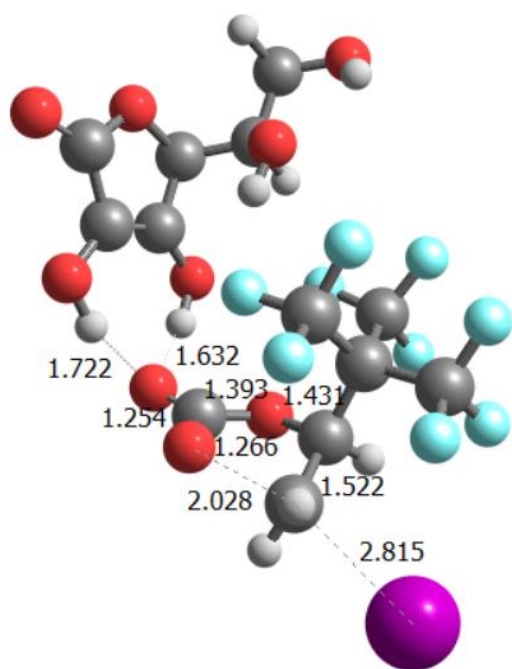
[287.7i]

EPO-CH₂Ph

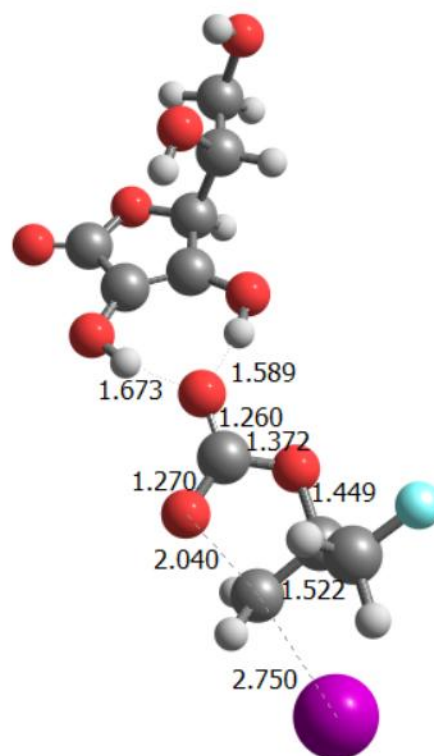


[299.8i]

EPO-CF₃



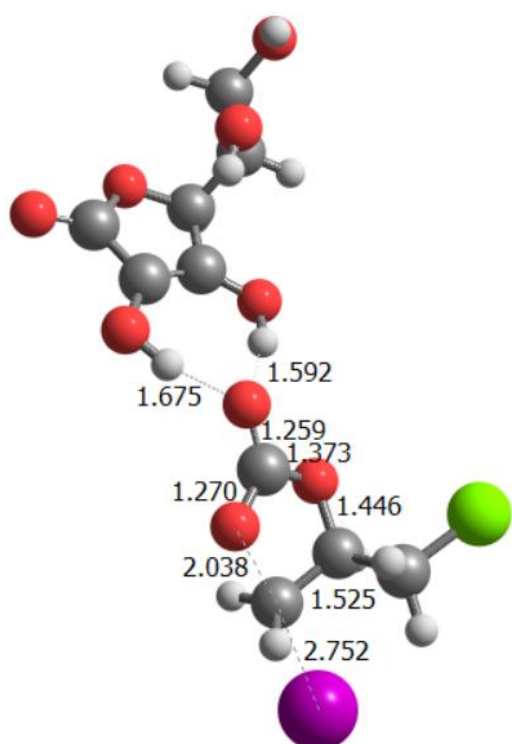
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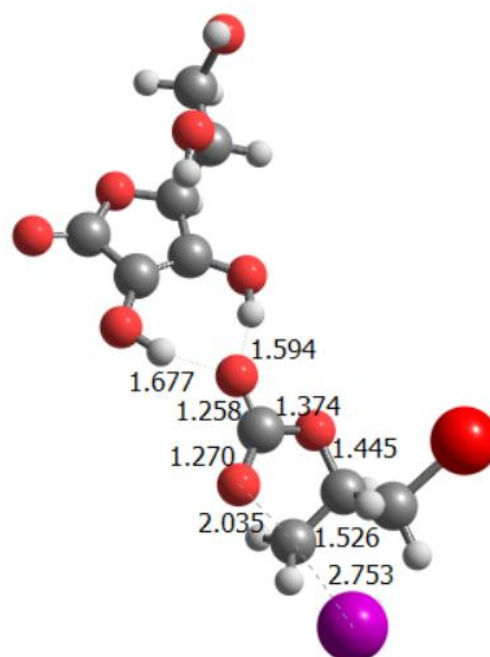
[283.5i]

EPO-C(CF₃)₃

EPO-CH₂F



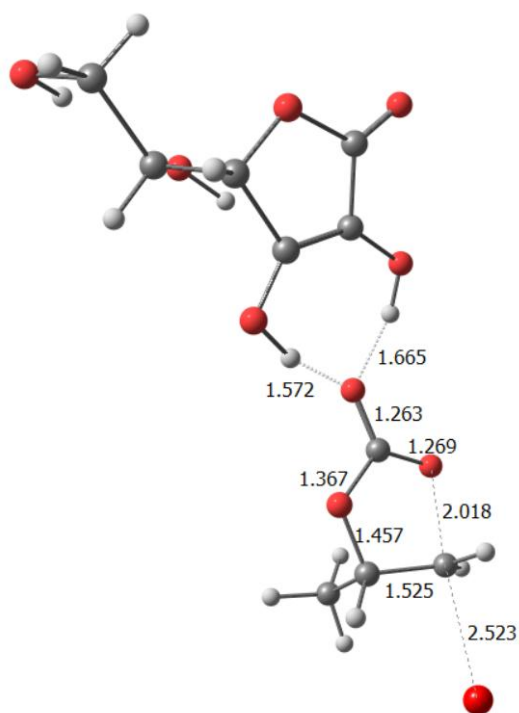
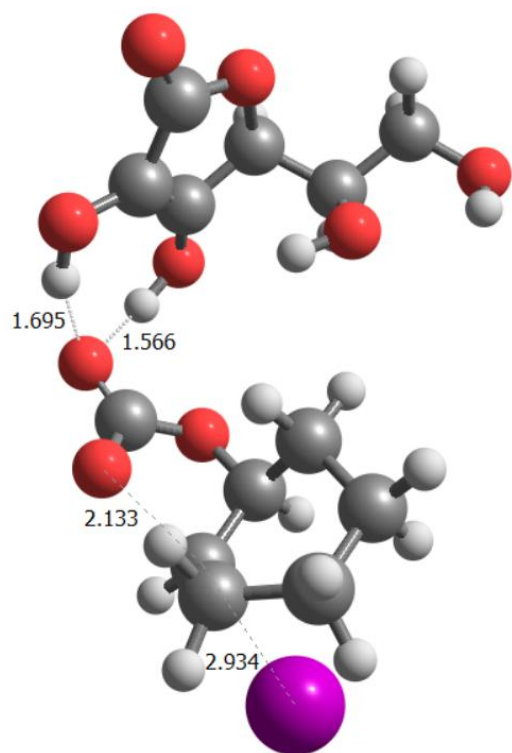
[285.4i]



[287.5i]

EPO-CH₂Cl

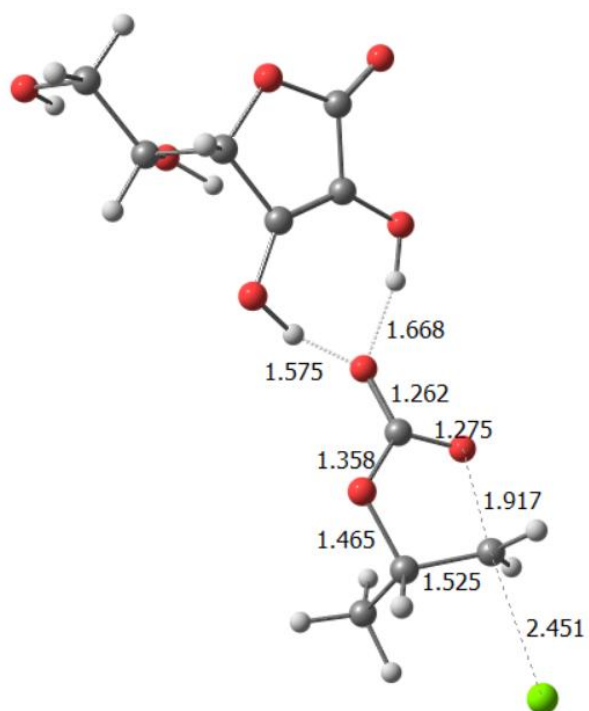
EPO-CH₂Br



[287.5i]

[231.7i]

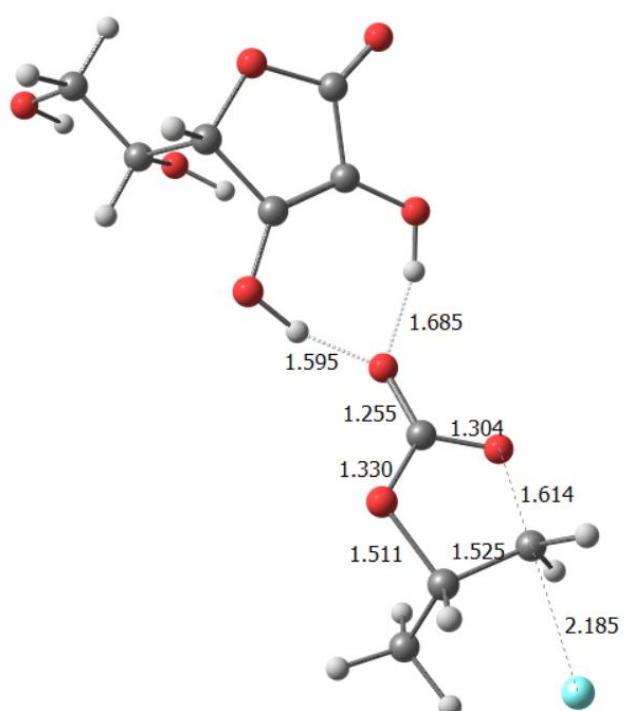
EPO-Cyc



[311.3i]

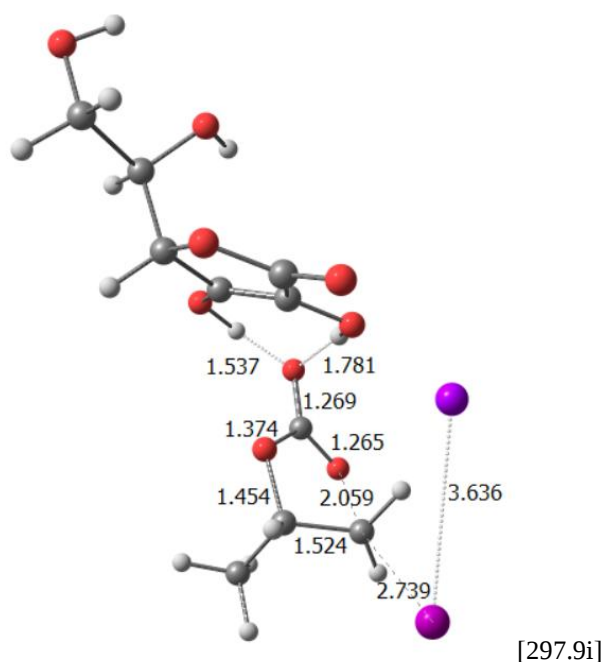
Cl-

Br-



[131.2i]

F-



KI

Figure S2. Transition state **TS-CD** of the cycloaddition of CO₂ for the series of epoxides under study (selected distances in Å, and imaginary frequencies for the transition states included within brackets).

Cations

Table S9. Relative Gibbs energies (in kcal/mol) obtained at various stages of the reaction of a methyl epoxide substrate with CO₂, catalyzed by ascorbic acid and iodine as a nucleophile.

Nucleophile	A+X ⁻	TS-AB	B	TS-BC	C	TS-CD	D
KI	-11.7	9.0	-6.5	-	-5.7	9.2	-20.8
TBAI	8.2	-	5.9	-	9.7	-	-0.2

Table S10. Selected distances for the free epoxide and for **TS-CD** (in Å).

Nucleophile	Distances				%V _{Bur}	
	d(C-O) epoxide	d(C-C) epoxide	d(C⋯O) TS-CD	d(C⋯X) TS-CD	epoxide	TS-CD
KI	1.434	1.480	2.059	2.739	36.9	46.4
TBAI	1.434	1.480	-	-	36.9	-

Table S11. %V_{Bur} global and by quadrants, whether or not considering the hydrogens for **TS-CD**.

Substrate	%V _{Bur}
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<i>Without</i>		global	SW	NW	NE	SE
<i>hydrogen</i>	KI	46.4	28.4	26.9	68.5	61.7
<i>atoms</i>	TBAI	-	-	-	-	-
<i>With</i>	Substrate	global	SW	NW	NE	SE
<i>hydrogen</i>	KI	48.9	30.7	29.2	71.5	64.1
<i>atoms</i>	TBAI	-	-	-	-	-

Table S12. Electronic parameters for intermediate **C** (H = HOMO, L = LUMO, η = chemical hardness, ϵ = electrophilicity, q = NPA charge).

Substrate	H	L	η	ϵ	q(O)	q(C)
KI	-0.193	-0.084	0.109	0.088	-0.835	-0.569
TBAI	-0.173	-0.077	0.096	0.082	-0.776	-0.568

Table S13. Xyz coordinates for optimized systems

EPO-H

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ACID-AB SCF Done: -849.606302929 A.U.

O	-1.282179	-0.823663	0.648564
O	-1.162267	2.028800	-0.815097
H	-0.322444	1.475449	-0.756793
C	-2.198741	0.129580	0.430757
O	-3.909916	3.030787	-0.507594
C	-2.159846	1.344687	-0.218423
O	-4.345340	1.064199	0.562199
C	-3.507613	1.956100	-0.115961
O	-4.203141	-1.112051	-1.318271
H	-3.381773	-0.617496	-1.524316
O	-6.217524	-2.660378	-0.344902

H	-5.931149	-2.446019	-1.256958
C	-3.622263	-0.138155	0.856297
H	-3.685685	-0.344675	1.951132
C	-4.225554	-1.334474	0.089222
H	-3.610337	-2.230530	0.359627
C	-5.690889	-1.601923	0.441293
H	-5.773575	-1.897414	1.510277
H	-6.252985	-0.645221	0.303670
H	-0.386482	-0.508238	0.258813
O	0.787588	0.340392	-0.309869
C	1.813801	0.706343	0.633151
H	1.994374	1.795918	0.720283
C	2.458437	-0.013237	-0.460796
H	2.816124	0.526945	-1.345716
H	2.554222	-1.105270	-0.425768
I	5.399812	-0.060795	0.332810
H	1.742713	0.204099	1.618566

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ACID-A+I SCF Done: -849.608984391 A.U.

O	-1.381559	-0.635109	0.935130
O	-1.237864	2.138577	-0.698674
H	-0.385927	1.646842	-0.535020
C	-2.309469	0.259919	0.554234
O	-4.038137	3.001473	-0.749298
C	-2.256228	1.431808	-0.163431
O	-4.495874	1.088547	0.404982
C	-3.635716	1.976405	-0.244288
O	-4.081265	-1.185304	-1.302633

H	-3.236879	-0.718032	-1.470940
O	-6.096931	-2.789662	-0.406454
H	-5.743264	-2.625591	-1.305036
C	-3.755652	-0.055236	0.849972
H	-3.922022	-0.195623	1.944300
C	-4.224450	-1.325873	0.107749
H	-3.597921	-2.171226	0.491560
C	-5.702352	-1.649444	0.339914
H	-5.873558	-1.870959	1.416081
H	-6.294447	-0.737905	0.077688
H	-0.475345	-0.326741	0.618451
O	0.786501	0.508275	-0.012552
C	2.081980	0.742510	0.662229
H	2.405307	1.796911	0.663596
C	2.063121	-0.002466	-0.591654
H	2.362426	0.497346	-1.527074
H	2.164676	-1.099615	-0.570293
I	5.504333	-0.351652	0.031481
H	2.208050	0.196326	1.612033

27

ACID-A SCF Done: -838.002193366 A.U.

O	-0.777518	-1.487180	0.250825
O	-1.459449	1.594654	0.972595
H	-2.064591	0.901913	1.327440
C	-0.188242	-0.305313	-0.049375
O	0.673624	3.058611	-0.371636
C	-0.464838	0.996682	0.269578
O	1.450999	1.024743	-1.055039

C	0.566875	1.854289	-0.375113
O	2.490593	-0.395700	1.204914
H	1.647691	-0.307506	1.690874
O	4.560651	-1.742959	-0.013269
H	4.528892	-1.320149	0.869083
C	1.107494	-0.346798	-0.821304
H	0.975770	-0.862145	-1.801659
C	2.229782	-1.056547	-0.028205
H	1.893683	-2.111811	0.137619
C	3.568042	-1.078065	-0.772261
H	3.451693	-1.626531	-1.731927
H	3.840025	-0.020943	-1.013691
H	-1.619391	-1.326121	0.747122
O	-3.140597	-0.539979	1.159889
C	-3.903306	-0.293060	-0.054853
C	-4.570650	-0.772199	1.172446
H	-3.962886	0.772901	-0.338812
H	-4.862667	-1.834374	1.258918
H	-5.142605	-0.063302	1.797740
H	-3.689670	-1.000957	-0.875824

31

ACID-B+CO2 SCF Done: -1038.10105176 A.U.

O	1.547875	-0.132638	-1.701631
O	0.652541	1.690832	0.723089
H	0.110562	0.882294	0.480092
C	2.228184	0.736913	-0.935461
O	3.183470	3.058856	1.493925
C	1.856819	1.517991	0.129204

O	4.151362	1.813139	-0.155388
C	3.058297	2.228395	0.615989
O	3.920843	-0.890746	0.794315
H	2.958647	-1.125284	0.830352
O	6.278605	-1.878825	0.013621
H	5.639225	-2.014634	0.750016
C	3.729288	0.754954	-1.023911
H	4.102994	0.959140	-2.055624
C	4.295180	-0.608277	-0.540534
H	3.898899	-1.380808	-1.247687
C	5.827860	-0.656024	-0.546733
H	6.209497	-0.578276	-1.589557
H	6.197858	0.235408	0.019998
H	0.676928	-0.346606	-1.223774
O	-0.493587	-0.560363	-0.153013
C	-1.864537	-0.607073	-0.497168
H	-2.018289	-0.068511	-1.460033
C	-2.630830	0.060632	0.640305
H	-2.330661	1.116479	0.786942
H	-2.520700	-0.519167	1.576217
I	-4.854154	0.139518	0.246173
O	-0.851528	-2.552649	1.199225
O	1.274235	-1.674963	0.984318
C	0.074665	-1.843472	0.871316
H	-2.201263	-1.661342	-0.614795

O	1.336985	-0.403223	-1.153593
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O	0.849947	2.122752	0.687921
H	0.128000	1.400443	0.571239
C	2.155432	0.569380	-0.745191
O	3.532467	3.394425	0.796537
C	1.958035	1.659455	0.078406
O	4.217391	1.669408	-0.529963
C	3.246486	2.371477	0.204762
O	4.123970	-0.772482	1.000431
H	3.174454	-0.664772	1.223011
O	6.294377	-2.024125	0.025372
H	5.838093	-1.982571	0.893604
C	3.628448	0.477301	-1.060296
H	3.811450	0.437435	-2.162022
C	4.258362	-0.777676	-0.416089
H	3.735169	-1.660378	-0.866965
C	5.762784	-0.902213	-0.666561
H	5.956387	-1.038000	-1.753611
H	6.238964	0.059077	-0.349808
H	0.375845	-0.225351	-0.666997
O	-0.677982	0.123624	0.155977
C	-1.917582	0.216462	-0.468799
H	-2.293358	1.270709	-0.539734
C	-2.849456	-0.613927	0.410574
H	-2.920110	-0.203317	1.436398
H	-2.550224	-1.678871	0.438744
I	-5.021321	-0.649168	-0.336069
O	-0.170675	-2.736245	0.718575
O	1.278483	-1.226711	1.788189
C	0.525839	-1.924324	1.208410

H	-1.918374	-0.193704	-1.512668
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ACID-B SCF Done: -849.627486968 A.U.

O	1.207459	-0.710910	0.759202
O	1.006756	2.436755	0.649899
H	0.375019	1.894543	1.202958
C	1.864612	0.174811	0.040939
O	3.303584	3.173615	-1.088465
C	1.822495	1.556576	-0.003765
O	3.648023	0.926172	-1.311453
C	2.937554	2.042494	-0.817471
O	3.843728	-1.227152	1.249084
H	2.868626	-1.237063	1.445160
O	6.163196	-2.111042	0.196491
H	5.738889	-2.109787	1.082161
C	2.986049	-0.274489	-0.883997
H	2.569167	-0.768827	-1.795203
C	3.914440	-1.301123	-0.174164
H	3.588771	-2.318890	-0.513926
C	5.396720	-1.146497	-0.516912
H	5.560684	-1.294754	-1.606581
H	5.696303	-0.098347	-0.273896
H	0.164125	-0.013280	1.450015
O	-0.663124	0.598165	1.762029
C	-1.609212	0.470929	0.720172
H	-2.488974	1.116981	0.939263
C	-2.011594	-1.001341	0.677036
H	-2.434132	-1.340509	1.642473

H	-1.151097	-1.632693	0.379481
I	-3.627334	-1.434061	-0.857034
H	-1.201008	0.784260	-0.272622

31

ACID-CD SCF Done: -1038.08656449 A.U.

O	2.258573	-0.874631	-0.356110
O	2.383095	2.140165	0.770889
H	1.543018	1.610342	0.924936
C	3.196557	0.079561	-0.386789
O	5.053319	3.025841	-0.066438
C	3.266934	1.362059	0.116967
O	5.306622	0.939049	-0.949886
C	4.586953	1.923302	-0.262029
O	5.425589	-0.999534	1.180521
H	4.658566	-0.441553	1.432262
O	7.271807	-2.687002	0.121641
H	7.114836	-2.357352	1.030935
C	4.538085	-0.269999	-0.985997
H	4.433193	-0.605694	-2.045184
C	5.240992	-1.383220	-0.179925
H	4.586635	-2.289441	-0.249997
C	6.637363	-1.722910	-0.706502
H	6.561040	-2.149761	-1.730755
H	7.216484	-0.768761	-0.772735
H	1.438426	-0.518498	0.140500
O	0.417843	0.383646	0.923700
C	-0.832265	0.423265	0.738680
O	-1.374939	-0.664378	0.107097

O	-1.621321	1.355080	1.071409
C	-3.385355	0.757946	0.191519
H	-3.212967	1.478912	-0.616873
H	-3.867115	1.120086	1.103068
C	-2.820257	-0.650207	0.087262
H	-3.105639	-1.133140	-0.865660
I	-5.882751	0.240968	-0.757057
H	-3.200713	-1.274868	0.924741

31

ACID-C SCF Done: -1038.10000114 A.U.

O	-2.667372	-0.953118	1.287263
O	-1.384675	1.335132	-0.613830
H	-0.684314	0.867799	-0.036198
C	-3.162990	0.090970	0.630998
O	-3.719140	2.966925	-1.287413
C	-2.632630	1.055119	-0.205797
O	-4.931167	1.499462	-0.034559
C	-3.736645	1.963927	-0.602465
O	-4.975483	-1.078828	-1.332205
H	-4.032731	-0.805595	-1.377918
O	-7.516964	-1.804399	-0.747908
H	-6.943359	-1.910750	-1.535741
C	-4.664187	0.287323	0.679149
H	-5.028064	0.391695	1.729738
C	-5.392749	-0.902597	0.020349
H	-5.139108	-1.806083	0.631367
C	-6.912156	-0.731526	-0.037071
H	-7.331617	-0.723024	0.993384

H	-7.124672	0.261836	-0.504492
H	-1.710975	-1.255187	0.955346
O	0.552657	0.206792	0.683850
C	0.542212	-1.051746	0.660819
O	-0.427202	-1.847969	0.596204
O	1.786461	-1.714984	0.711393
C	2.946008	-0.888251	0.790493
H	2.794910	-0.047327	1.500582
C	3.243607	-0.351600	-0.606234
H	2.472431	0.376884	-0.919555
H	3.350147	-1.166152	-1.348232
I	5.197979	0.770951	-0.678842
H	3.766048	-1.542152	1.154969

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ACID-DminusI SCF Done: -1026.49273631 A.U.

O	0.385378	-1.344971	2.057130
O	-0.852230	1.521591	1.458804
H	-0.974181	1.139798	2.352430
C	0.475486	-0.537444	0.984081
O	-0.399008	1.839519	-1.390294
C	-0.055669	0.694166	0.725845
O	0.957506	0.008443	-1.240474
C	0.126058	0.977741	-0.711955
O	3.275670	0.305354	0.428924
H	2.807550	0.579429	1.240954
O	5.003130	-1.390267	-0.892411
H	5.184541	-0.527172	-0.467287
C	1.279095	-0.959354	-0.221339

H	0.947913	-1.964493	-0.569864
C	2.800696	-0.980213	0.045939
H	2.980720	-1.741066	0.847055
C	3.620767	-1.368730	-1.188668
H	3.328884	-2.387400	-1.523385
H	3.361674	-0.653222	-2.008117
H	-0.543154	-1.270700	2.419878
O	-2.272649	-0.839526	2.493856
C	-2.776850	-0.445886	1.453335
O	-2.504629	-0.973378	0.239295
O	-3.634907	0.587996	1.366991
C	-3.647052	1.038353	-0.012664
H	-2.894904	1.849624	-0.113472
H	-4.661332	1.401248	-0.261638
C	-3.214271	-0.222503	-0.778764
H	-2.513931	-0.002480	-1.607032
H	-4.062610	-0.840523	-1.141829

31

ACID-D SCF Done: -1038.10696030 A.U.

O	2.452394	-0.809588	-0.691319
O	2.452024	2.137951	0.640228
H	1.592106	1.642773	0.635917
C	3.398751	0.128324	-0.511935
O	5.224327	2.996345	0.289209
C	3.408968	1.371530	0.075337
O	5.578584	0.969395	-0.693699
C	4.782987	1.922080	-0.055071
O	5.374691	-1.101034	1.290188

H	4.548155	-0.616171	1.494034
O	7.304508	-2.792944	0.366486
H	7.047904	-2.529086	1.274196
C	4.808797	-0.216522	-0.926613
H	4.857712	-0.477719	-2.010223
C	5.369922	-1.396783	-0.103459
H	4.717054	-2.279957	-0.322935
C	6.818888	-1.742808	-0.454830
H	6.878071	-2.082331	-1.512032
H	7.423989	-0.807457	-0.359311
H	1.581852	-0.485960	-0.315304
O	0.365456	0.418019	0.391429
C	-0.863257	0.377028	0.264160
O	-1.499264	-0.645983	-0.299757
O	-1.669742	1.346736	0.682381
C	-3.072853	0.986868	0.391353
H	-3.504258	1.765245	-0.263767
H	-3.634311	0.969032	1.342927
C	-2.955374	-0.396152	-0.283599
H	-3.324932	-0.414897	-1.324775
I	-6.422364	0.137192	-0.242559
H	-3.443962	-1.208944	0.283769

7

EPO SCF Done: -153.675645412 A.U.

O	0.956049	0.827556	-0.213475
C	-0.106397	0.144562	0.458717
C	1.057053	-0.592641	-0.078044
H	-0.185602	0.324996	1.550039

H	0.951745	-1.178928	-1.013514
H	1.841470	-0.961655	0.613588
H	-1.076542	0.106276	-0.076971

EPO-CH₃

31

ACID-AB SCF Done: -888.902621607 A.U.

O	-1.259545	-0.912283	0.490249
O	-1.151308	2.000028	-0.840300
H	-0.321496	1.425654	-0.847980
C	-2.166535	0.065875	0.367298
O	-3.859114	3.041755	-0.345706
C	-2.133377	1.310461	-0.224199
O	-4.283388	1.034446	0.650679
C	-3.460517	1.942115	-0.025622
O	-4.278372	-1.055351	-1.332351
H	-3.459266	-0.563714	-1.554217
O	-6.278106	-2.604918	-0.333289
H	-6.029952	-2.353585	-1.247126
C	-3.572235	-0.193985	0.852331
H	-3.584898	-0.450088	1.938433
C	-4.238240	-1.341553	0.063306
H	-3.630502	-2.261061	0.262570
C	-5.690466	-1.595739	0.474452
H	-5.728137	-1.939830	1.531372
H	-6.236986	-0.622503	0.409087

H	-0.366643	-0.575985	0.099870
O	0.789887	0.293238	-0.443591
C	1.726675	0.731973	0.569730
H	1.893901	1.829502	0.537705
C	1.493202	0.209346	1.969180
H	2.393202	0.406887	2.586339
H	0.614414	0.708455	2.426917
H	1.307713	-0.883935	1.956697
C	2.491689	-0.044823	-0.408308
H	2.917555	0.436679	-1.296475
H	2.571060	-1.133866	-0.298168
I	5.328960	-0.011647	0.623478

31

ACID-A+I SCF Done: -888.906219783 A.U.

O	-1.313656	-0.849853	0.558776
O	-1.216389	2.029967	-0.884756
H	-0.374494	1.495961	-0.853345
C	-2.226560	0.119377	0.372760
O	-3.941714	3.034602	-0.501602
C	-2.195833	1.338213	-0.263653
O	-4.360698	1.066121	0.571026
C	-3.539308	1.956106	-0.123870
O	-4.301395	-1.094771	-1.324515
H	-3.460371	-0.655853	-1.568910
O	-6.280348	-2.654637	-0.281457
H	-6.035278	-2.441673	-1.205566
C	-3.638526	-0.143120	0.836856
H	-3.670477	-0.355227	1.931782

C	-4.273293	-1.330388	0.080383
H	-3.655100	-2.232408	0.322391
C	-5.726627	-1.594200	0.481558
H	-5.773371	-1.885575	1.553626
H	-6.291275	-0.636837	0.360043
H	-0.429869	-0.546016	0.174811
O	0.804092	0.354655	-0.384269
C	1.798530	0.750707	0.645699
H	1.965488	1.844092	0.648052
C	1.667870	0.099631	1.993692
H	2.650776	0.177065	2.504697
H	0.886906	0.594808	2.606424
H	1.419014	-0.975849	1.893345
C	2.254533	0.019571	-0.537907
H	2.756470	0.554646	-1.359542
H	2.476027	-1.056760	-0.452764
I	5.536324	-0.135848	0.632265

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ACID-A SCF Done: -877.300217031 A.U.

O	-0.803063	-1.451902	0.334987
O	-1.454887	1.659355	0.882407
H	-2.023628	0.995269	1.333313
C	-0.202735	-0.300831	-0.042691
O	0.677082	3.034652	-0.561553
C	-0.468345	1.019110	0.203068
O	1.436529	0.959694	-1.133803
C	0.562413	1.832789	-0.495333
O	2.480695	-0.347753	1.197535

H	1.651942	-0.279527	1.709633
O	4.537501	-1.764621	0.035639
H	4.509095	-1.302603	0.898327
C	1.085937	-0.394449	-0.820907
H	0.941279	-0.962489	-1.769857
C	2.210354	-1.068170	0.000074
H	1.872663	-2.112875	0.219618
C	3.544607	-1.130769	-0.748862
H	3.420604	-1.722167	-1.681656
H	3.820276	-0.087359	-1.040498
H	-1.675999	-1.237088	0.764420
O	-3.155470	-0.457799	1.184490
C	-3.960538	-0.096376	0.009406
C	-4.512565	-0.959211	1.076174
H	-4.248116	0.972292	0.028477
H	-4.584378	-2.049660	0.906365
H	-5.215534	-0.544138	1.821108
C	-3.478745	-0.620030	-1.317294
H	-4.283965	-0.526355	-2.074904
H	-2.608247	-0.025440	-1.663062
H	-3.169891	-1.681430	-1.246145

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ACID-B+CO2 SCF Done: -1077.39018523 A.U.

O	1.528070	-0.250951	-1.594048
O	0.659021	1.687154	0.747799
H	0.079995	0.896932	0.482621
C	2.212644	0.662020	-0.890130
O	3.193945	3.097563	1.417801

C	1.852079	1.491206	0.145437
O	4.140867	1.796032	-0.199834
C	3.055603	2.232713	0.575172
O	4.006261	-0.914432	0.792601
H	3.041605	-1.097789	0.862444
O	6.369886	-1.842873	-0.066299
H	5.770531	-2.000812	0.697181
C	3.710691	0.712321	-1.031008
H	4.036429	0.907213	-2.081382
C	4.333883	-0.625080	-0.557731
H	3.942850	-1.415902	-1.247470
C	5.864967	-0.628870	-0.602225
H	6.216109	-0.532213	-1.653754
H	6.222965	0.268544	-0.038018
H	0.632574	-0.409229	-1.098824
O	-0.534331	-0.476830	-0.120059
C	-1.844996	-0.446782	-0.650085
H	-1.901185	0.374690	-1.409233
C	-2.209668	-1.773244	-1.327839
H	-3.215146	-1.738444	-1.795372
H	-1.462367	-1.989462	-2.118811
H	-2.181935	-2.598414	-0.588639
C	-2.725235	-0.063014	0.546195
H	-2.393412	0.894610	0.989475
H	-2.747469	-0.863807	1.308735
I	-4.911087	0.322176	0.037901
O	-0.904374	-2.437260	1.551492
O	1.257095	-1.677433	1.147821
C	0.074734	-1.866126	1.166859

ACID-BC SCF Done: -1077.38997190 A.U.

O	1.440014	-0.444344	-1.388338
O	0.691141	1.847381	0.653084
H	0.063791	1.051943	0.497809
C	2.165505	0.550388	-0.862225
O	3.271865	3.285325	1.015938
C	1.855385	1.534458	0.050292
O	4.134044	1.745222	-0.429945
C	3.085003	2.309732	0.315168
O	4.057842	-0.826327	0.899565
H	3.090647	-0.914410	1.040946
O	6.374377	-1.864940	0.019468
H	5.832221	-1.930332	0.836166
C	3.655012	0.568107	-1.088825
H	3.916182	0.625850	-2.173725
C	4.309325	-0.701453	-0.494385
H	3.883550	-1.569759	-1.059597
C	5.834645	-0.717035	-0.620476
H	6.126900	-0.742132	-1.693696
H	6.220536	0.237130	-0.182389
H	0.520418	-0.453224	-0.868846
O	-0.607264	-0.307291	0.050360
C	-1.868355	-0.281191	-0.566779
H	-2.011524	0.678051	-1.131826
C	-2.041203	-1.458998	-1.535139
H	-3.032998	-1.455556	-2.032979
H	-1.255616	-1.401118	-2.316744

H	-1.913406	-2.415549	-0.987646
C	-2.829309	-0.291929	0.627257
H	-2.635484	0.564147	1.300052
H	-2.781488	-1.248196	1.182118
I	-5.047656	-0.050808	0.099110
O	-0.746476	-2.735038	1.359177
O	1.236260	-1.499563	1.538974
C	0.177714	-1.994335	1.346849

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ACID-B SCF Done: -888.917764439 A.U.

O	1.466889	-1.243015	0.358891
O	0.672699	1.757646	0.928932
H	0.137663	0.983853	1.288631
C	1.986301	-0.108080	-0.069422
O	2.903574	3.269386	-0.337111
C	1.682144	1.215427	0.189702
O	3.681860	1.231532	-1.014612
C	2.740375	2.061830	-0.366886
O	4.136528	-1.355166	1.027928
H	3.177701	-1.589426	1.133735
O	6.621700	-1.628518	0.009797
H	6.164122	-1.879536	0.841615
C	3.232866	-0.129874	-0.938873
H	2.985133	-0.459599	-1.977752
C	4.287219	-1.120602	-0.371808
H	4.154360	-2.083557	-0.930493
C	5.736030	-0.667975	-0.555508
H	5.972870	-0.556858	-1.636212

H	5.841485	0.339510	-0.085148
H	0.311382	-0.934449	1.040304
O	-0.620136	-0.514928	1.447891
C	-1.568149	-0.548787	0.392734
H	-1.285525	0.164393	-0.424406
C	-1.688435	-1.959022	-0.194617
H	-2.410240	-2.003743	-1.035832
H	-0.687401	-2.269414	-0.557241
H	-2.005826	-2.672593	0.596052
C	-2.829075	-0.028157	1.085194
H	-2.660761	0.982250	1.502942
H	-3.171837	-0.722134	1.877787
I	-4.625911	0.243030	-0.274451

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ACID-CD SCF Done: -1077.37923928 A.U.

O	2.264735	-0.838661	-0.439792
O	2.389975	2.150220	0.758476
H	1.542427	1.625515	0.884148
C	3.211941	0.106748	-0.424339
O	5.088523	3.025814	0.009369
C	3.282033	1.376834	0.110083
O	5.343927	0.956976	-0.914699
C	4.616716	1.932754	-0.222875
O	5.389482	-1.029812	1.173934
H	4.622379	-0.468593	1.418175
O	7.245915	-2.712004	0.124242
H	7.069161	-2.401101	1.036500
C	4.564883	-0.242999	-0.997353

H	4.483573	-0.553881	-2.066130
C	5.236187	-1.381069	-0.199118
H	4.575098	-2.278732	-0.306265
C	6.642230	-1.723133	-0.697662
H	6.588054	-2.126104	-1.732938
H	7.232035	-0.773709	-0.727492
H	1.437341	-0.488654	0.048326
O	0.413505	0.402612	0.840185
C	-0.844407	0.412636	0.719792
O	-1.395680	-0.671767	0.088562
O	-1.640416	1.314114	1.117389
C	-3.390393	0.723409	0.194282
H	-3.155127	1.389642	-0.643944
H	-3.907590	1.146422	1.060251
C	-2.846883	-0.700438	0.205180
H	-3.171309	-1.237829	-0.706647
I	-5.862380	0.282332	-0.890308
C	-3.248397	-1.472913	1.459744
H	-4.350550	-1.585135	1.495826
H	-2.779785	-2.476692	1.457113
H	-2.913727	-0.923195	2.363861

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ACID-C SCF Done: -1077.38869021 A.U.

O	-2.661653	-1.060754	1.038718
O	-1.663200	1.678641	-0.377100
H	-0.895790	1.161384	0.055866
C	-3.266879	0.058043	0.654235
O	-4.140252	3.227452	-0.551537

C	-2.858783	1.219212	0.024060
O	-5.165685	1.431692	0.405293
C	-4.044955	2.101631	-0.105313
O	-5.121324	-0.799005	-1.426606
H	-4.205785	-0.443148	-1.456551
O	-7.565566	-1.831606	-0.894872
H	-7.038480	-1.717457	-1.713522
C	-4.771457	0.119068	0.819187
H	-5.071615	-0.036440	1.883496
C	-5.460469	-0.953832	-0.049837
H	-5.107792	-1.945267	0.333045
C	-6.988447	-0.895275	0.006512
H	-7.339730	-1.145065	1.032224
H	-7.296451	0.156102	-0.217436
H	-1.704918	-1.204940	0.610618
O	0.408814	0.472381	0.605461
C	0.500728	-0.750543	0.326068
O	-0.401865	-1.594538	0.095630
O	1.793504	-1.307790	0.261684
C	2.901645	-0.414758	0.460054
H	2.657326	0.576827	0.019654
C	3.188953	-0.251754	1.951934
H	4.063189	0.405774	2.134500
H	2.297400	0.205707	2.423546
H	3.375958	-1.242020	2.418574
C	3.995903	-1.108809	-0.353845
H	3.672947	-1.255542	-1.401237
H	4.296192	-2.077988	0.090535
I	5.909844	0.071104	-0.508456

ACID-DminusI SCF Done: -1065.78729410 A.U.

O	0.386210	-1.333081	2.042924
O	-0.847158	1.526111	1.396877
H	-0.954849	1.168287	2.302210
C	0.480797	-0.541275	0.959638
O	-0.372964	1.804878	-1.453909
C	-0.046883	0.687393	0.679814
O	0.976249	-0.029108	-1.270279
C	0.143527	0.950390	-0.760525
O	3.284683	0.293679	0.406044
H	2.795390	0.591151	1.197264
O	5.019653	-1.423360	-0.875804
H	5.198124	-0.552809	-0.464924
C	1.291415	-0.981000	-0.234899
H	0.962705	-1.991736	-0.569434
C	2.811276	-0.997917	0.042302
H	2.985502	-1.744754	0.857920
C	3.638780	-1.408186	-1.180127
H	3.349625	-2.433083	-1.497875
H	3.383987	-0.707828	-2.013881
H	-0.537847	-1.238864	2.415638
O	-2.247653	-0.794805	2.532193
C	-2.772375	-0.415482	1.494918
O	-2.514119	-0.946093	0.283419
O	-3.644986	0.607352	1.418662
C	-3.689827	1.046240	0.037733
H	-2.954520	1.869057	-0.083669

H	-4.716293	1.388672	-0.192776
C	-3.259561	-0.214392	-0.743561
H	-2.529762	0.042054	-1.537611
C	-4.394747	-1.082245	-1.263953
H	-4.924327	-0.558990	-2.086263
H	-4.002393	-2.041051	-1.656245
H	-5.123782	-1.300056	-0.456099

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ACID-D SCF Done: -1077.40103641 A.U.

O	2.553586	-0.371782	-1.355451
O	2.503031	2.393213	0.321563
H	1.627610	2.008196	0.057252
C	3.509630	0.405772	-0.818217
O	5.342867	2.910183	0.783837
C	3.491569	1.567951	-0.083587
O	5.734808	0.967184	-0.343719
C	4.900500	1.944032	0.202303
O	4.817740	-1.253302	1.233882
H	4.023397	-0.682927	1.293221
O	6.738786	-3.081399	0.589278
H	6.286012	-2.883034	1.434876
C	4.936783	-0.076816	-0.915113
H	5.239019	-0.228230	-1.978398
C	5.143031	-1.399750	-0.145227
H	4.482659	-2.161215	-0.633665
C	6.590677	-1.895937	-0.175847
H	6.885999	-2.127508	-1.222609
H	7.242299	-1.063996	0.189536

H	1.651386	0.009995	-1.144668
O	0.387870	0.932433	-0.553905
C	-0.765440	0.618759	-0.239361
O	-1.345176	-0.512918	-0.629602
O	-1.547481	1.385383	0.517391
C	-2.898458	0.797293	0.546544
H	-3.561897	1.383006	-0.118936
H	-3.285506	0.853820	1.579110
C	-2.661293	-0.644054	0.052438
H	-3.399721	-0.931664	-0.719241
I	-6.306108	-0.327411	0.477934
C	-2.553221	-1.692180	1.143835
H	-3.560128	-1.818041	1.593104
H	-2.221784	-2.662257	0.723275
H	-1.836309	-1.374124	1.930498

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ACID SCF Done: -958.106590964 A.U.

O	1.642076	0.061932	0.834422
O	1.093506	2.448450	-1.247251
H	0.500080	3.111406	-1.669997
C	0.581520	0.844998	0.584835
O	-1.663772	3.127359	-0.749964
C	0.324269	1.849363	-0.301894
O	-1.639204	1.539161	0.906276
C	-1.072561	2.268964	-0.118817
O	-1.417348	-1.014740	-0.380651
O	-3.274049	-1.909530	0.612386
C	-0.694307	0.543495	1.338372

H	-0.556962	0.639488	2.440322
C	-1.229683	-0.866410	1.018964
H	-0.459485	-1.593643	1.370451
C	-2.623758	-1.162871	1.628539
H	-2.572726	-1.782513	2.546447
H	-3.160878	-0.213388	1.862847
C	-2.788038	-1.412949	-0.637200
C	-3.592387	-0.198433	-1.115411
H	-4.642925	-0.489683	-1.315417
H	-3.573570	0.606788	-0.356545
H	-3.146236	0.208807	-2.044142
C	-2.779010	-2.565289	-1.634280
H	-3.812078	-2.921872	-1.815505
H	-2.339149	-2.233442	-2.594886
H	-2.174464	-3.396270	-1.222699
C	2.757432	0.161407	-0.084929
H	2.400160	-0.087257	-1.109461
H	3.125198	1.211248	-0.106588
C	3.838841	-0.801658	0.380742
H	4.124997	-0.539658	1.423661
H	3.409938	-1.827475	0.422521
C	5.077146	-0.782312	-0.528459
H	5.485526	0.252899	-0.572851
H	4.772905	-1.030734	-1.570620
C	6.172831	-1.750629	-0.065653
H	7.055827	-1.719317	-0.736652
H	6.520878	-1.503860	0.960126
H	5.802225	-2.797761	-0.046004

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EPO SCF Done: -192.969880692 A.U.

O	0.829754	0.794705	-0.247190
C	-0.151921	0.044878	0.487694
C	1.054318	-0.609725	-0.065524
H	-0.158399	0.258833	1.578567
H	0.960685	-1.236612	-0.976051
H	1.893856	-0.885741	0.604515
C	-1.515378	-0.098357	-0.148734
H	-2.094791	-0.911801	0.337543
H	-2.095981	0.842383	-0.043909
H	-1.421474	-0.325110	-1.230210

EPO-(CH₃)₂

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ACID-AB SCF Done: -928.198098586 A.U.

O	-1.224923	-0.942024	0.405740
O	-1.125599	1.998304	-0.848973
H	-0.302328	1.415589	-0.889336
C	-2.127666	0.041967	0.333179
O	-3.813522	3.049426	-0.258898
C	-2.100099	1.302514	-0.224290
O	-4.230327	1.018510	0.692579
C	-3.415734	1.938552	0.021975
O	-4.287342	-1.019112	-1.343822
H	-3.470853	-0.525776	-1.571513
O	-6.275092	-2.579164	-0.339747

H	-6.044454	-2.305494	-1.251778
C	-3.523884	-0.219867	0.845075
H	-3.511858	-0.504036	1.924115
C	-4.216765	-1.341770	0.042836
H	-3.611264	-2.270208	0.203735
C	-5.660887	-1.596600	0.481131
H	-5.676579	-1.969007	1.528971
H	-6.201166	-0.618051	0.454874
H	-0.326823	-0.584776	0.027496
O	0.814641	0.280192	-0.489755
C	1.709819	0.768446	0.550838
C	1.386729	0.250506	1.943577
H	2.252550	0.432957	2.611528
H	0.494096	0.773330	2.345656
H	1.175454	-0.836938	1.928065
C	2.525140	-0.079090	-0.332417
H	2.989784	0.344804	-1.230793
H	2.572495	-1.162485	-0.166704
I	5.271714	-0.017982	0.840517
C	1.927932	2.272132	0.490127
H	2.782154	2.551575	1.138822
H	2.153168	2.594292	-0.546214
H	1.011176	2.799318	0.824847

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ACID-A+I SCF Done: -928.203024936 A.U.

O	-1.232184	-0.967131	0.429294
O	-1.075243	1.978442	-0.870627
H	-0.261696	1.402617	-0.920125

C	-2.104668	0.051209	0.346246
O	-3.722517	3.084903	-0.276701
C	-2.050290	1.300851	-0.226055
O	-4.176481	1.082590	0.716412
C	-3.352290	1.970667	0.021996
O	-4.324443	-0.974451	-1.287411
H	-3.481538	-0.551485	-1.553084
O	-6.319253	-2.492584	-0.216073
H	-6.114382	-2.239660	-1.139912
C	-3.499847	-0.170573	0.878041
H	-3.480489	-0.439371	1.960671
C	-4.232220	-1.285503	0.100066
H	-3.646391	-2.226507	0.260504
C	-5.672710	-1.503296	0.569460
H	-5.675092	-1.851748	1.625399
H	-6.195221	-0.515552	0.531631
H	-0.346012	-0.674972	0.036878
O	0.885797	0.216840	-0.505110
C	1.794884	0.707797	0.591999
C	1.605938	0.002809	1.913496
H	2.544298	0.121385	2.495140
H	0.758058	0.443119	2.477961
H	1.420816	-1.080186	1.773987
C	2.352642	-0.027542	-0.549181
H	2.876624	0.521362	-1.348589
H	2.638494	-1.085331	-0.428147
I	5.552678	0.285438	0.941880
C	1.927013	2.210437	0.646472
H	1.058149	2.664611	1.165260

H	2.862048	2.448262	1.195376
H	2.003006	2.645982	-0.369089

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ACID-A SCF Done: -916.597147614 A.U.

O	-0.815079	-1.415194	0.374145
O	-1.403293	1.691591	0.978979
H	-2.012186	1.029466	1.378875
C	-0.197456	-0.272320	0.003690
O	0.725777	3.056933	-0.479877
C	-0.437493	1.047739	0.272445
O	1.450970	0.978750	-1.085184
C	0.595602	1.855755	-0.426785
O	2.496861	-0.388690	1.212477
H	1.676208	-0.321681	1.737582
O	4.517037	-1.817663	0.002415
H	4.504068	-1.372445	0.874284
C	1.080371	-0.374650	-0.791143
H	0.914888	-0.923255	-1.748094
C	2.201850	-1.082027	0.004865
H	1.849099	-2.124944	0.208590
C	3.526947	-1.152696	-0.759500
H	3.383234	-1.724171	-1.701833
H	3.817128	-0.108700	-1.034499
H	-1.693818	-1.182844	0.788527
O	-3.163328	-0.400590	1.170929
C	-3.985494	-0.059245	-0.018560
C	-4.484531	-0.983004	1.028182
H	-4.486395	-2.073411	0.843042

H	-5.224053	-0.626714	1.768878
C	-3.436523	-0.603975	-1.319904
H	-4.230399	-0.604274	-2.094661
H	-2.606332	0.040925	-1.675283
H	-3.047217	-1.633307	-1.201620
C	-4.444648	1.383436	-0.034652
H	-5.246919	1.517870	-0.788842
H	-4.832333	1.695816	0.954803
H	-3.593193	2.043113	-0.297890

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ACID-B+CO2 SCF Done: -1116.68428001 A.U.

O	1.492057	-0.349845	-1.537582
O	0.607678	1.702019	0.691386
H	0.055432	0.865455	0.500504
C	2.169776	0.609875	-0.892701
O	3.130314	3.180865	1.273584
C	1.802631	1.492127	0.095850
O	4.085714	1.808045	-0.278836
C	2.998322	2.271000	0.478917
O	3.996815	-0.867777	0.834306
H	3.037530	-1.068176	0.911326
O	6.378859	-1.782790	0.001524
H	5.788688	-1.925121	0.774785
C	3.665412	0.679084	-1.052831
H	3.974977	0.830290	-2.115252
C	4.317303	-0.624295	-0.528101
H	3.942495	-1.450325	-1.184525
C	5.847810	-0.598544	-0.574433

H	6.195570	-0.531090	-1.629233
H	6.187807	0.324998	-0.042453
H	0.602309	-0.494718	-1.010191
O	-0.540825	-0.516015	-0.044888
C	-1.821125	-0.404126	-0.655564
C	-2.181609	-1.716841	-1.371669
H	-3.179950	-1.665256	-1.852719
H	-1.421989	-1.916682	-2.155640
H	-2.168488	-2.558902	-0.652143
C	-2.712961	-0.119414	0.567700
H	-2.425082	0.830837	1.056304
H	-2.677563	-0.959820	1.284275
I	-4.951270	0.151998	0.171630
O	-0.899391	-2.622606	1.527823
O	1.247607	-1.747243	1.266974
C	0.085149	-2.013611	1.243195
C	-1.778555	0.779760	-1.641229
H	-1.033743	0.564867	-2.434720
H	-2.765722	0.963201	-2.113079
H	-1.445697	1.697137	-1.113680

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ACID-BC SCF Done: -1116.67788089 A.U.

O	1.425764	-0.567153	-1.329093
O	0.702692	1.904324	0.487353
H	0.069855	1.097077	0.420059
C	2.167044	0.455653	-0.892666
O	3.304240	3.339910	0.727722
C	1.869397	1.523562	-0.075929

O	4.147760	1.667511	-0.575701
C	3.105984	2.307221	0.117972
O	4.075803	-0.774938	0.970329
H	3.109204	-0.825309	1.130482
O	6.372392	-1.907992	0.152843
H	5.846694	-1.894856	0.982444
C	3.656015	0.441686	-1.127910
H	3.907111	0.404554	-2.216009
C	4.308175	-0.776129	-0.432800
H	3.867819	-1.687315	-0.913181
C	5.831339	-0.816287	-0.577733
H	6.107657	-0.938502	-1.648424
H	6.230433	0.169455	-0.230915
H	0.491954	-0.505249	-0.817165
O	-0.627692	-0.270101	0.053564
C	-1.869808	-0.252732	-0.626227
C	-1.947632	-1.448262	-1.594103
H	-2.933127	-1.512051	-2.100328
H	-1.158814	-1.334520	-2.366988
H	-1.760055	-2.392792	-1.044663
C	-2.815144	-0.412084	0.577462
H	-2.724962	0.446912	1.269134
H	-2.639436	-1.368454	1.102121
I	-5.082766	-0.478961	0.132526
O	-0.562985	-2.827315	1.254824
O	1.246901	-1.390739	1.663189
C	0.285109	-2.014769	1.377688
C	-2.071881	1.101746	-1.373951
H	-1.151173	1.706414	-1.257232

H	-2.259927	0.959614	-2.457834
H	-2.917658	1.689232	-0.962245

ACID-B SCF Done: -928.211015246 A.U.

O	1.437317	-1.148778	0.184560
O	0.723564	1.871255	0.770320
H	0.119446	1.117948	1.055348
C	2.026233	-0.027076	-0.182345
O	3.078034	3.318846	-0.330508
C	1.757142	1.302106	0.086977
O	3.826960	1.264454	-0.991027
C	2.876127	2.118358	-0.389852
O	4.054574	-1.368176	1.028824
H	3.083935	-1.570869	1.068939
O	6.589566	-1.718773	0.165295
H	6.072570	-1.965500	0.962800
C	3.325285	-0.080314	-0.969815
H	3.134067	-0.383891	-2.028366
C	4.303946	-1.118472	-0.353980
H	4.172683	-2.067088	-0.936929
C	5.776906	-0.716975	-0.436508
H	6.086424	-0.596708	-1.497678
H	5.887836	0.277986	0.058610
H	0.269257	-0.813942	0.830251
O	-0.659706	-0.379416	1.225533
C	-1.681667	-0.605477	0.252831
C	-1.721333	-2.101090	-0.109248
H	-2.523278	-2.331761	-0.840080

H	-0.739544	-2.378415	-0.544509
H	-1.877140	-2.710823	0.805090
C	-2.907641	-0.156927	1.068057
H	-2.839964	0.916441	1.329089
H	-3.015298	-0.770225	1.982174
I	-4.938416	-0.333162	0.047445
C	-1.449928	0.258518	-1.000964
H	-0.497693	-0.049525	-1.477755
H	-2.271975	0.148233	-1.737628
H	-1.344483	1.325565	-0.719411

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ACID-CD SCF Done: -1116.66538986 A.U.

O	2.138739	-0.964380	0.264024
O	2.294073	2.247574	0.159023
H	1.506065	1.822450	0.616479
C	3.015573	-0.106404	-0.269620
O	4.759966	2.720458	-1.364793
C	3.102725	1.270419	-0.295095
O	4.971867	0.451256	-1.440358
C	4.320695	1.631388	-1.060756
O	5.505765	-0.555523	1.207457
H	4.761909	0.067959	1.352547
O	7.244062	-2.542189	0.568392
H	7.213022	-1.895029	1.303485
C	4.263748	-0.673082	-0.903502
H	4.013296	-1.377776	-1.731981
C	5.132781	-1.415864	0.133820
H	4.518028	-2.273392	0.509487

C	6.445989	-1.947593	-0.445220
H	6.233146	-2.724672	-1.212048
H	6.963301	-1.095651	-0.951931
H	1.382216	-0.430328	0.706577
O	0.424255	0.699274	1.201427
C	-0.811698	0.654448	0.921628
O	-1.331285	-0.600442	0.758062
O	-1.600288	1.633002	0.800072
C	-3.430892	0.628820	0.705314
H	-3.686945	1.439669	0.021689
H	-3.548047	0.795511	1.782812
C	-2.697200	-0.628322	0.211296
I	-6.120521	0.090099	0.527861
C	-3.236678	-1.961155	0.746474
H	-4.200685	-2.227484	0.277371
H	-2.486217	-2.747127	0.525281
H	-3.375388	-1.909117	1.844503
C	-2.598412	-0.617283	-1.318570
H	-2.111194	0.318008	-1.661594
H	-1.999652	-1.481469	-1.668339
H	-3.614961	-0.671808	-1.757932

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ACID-C SCF Done: -1116.67661683 A.U.

O	-2.674246	-1.144081	0.946862
O	-1.799290	1.818710	-0.022415
H	-1.011872	1.266917	0.321940
C	-3.329399	-0.006100	0.742705
O	-4.339654	3.273472	0.045940

C	-2.973914	1.254796	0.301107
O	-5.284048	1.309762	0.712671
C	-4.195510	2.096814	0.311410
O	-5.164326	-0.605849	-1.443617
H	-4.261782	-0.217979	-1.421035
O	-7.559403	-1.811336	-1.073492
H	-7.044284	-1.550872	-1.865847
C	-4.833807	-0.033976	0.917035
H	-5.119163	-0.364848	1.944719
C	-5.485315	-0.986663	-0.107053
H	-5.089341	-2.009980	0.116574
C	-7.013859	-1.001561	-0.039693
H	-7.345962	-1.420797	0.935911
H	-7.366720	0.057922	-0.098172
H	-1.718823	-1.177317	0.494767
O	0.328197	0.553638	0.744587
C	0.469070	-0.597176	0.253526
O	-0.411403	-1.423068	-0.097068
O	1.769271	-1.091751	0.045156
C	2.951955	-0.289382	0.309788
C	3.064603	0.041359	1.805039
H	4.020874	0.556713	2.027177
H	2.217927	0.692694	2.090174
H	3.011469	-0.890786	2.404882
C	3.992361	-1.340474	-0.141215
H	3.857826	-1.592406	-1.209801
H	3.917463	-2.255943	0.475061
I	6.157525	-0.733900	0.021783
C	2.973803	0.967637	-0.571845

H	3.931194	1.514976	-0.457311
H	2.847198	0.685676	-1.637556
H	2.135741	1.627270	-0.280865

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ACID-DminusI SCF Done: -1105.08928297 A.U.

O	2.250769	0.076759	-2.152034
O	2.409737	3.060168	-1.003174
H	1.525507	2.791069	-1.365887
C	3.078581	0.678553	-1.262696
O	4.717953	2.945833	0.817052
C	3.132114	1.951021	-0.758963
O	4.835578	0.731481	0.272765
C	4.280234	2.011353	0.190509
O	2.407105	-0.692677	1.170187
H	2.252940	0.233544	0.880331
O	3.692814	-2.993412	1.991909
H	3.033340	-2.476590	2.496670
C	4.090033	-0.179887	-0.549121
H	4.788308	-0.678765	-1.260038
C	3.405978	-1.260935	0.314331
H	2.918952	-1.978956	-0.391050
C	4.382298	-2.037769	1.203880
H	5.108983	-2.588759	0.568669
H	4.954217	-1.300983	1.818002
H	1.585680	0.732919	-2.468055
O	0.100259	1.822691	-1.840009
C	-0.315164	1.031139	-1.001707
O	-1.209002	0.068355	-1.247609

O	0.114698	1.013993	0.278375
C	-0.615951	-0.006499	1.003496
H	-1.410709	0.490855	1.599011
H	0.099696	-0.535910	1.658909
C	-1.182577	-0.902499	-0.122336
C	-0.215826	-2.015368	-0.527117
H	-0.095548	-2.740648	0.302380
H	-0.599003	-2.547772	-1.419681
H	0.780000	-1.592583	-0.764309
C	-2.604031	-1.380626	0.128702
H	-3.282138	-0.525291	0.320077
H	-2.983639	-1.947165	-0.744235
H	-2.620454	-2.052783	1.010755

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ACID-D SCF Done: -1116.69344171 A.U.

O	2.490743	-0.910178	-0.520146
O	2.462776	2.094270	0.675515
H	1.624238	1.569945	0.750928
C	3.409524	0.068789	-0.448826
O	5.168973	3.036261	0.096980
C	3.409443	1.337738	0.080271
O	5.537439	0.979133	-0.815702
C	4.748837	1.931590	-0.167944
O	5.547581	-1.003296	1.267005
H	4.719995	-0.535886	1.504518
O	7.476662	-2.665539	0.287894
H	7.273454	-2.368733	1.198929
C	4.801374	-0.243664	-0.942890

H	4.788417	-0.553285	-2.014722
C	5.461948	-1.363084	-0.108744
H	4.831303	-2.278708	-0.244387
C	6.896804	-1.672218	-0.542846
H	6.898801	-2.057375	-1.585968
H	7.469774	-0.712207	-0.529285
H	1.633255	-0.595945	-0.107034
O	0.419656	0.300287	0.613765
C	-0.800354	0.232910	0.427660
O	-1.387145	-0.766174	-0.221386
O	-1.653616	1.157553	0.868498
C	-2.985027	0.853571	0.339033
H	-3.172815	1.525382	-0.523133
H	-3.751436	1.039744	1.114914
C	-2.878359	-0.635432	-0.068486
I	-6.783096	0.537831	0.557377
C	-3.301517	-1.579689	1.050786
H	-4.398999	-1.479683	1.196592
H	-3.051383	-2.626857	0.787803
H	-2.795382	-1.314950	2.002373
C	-3.519715	-0.955600	-1.405909
H	-3.097097	-0.316506	-2.207168
H	-3.360283	-2.020465	-1.669618
H	-4.610759	-0.758380	-1.322557

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EPO SCF Done: -232.263297409 A.U.

O	-3.074531	-0.839138	0.821204
C	-3.898450	0.075788	0.062715

C	-4.496841	-0.913615	0.990600
H	-4.987966	-1.821172	0.583551
H	-4.887490	-0.578802	1.973395
C	-3.920118	-0.181711	-1.433867
H	-2.999602	0.223121	-1.905631
H	-3.966730	-1.267765	-1.647602
H	-4.792423	0.314012	-1.909724
C	-3.782079	1.530935	0.481735
H	-4.647764	2.120804	0.113145
H	-3.732054	1.621911	1.584690
H	-2.859076	1.979333	0.056605

EPO-*cis*(CH₃)₂

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ACID-AB SCF Done: -928.192790955 A.U.

O	-1.164689	-0.947702	0.323249
O	-1.136907	2.068547	-0.717982
H	-0.316697	1.494520	-0.841042
C	-2.086534	0.020455	0.343537
O	-3.826187	3.036555	0.004172
C	-2.089181	1.316943	-0.125216
O	-4.191623	0.938127	0.821063
C	-3.406167	1.915132	0.196654
O	-4.268225	-0.957832	-1.350560
H	-3.473725	-0.419703	-1.554500
O	-6.215543	-2.606036	-0.411991
H	-6.011576	-2.264504	-1.307350

C	-3.465206	-0.297323	0.870221
H	-3.422220	-0.654742	1.926494
C	-4.162791	-1.371750	0.009447
H	-3.541963	-2.300264	0.093395
C	-5.593131	-1.675530	0.461850
H	-5.579920	-2.120733	1.480955
H	-6.144952	-0.704672	0.516795
H	-0.290248	-0.543560	-0.075493
O	0.822002	0.335646	-0.601777
C	1.753043	0.728611	0.428881
H	2.118736	1.767605	0.283848
C	1.317356	0.492663	1.860054
H	2.172881	0.683991	2.538706
H	0.489498	1.189094	2.107221
H	0.947863	-0.539467	2.017877
C	2.516020	-0.261515	-0.351450
H	3.055782	0.126235	-1.226848
I	5.285250	0.251688	0.925027
C	2.420810	-1.748576	-0.181831
H	1.836206	-2.032533	0.713961
H	1.940114	-2.200964	-1.075302
H	3.438873	-2.172837	-0.086427

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ACID-A+I SCF Done: -928.200872698 A.U.

O	-1.318096	-0.679090	0.775501
O	-1.251812	2.121890	-0.809689
H	-0.389295	1.636813	-0.689888
C	-2.263113	0.224968	0.467404

O	-4.046814	2.994982	-0.695144
C	-2.242686	1.409079	-0.232597
O	-4.451251	1.062406	0.446354
C	-3.621898	1.960027	-0.230241
O	-4.126106	-1.185558	-1.318522
H	-3.302883	-0.692168	-1.516305
O	-6.104074	-2.795134	-0.354131
H	-5.795975	-2.613174	-1.265948
C	-3.692894	-0.090680	0.833196
H	-3.803240	-0.249337	1.932107
C	-4.202382	-1.347644	0.094933
H	-3.560294	-2.200408	0.434124
C	-5.668285	-1.670890	0.394029
H	-5.787113	-1.913076	1.472816
H	-6.268985	-0.752685	0.179037
H	-0.430101	-0.352786	0.414801
O	0.800805	0.505432	-0.186358
C	1.973842	0.691780	0.715782
H	2.364835	1.724457	0.671778
C	1.865191	0.109036	2.096903
H	2.893153	0.044926	2.512336
H	1.248745	0.763003	2.747442
H	1.417763	-0.903425	2.092528
C	2.127120	-0.090726	-0.520816
H	2.615228	0.439970	-1.358142
I	5.650839	0.142657	0.599033
C	2.197923	-1.590216	-0.586183
H	1.657551	-2.073412	0.250738
H	1.775994	-1.960308	-1.543515

H	3.270339	-1.873686	-0.527865
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ACID-A SCF Done: -916.594965874 A.U.

O	-0.847307	-1.431213	0.307620
O	-1.467756	1.689166	0.799372
H	-2.041708	1.038500	1.263396
C	-0.220021	-0.296504	-0.073147
O	0.709440	3.020595	-0.623559
C	-0.472546	1.029942	0.151726
O	1.453426	0.928428	-1.152184
C	0.578980	1.821312	-0.540849
O	2.441643	-0.352423	1.215480
H	1.597015	-0.225307	1.689609
O	4.498513	-1.817336	0.117181
H	4.463576	-1.335869	0.968863
C	1.081369	-0.416853	-0.825626
H	0.947937	-0.997766	-1.768411
C	2.181589	-1.090871	0.027087
H	1.823603	-2.126076	0.260229
C	3.527246	-1.187432	-0.697286
H	3.411005	-1.797416	-1.619097
H	3.821922	-0.154257	-1.006274
H	-1.714269	-1.187470	0.739967
O	-3.172105	-0.418029	1.180168
C	-4.011087	-0.099865	0.014516
C	-4.483083	-1.056627	1.047745
H	-4.417216	0.928268	0.081421
H	-5.208784	-0.661937	1.786025

C	-3.471734	-0.470770	-1.342274
H	-4.280125	-0.397395	-2.098723
H	-2.669609	0.241064	-1.625827
H	-3.044240	-1.490376	-1.364768
C	-4.490017	-2.554941	0.885920
H	-3.735349	-2.900162	0.153705
H	-4.280546	-3.046393	1.857961
H	-5.492021	-2.890530	0.546339

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ACID-B+CO2 SCF Done: -1116.67942289 A.U.

O	1.462870	-0.461632	-1.374387
O	0.567477	0.685396	1.406363
H	-0.016524	0.058443	0.832509
C	2.074834	0.360578	-0.534968
O	2.924573	2.320596	2.246664
C	1.713225	0.860993	0.699570
O	3.866030	1.649924	0.276902
C	2.818622	1.681706	1.216627
O	4.355540	-1.184880	0.464761
H	3.414727	-1.366999	0.673628
O	6.690639	-1.349799	-0.860040
H	6.278285	-1.819369	-0.103063
C	3.512044	0.756880	-0.784982
H	3.634058	1.281350	-1.763475
C	4.421061	-0.491923	-0.777123
H	4.070014	-1.142610	-1.618842
C	5.904610	-0.170367	-0.969222
H	6.070400	0.267732	-1.978308

H	6.184800	0.600720	-0.209045
H	0.520604	-0.792083	-0.879301
O	-0.587794	-1.020405	-0.142766
C	-1.740531	-0.680307	-0.867908
H	-1.481769	-0.058797	-1.765661
C	-2.466295	-1.944901	-1.349754
H	-3.398240	-1.714910	-1.907111
H	-1.784508	-2.513808	-2.014429
H	-2.710807	-2.599805	-0.487866
C	-2.558001	0.219872	0.089905
H	-1.945081	1.109689	0.335243
I	-4.334064	1.240883	-1.018520
O	-0.292737	-2.096203	2.740936
O	1.637578	-2.201841	1.405173
C	0.647716	-2.103132	2.034670
C	-3.071263	-0.460895	1.343582
H	-3.844390	-1.224024	1.122953
H	-2.193219	-0.978348	1.785189
H	-3.474256	0.261387	2.079304

37

ACID-BC SCF Done: -1116.67340571 A.U.

O	1.373977	-0.664292	-1.133261
O	0.642645	1.801032	0.690459
H	0.005080	0.994517	0.588032
C	2.095953	0.390901	-0.740779
O	3.184853	3.346957	0.782432
C	1.790263	1.458334	0.077900
O	4.034275	1.695188	-0.542194

C	3.001134	2.298488	0.195556
O	4.191287	-0.739008	1.000129
H	3.235935	-0.725043	1.222802
O	6.479515	-1.763665	0.024734
H	6.025797	-1.766215	0.895173
C	3.567996	0.446151	-1.064219
H	3.750418	0.419603	-2.166451
C	4.325072	-0.734786	-0.416435
H	3.896140	-1.668611	-0.863957
C	5.834115	-0.703629	-0.667889
H	6.039987	-0.820282	-1.754862
H	6.208492	0.302193	-0.352952
H	0.412054	-0.578860	-0.635932
O	-0.687867	-0.338618	0.191268
C	-1.891549	-0.236643	-0.518443
H	-1.986005	0.758994	-1.028648
C	-2.015676	-1.336275	-1.582654
H	-2.967183	-1.268132	-2.148728
H	-1.170893	-1.234471	-2.294726
H	-1.936260	-2.341860	-1.120734
C	-2.939352	-0.275419	0.612911
H	-2.797172	0.623498	1.241659
I	-5.076767	0.246962	-0.235777
O	0.126559	-3.150122	0.714887
O	1.398820	-1.494119	1.792902
C	0.730125	-2.269719	1.209917
C	-2.984979	-1.563378	1.444179
H	-3.975142	-2.057860	1.435596
H	-2.237369	-2.284684	1.060458

H	-2.730503	-1.349931	2.502177
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ACID-B SCF Done: -928.208155737 A.U.

O	1.574971	-1.428626	0.028190
O	0.494055	1.119421	1.531061
H	0.071550	0.216282	1.628091
C	1.971609	-0.176830	-0.000046
O	2.541957	3.181651	0.862676
C	1.545495	0.956906	0.667012
O	3.507551	1.564731	-0.431969
C	2.499531	2.039907	0.437045
O	4.246316	-1.508537	0.644254
H	3.313803	-1.851494	0.641900
O	6.737092	-1.155837	-0.331493
H	6.315550	-1.721736	0.351431
C	3.198728	0.214923	-0.811643
H	2.959937	0.219437	-1.903084
C	4.358789	-0.794976	-0.586697
H	4.327185	-1.517280	-1.443617
C	5.748596	-0.157809	-0.562784
H	5.963700	0.339539	-1.533680
H	5.748217	0.633932	0.224948
H	0.412950	-1.503649	0.817704
O	-0.531405	-1.390987	1.335678
C	-1.518442	-1.401043	0.310834
H	-1.015756	-1.352144	-0.684703
C	-2.342180	-2.690638	0.395567
H	-3.149315	-2.725654	-0.364992

H	-1.667838	-3.556606	0.238407
H	-2.792533	-2.798322	1.404061
C	-2.312318	-0.089340	0.502319
H	-1.608558	0.760825	0.405479
I	-3.717110	0.286930	-1.292565
C	-3.107982	0.002753	1.791259
H	-3.531387	1.014049	1.946608
H	-3.926831	-0.743015	1.841964
H	-2.397050	-0.212497	2.619105

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ACID-CD SCF Done: -1116.67590212 A.U.

O	2.013124	-0.089362	-2.140761
O	2.214640	3.014765	-1.534232
H	1.302687	2.646947	-1.739571
C	2.871456	0.631289	-1.385085
O	4.584007	3.186631	0.259652
C	2.955868	1.971242	-1.110033
O	4.642765	0.910506	0.107336
C	4.102662	2.168315	-0.189158
O	2.240850	0.084543	1.418354
H	1.530472	0.506108	0.865983
O	3.116720	-2.148990	2.679509
H	2.502702	-1.429213	2.939540
C	3.807370	-0.101656	-0.466257
H	4.445547	-0.845336	-0.999131
C	3.000503	-0.828161	0.644437
H	2.342769	-1.574371	0.129000
C	3.894443	-1.564736	1.647075

H	4.450979	-2.378145	1.132115
H	4.642461	-0.830051	2.036674
H	1.250636	0.511991	-2.382744
O	-0.020840	1.609148	-1.994624
C	-0.500031	0.989948	-1.010116
O	-1.605046	0.221326	-1.237245
O	-0.053892	0.976636	0.191210
C	-1.655100	0.042364	1.174048
H	-2.097930	1.043018	1.241454
C	-1.849924	-0.701499	-0.141203
H	-2.914424	-0.980578	-0.249550
I	-4.371309	-0.409266	2.369309
C	-0.956352	-1.931939	-0.308149
H	-1.191482	-2.700662	0.453921
H	-1.118682	-2.368858	-1.312547
H	0.111448	-1.649950	-0.214769
C	-0.922308	-0.540616	2.342494
H	-1.063946	0.075901	3.248145
H	-1.265976	-1.569369	2.563571
H	0.163790	-0.595775	2.108894

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ACID-C SCF Done: -1116.67858601 A.U.

O	-2.662143	-1.038982	1.066555
O	-1.652920	1.659262	-0.418058
H	-0.887299	1.150096	0.026984
C	-3.263032	0.072781	0.655206
O	-4.123021	3.214954	-0.628554
C	-2.850109	1.215865	-0.004032

O	-5.155668	1.448422	0.373859
C	-4.032411	2.100283	-0.154410
O	-5.123550	-0.828436	-1.400972
H	-4.206814	-0.476643	-1.440916
O	-7.571820	-1.836195	-0.840528
H	-7.045287	-1.745164	-1.662436
C	-4.767013	0.144853	0.820375
H	-5.066589	0.017750	1.888630
C	-5.461937	-0.946547	-0.020365
H	-5.113398	-1.929560	0.387268
C	-6.989578	-0.879683	0.036033
H	-7.340790	-1.101629	1.068159
H	-7.293202	0.166987	-0.214365
H	-1.708229	-1.197371	0.638650
O	0.416277	0.468443	0.593117
C	0.500204	-0.760798	0.341566
O	-0.407465	-1.604047	0.128017
O	1.788355	-1.329021	0.290613
C	2.907406	-0.445020	0.487191
H	2.672563	0.539834	0.029603
C	3.172267	-0.251773	1.980202
H	4.070110	0.374419	2.156856
H	2.290643	0.258417	2.414565
H	3.303720	-1.227315	2.491369
C	4.011314	-1.145689	-0.327586
H	3.674089	-1.210603	-1.380508
I	5.834383	0.233431	-0.532377
C	4.450967	-2.500490	0.196762
H	3.530424	-3.118356	0.283619

H	5.157805	-3.004834	-0.490844
H	4.914956	-2.433562	1.200934

ACID-DminusI SCF Done: -1105.09072863 A.U.

O	2.123080	0.059513	-1.966593
O	1.976696	3.065990	-0.829164
H	1.200408	2.762954	-1.366145
C	2.818781	0.726217	-1.016390
O	4.011032	3.056613	1.282602
C	2.750095	2.002929	-0.528965
O	4.426417	0.893577	0.670717
C	3.749673	2.126906	0.557338
O	2.506099	-0.914743	1.510054
H	2.947944	-0.166854	1.970037
O	4.014406	-3.221463	1.773685
H	3.304853	-2.823719	2.321117
C	3.897882	-0.032936	-0.292725
H	4.710311	-0.328875	-0.998277
C	3.399757	-1.286150	0.450770
H	2.805373	-1.906670	-0.254557
C	4.538036	-2.137280	1.033116
H	5.161846	-2.550281	0.210556
H	5.198057	-1.469594	1.645837
H	1.433479	0.655521	-2.350899
O	-0.070022	1.708849	-2.079064
C	-0.616024	1.058302	-1.192736
O	-1.324184	-0.059913	-1.413161
O	-0.536591	1.365657	0.108508

C	-1.348517	0.417360	0.875515
H	-2.336579	0.906592	1.027152
C	-1.491628	-0.755890	-0.131549
H	-2.520757	-1.167013	-0.127004
C	-0.443072	-1.853644	-0.039399
H	-0.568025	-2.436214	0.894767
H	-0.546227	-2.541424	-0.900987
H	0.576393	-1.421176	-0.044397
C	-0.669519	0.126425	2.198294
H	-1.262048	-0.615870	2.771021
H	0.351637	-0.269155	2.031740
H	-0.603434	1.053534	2.800605

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ACID-D SCF Done: -1116.69400217 A.U.

O	2.519161	-0.296467	-1.519973
O	2.429490	2.512041	0.076620
H	1.565962	2.145320	-0.249604
C	3.454813	0.459147	-0.920110
O	5.237836	2.940403	0.772614
C	3.417863	1.640982	-0.217864
O	5.650774	0.953817	-0.268228
C	4.810206	1.974653	0.179326
O	4.516487	-1.187534	1.277984
H	3.747159	-0.581313	1.253351
O	6.415943	-3.100287	0.849171
H	5.900173	-2.862277	1.647098
C	4.865639	-0.076685	-0.880687
H	5.252206	-0.268485	-1.909585

C	4.954294	-1.384059	-0.063352
H	4.309913	-2.134635	-0.588557
C	6.379263	-1.932255	0.044782
H	6.754715	-2.203536	-0.966168
H	7.028064	-1.114130	0.444760
H	1.615416	0.117229	-1.383244
O	0.344625	1.073202	-0.883062
C	-0.742947	0.707602	-0.417893
O	-1.246377	-0.503814	-0.623799
O	-1.511550	1.490903	0.327435
C	-2.747405	0.772372	0.713876
H	-3.595534	1.294435	0.226363
C	-2.557784	-0.631559	0.051962
H	-3.321902	-0.768950	-0.739601
I	-6.279735	-0.410722	0.334110
C	-2.529642	-1.842306	0.962681
H	-3.533103	-1.952500	1.421596
H	-2.318146	-2.753144	0.368249
H	-1.760406	-1.747393	1.755279
C	-2.900753	0.826989	2.220412
H	-3.853323	0.327013	2.489453
H	-2.055328	0.334139	2.741162
H	-2.956543	1.882467	2.552796

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EPO SCF Done: -232.262435806 A.U.

O	-3.183177	-0.413089	1.173096
C	-3.995913	-0.086286	0.030505
C	-4.468536	-1.051160	1.056201

H	-4.436993	0.933882	0.074359
H	-5.222651	-0.670053	1.779582
C	-3.469324	-0.468438	-1.334468
H	-4.273282	-0.393817	-2.097352
H	-2.653031	0.221578	-1.634932
H	-3.061336	-1.497527	-1.348009
C	-4.490660	-2.552926	0.881472
H	-3.745315	-2.894581	0.137573
H	-4.257966	-3.052347	1.845400
H	-5.497732	-2.892929	0.558781

EPO-*trans*(CH₃)₂

34

ACID-AB SCF Done: -928.193439100 A.U.

O	-1.259499	-0.907714	0.508977
O	-1.146467	2.007250	-0.801418
H	-0.318161	1.422279	-0.808366
C	-2.168860	0.066337	0.384940
O	-3.863761	3.043687	-0.321303
C	-2.134550	1.315317	-0.199279
O	-4.290863	1.028091	0.657281
C	-3.463895	1.942632	-0.006261
O	-4.257039	-1.050075	-1.340610
H	-3.448070	-0.533020	-1.542815
O	-6.269888	-2.601888	-0.377852
H	-6.009102	-2.341245	-1.285606
C	-3.577960	-0.199966	0.856764

H	-3.599513	-0.463500	1.940950
C	-4.233921	-1.343702	0.054195
H	-3.626904	-2.263351	0.254788
C	-5.690551	-1.601576	0.447259
H	-5.739974	-1.956856	1.500037
H	-6.236163	-0.627570	0.386004
H	-0.363662	-0.566755	0.116325
O	0.771037	0.293904	-0.439611
C	1.730983	0.732795	0.540130
H	1.860572	1.838759	0.531315
C	1.521000	0.190118	1.938002
H	2.382011	0.454475	2.583232
H	0.589755	0.616015	2.365704
H	1.421808	-0.914254	1.919770
C	2.576838	0.023079	-0.437201
H	2.651099	-1.068124	-0.318062
I	5.272247	-0.106039	1.040376
C	3.063910	0.652969	-1.709312
H	4.133059	0.417268	-1.868187
H	2.486948	0.253072	-2.570495
H	2.943614	1.754200	-1.683957

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ACID-A+I SCF Done: -928.202483679 A.U.

O	-1.311520	-0.851994	0.573598
O	-1.211645	2.009815	-0.910941
H	-0.370797	1.472926	-0.870938
C	-2.222996	0.115114	0.369612
O	-3.938602	3.016584	-0.548784

C	-2.192020	1.325347	-0.283333
O	-4.358626	1.062842	0.549997
C	-3.536509	1.943508	-0.155207
O	-4.292421	-1.121815	-1.317320
H	-3.448756	-0.690130	-1.565382
O	-6.273326	-2.669470	-0.260400
H	-6.023371	-2.469316	-1.186074
C	-3.636156	-0.142229	0.833465
H	-3.670726	-0.340109	1.930920
C	-4.268086	-1.339684	0.090619
H	-3.649989	-2.238045	0.345869
C	-5.722425	-1.599205	0.490821
H	-5.772000	-1.876984	1.566361
H	-6.287321	-0.643797	0.355593
H	-0.426742	-0.561246	0.186143
O	0.802827	0.347982	-0.390615
C	1.776239	0.802572	0.633268
H	1.857421	1.907023	0.645678
C	1.702458	0.128342	1.973595
H	2.678643	0.262753	2.485711
H	0.886799	0.556193	2.592319
H	1.537368	-0.961189	1.858838
C	2.270606	0.123700	-0.573855
H	2.550353	-0.938504	-0.451285
I	5.554602	-0.605903	0.950335
C	2.900553	0.848263	-1.727677
H	4.001442	0.813335	-1.585348
H	2.651104	0.351509	-2.688217
H	2.569193	1.905750	-1.771164

ACID-A SCF Done: -916.596132341 A.U.

O	-0.807889	-1.453472	0.303347
O	-1.447315	1.646731	0.925144
H	-2.036381	0.971208	1.334270
C	-0.201399	-0.296221	-0.043266
O	0.695116	3.046980	-0.479876
C	-0.462106	1.019207	0.233518
O	1.448635	0.982838	-1.096922
C	0.574805	1.844289	-0.441978
O	2.475624	-0.382362	1.207524
H	1.637508	-0.291556	1.701035
O	4.531479	-1.782049	0.025896
H	4.500606	-1.337425	0.897559
C	1.090562	-0.376727	-0.817796
H	0.948566	-0.921786	-1.780514
C	2.207305	-1.074547	-0.006836
H	1.861806	-2.121663	0.188352
C	3.544689	-1.128700	-0.750634
H	3.422526	-1.701570	-1.695202
H	3.826390	-0.081069	-1.020597
H	-1.680842	-1.245357	0.737782
O	-3.147387	-0.461581	1.166894
C	-3.953477	-0.091611	-0.007308
C	-4.536923	-0.913382	1.077686
H	-4.204086	0.987204	-0.000522
H	-4.605966	-2.003256	0.888517
C	-3.496602	-0.644529	-1.331029

H	-4.300000	-0.526197	-2.087247
H	-2.605185	-0.087098	-1.685483
H	-3.228263	-1.716296	-1.252473
C	-5.478994	-0.361954	2.114931
H	-6.529186	-0.554429	1.811309
H	-5.312598	-0.853467	3.095347
H	-5.340545	0.730406	2.239669

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ACID-B+CO2 SCF Done: -1116.68105540 A.U.

O	1.562066	-0.190611	-1.732247
O	0.731883	1.891237	0.489482
H	0.160503	1.085234	0.321728
C	2.277600	0.723610	-1.054302
O	3.310821	3.235188	1.143112
C	1.933743	1.615746	-0.071931
O	4.236264	1.800201	-0.371570
C	3.158370	2.327787	0.349764
O	3.898293	-0.780918	0.843349
H	2.929241	-0.991472	0.892374
O	6.218635	-1.932292	0.188272
H	5.568880	-1.965837	0.927693
C	3.778353	0.676424	-1.133681
H	4.164586	0.762002	-2.177203
C	4.288720	-0.651828	-0.509422
H	3.864436	-1.476288	-1.137205
C	5.818743	-0.758684	-0.500535
H	6.206367	-0.805446	-1.543082
H	6.221849	0.172301	-0.027585

H	0.704684	-0.346497	-1.213521
O	-0.479512	-0.413827	-0.115363
C	-1.837005	-0.425996	-0.584423
H	-1.897000	0.445977	-1.277488
C	-2.124584	-1.720672	-1.350466
H	-3.127117	-1.707486	-1.822063
H	-1.363833	-1.845984	-2.147480
H	-2.057544	-2.584019	-0.659669
C	-2.785946	-0.147893	0.606313
H	-2.973168	-1.072107	1.182100
I	-4.893638	0.324051	-0.218131
O	-0.896340	-2.150207	1.498743
O	1.251905	-1.473603	1.033961
C	0.032169	-1.542430	0.993033
C	-2.352814	0.998511	1.500610
H	-3.105386	1.218281	2.282622
H	-1.412181	0.700614	2.009764
H	-2.141073	1.923472	0.926707

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ACID-BC SCF Done: -1116.67982750 A.U.

O	1.417043	-0.554845	-1.307677
O	0.749781	2.070165	0.328865
H	0.059355	1.311985	0.224484
C	2.183700	0.467277	-0.910852
O	3.390692	3.419471	0.527636
C	1.906939	1.599107	-0.172300
O	4.200549	1.631502	-0.634893
C	3.168539	2.352929	-0.011736

O	4.052273	-0.692521	1.060173
H	3.086788	-0.606662	1.213799
O	6.308199	-1.959608	0.329397
H	5.791992	-1.866208	1.159290
C	3.675702	0.389929	-1.117035
H	3.938442	0.276492	-2.197235
C	4.283554	-0.799306	-0.339108
H	3.810276	-1.725357	-0.756726
C	5.803964	-0.904525	-0.478023
H	6.074746	-1.113995	-1.536531
H	6.238163	0.088750	-0.202118
H	0.445250	-0.397150	-0.883027
O	-0.657464	-0.031336	-0.058546
C	-1.964259	-0.090843	-0.556099
H	-2.296956	0.908706	-0.950468
C	-2.071789	-1.134747	-1.676698
H	-3.085574	-1.195801	-2.121304
H	-1.350117	-0.867798	-2.476131
H	-1.785314	-2.132347	-1.283454
C	-2.807317	-0.399945	0.701207
H	-2.605340	-1.435537	1.043310
I	-5.088336	-0.537006	0.202166
O	-0.280397	-2.725964	0.874618
O	1.184039	-1.109855	1.747771
C	0.411086	-1.845695	1.243456
C	-2.650699	0.620707	1.816800
H	-3.239656	0.354831	2.716542
H	-1.574076	0.656385	2.085068
H	-2.944542	1.636085	1.478801

ACID-B SCF Done: -928.208381282 A.U.

O	1.492544	-1.268465	0.450793
O	0.677524	1.715395	1.049775
H	0.160585	0.931667	1.408879
C	1.976870	-0.130644	-0.001286
O	2.834314	3.261532	-0.307196
C	1.664009	1.190441	0.263163
O	3.613227	1.234148	-1.016715
C	2.686500	2.051615	-0.331872
O	4.179001	-1.362702	0.996785
H	3.225239	-1.604986	1.134185
O	6.631370	-1.580981	-0.107462
H	6.205953	-1.847797	0.736463
C	3.186382	-0.133573	-0.924237
H	2.896847	-0.464874	-1.951502
C	4.277000	-1.111469	-0.404664
H	4.142045	-2.071133	-0.968577
C	5.710507	-0.631348	-0.633666
H	5.908379	-0.506620	-1.720704
H	5.814529	0.373741	-0.157870
H	0.301639	-0.977203	1.147229
O	-0.625846	-0.570450	1.533831
C	-1.525584	-0.560538	0.430884
H	-1.150587	0.120202	-0.377448
C	-1.673598	-1.977908	-0.134019
H	-2.320093	-2.016389	-1.033492
H	-0.660594	-2.340050	-0.403411

H	-2.089467	-2.654150	0.643484
C	-2.812510	0.057385	1.010050
H	-3.305397	-0.660815	1.698310
I	-4.416295	0.271437	-0.639016
C	-2.608169	1.416622	1.657668
H	-3.560723	1.876411	1.986661
H	-1.965438	1.259446	2.549442
H	-2.066720	2.110327	0.983371

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ACID-CD SCF Done: -1116.66732223 A.U.

O	2.221430	-0.969384	-0.173721
O	2.314980	2.020470	1.018268
H	1.512092	1.450795	1.222496
C	3.113906	0.024635	-0.256686
O	4.867858	3.040338	-0.012006
C	3.172783	1.297351	0.272322
O	5.133237	0.986674	-0.966876
C	4.432905	1.923416	-0.197877
O	5.507395	-0.992563	1.094421
H	4.741753	-0.473973	1.422699
O	7.326409	-2.575861	-0.155637
H	7.233277	-2.273227	0.771628
C	4.414379	-0.253181	-0.972379
H	4.236150	-0.568483	-2.027970
C	5.226442	-1.353292	-0.255820
H	4.605999	-2.284850	-0.295486
C	6.586930	-1.621340	-0.903770
H	6.443104	-2.028137	-1.928907

H	7.119495	-0.642259	-0.992849
H	1.424366	-0.654041	0.384102
O	0.416608	0.199018	1.239831
C	-0.817091	0.294807	0.974977
O	-1.356310	-0.728259	0.238499
O	-1.597323	1.235176	1.307507
C	-3.232196	0.800331	0.028605
H	-3.834883	1.286972	0.802608
C	-2.812822	-0.657546	0.207360
H	-3.081207	-1.228726	-0.702997
I	-5.862203	0.220008	-1.007210
C	-3.382801	-1.317581	1.460148
H	-4.486601	-1.376940	1.393910
H	-2.968286	-2.339523	1.565766
H	-3.108375	-0.723466	2.355585
C	-2.752214	1.595459	-1.155956
H	-1.813626	2.124961	-0.885082
H	-2.543642	0.939906	-2.023951
H	-3.496042	2.356942	-1.453858

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ACID-C SCF Done: -1116.67866399 A.U.

O	-2.674100	-1.048985	1.074417
O	-1.663220	1.667685	-0.372672
H	-0.900691	1.156983	0.076194
C	-3.276791	0.063494	0.668148
O	-4.138807	3.213838	-0.594492
C	-2.862902	1.214861	0.024039
O	-5.173014	1.433081	0.380875

C	-4.047665	2.095156	-0.129869
O	-5.111556	-0.826599	-1.415266
H	-4.196304	-0.469711	-1.442022
O	-7.561046	-1.850399	-0.890198
H	-7.026451	-1.749046	-1.705660
C	-4.782729	0.127028	0.818828
H	-5.092497	-0.011721	1.882694
C	-5.463874	-0.959393	-0.039433
H	-5.115045	-1.944658	0.362442
C	-6.992306	-0.899852	0.001586
H	-7.353270	-1.133315	1.027783
H	-7.298032	0.147837	-0.241902
H	-1.717413	-1.200409	0.648424
O	0.399409	0.470059	0.641847
C	0.488221	-0.752190	0.359923
O	-0.417183	-1.594382	0.130396
O	1.777218	-1.313371	0.285603
C	2.896649	-0.423215	0.449978
H	2.634379	0.572210	0.027141
C	3.208623	-0.284539	1.939778
H	4.060463	0.397058	2.132770
H	2.307335	0.131456	2.431035
H	3.431820	-1.279076	2.380424
C	3.980267	-1.089233	-0.419466
H	4.313770	-2.041683	0.041887
I	5.916122	0.142114	-0.361448
C	3.571138	-1.276434	-1.871162
H	4.365440	-1.761952	-2.471349
H	2.666970	-1.920783	-1.877219

H	3.300425	-0.309332	-2.341884
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ACID-DminusI SCF Done: -1105.09153285 A.U.

O	2.305369	0.050434	-2.162035
O	2.236769	3.105597	-1.229915
H	1.433194	2.792274	-1.723008
C	2.971089	0.730707	-1.196141
O	4.115891	3.145379	1.036354
C	2.935341	2.037608	-0.798369
O	4.434799	0.922345	0.609729
C	3.852606	2.182945	0.356345
O	2.281647	-0.699760	1.360716
H	2.694094	0.073424	1.804969
O	3.627263	-3.041383	1.988183
H	2.887152	-2.570104	2.425165
C	3.926024	-0.041370	-0.328425
H	4.773817	-0.446077	-0.930760
C	3.276641	-1.197656	0.455525
H	2.740176	-1.857819	-0.259639
C	4.291786	-2.041149	1.241347
H	4.991605	-2.544477	0.539283
H	4.902007	-1.352590	1.881021
H	1.698038	0.668090	-2.633796
O	0.098762	1.786401	-2.369461
C	-0.359450	1.072775	-1.482726
O	-1.192517	0.042250	-1.700268
O	-0.045426	1.210324	-0.187533
C	-0.729232	0.189262	0.602344

H	0.061300	-0.274352	1.225552
C	-1.217965	-0.793073	-0.497364
H	-2.275242	-1.089804	-0.341196
C	-0.310089	-1.992778	-0.718832
H	-0.264991	-2.615133	0.197888
H	-0.679179	-2.614769	-1.557502
H	0.713927	-1.642117	-0.959648
C	-1.830280	0.834300	1.427701
H	-2.604785	1.283356	0.771704
H	-2.313705	0.072216	2.073021
H	-1.413577	1.628599	2.077664

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ACID-D SCF Done: -1116.69446877 A.U.

O	2.473063	-0.810981	-0.694485
O	2.422176	2.078318	0.759990
H	1.578850	1.555448	0.762340
C	3.395536	0.147740	-0.500531
O	5.156249	3.035700	0.370772
C	3.385139	1.365418	0.137945
O	5.543559	1.062352	-0.704450
C	4.738021	1.963114	-0.005954
O	5.456235	-1.091670	1.197214
H	4.621997	-0.640484	1.442651
O	7.408571	-2.685610	0.153576
H	7.170608	-2.466354	1.078065
C	4.803359	-0.136414	-0.965782
H	4.830282	-0.352030	-2.060111
C	5.421595	-1.331076	-0.206780

H	4.789217	-2.224244	-0.444988
C	6.869832	-1.618239	-0.610332
H	6.909695	-1.912532	-1.681890
H	7.449587	-0.669522	-0.492135
H	1.603880	-0.530508	-0.283035
O	0.382688	0.305010	0.498852
C	-0.847523	0.239088	0.403172
O	-1.478062	-0.736005	-0.250663
O	-1.672531	1.130816	0.947941
C	-3.040787	0.863041	0.427956
H	-3.747446	1.027278	1.263199
C	-2.928076	-0.632918	0.066410
H	-3.485703	-0.870742	-0.859040
I	-6.728060	-0.128386	-0.044127
C	-3.254394	-1.598265	1.190541
H	-4.349401	-1.563005	1.371648
H	-2.967420	-2.630330	0.907536
H	-2.717973	-1.314812	2.120814
C	-3.313715	1.793518	-0.738811
H	-2.620624	1.582684	-1.580551
H	-4.359664	1.631595	-1.074721
H	-3.192013	2.849472	-0.426406

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ACID-AB SCF Done: -928.193439100 A.U.

O	-1.259499	-0.907714	0.508977
O	-1.146467	2.007250	-0.801418
H	-0.318161	1.422279	-0.808366
C	-2.168860	0.066337	0.384940

O	-3.863761	3.043687	-0.321303
C	-2.134550	1.315317	-0.199279
O	-4.290863	1.028091	0.657281
C	-3.463895	1.942632	-0.006261
O	-4.257039	-1.050075	-1.340610
H	-3.448070	-0.533020	-1.542815
O	-6.269888	-2.601888	-0.377852
H	-6.009102	-2.341245	-1.285606
C	-3.577960	-0.199966	0.856764
H	-3.599513	-0.463500	1.940950
C	-4.233921	-1.343702	0.054195
H	-3.626904	-2.263351	0.254788
C	-5.690551	-1.601576	0.447259
H	-5.739974	-1.956856	1.500037
H	-6.236163	-0.627570	0.386004
H	-0.363662	-0.566755	0.116325
O	0.771037	0.293904	-0.439611
C	1.730983	0.732795	0.540130
H	1.860572	1.838759	0.531315
C	1.521000	0.190118	1.938002
H	2.382011	0.454475	2.583232
H	0.589755	0.616015	2.365704
H	1.421808	-0.914254	1.919770
C	2.576838	0.023079	-0.437201
H	2.651099	-1.068124	-0.318062
I	5.272247	-0.106039	1.040376
C	3.063910	0.652969	-1.709312
H	4.133059	0.417268	-1.868187
H	2.486948	0.253072	-2.570495

H	2.943614	1.754200	-1.683957
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ACID-A+I SCF Done: -928.202483679 A.U.

O	-1.311520	-0.851994	0.573598
O	-1.211645	2.009815	-0.910941
H	-0.370797	1.472926	-0.870938
C	-2.222996	0.115114	0.369612
O	-3.938602	3.016584	-0.548784
C	-2.192020	1.325347	-0.283333
O	-4.358626	1.062842	0.549997
C	-3.536509	1.943508	-0.155207
O	-4.292421	-1.121815	-1.317320
H	-3.448756	-0.690130	-1.565382
O	-6.273326	-2.669470	-0.260400
H	-6.023371	-2.469316	-1.186074
C	-3.636156	-0.142229	0.833465
H	-3.670726	-0.340109	1.930920
C	-4.268086	-1.339684	0.090619
H	-3.649989	-2.238045	0.345869
C	-5.722425	-1.599205	0.490821
H	-5.772000	-1.876984	1.566361
H	-6.287321	-0.643797	0.355593
H	-0.426742	-0.561246	0.186143
O	0.802827	0.347982	-0.390615
C	1.776239	0.802572	0.633268
H	1.857421	1.907023	0.645678
C	1.702458	0.128342	1.973595
H	2.678643	0.262753	2.485711

H	0.886799	0.556193	2.592319
H	1.537368	-0.961189	1.858838
C	2.270606	0.123700	-0.573855
H	2.550353	-0.938504	-0.451285
I	5.554602	-0.605903	0.950335
C	2.900553	0.848263	-1.727677
H	4.001442	0.813335	-1.585348
H	2.651104	0.351509	-2.688217
H	2.569193	1.905750	-1.771164

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ACID-A SCF Done: -916.596132341 A.U.

O	-0.807889	-1.453472	0.303347
O	-1.447315	1.646731	0.925144
H	-2.036381	0.971208	1.334270
C	-0.201399	-0.296221	-0.043266
O	0.695116	3.046980	-0.479876
C	-0.462106	1.019207	0.233518
O	1.448635	0.982838	-1.096922
C	0.574805	1.844289	-0.441978
O	2.475624	-0.382362	1.207524
H	1.637508	-0.291556	1.701035
O	4.531479	-1.782049	0.025896
H	4.500606	-1.337425	0.897559
C	1.090562	-0.376727	-0.817796
H	0.948566	-0.921786	-1.780514
C	2.207305	-1.074547	-0.006836
H	1.861806	-2.121663	0.188352
C	3.544689	-1.128700	-0.750634

H	3.422526	-1.701570	-1.695202
H	3.826390	-0.081069	-1.020597
H	-1.680842	-1.245357	0.737782
O	-3.147387	-0.461581	1.166894
C	-3.953477	-0.091611	-0.007308
C	-4.536923	-0.913382	1.077686
H	-4.204086	0.987204	-0.000522
H	-4.605966	-2.003256	0.888517
C	-3.496602	-0.644529	-1.331029
H	-4.300000	-0.526197	-2.087247
H	-2.605185	-0.087098	-1.685483
H	-3.228263	-1.716296	-1.252473
C	-5.478994	-0.361954	2.114931
H	-6.529186	-0.554429	1.811309
H	-5.312598	-0.853467	3.095347
H	-5.340545	0.730406	2.239669

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ACID-B+CO2 SCF Done: -1116.68105540 A.U.

O	1.562066	-0.190611	-1.732247
O	0.731883	1.891237	0.489482
H	0.160503	1.085234	0.321728
C	2.277600	0.723610	-1.054302
O	3.310821	3.235188	1.143112
C	1.933743	1.615746	-0.071931
O	4.236264	1.800201	-0.371570
C	3.158370	2.327787	0.349764
O	3.898293	-0.780918	0.843349
H	2.929241	-0.991472	0.892374

O	6.218635	-1.932292	0.188272
H	5.568880	-1.965837	0.927693
C	3.778353	0.676424	-1.133681
H	4.164586	0.762002	-2.177203
C	4.288720	-0.651828	-0.509422
H	3.864436	-1.476288	-1.137205
C	5.818743	-0.758684	-0.500535
H	6.206367	-0.805446	-1.543082
H	6.221849	0.172301	-0.027585
H	0.704684	-0.346497	-1.213521
O	-0.479512	-0.413827	-0.115363
C	-1.837005	-0.425996	-0.584423
H	-1.897000	0.445977	-1.277488
C	-2.124584	-1.720672	-1.350466
H	-3.127117	-1.707486	-1.822063
H	-1.363833	-1.845984	-2.147480
H	-2.057544	-2.584019	-0.659669
C	-2.785946	-0.147893	0.606313
H	-2.973168	-1.072107	1.182100
I	-4.893638	0.324051	-0.218131
O	-0.896340	-2.150207	1.498743
O	1.251905	-1.473603	1.033961
C	0.032169	-1.542430	0.993033
C	-2.352814	0.998511	1.500610
H	-3.105386	1.218281	2.282622
H	-1.412181	0.700614	2.009764
H	-2.141073	1.923472	0.926707

ACID-BC SCF Done: -1116.67982750 A.U.

O	1.417043	-0.554845	-1.307677
O	0.749781	2.070165	0.328865
H	0.059355	1.311985	0.224484
C	2.183700	0.467277	-0.910852
O	3.390692	3.419471	0.527636
C	1.906939	1.599107	-0.172300
O	4.200549	1.631502	-0.634893
C	3.168539	2.352929	-0.011736
O	4.052273	-0.692521	1.060173
H	3.086788	-0.606662	1.213799
O	6.308199	-1.959608	0.329397
H	5.791992	-1.866208	1.159290
C	3.675702	0.389929	-1.117035
H	3.938442	0.276492	-2.197235
C	4.283554	-0.799306	-0.339108
H	3.810276	-1.725357	-0.756726
C	5.803964	-0.904525	-0.478023
H	6.074746	-1.113995	-1.536531
H	6.238163	0.088750	-0.202118
H	0.445250	-0.397150	-0.883027
O	-0.657464	-0.031336	-0.058546
C	-1.964259	-0.090843	-0.556099
H	-2.296956	0.908706	-0.950468
C	-2.071789	-1.134747	-1.676698
H	-3.085574	-1.195801	-2.121304
H	-1.350117	-0.867798	-2.476131
H	-1.785314	-2.132347	-1.283454
C	-2.807317	-0.399945	0.701207

H	-2.605340	-1.435537	1.043310
I	-5.088336	-0.537006	0.202166
O	-0.280397	-2.725964	0.874618
O	1.184039	-1.109855	1.747771
C	0.411086	-1.845695	1.243456
C	-2.650699	0.620707	1.816800
H	-3.239656	0.354831	2.716542
H	-1.574076	0.656385	2.085068
H	-2.944542	1.636085	1.478801

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ACID-B SCF Done: -928.208381282 A.U.

O	1.492544	-1.268465	0.450793
O	0.677524	1.715395	1.049775
H	0.160585	0.931667	1.408879
C	1.976870	-0.130644	-0.001286
O	2.834314	3.261532	-0.307196
C	1.664009	1.190441	0.263163
O	3.613227	1.234148	-1.016715
C	2.686500	2.051615	-0.331872
O	4.179001	-1.362702	0.996785
H	3.225239	-1.604986	1.134185
O	6.631370	-1.580981	-0.107462
H	6.205953	-1.847797	0.736463
C	3.186382	-0.133573	-0.924237
H	2.896847	-0.464874	-1.951502
C	4.277000	-1.111469	-0.404664
H	4.142045	-2.071133	-0.968577
C	5.710507	-0.631348	-0.633666

H	5.908379	-0.506620	-1.720704
H	5.814529	0.373741	-0.157870
H	0.301639	-0.977203	1.147229
O	-0.625846	-0.570450	1.533831
C	-1.525584	-0.560538	0.430884
H	-1.150587	0.120202	-0.377448
C	-1.673598	-1.977908	-0.134019
H	-2.320093	-2.016389	-1.033492
H	-0.660594	-2.340050	-0.403411
H	-2.089467	-2.654150	0.643484
C	-2.812510	0.057385	1.010050
H	-3.305397	-0.660815	1.698310
I	-4.416295	0.271437	-0.639016
C	-2.608169	1.416622	1.657668
H	-3.560723	1.876411	1.986661
H	-1.965438	1.259446	2.549442
H	-2.066720	2.110327	0.983371

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ACID-CD SCF Done: -1116.66732223 A.U.

O	2.221430	-0.969384	-0.173721
O	2.314980	2.020470	1.018268
H	1.512092	1.450795	1.222496
C	3.113906	0.024635	-0.256686
O	4.867858	3.040338	-0.012006
C	3.172783	1.297351	0.272322
O	5.133237	0.986674	-0.966876
C	4.432905	1.923416	-0.197877
O	5.507395	-0.992563	1.094421

H	4.741753	-0.473973	1.422699
O	7.326409	-2.575861	-0.155637
H	7.233277	-2.273227	0.771628
C	4.414379	-0.253181	-0.972379
H	4.236150	-0.568483	-2.027970
C	5.226442	-1.353292	-0.255820
H	4.605999	-2.284850	-0.295486
C	6.586930	-1.621340	-0.903770
H	6.443104	-2.028137	-1.928907
H	7.119495	-0.642259	-0.992849
H	1.424366	-0.654041	0.384102
O	0.416608	0.199018	1.239831
C	-0.817091	0.294807	0.974977
O	-1.356310	-0.728259	0.238499
O	-1.597323	1.235176	1.307507
C	-3.232196	0.800331	0.028605
H	-3.834883	1.286972	0.802608
C	-2.812822	-0.657546	0.207360
H	-3.081207	-1.228726	-0.702997
I	-5.862203	0.220008	-1.007210
C	-3.382801	-1.317581	1.460148
H	-4.486601	-1.376940	1.393910
H	-2.968286	-2.339523	1.565766
H	-3.108375	-0.723466	2.355585
C	-2.752214	1.595459	-1.155956
H	-1.813626	2.124961	-0.885082
H	-2.543642	0.939906	-2.023951
H	-3.496042	2.356942	-1.453858

ACID-C SCF Done: -1116.67866399 A.U.

O	-2.674100	-1.048985	1.074417
O	-1.663220	1.667685	-0.372672
H	-0.900691	1.156983	0.076194
C	-3.276791	0.063494	0.668148
O	-4.138807	3.213838	-0.594492
C	-2.862902	1.214861	0.024039
O	-5.173014	1.433081	0.380875
C	-4.047665	2.095156	-0.129869
O	-5.111556	-0.826599	-1.415266
H	-4.196304	-0.469711	-1.442022
O	-7.561046	-1.850399	-0.890198
H	-7.026451	-1.749046	-1.705660
C	-4.782729	0.127028	0.818828
H	-5.092497	-0.011721	1.882694
C	-5.463874	-0.959393	-0.039433
H	-5.115045	-1.944658	0.362442
C	-6.992306	-0.899852	0.001586
H	-7.353270	-1.133315	1.027783
H	-7.298032	0.147837	-0.241902
H	-1.717413	-1.200409	0.648424
O	0.399409	0.470059	0.641847
C	0.488221	-0.752190	0.359923
O	-0.417183	-1.594382	0.130396
O	1.777218	-1.313371	0.285603
C	2.896649	-0.423215	0.449978
H	2.634379	0.572210	0.027141
C	3.208623	-0.284539	1.939778

H	4.060463	0.397058	2.132770
H	2.307335	0.131456	2.431035
H	3.431820	-1.279076	2.380424
C	3.980267	-1.089233	-0.419466
H	4.313770	-2.041683	0.041887
I	5.916122	0.142114	-0.361448
C	3.571138	-1.276434	-1.871162
H	4.365440	-1.761952	-2.471349
H	2.666970	-1.920783	-1.877219
H	3.300425	-0.309332	-2.341884

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ACID-DminusI SCF Done: -1105.09153285 A.U.

O	2.305369	0.050434	-2.162035
O	2.236769	3.105597	-1.229915
H	1.433194	2.792274	-1.723008
C	2.971089	0.730707	-1.196141
O	4.115891	3.145379	1.036354
C	2.935341	2.037608	-0.798369
O	4.434799	0.922345	0.609729
C	3.852606	2.182945	0.356345
O	2.281647	-0.699760	1.360716
H	2.694094	0.073424	1.804969
O	3.627263	-3.041383	1.988183
H	2.887152	-2.570104	2.425165
C	3.926024	-0.041370	-0.328425
H	4.773817	-0.446077	-0.930760
C	3.276641	-1.197656	0.455525
H	2.740176	-1.857819	-0.259639

C	4.291786	-2.041149	1.241347
H	4.991605	-2.544477	0.539283
H	4.902007	-1.352590	1.881021
H	1.698038	0.668090	-2.633796
O	0.098762	1.786401	-2.369461
C	-0.359450	1.072775	-1.482726
O	-1.192517	0.042250	-1.700268
O	-0.045426	1.210324	-0.187533
C	-0.729232	0.189262	0.602344
H	0.061300	-0.274352	1.225552
C	-1.217965	-0.793073	-0.497364
H	-2.275242	-1.089804	-0.341196
C	-0.310089	-1.992778	-0.718832
H	-0.264991	-2.615133	0.197888
H	-0.679179	-2.614769	-1.557502
H	0.713927	-1.642117	-0.959648
C	-1.830280	0.834300	1.427701
H	-2.604785	1.283356	0.771704
H	-2.313705	0.072216	2.073021
H	-1.413577	1.628599	2.077664

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ACID-D SCF Done: -1116.69446877 A.U.

O	2.473063	-0.810981	-0.694485
O	2.422176	2.078318	0.759990
H	1.578850	1.555448	0.762340
C	3.395536	0.147740	-0.500531
O	5.156249	3.035700	0.370772
C	3.385139	1.365418	0.137945

O	5.543559	1.062352	-0.704450
C	4.738021	1.963114	-0.005954
O	5.456235	-1.091670	1.197214
H	4.621997	-0.640484	1.442651
O	7.408571	-2.685610	0.153576
H	7.170608	-2.466354	1.078065
C	4.803359	-0.136414	-0.965782
H	4.830282	-0.352030	-2.060111
C	5.421595	-1.331076	-0.206780
H	4.789217	-2.224244	-0.444988
C	6.869832	-1.618239	-0.610332
H	6.909695	-1.912532	-1.681890
H	7.449587	-0.669522	-0.492135
H	1.603880	-0.530508	-0.283035
O	0.382688	0.305010	0.498852
C	-0.847523	0.239088	0.403172
O	-1.478062	-0.736005	-0.250663
O	-1.672531	1.130816	0.947941
C	-3.040787	0.863041	0.427956
H	-3.747446	1.027278	1.263199
C	-2.928076	-0.632918	0.066410
H	-3.485703	-0.870742	-0.859040
I	-6.728060	-0.128386	-0.044127
C	-3.254394	-1.598265	1.190541
H	-4.349401	-1.563005	1.371648
H	-2.967420	-2.630330	0.907536
H	-2.717973	-1.314812	2.120814
C	-3.313715	1.793518	-0.738811
H	-2.620624	1.582684	-1.580551

H	-4.359664	1.631595	-1.074721
H	-3.192013	2.849472	-0.426406

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EPO SCF Done: -232.264106384 A.U.

O	-3.155560	-0.452285	1.157412
C	-3.934713	-0.076746	0.005674
C	-4.518471	-0.911901	1.080398
H	-4.226425	0.996112	-0.008597
H	-4.614165	-1.999960	0.872360
C	-3.495359	-0.640491	-1.326215
H	-4.294640	-0.521758	-2.088339
H	-2.591936	-0.110764	-1.695331
H	-3.247077	-1.717262	-1.234898
C	-5.479042	-0.368545	2.113238
H	-6.531263	-0.560296	1.813479
H	-5.311346	-0.855853	3.096821
H	-5.339216	0.723560	2.244290

EPO-tBu

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ACID-AB SCF Done: -1006.76722150 A.U.

O	-1.311489	-1.030263	0.525859
O	-1.090282	2.072728	-0.185627
H	-0.291919	1.472605	-0.332918
C	-2.203301	-0.030334	0.553871
O	-3.803354	3.073344	0.388238

C	-2.118108	1.305561	0.230686
O	-4.308976	0.920006	0.945312
C	-3.440628	1.921255	0.496161
O	-4.264986	-0.739425	-1.409471
H	-3.416280	-0.258924	-1.510816
O	-6.329123	-2.407604	-0.807539
H	-6.036431	-1.993229	-1.645675
C	-3.631316	-0.343847	0.925995
H	-3.691894	-0.807315	1.939230
C	-4.285936	-1.295854	-0.097712
H	-3.704052	-2.252330	-0.061592
C	-5.758022	-1.588320	0.201627
H	-5.845158	-2.128635	1.169781
H	-6.284256	-0.607283	0.305989
H	-0.395975	-0.643687	0.245273
O	0.776633	0.243151	-0.219539
C	1.972010	0.499776	0.536946
H	2.321075	1.546817	0.393700
C	1.934538	0.148657	2.037344
C	2.376465	-0.425405	-0.534693
H	2.667734	-0.032011	-1.514851
H	2.226793	-1.504143	-0.414624
I	5.266856	-1.181778	-0.419187
C	1.755017	-1.364948	2.262642
H	2.624671	-1.930814	1.868800
H	1.672385	-1.579969	3.349098
H	0.827523	-1.739245	1.782346
C	0.745273	0.921665	2.652487
H	-0.221413	0.566998	2.246156

H	0.724790	0.785320	3.754426
H	0.815287	2.010150	2.442385
C	3.253493	0.623310	2.682849
H	3.245463	0.398886	3.771249
H	4.132189	0.124625	2.225610
H	3.383664	1.721247	2.566885

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ACID-A+I SCF Done: -1006.77202245 A.U.

O	-1.424405	-1.063777	0.431781
O	-1.184378	2.041177	-0.345236
H	-0.396299	1.453159	-0.506390
C	-2.302002	-0.044528	0.448782
O	-3.873104	3.066770	0.232810
C	-2.207573	1.280916	0.101418
O	-4.390919	0.932905	0.850084
C	-3.523953	1.914449	0.366469
O	-4.416439	-0.772487	-1.465411
H	-3.539169	-0.369366	-1.629197
O	-6.468442	-2.433124	-0.774128
H	-6.202819	-2.045334	-1.633491
C	-3.726643	-0.337865	0.847852
H	-3.774059	-0.777650	1.871990
C	-4.408716	-1.305084	-0.144099
H	-3.834622	-2.265865	-0.101767
C	-5.875615	-1.581826	0.193566
H	-5.944048	-2.088441	1.180970
H	-6.396488	-0.595857	0.276001
H	-0.515451	-0.713251	0.162335

O	0.754680	0.209435	-0.289692
C	1.859233	0.629248	0.596797
H	2.061501	1.712700	0.480302
C	1.809667	0.177975	2.055202
C	2.160271	-0.217845	-0.564409
H	2.604082	0.224639	-1.470569
H	2.329979	-1.296751	-0.430052
I	5.502095	-1.243628	-0.233530
C	1.724077	-1.355024	2.182575
H	2.632928	-1.838711	1.767398
H	1.645082	-1.637191	3.253213
H	0.825618	-1.758062	1.670543
C	0.573053	0.842523	2.703548
H	-0.366289	0.471769	2.247081
H	0.537592	0.617072	3.790069
H	0.593189	1.946581	2.583024
C	3.107409	0.685195	2.723401
H	3.120083	0.387066	3.793258
H	4.004438	0.259066	2.225362
H	3.176147	1.793925	2.681101

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ACID-A SCF Done: -995.165619127 A.U.

O	-0.494343	-1.459723	0.109414
O	-1.273474	1.609546	0.655428
H	-1.880158	0.911960	0.999470
C	0.147249	-0.291009	-0.122708
O	1.036509	3.070526	-0.389619
C	-0.175460	1.015192	0.127282

O	1.910758	1.026119	-0.905649
C	0.934690	1.865738	-0.379488
O	2.611037	-0.348119	1.511020
H	1.703098	-0.236344	1.854550
O	4.841613	-1.705488	0.635699
H	4.680257	-1.265469	1.495123
C	1.540344	-0.343332	-0.696241
H	1.552129	-0.878262	-1.674703
C	2.536143	-1.032270	0.265463
H	2.181161	-2.086018	0.399772
C	3.969021	-1.061161	-0.273804
H	3.996009	-1.629149	-1.228789
H	4.270696	-0.007501	-0.494139
H	-1.415387	-1.270213	0.435921
O	-2.924299	-0.544125	0.850989
C	-3.996986	-0.189554	-0.081621
C	-4.268712	-1.032899	1.102243
H	-4.266842	0.881719	0.007863
H	-4.378337	-2.125263	0.987154
H	-4.758114	-0.594130	1.990484
C	-3.899579	-0.673200	-1.527655
C	-5.293453	-0.452868	-2.158412
H	-5.278860	-0.749198	-3.227465
H	-6.070721	-1.059289	-1.647120
H	-5.600198	0.613442	-2.111200
C	-2.843458	0.201736	-2.241407
H	-1.836908	0.051199	-1.803061
H	-2.789566	-0.058697	-3.318425
H	-3.084577	1.281956	-2.161236

C	-3.497964	-2.157746	-1.627590
H	-2.514655	-2.344751	-1.151665
H	-4.254824	-2.828515	-1.170446
H	-3.407035	-2.447292	-2.694130

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ACID-B+CO2 SCF Done: -1195.24791705 A.U.

O	1.542523	-0.445789	-1.410371
O	0.594403	1.426449	0.930460
H	0.012363	0.672980	0.550579
C	2.186622	0.502211	-0.725466
O	3.068781	2.949505	1.615110
C	1.792394	1.311532	0.316369
O	4.057729	1.743646	-0.051394
C	2.958831	2.104322	0.748024
O	4.192939	-1.053726	0.747355
H	3.231305	-1.194999	0.870823
O	6.586549	-1.696043	-0.296626
H	6.063952	-1.971103	0.487834
C	3.670615	0.678348	-0.926550
H	3.918200	0.964325	-1.978224
C	4.429167	-0.624720	-0.589185
H	4.076625	-1.392341	-1.324820
C	5.949962	-0.488975	-0.692296
H	6.240864	-0.267246	-1.742872
H	6.255588	0.382187	-0.060805
H	0.593606	-0.584020	-0.941306
O	-0.591911	-0.621071	-0.136104
C	-1.799310	-0.475762	-0.830986

H	-1.695241	0.254076	-1.679108
C	-2.272942	-1.840795	-1.462044
C	-2.650973	0.160750	0.278479
H	-2.192283	1.115488	0.592291
H	-2.755621	-0.517365	1.145254
I	-4.813811	0.846293	-0.136650
O	-0.811122	-1.976398	2.426865
O	1.341372	-1.521825	1.607358
C	0.227729	-1.704711	1.942715
C	-2.861153	-2.772266	-0.385263
H	-3.826514	-2.386273	0.004754
H	-3.050021	-3.785125	-0.803086
H	-2.159402	-2.874752	0.467207
C	-1.025118	-2.509388	-2.084383
H	-0.276190	-2.760602	-1.308467
H	-1.312572	-3.442094	-2.616505
H	-0.526815	-1.835932	-2.814000
C	-3.300534	-1.614796	-2.591514
H	-2.897955	-0.924051	-3.363887
H	-3.533783	-2.579377	-3.094506
H	-4.254977	-1.190791	-2.224537

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ACID-B SCF Done: -1006.77694730 A.U.

O	1.718169	-1.130007	-0.280689
O	0.907784	0.890864	2.001917
H	0.394434	0.047889	1.829783
C	2.204663	0.048288	0.046690
O	3.068821	2.933803	1.852123

C	1.896579	0.940521	1.055988
O	3.846207	1.743805	0.063348
C	2.919740	1.985346	1.101538
O	4.418821	-1.527108	0.126817
H	3.471296	-1.818602	0.092168
O	6.859518	-1.051066	-0.928634
H	6.444289	-1.766036	-0.398977
C	3.417712	0.598116	-0.688231
H	3.131602	0.952890	-1.708452
C	4.505176	-0.497659	-0.858485
H	4.356749	-0.939934	-1.877757
C	5.939793	0.024724	-0.777452
H	6.126341	0.769100	-1.582053
H	6.056286	0.552832	0.199763
H	0.601805	-1.340613	0.487536
O	-0.336699	-1.324057	1.058409
C	-1.340720	-1.013759	0.102178
H	-0.860182	-0.696225	-0.856592
C	-2.177051	-2.308564	-0.194633
C	-2.052227	0.201707	0.721172
H	-1.285436	0.917413	1.071939
H	-2.726691	-0.070052	1.555676
I	-3.324122	1.507871	-0.635940
C	-2.873842	-2.793789	1.092113
H	-2.135325	-2.858054	1.917216
H	-3.690410	-2.107303	1.402948
H	-3.326645	-3.797505	0.941259
C	-1.166064	-3.384826	-0.657625
H	-0.432933	-3.605776	0.142251

H	-1.693691	-4.325167	-0.927408
H	-0.594631	-3.039237	-1.545409
C	-3.214161	-2.102160	-1.315742
H	-2.747354	-1.660735	-2.221951
H	-3.658764	-3.079590	-1.606113
H	-4.044488	-1.437032	-1.007207

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ACID-CD SCF Done: -1195.24924969 A.U.

O	1.584330	-0.048750	-1.615913
O	1.796194	2.615877	0.151380
H	0.968027	2.470115	-0.398221
C	2.523072	0.419903	-0.781653
O	4.428760	2.335928	1.434876
C	2.614357	1.556044	-0.010983
O	4.577000	0.337754	0.345260
C	3.919979	1.524389	0.690915
O	2.676178	-1.474325	1.478972
H	2.019576	-0.762144	1.332265
O	4.068898	-3.805751	1.291675
H	3.456456	-3.452429	1.969972
C	3.721169	-0.450805	-0.490536
H	4.266366	-0.717860	-1.427136
C	3.311534	-1.752203	0.234250
H	2.617712	-2.302054	-0.450961
C	4.497266	-2.655102	0.579007
H	4.993037	-2.997150	-0.355757
H	5.234292	-2.042775	1.155640
H	0.799613	0.611641	-1.638995

O	-0.240640	1.759509	-1.321751
C	-1.198215	1.293674	-0.631661
O	-1.519893	-0.018146	-0.878415
O	-1.863514	1.896416	0.257671
C	-3.258631	0.430805	0.723126
H	-3.907029	0.934191	0.001096
H	-3.265699	0.782903	1.759910
C	-2.265035	-0.607698	0.221087
H	-2.819702	-1.445213	-0.245840
I	-5.540294	-1.035801	1.272525
C	-1.259973	-1.211136	1.257332
C	-0.356392	-0.131189	1.895830
H	0.293371	-0.603395	2.662608
H	0.303242	0.365227	1.152724
H	-0.935588	0.672681	2.390207
C	-2.034378	-1.943563	2.371293
H	-2.719615	-2.710277	1.956252
H	-1.315639	-2.448435	3.051569
H	-2.651252	-1.249877	2.977216
C	-0.371517	-2.224928	0.498607
H	0.381277	-2.666286	1.182998
H	-0.982665	-3.048891	0.072236
H	0.168994	-1.729701	-0.333384

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ACID-C SCF Done: -1195.24700922 A.U.

O	-2.772817	-0.730300	1.155975
O	-1.707212	1.523662	-0.913568
H	-0.957525	1.140919	-0.338131

C	-3.353689	0.256235	0.480108
O	-4.154429	3.005008	-1.535151
C	-2.916535	1.204154	-0.425847
O	-5.223858	1.540648	-0.155318
C	-4.085194	2.036739	-0.805280
O	-5.198675	-1.096506	-1.329137
H	-4.276268	-0.776023	-1.438128
O	-7.667052	-1.917278	-0.579181
H	-7.130791	-2.032128	-1.391711
C	-4.858579	0.379441	0.598327
H	-5.174233	0.516507	1.660669
C	-5.556351	-0.875698	0.033825
H	-5.226240	-1.735039	0.671410
C	-7.083624	-0.782676	0.048672
H	-7.450653	-0.744920	1.098285
H	-7.370481	0.175149	-0.452004
H	-1.813351	-0.986754	0.801904
O	0.329194	0.616627	0.421094
C	0.411694	-0.634938	0.482764
O	-0.492760	-1.506046	0.443514
O	1.695693	-1.207965	0.639144
C	2.828020	-0.324794	0.715341
H	2.481286	0.713178	0.520361
C	3.401444	-0.401250	2.168071
C	3.677414	-0.826662	-0.460013
H	3.025349	-0.932435	-1.345169
H	4.188284	-1.786143	-0.254084
I	5.311646	0.536779	-1.231348
C	3.933336	-1.816222	2.474130

H	3.162140	-2.576386	2.233197
H	4.852643	-2.049257	1.895178
H	4.191403	-1.910082	3.550678
C	2.227811	-0.083581	3.127789
H	1.452974	-0.874257	3.086536
H	2.595912	-0.012665	4.173566
H	1.738223	0.874522	2.857740
C	4.511905	0.645158	2.394316
H	4.791074	0.669564	3.470118
H	5.430405	0.421356	1.817141
H	4.170420	1.662961	2.110686

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ACID-DminusI SCF Done: -1183.65590484 A.U.

O	0.299986	-0.584087	2.102845
O	-0.951774	1.899039	0.561980
H	-0.886938	1.953984	1.537396
C	0.301406	-0.244646	0.805767
O	-0.614627	1.162219	-2.241485
C	-0.224052	0.824901	0.135360
O	0.638657	-0.588775	-1.483897
C	-0.106695	0.566317	-1.311713
O	3.079750	0.179451	-0.179532
H	2.677803	0.760772	0.494244
O	4.654398	-1.975292	-0.869032
H	4.890061	-1.027093	-0.805857
C	1.003358	-1.124339	-0.198783
H	0.620441	-2.168614	-0.126168
C	2.538973	-1.128197	-0.027758

H	2.752938	-1.545929	0.988461
C	3.254928	-1.990662	-1.072057
H	2.910240	-3.043539	-0.984380
H	2.957037	-1.617552	-2.083232
H	-0.523577	-0.207394	2.539614
O	-2.075381	0.457090	2.877294
C	-2.850110	0.397760	1.930770
O	-2.723177	-0.460471	0.905092
O	-3.916230	1.205307	1.781568
C	-4.591536	0.854784	0.544371
H	-4.883413	1.788161	0.029122
H	-5.496811	0.261887	0.793995
C	-3.521793	0.049885	-0.213255
H	-2.854674	0.744309	-0.772072
C	-3.961569	-1.096187	-1.139442
C	-4.871955	-0.486586	-2.228132
H	-4.356865	0.331606	-2.774188
H	-5.147470	-1.263788	-2.970158
H	-5.817267	-0.084317	-1.804609
C	-2.690112	-1.685736	-1.791871
H	-1.980277	-2.048288	-1.020959
H	-2.953454	-2.541048	-2.447445
H	-2.163161	-0.926820	-2.405186
C	-4.710243	-2.192858	-0.355482
H	-5.649858	-1.819290	0.103451
H	-4.987036	-3.022939	-1.037049
H	-4.074359	-2.609256	0.451731

ACID-D SCF Done: -1195.26911813 A.U.

O	2.000489	-0.158181	-1.664327
O	2.180242	2.772360	-0.329224
H	1.318471	2.519814	-0.756699
C	2.929114	0.460347	-0.906436
O	4.818248	2.738402	0.942448
C	2.999706	1.701414	-0.323706
O	4.995743	0.595347	0.182437
C	4.321847	1.806021	0.350512
O	3.183365	-1.041342	1.649176
H	2.518244	-0.360506	1.420654
O	4.602819	-3.373123	1.760966
H	4.031949	-2.930242	2.422210
C	4.143654	-0.334511	-0.497773
H	4.678414	-0.739623	-1.389060
C	3.772886	-1.507731	0.439316
H	3.061456	-2.162690	-0.125472
C	4.984338	-2.337426	0.871125
H	5.450872	-2.809965	-0.020650
H	5.731988	-1.637007	1.319769
H	1.221688	0.456342	-1.803586
O	0.019178	1.610392	-1.488580
C	-0.857351	1.094155	-0.782032
O	-1.420587	-0.076529	-1.067088
O	-1.307919	1.638978	0.344587
C	-2.370787	0.782621	0.882877
H	-3.360230	1.245438	0.686500
H	-2.216667	0.697810	1.973427
C	-2.191185	-0.537318	0.109278

H	-3.174482	-0.900998	-0.253975
I	-5.935056	-0.473291	0.988182
C	-1.406422	-1.678462	0.802544
C	-2.198395	-2.126175	2.049121
H	-3.249316	-2.377378	1.795305
H	-1.710042	-3.017032	2.497856
H	-2.229334	-1.337179	2.828757
C	-1.298657	-2.854183	-0.193758
H	-0.736120	-3.695144	0.263042
H	-2.305562	-3.225893	-0.476225
H	-0.768064	-2.545855	-1.117598
C	0.012327	-1.211369	1.194786
H	0.562997	-2.020137	1.716003
H	0.605977	-0.946152	0.294331
H	-0.010073	-0.335949	1.878548

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EPO SCF Done: -310.832572478 A.U.

O	0.852109	0.723028	-0.056987
C	-0.207764	-0.045647	0.531724
C	1.042582	-0.694557	0.083392
H	-0.324247	0.119222	1.625794
H	1.063376	-1.270583	-0.861325
H	1.795576	-1.008014	0.834104
C	-1.549267	-0.102903	-0.211518
C	-1.350611	-0.371380	-1.715905
H	-0.616194	0.342356	-2.142302
H	-0.986826	-1.402721	-1.905255
H	-2.310039	-0.253205	-2.260439

C	-2.234399	1.269419	-0.019101
H	-3.228929	1.289268	-0.512631
H	-2.385735	1.497294	1.057747
H	-1.613320	2.079193	-0.454844
C	-2.401862	-1.219044	0.426694
H	-3.399320	-1.275934	-0.057990
H	-1.912314	-2.209988	0.317246
H	-2.565739	-1.037289	1.510653

EPO-CH₂-nBu

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ACID-AB SCF Done: -1046.04696340 A.U.

O	-0.974460	2.936294	1.007173
O	1.386704	4.786224	-0.110000
H	1.369462	3.807834	-0.356181
C	-0.693036	4.237239	1.155094
O	0.753418	7.419248	1.045194
C	0.309414	5.043371	0.660821
O	-1.066739	6.403570	1.971493
C	0.095681	6.411051	1.192293
O	-2.930593	5.662233	-0.096702
H	-2.083266	5.333706	-0.465321
O	-5.258661	6.155006	1.220536
H	-4.979416	6.301324	0.292924
C	-1.662720	5.100274	1.925483
H	-1.799592	4.723363	2.966851
C	-3.040522	5.158160	1.231988

H	-3.440199	4.111837	1.227882
C	-4.037491	6.077905	1.940966
H	-4.263611	5.678778	2.954098
H	-3.549431	7.076214	2.064821
H	-0.213743	2.502230	0.460399
O	1.106455	2.194730	-0.279249
C	2.103192	1.532071	0.525289
H	3.101437	2.014798	0.438731
C	1.704507	1.287563	1.971782
H	1.403367	2.273395	2.394469
H	0.791528	0.652356	1.994531
C	1.767522	0.590767	-0.553197
H	2.275818	0.651875	-1.522061
H	0.907090	-0.080015	-0.437493
I	3.349164	-1.951942	-0.326686
C	2.816830	0.667473	2.827629
H	3.158828	-0.280877	2.358698
H	3.702114	1.345144	2.824368
C	2.382471	0.405360	4.275891
H	2.026309	1.355181	4.741445
H	1.500141	-0.276455	4.275411
C	3.490068	-0.206173	5.146716
H	4.372927	0.473694	5.144765
H	3.840074	-1.151650	4.674652
C	3.050586	-0.477404	6.591233
H	2.191871	-1.182754	6.623649
H	2.724827	0.458000	7.096766
H	3.869127	-0.919105	7.198392

ACID-A+I SCF Done: -1046.05158540 A.U.

O	-0.980924	2.712528	1.319584
O	1.008113	4.616906	-0.358879
H	1.083336	3.632019	-0.493323
C	-0.801136	4.044692	1.269702
O	0.276954	7.294115	0.576623
C	0.030259	4.861266	0.540476
O	-1.268824	6.254395	1.892140
C	-0.245837	6.264416	0.942589
O	-3.338358	5.128965	0.244635
H	-2.568041	4.766518	-0.239688
O	-5.483744	5.549556	1.876145
H	-5.379628	5.614869	0.904397
C	-1.730562	4.911094	2.084087
H	-1.672357	4.655376	3.168520
C	-3.195429	4.769851	1.615938
H	-3.484054	3.700572	1.782354
C	-4.163534	5.676219	2.380069
H	-4.179554	5.387566	3.453745
H	-3.775349	6.722484	2.310765
H	-0.301123	2.264753	0.723768
O	1.036333	1.956853	-0.170606
C	2.185361	1.496844	0.636175
H	3.075893	2.136390	0.479814
C	1.890081	1.134356	2.071577
H	1.581803	2.056002	2.616258
H	1.017773	0.445131	2.096968
C	1.739617	0.678617	-0.499070

H	2.291348	0.696315	-1.452413
H	1.140301	-0.226563	-0.308459
I	3.622327	-2.296094	-0.383752
C	3.103107	0.480820	2.752846
H	3.438580	-0.384349	2.136928
H	3.952871	1.202286	2.763154
C	2.808817	0.016613	4.184918
H	2.453576	0.877633	4.800689
H	1.963014	-0.709318	4.165027
C	4.017810	-0.640002	4.867581
H	4.863549	0.085302	4.889007
H	4.366301	-1.488995	4.238505
C	3.721205	-1.130235	6.290381
H	2.905815	-1.885744	6.291925
H	3.395482	-0.294296	6.947912
H	4.611424	-1.599356	6.760328

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ACID-A SCF Done: -1034.44550103 A.U.

O	-1.219036	2.296629	-0.509602
O	-3.988111	3.862601	0.005926
H	-3.770500	3.121708	0.614937
C	-1.786298	3.381723	-1.081774
O	-3.907321	6.001029	-1.981306
C	-2.953737	4.057944	-0.852452
O	-1.880970	5.154311	-2.603235
C	-3.031562	5.182513	-1.822253
O	0.039589	5.640580	-0.526997
H	-0.477368	5.178476	0.160854
O	2.283118	6.041884	-2.073399

H	1.999746	6.500155	-1.255980
C	-1.005480	4.117182	-2.141927
H	-0.756371	3.443475	-2.995256
C	0.302960	4.722671	-1.582424
H	0.933791	3.866872	-1.231090
C	1.091257	5.517049	-2.627625
H	1.374292	4.847539	-3.468412
H	0.414746	6.308604	-3.034491
H	-1.882057	1.866585	0.098321
O	-3.350176	1.324521	0.814452
C	-4.260126	0.709017	-0.160244
C	-3.785467	-0.045352	1.019234
H	-5.276568	1.144751	-0.105758
H	-2.988587	-0.801012	0.888592
H	-4.444771	-0.190386	1.894061
C	-3.718501	0.492157	-1.552112
H	-3.687052	1.479343	-2.064483
H	-2.665400	0.143254	-1.486173
C	-4.571819	-0.496415	-2.363195
H	-4.603949	-1.477942	-1.836945
H	-5.625341	-0.136245	-2.398720
C	-4.054174	-0.696697	-3.794908
H	-4.021166	0.289039	-4.313468
H	-2.997949	-1.050916	-3.757807
C	-4.894584	-1.681537	-4.621228
H	-5.948838	-1.323332	-4.652995
H	-4.927204	-2.663751	-4.096416
C	-4.369865	-1.874078	-6.049409
H	-3.329498	-2.264419	-6.047421

H	-4.360565	-0.913525	-6.607658
H	-4.994848	-2.589003	-6.623318

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ACID-B+CO2 SCF Done: -1234.54447649 A.U.

O	-3.012573	2.519694	-1.758467
O	-2.655296	3.155365	1.304855
H	-3.126426	2.307179	0.981250
C	-2.345885	3.486773	-1.136152
O	-0.854118	5.527922	1.288419
C	-2.159891	3.764976	0.201669
O	-0.898116	5.330802	-0.986196
C	-1.263013	4.930156	0.311903
O	0.470385	2.898262	-1.749417
H	-0.087407	2.435349	-1.086965
O	1.576543	3.636698	-4.111718
H	1.829553	3.007951	-3.402623
C	-1.460023	4.414999	-1.932726
H	-2.040614	4.987564	-2.696015
C	-0.364039	3.609743	-2.659121
H	-0.900870	2.901881	-3.339788
C	0.593758	4.458269	-3.493509
H	0.032025	4.986190	-4.295309
H	1.043708	5.230587	-2.820783
H	-3.271065	1.780807	-0.989619
O	-3.408773	0.994628	0.124884
C	-4.492360	0.112197	0.082743
H	-5.388557	0.587105	-0.405689
C	-4.157218	-1.168596	-0.710241

H	-3.373163	-1.733428	-0.154315
H	-5.058288	-1.818590	-0.741230
C	-4.809592	-0.118391	1.563198
H	-5.025093	0.838396	2.074017
H	-3.992216	-0.654516	2.082455
I	-6.681251	-1.369603	1.993340
O	-1.570281	0.239194	2.309150
O	-0.504853	1.104429	0.403192
C	-1.109631	0.701303	1.330861
C	-3.664231	-0.867491	-2.143382
H	-3.937318	-1.707495	-2.822571
H	-4.211809	0.021318	-2.534697
C	-2.151571	-0.608232	-2.250974
H	-1.857549	0.110208	-1.460953
H	-1.602063	-1.554847	-2.031087
C	-1.709282	-0.048085	-3.608936
H	-2.219473	0.931174	-3.749409
H	-2.067694	-0.710937	-4.432367
C	-0.190002	0.145585	-3.709185
H	0.347304	-0.827023	-3.654138
H	0.181119	0.780418	-2.877693
H	0.109756	0.649540	-4.652489

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ACID-BC SCF Done: -1234.53064434 A.U.

O	-0.996827	2.872189	-1.581808
O	-2.778947	3.907031	0.810721
H	-2.716433	2.907939	0.590379
C	-1.077954	4.069094	-0.986958

O	-1.863960	6.718084	1.156590
C	-1.828979	4.518971	0.076327
O	-0.423670	6.277186	-0.557184
C	-1.440723	5.919428	0.343897
O	1.493225	4.323001	0.392050
H	0.883241	3.583074	0.599307
O	3.711933	5.236208	-0.821113
H	3.504328	4.776009	0.021529
C	-0.065486	5.129499	-1.334234
H	-0.093209	5.400109	-2.418019
C	1.363665	4.651422	-0.985643
H	1.564369	3.759181	-1.632420
C	2.439503	5.710028	-1.239384
H	2.491545	5.945761	-2.325420
H	2.132314	6.641088	-0.700925
H	-1.575366	2.206659	-0.998925
O	-2.349767	1.485914	0.005722
C	-3.368284	0.657613	-0.494233
H	-4.217035	1.265045	-0.909127
C	-2.809846	-0.240442	-1.620605
H	-2.203732	0.444304	-2.255723
H	-2.086441	-0.958293	-1.175022
C	-3.829370	-0.041281	0.791965
H	-4.082407	0.712290	1.559355
H	-3.063028	-0.743934	1.170397
I	-5.755928	-1.297436	0.722809
O	-0.548315	-0.427920	0.925589
O	0.045099	1.828611	1.155852
C	-0.386307	0.742962	0.971477

C	-3.813014	-0.965404	-2.528746
H	-4.349531	-1.761101	-1.969890
H	-4.600370	-0.247419	-2.856557
C	-3.149967	-1.587993	-3.767205
H	-2.617384	-0.794649	-4.342642
H	-2.356029	-2.300155	-3.440513
C	-4.131545	-2.316514	-4.697506
H	-4.925205	-1.603538	-5.019035
H	-4.660904	-3.109978	-4.121769
C	-3.460995	-2.933541	-5.931854
H	-2.685789	-3.674974	-5.639470
H	-2.954087	-2.156549	-6.544507
H	-4.191796	-3.453478	-6.587343

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ACID-B SCF Done: -1046.08474372 A.U.

O	-0.502900	1.742911	-0.584777
O	-3.618305	1.945111	-1.070713
H	-3.271126	1.652545	-0.180536
C	-1.203247	1.801183	-1.691194
O	-3.810083	2.005081	-4.038389
C	-2.561751	1.907324	-1.940207
O	-1.523381	1.919691	-4.031321
C	-2.782718	1.955374	-3.382135
O	1.537877	2.645317	-2.083264
H	0.979519	2.356560	-1.298645
O	1.146857	5.182500	-2.899131
H	1.745239	4.665573	-2.309872
C	-0.501730	1.769142	-3.038654

H	-0.007099	0.776745	-3.174955
C	0.590762	2.850537	-3.138021
H	1.143098	2.744118	-4.100653
C	0.051372	4.290388	-3.050404
H	-0.510305	4.549912	-3.973237
H	-0.667546	4.355217	-2.193352
H	-1.429125	1.374890	0.499107
O	-2.231425	1.053039	1.110791
C	-2.040710	-0.321744	1.433670
H	-2.994802	-0.692321	1.877197
C	-1.671023	-1.177505	0.209141
H	-0.793344	-0.689619	-0.270392
H	-1.339325	-2.186026	0.538135
C	-0.962171	-0.273095	2.523049
H	-1.244016	0.440363	3.318791
H	0.030207	-0.013597	2.102612
I	-0.616292	-2.227172	3.642285
C	-2.823348	-1.284771	-0.804729
H	-3.552330	-2.060514	-0.473509
H	-3.380201	-0.326082	-0.810581
C	-2.367183	-1.561102	-2.243887
H	-1.567927	-0.829037	-2.495748
H	-1.892930	-2.568805	-2.322077
C	-3.491094	-1.418763	-3.282206
H	-4.033435	-0.466128	-3.094536
H	-4.236937	-2.235993	-3.141294
C	-2.973389	-1.403832	-4.725856
H	-2.396120	-2.324749	-4.966600
H	-2.308534	-0.527869	-4.884090

H	-3.803727	-1.319326	-5.457947
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ACID-CD SCF Done: -1234.53895988 A.U.

O	-6.793191	-0.314720	-5.165733
O	-4.460881	-1.134972	-7.147506
H	-4.270991	-0.401888	-6.488368
C	-6.517129	-1.469918	-5.810420
O	-5.080018	-3.979719	-7.760917
C	-5.502234	-1.834963	-6.654806
O	-6.829849	-3.727495	-6.318230
C	-5.702601	-3.262195	-7.007795
O	-5.756181	-3.302767	-3.635659
H	-5.172708	-2.559577	-3.936341
O	-7.639769	-4.616412	-2.173798
H	-6.676351	-4.473266	-2.053391
C	-7.316108	-2.692942	-5.455371
H	-8.408513	-2.552695	-5.637711
C	-7.112621	-3.054604	-3.963944
H	-7.516175	-2.182311	-3.385489
C	-7.871225	-4.315453	-3.544460
H	-8.964015	-4.164543	-3.679638
H	-7.548922	-5.147941	-4.216665
H	-5.986927	0.274908	-5.235656
O	-4.307588	0.627552	-5.108669
C	-4.042874	-0.014456	-4.059796
O	-3.971104	0.667438	-2.885916
O	-3.848258	-1.284012	-3.978997
C	-3.143984	-1.459184	-2.119399

H	-2.119213	-1.313822	-2.477661
H	-3.531799	-2.480831	-2.044787
C	-3.993524	-0.255390	-1.746854
H	-3.528434	0.314331	-0.921013
I	-1.847066	-1.967774	0.346509
C	-5.458538	-0.597464	-1.440829
H	-5.998372	0.361659	-1.286179
H	-5.888949	-1.056772	-2.355345
C	-5.689492	-1.543581	-0.257197
H	-5.308851	-1.086302	0.682938
H	-5.082132	-2.464094	-0.394625
C	-7.162722	-1.947707	-0.115139
H	-7.796048	-1.043221	0.043797
H	-7.501638	-2.401739	-1.071787
C	-7.421168	-2.966186	1.004800
H	-7.191054	-2.506620	1.993664
H	-6.702237	-3.809486	0.892907
C	-8.851549	-3.520293	0.981400
H	-9.032836	-4.045059	0.019573
H	-9.603185	-2.705536	1.074600
H	-9.032205	-4.239902	1.808297

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ACID-C SCF Done: -1234.53405295 A.U.

O	6.364977	3.630147	4.456921
O	4.150701	5.099857	2.602630
H	4.021777	4.087428	2.634997
C	6.299386	4.811828	3.851849
O	5.445324	7.652618	1.991538

C	5.350536	5.460949	3.083993
O	7.175796	6.923886	3.282388
C	5.910897	6.779166	2.695661
O	6.325896	6.745284	6.035428
H	5.596492	6.322601	5.530575
O	8.601257	7.585682	7.236714
H	7.647268	7.726908	7.412693
C	7.448269	5.770766	4.086124
H	8.422331	5.324876	3.770816
C	7.542104	6.157886	5.576796
H	7.757610	5.212058	6.136184
C	8.633653	7.188875	5.871589
H	9.635013	6.749904	5.665566
H	8.484304	8.050347	5.174466
H	5.432872	3.142145	4.551982
O	3.636706	2.558201	2.623610
C	3.617007	2.028142	3.763742
O	4.243534	2.337537	4.808019
O	2.786736	0.901437	3.943698
C	1.998496	0.481329	2.816252
H	1.684220	1.375754	2.236464
C	2.821800	-0.433592	1.896502
H	2.218471	-0.692263	0.998430
H	3.666352	0.192919	1.537912
C	0.795015	-0.150841	3.518710
H	0.275848	0.591588	4.152281
H	1.079843	-1.029977	4.127384
I	-0.791788	-0.911035	2.115287
C	3.351141	-1.704091	2.572076

H	3.839091	-1.417969	3.530208
H	2.502695	-2.375220	2.841367
C	4.342792	-2.485019	1.698993
H	3.857584	-2.748941	0.729739
H	5.197765	-1.820894	1.433300
C	4.879243	-3.762488	2.361917
H	4.022603	-4.425409	2.624383
H	5.357032	-3.494028	3.331727
C	5.878565	-4.531340	1.488039
H	6.761571	-3.903013	1.241033
H	5.416699	-4.839467	0.524717
H	6.250524	-5.449407	1.990547

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ACID-DminusI SCF Done: -1222.94874203 A.U.

O	-4.830044	-2.202468	-0.953238
O	-4.781332	0.945651	-0.276148
H	-5.219541	0.668431	-1.110994
C	-4.318346	-1.492303	0.067040
O	-3.201728	1.055194	2.171684
C	-4.301399	-0.156394	0.364618
O	-3.169451	-1.221884	2.089449
C	-3.532294	0.027741	1.614794
O	-5.788766	-2.365903	2.473099
H	-6.287265	-1.997741	1.719149
O	-5.057408	-4.657518	3.818033
H	-5.834466	-4.075284	3.945508
C	-3.685545	-2.238649	1.215403
H	-2.838251	-2.869498	0.858795

C	-4.701416	-3.131787	1.963536
H	-5.052248	-3.906609	1.236712
C	-4.095851	-3.839910	3.179510
H	-3.257482	-4.491657	2.851832
H	-3.673094	-3.055766	3.855135
H	-4.938120	-1.604837	-1.747579
O	-4.745065	-0.262405	-2.814605
C	-3.607958	0.199969	-2.828022
O	-2.503612	-0.526439	-2.585892
O	-3.330405	1.490284	-3.047215
C	-1.948778	1.744775	-2.618537
H	-1.526827	2.455955	-3.357864
C	-1.325696	0.330718	-2.738361
H	-0.668602	0.107105	-1.873893
C	-0.641396	0.031636	-4.062764
H	0.284649	0.635597	-4.153228
H	-0.369776	-1.040128	-4.129696
H	-1.309018	0.283634	-4.912473
C	-1.937570	2.315238	-1.203996
H	-2.278687	1.528939	-0.496688
H	-0.875659	2.531280	-0.946047
C	-2.806878	3.564249	-1.019094
H	-2.461254	4.372102	-1.706232
H	-3.844878	3.312969	-1.324530
C	-2.817016	4.061465	0.433791
H	-1.776795	4.313350	0.744330
H	-3.138493	3.223325	1.089440
C	-3.730097	5.274933	0.640960
H	-4.781489	5.031947	0.375642

H	-3.419776	6.136755	0.010375
H	-3.723829	5.612712	1.697854

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ACID-D SCF Done: -1234.54595160 A.U.

O	-8.358918	2.189292	-1.685363
O	-10.329425	-0.024365	-2.978418
H	-9.383489	-0.287586	-2.836210
C	-9.669807	2.174455	-1.982817
O	-12.896562	1.372482	-3.052289
C	-10.516552	1.227622	-2.508810
O	-11.803305	3.135864	-2.105892
C	-11.868143	1.836506	-2.611452
O	-11.071892	2.469383	0.591568
H	-10.739871	1.664902	0.141888
O	-11.413335	4.910580	1.764558
H	-11.609096	4.003970	2.079334
C	-10.484492	3.388110	-1.605465
H	-10.080179	4.309542	-2.087464
C	-10.515902	3.598522	-0.075784
H	-9.457210	3.772473	0.245663
C	-11.373572	4.792053	0.351483
H	-10.939582	5.731007	-0.056620
H	-12.388790	4.658601	-0.097749
H	-7.957673	1.294043	-1.889773
O	-7.716707	-0.314358	-2.290205
C	-7.052213	-1.155968	-1.676106
O	-6.064963	-0.838858	-0.839973
O	-7.249149	-2.467822	-1.789730

C	-6.160745	-3.161027	-1.082426
H	-5.410342	-3.516077	-1.817480
H	-6.590300	-4.030496	-0.553085
C	-5.615686	-2.068928	-0.145257
H	-4.508418	-2.066809	-0.144936
I	-2.968394	-4.829713	-0.471133
C	-6.203875	-2.066818	1.265984
H	-6.049474	-1.052999	1.696316
H	-7.305454	-2.209766	1.179271
C	-5.584726	-3.133192	2.188718
H	-5.515278	-4.104221	1.648517
H	-6.270002	-3.298465	3.050172
C	-4.187300	-2.767901	2.709470
H	-3.509948	-2.578924	1.847089
H	-4.244750	-1.817993	3.293289
C	-3.559377	-3.876160	3.564762
H	-3.484168	-4.791632	2.936545
H	-4.238753	-4.122912	4.414858
C	-2.168140	-3.508262	4.093143
H	-2.198686	-2.592739	4.725156
H	-1.471200	-3.312791	3.250759
H	-1.731157	-4.325573	4.705169

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EPO SCF Done: -350.114328349 A.U.

O	-3.356450	1.298142	0.818440
C	-4.255802	0.736573	-0.149673
C	-3.778528	-0.060471	1.001436
H	-5.290923	1.139138	-0.098376

H	-3.001154	-0.834317	0.835815
H	-4.447689	-0.250117	1.864740
C	-3.720347	0.520393	-1.550233
H	-3.680105	1.502263	-2.074453
H	-2.668656	0.166046	-1.475614
C	-4.566873	-0.470526	-2.364203
H	-4.600860	-1.447780	-1.829946
H	-5.622208	-0.113902	-2.403438
C	-4.052429	-0.686558	-3.794413
H	-4.018765	0.293009	-4.325640
H	-2.995938	-1.040492	-3.756047
C	-4.892320	-1.680107	-4.611037
H	-5.947337	-1.323689	-4.645342
H	-4.924417	-2.656633	-4.075696
C	-4.370203	-1.889185	-6.037965
H	-3.329419	-2.278777	-6.032850
H	-4.360962	-0.934774	-6.607201
H	-4.995064	-2.610766	-6.604224

EPO-OH

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ACID-AB SCF Done: -924.782102209 A.U.

O	-1.112498	-1.024397	0.119816
O	-1.053361	2.013633	-0.828556
H	-0.337581	1.391054	-1.136311
C	-1.992399	-0.033298	0.247334
O	-3.639376	3.053139	0.144426

C	-1.992518	1.275531	-0.176005
O	-4.011620	0.944100	0.934450
C	-3.250778	1.911159	0.270190
O	-4.374774	-0.871462	-1.265819
H	-3.555095	-0.431101	-1.571663
O	-6.262198	-2.509555	-0.186086
H	-6.141059	-2.151605	-1.089830
C	-3.332003	-0.318500	0.884174
H	-3.203200	-0.707490	1.921338
C	-4.144987	-1.339909	0.060944
H	-3.551694	-2.289684	0.052202
C	-5.533101	-1.617594	0.642865
H	-5.432783	-2.088076	1.645283
H	-6.049223	-0.634418	0.773851
H	-0.237418	-0.628642	-0.255392
O	0.929804	0.234478	-0.853987
C	1.592726	0.980661	0.203922
H	1.931791	1.981222	-0.142281
C	2.408365	-0.177141	-0.137078
H	3.185508	-0.114493	-0.906335
H	2.262831	-1.109600	0.424161
I	5.046919	0.029197	1.510711
O	0.942375	0.987260	1.417855
H	0.290465	1.716202	1.383673

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ACID-A+I SCF Done: -924.802478569 A.U.

O	-1.337915	-0.472079	1.045318
O	-1.296529	2.219435	-0.732176

H	-0.427958	1.771075	-0.515163
C	-2.295735	0.351546	0.593348
O	-4.139500	2.920258	-0.896168
C	-2.290540	1.486193	-0.185651
O	-4.521380	1.050321	0.351860
C	-3.693674	1.946951	-0.326316
O	-3.940057	-1.278055	-1.226321
H	-3.095669	-0.811400	-1.395257
O	-5.891711	-2.939358	-0.305186
H	-5.500089	-2.806055	-1.193222
C	-3.731042	-0.026553	0.872371
H	-3.916185	-0.120113	1.968565
C	-4.112199	-1.356777	0.186620
H	-3.452487	-2.146720	0.627284
C	-5.577139	-1.746606	0.396409
H	-5.766570	-1.925696	1.477416
H	-6.207891	-0.880860	0.075142
H	-0.433760	-0.153083	0.737855
O	0.770118	0.734188	0.021722
C	2.189438	1.121431	0.544621
H	2.268219	2.223342	0.470263
C	1.975068	0.347037	-0.695843
H	2.100822	0.835611	-1.682275
H	2.198971	-0.736980	-0.675985
I	3.991787	-2.405576	1.290368
O	2.601374	0.632533	1.702764
H	2.947619	-0.334388	1.610810

ACID-A SCF Done: -913.195590929 A.U.

O	-0.854980	-1.388843	0.157708
O	-1.532987	1.787336	0.143786
H	-1.269503	2.717392	-0.069410
C	-0.234262	-0.310743	-0.313206
O	0.731828	2.931096	-1.122249
C	-0.474053	1.032290	-0.306256
O	1.577038	0.804608	-1.351385
C	0.642626	1.725669	-0.952415
O	2.221543	-0.334008	1.259030
H	1.423088	-0.506369	1.792246
O	4.431343	-1.795213	0.470621
H	4.269411	-1.301110	1.300722
C	1.137681	-0.505877	-0.935261
H	1.076772	-1.157685	-1.836754
C	2.138680	-1.116364	0.068694
H	1.784432	-2.152873	0.289267
C	3.568936	-1.195556	-0.475895
H	3.584572	-1.817711	-1.396387
H	3.885576	-0.162103	-0.760917
H	-1.719452	-1.161512	0.642660
O	-3.081121	-0.907919	1.462365
C	-4.020534	-0.069584	0.691945
C	-4.306641	-1.491669	0.935378
H	-4.474270	0.709706	1.339311
H	-4.165803	-2.183143	0.083661
H	-5.034283	-1.807918	1.705233
O	-3.634347	0.297912	-0.556213
H	-2.994173	1.053169	-0.448643

ACID-B+CO2 SCF Done: -1113.27362079 A.U.

O	1.530208	-0.231552	-1.561020
O	0.618967	1.354361	1.032023
H	-0.018573	0.739114	0.527231
C	2.185085	0.590585	-0.741078
O	3.116714	2.720739	1.876362
C	1.812300	1.267843	0.399784
O	4.085458	1.696383	0.081682
C	2.993929	1.982338	0.918150
O	4.129781	-1.132933	0.629773
H	3.161605	-1.243026	0.743998
O	6.500681	-1.785664	-0.455035
H	5.960304	-2.098908	0.302845
C	3.678445	0.738988	-0.901387
H	3.954010	1.115813	-1.916184
C	4.385589	-0.616751	-0.670642
H	4.004336	-1.311176	-1.462309
C	5.910845	-0.530765	-0.764556
H	6.212002	-0.246497	-1.797176
H	6.247647	0.281325	-0.072850
H	0.567989	-0.402989	-1.147651
O	-0.624838	-0.451065	-0.327661
C	-1.870754	-0.508591	-0.865769
H	-1.956993	0.063234	-1.838709
C	-2.763049	0.156949	0.199070
H	-2.492616	1.216925	0.364206
H	-2.736802	-0.422788	1.140896

I	-4.988787	0.258830	-0.369260
O	-0.755065	-1.507765	2.372017
O	1.284289	-1.807116	1.246964
C	0.232570	-1.606850	1.741066
O	-2.224772	-1.875684	-1.091223
H	-3.081157	-1.872069	-1.563865

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ACID-BC SCF Done: -1113.27640960 A.U.

O	1.170139	-0.842651	-0.953956
O	0.661067	1.954601	0.390337
H	0.093006	1.127292	0.634753
C	1.948385	0.228904	-0.841335
O	3.260112	3.375165	-0.037817
C	1.756830	1.453685	-0.242382
O	3.938855	1.449949	-1.059738
C	2.993025	2.240319	-0.383743
O	4.121562	-0.587986	0.959427
H	3.188057	-0.670329	1.272597
O	6.321641	-1.886765	0.089867
H	5.920840	-1.684504	0.963728
C	3.393540	0.141548	-1.268107
H	3.496124	-0.126765	-2.347471
C	4.162416	-0.907398	-0.425202
H	3.687554	-1.902299	-0.621770
C	5.650392	-0.983553	-0.778043
H	5.773528	-1.342986	-1.823623
H	6.066237	0.053491	-0.720790
H	0.284911	-0.649606	-0.379943

O	-0.721362	-0.193347	0.547249
C	-1.918704	0.177788	-0.044081
H	-2.582158	0.687305	0.711358
C	-2.557964	-1.136494	-0.493832
H	-2.646892	-1.833444	0.358900
H	-1.973222	-1.574075	-1.326416
I	-4.683174	-0.960273	-1.294282
O	-0.627057	-1.810526	3.015957
O	1.396508	-1.081705	2.055840
C	0.338035	-1.326223	2.516415
O	-1.728282	1.008710	-1.179353
H	-1.056145	1.670265	-0.898121

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ACID-B SCF Done: -924.804919542 A.U.

O	1.443228	-1.351151	0.139489
O	0.545625	1.461760	1.263849
H	0.043044	0.619138	1.464324
C	1.930098	-0.140784	-0.049952
O	2.741627	3.250693	0.351699
C	1.581754	1.099771	0.447874
O	3.595700	1.403653	-0.686176
C	2.619458	2.067743	0.086788
O	4.129953	-1.465237	0.862162
H	3.189840	-1.770189	0.920859
O	6.616747	-1.517173	-0.200296
H	6.175120	-1.912373	0.582456
C	3.191322	0.039835	-0.878988
H	2.971692	-0.096232	-1.966162
C	4.268438	-1.004947	-0.482577

H	4.151670	-1.867157	-1.188755
C	5.705999	-0.496550	-0.593105
H	5.931554	-0.202160	-1.641303
H	5.793374	0.420856	0.037909
H	0.319968	-1.241089	0.823851
O	-0.658581	-0.959647	1.320198
C	-1.646876	-1.013378	0.338402
H	-1.211017	-1.066148	-0.689872
C	-2.435408	0.297606	0.507515
H	-1.774024	1.174884	0.369293
H	-2.922498	0.331829	1.502743
I	-4.109570	0.577039	-0.979657
O	-2.450106	-2.174341	0.482799
H	-2.472667	-2.316704	1.450984

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ACID-CD SCF Done: -1113.25952269 A.U.

O	-0.063369	-3.716562	-2.871105
O	2.619578	-2.472583	-1.588333
H	1.747728	-2.282045	-1.130025
C	1.230825	-3.775118	-3.209178
O	4.702770	-3.418663	-3.423606
C	2.385304	-3.268321	-2.649820
O	3.024118	-4.468418	-4.554720
C	3.521186	-3.676966	-3.512861
O	1.958686	-6.601366	-2.934405
H	2.005641	-5.850503	-2.304420
O	1.478595	-8.426787	-4.889068
H	1.824998	-8.506578	-3.975996

C	1.613564	-4.650069	-4.379106
H	1.085047	-4.334691	-5.310099
C	1.288305	-6.133536	-4.102039
H	0.177566	-6.197811	-3.973244
C	1.723038	-7.070229	-5.231724
H	1.145604	-6.841887	-6.154502
H	2.802744	-6.870048	-5.442206
H	-0.159667	-3.156313	-2.022927
O	0.116327	-2.258093	-0.756921
C	-0.651699	-1.393505	-0.254285
O	-1.964956	-1.436137	-0.671299
O	-0.349013	-0.490731	0.578211
C	-2.077546	0.571939	0.701424
H	-1.657276	1.297058	-0.001459
H	-1.894979	0.677821	1.774075
C	-2.830053	-0.641183	0.180996
H	-3.658562	-0.351282	-0.500395
I	-4.204417	2.308378	1.025118
O	-3.254918	-1.393557	1.277175
H	-3.819427	-2.109625	0.929625

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ACID-C SCF Done: -1113.28138639 A.U.

O	-2.601493	-1.127648	0.942286
O	-1.647676	1.713968	-0.288555
H	-0.873584	1.172171	0.087627
C	-3.220184	0.016815	0.663345
O	-4.129674	3.264336	-0.274635
C	-2.831580	1.222798	0.113158

O	-5.124694	1.399886	0.577485
C	-4.021773	2.109306	0.084318
O	-5.144881	-0.686490	-1.415678
H	-4.225289	-0.343580	-1.454351
O	-7.567749	-1.770040	-0.874192
H	-7.073853	-1.594850	-1.702568
C	-4.718263	0.060733	0.879998
H	-4.983972	-0.173504	1.938918
C	-5.435452	-0.946023	-0.043705
H	-5.069825	-1.962498	0.251300
C	-6.960604	-0.897161	0.069556
H	-7.275119	-1.219761	1.086753
H	-7.277478	0.166266	-0.068654
H	-1.667525	-1.227819	0.476512
O	0.457805	0.435976	0.566646
C	0.556618	-0.763793	0.151759
O	-0.359661	-1.567140	-0.131313
O	1.844723	-1.275743	-0.013165
C	2.919061	-0.313383	0.149197
H	2.810183	0.443880	-0.670054
C	4.158426	-1.178187	-0.052726
H	4.086958	-1.754380	-0.992844
H	4.295770	-1.848346	0.816933
I	6.045833	0.010440	-0.215150
O	2.930678	0.271481	1.404078
H	2.024963	0.689671	1.429154

O	0.436149	-1.057755	2.181816
O	-0.768543	1.620964	1.121204
H	-0.835997	1.383669	2.068900
C	0.545039	-0.478084	0.975820
O	-0.574356	1.265984	-1.792183
C	0.004288	0.684992	0.502189
O	0.903431	-0.400631	-1.331013
C	0.067544	0.625048	-0.967809
O	3.299754	0.265277	0.099285
H	2.872210	0.699577	0.862464
O	4.994561	-1.655179	-0.929430
H	5.182385	-0.718730	-0.714443
C	1.303901	-1.133556	-0.150326
H	0.975082	-2.190338	-0.271861
C	2.837617	-1.077957	0.025541
H	3.079144	-1.649865	0.956983
C	3.598846	-1.710899	-1.144566
H	3.312036	-2.780209	-1.239572
H	3.280540	-1.188374	-2.080776
H	-0.520093	-0.950827	2.481074
O	-2.239110	-0.670567	2.558266
C	-2.871870	-0.393586	1.546539
O	-2.432342	-0.542895	0.294999
O	-4.111968	0.158987	1.572985
C	-4.526487	0.396906	0.200643
H	-5.118941	1.329879	0.170151
H	-5.126797	-0.459935	-0.174878
C	-3.188511	0.488137	-0.527829
H	-2.651102	1.437741	-0.305818

O	-3.192853	0.172049	-1.839591
H	-2.336234	0.521947	-2.199386

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ACID-D SCF Done: -1113.27837187 A.U.

O	2.539842	-0.367352	-1.379904
O	2.454780	2.372760	0.338279
H	1.585244	1.991595	0.051570
C	3.484856	0.406865	-0.818449
O	5.285066	2.894208	0.846254
C	3.452108	1.557431	-0.066613
O	5.701083	0.971813	-0.307747
C	4.855543	1.935534	0.243275
O	4.777266	-1.277076	1.223349
H	3.981245	-0.709020	1.281284
O	6.716234	-3.085747	0.571908
H	6.254909	-2.903511	1.416437
C	4.915648	-0.067120	-0.905524
H	5.231446	-0.199795	-1.967276
C	5.119815	-1.400891	-0.153996
H	4.469301	-2.158124	-0.661665
C	6.570458	-1.888851	-0.175386
H	6.879207	-2.101866	-1.222182
H	7.213186	-1.059474	0.210961
H	1.633137	0.002955	-1.173971
O	0.351431	0.912520	-0.575881
C	-0.796441	0.596385	-0.248101
O	-1.385338	-0.537340	-0.616525
O	-1.568454	1.370070	0.520688

C	-2.918946	0.788618	0.548945
H	-3.573051	1.320315	-0.170474
H	-3.345025	0.904084	1.562018
C	-2.686990	-0.676341	0.145969
H	-3.434800	-1.064999	-0.569065
I	-6.366175	-0.031876	0.241602
O	-2.525840	-1.581813	1.161742
H	-2.099068	-1.141787	1.923760

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EPO SCF Done: -228.850879598 A.U.

O	-0.668674	0.546681	1.703631
C	-0.135563	0.084821	0.462798
C	0.586645	1.096832	1.245360
H	0.189885	-0.979562	0.477656
H	0.545717	2.145012	0.889430
H	1.484382	0.824694	1.835742
O	-0.752573	0.497882	-0.704910
H	-1.504099	-0.103652	-0.872325

EPO-CH₂-OH

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ACID-AB SCF Done: -964.068016437 A.U.

O	-1.300059	-0.816296	0.621428
O	-1.198141	2.027378	-0.851193
H	-0.356497	1.471599	-0.796411
C	-2.223485	0.131545	0.405406

O	-3.951023	3.020794	-0.539580
C	-2.191474	1.344605	-0.247568
O	-4.372605	1.058462	0.543522
C	-3.541639	1.950531	-0.142974
O	-4.228176	-1.132615	-1.322015
H	-3.414896	-0.626220	-1.532126
O	-6.235941	-2.676288	-0.331277
H	-5.952200	-2.466287	-1.245192
C	-3.642712	-0.138958	0.842188
H	-3.698300	-0.337307	1.938923
C	-4.245511	-1.343211	0.087622
H	-3.626309	-2.234989	0.362944
C	-5.708741	-1.612124	0.447218
H	-5.786591	-1.901786	1.518151
H	-6.273798	-0.657677	0.306264
H	-0.406137	-0.495259	0.226456
O	0.754594	0.361897	-0.350637
C	1.725933	0.799301	0.611995
H	1.881418	1.899775	0.626720
C	1.557060	0.251718	2.028608
H	0.566249	0.588703	2.407562
H	1.509021	-0.868203	1.972482
C	2.502096	0.047656	-0.380769
H	2.874775	0.541193	-1.286911
H	2.561330	-1.045410	-0.299659
I	5.307421	0.000709	0.600731
O	2.544233	0.734149	2.908803
H	3.420747	0.493882	2.519381

ACID-A+I SCF Done: -964.074390978 A.U.

O	-1.321305	-0.746845	0.638242
O	-1.280167	2.069496	-0.936385
H	-0.422821	1.568338	-0.857037
C	-2.258596	0.184530	0.383357
O	-4.044253	2.996497	-0.667443
C	-2.251389	1.372980	-0.307137
O	-4.425012	1.069628	0.491401
C	-3.617582	1.951329	-0.227870
O	-4.258639	-1.172831	-1.296955
H	-3.418330	-0.736642	-1.547670
O	-6.207662	-2.748043	-0.219975
H	-5.947304	-2.572920	-1.147830
C	-3.671538	-0.101836	0.830173
H	-3.720811	-0.262547	1.933024
C	-4.252187	-1.343055	0.117811
H	-3.611391	-2.212438	0.413883
C	-5.704738	-1.634995	0.501888
H	-5.765039	-1.876225	1.585607
H	-6.296864	-0.703525	0.323086
H	-0.443880	-0.453632	0.244034
O	0.790551	0.472040	-0.353432
C	1.784168	0.904538	0.652143
H	1.893961	2.004287	0.708142
C	1.729358	0.208808	2.005836
H	0.769246	0.486568	2.498735
H	1.700251	-0.898622	1.836933
C	2.233419	0.216762	-0.565022

H	2.670468	0.791525	-1.399322
H	2.526665	-0.845038	-0.498013
I	5.381570	-0.870366	0.954859
O	2.784566	0.633238	2.823527
H	3.622641	0.251726	2.430720

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ACID-A SCF Done: -952.454499874 A.U.

O	-0.809215	-1.457133	0.366972
O	-1.464824	1.654952	0.900499
H	-2.015665	0.993515	1.375627
C	-0.215440	-0.306849	-0.024562
O	0.644097	3.027746	-0.578817
C	-0.482070	1.013387	0.215283
O	1.405708	0.951482	-1.143784
C	0.536809	1.825830	-0.501253
O	2.480406	-0.340733	1.185225
H	1.671642	-0.322111	1.731618
O	4.531540	-1.751528	0.002461
H	4.510167	-1.289467	0.865383
C	1.063671	-0.402051	-0.817701
H	0.908711	-0.976259	-1.761208
C	2.201325	-1.066645	-0.007254
H	1.874034	-2.113019	0.218522
C	3.527649	-1.122233	-0.771044
H	3.396139	-1.713508	-1.702803
H	3.794969	-0.077407	-1.065354
H	-1.678534	-1.243932	0.804102
O	-3.167644	-0.466738	1.210901

C	-3.944948	-0.066996	0.037867
C	-4.530751	-0.953620	1.060885
H	-4.225108	1.004525	0.057714
H	-4.609865	-2.036582	0.852637
H	-5.241638	-0.551215	1.804550
C	-3.460106	-0.586866	-1.307479
H	-2.547787	-0.015630	-1.603845
H	-3.149713	-1.647920	-1.196742
O	-4.498722	-0.528431	-2.269634
H	-4.535616	0.381792	-2.618349

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ACID-B+CO2 SCF Done: -1152.55059280 A.U.

O	0.217610	0.243432	1.324081
O	-0.493744	-2.316181	3.042050
H	-0.886333	-2.156405	2.111892
C	0.657360	-0.182249	2.509169
O	1.278328	-2.032996	5.415065
C	0.376126	-1.303158	3.259334
O	2.027049	-0.123468	4.413598
C	1.218413	-1.270722	4.469885
O	3.465316	-0.914730	2.046970
H	2.717216	-1.395778	1.633124
O	5.453251	0.895933	2.072221
H	5.355606	-0.038628	1.787177
C	1.816258	0.532899	3.158991
H	1.592332	1.611602	3.342737
C	3.079220	0.435470	2.271785
H	2.829273	0.949466	1.308458

C	4.311400	1.097124	2.893267
H	4.142560	2.191898	2.996608
H	4.443090	0.671551	3.919364
H	-0.394815	-0.520423	0.915057
O	-1.103042	-1.743247	0.598389
C	-2.335597	-1.752797	-0.056559
H	-2.893000	-0.782623	0.036738
C	-2.111110	-2.012279	-1.565111
H	-1.275575	-1.342027	-1.861152
H	-1.737722	-3.062581	-1.686575
C	-3.075699	-2.852411	0.710211
H	-3.202403	-2.585546	1.775448
H	-2.562999	-3.828069	0.607430
I	-5.250889	-3.315909	0.064209
O	-0.045383	-4.361492	0.228601
O	1.526990	-2.648565	0.555803
C	0.659148	-3.434712	0.411965
O	-3.202083	-1.707030	-2.421381
H	-3.949393	-2.276268	-2.147076

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ACID-BC SCF Done: -1152.54981097 A.U.

O	0.633563	0.155420	0.313844
O	-0.582465	-1.094291	2.950975
H	-0.820141	-1.470198	2.027029
C	0.919071	0.353153	1.607709
O	1.044501	0.166612	5.097153
C	0.414651	-0.209242	2.759318
O	2.146901	1.224084	3.402573

C	1.168827	0.348352	3.901929
O	3.609978	-0.777625	1.913917
H	2.843826	-1.328038	1.645990
O	5.841824	0.612804	1.345234
H	5.624785	-0.327600	1.526453
C	2.123260	1.182654	1.971732
H	2.048437	2.225517	1.577768
C	3.417719	0.542122	1.419016
H	3.319454	0.543053	0.303099
C	4.688570	1.298109	1.813289
H	4.679132	2.315957	1.364467
H	4.682614	1.413677	2.925810
H	-0.061220	-0.634737	0.272810
O	-0.919844	-1.807264	0.489815
C	-2.168720	-1.821415	-0.141039
H	-2.904403	-1.120227	0.334341
C	-2.023912	-1.405972	-1.623469
H	-1.403030	-0.483908	-1.624841
H	-1.430768	-2.193852	-2.154377
C	-2.588220	-3.271560	0.113611
H	-2.660287	-3.483169	1.195994
H	-1.906639	-3.982762	-0.390119
I	-4.684696	-3.927900	-0.641022
O	0.548707	-3.685605	-1.043840
O	1.630419	-2.739792	0.811866
C	0.988168	-3.141759	-0.092844
O	-3.233439	-1.072879	-2.289244
H	-3.803147	-1.868031	-2.268337

ACID-B SCF Done: -964.070233561 A.U.

O	-0.431902	0.218516	1.894021
O	-2.734561	-0.427595	3.948699
H	-2.266376	-1.149050	3.428095
C	-1.215939	1.012262	2.599831
O	-3.361639	2.252068	5.084769
C	-2.205031	0.756950	3.530498
O	-1.823229	3.058678	3.601506
C	-2.575495	2.014825	4.184349
O	1.264837	1.865571	3.308171
H	1.021118	1.028827	2.833037
O	2.185264	4.398163	3.481767
H	2.545076	3.500154	3.650114
C	-1.011718	2.517288	2.548380
H	-1.390540	2.936524	1.583887
C	0.496451	2.875511	2.655091
H	0.867945	3.010675	1.605807
C	0.781916	4.166102	3.423480
H	0.298045	5.031425	2.920044
H	0.322170	4.069192	4.436683
H	-0.906214	-1.070000	2.047241
O	-1.461494	-2.004302	2.198436
C	-2.408757	-2.113044	1.147165
H	-3.197490	-1.320507	1.204479
C	-1.667862	-1.956852	-0.190698
H	-1.078076	-1.014157	-0.092788
H	-0.932995	-2.801647	-0.271828
C	-3.029138	-3.485714	1.419748

H	-3.377754	-3.530348	2.468433
H	-2.302452	-4.299545	1.226393
I	-4.875560	-4.041885	0.239791
O	-2.573031	-1.912159	-1.287717
H	-2.076946	-1.560297	-2.048016

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ACID-CD SCF Done: -1152.54140929 A.U.

O	2.169832	1.373698	4.069554
O	3.077965	-1.577685	4.922543
H	2.173533	-1.258959	5.212788
C	3.179036	0.587446	3.684845
O	5.508896	-1.993846	3.311958
C	3.560044	-0.693997	4.023073
O	5.095357	0.071120	2.434184
C	4.797929	-1.012120	3.271209
O	2.640926	-0.016559	0.881951
H	2.441099	-0.508732	1.707592
O	3.370043	1.677846	-1.136517
H	2.847190	0.849318	-1.139600
C	4.069608	1.064639	2.563509
H	4.541808	2.046509	2.803720
C	3.270527	1.210643	1.250415
H	2.501080	2.001600	1.434771
C	4.138109	1.609643	0.054467
H	4.580646	2.614968	0.230954
H	4.976461	0.872860	-0.016066
H	1.499932	0.797297	4.592605
O	0.708691	-0.406036	5.207722

C	-0.192497	-0.860631	4.440573
O	-0.618483	-0.004915	3.452576
O	-0.741977	-1.996861	4.495277
C	-2.344257	-1.693238	3.190339
H	-2.942611	-1.402985	4.061204
H	-2.246960	-2.760723	2.968480
C	-1.483231	-0.651779	2.484211
H	-2.108002	0.166060	2.073908
I	-4.636788	-1.702464	1.728795
C	-0.613476	-1.235384	1.350656
H	0.183419	-0.495345	1.126900
H	-0.104396	-2.151736	1.751991
O	-1.316629	-1.471581	0.149891
H	-2.151399	-1.939888	0.365285

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ACID-C SCF Done: -1152.54131934 A.U.

O	-1.713493	-1.719371	-1.098197
O	0.492986	-0.412313	-3.081426
H	0.845083	-0.523841	-2.129465
C	-1.773783	-1.093758	-2.269539
O	-1.165311	0.629147	-5.256244
C	-0.839977	-0.558382	-3.137145
O	-2.946471	-0.221286	-4.117893
C	-1.576312	0.022020	-4.287852
O	-2.808362	-3.104775	-4.111352
H	-1.896273	-2.820180	-3.881858
O	-5.446187	-3.655613	-4.367464
H	-4.629318	-4.057798	-4.730771

C	-3.136179	-0.986202	-2.922661
H	-3.865192	-0.459220	-2.260877
C	-3.694691	-2.385327	-3.256323
H	-3.817608	-2.918073	-2.279060
C	-5.035654	-2.346892	-3.992341
H	-5.819603	-1.918305	-3.329302
H	-4.920065	-1.668294	-4.873563
H	-0.748642	-2.062797	-0.839908
O	1.563474	-0.668703	-0.732400
C	1.408033	-1.789442	-0.183053
O	0.488730	-2.634435	-0.320373
O	2.384789	-2.197675	0.749972
C	3.522476	-1.341013	0.932635
H	3.791015	-0.849953	-0.027800
C	3.122688	-0.265015	1.950436
H	2.264387	0.276364	1.489943
H	2.744775	-0.794450	2.864611
C	4.608761	-2.320245	1.388456
H	4.562974	-3.230259	0.762168
H	4.512650	-2.592475	2.458095
I	6.729653	-1.610344	1.152868
O	4.217634	0.595217	2.236929
H	3.849810	1.403774	2.635510

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ACID-DminusI SCF Done: -1140.94385459 A.U.

O	-4.011974	-1.892518	4.416726
O	-6.891323	-1.665320	3.076009
H	-6.621068	-2.539591	3.424244

C	-4.755146	-0.830321	4.061056
O	-7.073529	1.156701	2.396694
C	-5.992397	-0.725634	3.491637
O	-5.165123	1.432800	3.623472
C	-6.206106	0.682652	3.101242
O	-5.453917	0.847443	6.419208
H	-5.799672	-0.058006	6.299481
O	-3.621928	2.632088	7.447399
H	-4.498991	2.371941	7.796120
C	-4.240056	0.566832	4.307288
H	-3.230884	0.689593	3.850801
C	-4.170580	0.924410	5.809123
H	-3.447799	0.211597	6.281183
C	-3.682444	2.354418	6.061984
H	-2.659254	2.477009	5.645970
H	-4.361597	3.048545	5.507610
H	-4.191934	-2.637759	3.772650
O	-4.737798	-3.538797	2.365457
C	-5.107809	-2.853926	1.423375
O	-4.535005	-1.676599	1.085004
O	-6.144499	-3.156009	0.623056
C	-6.545550	-1.941982	-0.065965
H	-7.367702	-1.476941	0.514972
H	-6.866453	-2.187978	-1.094925
C	-5.264956	-1.088303	-0.023202
H	-5.485393	-0.031673	0.228949
C	-4.409781	-1.181491	-1.287273
H	-3.448884	-0.641405	-1.106858
H	-4.161328	-2.259685	-1.463534

O	-5.187671	-0.616917	-2.326757
H	-4.676879	-0.664015	-3.154910

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ACID-D SCF Done: -1152.56537696 A.U.

O	3.463338	-0.646593	0.256536
O	4.384190	-2.999016	2.200735
H	3.685374	-2.394976	2.571207
C	3.945577	-1.889247	0.026088
O	5.221226	-5.121656	0.299731
C	4.323649	-2.910562	0.855908
O	4.534962	-3.688741	-1.340817
C	4.747912	-4.050807	-0.003338
O	1.733672	-3.537480	-0.968762
H	1.846033	-3.320778	-0.015543
O	0.664233	-3.032440	-3.382591
H	0.357856	-3.656373	-2.688404
C	3.880567	-2.419747	-1.382405
H	4.393590	-1.757736	-2.117754
C	2.387129	-2.568228	-1.768830
H	1.949062	-1.548275	-1.621409
C	2.083391	-2.974897	-3.205687
H	2.479111	-2.220761	-3.917109
H	2.566406	-3.956694	-3.422287
H	3.240277	-0.563125	1.221413
O	2.328592	-1.211069	2.629497
C	1.249653	-1.500649	2.105793
O	0.272308	-0.628226	1.870352
O	0.963461	-2.735420	1.650308

C	-0.436830	-2.741367	1.193391
H	-1.076658	-3.153244	2.003846
H	-0.496322	-3.332581	0.262671
C	-0.704467	-1.256095	0.962791
H	-1.720263	-0.980482	1.318090
I	-3.453349	-2.071553	3.594805
C	-0.373036	-0.759009	-0.461812
H	-0.698207	0.305832	-0.548667
H	0.739819	-0.754750	-0.554492
O	-0.999162	-1.578792	-1.426220
H	-0.356185	-1.806093	-2.136894

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EPO SCF Done: -268.124585325 A.U.

O	0.720500	0.308092	-1.160036
C	-0.067607	-0.464688	-0.247127
C	0.503785	-1.079991	-1.461465
H	0.408458	-0.685226	0.731318
H	-0.158859	-1.289412	-2.325140
H	1.391905	-1.737121	-1.378557
C	-1.535457	-0.098591	-0.165069
H	-1.633135	0.829817	0.453191
H	-1.885781	0.161886	-1.196506
O	-2.228544	-1.202501	0.400012
H	-3.133875	-0.908809	0.607755

EPO-Glyc

41

ACID-AB SCF Done: -1193.96159799 A.U.

O	-0.779742	-0.087059	0.917406
O	-0.866610	2.057504	-1.450670
H	0.025330	1.707288	-1.157305
C	-1.782870	0.598898	0.356123
O	-3.707790	2.798671	-1.556828
C	-1.828776	1.502730	-0.679977
O	-4.011414	1.278857	0.117736
C	-3.230176	1.966301	-0.816087
O	-3.568920	-1.377102	-0.896291
H	-2.758324	-0.948726	-1.242311
O	-5.455579	-2.722179	0.539991
H	-5.150551	-2.810381	-0.386707
C	-3.193096	0.333356	0.820740
H	-3.294328	0.508620	1.917645
C	-3.634505	-1.111191	0.501602
H	-2.947597	-1.788464	1.071004
C	-5.080782	-1.404073	0.907890
H	-5.186354	-1.315038	2.011303
H	-5.729617	-0.625138	0.436095
H	0.097043	0.218531	0.470445
O	1.237861	0.862651	-0.341459
C	2.502839	1.054157	0.314117
H	3.045081	1.969784	-0.000749
C	2.641742	-0.118161	-0.556540
H	2.950952	-0.000909	-1.601251
I	5.461864	-1.090808	-0.158651
C	-1.028054	2.393690	3.045339
C	0.273154	2.718858	2.360171

C	0.370287	3.283055	1.136251
C	1.518226	2.580760	3.197865
O	1.575708	3.018490	4.332188
O	2.640295	2.039397	2.625304
C	2.556071	0.842445	1.819719
H	-0.520576	3.532006	0.540155
H	1.349334	3.532739	0.700007
H	-1.101171	1.298732	3.219599
H	-1.072844	2.896260	4.033797
H	-1.894145	2.702084	2.427498
H	1.694899	0.214070	2.137255
H	3.494679	0.289492	2.035823
H	2.366730	-1.114203	-0.185989

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ACID-A+I SCF Done: -1193.97352651 A.U.

O	0.272117	0.558416	1.533287
O	-0.755778	3.192545	0.008016
H	0.202897	2.978303	-0.082485
C	-0.953396	0.985492	1.167635
O	-3.649168	2.759757	-0.160758
C	-1.394866	2.099407	0.507628
O	-3.275103	0.809454	0.958338
C	-2.863438	1.991388	0.355967
O	-1.731824	-1.138581	-0.655090
H	-0.875547	-1.622193	-0.834243
O	-3.162222	-3.367259	0.217371
H	-2.706257	-3.143997	-0.623707
C	-2.126818	0.080218	1.432318

H	-2.259218	-0.099068	2.526543
C	-2.003621	-1.290338	0.732495
H	-1.160831	-1.830781	1.226259
C	-3.289185	-2.123460	0.879046
H	-3.496156	-2.323529	1.954735
H	-4.137184	-1.510904	0.481441
H	0.962912	1.031398	0.997523
O	1.508560	1.821670	-0.498305
C	2.395948	1.382298	-1.568768
H	2.778869	2.227876	-2.172556
C	0.956048	1.059119	-1.618566
H	0.284652	1.648147	-2.267929
H	0.612988	0.043085	-1.348520
I	1.223679	-2.917016	-0.974413
C	3.398188	-0.660910	1.782704
C	3.590970	0.839337	1.732782
C	3.006765	1.686531	2.611725
C	4.523140	1.464841	0.717258
O	5.288095	2.370842	0.992332
O	4.563513	0.957751	-0.560710
C	3.419313	0.343824	-1.187090
H	2.325059	1.311859	3.391653
H	3.181725	2.771876	2.547755
H	4.249316	-1.205593	1.327660
H	3.288526	-0.997053	2.833250
H	2.480172	-0.994753	1.248213
H	2.950008	-0.462671	-0.588006
H	3.809312	-0.134742	-2.108120

ACID-A SCF Done: -1182.35651039 A.U.

O	-1.217895	-1.076876	0.270282
O	-1.496087	1.924432	1.297005
H	-1.253742	2.879831	1.266021
C	-0.511073	0.046086	0.019849
O	0.606779	3.326948	-0.077284
C	-0.611410	1.328913	0.462713
O	1.156127	1.317798	-1.043329
C	0.423570	2.130731	-0.214720
O	2.269965	-0.551612	0.842734
H	1.510786	-0.451899	1.449936
O	3.973599	-1.910492	-0.844052
H	4.103701	-1.639475	0.087643
C	0.662046	-0.031334	-0.932245
H	0.324060	-0.361664	-1.942375
C	1.773409	-0.970836	-0.423990
H	1.326486	-1.996375	-0.366824
C	2.993292	-1.021998	-1.347786
H	2.685551	-1.388717	-2.350757
H	3.373619	0.022180	-1.468767
H	-2.002167	-0.859385	0.854666
O	-3.424671	-0.335619	1.583879
C	-4.349728	0.320154	0.688071
C	-4.792060	-0.786646	1.564911
H	-4.565452	1.367138	0.971224
H	-4.961851	-1.790865	1.130203
H	-5.366132	-0.564735	2.483174
C	-3.077968	-0.106585	-4.681167

C	-2.647730	-0.416180	-3.268167
C	-2.305882	-1.646709	-2.824394
C	-2.434773	0.811455	-2.411560
O	-1.658634	1.684496	-2.742237
O	-3.121485	0.966622	-1.236796
C	-4.147476	0.072212	-0.786966
H	-2.346646	-2.515894	-3.502346
H	-1.939121	-1.812910	-1.797858
H	-2.361304	0.608064	-5.138184
H	-3.124536	-1.022740	-5.301786
H	-4.074589	0.385823	-4.700747
H	-3.877224	-0.988735	-0.959648
H	-5.098053	0.280018	-1.331021

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ACID-B+CO2 SCF Done: -1382.45546437 A.U.

O	0.876283	0.230452	-1.921160
O	0.583032	1.467718	0.949424
H	-0.215575	1.027696	0.480293
C	1.792756	0.601110	-1.033969
O	3.409836	1.758789	1.847904
C	1.682071	1.127753	0.234073
O	3.962240	0.864117	-0.180770
C	3.039967	1.307022	0.781812
O	3.145105	-1.874996	-0.120002
H	2.338609	-1.465392	0.260327
O	5.078283	-3.039907	-1.579228
H	4.558048	-3.295019	-0.787887
C	3.248110	0.291674	-1.285059

H	3.613597	0.746893	-2.235831
C	3.464937	-1.237586	-1.353118
H	2.801658	-1.613841	-2.173337
C	4.916391	-1.629715	-1.638446
H	5.206334	-1.290843	-2.657509
H	5.564625	-1.095675	-0.898778
H	-0.036123	0.119444	-1.381031
O	-1.011540	-0.068429	-0.332126
C	-2.323312	-0.219952	-0.761486
H	-2.684077	0.650115	-1.374395
C	-3.134300	-0.302935	0.534782
H	-2.956321	0.587800	1.163811
H	-2.901474	-1.218212	1.113035
I	-5.409450	-0.338291	0.282475
O	-0.896285	-0.284165	2.896305
O	0.935733	-1.338827	1.870226
C	0.024174	-0.759085	2.339637
C	0.467233	-4.411144	-2.944284
C	0.006908	-3.144885	-2.258290
C	0.305911	-2.852479	-0.972194
C	-0.638561	-2.155129	-3.202441
O	-0.259017	-2.070767	-4.358999
O	-1.661894	-1.341089	-2.809281
C	-2.469849	-1.486499	-1.627618
H	0.903725	-3.553156	-0.366949
H	0.002425	-1.897903	-0.510195
H	1.140836	-4.157505	-3.788846
H	1.001456	-5.078869	-2.239637
H	-0.389982	-4.967519	-3.383294

H	-2.178794	-2.383894	-1.042143
H	-3.517286	-1.609971	-1.977901

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ACID-BC SCF Done: -1382.44945033 A.U.

O	1.153335	-0.313541	-1.218982
O	0.900297	1.965877	0.963075
H	0.113572	1.360296	0.730879
C	2.051203	0.545004	-0.714447
O	3.668807	3.017863	1.155533
C	1.952635	1.525711	0.245169
O	4.187870	1.464821	-0.433008
C	3.295221	2.118537	0.429977
O	3.937316	-1.123602	0.798667
H	3.003426	-0.984391	1.065195
O	5.984456	-2.415869	-0.378300
H	5.551567	-2.445290	0.502320
C	3.503120	0.391858	-1.088659
H	3.663706	0.474732	-2.190959
C	4.045310	-0.975368	-0.610991
H	3.446819	-1.756425	-1.146980
C	5.530837	-1.181326	-0.915494
H	5.693921	-1.198070	-2.015843
H	6.086597	-0.304437	-0.499036
H	0.269597	-0.243785	-0.615605
O	-0.730567	0.050960	0.353432
C	-2.078966	0.145243	0.033237
H	-2.635612	0.762726	0.783330
C	-2.555930	-1.308209	0.109423

H	-2.377569	-1.706936	1.124334
H	-2.065907	-1.944906	-0.653769
I	-4.805874	-1.662049	-0.205635
O	-0.758169	-0.378265	3.144256
O	1.201791	-1.035548	2.030304
C	0.185896	-0.660958	2.499333
C	-1.769705	3.017683	-4.857844
C	-1.171450	2.350344	-3.642941
C	-0.187087	1.425142	-3.696799
C	-1.617591	2.943025	-2.324825
O	-1.756608	4.148075	-2.201957
O	-1.809903	2.138452	-1.245372
C	-2.282702	0.778410	-1.347930
H	0.215434	1.100460	-4.672377
H	0.260802	0.970249	-2.796866
H	-1.612373	4.114795	-4.797024
H	-1.323537	2.632411	-5.796408
H	-2.869836	2.859196	-4.899624
H	-1.714823	0.198719	-2.104590
H	-3.355518	0.795802	-1.642126

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ACID-B SCF Done: -1193.98025674 A.U.

O	1.118969	-1.328216	-0.459548
O	0.187984	1.097514	1.322530
H	-0.405663	0.287778	1.138554
C	1.718472	-0.175681	-0.155849
O	2.608463	2.833569	1.391858
C	1.341681	0.876716	0.645907

O	3.549745	1.282295	0.007419
C	2.484943	1.796338	0.769575
O	3.803627	-1.631961	1.056986
H	2.886011	-1.973903	1.051690
O	6.306562	-1.957695	0.045631
H	5.810440	-2.337283	0.802375
C	3.136712	0.060170	-0.619477
H	3.184310	0.203214	-1.727399
C	4.046991	-1.133225	-0.261100
H	3.834230	-1.929329	-1.018064
C	5.540950	-0.810479	-0.298279
H	5.833044	-0.486004	-1.320878
H	5.721109	0.048710	0.392897
H	0.114673	-1.303409	-0.016692
O	-1.123414	-1.031901	0.528327
C	-1.990044	-0.769989	-0.535286
H	-1.436066	-0.688363	-1.507930
C	-2.630967	0.584227	-0.201813
H	-1.847613	1.347506	-0.037450
H	-3.287025	0.518310	0.689287
I	-3.956044	1.492870	-1.823997
C	-3.623565	-5.534397	1.475201
C	-2.844965	-4.287496	1.121853
C	-2.449514	-3.364982	2.028806
C	-2.376365	-4.260492	-0.318254
O	-1.987444	-5.287926	-0.853452
O	-2.380230	-3.117431	-1.050579
C	-3.037226	-1.885296	-0.696310
H	-2.713384	-3.496983	3.093637

H	-1.858948	-2.475805	1.728449
H	-3.037583	-6.435563	1.198691
H	-3.865820	-5.568514	2.556425
H	-4.573831	-5.590097	0.899421
H	-3.628103	-1.994797	0.237208
H	-3.729074	-1.657567	-1.534804

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ACID-CD SCF Done: -1382.44912771 A.U.

O	-0.810409	-3.046662	-4.001703
O	1.386286	-0.951422	-3.230249
H	0.434017	-0.692300	-3.123006
C	0.456743	-3.211268	-3.572387
O	3.690442	-2.661488	-2.383851
C	1.414481	-2.304071	-3.216452
O	2.297911	-4.422659	-2.802891
C	2.603267	-3.054587	-2.746930
O	0.119837	-4.415270	-0.865713
H	0.009522	-3.444008	-1.035026
O	-0.446930	-7.058355	-0.642325
H	-0.478219	-6.309446	-0.008761
C	0.933146	-4.588934	-3.202409
H	0.892186	-5.296410	-4.065306
C	0.055244	-5.166040	-2.066259
H	-0.985960	-5.173675	-2.477407
C	0.420682	-6.596179	-1.670468
H	0.306878	-7.275865	-2.542604
H	1.494029	-6.607765	-1.357690
H	-1.131845	-2.157788	-3.657122

O	-1.391365	-0.868987	-2.632723
C	-1.325743	-1.159458	-1.415997
O	-2.377398	-0.868690	-0.607718
O	-0.317897	-1.705879	-0.821944
C	-0.664651	-1.327628	1.060184
H	-0.100995	-0.387822	1.038114
H	-0.135344	-2.237671	1.361243
C	-2.155406	-1.332999	0.761524
H	-2.712248	-0.612478	1.387608
I	-0.857772	-0.885400	3.857558
C	-3.595067	-5.475766	-0.721467
C	-3.833818	-4.094238	-1.293202
C	-3.419765	-3.675305	-2.505923
C	-4.686278	-3.172828	-0.447920
O	-5.831771	-2.875788	-0.716559
O	-4.140933	-2.734913	0.730934
C	-2.724296	-2.741546	0.937470
H	-2.823697	-4.316237	-3.172584
H	-3.638321	-2.654584	-2.857681
H	-3.426800	-5.437363	0.375530
H	-4.496704	-6.108960	-0.874728
H	-2.720599	-5.986707	-1.172279
H	-2.191290	-3.426826	0.242312
H	-2.539108	-3.061837	1.982892

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ACID-C SCF Done: -1382.44921634 A.U.

O	-2.066561	-1.443119	-0.126748
O	-1.001089	0.868608	-2.098036

H	-0.182288	0.271476	-1.920182
C	-2.264382	-0.131240	-0.192262
O	-2.148953	3.291934	-0.890615
C	-1.821330	0.871166	-1.034795
O	-3.244010	1.887094	0.528264
C	-2.371196	2.150079	-0.526716
O	-5.098742	0.164159	-0.853959
H	-4.293407	0.124928	-1.413702
O	-7.060859	0.063552	1.015146
H	-7.068585	0.120715	0.036846
C	-3.278937	0.470289	0.758328
H	-3.004002	0.268090	1.820245
C	-4.691594	-0.087328	0.489808
H	-4.642508	-1.188201	0.688677
C	-5.771728	0.541808	1.373289
H	-5.591352	0.275626	2.438026
H	-5.686473	1.652463	1.276094
H	-1.131678	-1.754176	-0.483876
O	1.126749	-0.368136	-1.505026
C	1.137900	-1.375589	-0.748538
O	0.263955	-2.254540	-0.564040
O	2.297494	-1.563118	0.036120
C	3.223933	-0.463645	0.073147
H	3.294985	0.013042	-0.927953
C	4.537650	-1.144159	0.458269
H	4.700597	-2.021674	-0.194734
H	4.548738	-1.460095	1.520066
I	6.376689	0.107315	0.189956
C	0.540724	4.133132	1.133673

C	1.485041	3.192940	0.421329
C	1.232151	2.671993	-0.801198
C	2.823430	3.008387	1.091166
O	3.433477	3.943478	1.579083
O	3.410548	1.764381	1.127330
C	2.654694	0.547642	1.082710
H	0.284916	2.881679	-1.324982
H	1.939405	1.996138	-1.305019
H	1.033873	5.115308	1.294116
H	-0.395478	4.265572	0.556789
H	0.280035	3.742819	2.142198
H	1.600221	0.741507	0.801434
H	2.673615	0.091780	2.099077

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ACID-DminusI SCF Done: -1370.84137383 A.U.

O	0.315387	-1.632787	1.715070
O	-0.923420	1.287288	1.429333
H	-0.991111	0.863979	2.309277
C	0.491808	-0.671701	0.797398
O	-0.040222	2.112587	-1.219671
C	-0.026528	0.587353	0.672438
O	1.247189	0.227761	-1.227369
C	0.362069	1.117218	-0.646626
O	3.320179	0.245386	0.764172
H	2.806049	0.334162	1.588906
O	5.239578	-1.204542	-0.588086
H	5.346799	-0.426759	-0.002984
C	1.452320	-0.892791	-0.344993

H	1.193320	-1.828154	-0.892114
C	2.927707	-0.957578	0.112157
H	3.021909	-1.842558	0.790229
C	3.907200	-1.129480	-1.053816
H	3.681237	-2.074485	-1.593056
H	3.740666	-0.283270	-1.765667
H	-0.606741	-1.545908	2.104357
O	-2.254617	-1.148415	2.407308
C	-2.858446	-0.641504	1.473446
O	-2.549280	-0.846404	0.174147
O	-3.892391	0.204360	1.615127
C	-4.343961	0.625422	0.301894
H	-4.522849	1.715450	0.319591
H	-5.288597	0.093666	0.058612
C	-3.172581	0.208957	-0.607742
H	-2.429609	1.031042	-0.704721
C	-2.832293	0.567247	-5.989214
C	-2.827551	0.986028	-4.539560
C	-1.731555	1.419349	-3.875659
C	-4.195360	1.073663	-3.913864
O	-5.153128	1.532019	-4.497763
O	-4.372170	0.663032	-2.601626
C	-3.570044	-0.338271	-1.969900
H	-0.748443	1.467841	-4.371672
H	-1.754228	1.780352	-2.835816
H	-3.515713	1.224383	-6.566476
H	-1.817478	0.619492	-6.428837
H	-3.216867	-0.469036	-6.106410
H	-2.668892	-0.601427	-2.560337

H	-4.189636	-1.253411	-1.832815
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ACID-D SCF Done: -1382.46481536 A.U.

O	1.870465	-0.384932	-1.984601
O	1.863238	1.958033	0.220380
H	1.028122	1.814799	-0.296201
C	2.766469	0.018302	-1.069196
O	4.489021	1.653484	1.489467
C	2.765737	1.015197	-0.125648
O	4.829708	-0.077795	0.036467
C	4.058225	0.972003	0.586921
O	3.557864	-2.366206	0.754832
H	4.108616	-1.712560	1.240995
O	5.123621	-4.326415	-0.361548
H	4.625417	-4.223168	0.478231
C	4.069815	-0.733318	-0.992945
H	4.620699	-0.651725	-1.960406
C	3.936199	-2.225836	-0.619951
H	3.113157	-2.676647	-1.215921
C	5.239220	-3.007256	-0.854293
H	5.461705	-3.057545	-1.943554
H	6.077498	-2.437763	-0.371147
H	1.015955	0.123182	-1.869305
O	-0.235783	1.096826	-1.277920
C	-1.327600	0.740034	-0.822387
O	-1.976202	-0.346363	-1.248024
O	-1.967413	1.393254	0.141247
C	-3.289694	0.766496	0.345477

H	-4.069069	1.401920	-0.116382
H	-3.482006	0.699669	1.430711
C	-3.125513	-0.597355	-0.351276
H	-3.991777	-0.863963	-0.984179
I	-6.564446	-0.346174	0.960661
C	0.434120	-4.137114	1.752420
C	-0.234342	-3.267663	0.716798
C	0.351541	-2.180016	0.167433
C	-1.535249	-3.802760	0.163443
O	-1.664082	-4.979023	-0.119600
O	-2.573237	-2.946376	-0.092745
C	-2.792302	-1.722029	0.619589
H	1.363603	-1.870717	0.474892
H	-0.142126	-1.621557	-0.638390
H	0.454557	-5.187715	1.394660
H	1.468510	-3.792492	1.946780
H	-0.137006	-4.136003	2.706814
H	-1.917859	-1.444678	1.247276
H	-3.690740	-1.845456	1.266258

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EPO SCF Done: -498.024303441 A.U.

C	4.114329	-5.195700	-2.197889
C	3.413338	-4.745497	-0.939633
C	2.967996	-5.582291	0.025494
C	3.421878	-3.250302	-0.729273
O	4.406091	-2.580952	-0.972346
O	2.317116	-2.610874	-0.218552
C	0.983899	-3.131505	-0.252745

C	0.387903	-3.222487	1.140675
C	0.998840	-2.546160	2.303352
O	1.109066	-3.971857	2.126252
H	3.089689	-6.673423	-0.083012
H	2.500399	-5.204644	0.949646
H	5.137422	-4.766706	-2.230299
H	4.177605	-6.299940	-2.255040
H	3.588295	-4.823746	-3.103830
H	0.944088	-4.124635	-0.749722
H	0.369561	-2.421433	-0.851271
H	0.358292	-2.218697	3.145312
H	1.934242	-1.976575	2.152620
H	-0.709696	-3.393485	1.136267

EPO-Ph

38

ACID-AB SCF Done: -1080.51206329 A.U.

O	-0.899129	-0.800830	1.205033
O	-0.882062	2.374127	1.141588
H	-0.267055	1.871490	0.529636
C	-1.428199	0.108762	2.024816
O	-2.183499	3.089721	3.682689
C	-1.439829	1.484497	1.997073
O	-2.470466	0.847901	3.989480
C	-2.049569	1.960731	3.257344
O	-4.323808	-0.394509	2.153750
H	-3.787051	0.218617	1.607602
O	-5.407388	-2.229652	3.838689

H	-5.794504	-1.652756	3.147831
C	-2.143831	-0.352098	3.268995
H	-1.449941	-0.967435	3.889109
C	-3.415031	-1.157072	2.947621
H	-3.082875	-2.072676	2.394991
C	-4.197871	-1.576096	4.194848
H	-3.591340	-2.284886	4.800096
H	-4.372702	-0.659148	4.810308
H	-0.192929	-0.315335	0.628214
O	0.838259	0.688241	0.046822
C	2.033170	0.774442	0.879079
H	2.442621	1.806268	0.891194
C	2.387071	-0.023875	-0.296717
H	2.751730	0.468108	-1.204739
H	2.200901	-1.104202	-0.309888
I	5.275690	-0.829743	-0.063880
C	1.884965	0.205888	2.265493
C	1.318122	1.031399	3.261290
C	2.195028	-1.132691	2.577082
C	1.038228	0.523434	4.540360
C	1.923026	-1.640047	3.858659
C	1.335743	-0.818505	4.838902
H	1.059110	2.073979	3.015129
H	2.678658	-1.770833	1.821775
H	0.566126	1.172770	5.294184
H	2.175805	-2.686429	4.093570
H	1.115458	-1.222810	5.840492

ACID-A+I SCF Done: -1080.51666862 A.U.

O	-0.626365	-0.911579	-0.203401
O	-0.904668	2.202759	-0.867108
H	-0.082721	1.737593	-1.162479
C	-1.505517	0.019601	0.186263
O	-3.116962	3.041675	0.857243
C	-1.640833	1.353404	-0.107371
O	-3.269980	0.852976	1.480575
C	-2.725451	1.899773	0.739731
O	-4.194608	-0.912426	-0.601715
H	-3.534058	-0.376015	-1.087348
O	-5.607406	-2.673939	0.922659
H	-5.784032	-2.278749	0.044018
C	-2.585002	-0.369751	1.163223
H	-2.114719	-0.770803	2.091874
C	-3.561754	-1.405690	0.577942
H	-2.960011	-2.323065	0.353401
C	-4.698057	-1.773303	1.535567
H	-4.281536	-2.270203	2.438679
H	-5.189196	-0.822912	1.860860
H	0.187178	-0.436461	-0.570818
O	1.341050	0.684619	-0.914818
C	2.013172	1.184662	0.330310
H	2.194670	2.272940	0.250608
C	2.744354	0.316139	-0.601575
H	3.499570	0.752008	-1.276055
H	2.893582	-0.749919	-0.364969
I	5.738040	-0.894126	0.904029
C	1.411045	0.737728	1.620951

C	0.393616	1.532891	2.195735
C	1.786484	-0.471534	2.242644
C	-0.270397	1.109039	3.357725
C	1.125691	-0.889234	3.410085
C	0.092188	-0.109353	3.961814
H	0.100825	2.475837	1.706075
H	2.620761	-1.064925	1.832080
H	-1.083111	1.722139	3.777371
H	1.430068	-1.829651	3.896169
H	-0.426889	-0.446465	4.874025

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ACID-A SCF Done: -1068.91237154 A.U.

O	-0.545857	-2.229653	-1.997902
O	-0.125896	0.818184	-2.891807
H	0.575602	0.396311	-2.348922
C	-1.315419	-1.370494	-2.695077
O	-2.705909	1.521248	-4.049664
C	-1.133374	-0.072989	-3.087559
O	-3.292840	-0.658486	-3.718668
C	-2.402621	0.406587	-3.685230
O	-1.877303	-2.528354	-5.377919
H	-1.042880	-2.109957	-5.087154
O	-3.839628	-4.434882	-5.686327
H	-3.194027	-4.095085	-6.339104
C	-2.671152	-1.829688	-3.166864
H	-3.273608	-2.175558	-2.294712
C	-2.588669	-2.952847	-4.220887
H	-2.083277	-3.822352	-3.727406

C	-3.962694	-3.405014	-4.723405
H	-4.556137	-3.805622	-3.873094
H	-4.494183	-2.503322	-5.116720
H	0.110568	-1.702738	-1.463212
O	0.884262	-0.392857	-0.621263
C	-0.056724	0.439611	0.187217
C	1.089734	-0.262520	0.802047
H	0.080236	1.512694	-0.038692
H	0.925695	-1.189491	1.380843
H	1.987627	0.314618	1.091325
C	-1.477812	-0.009179	0.228526
C	-1.876081	-1.232882	0.808221
C	-2.439619	0.780413	-0.440473
H	-1.141702	-1.873770	1.320034
H	-2.126489	1.708699	-0.944410
C	-3.212477	-1.653064	0.725144
C	-3.775167	0.358295	-0.529111
H	-3.513173	-2.609935	1.179480
H	-4.502761	0.969326	-1.083899
C	-4.163096	-0.859980	0.055267
H	-5.208659	-1.198137	-0.018596

41

ACID-B+CO2 SCF Done: -1268.99710624 A.U.

O	1.373827	-0.478650	-1.407359
O	0.667684	1.803468	0.665594
H	0.017553	1.034451	0.480574
C	2.119208	0.488901	-0.858304
O	3.284818	3.152320	1.085835

C	1.828905	1.465142	0.068317
O	4.118029	1.614461	-0.379181
C	3.078289	2.196734	0.363412
O	3.928072	-0.989930	0.892487
H	2.958991	-1.092823	1.003884
O	6.235662	-2.071486	0.034814
H	5.670685	-2.145913	0.835207
C	3.611240	0.465909	-1.067680
H	3.888522	0.537672	-2.147623
C	4.216619	-0.836251	-0.491979
H	3.780582	-1.677368	-1.088593
C	5.743576	-0.890981	-0.583306
H	6.060260	-0.893089	-1.649853
H	6.145398	0.038924	-0.108892
H	0.469320	-0.504835	-0.869253
O	-0.673273	-0.314787	0.039488
C	-1.905163	-0.271608	-0.632507
H	-1.912698	0.551295	-1.395804
C	-2.912781	0.083474	0.461125
H	-2.651806	1.055803	0.917930
H	-2.976116	-0.698240	1.241031
I	-5.045060	0.384884	-0.278488
O	-1.140146	-2.245295	1.956900
O	1.084639	-1.692580	1.471510
C	-0.079821	-1.861217	1.598631
C	-2.136912	-1.586744	-1.376590
C	-1.532169	-1.748951	-2.641630
C	-2.830423	-2.679520	-0.818647
C	-1.624611	-2.965362	-3.337327

C	-2.929209	-3.897744	-1.512802
C	-2.329643	-4.045548	-2.776146
H	-0.955737	-0.912286	-3.069603
H	-3.296578	-2.584282	0.172882
H	-1.140815	-3.071612	-4.322125
H	-3.479985	-4.739176	-1.061030
H	-2.407717	-5.001339	-3.319921

41

ACID-BC SCF Done: -1268.99917667 A.U.

O	1.733738	-0.561933	-1.428867
O	0.544541	1.286953	0.830950
H	-0.004874	0.557794	0.349198
C	2.287072	0.400349	-0.692768
O	2.898626	2.919481	1.662556
C	1.790813	1.204744	0.310918
O	4.056535	1.723507	0.100358
C	2.888493	2.053489	0.809137
O	4.197359	-0.994697	1.043833
H	3.222785	-1.078819	1.114825
O	6.680666	-1.644960	0.237456
H	6.106288	-1.880451	0.997854
C	3.778956	0.617572	-0.765694
H	4.115153	0.868517	-1.800720
C	4.532502	-0.647614	-0.294712
H	4.250986	-1.466262	-1.005630
C	6.053837	-0.483042	-0.288185
H	6.422579	-0.326345	-1.326038
H	6.292528	0.435458	0.303878

H	0.735910	-0.712943	-1.069902
O	-0.525220	-0.697594	-0.394472
C	-1.663320	-0.506615	-1.172998
H	-1.486752	0.191267	-2.035589
C	-2.636870	0.170196	-0.188615
H	-2.211530	1.120168	0.186893
H	-2.884142	-0.504912	0.652973
I	-4.656284	0.795784	-1.049341
O	-0.861102	-1.172927	2.523443
O	1.288301	-1.601787	1.677501
C	0.199486	-1.347197	2.047520
C	-2.209095	-1.821440	-1.733147
C	-2.847745	-1.890592	-2.986905
C	-2.079216	-3.000771	-0.972043
C	-3.364245	-3.108321	-3.464075
C	-2.596294	-4.218743	-1.442442
C	-3.243591	-4.276938	-2.691191
H	-2.942194	-0.975477	-3.594384
H	-1.548970	-2.937768	-0.009276
H	-3.861021	-3.145373	-4.447768
H	-2.487793	-5.132681	-0.834920
H	-3.645677	-5.233256	-3.064633

38

ACID-B SCF Done: -1080.52615704 A.U.

O	1.644166	-1.312145	0.267494
O	0.617150	1.464830	1.350628
H	0.121113	0.607393	1.515765
C	2.080214	-0.086286	0.060296

O	2.733956	3.344052	0.427738
C	1.670649	1.144126	0.539552
O	3.677245	1.526534	-0.584781
C	2.666421	2.154038	0.174734
O	4.316272	-1.326907	0.980838
H	3.383126	-1.659127	1.027254
O	6.819574	-1.250797	-0.035090
H	6.382483	-1.670761	0.737350
C	3.335261	0.143973	-0.767102
H	3.126067	-0.009787	-1.854030
C	4.455138	-0.850958	-0.357709
H	4.393259	-1.712928	-1.071616
C	5.868147	-0.272987	-0.440393
H	6.098303	0.037603	-1.482911
H	5.899651	0.644207	0.196186
H	0.402459	-1.211628	0.918961
O	-0.589426	-0.928859	1.262892
C	-1.338648	-0.778065	0.059032
H	-0.681998	-0.377296	-0.752491
C	-2.373456	0.292925	0.394990
H	-1.846692	1.218584	0.694495
H	-3.076359	-0.030485	1.187198
I	-3.655271	0.924705	-1.348178
C	-1.852611	-2.143477	-0.392484
C	-0.923397	-3.014617	-1.004737
C	-3.160756	-2.608802	-0.156183
H	0.113679	-2.662931	-1.141527
H	-3.903451	-1.951037	0.321876
C	-1.299351	-4.313010	-1.383123

C	-3.540789	-3.908761	-0.536819
H	-0.560816	-4.979620	-1.858264
H	-4.571678	-4.252807	-0.350582
C	-2.613170	-4.764573	-1.155391
H	-2.911993	-5.782103	-1.456938

41

ACID-CD SCF Done: -1268.98444346 A.U.

O	2.235646	-0.834427	-0.382650
O	2.485693	2.200186	0.679183
H	1.628488	1.709136	0.854556
C	3.207837	0.084440	-0.441025
O	5.177911	2.963286	-0.198731
C	3.331564	1.373327	0.034089
O	5.342919	0.851202	-1.041875
C	4.668719	1.875556	-0.367888
O	5.413768	-1.044225	1.127335
H	4.663019	-0.466141	1.381800
O	7.178725	-2.827705	0.084268
H	7.044970	-2.475655	0.988825
C	4.529171	-0.328311	-1.044974
H	4.400715	-0.681823	-2.095699
C	5.197929	-1.450238	-0.221897
H	4.508707	-2.331944	-0.265053
C	6.574003	-1.855000	-0.755671
H	6.469600	-2.297688	-1.770646
H	7.189541	-0.925966	-0.846314
H	1.436146	-0.443099	0.115071
O	0.453588	0.520249	0.897014

C	-0.803300	0.569807	0.804903
O	-1.409711	-0.520585	0.244667
O	-1.556583	1.521335	1.179462
C	-3.338010	0.979947	0.348682
H	-3.124670	1.631303	-0.506510
H	-3.830944	1.411241	1.224305
C	-2.868060	-0.471646	0.328125
H	-3.197539	-0.960812	-0.607422
I	-5.856851	0.600801	-0.687307
C	-3.347247	-1.278580	1.524221
C	-4.119544	-2.439718	1.333396
C	-3.020485	-0.878615	2.838445
H	-4.396285	-2.739422	0.310070
H	-2.429456	0.037651	2.993252
C	-4.556211	-3.196961	2.434001
C	-3.451963	-1.637350	3.938173
H	-5.166044	-4.099885	2.269468
H	-3.189160	-1.316453	4.959177
C	-4.220782	-2.799149	3.739632
H	-4.561917	-3.391626	4.604143

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ACID-C SCF Done: -1268.99765314 A.U.

O	-3.155732	0.037137	1.359562
O	-1.659869	1.025419	-1.338700
H	-1.031998	0.987048	-0.536784
C	-3.571250	0.542428	0.201581
O	-3.897432	1.914559	-3.002674
C	-2.946940	0.939216	-0.965544

O	-5.247468	1.280248	-1.280124
C	-3.995951	1.433763	-1.891836
O	-5.167562	-1.590397	-0.988900
H	-4.222560	-1.338568	-1.082007
O	-7.762164	-2.024791	-0.346059
H	-7.109776	-2.506386	-0.896837
C	-5.067362	0.653105	-0.005689
H	-5.542758	1.283085	0.784275
C	-5.727192	-0.741578	0.011437
H	-5.546891	-1.164337	1.032574
C	-7.230505	-0.708176	-0.271729
H	-7.758222	-0.170965	0.547220
H	-7.385224	-0.132623	-1.217883
H	-2.174948	-0.341843	1.329746
O	0.118238	0.884379	0.548763
C	0.104161	-0.199395	1.186587
O	-0.849638	-0.968281	1.456051
O	1.336788	-0.670116	1.697854
C	2.501591	0.127087	1.441461
H	2.237138	1.206158	1.465807
C	2.923998	-0.246518	0.011298
H	2.113942	0.023625	-0.691841
H	3.190761	-1.318583	-0.061628
I	4.726098	0.863453	-0.752495
C	3.538286	-0.200971	2.500582
C	3.668669	-1.519708	2.984593
C	4.403472	0.795792	2.993819
H	2.968038	-2.287436	2.622281
H	4.298198	1.830153	2.629217

C	4.656458	-1.836553	3.931460
C	5.395067	0.479691	3.938672
H	4.744617	-2.869959	4.304887
H	6.065477	1.270190	4.313375
C	5.526684	-0.838846	4.408366
H	6.301795	-1.087737	5.151527

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ACID-DminusI SCF Done: -1257.39736833 A.U.

O	0.282227	-0.739287	2.108226
O	-0.859234	1.888906	0.740686
H	-0.757358	1.886552	1.714467
C	0.256645	-0.340453	0.828489
O	-0.739409	1.244878	-2.100912
C	-0.224167	0.791772	0.231787
O	0.463773	-0.595734	-1.488924
C	-0.207421	0.583284	-1.228014
O	3.006591	-0.039259	-0.276027
H	2.674058	0.533858	0.441216
O	4.409650	-2.250964	-1.133907
H	4.706641	-1.322535	-1.042176
C	0.854324	-1.213642	-0.247098
H	0.408606	-2.233747	-0.203820
C	2.392825	-1.317596	-0.153673
H	2.628074	-1.793783	0.831683
C	3.004036	-2.173029	-1.268124
H	2.598829	-3.206055	-1.208590
H	2.683238	-1.736860	-2.246568
H	-0.511718	-0.349897	2.586421

O	-2.026763	0.375104	2.997764
C	-2.821617	0.444299	2.068947
O	-2.794273	-0.354693	0.988695
O	-3.812443	1.355709	1.997482
C	-4.537446	1.146286	0.757993
H	-4.775795	2.131312	0.315684
H	-5.476273	0.595414	0.980177
C	-3.543779	0.329123	-0.085784
H	-2.816124	1.008518	-0.578471
C	-4.091104	-0.655885	-1.078264
C	-3.616928	-0.625183	-2.406899
C	-5.042789	-1.627137	-0.698119
H	-2.842471	0.106926	-2.691217
H	-5.392529	-1.679561	0.345756
C	-4.111366	-1.542219	-3.350427
C	-5.529320	-2.544956	-1.641278
H	-3.737544	-1.513288	-4.385801
H	-6.269130	-3.302747	-1.338827
C	-5.068306	-2.499054	-2.970825
H	-5.452557	-3.219026	-3.710742

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ACID-D SCF Done: -1269.01729206 A.U.

O	2.100615	0.028964	-1.704688
O	2.257870	2.917422	-0.267141
H	1.414855	2.700251	-0.740907
C	2.950497	0.580500	-0.808174
O	4.615274	2.647423	1.453232
C	3.009478	1.796947	-0.183396

O	4.796286	0.529192	0.627673
C	4.180441	1.778579	0.729849
O	2.624997	-1.032861	1.633146
H	1.688890	-1.002148	1.349990
O	3.803450	-3.472512	1.868164
H	3.133972	-2.985898	2.398735
C	4.025591	-0.306444	-0.241270
H	4.690223	-0.707903	-1.043638
C	3.417780	-1.490484	0.539619
H	2.800490	-2.064975	-0.192004
C	4.456548	-2.440132	1.143964
H	5.060480	-2.910589	0.338436
H	5.147901	-1.839072	1.784855
H	1.348370	0.662945	-1.876968
O	0.108819	1.782015	-1.512659
C	-0.753966	1.218473	-0.833282
O	-1.258559	0.021420	-1.152704
O	-1.269254	1.724216	0.283494
C	-2.354612	0.851732	0.739695
H	-3.332887	1.313178	0.493700
H	-2.263460	0.728911	1.833691
C	-2.107655	-0.453032	-0.055709
H	-3.067323	-0.810381	-0.489988
I	-5.786943	-0.561705	0.892093
C	-1.421122	-1.568341	0.709281
C	-2.109219	-2.131056	1.807401
C	-0.157939	-2.078739	0.338693
H	-3.113446	-1.753705	2.071011
H	0.370858	-1.653837	-0.531520

C	-1.530595	-3.184317	2.532534
C	0.413469	-3.140669	1.071454
H	-2.078064	-3.618660	3.384379
H	1.405378	-3.536913	0.801269
C	-0.268752	-3.689531	2.169912
H	0.185262	-4.516359	2.739473

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EPO SCF Done: -384.579093593 A.U.

O	1.305676	0.438664	-0.396816
C	0.053189	0.400723	0.305788
C	0.889291	-0.818758	0.142042
H	0.065053	0.894427	1.299671
H	0.571256	-1.580311	-0.598134
H	1.481170	-1.202419	0.997544
C	-1.194946	0.609433	-0.494275
C	-1.161079	0.548942	-1.903695
C	-2.422149	0.854621	0.156070
H	-0.191281	0.387947	-2.400417
H	-2.453438	0.918182	1.256645
C	-2.339824	0.715809	-2.647906
C	-3.601684	1.018622	-0.589771
H	-2.302716	0.671825	-3.748233
H	-4.555346	1.208256	-0.071713
C	-3.564134	0.947583	-1.993919
H	-4.487893	1.080690	-2.579084

EPO-(Ph)₂

ACID-AB SCF Done: -1311.41709020 A.U.

O	-0.892990	-0.653412	-0.548600
O	-1.234942	2.466209	-0.205790
H	-0.399475	2.104278	-0.614359
C	-1.769018	0.064244	0.153631
O	-3.492461	2.680384	1.703299
C	-1.923747	1.418931	0.314840
O	-3.524257	0.393172	1.667657
C	-3.018370	1.652966	1.265039
O	-4.600273	-0.946221	-0.489613
H	-4.865495	-0.154086	0.028619
O	-5.478478	-3.229656	0.677966
H	-5.777713	-2.600268	-0.016704
C	-2.735989	-0.648216	1.057930
H	-2.155364	-1.174134	1.854079
C	-3.680143	-1.637992	0.361728
H	-3.075415	-2.299146	-0.296618
C	-4.481649	-2.491777	1.361053
H	-3.806701	-3.203058	1.887529
H	-4.913426	-1.806131	2.137187
H	-0.113612	-0.029240	-0.799029
O	0.974643	1.092946	-0.898889
C	1.892427	1.055767	0.224151
C	2.539563	0.300779	-0.868605
H	3.142547	0.845279	-1.603285
H	2.314132	-0.760954	-1.024701
I	5.203740	-0.695590	0.030317

C	2.507066	2.404342	0.557650
C	2.167064	3.557919	-0.171925
C	3.449657	2.494447	1.603100
C	2.751253	4.796617	0.148603
C	4.040824	3.729011	1.912795
C	3.689353	4.885323	1.191114
H	1.443011	3.475911	-0.995667
H	3.728931	1.584880	2.155985
H	2.469641	5.696636	-0.421889
H	4.785399	3.787255	2.722956
H	4.149850	5.855211	1.440998
C	1.323339	0.332219	1.433964
C	0.415151	1.035883	2.255858
C	1.603514	-1.017954	1.717709
C	-0.218677	0.395825	3.332351
C	0.974354	-1.657167	2.800481
C	0.058080	-0.956516	3.605769
H	0.186876	2.088303	2.025733
H	2.338295	-1.564848	1.107556
H	-0.945263	0.951937	3.945615
H	1.207405	-2.712212	3.016556
H	-0.438147	-1.462300	4.450258

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ACID-A+I SCF Done: -1311.42130085 A.U.

O	-0.608785	-0.930492	-0.135718
O	-1.128899	1.988429	-1.262492
H	-0.234447	1.588981	-1.407703
C	-1.579756	-0.041938	0.108455

O	-3.467670	2.888836	0.284221
C	-1.813558	1.218542	-0.377170
O	-3.454168	0.807559	1.220287
C	-2.972443	1.784000	0.349355
O	-4.157670	-1.279727	-0.636769
H	-3.511476	-0.784934	-1.181554
O	-5.488880	-2.943693	1.061402
H	-5.658661	-2.682614	0.132760
C	-2.665905	-0.388182	1.092466
H	-2.209775	-0.629276	2.080822
C	-3.536067	-1.565640	0.615005
H	-2.857837	-2.452868	0.530977
C	-4.679129	-1.898852	1.577060
H	-4.262677	-2.237796	2.550476
H	-5.255803	-0.958115	1.757958
H	0.176163	-0.412928	-0.505746
O	1.270757	0.778306	-0.875157
C	1.947227	1.315466	0.352464
C	2.631460	0.324511	-0.500448
H	3.431974	0.670572	-1.174138
H	2.691891	-0.732306	-0.194544
I	5.631994	-0.567176	1.181170
C	1.265910	0.910486	1.635040
C	0.157767	1.658587	2.093015
C	1.692680	-0.217046	2.365747
C	-0.541939	1.261124	3.243037
C	0.996969	-0.605430	3.523919
C	-0.125204	0.122466	3.958381
H	-0.166544	2.552669	1.539779

H	2.593950	-0.768530	2.047841
H	-1.422878	1.835538	3.569789
H	1.344496	-1.482013	4.093438
H	-0.670996	-0.189533	4.863904
C	2.379472	2.755449	0.245342
C	3.677213	3.088808	0.688901
C	1.519533	3.762162	-0.241070
C	4.106817	4.425560	0.645156
C	1.958089	5.097332	-0.280386
C	3.250010	5.432299	0.163342
H	4.346931	2.288864	1.052951
H	0.508098	3.504351	-0.590783
H	5.124228	4.677104	0.985475
H	1.282184	5.879246	-0.662820
H	3.590735	6.480219	0.130036

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ACID-A SCF Done: -1299.81109294 A.U.

O	-1.193424	-1.490024	0.484045
O	-1.956119	1.446964	1.449365
H	-2.654811	0.764501	1.601273
C	-0.810022	-0.265071	0.054377
O	-0.536986	3.167083	-0.471766
C	-1.128319	0.995699	0.479594
O	0.342445	1.237208	-1.310564
C	-0.446337	1.959983	-0.423653
O	2.094847	-0.056671	0.557354
H	1.413454	-0.081395	1.257261
O	3.905266	-1.155953	-1.202628

H	4.057615	-0.744988	-0.327164
C	0.229216	-0.167115	-1.031440
H	-0.103559	-0.693760	-1.956405
C	1.592791	-0.742418	-0.583609
H	1.432474	-1.829959	-0.369462
C	2.680501	-0.608850	-1.653448
H	2.375750	-1.165376	-2.565961
H	2.760236	0.473061	-1.923818
H	-2.061456	-1.391635	0.952025
O	-3.691522	-0.678361	1.145542
C	-4.700983	-0.252768	0.124150
C	-5.089869	-0.915047	1.400878
H	-5.390246	-1.978716	1.363855
H	-5.512159	-0.325303	2.234561
C	-4.696740	-1.065575	-1.145890
C	-3.914414	-2.230624	-1.283749
C	-5.526798	-0.661980	-2.214922
C	-3.963777	-2.979861	-2.471237
C	-5.581085	-1.419035	-3.396078
C	-4.799317	-2.580414	-3.528585
H	-3.234772	-2.533838	-0.476151
H	-6.127669	0.255594	-2.119143
H	-3.336379	-3.879565	-2.570976
H	-6.233490	-1.093776	-4.221635
H	-4.835247	-3.168840	-4.458861
C	-4.793419	1.241364	-0.018087
C	-3.861375	1.890907	-0.857048
C	-5.729832	2.011381	0.700541
C	-3.823023	3.289314	-0.930260

C	-5.716013	3.413466	0.598823
C	-4.754849	4.052425	-0.203493
H	-3.135056	1.287752	-1.423101
H	-6.481390	1.518458	1.337126
H	-3.043409	3.779780	-1.531399
H	-6.454016	4.009065	1.158813
H	-4.727225	5.151979	-0.259098

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ACID-B+CO2 SCF Done: -1499.89938923 A.U.

O	1.364060	-0.854951	-1.347567
O	0.558530	1.527001	0.570511
H	-0.086215	0.753458	0.364212
C	2.021489	0.245888	-0.970541
O	2.996173	3.227338	0.578862
C	1.690070	1.278209	-0.122040
O	3.882364	1.665426	-0.829207
C	2.850088	2.187658	-0.032867
O	4.209494	-0.768131	0.686647
H	3.261442	-0.813153	0.933938
O	6.531594	-1.653278	-0.353063
H	6.099985	-1.693403	0.527541
C	3.472926	0.396177	-1.350336
H	3.619905	0.389548	-2.457419
C	4.312397	-0.746006	-0.732504
H	3.927425	-1.698503	-1.178958
C	5.810910	-0.623910	-1.016491
H	5.998050	-0.715232	-2.109258
H	6.134168	0.397964	-0.696689

H	0.446504	-0.870331	-0.814602
O	-0.714157	-0.648923	0.030719
C	-1.957928	-0.599697	-0.619502
C	-2.892167	-0.688217	0.607536
H	-2.763479	0.183987	1.275191
H	-2.671294	-1.621374	1.154355
I	-5.160910	-0.822969	0.274896
O	-0.473060	-0.332919	3.012351
O	1.436941	-1.144807	1.910504
C	0.461269	-0.711554	2.409164
C	-2.162617	-1.829655	-1.528696
C	-1.444488	-3.009016	-1.249320
C	-3.069174	-1.824952	-2.608288
C	-1.631899	-4.164014	-2.027403
C	-3.258591	-2.978352	-3.388151
C	-2.541702	-4.153776	-3.099807
H	-0.723164	-2.992581	-0.417847
H	-3.626022	-0.904383	-2.840681
H	-1.056780	-5.076587	-1.799110
H	-3.970150	-2.957588	-4.230045
H	-2.686661	-5.057344	-3.714762
C	-2.030898	0.716401	-1.417017
C	-1.177123	0.841681	-2.537801
C	-2.773316	1.841768	-1.013433
C	-1.080153	2.050959	-3.239467
C	-2.682122	3.055850	-1.719597
C	-1.838111	3.166230	-2.835585
H	-0.557498	-0.018119	-2.836108
H	-3.434150	1.787576	-0.136334

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ACID-BC

H	-0.397263	2.128237	-4.101065
H	-3.271987	3.924335	-1.383733
H	-1.759617	4.120182	-3.382047
O	1.509181	-0.285218	-1.486610
O	0.653566	1.817578	0.643843
H	0.082097	1.015211	0.499924
C	2.224059	0.635907	-0.830207
O	3.199343	3.229451	1.261532
C	1.865732	1.551451	0.102286
O	4.148816	1.780939	-0.203897
C	3.064734	2.298633	0.496784
O	4.058460	-1.014360	0.771420
H	3.113231	-1.225088	0.857257
O	6.475822	-1.837753	-0.233984
H	5.996369	-2.105715	0.565110
C	3.714158	0.671126	-1.006501
H	4.002370	0.872981	-2.048445
C	4.377678	-0.650523	-0.564840
H	4.024428	-1.423946	-1.264498
C	5.902404	-0.589354	-0.618693
H	6.238679	-0.386541	-1.640848
H	6.253144	0.219373	0.035659
H	0.626927	-0.434054	-0.987555
O	-0.553572	-0.506884	0.005304
C	-1.848037	-0.468175	-0.572763
C	-2.819653	-0.134803	0.564818

H	-2.511283	0.764976	1.093763
H	-2.960287	-0.964257	1.253849
I	-4.887487	0.369563	-0.134786
O	-1.014768	-2.451066	1.623003
O	1.163759	-1.733417	1.307423
C	-0.020026	-1.891358	1.273575
C	-2.180488	-1.759241	-1.323447
C	-1.235584	-2.368918	-2.165931
C	-3.439378	-2.368918	-1.189949
C	-1.538155	-3.545097	-2.849946
C	-3.742542	-3.545097	-1.873701
C	-2.793243	-4.138859	-2.707063
H	-0.256384	-1.915435	-2.284195
H	-4.185033	-1.915435	-0.544335
H	-0.791663	-3.998477	-3.495859
H	-4.722526	-3.998477	-1.755019
H	-3.029218	-5.055263	-3.239902
C	-1.876362	0.699167	-1.576810
C	-0.924357	0.789981	-2.606261
C	-2.854945	1.703697	-1.489478
C	-0.949734	1.846419	-3.515173
C	-2.880841	2.760380	-2.398089
C	-1.928229	2.836774	-3.415394
H	-0.158961	0.025047	-2.692922
H	-3.600571	1.653906	-0.702061
H	-0.203395	1.895782	-4.302921
H	-3.646944	3.525558	-2.310938
H	-1.948204	3.659978	-4.123443

ACID-B SCF Done: -1311.43047107 A.U.

O	1.526660	-1.444944	0.382808
O	0.265888	1.269760	1.307385
H	-0.253740	0.374900	1.349304
C	1.889273	-0.187178	0.139898
O	1.899379	3.300385	-0.143734
C	1.351270	1.016970	0.550404
O	3.135137	1.525315	-0.870624
C	2.084680	2.099014	-0.135875
O	4.568186	0.154782	1.245224
H	3.672558	0.409590	1.561481
O	6.828194	-0.414365	-0.124275
H	6.644200	-0.103042	0.787072
C	3.099503	0.097237	-0.713781
H	2.981914	-0.372476	-1.718751
C	4.396973	-0.407266	-0.056274
H	4.308509	-1.521484	0.012726
C	5.659015	-0.043074	-0.843521
H	5.668530	-0.582206	-1.816680
H	5.621451	1.053761	-1.056958
H	0.508644	-1.406659	0.711863
O	-0.840274	-1.041413	1.085410
C	-1.771573	-1.001990	0.030551
C	-2.891559	-0.190606	0.725133
H	-2.521887	0.804485	1.034999
H	-3.262283	-0.757260	1.597521
I	-4.808061	0.293375	-0.443944
C	-2.292996	-2.415713	-0.303099

C	-2.970809	-2.711942	-1.504597
C	-2.118597	-3.441420	0.646441
C	-3.468561	-4.003831	-1.745686
C	-2.615520	-4.734524	0.408136
C	-3.294664	-5.021164	-0.789558
H	-3.099958	-1.923672	-2.261581
H	-1.572110	-3.190146	1.568503
H	-3.994605	-4.218073	-2.690746
H	-2.466296	-5.526186	1.161394
H	-3.682269	-6.035535	-0.981252
C	-1.135221	-0.306954	-1.192884
C	-0.295350	-1.056018	-2.046299
C	-1.176853	1.092162	-1.362788
C	0.489505	-0.426688	-3.025597
C	-0.381062	1.727433	-2.329989
C	0.461117	0.972349	-3.162774
H	-0.224996	-2.145529	-1.909499
H	-1.798854	1.713148	-0.704563
H	1.147803	-1.033363	-3.669369
H	-0.390560	2.825786	-2.402171
H	1.105784	1.474155	-3.901698

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ACID-CD SCF Done: -1499.88271140 A.U.

O	1.737087	-0.127753	-1.295870
O	2.106362	2.627997	0.325062
H	1.218547	2.450691	-0.107130
C	2.740877	0.382710	-0.567220
O	4.848322	2.410500	1.346711

C	2.896314	1.553259	0.143094
O	4.901142	0.362252	0.345902
C	4.272610	1.561478	0.700736
O	3.137518	-1.444545	1.707894
H	2.561480	-0.654588	1.616137
O	4.590429	-3.745299	1.466887
H	4.075905	-3.383728	2.217410
C	3.976582	-0.462232	-0.374889
H	4.425486	-0.745360	-1.356653
C	3.669669	-1.749404	0.418304
H	2.929704	-2.333921	-0.184537
C	4.908406	-2.610062	0.676201
H	5.317938	-2.975156	-0.290962
H	5.681002	-1.957656	1.153288
H	0.964654	0.544926	-1.303295
O	-0.028655	1.717790	-0.952260
C	-1.125523	1.311651	-0.472477
O	-1.535332	0.076961	-0.918058
O	-1.883663	1.904533	0.344689
C	-3.519264	0.682320	0.293364
H	-3.942622	1.297420	-0.507824
H	-3.681195	0.966853	1.334661
C	-2.598624	-0.492845	-0.089364
I	-6.137810	-0.299850	0.528450
C	-3.256754	-1.525581	-1.021484
C	-3.574868	-1.137300	-2.339406
C	-3.537525	-2.839786	-0.609117
C	-4.188280	-2.039837	-3.219438
C	-4.149423	-3.745586	-1.492381

C	-4.482431	-3.349203	-2.797376
H	-3.333070	-0.117585	-2.674746
H	-3.287115	-3.157492	0.412955
H	-4.439265	-1.718146	-4.243108
H	-4.370966	-4.769414	-1.150811
H	-4.967585	-4.058800	-3.487054
C	-1.955023	-1.129855	1.152312
C	-2.724057	-1.408127	2.302163
C	-0.592412	-1.497277	1.133062
C	-2.139628	-2.043414	3.411265
C	-0.009314	-2.127935	2.246588
C	-0.781716	-2.404768	3.388004
H	-3.793827	-1.148561	2.325804
H	0.021935	-1.276318	0.246317
H	-2.755645	-2.254999	4.300403
H	1.061053	-2.385372	2.218022
H	-0.322762	-2.898320	4.260126

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ACID-C SCF Done: -1499.89958812 A.U.

O	-3.506152	0.221758	2.478793
O	-1.825332	2.641916	1.384318
H	-1.256613	2.008266	1.916676
C	-3.586132	0.900909	1.323631
O	-2.970359	3.105108	-1.325352
C	-2.837667	1.940127	0.833998
O	-4.327001	1.343578	-0.860386
C	-3.317934	2.243508	-0.536373
O	-2.616521	-1.078845	-0.546122

H	-2.110273	-1.203197	0.307558
O	-4.206708	-2.786297	-1.876721
H	-3.243186	-2.666061	-1.712142
C	-4.464630	0.391781	0.207077
H	-5.540820	0.335444	0.497469
C	-4.002927	-1.021693	-0.234297
H	-4.237678	-1.699759	0.623416
C	-4.730125	-1.527281	-1.487190
H	-5.817841	-1.639882	-1.280242
H	-4.615477	-0.751230	-2.284974
H	-2.608340	-0.299424	2.445857
O	-0.156700	0.768096	2.346487
C	-0.381999	-0.333781	1.813813
O	-1.418587	-1.071653	1.902373
O	0.555975	-0.918940	0.951598
C	1.818316	-0.268311	0.618321
C	2.191991	-1.208036	-0.560180
H	1.452687	-1.070712	-1.369841
H	2.201363	-2.266362	-0.240196
I	4.172316	-0.856771	-1.536632
C	1.630246	1.153871	0.071012
C	0.415413	1.518943	-0.544672
C	2.693771	2.080584	0.082408
C	0.249563	2.798322	-1.098738
C	2.537707	3.353245	-0.492106
C	1.312893	3.717229	-1.076257
H	-0.429176	0.811348	-0.570826
H	3.653776	1.807004	0.544605
H	-0.732871	3.081501	-1.505621

H	3.379467	4.065116	-0.472181
H	1.179094	4.723858	-1.505092
C	2.744776	-0.376195	1.842165
C	2.742691	0.634910	2.829598
C	3.534853	-1.523376	2.065178
C	3.522174	0.507074	3.990403
C	4.316058	-1.653174	3.226190
C	4.316922	-0.634673	4.193762
H	2.097081	1.511229	2.688659
H	3.554737	-2.337658	1.326349
H	3.500157	1.307972	4.747186
H	4.928531	-2.557968	3.371142
H	4.929675	-0.733009	5.104862

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ACID-DminusI SCF Done: -1488.30670022 A.U.

O	2.363096	-0.856540	-1.733152
O	2.411566	2.344295	-1.964855
H	1.725213	1.900224	-2.526907
C	2.808959	0.121879	-0.910959
O	3.654044	3.158588	0.572301
C	2.828908	1.486304	-1.011657
O	3.811753	0.926013	1.038565
C	3.449524	2.020974	0.223055
O	1.425891	-0.086448	1.840086
H	1.938772	0.704271	2.122620
O	2.143328	-2.214657	3.444673
H	1.415135	-1.556842	3.442237
C	3.396979	-0.297567	0.408162

H	4.288193	-0.949593	0.250980
C	2.403059	-1.015970	1.348225
H	1.839064	-1.776756	0.770101
C	3.096960	-1.685610	2.543652
H	3.740369	-2.519496	2.186060
H	3.769874	-0.931806	3.029907
H	1.935512	-0.451483	-2.525559
O	0.488262	0.714381	-3.068633
C	-0.234432	0.422583	-2.121269
O	-0.796149	-0.781263	-1.965457
O	-0.517008	1.258722	-1.112824
C	-1.108934	0.512228	-0.023620
H	-1.983052	1.073176	0.355631
H	-0.329837	0.395492	0.757973
C	-1.492441	-0.868873	-0.663789
C	-2.985221	-1.010797	-0.966437
C	-3.665558	0.066615	-1.578158
C	-3.690242	-2.198962	-0.693710
C	-5.025056	-0.041725	-1.905059
C	-5.054799	-2.305439	-1.017301
C	-5.725134	-1.229481	-1.621579
H	-3.127728	1.000287	-1.811714
H	-3.168746	-3.046322	-0.224379
H	-5.541629	0.805149	-2.383330
H	-5.594839	-3.239430	-0.796112
H	-6.793786	-1.314109	-1.874192
C	-0.899329	-2.030220	0.121340
C	-1.148558	-2.118016	1.507990
C	-0.112177	-3.014943	-0.503167

C	-0.600175	-3.165058	2.261469
C	0.434097	-4.066590	0.256830
C	0.198513	-4.141087	1.638101
H	-1.769843	-1.355330	2.004650
H	0.097057	-2.940425	-1.578778
H	-0.781309	-3.215028	3.345980
H	1.062188	-4.823070	-0.239168
H	0.650206	-4.944803	2.238438

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ACID-D SCF Done: -1499.91247051 A.U.

O	2.037408	0.294648	-1.673248
O	2.339106	3.002564	0.056462
H	1.460693	2.853087	-0.371284
C	2.938531	0.719967	-0.759160
O	4.760644	2.490491	1.628650
C	3.058869	1.859004	-0.010194
O	4.833035	0.462459	0.587122
C	4.265439	1.713321	0.843005
O	2.625006	-1.084797	1.531135
H	1.685363	-0.975868	1.282261
O	3.705708	-3.573658	1.534776
H	3.085895	-3.100067	2.133211
C	3.995267	-0.257468	-0.322160
H	4.611456	-0.611457	-1.183127
C	3.361083	-1.480149	0.375977
H	2.695670	-1.964929	-0.378163
C	4.377390	-2.517494	0.863396
H	4.927628	-2.949919	0.000199

H	5.119461	-1.998448	1.518785
H	1.297497	0.962543	-1.732033
O	0.086350	2.050293	-1.203415
C	-0.857721	1.406113	-0.744481
O	-1.232568	0.223766	-1.250837
O	-1.608121	1.792090	0.281869
C	-2.731365	0.867168	0.410274
H	-3.611745	1.326749	-0.081973
H	-2.963288	0.710785	1.481199
C	-2.228850	-0.390247	-0.348625
I	-5.546810	0.012297	3.030650
C	-3.291571	-1.081232	-1.193378
C	-2.961188	-1.610287	-2.457754
C	-4.592090	-1.248876	-0.677512
C	-3.933455	-2.291911	-3.208300
C	-5.556700	-1.937808	-1.431914
C	-5.233491	-2.458722	-2.697017
H	-1.942696	-1.482192	-2.853934
H	-4.867155	-0.855294	0.320702
H	-3.671124	-2.697212	-4.198998
H	-6.568952	-2.061427	-1.015497
H	-5.993919	-2.996709	-3.286157
C	-1.511268	-1.415469	0.539279
C	-2.154350	-1.872959	1.707801
C	-0.276694	-1.981226	0.149538
C	-1.563157	-2.883514	2.482936
C	0.300706	-3.007151	0.924751
C	-0.340564	-3.456497	2.092442
H	-3.124637	-1.448249	2.026838

H	0.231223	-1.616074	-0.757886
H	-2.073905	-3.220276	3.398855
H	1.265971	-3.451624	0.633328
H	0.119108	-4.254592	2.697411

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EPO SCF Done: -615.477964856 A.U.

O	-2.528104	-0.321024	0.319821
C	-3.625236	0.500738	-0.142661
C	-3.856556	-0.757113	0.622387
H	-4.205495	-1.655673	0.075415
H	-4.155453	-0.694520	1.687833
C	-3.829342	0.505797	-1.640811
C	-3.178543	-0.460377	-2.438622
C	-4.669639	1.454130	-2.261458
C	-3.378511	-0.487220	-3.827823
C	-4.870770	1.423039	-3.652162
C	-4.228517	0.452049	-4.440050
H	-2.498297	-1.175909	-1.951226
H	-5.165152	2.225754	-1.652175
H	-2.860322	-1.243470	-4.439115
H	-5.530468	2.168995	-4.123535
H	-4.383393	0.431842	-5.530519
C	-3.771990	1.820658	0.572838
C	-5.009089	2.212986	1.121633
C	-2.665155	2.687794	0.668215
C	-5.141310	3.461821	1.754660
C	-2.794924	3.932130	1.305892
C	-4.033936	4.323092	1.847260

H	-5.872884	1.532066	1.049707
H	-1.699006	2.369928	0.246259
H	-6.111694	3.760864	2.182031
H	-1.924041	4.602563	1.382372
H	-4.134834	5.300094	2.346120

EPO-*cis*(Ph)₂

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ACID-AB SCF Done: -1311.40883780 A.U.

O	-1.599657	-1.030196	-1.865377
O	-0.528094	1.836633	-2.602756
H	0.139340	1.101150	-2.446987
C	-2.152648	0.181498	-1.724227
O	-2.783605	3.616175	-1.818007
C	-1.689259	1.435550	-2.034502
O	-3.810117	1.705840	-1.093197
C	-2.731588	2.413575	-1.674934
O	-5.009443	-0.018103	-2.865499
H	-4.977374	0.959488	-2.764469
O	-6.951674	-1.128368	-1.331124
H	-6.842838	-0.809534	-2.255650
C	-3.466449	0.308595	-1.002868
H	-3.314020	0.040180	0.070934
C	-4.621146	-0.518891	-1.581538
H	-4.264074	-1.559734	-1.741084
C	-5.856092	-0.529286	-0.662975
H	-5.640846	-1.106964	0.263555

H	-6.069692	0.527770	-0.353578
H	-0.587317	-0.905266	-1.838061
O	0.815359	-0.184873	-1.563530
C	0.940467	0.428446	-0.256785
H	1.011634	1.533997	-0.310439
C	2.230571	-0.247345	-0.507055
H	2.959918	0.334773	-1.085531
I	3.910558	1.234877	1.695640
C	-0.084544	0.018626	0.770964
C	-0.647030	1.013309	1.597184
C	-0.570817	-1.303108	0.871682
C	-1.665751	0.698509	2.511854
C	-1.586719	-1.621148	1.787074
C	-2.138929	-0.622465	2.609945
H	-0.284993	2.050088	1.510884
H	-0.165486	-2.083546	0.214010
H	-2.096764	1.491143	3.143673
H	-1.957446	-2.656881	1.849102
H	-2.943020	-0.872167	3.321126
C	2.556944	-1.655692	-0.182262
C	3.021176	-2.499330	-1.217090
C	2.415836	-2.181977	1.121924
C	3.325603	-3.845723	-0.959530
C	2.722361	-3.526942	1.376681
C	3.175079	-4.363894	0.339342
H	3.125109	-2.089506	-2.234112
H	2.103011	-1.511063	1.934014
H	3.683093	-4.493045	-1.776723
H	2.618085	-3.921678	2.399970

H	3.419346	-5.418769	0.545775
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ACID-A+I SCF Done: -1311.41755617 A.U.

O	0.401919	-0.318123	2.274390
O	0.171836	2.713456	1.288858
H	0.485451	2.044143	0.631353
C	0.179121	0.831543	2.929002
O	-0.088517	4.199958	3.798985
C	0.069215	2.132351	2.507570
O	-0.061892	2.168306	4.834478
C	-0.043226	2.992211	3.709994
O	-2.391471	0.534583	4.346853
H	-2.180800	0.888220	3.457469
O	-2.561460	-0.696462	6.772563
H	-3.247196	-0.330869	6.176300
C	0.043257	0.794525	4.429149
H	0.968339	0.358024	4.874139
C	-1.188008	-0.006663	4.888221
H	-1.033697	-1.059367	4.538013
C	-1.376003	-0.006882	6.407536
H	-0.518423	-0.522799	6.891946
H	-1.375800	1.057335	6.750285
H	0.814289	-0.093075	1.380771
O	1.542101	0.669641	0.116515
C	2.919136	1.160442	0.513856
H	3.098067	2.182657	0.132622
C	2.741649	0.155602	-0.556797
H	2.887885	0.577230	-1.573172

I	5.570589	1.934026	-2.227694
C	3.288495	0.964190	1.947064
C	3.152431	2.089298	2.793839
C	3.679364	-0.269774	2.511526
C	3.382680	1.985609	4.174303
C	3.919691	-0.370909	3.891225
C	3.765450	0.750593	4.727040
H	2.825774	3.049137	2.363314
H	3.794761	-1.154987	1.872743
H	3.242010	2.867371	4.818120
H	4.226817	-1.339322	4.317335
H	3.944881	0.662330	5.810849
C	3.027612	-1.307974	-0.447093
C	2.054793	-2.232903	-0.017354
C	4.315437	-1.762193	-0.813053
C	2.372975	-3.598689	0.079113
C	4.624518	-3.128275	-0.713587
C	3.660036	-4.049597	-0.262599
H	1.045884	-1.886357	0.251039
H	5.065476	-1.031407	-1.163934
H	1.607979	-4.312914	0.424164
H	5.632620	-3.476019	-0.991533
H	3.910350	-5.119992	-0.182407

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ACID-A SCF Done: -1299.81342703 A.U.

O	-2.448182	-0.911978	-0.372015
O	-1.586973	2.067783	-1.108615
H	-0.932820	1.346932	-1.229155

C	-3.119338	0.257667	-0.335740
O	-3.905668	3.650757	-0.286135
C	-2.754075	1.534053	-0.659409
O	-4.913900	1.658532	0.188481
C	-3.861695	2.440826	-0.272424
O	-5.454129	0.099505	-2.163313
H	-4.518355	0.242368	-2.408726
O	-7.774302	-1.143517	-1.359129
H	-7.538129	-0.773684	-2.234211
C	-4.557496	0.268939	0.112387
H	-4.643051	-0.179091	1.129108
C	-5.488533	-0.480069	-0.864248
H	-5.144289	-1.546137	-0.884861
C	-6.958228	-0.447427	-0.435471
H	-7.068416	-0.942760	0.553583
H	-7.253320	0.624400	-0.316332
H	-1.471336	-0.710080	-0.333141
O	0.094124	0.014085	-0.155077
C	0.268898	0.876470	1.047685
C	1.072412	-0.363040	0.844167
H	0.785307	1.816210	0.777622
H	2.114223	-0.201066	0.496161
C	-0.914073	1.091699	1.928777
C	-1.659901	0.048753	2.524297
C	-1.375164	2.422369	2.055581
H	-1.340460	-0.995573	2.419735
H	-0.829790	3.236487	1.553737
C	-2.845255	0.340262	3.216811
C	-2.565812	2.708491	2.738444

H	-3.422452	-0.481516	3.669252
H	-2.935711	3.743614	2.779613
C	-3.308778	1.664629	3.314901
H	-4.257487	1.882263	3.829404
C	0.864137	-1.648121	1.584956
C	0.176482	-2.726617	0.993493
C	1.380799	-1.780542	2.890752
C	-0.010771	-3.919850	1.711471
C	1.193981	-2.975264	3.604367
C	0.494434	-4.045779	3.017611
H	-0.225872	-2.628476	-0.026057
H	1.911202	-0.934294	3.356272
H	-0.556684	-4.755647	1.246581
H	1.588976	-3.068197	4.628206
H	0.342653	-4.980151	3.580393

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ACID-B+CO2 SCF Done: -1499.89785485 A.U.

O	0.618751	-1.360402	-0.232657
O	0.416560	1.517648	-1.528169
H	-0.376259	1.107944	-1.020901
C	1.533505	-0.584957	-0.811884
O	3.221914	2.074005	-2.337908
C	1.467475	0.681786	-1.349180
O	3.701692	0.015692	-1.476799
C	2.822219	1.066245	-1.787649
O	3.322453	0.094795	1.400137
H	2.370982	0.327681	1.413163
O	5.364601	-1.487332	2.163054

H	4.896490	-0.711194	2.540727
C	2.982160	-1.003834	-0.774731
H	3.141997	-1.983277	-1.287450
C	3.475673	-1.126391	0.684380
H	2.872133	-1.944238	1.154215
C	4.963067	-1.466058	0.800352
H	5.157945	-2.469415	0.361289
H	5.530891	-0.712842	0.199298
H	-0.285306	-0.787972	-0.174024
O	-1.336483	0.179837	-0.201752
C	-2.555564	-0.258117	-0.739149
H	-3.079352	0.585120	-1.261657
C	-3.377991	-0.532656	0.530594
H	-3.516387	0.441437	1.031095
I	-5.709997	-0.852312	0.031167
O	-1.750109	1.559300	2.371057
O	0.412952	0.762067	1.926555
C	-0.694259	1.130731	2.077650
C	-2.354255	-1.343910	-1.810431
C	-1.398364	-1.055797	-2.812430
C	-3.018810	-2.585825	-1.860010
C	-1.122918	-1.974862	-3.835284
C	-2.741933	-3.510617	-2.884531
C	-1.795074	-3.210537	-3.877399
H	-0.850355	-0.101187	-2.772146
H	-3.757746	-2.848544	-1.090479
H	-0.367949	-1.725721	-4.598533
H	-3.271760	-4.477461	-2.898460
H	-1.576303	-3.937636	-4.676726

C	-2.919716	-1.546723	1.532579
C	-3.403083	-1.446374	2.861432
C	-1.964892	-2.549663	1.244469
C	-2.970968	-2.328096	3.860531
C	-1.522262	-3.425459	2.249556
C	-2.025881	-3.327275	3.557281
H	-4.137142	-0.660285	3.101374
H	-1.528081	-2.629093	0.241481
H	-3.365022	-2.230211	4.885220
H	-0.761279	-4.182601	2.002638
H	-1.674987	-4.016891	4.342208

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ACID-BC SCF Done: -1499.89979315 A.U.

O	-0.032454	-2.094271	-2.945168
O	0.539492	0.757847	-1.707762
H	-0.312826	0.217401	-1.480826
C	1.036926	-1.291457	-3.010133
O	3.308048	1.342219	-2.630103
C	1.302371	-0.055760	-2.457451
O	3.227413	-0.714581	-3.614013
C	2.674706	0.329825	-2.854141
O	3.149304	-2.739327	-1.557790
H	2.423575	-2.189845	-1.189681
O	4.668477	-4.635251	-2.724443
H	4.546788	-4.319048	-1.803985
C	2.295598	-1.801728	-3.665193
H	2.120666	-2.083732	-4.731754
C	2.850265	-3.034210	-2.917621

H	2.061783	-3.827527	-2.990416
C	4.157997	-3.565452	-3.508754
H	3.981473	-3.945718	-4.539193
H	4.872020	-2.707188	-3.575257
H	-0.779960	-1.592668	-2.385135
O	-1.476745	-0.788628	-1.400191
C	-2.734710	-0.226829	-1.543972
H	-2.737444	0.677468	-2.210541
C	-2.990837	0.298339	-0.093219
H	-2.221864	1.069774	0.099745
I	-4.904160	1.638325	0.083220
O	-0.949126	-3.542202	-0.054072
O	0.757990	-1.935886	0.112200
C	-0.125025	-2.706363	-0.003084
C	-3.780895	-1.197752	-2.089043
C	-4.914624	-0.735554	-2.789686
C	-3.618181	-2.586549	-1.904789
C	-5.882292	-1.636499	-3.266519
C	-4.582814	-3.489553	-2.382719
C	-5.722496	-3.018989	-3.059624
H	-5.039302	0.345576	-2.961506
H	-2.724087	-2.945900	-1.378446
H	-6.763443	-1.256707	-3.809737
H	-4.439662	-4.571396	-2.225975
H	-6.478757	-3.727468	-3.436426
C	-2.973678	-0.742955	0.987344
C	-3.978698	-1.727720	1.115646
C	-1.855663	-0.799626	1.850079
C	-3.856298	-2.750419	2.068401

C	-1.732923	-1.824231	2.803210
C	-2.732076	-2.806951	2.912018
H	-4.861656	-1.682573	0.462061
H	-1.054837	-0.052002	1.738714
H	-4.645188	-3.515787	2.147258
H	-0.844129	-1.860306	3.453687
H	-2.635950	-3.616215	3.653958

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ACID-B SCF Done: -1311.42943336 A.U.

O	1.913690	-1.276630	-0.169310
O	0.516612	0.454487	2.060425
H	0.118336	-0.405227	1.732065
C	2.207421	-0.090150	0.313938
O	2.424496	2.709536	2.425469
C	1.640591	0.681577	1.309973
O	3.624331	1.752129	0.731993
C	2.515889	1.815542	1.602395
O	4.552128	-1.415418	0.724564
H	3.675221	-1.821958	0.511082
O	7.058923	-0.631601	0.076086
H	6.654469	-1.415524	0.507103
C	3.459768	0.635413	-0.155908
H	3.314871	1.042419	-1.186213
C	4.673242	-0.330252	-0.195874
H	4.728732	-0.728815	-1.241652
C	6.012727	0.331465	0.128500
H	6.232825	1.136705	-0.605928
H	5.922237	0.810960	1.133202

H	0.713554	-1.649474	0.358218
O	-0.316711	-1.754183	0.742381
C	-1.141734	-1.513075	-0.376489
H	-0.510514	-1.355289	-1.283034
C	-1.861772	-0.156279	-0.080503
H	-1.070453	0.576809	0.161763
I	-2.694224	0.800840	-2.032991
C	-2.082484	-2.686235	-0.625152
C	-2.615730	-2.952688	-1.902827
C	-2.454993	-3.514322	0.454062
H	-2.314992	-2.325180	-2.756189
H	-2.006921	-3.310347	1.437560
C	-3.533894	-4.001200	-2.090468
C	-3.369076	-4.563803	0.268552
H	-3.945289	-4.194329	-3.094913
H	-3.656873	-5.196414	1.124403
C	-3.919979	-4.806127	-1.003391
H	-4.639877	-5.628169	-1.150308
C	-2.919713	-0.166726	0.983092
C	-4.145018	-0.860681	0.832317
C	-2.656498	0.490725	2.207667
C	-5.076023	-0.900232	1.879543
C	-3.590736	0.443410	3.257173
C	-4.802006	-0.250750	3.098523
H	-4.371023	-1.356035	-0.123282
H	-1.696135	1.014444	2.341538
H	-6.024764	-1.444036	1.742369
H	-3.364020	0.955259	4.206392
H	-5.535610	-0.283768	3.920851

ACID-CD SCF Done: -1499.88017090 A.U.

O	2.266464	-0.790016	-0.402151
O	2.576247	2.059342	1.077096
H	1.718197	1.554721	1.201884
C	3.247221	0.120454	-0.352414
O	5.254950	2.919230	0.250016
C	3.396870	1.326838	0.298933
O	5.375543	0.949079	-0.891482
C	4.729684	1.871126	-0.060764
O	5.476896	-1.238466	0.980693
H	4.740589	-0.694124	1.333059
O	7.197113	-2.866388	-0.351267
H	7.089948	-2.645809	0.597356
C	4.548578	-0.211470	-1.043240
H	4.390489	-0.408970	-2.130130
C	5.224528	-1.445051	-0.407037
H	4.524816	-2.306254	-0.558620
C	6.582787	-1.779330	-1.028215
H	6.448890	-2.071842	-2.092882
H	7.206093	-0.851457	-1.001299
H	1.482735	-0.468809	0.163692
O	0.529369	0.383234	1.104099
C	-0.728929	0.462759	1.071995
O	-1.373503	-0.540659	0.393863
O	-1.452995	1.359666	1.596969
C	-3.289566	0.952548	0.590704
H	-2.887377	1.577273	-0.217802

C	-2.820627	-0.508892	0.535771
H	-3.178472	-0.943966	-0.413263
I	-5.503561	0.626775	-1.341285
C	-3.266411	-1.403583	1.679103
C	-4.213503	-2.416180	1.428157
C	-2.778565	-1.225114	2.992022
H	-4.608072	-2.540003	0.406704
H	-2.070289	-0.410237	3.200812
C	-4.677379	-3.234557	2.473156
C	-3.234914	-2.048927	4.032340
H	-5.424746	-4.016941	2.264652
H	-2.852456	-1.896901	5.054450
C	-4.187711	-3.053354	3.778175
H	-4.549100	-3.693749	4.599156
C	-4.127122	1.633476	1.591379
C	-5.076982	0.986417	2.419428
C	-3.938081	3.030526	1.747617
C	-5.802566	1.713548	3.372281
C	-4.661942	3.753307	2.703865
C	-5.598752	3.097530	3.523993
H	-5.282832	-0.082268	2.282758
H	-3.189705	3.539197	1.121190
H	-6.546473	1.192602	3.995990
H	-4.492293	4.836585	2.812122
H	-6.173610	3.664812	4.273862

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ACID-C SCF Done: -1499.91396740 A.U.

O	-3.352208	1.791211	0.049953
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O	-0.564065	2.342956	-1.321749
H	-0.590931	2.496323	-0.325735
C	-2.800946	1.296472	-1.071697
O	-0.552471	0.506849	-3.634036
C	-1.580745	1.517417	-1.653973
O	-2.607640	-0.161388	-2.904787
C	-1.454254	0.622238	-2.830208
O	-2.464432	-1.452028	-0.194918
H	-2.238512	-0.820321	0.550169
O	-4.150691	-3.424589	-0.697316
H	-3.357489	-3.246866	-0.140110
C	-3.467449	0.151889	-1.797591
H	-4.470899	0.434810	-2.199262
C	-3.660060	-1.058192	-0.849876
H	-4.430982	-0.742108	-0.103580
C	-4.142461	-2.318459	-1.584231
H	-5.171070	-2.161981	-1.979401
H	-3.464702	-2.481111	-2.459549
H	-2.779784	1.428496	0.833286
O	-0.337298	2.159382	1.283869
C	-0.665532	0.981592	1.545588
O	-1.838500	0.487301	1.619076
O	0.327325	0.029410	1.781045
C	1.687690	0.435758	1.540798
H	1.797813	1.508290	1.803485
C	1.902789	0.296132	-0.001917
H	1.165353	0.956910	-0.500423
I	3.842019	1.338896	-0.601656
C	2.587958	-0.431531	2.395280

C	2.266820	-1.787013	2.624721
C	3.775603	0.091943	2.944387
H	1.333676	-2.189171	2.204768
H	4.025870	1.151118	2.774954
C	3.126363	-2.603142	3.377636
C	4.639807	-0.726312	3.692659
H	2.864796	-3.660572	3.545058
H	5.566623	-0.302856	4.112912
C	4.318414	-2.078074	3.909153
H	4.994345	-2.720882	4.496824
C	1.791809	-1.113497	-0.510060
C	2.832446	-2.067453	-0.455017
C	0.506587	-1.532664	-0.915825
C	2.590075	-3.404091	-0.808231
C	0.255979	-2.875429	-1.238325
C	1.299756	-3.814846	-1.194974
H	3.837834	-1.754105	-0.135766
H	-0.331880	-0.824422	-0.931708
H	3.415291	-4.133909	-0.769085
H	-0.770413	-3.165468	-1.510402
H	1.110991	-4.867939	-1.461231

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ACID-DminusI SCF Done: -1488.29787927 A.U.

O	0.289508	-0.711603	2.104197
O	-0.882165	1.895153	0.715944
H	-0.765208	1.911034	1.687934
C	0.241926	-0.329594	0.819600
O	-0.782129	1.223744	-2.118953

C	-0.249029	0.793310	0.214279
O	0.425176	-0.611925	-1.497264
C	-0.245311	0.569785	-1.244382
O	2.980005	-0.041689	-0.315745
H	2.650154	0.541123	0.394906
O	4.374273	-2.262468	-1.163086
H	4.671643	-1.332948	-1.084682
C	0.827852	-1.215222	-0.252574
H	0.382591	-2.234737	-0.192779
C	2.367117	-1.318435	-0.173142
H	2.612111	-1.783488	0.815195
C	2.967190	-2.186393	-1.283895
H	2.562952	-3.218754	-1.208466
H	2.636353	-1.761519	-2.263914
H	-0.488296	-0.308436	2.595879
O	-1.995685	0.439528	3.032365
C	-2.799549	0.465628	2.108690
O	-2.792419	-0.393693	1.077262
O	-3.780392	1.383026	1.995461
C	-4.545069	1.117230	0.783386
H	-4.687847	2.088334	0.269587
C	-3.526452	0.241381	-0.024822
H	-2.808861	0.928756	-0.519835
C	-4.022739	-0.771879	-1.011829
C	-3.714686	-0.591796	-2.376752
C	-4.777516	-1.894504	-0.606126
H	-3.071955	0.250300	-2.682815
H	-5.000361	-2.048258	0.460146
C	-4.189374	-1.507687	-3.331670

C	-5.239848	-2.811013	-1.561480
H	-3.943515	-1.363017	-4.395265
H	-5.827834	-3.684951	-1.239954
C	-4.955367	-2.614032	-2.926280
H	-5.322569	-3.334500	-3.674481
C	-5.878017	0.475501	1.096889
C	-6.871557	0.464047	0.095833
C	-6.120651	-0.176627	2.321211
C	-8.084601	-0.208029	0.308393
C	-7.337551	-0.848115	2.533415
C	-8.318781	-0.870093	1.527303
H	-6.681885	0.964809	-0.867366
H	-5.360237	-0.153105	3.116129
H	-8.850280	-0.217348	-0.482926
H	-7.519775	-1.354792	3.494181
H	-9.270474	-1.398395	1.695057

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ACID-D SCF Done: -1499.92916450 A.U.

O	2.055982	-0.004792	-1.446322
O	1.711651	2.920883	-0.130376
H	1.064735	2.666438	-0.840554
C	2.652755	0.623980	-0.413465
O	3.553166	2.814525	2.143739
C	2.506685	1.861124	0.152766
O	4.177947	0.766105	1.355354
C	3.418703	1.934266	1.320267
O	2.152182	-0.961454	2.146258
H	1.306348	-0.612708	1.795871

O	3.373491	-3.321366	2.486213
H	2.645678	-2.849423	2.949351
C	3.665068	-0.154125	0.387150
H	4.498846	-0.512883	-0.261831
C	3.023100	-1.367386	1.103430
H	2.487340	-1.957145	0.318954
C	4.043260	-2.284895	1.785503
H	4.705620	-2.751104	1.024738
H	4.678280	-1.657694	2.459923
H	1.325692	0.569281	-1.816227
O	-0.004961	1.675767	-1.856742
C	-0.876425	1.136602	-1.162741
O	-1.173211	-0.157235	-1.258987
O	-1.574045	1.771544	-0.226465
C	-2.221591	0.785850	0.645570
H	-3.289103	1.074992	0.774938
C	-2.169764	-0.517773	-0.242622
H	-3.156894	-0.636590	-0.740968
I	-5.918780	-0.132633	0.721581
C	-1.748798	-1.788740	0.450561
C	-2.726238	-2.588310	1.076485
C	-0.387455	-2.141375	0.549496
H	-3.791125	-2.309215	0.990329
H	0.362690	-1.542967	0.006315
C	-2.333202	-3.710359	1.824445
C	0.002348	-3.264183	1.299733
H	-3.101901	-4.325191	2.319776
H	1.069170	-3.523891	1.395247
C	-0.972364	-4.043986	1.947510

H	-0.667272	-4.919194	2.543867
C	-1.497430	0.724292	1.970323
C	-2.093333	0.003878	3.028241
C	-0.246033	1.344587	2.167938
C	-1.415134	-0.131175	4.249393
C	0.421451	1.221930	3.401565
C	-0.154311	0.467219	4.436826
H	-3.089726	-0.444147	2.883660
H	0.200328	1.966851	1.379283
H	-1.880357	-0.707244	5.065289
H	1.398260	1.713317	3.531707
H	0.375274	0.353901	5.396270

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EPO SCF Done: -615.480898818 A.U.

O	0.141575	-0.204545	-0.378112
C	0.137781	0.817630	0.625760
C	1.078936	-0.351363	0.695765
H	0.582689	1.782467	0.301540
H	2.133955	-0.144514	0.416625
C	-1.056783	0.943570	1.516470
C	-2.219282	0.177847	1.297892
C	-1.017923	1.845821	2.601167
H	-2.248347	-0.504464	0.435945
H	-0.114063	2.454019	2.772207
C	-3.321909	0.302480	2.159882
C	-2.118286	1.966106	3.464568
H	-4.227163	-0.298895	1.979212
H	-2.075490	2.668258	4.312443

C	-3.273581	1.192316	3.247027
H	-4.137732	1.287640	3.923502
C	0.893917	-1.476622	1.662735
C	-0.112167	-2.446045	1.479105
C	1.742352	-1.566570	2.787151
C	-0.276313	-3.482132	2.413884
C	1.574482	-2.599437	3.722955
C	0.562125	-3.559745	3.539544
H	-0.751849	-2.381282	0.587151
H	2.537609	-0.816279	2.931386
H	-1.064320	-4.236556	2.260081
H	2.237963	-2.657084	4.600574
H	0.431241	-4.371423	4.272697

EPO-*trans*(Ph)₂

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ACID-AB SCF Done: -1311.41518489 A.U.

O	-1.073715	-0.554403	1.084763
O	-0.570056	2.574677	1.290159
H	-0.061327	2.042773	0.610889
C	-1.453006	0.350315	1.987574
O	-1.857493	3.278650	3.851734
C	-1.233970	1.703071	2.089738
O	-2.421347	1.066761	3.997106
C	-1.824997	2.174224	3.349621
O	-4.476278	0.046500	2.462776
H	-4.351738	0.873366	2.979490

O	-5.362091	-1.979244	4.032883
H	-5.743553	-1.289356	3.444055
C	-2.163048	-0.122958	3.225997
H	-1.468893	-0.781767	3.801706
C	-3.491565	-0.852537	2.984370
H	-3.330290	-1.630945	2.207022
C	-4.048565	-1.503303	4.263452
H	-3.406386	-2.358540	4.571322
H	-4.007559	-0.742868	5.087425
H	-0.308346	-0.143727	0.533803
O	0.860917	0.757932	0.015944
C	2.051713	0.667227	0.846928
H	2.523433	1.661173	0.996577
C	2.392521	-0.001991	-0.415895
H	2.158167	-1.071101	-0.500637
I	5.177867	-1.444087	0.182664
C	1.851715	-0.038853	2.162546
C	1.460449	0.747779	3.267706
C	1.922751	-1.438244	2.307904
C	1.136921	0.149950	4.497009
C	1.604153	-2.037670	3.537266
C	1.205754	-1.248165	4.632174
H	1.377095	1.840200	3.148430
H	2.263443	-2.061134	1.468007
H	0.812384	0.777843	5.341650
H	1.675769	-3.132018	3.641353
H	0.953346	-1.723185	5.594354
C	2.927600	0.677167	-1.608211
C	3.120349	2.077691	-1.655772

C	3.200825	-0.083936	-2.769320
C	3.592876	2.693480	-2.823900
C	3.670927	0.531859	-3.935982
C	3.873709	1.924874	-3.968123
H	2.888387	2.693921	-0.774311
H	3.074626	-1.176694	-2.730523
H	3.741760	3.785173	-2.841223
H	3.892165	-0.080319	-4.824869
H	4.249685	2.410188	-4.883335

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ACID-A+I SCF Done: -1311.42423826 A.U.

O	-0.507497	-1.197484	-0.075815
O	-0.746202	1.733834	-1.349711
H	0.083411	1.219529	-1.516348
C	-1.373961	-0.192185	0.111733
O	-2.959924	2.916728	0.161826
C	-1.488918	1.061765	-0.433895
O	-3.148016	0.890566	1.191140
C	-2.580707	1.769592	0.273726
O	-4.069244	-1.218923	-0.539406
H	-3.376256	-0.858132	-1.129594
O	-5.528032	-2.652626	1.259321
H	-5.673313	-2.436677	0.314994
C	-2.476721	-0.378220	1.122737
H	-2.031247	-0.604233	2.119558
C	-3.459762	-1.493414	0.721249
H	-2.869446	-2.443967	0.682688
C	-4.617233	-1.661670	1.708436

H	-4.222347	-1.982070	2.696980
H	-5.100938	-0.661830	1.838407
H	0.347392	-0.825719	-0.448880
O	1.497378	0.347114	-0.880573
C	1.896101	1.201033	0.272321
H	1.811146	2.272502	0.007221
C	2.914368	0.421420	-0.477179
H	3.298894	-0.517457	-0.021847
I	4.912732	-2.589424	1.083230
C	1.306796	0.844240	1.593999
C	0.304857	1.692575	2.118949
C	1.642572	-0.344250	2.277065
C	-0.360052	1.359696	3.309401
C	0.977730	-0.672284	3.470154
C	-0.023276	0.171858	3.985699
H	0.020037	2.603429	1.567015
H	2.429132	-1.018900	1.893236
H	-1.156606	2.015928	3.692927
H	1.250875	-1.600498	3.996224
H	-0.545221	-0.096444	4.918872
C	3.838140	1.075964	-1.450772
C	5.196726	0.694152	-1.456389
C	3.384779	2.064380	-2.351987
C	6.092769	1.314535	-2.344143
C	4.283602	2.676212	-3.239667
C	5.641967	2.305407	-3.234408
H	5.533920	-0.099825	-0.766943
H	2.318130	2.341830	-2.366741
H	7.151836	1.010107	-2.344482

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ACID-A SCF Done: -1299.81650968 A.U.

H	3.921869	3.444020	-3.942753
H	6.347239	2.785952	-3.932114
O	-0.587713	-2.635699	-1.853052
O	0.883537	0.012462	-2.838803
H	1.266585	-0.462603	-2.063876
C	-1.002480	-1.598346	-2.614031
O	-1.263830	1.496291	-4.195400
C	-0.375171	-0.460182	-3.037869
O	-2.574108	-0.324918	-3.779503
C	-1.377718	0.378983	-3.743090
O	-1.819971	-2.672180	-5.264696
H	-0.895855	-2.656490	-4.948482
O	-4.308188	-3.806938	-5.594018
H	-3.553232	-3.762624	-6.215933
C	-2.413456	-1.600692	-3.138286
H	-3.132570	-1.668385	-2.289070
C	-2.680024	-2.749323	-4.132936
H	-2.531036	-3.706011	-3.570227
C	-4.103394	-2.731727	-4.697124
H	-4.833326	-2.838210	-3.865765
H	-4.268903	-1.732464	-5.170717
H	0.087740	-2.299209	-1.211269
O	0.814065	-0.910544	-0.288192
C	-0.168312	0.139263	0.030645
C	0.922463	-0.209067	0.986551
H	-0.007867	1.053371	-0.571231

H	0.642241	-0.836226	1.854683
C	-1.593915	-0.275517	0.151302
C	-1.968248	-1.496443	0.751950
C	-2.587000	0.547831	-0.421214
H	-1.197664	-2.167949	1.162138
H	-2.294489	1.478442	-0.933496
C	-3.318431	-1.876775	0.794617
C	-3.937835	0.168173	-0.375788
H	-3.602030	-2.834583	1.257955
H	-4.700959	0.811504	-0.839685
C	-4.306022	-1.044534	0.234836
H	-5.363958	-1.349180	0.263337
C	2.120341	0.659558	1.179595
C	2.666506	0.812788	2.470612
C	2.706530	1.346819	0.092567
C	3.775440	1.650490	2.678063
C	3.817609	2.177341	0.301513
C	4.353205	2.333448	1.593986
H	2.218810	0.272154	3.320690
H	2.294305	1.229806	-0.922545
H	4.193301	1.764989	3.690558
H	4.268587	2.707617	-0.551748
H	5.224916	2.987130	1.754542

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ACID-B+CO2 SCF Done: -1499.90089831 A.U.

O	1.511076	-1.184095	-0.937572
O	0.937227	1.926992	-0.945507
H	0.194665	1.231846	-0.768119

C	2.328474	-0.123772	-0.965053
O	3.668956	3.107157	-0.997514
C	2.090573	1.234204	-0.946147
O	4.412082	0.950225	-0.953193
C	3.398865	1.922626	-0.964464
O	3.764337	-0.160211	1.617590
H	2.823915	0.094528	1.497232
O	5.924544	-1.708128	2.034094
H	5.330753	-1.171457	2.602062
C	3.813897	-0.345698	-0.835119
H	4.206149	-1.005653	-1.646510
C	4.161595	-0.984396	0.528980
H	3.634760	-1.973289	0.558038
C	5.662253	-1.206795	0.730634
H	6.038807	-1.947000	-0.009556
H	6.177248	-0.232970	0.536455
H	0.520569	-0.829391	-0.902218
O	-0.661679	-0.028727	-0.569859
C	-1.927747	-0.001262	-1.139719
H	-2.058327	0.861030	-1.847831
C	-2.865264	0.202126	0.080123
H	-2.990078	-0.756688	0.620089
I	-5.084590	0.578626	-0.620583
O	-0.720005	-1.572462	1.888547
O	0.803837	0.215173	1.836129
C	0.017154	-0.659388	1.782738
C	-2.254205	-1.285319	-1.901772
C	-2.932772	-1.268541	-3.135371
C	-1.859379	-2.526050	-1.357682

C	-3.223890	-2.466802	-3.811142
C	-2.151516	-3.724607	-2.028257
C	-2.836791	-3.699964	-3.257647
H	-3.239592	-0.301862	-3.566746
H	-1.307321	-2.534205	-0.404758
H	-3.754722	-2.436495	-4.777008
H	-1.835470	-4.686481	-1.591889
H	-3.061920	-4.640628	-3.786809
C	-2.473496	1.297429	1.021895
C	-2.653207	1.114449	2.411986
C	-1.850636	2.483935	0.572804
C	-2.217272	2.083706	3.329546
C	-1.404535	3.447150	1.487037
C	-1.586522	3.252957	2.868985
H	-3.124910	0.185937	2.772753
H	-1.680999	2.643770	-0.501667
H	-2.356983	1.917710	4.410164
H	-0.884875	4.343968	1.115715
H	-1.223393	4.006624	3.586282

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ACID-BC SCF Done: -1499.90617854 A.U.

O	1.630688	-0.152054	-1.159499
O	0.245788	-0.429406	1.662812
H	-0.245854	-0.707473	0.805123
C	1.914791	0.389480	0.017251
O	1.853646	1.403780	3.365941
C	1.334028	0.274672	1.261104
O	3.148599	1.715567	1.511625

C	2.065083	1.138931	2.196818
O	4.470877	-0.775019	0.745794
H	3.647242	-1.291811	0.620279
O	6.839894	0.240422	-0.053300
H	6.544016	-0.595694	0.367081
C	3.161111	1.224134	0.165578
H	3.148509	2.091842	-0.537094
C	4.416694	0.367846	-0.104734
H	4.364872	0.063043	-1.181224
C	5.731698	1.107781	0.145769
H	5.824891	1.962386	-0.560118
H	5.694700	1.522788	1.183489
H	0.665891	-0.649327	-1.043810
O	-0.558134	-1.168063	-0.660545
C	-1.639731	-0.775059	-1.444945
H	-1.318135	-0.386290	-2.446902
C	-2.287057	0.394727	-0.654514
H	-2.765476	-0.005915	0.261184
I	-4.196752	1.258821	-1.763645
O	-0.111404	-3.476803	1.479064
O	1.924486	-2.697513	0.601540
C	0.883855	-3.032511	1.039148
C	-2.603316	-1.939884	-1.681108
C	-3.276610	-2.123114	-2.904741
C	-2.810249	-2.874343	-0.645183
C	-4.157973	-3.203474	-3.086031
C	-3.695567	-3.950703	-0.819881
C	-4.376306	-4.118194	-2.040502
H	-3.109457	-1.406678	-3.725415

H	-2.240137	-2.758647	0.289290
H	-4.677128	-3.331628	-4.050354
H	-3.847352	-4.671769	0.000423
H	-5.067660	-4.965797	-2.180004
C	-1.385094	1.546141	-0.339191
C	-1.323776	2.040114	0.983431
C	-0.536134	2.117200	-1.313968
C	-0.418001	3.052524	1.332693
C	0.356458	3.141451	-0.970458
C	0.427448	3.605606	0.356189
H	-1.952057	1.578229	1.760346
H	-0.562844	1.738155	-2.346313
H	-0.332991	3.370359	2.382679
H	1.025795	3.560176	-1.739144
H	1.163389	4.375561	0.636181

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ACID-B SCF Done: -1311.42710948 A.U.

O	1.662685	-1.286648	0.284853
O	0.903294	1.046798	2.250741
H	0.190829	0.392582	1.999479
C	2.144562	-0.072316	0.406642
O	2.893690	3.153151	1.582940
C	1.854943	0.961810	1.281312
O	3.715073	1.658462	0.061735
C	2.802983	2.051068	1.063987
O	4.401904	-1.560667	0.616788
H	3.464625	-1.878761	0.672752
O	6.789553	-1.172437	-0.589242

H	6.422192	-1.812802	0.057967
C	3.301031	0.387057	-0.467610
H	2.954505	0.562069	-1.515428
C	4.419802	-0.688751	-0.513164
H	4.255910	-1.283055	-1.449228
C	5.836662	-0.116049	-0.563128
H	5.969882	0.506701	-1.474462
H	5.965163	0.554229	0.321092
H	0.386119	-1.247445	0.916950
O	-0.607116	-0.967613	1.224369
C	-1.306107	-0.830199	-0.006584
H	-0.595980	-0.531057	-0.814206
C	-2.294542	0.325925	0.207849
H	-3.047857	0.064269	0.976210
I	-3.653176	0.543034	-1.696981
C	-1.878223	-2.192722	-0.387218
C	-1.047103	-3.069858	-1.115553
C	-3.131623	-2.660058	0.055340
H	-0.044655	-2.718793	-1.412756
H	-3.793252	-1.995685	0.633097
C	-1.468608	-4.375302	-1.418019
C	-3.558322	-3.964008	-0.247156
H	-0.806296	-5.046406	-1.989266
H	-4.547130	-4.309258	0.097281
C	-2.730421	-4.825844	-0.989632
H	-3.066850	-5.847982	-1.229277
C	-1.650358	1.638652	0.506678
C	-2.034424	2.360835	1.659213
C	-0.606665	2.151962	-0.299869

C	-1.351049	3.526889	2.032941
C	0.067434	3.321223	0.069220
C	-0.282738	3.997383	1.250421
H	-2.850578	1.971442	2.290481
H	-0.310178	1.612641	-1.212494
H	-1.631750	4.052875	2.959573
H	0.911572	3.683004	-0.536524
H	0.298202	4.876768	1.565902

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ACID-CD SCF Done: -1499.89487559 A.U.

O	2.162742	-0.703347	1.100805
O	1.611737	2.450140	1.199956
H	1.138885	1.864260	1.860420
C	2.506841	0.305146	0.295583
O	2.926169	3.407156	-1.256794
C	2.267929	1.660168	0.325720
O	3.510970	1.225849	-1.611801
C	2.887790	2.259780	-0.865093
O	5.545626	0.198352	-0.042921
H	5.412557	1.057017	-0.502165
O	6.629364	-1.639371	-1.718723
H	6.940453	-0.984650	-1.053450
C	3.286589	-0.029316	-0.946635
H	2.675809	-0.688392	-1.611645
C	4.645072	-0.704089	-0.691943
H	4.489771	-1.552646	0.009410
C	5.306244	-1.211999	-1.986021
H	4.731514	-2.069238	-2.402849

H	5.268286	-0.385790	-2.744172
H	1.485958	-0.364912	1.788291
O	0.386211	0.490883	2.539229
C	-0.747175	0.391382	1.987126
O	-1.050588	-0.818428	1.428654
O	-1.611982	1.316066	1.868112
C	-2.636884	0.590078	0.253493
H	-3.538392	1.115292	0.585539
C	-2.362777	-0.819293	0.770987
H	-2.227755	-1.507011	-0.084916
I	-4.765943	-0.404932	-1.677625
C	-3.420421	-1.379473	1.705689
C	-3.996542	-2.634997	1.431258
C	-3.824126	-0.678414	2.862594
H	-3.705939	-3.170227	0.513644
H	-3.379624	0.304644	3.078490
C	-4.957134	-3.186694	2.294410
C	-4.783749	-1.230525	3.727121
H	-5.405936	-4.165052	2.058861
H	-5.092087	-0.672074	4.625907
C	-5.353337	-2.485564	3.446778
H	-6.110275	-2.914469	4.123614
C	-1.793379	1.218642	-0.763506
C	-0.662305	0.568303	-1.318673
C	-2.040262	2.570437	-1.114901
C	0.184377	1.250342	-2.202562
C	-1.179687	3.252559	-1.979877
C	-0.057655	2.597234	-2.523398
H	-0.427884	-0.469308	-1.038388

H	-2.916656	3.080105	-0.685315
H	1.066025	0.743892	-2.623980
H	-1.373114	4.308645	-2.225753
H	0.644486	3.139511	-3.174254

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ACID-C SCF Done: -1499.91403905 A.U.

O	-3.253732	-2.936517	0.296286
O	-2.817986	0.173381	0.101664
H	-2.086714	-0.295440	0.620317
C	-3.572138	-2.057024	-0.668153
O	-3.857661	0.848027	-2.596312
C	-3.355185	-0.706750	-0.766015
O	-4.257368	-1.381175	-2.810150
C	-3.822749	-0.265412	-2.100908
O	-1.629450	-2.743045	-2.673571
H	-1.215147	-2.761833	-1.769305
O	-2.028101	-4.529172	-4.614325
H	-1.276457	-4.034321	-4.213463
C	-4.008115	-2.556826	-2.023145
H	-4.941598	-3.167322	-1.986936
C	-2.875703	-3.421822	-2.638253
H	-2.811504	-4.338368	-2.000112
C	-3.147548	-3.833355	-4.090732
H	-4.039891	-4.496547	-4.141326
H	-3.381673	-2.904739	-4.669726
H	-2.217438	-2.932024	0.345448
O	-0.654499	-0.923022	1.159590
C	-0.157540	-1.897057	0.555044

O	-0.739228	-2.874012	-0.012167
O	1.237181	-2.007451	0.469973
C	2.031890	-0.861890	0.821495
H	1.385896	-0.106224	1.314594
C	2.534324	-0.340209	-0.548014
H	3.281821	-1.044762	-0.962846
I	3.868307	1.545803	-0.207641
C	3.135929	-1.311681	1.760900
C	3.809040	-2.528459	1.522274
C	3.510950	-0.530606	2.871153
H	3.488757	-3.155215	0.675388
H	2.981551	0.414842	3.068269
C	4.850521	-2.945021	2.367031
C	4.553636	-0.944948	3.717580
H	5.366834	-3.898899	2.170573
H	4.837375	-0.321729	4.581145
C	5.229694	-2.151636	3.465678
H	6.047078	-2.477913	4.129330
C	1.452447	-0.048763	-1.533677
C	1.483089	-0.683075	-2.797900
C	0.337599	0.754741	-1.201294
C	0.410791	-0.545329	-3.691810
C	-0.728273	0.899114	-2.097675
C	-0.701300	0.237675	-3.338570
H	2.342455	-1.322617	-3.060122
H	0.287673	1.242210	-0.217049
H	0.424909	-1.083265	-4.652659
H	-1.619711	1.474029	-1.809589
H	-1.572859	0.318352	-4.005389

ACID-DminusI SCF Done: -1488.30158568 A.U.

O	0.294908	-0.779838	2.080588
O	-0.801966	1.960281	0.894094
H	-0.751524	1.871013	1.868436
C	0.248079	-0.303084	0.828996
O	-0.758869	1.487224	-1.977265
C	-0.212940	0.874687	0.310694
O	0.401347	-0.421615	-1.505308
C	-0.228016	0.758313	-1.159066
O	2.985857	-0.034398	-0.304925
H	2.716245	0.486679	0.475361
O	4.287928	-2.234164	-1.336337
H	4.621339	-1.325994	-1.185378
C	0.791418	-1.128599	-0.311626
H	0.307207	-2.131903	-0.321513
C	2.325984	-1.294959	-0.256568
H	2.560689	-1.845495	0.689138
C	2.884497	-2.094387	-1.438319
H	2.440033	-3.112838	-1.441593
H	2.564862	-1.580291	-2.378546
H	-0.472341	-0.395916	2.605476
O	-1.955049	0.360538	3.070219
C	-2.763492	0.431627	2.150131
O	-2.772024	-0.407335	1.097610
O	-3.710331	1.377210	2.055720
C	-4.457128	1.179243	0.799421
H	-5.389260	0.634203	1.063100

C	-3.489359	0.271361	0.007158
H	-2.740994	0.904621	-0.512198
C	-4.088078	-0.700554	-0.965188
C	-3.700938	-0.632470	-2.319587
C	-5.020373	-1.674760	-0.549724
H	-2.949227	0.112141	-2.631498
H	-5.301939	-1.748580	0.513287
C	-4.260480	-1.520308	-3.254453
C	-5.570744	-2.565040	-1.484338
H	-3.956765	-1.462855	-4.311356
H	-6.294277	-3.327931	-1.156289
C	-5.195455	-2.484271	-2.839093
H	-5.630355	-3.182275	-3.571991
C	-4.773202	2.491333	0.133844
C	-3.731394	3.365097	-0.250494
C	-6.111409	2.839207	-0.136742
C	-4.036234	4.572408	-0.897291
C	-6.411944	4.045543	-0.791621
C	-5.373960	4.914127	-1.170586
H	-2.681787	3.098910	-0.048180
H	-6.923892	2.157305	0.163331
H	-3.220358	5.248323	-1.197305
H	-7.460151	4.308140	-1.004131
H	-5.607446	5.860678	-1.683423

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ACID-D SCF Done: -1499.91103027 A.U.

O	2.056026	-0.359728	-1.881563
O	2.015057	2.728834	-0.946277

H	1.194587	2.381355	-1.379522
C	2.836088	0.375559	-1.053669
O	4.280493	2.865805	0.912268
C	2.810389	1.679018	-0.639798
O	4.596713	0.652943	0.459984
C	3.925804	1.869041	0.322184
O	2.426957	-0.845675	1.581380
H	1.506748	-0.982142	1.274353
O	3.694381	-3.171991	2.254612
H	2.957207	-2.660376	2.656176
C	3.914859	-0.351566	-0.298494
H	4.642990	-0.839078	-0.990382
C	3.313235	-1.427469	0.628047
H	2.772440	-2.140593	-0.038388
C	4.349350	-2.216302	1.434568
H	5.036553	-2.760146	0.750822
H	4.959217	-1.488234	2.024977
H	1.275918	0.185983	-2.169714
O	-0.065304	1.259796	-1.950143
C	-0.861770	0.831786	-1.114486
O	-1.552806	-0.299961	-1.260619
O	-1.115736	1.450599	0.046306
C	-2.281162	0.814118	0.658095
H	-2.069479	0.746103	1.744246
C	-2.234212	-0.600782	-0.000899
H	-3.251102	-0.989446	-0.241040
I	-5.606252	-2.739419	0.747783
C	-1.465650	-1.628026	0.805206
C	-2.052408	-2.068365	2.011461

C	-0.234502	-2.174015	0.385326
H	-3.045499	-1.692072	2.306717
H	0.216233	-1.857722	-0.570152
C	-1.400883	-3.026564	2.803152
C	0.409174	-3.143932	1.183285
H	-1.875641	-3.369401	3.735736
H	1.376752	-3.569170	0.875160
C	-0.167755	-3.562811	2.393769
H	0.345148	-4.317837	3.010730
C	-3.533504	1.631028	0.389396
C	-3.465617	2.915565	-0.187863
C	-4.784701	1.094600	0.757780
C	-4.643214	3.653564	-0.401689
C	-5.956919	1.834932	0.537418
C	-5.890720	3.115587	-0.040001
H	-2.489665	3.339518	-0.467880
H	-4.866889	0.076449	1.180213
H	-4.581463	4.655292	-0.856842
H	-6.925940	1.388470	0.810626
H	-6.813072	3.693245	-0.214170

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ACID-AB SCF Done: -1311.41518489 A.U.

O	-1.073715	-0.554403	1.084763
O	-0.570056	2.574677	1.290159
H	-0.061327	2.042773	0.610889
C	-1.453006	0.350315	1.987574
O	-1.857493	3.278650	3.851734
C	-1.233970	1.703071	2.089738

O	-2.421347	1.066761	3.997106
C	-1.824997	2.174224	3.349621
O	-4.476278	0.046500	2.462776
H	-4.351738	0.873366	2.979490
O	-5.362091	-1.979244	4.032883
H	-5.743553	-1.289356	3.444055
C	-2.163048	-0.122958	3.225997
H	-1.468893	-0.781767	3.801706
C	-3.491565	-0.852537	2.984370
H	-3.330290	-1.630945	2.207022
C	-4.048565	-1.503303	4.263452
H	-3.406386	-2.358540	4.571322
H	-4.007559	-0.742868	5.087425
H	-0.308346	-0.143727	0.533803
O	0.860917	0.757932	0.015944
C	2.051713	0.667227	0.846928
H	2.523433	1.661173	0.996577
C	2.392521	-0.001991	-0.415895
H	2.158167	-1.071101	-0.500637
I	5.177867	-1.444087	0.182664
C	1.851715	-0.038853	2.162546
C	1.460449	0.747779	3.267706
C	1.922751	-1.438244	2.307904
C	1.136921	0.149950	4.497009
C	1.604153	-2.037670	3.537266
C	1.205754	-1.248165	4.632174
H	1.377095	1.840200	3.148430
H	2.263443	-2.061134	1.468007
H	0.812384	0.777843	5.341650

H	1.675769	-3.132018	3.641353
H	0.953346	-1.723185	5.594354
C	2.927600	0.677167	-1.608211
C	3.120349	2.077691	-1.655772
C	3.200825	-0.083936	-2.769320
C	3.592876	2.693480	-2.823900
C	3.670927	0.531859	-3.935982
C	3.873709	1.924874	-3.968123
H	2.888387	2.693921	-0.774311
H	3.074626	-1.176694	-2.730523
H	3.741760	3.785173	-2.841223
H	3.892165	-0.080319	-4.824869
H	4.249685	2.410188	-4.883335

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ACID-A+I SCF Done: -1311.42423826 A.U.

O	-0.507497	-1.197484	-0.075815
O	-0.746202	1.733834	-1.349711
H	0.083411	1.219529	-1.516348
C	-1.373961	-0.192185	0.111733
O	-2.959924	2.916728	0.161826
C	-1.488918	1.061765	-0.433895
O	-3.148016	0.890566	1.191140
C	-2.580707	1.769592	0.273726
O	-4.069244	-1.218923	-0.539406
H	-3.376256	-0.858132	-1.129594
O	-5.528032	-2.652626	1.259321
H	-5.673313	-2.436677	0.314994
C	-2.476721	-0.378220	1.122737

H	-2.031247	-0.604233	2.119558
C	-3.459762	-1.493414	0.721249
H	-2.869446	-2.443967	0.682688
C	-4.617233	-1.661670	1.708436
H	-4.222347	-1.982070	2.696980
H	-5.100938	-0.661830	1.838407
H	0.347392	-0.825719	-0.448880
O	1.497378	0.347114	-0.880573
C	1.896101	1.201033	0.272321
H	1.811146	2.272502	0.007221
C	2.914368	0.421420	-0.477179
H	3.298894	-0.517457	-0.021847
I	4.912732	-2.589424	1.083230
C	1.306796	0.844240	1.593999
C	0.304857	1.692575	2.118949
C	1.642572	-0.344250	2.277065
C	-0.360052	1.359696	3.309401
C	0.977730	-0.672284	3.470154
C	-0.023276	0.171858	3.985699
H	0.020037	2.603429	1.567015
H	2.429132	-1.018900	1.893236
H	-1.156606	2.015928	3.692927
H	1.250875	-1.600498	3.996224
H	-0.545221	-0.096444	4.918872
C	3.838140	1.075964	-1.450772
C	5.196726	0.694152	-1.456389
C	3.384779	2.064380	-2.351987
C	6.092769	1.314535	-2.344143
C	4.283602	2.676212	-3.239667

C	5.641967	2.305407	-3.234408
H	5.533920	-0.099825	-0.766943
H	2.318130	2.341830	-2.366741
H	7.151836	1.010107	-2.344482
H	3.921869	3.444020	-3.942753
H	6.347239	2.785952	-3.932114

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ACID-A SCF Done: -1299.81650968 A.U.

O	-0.587713	-2.635699	-1.853052
O	0.883537	0.012462	-2.838803
H	1.266585	-0.462603	-2.063876
C	-1.002480	-1.598346	-2.614031
O	-1.263830	1.496291	-4.195400
C	-0.375171	-0.460182	-3.037869
O	-2.574108	-0.324918	-3.779503
C	-1.377718	0.378983	-3.743090
O	-1.819971	-2.672180	-5.264696
H	-0.895855	-2.656490	-4.948482
O	-4.308188	-3.806938	-5.594018
H	-3.553232	-3.762624	-6.215933
C	-2.413456	-1.600692	-3.138286
H	-3.132570	-1.668385	-2.289070
C	-2.680024	-2.749323	-4.132936
H	-2.531036	-3.706011	-3.570227
C	-4.103394	-2.731727	-4.697124
H	-4.833326	-2.838210	-3.865765
H	-4.268903	-1.732464	-5.170717
H	0.087740	-2.299209	-1.211269

O	0.814065	-0.910544	-0.288192
C	-0.168312	0.139263	0.030645
C	0.922463	-0.209067	0.986551
H	-0.007867	1.053371	-0.571231
H	0.642241	-0.836226	1.854683
C	-1.593915	-0.275517	0.151302
C	-1.968248	-1.496443	0.751950
C	-2.587000	0.547831	-0.421214
H	-1.197664	-2.167949	1.162138
H	-2.294489	1.478442	-0.933496
C	-3.318431	-1.876775	0.794617
C	-3.937835	0.168173	-0.375788
H	-3.602030	-2.834583	1.257955
H	-4.700959	0.811504	-0.839685
C	-4.306022	-1.044534	0.234836
H	-5.363958	-1.349180	0.263337
C	2.120341	0.659558	1.179595
C	2.666506	0.812788	2.470612
C	2.706530	1.346819	0.092567
C	3.775440	1.650490	2.678063
C	3.817609	2.177341	0.301513
C	4.353205	2.333448	1.593986
H	2.218810	0.272154	3.320690
H	2.294305	1.229806	-0.922545
H	4.193301	1.764989	3.690558
H	4.268587	2.707617	-0.551748
H	5.224916	2.987130	1.754542

ACID-B+CO2 SCF Done: -1499.90089831 A.U.

O	1.511076	-1.184095	-0.937572
O	0.937227	1.926992	-0.945507
H	0.194665	1.231846	-0.768119
C	2.328474	-0.123772	-0.965053
O	3.668956	3.107157	-0.997514
C	2.090573	1.234204	-0.946147
O	4.412082	0.950225	-0.953193
C	3.398865	1.922626	-0.964464
O	3.764337	-0.160211	1.617590
H	2.823915	0.094528	1.497232
O	5.924544	-1.708128	2.034094
H	5.330753	-1.171457	2.602062
C	3.813897	-0.345698	-0.835119
H	4.206149	-1.005653	-1.646510
C	4.161595	-0.984396	0.528980
H	3.634760	-1.973289	0.558038
C	5.662253	-1.206795	0.730634
H	6.038807	-1.947000	-0.009556
H	6.177248	-0.232970	0.536455
H	0.520569	-0.829391	-0.902218
O	-0.661679	-0.028727	-0.569859
C	-1.927747	-0.001262	-1.139719
H	-2.058327	0.861030	-1.847831
C	-2.865264	0.202126	0.080123
H	-2.990078	-0.756688	0.620089
I	-5.084590	0.578626	-0.620583
O	-0.720005	-1.572462	1.888547
O	0.803837	0.215173	1.836129

C	0.017154	-0.659388	1.782738
C	-2.254205	-1.285319	-1.901772
C	-2.932772	-1.268541	-3.135371
C	-1.859379	-2.526050	-1.357682
C	-3.223890	-2.466802	-3.811142
C	-2.151516	-3.724607	-2.028257
C	-2.836791	-3.699964	-3.257647
H	-3.239592	-0.301862	-3.566746
H	-1.307321	-2.534205	-0.404758
H	-3.754722	-2.436495	-4.777008
H	-1.835470	-4.686481	-1.591889
H	-3.061920	-4.640628	-3.786809
C	-2.473496	1.297429	1.021895
C	-2.653207	1.114449	2.411986
C	-1.850636	2.483935	0.572804
C	-2.217272	2.083706	3.329546
C	-1.404535	3.447150	1.487037
C	-1.586522	3.252957	2.868985
H	-3.124910	0.185937	2.772753
H	-1.680999	2.643770	-0.501667
H	-2.356983	1.917710	4.410164
H	-0.884875	4.343968	1.115715
H	-1.223393	4.006624	3.586282

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ACID-B SCF Done: -1311.42710948 A.U.

O	1.662685	-1.286648	0.284853
O	0.903294	1.046798	2.250741
H	0.190829	0.392582	1.999479

C	2.144562	-0.072316	0.406642
O	2.893690	3.153151	1.582940
C	1.854943	0.961810	1.281312
O	3.715073	1.658462	0.061735
C	2.802983	2.051068	1.063987
O	4.401904	-1.560667	0.616788
H	3.464625	-1.878761	0.672752
O	6.789553	-1.172437	-0.589242
H	6.422192	-1.812802	0.057967
C	3.301031	0.387057	-0.467610
H	2.954505	0.562069	-1.515428
C	4.419802	-0.688751	-0.513164
H	4.255910	-1.283055	-1.449228
C	5.836662	-0.116049	-0.563128
H	5.969882	0.506701	-1.474462
H	5.965163	0.554229	0.321092
H	0.386119	-1.247445	0.916950
O	-0.607116	-0.967613	1.224369
C	-1.306107	-0.830199	-0.006584
H	-0.595980	-0.531057	-0.814206
C	-2.294542	0.325925	0.207849
H	-3.047857	0.064269	0.976210
I	-3.653176	0.543034	-1.696981
C	-1.878223	-2.192722	-0.387218
C	-1.047103	-3.069858	-1.115553
C	-3.131623	-2.660058	0.055340
H	-0.044655	-2.718793	-1.412756
H	-3.793252	-1.995685	0.633097
C	-1.468608	-4.375302	-1.418019

C	-3.558322	-3.964008	-0.247156
H	-0.806296	-5.046406	-1.989266
H	-4.547130	-4.309258	0.097281
C	-2.730421	-4.825844	-0.989632
H	-3.066850	-5.847982	-1.229277
C	-1.650358	1.638652	0.506678
C	-2.034424	2.360835	1.659213
C	-0.606665	2.151962	-0.299869
C	-1.351049	3.526889	2.032941
C	0.067434	3.321223	0.069220
C	-0.282738	3.997383	1.250421
H	-2.850578	1.971442	2.290481
H	-0.310178	1.612641	-1.212494
H	-1.631750	4.052875	2.959573
H	0.911572	3.683004	-0.536524
H	0.298202	4.876768	1.565902

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ACID-CD3 SCF Done: -1499.89487559 A.U.

O	2.162742	-0.703347	1.100805
O	1.611737	2.450140	1.199956
H	1.138885	1.864260	1.860420
C	2.506841	0.305146	0.295583
O	2.926169	3.407156	-1.256794
C	2.267929	1.660168	0.325720
O	3.510970	1.225849	-1.611801
C	2.887790	2.259780	-0.865093
O	5.545626	0.198352	-0.042921
H	5.412557	1.057017	-0.502165

O	6.629364	-1.639371	-1.718723
H	6.940453	-0.984650	-1.053450
C	3.286589	-0.029316	-0.946635
H	2.675809	-0.688392	-1.611645
C	4.645072	-0.704089	-0.691943
H	4.489771	-1.552646	0.009410
C	5.306244	-1.211999	-1.986021
H	4.731514	-2.069238	-2.402849
H	5.268286	-0.385790	-2.744172
H	1.485958	-0.364912	1.788291
O	0.386211	0.490883	2.539229
C	-0.747175	0.391382	1.987126
O	-1.050588	-0.818428	1.428654
O	-1.611982	1.316066	1.868112
C	-2.636884	0.590078	0.253493
H	-3.538392	1.115292	0.585539
C	-2.362777	-0.819293	0.770987
H	-2.227755	-1.507011	-0.084916
I	-4.765943	-0.404932	-1.677625
C	-3.420421	-1.379473	1.705689
C	-3.996542	-2.634997	1.431258
C	-3.824126	-0.678414	2.862594
H	-3.705939	-3.170227	0.513644
H	-3.379624	0.304644	3.078490
C	-4.957134	-3.186694	2.294410
C	-4.783749	-1.230525	3.727121
H	-5.405936	-4.165052	2.058861
H	-5.092087	-0.672074	4.625907
C	-5.353337	-2.485564	3.446778

H	-6.110275	-2.914469	4.123614
C	-1.793379	1.218642	-0.763506
C	-0.662305	0.568303	-1.318673
C	-2.040262	2.570437	-1.114901
C	0.184377	1.250342	-2.202562
C	-1.179687	3.252559	-1.979877
C	-0.057655	2.597234	-2.523398
H	-0.427884	-0.469308	-1.038388
H	-2.916656	3.080105	-0.685315
H	1.066025	0.743892	-2.623980
H	-1.373114	4.308645	-2.225753
H	0.644486	3.139511	-3.174254

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ACID-CD SCF Done: -1499.90269957 A.U.

O	1.889975	-0.783495	0.665252
O	1.860003	2.242964	1.517336
H	1.333646	1.570645	2.050278
C	2.442648	0.281605	0.098801
O	3.392081	3.565821	-0.645870
C	2.437224	1.610251	0.469225
O	3.656968	1.466802	-1.520467
C	3.176196	2.373637	-0.533991
O	5.429998	-0.293172	-0.366496
H	5.433951	0.669842	-0.566127
O	6.167215	-1.795127	-2.487917
H	6.577678	-1.393595	-1.688143
C	3.179816	0.144744	-1.204969
H	2.461210	-0.174648	-1.999105
C	4.376105	-0.818030	-1.180911

H	4.052837	-1.770954	-0.707622
C	4.939901	-1.095007	-2.586832
H	4.222728	-1.709456	-3.176402
H	5.050894	-0.112153	-3.116714
H	1.300224	-0.387246	1.446174
O	0.488195	0.158147	2.520781
C	-0.759958	0.296902	2.249142
O	-1.188569	-0.722958	1.377099
O	-1.535338	1.175118	2.644554
C	-2.787103	0.714657	0.199135
H	-3.084978	1.428037	0.983693
C	-2.505610	-0.687724	0.788416
H	-2.401546	-1.393228	-0.063136
I	-4.756874	0.579050	-1.042383
C	-3.581745	-1.244528	1.714417
C	-4.191270	-2.474958	1.392925
C	-3.987979	-0.573268	2.889048
H	-3.880433	-3.006105	0.477895
H	-3.484366	0.368123	3.154628
C	-5.192889	-3.023639	2.211453
C	-4.987862	-1.121810	3.708801
H	-5.659588	-3.984262	1.938442
H	-5.293189	-0.586359	4.622791
C	-5.597303	-2.344963	3.373963
H	-6.383986	-2.769617	4.019164
C	-1.673440	1.251052	-0.648313
C	-1.040989	2.458142	-0.272459
C	-1.185654	0.548092	-1.774464
C	0.041907	2.957240	-1.013392

C	-0.115812	1.056000	-2.523320
C	0.500919	2.264384	-2.145789
H	-1.365733	2.968239	0.647153
H	-1.671330	-0.393214	-2.077778
H	0.576038	3.856643	-0.672293
H	0.247768	0.502043	-3.404284
H	1.367209	2.647004	-2.707057

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ACID-C SCF Done: -1499.91403905 A.U.

O	-3.253732	-2.936517	0.296286
O	-2.817986	0.173381	0.101664
H	-2.086714	-0.295440	0.620317
C	-3.572138	-2.057024	-0.668153
O	-3.857661	0.848027	-2.596312
C	-3.355185	-0.706750	-0.766015
O	-4.257368	-1.381175	-2.810150
C	-3.822749	-0.265412	-2.100908
O	-1.629450	-2.743045	-2.673571
H	-1.215147	-2.761833	-1.769305
O	-2.028101	-4.529172	-4.614325
H	-1.276457	-4.034321	-4.213463
C	-4.008115	-2.556826	-2.023145
H	-4.941598	-3.167322	-1.986936
C	-2.875703	-3.421822	-2.638253
H	-2.811504	-4.338368	-2.000112
C	-3.147548	-3.833355	-4.090732
H	-4.039891	-4.496547	-4.141326
H	-3.381673	-2.904739	-4.669726
H	-2.217438	-2.932024	0.345448

O	-0.654499	-0.923022	1.159590
C	-0.157540	-1.897057	0.555044
O	-0.739228	-2.874012	-0.012167
O	1.237181	-2.007451	0.469973
C	2.031890	-0.861890	0.821495
H	1.385896	-0.106224	1.314594
C	2.534324	-0.340209	-0.548014
H	3.281821	-1.044762	-0.962846
I	3.868307	1.545803	-0.207641
C	3.135929	-1.311681	1.760900
C	3.809040	-2.528459	1.522274
C	3.510950	-0.530606	2.871153
H	3.488757	-3.155215	0.675388
H	2.981551	0.414842	3.068269
C	4.850521	-2.945021	2.367031
C	4.553636	-0.944948	3.717580
H	5.366834	-3.898899	2.170573
H	4.837375	-0.321729	4.581145
C	5.229694	-2.151636	3.465678
H	6.047078	-2.477913	4.129330
C	1.452447	-0.048763	-1.533677
C	1.483089	-0.683075	-2.797900
C	0.337599	0.754741	-1.201294
C	0.410791	-0.545329	-3.691810
C	-0.728273	0.899114	-2.097675
C	-0.701300	0.237675	-3.338570
H	2.342455	-1.322617	-3.060122
H	0.287673	1.242210	-0.217049
H	0.424909	-1.083265	-4.652659

H	-1.619711	1.474029	-1.809589
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H	-1.572859	0.318352	-4.005389
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ACID-DminusI SCF Done: -1488.30158568 A.U.

O	0.294908	-0.779838	2.080588
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O	-0.801966	1.960281	0.894094
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H	-0.751524	1.871013	1.868436
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C	0.248079	-0.303084	0.828996
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O	-0.758869	1.487224	-1.977265
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C	-0.212940	0.874687	0.310694
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O	0.401347	-0.421615	-1.505308
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C	-0.228016	0.758313	-1.159066
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O	2.985857	-0.034398	-0.304925
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H	2.716245	0.486679	0.475361
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O	4.287928	-2.234164	-1.336337
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H	4.621339	-1.325994	-1.185378
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C	0.791418	-1.128599	-0.311626
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H	0.307207	-2.131903	-0.321513
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C	2.325984	-1.294959	-0.256568
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H	2.560689	-1.845495	0.689138
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C	2.884497	-2.094387	-1.438319
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H	2.440033	-3.112838	-1.441593
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H	2.564862	-1.580291	-2.378546
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H	-0.472341	-0.395916	2.605476
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O	-1.955049	0.360538	3.070219
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C	-2.763492	0.431627	2.150131
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O	-2.772024	-0.407335	1.097610
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O	-3.710331	1.377210	2.055720
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C	-4.457128	1.179243	0.799421
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H	-5.389260	0.634203	1.063100
C	-3.489359	0.271361	0.007158
H	-2.740994	0.904621	-0.512198
C	-4.088078	-0.700554	-0.965188
C	-3.700938	-0.632470	-2.319587
C	-5.020373	-1.674760	-0.549724
H	-2.949227	0.112141	-2.631498
H	-5.301939	-1.748580	0.513287
C	-4.260480	-1.520308	-3.254453
C	-5.570744	-2.565040	-1.484338
H	-3.956765	-1.462855	-4.311356
H	-6.294277	-3.327931	-1.156289
C	-5.195455	-2.484271	-2.839093
H	-5.630355	-3.182275	-3.571991
C	-4.773202	2.491333	0.133844
C	-3.731394	3.365097	-0.250494
C	-6.111409	2.839207	-0.136742
C	-4.036234	4.572408	-0.897291
C	-6.411944	4.045543	-0.791621
C	-5.373960	4.914127	-1.170586
H	-2.681787	3.098910	-0.048180
H	-6.923892	2.157305	0.163331
H	-3.220358	5.248323	-1.197305
H	-7.460151	4.308140	-1.004131
H	-5.607446	5.860678	-1.683423

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ACID-D SCF Done: -1499.91103027 A.U.

O	2.056026	-0.359728	-1.881563
O	2.015057	2.728834	-0.946277

H	1.194587	2.381355	-1.379522
C	2.836088	0.375559	-1.053669
O	4.280493	2.865805	0.912268
C	2.810389	1.679018	-0.639798
O	4.596713	0.652943	0.459984
C	3.925804	1.869041	0.322184
O	2.426957	-0.845675	1.581380
H	1.506748	-0.982142	1.274353
O	3.694381	-3.171991	2.254612
H	2.957207	-2.660376	2.656176
C	3.914859	-0.351566	-0.298494
H	4.642990	-0.839078	-0.990382
C	3.313235	-1.427469	0.628047
H	2.772440	-2.140593	-0.038388
C	4.349350	-2.216302	1.434568
H	5.036553	-2.760146	0.750822
H	4.959217	-1.488234	2.024977
H	1.275918	0.185983	-2.169714
O	-0.065304	1.259796	-1.950143
C	-0.861770	0.831786	-1.114486
O	-1.552806	-0.299961	-1.260619
O	-1.115736	1.450599	0.046306
C	-2.281162	0.814118	0.658095
H	-2.069479	0.746103	1.744246
C	-2.234212	-0.600782	-0.000899
H	-3.251102	-0.989446	-0.241040
I	-5.606252	-2.739419	0.747783
C	-1.465650	-1.628026	0.805206
C	-2.052408	-2.068365	2.011461

C	-0.234502	-2.174015	0.385326
H	-3.045499	-1.692072	2.306717
H	0.216233	-1.857722	-0.570152
C	-1.400883	-3.026564	2.803152
C	0.409174	-3.143932	1.183285
H	-1.875641	-3.369401	3.735736
H	1.376752	-3.569170	0.875160
C	-0.167755	-3.562811	2.393769
H	0.345148	-4.317837	3.010730
C	-3.533504	1.631028	0.389396
C	-3.465617	2.915565	-0.187863
C	-4.784701	1.094600	0.757780
C	-4.643214	3.653564	-0.401689
C	-5.956919	1.834932	0.537418
C	-5.890720	3.115587	-0.040001
H	-2.489665	3.339518	-0.467880
H	-4.866889	0.076449	1.180213
H	-4.581463	4.655292	-0.856842
H	-6.925940	1.388470	0.810626
H	-6.813072	3.693245	-0.214170

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EPO SCF Done: -615.483574090 A.U.

O	0.844829	-0.951483	-0.317745
C	-0.123882	0.088969	-0.123771
C	0.909512	-0.227149	0.919049
H	0.059220	1.007061	-0.719670
H	0.544521	-0.789753	1.803225
C	-1.554217	-0.310573	0.034051
C	-1.902470	-1.658027	0.268612

C	-2.571507	0.665153	-0.028244
H	-1.102065	-2.414464	0.286515
H	-2.306312	1.717458	-0.223975
C	-3.246825	-2.019462	0.451186
C	-3.915695	0.302008	0.157677
H	-3.510138	-3.074484	0.628777
H	-4.702699	1.071378	0.108423
C	-4.256943	-1.041076	0.399828
H	-5.311439	-1.326348	0.541557
C	2.093900	0.652688	1.150669
C	2.339056	1.184364	2.434419
C	2.965220	0.979197	0.089475
C	3.429615	2.042959	2.650725
C	4.056438	1.835122	0.308367
C	4.290318	2.372221	1.587835
H	1.669018	0.922312	3.270102
H	2.779743	0.535054	-0.901230
H	3.611998	2.453913	3.656502
H	4.734532	2.080628	-0.524615
H	5.147860	3.042240	1.758497

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EPO SCF Done: -615.483574090 A.U.

O	0.844829	-0.951483	-0.317745
C	-0.123882	0.088969	-0.123771
C	0.909512	-0.227149	0.919049
H	0.059220	1.007061	-0.719670
H	0.544521	-0.789753	1.803225
C	-1.554217	-0.310573	0.034051
C	-1.902470	-1.658027	0.268612

C	-2.571507	0.665153	-0.028244
H	-1.102065	-2.414464	0.286515
H	-2.306312	1.717458	-0.223975
C	-3.246825	-2.019462	0.451186
C	-3.915695	0.302008	0.157677
H	-3.510138	-3.074484	0.628777
H	-4.702699	1.071378	0.108423
C	-4.256943	-1.041076	0.399828
H	-5.311439	-1.326348	0.541557
C	2.093900	0.652688	1.150669
C	2.339056	1.184364	2.434419
C	2.965220	0.979197	0.089475
C	3.429615	2.042959	2.650725
C	4.056438	1.835122	0.308367
C	4.290318	2.372221	1.587835
H	1.669018	0.922312	3.270102
H	2.779743	0.535054	-0.901230
H	3.611998	2.453913	3.656502
H	4.734532	2.080628	-0.524615
H	5.147860	3.042240	1.758497

EPO-CH₂Ph

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ACID-AB SCF Done: -1119.80607736 A.U.

O	-0.548649	-1.000352	0.089490
O	0.154473	2.089715	-0.298742
H	0.676722	1.397080	-0.807063

C	-1.030066	0.113833	0.653630
O	-1.519516	3.399150	1.731777
C	-0.743535	1.448517	0.480265
O	-2.352456	1.320492	2.165392
C	-1.529668	2.213291	1.472971
O	-3.877445	0.265773	-0.050582
H	-3.078076	0.672678	-0.449176
O	-5.797433	-1.044677	1.356192
H	-5.826304	-0.499618	0.542462
C	-2.144265	-0.007862	1.661536
H	-1.831969	-0.666498	2.504584
C	-3.437337	-0.556813	1.028185
H	-3.201529	-1.589456	0.664134
C	-4.609755	-0.622785	2.010576
H	-4.385534	-1.355188	2.817037
H	-4.715894	0.385982	2.480972
H	0.277822	-0.748548	-0.463983
O	1.467724	-0.012845	-1.175198
C	2.766694	-0.034376	-0.546525
H	3.232464	0.973052	-0.516189
C	2.869630	-0.778141	0.774191
H	2.517843	-1.821045	0.627070
H	3.953006	-0.847563	1.022397
C	2.899161	-0.734584	-1.822994
H	3.145796	-0.185122	-2.739108
H	2.690343	-1.810459	-1.880648
I	5.808848	-1.576041	-1.888943
C	2.079645	-0.132625	1.900875
C	1.315750	-0.933929	2.776620

C	2.050790	1.266782	2.087676
C	0.540183	-0.360300	3.797771
C	1.255800	1.846713	3.090130
C	0.494221	1.036584	3.948956
H	1.308434	-2.026703	2.633172
H	2.614769	1.925778	1.410861
H	-0.053368	-1.008382	4.463504
H	1.194850	2.942683	3.170224
H	-0.153673	1.494830	4.711942

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ACID-A+I SCF Done: -1119.80092640 A.U.

O	-1.211397	-1.049400	0.231062
O	-0.960334	1.967507	-0.885444
H	-0.216188	1.338040	-1.085556
C	-1.999201	0.038882	0.321325
O	-3.412364	3.224739	0.101238
C	-1.904543	1.318723	-0.168923
O	-3.912110	1.197046	1.017673
C	-3.107004	2.066719	0.281392
O	-4.489792	-0.686693	-1.074172
H	-3.639478	-0.377213	-1.447865
O	-6.450089	-2.135013	0.155744
H	-6.342850	-1.839979	-0.772063
C	-3.332502	-0.113691	1.011476
H	-3.203753	-0.462032	2.063546
C	-4.249193	-1.107973	0.265170
H	-3.732165	-2.101195	0.287582
C	-5.633071	-1.248910	0.903586

H	-5.531772	-1.663353	1.930326
H	-6.073690	-0.224749	0.988075
H	-0.360329	-0.802216	-0.246937
O	0.908816	0.054923	-0.858032
C	1.912448	0.421500	0.154746
H	2.091535	1.513134	0.189366
C	1.740597	-0.242178	1.508000
H	0.769725	0.089764	1.934347
H	1.666844	-1.341591	1.359912
C	2.339120	-0.304341	-1.053737
H	2.838023	0.223841	-1.882380
H	2.550846	-1.385210	-0.992078
I	5.755490	-1.346886	-1.478614
C	2.875765	0.101094	2.456987
C	2.623103	0.772312	3.672143
C	4.206811	-0.231415	2.121803
C	3.676914	1.096985	4.544971
C	5.259430	0.099123	2.990916
C	4.999424	0.760517	4.205119
H	1.586986	1.042780	3.938140
H	4.439485	-0.738168	1.166997
H	3.462560	1.619001	5.492007
H	6.289503	-0.163941	2.701861
H	5.827649	1.018075	4.885585

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ACID-A SCF Done: -1108.19438835 A.U.

O	-0.887725	-1.307746	0.537054
O	-1.313732	1.886157	0.514119

H	-1.909847	1.357909	1.090586
C	-0.215582	-0.291165	-0.047814
O	0.871933	2.823773	-1.180122
C	-0.385434	1.066545	-0.044772
O	1.477728	0.631223	-1.369495
C	0.679926	1.665153	-0.892107
O	2.488621	-0.307621	1.147445
H	1.682101	-0.099259	1.657027
O	4.413750	-2.054178	0.235178
H	4.438043	-1.444588	1.000903
C	1.043518	-0.616023	-0.811627
H	0.835392	-1.333266	-1.640016
C	2.139751	-1.210118	0.103394
H	1.737598	-2.171701	0.512236
C	3.447388	-1.501372	-0.638533
H	3.259759	-2.239602	-1.447846
H	3.786464	-0.549579	-1.116947
H	-1.738041	-0.956209	0.921133
O	-3.157896	-0.023445	1.194890
C	-3.922314	0.215608	-0.034189
C	-4.540549	-0.466962	1.119186
H	-4.157386	1.286785	-0.181757
H	-4.666515	-1.565098	1.090247
H	-5.233667	0.077930	1.784827
C	-3.463883	-0.518550	-1.279624
H	-2.542645	-0.019980	-1.649495
H	-3.183299	-1.557272	-1.008857
C	-4.551950	-0.493452	-2.336627
C	-4.643112	0.581652	-3.246504

C	-5.526586	-1.512946	-2.389570
C	-5.682982	0.634583	-4.190367
C	-6.565979	-1.463393	-3.333594
C	-6.647306	-0.387692	-4.235863
H	-3.884751	1.381808	-3.219272
H	-5.463045	-2.361553	-1.687962
H	-5.736683	1.477012	-4.897945
H	-7.313914	-2.271403	-3.368247
H	-7.459782	-0.349143	-4.978478

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ACID-B+CO2 SCF Done: -1308.28333177 A.U.

O	-4.877805	0.316823	0.544550
O	-2.924302	2.798709	0.692641
H	-2.704976	1.979209	0.127471
C	-5.038079	1.549447	1.042672
O	-4.608140	4.894138	1.969760
C	-4.205275	2.644173	1.089521
O	-6.257961	3.317548	1.978064
C	-4.955596	3.761605	1.698014
O	-6.938629	2.814949	-0.786728
H	-6.079227	2.481317	-1.124276
O	-9.598757	2.511983	-0.559739
H	-8.978880	2.855216	-1.240412
C	-6.414334	1.987760	1.471379
H	-6.835155	1.337710	2.276468
C	-7.384123	1.969285	0.265199
H	-7.446569	0.903401	-0.073009
C	-8.788747	2.473283	0.606433

H	-9.267429	1.793153	1.345480
H	-8.681202	3.478498	1.085350
H	-3.980076	0.316095	0.006436
O	-2.724286	0.627861	-0.725232
C	-1.648733	-0.266476	-0.638642
H	-1.523661	-0.632004	0.414202
C	-1.917628	-1.493556	-1.555482
H	-2.974759	-1.769050	-1.346182
H	-1.884485	-1.151563	-2.610005
C	-0.439088	0.600052	-1.012158
H	-0.394516	1.487379	-0.354218
H	-0.479423	0.908409	-2.074066
I	1.622465	-0.321361	-0.739521
O	-2.631699	1.156203	-3.373307
O	-4.509813	1.856125	-2.167782
C	-3.489913	1.427019	-2.597885
C	-1.044169	-2.711254	-1.353635
C	-1.042957	-3.398639	-0.118551
C	-0.213117	-3.200041	-2.383774
C	-0.219503	-4.516769	0.088607
C	0.607010	-4.323342	-2.186303
C	0.613191	-4.983391	-0.945094
H	-1.694155	-3.042258	0.696899
H	-0.202235	-2.677669	-3.354356
H	-0.228561	-5.029804	1.064350
H	1.252795	-4.680250	-3.005380
H	1.261563	-5.860079	-0.783858

ACID-BC SCF Done: -1308.28059704 A.U.

O	-4.418817	0.227991	-1.287833
O	-3.467416	2.507902	0.657915
H	-3.029375	2.359416	-0.235892
C	-4.708323	0.454930	-0.040076
O	-4.764579	1.766267	3.230323
C	-4.326813	1.463907	0.843214
O	-5.716056	0.047701	2.066344
C	-4.904202	1.193658	2.162671
O	-7.592817	0.909148	0.041029
H	-6.824501	1.518227	0.110350
O	-9.404759	-1.065209	0.305546
H	-9.455990	-0.093805	0.180050
C	-5.670693	-0.448336	0.720105
H	-5.287295	-1.496048	0.733614
C	-7.069703	-0.421186	0.084226
H	-6.953156	-0.819346	-0.955428
C	-8.103126	-1.255089	0.847407
H	-7.852037	-2.336331	0.770468
H	-8.046029	-0.963124	1.925367
H	-3.333984	1.047609	-1.609951
O	-2.396690	1.605562	-1.614679
C	-1.449128	0.654240	-1.154946
H	-1.896069	0.027420	-0.344496
C	-1.004115	-0.300998	-2.309142
H	-1.691118	-0.076880	-3.151738
H	0.018672	-0.045200	-2.659791
C	-0.338415	1.508712	-0.546250
H	-0.723859	2.085306	0.316306

H	0.118716	2.177313	-1.301873
I	1.377931	0.319326	0.303296
O	-2.498954	-1.009948	2.171713
O	-1.502460	1.068149	2.636000
C	-2.017616	0.040322	2.397069
C	-1.093370	-1.774962	-1.969218
C	-2.341595	-2.332730	-1.601875
C	0.038805	-2.614618	-1.997695
C	-2.443747	-3.694199	-1.273577
C	-0.064346	-3.979365	-1.672949
C	-1.307575	-4.524592	-1.308384
H	-3.233165	-1.679493	-1.567800
H	1.019321	-2.184589	-2.260917
H	-3.422712	-4.110283	-0.983978
H	0.834710	-4.617420	-1.697015
H	-1.390642	-5.592343	-1.046593

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ACID-B SCF Done: -1119.81404970 A.U.

O	0.495397	0.030495	-1.562257
O	-1.060164	2.532901	-0.456496
H	-0.560028	1.911996	0.152475
C	-0.380633	0.825524	-2.137600
O	-2.409051	3.591168	-2.892060
C	-1.063384	1.941274	-1.686181
O	-1.515383	1.785887	-3.969186
C	-1.746861	2.571199	-2.819978
O	1.702393	0.963748	-3.874846
H	1.714198	0.601349	-2.952299

O	1.660127	0.758600	-6.569217
H	2.344141	0.916702	-5.882842
C	-0.745321	0.630202	-3.600384
H	-1.403610	-0.264902	-3.720970
C	0.526404	0.404525	-4.461224
H	0.649248	-0.704428	-4.565176
C	0.447202	1.002782	-5.865963
H	-0.392355	0.545501	-6.433534
H	0.225457	2.092505	-5.761400
H	0.318596	0.195897	-0.157816
O	-0.018482	0.422166	0.839531
C	-1.268212	-0.224961	1.051997
H	-2.100986	0.414990	0.667854
C	-1.344488	-1.614214	0.352837
H	-0.633329	-1.555008	-0.500146
H	-0.970283	-2.406599	1.036072
C	-1.335644	-0.272457	2.578747
H	-1.247961	0.743274	3.007462
H	-0.545262	-0.929492	2.992367
I	-3.273534	-1.059555	3.432162
C	-2.703759	-1.980660	-0.203738
C	-3.308913	-1.153172	-1.179087
C	-3.386277	-3.148362	0.195695
C	-4.560123	-1.480241	-1.726023
C	-4.635805	-3.483371	-0.354859
C	-5.230495	-2.648085	-1.316880
H	-2.786928	-0.237887	-1.509503
H	-2.932085	-3.799693	0.960338
H	-5.011289	-0.816190	-2.481101

H	-5.151034	-4.400495	-0.023978
H	-6.212198	-2.905980	-1.747108

ACID-CD SCF Done: -1308.27948257 A.U.

O	2.201671	1.052213	-1.486733
O	1.124696	2.414074	1.185264
H	0.867293	2.797903	0.302493
C	2.309302	0.715602	-0.203407
O	2.078304	0.570057	3.283161
C	1.850660	1.291783	0.957410
O	3.008660	-0.642882	1.579324
C	2.266304	0.455269	2.091581
O	1.234765	-2.185263	0.216243
H	1.415396	-2.041416	1.172800
O	2.768718	-4.214210	-0.791385
H	1.866301	-4.131620	-0.411638
C	3.056085	-0.545948	0.146904
H	4.121765	-0.469392	-0.178657
C	2.448014	-1.829822	-0.456748
H	2.171846	-1.628762	-1.514120
C	3.413428	-3.024409	-0.381244
H	4.288048	-2.850415	-1.047607
H	3.805360	-3.087838	0.669193
H	1.472673	1.777773	-1.575713
O	0.302882	2.796703	-1.374519
C	-0.782246	2.172204	-1.172570
O	-0.782836	0.833014	-1.454636
O	-1.858346	2.654053	-0.702136

C	-3.086042	1.068019	-0.832063
H	-3.432533	1.413753	-1.811311
H	-3.634321	1.383592	0.061468
C	-1.864247	0.171679	-0.736549
H	-2.022422	-0.781608	-1.274212
I	-5.156617	-0.827982	-1.167908
C	-1.364847	-0.089618	0.700738
H	-0.348963	-0.514756	0.580718
H	-1.251775	0.887418	1.215784
C	-2.224361	-1.037626	1.501762
C	-2.055542	-2.432384	1.358562
C	-3.218248	-0.565338	2.382693
C	-2.871931	-3.329777	2.064759
C	-4.035852	-1.460099	3.092082
C	-3.868297	-2.846152	2.931751
H	-1.268740	-2.804976	0.681733
H	-3.352802	0.521583	2.509387
H	-2.732619	-4.415609	1.935397
H	-4.814823	-1.071998	3.768123
H	-4.514746	-3.549757	3.481075

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ACID-C SCF Done: -1308.28381982 A.U.

O	-1.899400	-1.396119	-0.482084
O	0.121760	0.391790	-2.277812
H	0.573913	-0.000113	-1.452671
C	-2.065679	-0.458169	-1.410040
O	-1.724622	2.040918	-3.838056
C	-1.215079	0.289871	-2.201651

O	-3.401055	0.929013	-2.767700
C	-2.050470	1.188456	-3.036740
O	-3.418626	-1.834906	-3.598380
H	-2.471237	-1.649004	-3.416546
O	-6.094809	-2.245554	-3.652075
H	-5.351866	-2.539946	-4.219759
C	-3.488312	-0.144500	-1.824319
H	-4.104116	0.182138	-0.951990
C	-4.156388	-1.378373	-2.466288
H	-4.189906	-2.168410	-1.673408
C	-5.571935	-1.106908	-2.979980
H	-6.246125	-0.872938	-2.126470
H	-5.526526	-0.206113	-3.640963
H	-0.932484	-1.811281	-0.458101
O	1.454528	-0.552025	-0.257089
C	1.313934	-1.787315	-0.047514
O	0.336091	-2.534372	-0.292366
O	2.387277	-2.467642	0.559919
C	3.575304	-1.701261	0.806887
H	3.747961	-1.008770	-0.045065
C	3.435631	-0.873411	2.114137
H	2.349082	-0.678941	2.223499
H	3.746116	-1.487230	2.986905
C	4.637811	-2.799569	0.826197
H	4.627148	-3.366698	-0.122766
H	4.498162	-3.490622	1.680361
I	6.744755	-2.049973	1.016510
C	4.152111	0.462082	2.107709
C	5.164500	0.773853	3.037547

C	3.787562	1.437497	1.150353
C	5.808476	2.023384	3.011874
C	4.434110	2.683706	1.119439
C	5.448873	2.981855	2.048221
H	5.458648	0.020750	3.786899
H	2.981637	1.198159	0.436239
H	6.600294	2.246534	3.745977
H	4.138149	3.430846	0.365071
H	5.955752	3.960450	2.022616

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ACID-DminusI SCF Done: -1296.68734712 A.U.

O	0.394158	-0.817439	2.078410
O	-0.963943	1.729743	0.765134
H	-0.898518	1.693395	1.741349
C	0.367476	-0.377810	0.811994
O	-0.701224	1.204449	-2.093929
C	-0.207881	0.722058	0.238570
O	0.651181	-0.537073	-1.505105
C	-0.134171	0.566103	-1.226351
O	3.088913	0.257623	-0.218645
H	2.685204	0.768389	0.509146
O	4.747146	-1.761434	-1.099587
H	4.938766	-0.808935	-0.978771
C	1.080487	-1.147388	-0.271877
H	0.750889	-2.211503	-0.268526
C	2.619455	-1.083628	-0.144124
H	2.885441	-1.558969	0.833748
C	3.344888	-1.834123	-1.265775

H	3.055098	-2.906717	-1.243373
H	2.998559	-1.407695	-2.239820
H	-0.457527	-0.539456	2.535202
O	-2.060975	-0.014324	2.901739
C	-2.827823	0.014423	1.948010
O	-2.662782	-0.702745	0.821082
O	-3.924651	0.794319	1.889162
C	-4.572689	0.576660	0.605824
H	-4.930361	1.547609	0.217901
H	-5.432602	-0.114110	0.749231
C	-3.446145	-0.044345	-0.229374
H	-2.795738	0.754242	-0.648852
C	-3.837936	-1.028649	-1.319567
H	-2.904543	-1.481803	-1.714705
H	-4.451116	-1.844793	-0.882503
C	-4.587175	-0.300605	-2.421668
C	-3.892392	0.582675	-3.279664
C	-5.983000	-0.441764	-2.567254
C	-4.587364	1.302409	-4.265613
C	-6.676591	0.277975	-3.556563
C	-5.979341	1.152588	-4.407587
H	-2.801910	0.711595	-3.168965
H	-6.532467	-1.131335	-1.904478
H	-4.034429	1.985355	-4.929807
H	-7.765784	0.152008	-3.663573
H	-6.520437	1.716617	-5.183829

O	2.177746	-0.092667	-1.714693
O	2.479616	2.972916	-0.854824
H	1.697861	2.757326	-1.433798
C	2.781033	0.513139	-0.665139
O	4.050928	2.804367	1.637421
C	2.895583	1.824960	-0.285589
O	3.955684	0.542799	1.353428
C	3.672061	1.859707	0.983172
O	1.162891	-0.358088	1.578748
H	1.038162	0.395811	0.960888
O	1.674834	-2.743830	2.901708
H	0.926076	-2.123271	3.025209
C	3.340021	-0.360670	0.425794
H	4.114057	-1.065470	0.040989
C	2.218798	-1.182135	1.102665
H	1.845765	-1.893091	0.319630
C	2.715630	-1.983776	2.308778
H	3.504556	-2.696123	1.982824
H	3.178645	-1.262309	3.025058
H	1.661011	0.589328	-2.217448
O	0.397780	1.878770	-2.217083
C	-0.446921	1.370376	-1.473067
O	-1.437448	0.594119	-1.896552
O	-0.430345	1.514173	-0.136454
C	-1.644131	0.889516	0.409261
H	-2.402268	1.677355	0.604227
H	-1.367328	0.360678	1.339612
C	-2.071608	-0.047837	-0.727093
H	-3.171583	0.007242	-0.879417

I	-5.574650	1.259576	0.135296
C	-1.530975	-1.477012	-0.625518
H	-1.833411	-2.022398	-1.546639
H	-0.419470	-1.433501	-0.628077
C	-2.006849	-2.208658	0.617330
C	-3.347056	-2.130070	1.058121
C	-1.088401	-2.968286	1.372221
C	-3.748774	-2.801175	2.226823
C	-1.489834	-3.639646	2.539387
C	-2.826195	-3.557931	2.970710
H	-4.088632	-1.516336	0.517617
H	-0.034991	-3.029662	1.061299
H	-4.795236	-2.712033	2.559511
H	-0.741628	-4.210959	3.112202
H	-3.145319	-4.074384	3.890805

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EPO SCF Done: -423.863804194 A.U.

O	-3.178063	-0.052408	1.192781
C	-3.918437	0.222356	-0.002880
C	-4.530830	-0.528837	1.111846
H	-4.213610	1.284920	-0.136541
H	-4.650624	-1.627628	1.021389
H	-5.262047	-0.033439	1.780915
C	-3.455437	-0.471537	-1.277693
H	-2.545825	0.045854	-1.652040
H	-3.155258	-1.508898	-1.019561
C	-4.540663	-0.464998	-2.336183
C	-4.619632	0.572951	-3.289280

C	-5.537994	-1.464899	-2.348166
C	-5.661825	0.609727	-4.232082
C	-6.580219	-1.433437	-3.289343
C	-6.645889	-0.394121	-4.235023
H	-3.847936	1.360880	-3.294779
H	-5.490800	-2.281923	-1.609056
H	-5.703106	1.425822	-4.971161
H	-7.344850	-2.226744	-3.287001
H	-7.461201	-0.369151	-4.975343

EPO-CF₃

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ACID-AB SCF Done: -1186.40716899 A.U.

O	-1.292984	-1.019776	0.403516
O	-1.111356	1.946444	-0.834038
H	-0.298013	1.367106	-0.866726
C	-2.164364	-0.001688	0.323102
O	-3.773272	3.042538	-0.271012
C	-2.099967	1.259469	-0.220532
O	-4.243734	1.020869	0.673975
C	-3.406291	1.923319	0.014382
O	-4.356212	-1.022427	-1.349191
H	-3.517214	-0.578202	-1.592353
O	-6.369453	-2.542405	-0.322225
H	-6.146206	-2.280970	-1.239482
C	-3.565495	-0.232350	0.833206
H	-3.555657	-0.508715	1.913988

C	-4.285758	-1.341916	0.038177
H	-3.702183	-2.283866	0.200931
C	-5.733182	-1.562769	0.484182
H	-5.751668	-1.922723	1.536122
H	-6.254033	-0.574060	0.449149
H	-0.387042	-0.701964	0.093267
O	0.871304	0.235214	-0.406872
C	1.763329	0.758698	0.583034
H	1.888045	1.859667	0.584722
C	1.482385	0.245881	1.990889
C	2.505512	-0.044709	-0.384624
H	2.960761	0.438361	-1.256538
H	2.672852	-1.112367	-0.196999
I	5.524985	0.146112	0.384732
F	2.403816	0.676948	2.868359
F	1.433649	-1.106526	2.037856
F	0.266914	0.711145	2.398734

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ACID-A+I SCF Done: -1186.40788497 A.U.

O	-1.310172	-1.045862	0.369642
O	-1.115002	1.938387	-0.852733
H	-0.309698	1.361596	-0.915228
C	-2.168940	-0.012544	0.305479
O	-3.754146	3.048587	-0.253681
C	-2.098454	1.250055	-0.229358
O	-4.231855	1.028567	0.691119
C	-3.396930	1.925113	0.024218
O	-4.404211	-0.997970	-1.340090

H	-3.549110	-0.605297	-1.611351
O	-6.405118	-2.519101	-0.279415
H	-6.203083	-2.258515	-1.201696
C	-3.565144	-0.232482	0.833455
H	-3.541827	-0.514848	1.912351
C	-4.309101	-1.329854	0.042545
H	-3.732139	-2.278645	0.188024
C	-5.749923	-1.541867	0.513519
H	-5.751669	-1.900120	1.566058
H	-6.265511	-0.550152	0.486634
H	-0.406610	-0.747657	0.059679
O	0.902456	0.214725	-0.423894
C	1.751551	0.762265	0.611960
H	1.850322	1.863439	0.615854
C	1.464624	0.200430	1.995603
C	2.406246	-0.033981	-0.426703
H	2.941360	0.478023	-1.239867
H	2.672338	-1.081538	-0.221568
I	5.722825	0.201830	0.158045
F	1.400761	-1.151610	1.988981
F	0.257086	0.662451	2.428263
F	2.397503	0.589234	2.879134

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ACID-A SCF Done: -1174.79866898 A.U.

O	-0.708652	-1.526196	0.275697
O	-1.454577	1.510640	1.113725
H	-2.012447	0.788146	1.477551
C	-0.144165	-0.321987	0.021934

O	0.656099	3.066919	-0.160835
C	-0.445436	0.959991	0.385372
O	1.469713	1.077441	-0.928836
C	0.571111	1.862076	-0.217891
O	2.551536	-0.469203	1.236400
H	1.735191	-0.507460	1.770365
O	4.621842	-1.706276	-0.095721
H	4.591724	-1.349243	0.815408
C	1.141824	-0.308628	-0.765612
H	0.991241	-0.768296	-1.770496
C	2.283768	-1.051424	-0.035361
H	1.967877	-2.120779	0.063565
C	3.612788	-1.002174	-0.794793
H	3.490828	-1.481833	-1.789796
H	3.868977	0.072790	-0.963621
H	-1.604135	-1.407335	0.671942
O	-3.189345	-0.600810	1.048897
C	-3.890838	-0.068688	-0.091437
C	-4.634865	-0.717389	1.005093
H	-3.855504	1.032039	-0.190296
H	-5.004959	-1.748746	0.868912
H	-5.171837	-0.087523	1.735819
C	-3.663365	-0.804202	-1.406499
F	-3.600571	-2.141631	-1.217520
F	-2.516098	-0.402810	-1.989098
F	-4.685351	-0.534161	-2.248285

O	1.533941	-0.208457	-1.561207
O	0.634984	1.385473	1.035654
H	-0.017669	0.793769	0.518757
C	2.194658	0.606959	-0.736845
O	3.144986	2.721136	1.885249
C	1.826609	1.286595	0.403437
O	4.104819	1.691562	0.089092
C	3.016358	1.987145	0.924776
O	4.123485	-1.140973	0.624137
H	3.154704	-1.248145	0.733732
O	6.491023	-1.807278	-0.465704
H	5.950945	-2.121416	0.291859
C	3.688816	0.741917	-0.897901
H	3.966747	1.121162	-1.911093
C	4.385095	-0.620543	-0.673598
H	3.999663	-1.308176	-1.469032
C	5.911024	-0.545744	-0.765847
H	6.214929	-0.256241	-1.796137
H	6.253712	0.258652	-0.068105
H	0.573170	-0.364530	-1.161391
O	-0.640776	-0.372782	-0.331118
C	-1.906262	-0.450021	-0.864749
H	-2.059624	0.163323	-1.795084
C	-2.172814	-1.910743	-1.291899
C	-2.830505	0.039668	0.258882
H	-2.490581	1.038311	0.586472
H	-2.828935	-0.665984	1.110109
I	-5.026147	0.381985	-0.248932
O	-0.745269	-1.439371	2.378567

O	1.262671	-1.793003	1.213306
C	0.229116	-1.565915	1.732638
F	-2.209801	-2.752804	-0.222471
F	-3.342571	-2.069822	-1.967082
F	-1.183065	-2.345829	-2.112589

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ACID-B SCF Done: -1186.43092297 A.U.

O	1.522210	-1.313553	0.074234
O	0.606821	1.405215	1.389080
H	0.116806	0.545079	1.541000
C	1.998222	-0.089509	-0.037964
O	2.777846	3.276299	0.583335
C	1.643563	1.110359	0.545658
O	3.643188	1.511341	-0.580581
C	2.667159	2.112429	0.241698
O	4.242349	-1.407113	0.796639
H	3.316428	-1.745980	0.862356
O	6.700118	-1.409408	-0.340799
H	6.285847	-1.837594	0.439443
C	3.252996	0.158304	-0.858926
H	3.030580	0.088660	-1.951921
C	4.342524	-0.895399	-0.533115
H	4.207236	-1.729755	-1.268446
C	5.774994	-0.377596	-0.663232
H	5.968599	-0.039100	-1.704480
H	5.877804	0.513201	0.002683
H	0.417435	-1.256880	0.785892
O	-0.571088	-1.031058	1.294025

C	-1.521771	-1.045163	0.267081
H	-1.045518	-1.148439	-0.739336
C	-2.414749	-2.290217	0.446861
C	-2.280776	0.283704	0.374947
H	-1.543454	1.108430	0.387885
H	-2.902520	0.306712	1.290173
I	-3.680260	0.810647	-1.316879
F	-1.657172	-3.402491	0.595650
F	-3.212488	-2.189735	1.545515
F	-3.231554	-2.507222	-0.619419

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ACID-CD SCF Done: -1374.88326721 A.U.

O	2.277315	-0.818791	-0.503194
O	2.391134	2.172991	0.702641
H	1.538062	1.660661	0.807866
C	3.229703	0.123500	-0.459849
O	5.111856	3.028246	0.029943
C	3.292982	1.391573	0.076206
O	5.377713	0.960762	-0.894033
C	4.640903	1.938958	-0.218751
O	5.367982	-1.027152	1.189813
H	4.580599	-0.494898	1.431796
O	7.226964	-2.732330	0.173097
H	7.036112	-2.426846	1.084235
C	4.594338	-0.234538	-0.998404
H	4.537862	-0.542934	-2.069423
C	5.239208	-1.377906	-0.185512
H	4.574444	-2.270973	-0.307435

C	6.652745	-1.731047	-0.654002
H	6.617710	-2.125556	-1.693256
H	7.252635	-0.787516	-0.663492
H	1.442651	-0.472123	-0.042049
O	0.374113	0.439946	0.731739
C	-0.878185	0.436381	0.661394
O	-1.447235	-0.671221	0.052740
O	-1.682262	1.327140	1.067976
C	-3.417895	0.733071	0.257309
H	-3.225015	1.394520	-0.591789
H	-3.967823	1.120123	1.120083
C	-2.873388	-0.685394	0.216476
H	-3.277732	-1.251755	-0.643510
I	-5.898221	0.385881	-0.990027
C	-3.189978	-1.509870	1.485270
F	-2.554651	-1.012940	2.576031
F	-4.510736	-1.532180	1.753840
F	-2.773815	-2.788483	1.320477

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ACID-C SCF Done: -1374.89843476 A.U.

O	-2.793814	-0.669515	1.394316
O	-1.516521	1.398156	-0.753060
H	-0.824357	1.045552	-0.097434
C	-3.298199	0.261721	0.587828
O	-3.875165	2.833751	-1.714909
C	-2.768719	1.126576	-0.349723
O	-5.084296	1.502844	-0.315407
C	-3.887065	1.931978	-0.902035

O	-5.002133	-1.221762	-1.261224
H	-4.062867	-0.939111	-1.310414
O	-7.538049	-1.960385	-0.655637
H	-6.939684	-2.150255	-1.408408
C	-4.805336	0.405965	0.561522
H	-5.210618	0.634723	1.576466
C	-5.470882	-0.886252	0.043234
H	-5.210301	-1.692327	0.775538
C	-6.992215	-0.779969	-0.081581
H	-7.446040	-0.647079	0.925404
H	-7.220521	0.132621	-0.686110
H	-1.826611	-0.973022	1.135996
O	0.426558	0.519491	0.743436
C	0.445512	-0.729274	0.874538
O	-0.484348	-1.565649	0.888436
O	1.724592	-1.341028	1.022665
C	2.842974	-0.464247	1.038224
H	2.592093	0.500378	1.529370
C	3.909866	-1.172979	1.887788
C	3.214244	-0.247062	-0.429764
H	2.332340	0.189959	-0.932572
H	3.521352	-1.198805	-0.902258
I	4.864184	1.216896	-0.858077
F	3.398135	-1.569511	3.073831
F	4.411821	-2.271304	1.264076
F	4.955167	-0.350095	2.157080

O	0.477576	-1.238599	2.124034
O	-0.891028	1.486968	1.255850
H	-0.901284	1.250963	2.205784
C	0.525053	-0.545683	0.970546
O	-0.498230	1.522810	-1.619619
C	-0.061413	0.628185	0.595382
O	0.959670	-0.207106	-1.303717
C	0.086324	0.767038	-0.865986
O	3.275367	0.374210	0.295699
H	2.852240	0.681747	1.119749
O	5.072766	-1.359451	-0.881635
H	5.218414	-0.449940	-0.549769
C	1.340397	-1.048752	-0.195344
H	1.057651	-2.098847	-0.437042
C	2.864386	-0.965704	0.047702
H	3.094784	-1.634542	0.914806
C	3.688413	-1.431153	-1.157801
H	3.442127	-2.489454	-1.390162
H	3.385981	-0.810359	-2.037336
H	-0.451834	-1.174600	2.480967
O	-2.226629	-0.818273	2.530420
C	-2.780522	-0.411896	1.526568
O	-2.537200	-0.906126	0.281689
O	-3.669215	0.596309	1.493075
C	-3.801186	1.050783	0.128488
H	-3.140134	1.929582	-0.011622
H	-4.858201	1.306183	-0.071329
C	-3.279883	-0.149189	-0.689251
H	-2.599086	0.160302	-1.507830

C	-4.394216	-1.033135	-1.263600
F	-5.122941	-0.306612	-2.145365
F	-3.894058	-2.106628	-1.899441
F	-5.224082	-1.464059	-0.283673

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ACID-D SCF Done: -1374.90708059 A.U.

O	2.285665	0.138540	-1.957697
O	2.298860	2.826780	-0.164328
H	1.497326	2.656884	-0.715382
C	3.149910	0.652117	-1.059735
O	4.835851	2.616528	1.278424
C	3.153916	1.782586	-0.286511
O	5.145012	0.652532	0.160770
C	4.416687	1.793961	0.493448
O	3.402291	-1.313486	1.217900
H	2.518796	-0.917762	1.089178
O	4.891117	-3.558332	0.915009
H	4.241364	-3.256532	1.585496
C	4.372283	-0.163466	-0.726359
H	4.970481	-0.373288	-1.645350
C	4.019510	-1.508896	-0.047720
H	3.346018	-2.064066	-0.747444
C	5.255480	-2.366266	0.243027
H	5.754608	-2.643242	-0.711343
H	5.970655	-1.739731	0.833372
H	1.476699	0.717661	-2.014291
O	0.160924	1.765447	-1.562651
C	-0.579800	1.131183	-0.815120

O	-0.759036	-0.200547	-0.927178
O	-1.273554	1.663126	0.189320
C	-2.067785	0.614570	0.822996
H	-3.131854	0.698645	0.511831
H	-1.978009	0.717273	1.919861
C	-1.445285	-0.670082	0.257184
H	-2.238005	-1.415313	-0.005645
I	-4.998111	-1.723245	0.104377
C	-0.386808	-1.298766	1.164395
F	0.217788	-2.351812	0.589956
F	0.602052	-0.370872	1.443819
F	-0.921446	-1.679022	2.336161

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EPO SCF Done: -490.475666888 A.U.

O	0.773957	0.782068	-0.464456
C	-0.145658	0.164817	0.426648
C	1.080937	-0.539299	0.005498
H	-0.232571	0.599287	1.442846
H	1.010629	-1.344197	-0.750185
H	1.922450	-0.617422	0.720668
C	-1.495078	-0.210369	-0.162891
F	-2.287284	0.879096	-0.292747
F	-1.377587	-0.786883	-1.380111
F	-2.127868	-1.084964	0.660738

EPO-C(CF₃)₃

ACID-AB SCF Done: -1899.27107983 A.U.

O	-1.607816	-0.974456	0.867269
O	-1.141768	1.810212	-0.639273
H	-0.367280	1.190939	-0.483868
C	-2.437617	0.016649	0.499656
O	-3.853121	2.961611	-0.734005
C	-2.247969	1.206077	-0.160816
O	-4.527748	1.055635	0.321936
C	-3.564547	1.883987	-0.261296
O	-4.276420	-1.199428	-1.448440
H	-3.392988	-0.794205	-1.573388
O	-6.470557	-2.616027	-0.669985
H	-6.070019	-2.458891	-1.550031
C	-3.913602	-0.168375	0.746971
H	-4.122489	-0.324828	1.831893
C	-4.480931	-1.363888	-0.048172
H	-3.954064	-2.278169	0.327745
C	-5.990392	-1.545410	0.128437
H	-6.218688	-1.783289	1.190465
H	-6.480526	-0.571522	-0.119351
H	-0.658489	-0.703544	0.696918
O	0.731826	0.106353	0.149497
C	1.789583	0.816792	0.772881
H	1.756676	1.914345	0.615321
C	2.358558	0.031838	-0.334539
H	2.410224	0.497601	-1.324061
H	2.697864	-0.997826	-0.193388
I	5.350283	0.507153	-0.966941

C	1.990504	0.557933	2.294349
C	0.882018	1.399684	3.018489
F	1.154089	2.720120	2.906064
F	-0.328856	1.190764	2.457231
F	0.777961	1.105888	4.329974
C	1.842859	-0.940370	2.710971
F	2.258000	-1.134412	3.983850
F	0.553514	-1.340210	2.643480
F	2.565991	-1.759767	1.922966
C	3.405308	1.081937	2.732385
F	3.706303	2.222981	2.088566
F	3.436831	1.346231	4.064975
F	4.350904	0.170334	2.476184

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ACID-A+I SCF Done: -1899.27400645 A.U.

O	-1.521963	-1.107730	0.588348
O	-1.131902	2.005080	-0.150899
H	-0.357838	1.399539	-0.279494
C	-2.358330	-0.053897	0.553168
O	-3.819163	3.101786	0.243963
C	-2.201361	1.268927	0.225738
O	-4.442622	0.981534	0.807706
C	-3.515370	1.939388	0.396731
O	-4.362494	-0.713026	-1.511276
H	-3.451731	-0.376522	-1.633936
O	-6.498595	-2.323940	-0.963292
H	-6.165484	-1.946060	-1.803369
C	-3.816317	-0.307189	0.845523

H	-3.947041	-0.748035	1.862049
C	-4.456497	-1.251061	-0.195731
H	-3.915608	-2.228881	-0.120561
C	-5.950071	-1.486575	0.041371
H	-6.099067	-1.988153	1.022409
H	-6.447875	-0.486429	0.087701
H	-0.583876	-0.797272	0.463558
O	0.813505	0.128458	-0.026434
C	2.035259	0.500188	0.641309
H	2.317450	1.556496	0.477800
C	2.157513	0.132467	2.133430
C	2.134054	-0.411917	-0.508059
H	2.475419	-0.010535	-1.475357
H	2.253623	-1.495630	-0.363479
I	5.303335	-1.215982	-1.692992
C	2.116955	-1.405658	2.405346
F	1.086738	-1.992787	1.749629
F	3.249921	-1.995404	1.998840
F	1.951488	-1.662433	3.722501
C	0.981062	0.839956	2.894133
F	0.777308	2.081247	2.407073
F	-0.169708	0.149328	2.736060
F	1.220348	0.945645	4.216316
C	3.528747	0.715113	2.630277
F	3.462727	2.071696	2.657741
F	3.831511	0.293376	3.875426
F	4.518869	0.366875	1.806098

ACID-A SCF Done: -1887.66596186 A.U.

O	-0.322544	-1.455555	-0.324711
O	-1.542097	0.944328	1.416496
H	-1.995439	0.070221	1.395870
C	0.089415	-0.187635	-0.087853
O	0.412630	3.100344	1.026117
C	-0.414174	0.834016	0.662817
O	1.549156	1.623773	-0.293773
C	0.501177	1.996934	0.539518
O	2.686536	-0.490746	1.292554
H	1.868168	-0.856005	1.678952
O	5.000619	-0.911940	-0.144804
H	4.856401	-0.926749	0.823510
C	1.410068	0.246553	-0.669683
H	1.394568	0.173396	-1.782540
C	2.594602	-0.584351	-0.125673
H	2.432336	-1.641633	-0.455235
C	3.951674	-0.110881	-0.654777
H	3.968525	-0.193242	-1.762855
H	4.061332	0.970093	-0.391944
H	-1.252907	-1.576146	-0.031281
O	-3.055293	-1.158304	0.504569
C	-3.911743	-0.265903	-0.231891
C	-4.453849	-1.057410	0.891657
H	-3.693488	0.802246	-0.047931
H	-5.050349	-1.960759	0.690325
H	-4.630982	-0.546779	1.854982
C	-4.194217	-0.571656	-1.716854
C	-3.836078	-2.043173	-2.120435

F	-2.503165	-2.231487	-2.091197
F	-4.395572	-2.939296	-1.276379
F	-4.277268	-2.321034	-3.359871
C	-5.714928	-0.293151	-1.970278
F	-6.000572	-0.179588	-3.275531
F	-6.467239	-1.292228	-1.454861
F	-6.083157	0.849433	-1.351100
C	-3.318860	0.425044	-2.558379
F	-2.037823	0.374644	-2.134435
F	-3.344647	0.149293	-3.870132
F	-3.758351	1.688498	-2.376196

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ACID-B+CO2 SCF Done: -2087.76569720 A.U.

O	1.617151	-0.308362	-1.409371
O	0.557362	0.609649	1.423523
H	-0.004004	0.028578	0.795409
C	2.159132	0.464479	-0.470051
O	2.826056	2.207807	2.492390
C	1.723064	0.858768	0.774740
O	3.877412	1.714743	0.526932
C	2.788597	1.653777	1.411342
O	4.411706	-1.119367	0.530060
H	3.476985	-1.396983	0.632587
O	6.820204	-1.138137	-0.677233
H	6.380915	-1.677077	0.015685
C	3.597260	0.898710	-0.615803
H	3.760474	1.498049	-1.543594
C	4.531125	-0.333102	-0.650198

H	4.244880	-0.923194	-1.557889
C	6.015277	0.031059	-0.731283
H	6.224646	0.555730	-1.689539
H	6.236145	0.741062	0.104280
H	0.685659	-0.660821	-1.029438
O	-0.552814	-0.909022	-0.343654
C	-1.638715	-0.542478	-1.095842
H	-1.365419	-0.096608	-2.088476
C	-2.452461	-1.887158	-1.469108
C	-2.411987	0.524104	-0.267595
H	-1.649061	1.088322	0.297883
H	-3.167524	0.106385	0.418803
I	-3.481450	2.211137	-1.353082
O	-0.205945	-2.273413	2.534863
O	1.677558	-2.282169	1.130670
C	0.719580	-2.239176	1.815209
C	-1.637499	-2.631352	-2.579293
F	-1.732280	-1.964920	-3.758635
F	-0.332289	-2.740832	-2.291762
F	-2.108754	-3.888637	-2.788511
C	-2.559765	-2.817918	-0.212563
F	-2.861024	-2.123160	0.903885
F	-3.542895	-3.748340	-0.367830
F	-1.421913	-3.503103	0.015159
C	-3.879028	-1.604243	-2.022089
F	-3.853039	-0.646385	-2.968421
F	-4.464508	-2.690908	-2.585465
F	-4.700555	-1.188001	-1.025193

ACID-BC SCF Done: -2087.76527326 A.U.

O	1.614016	-0.277957	-1.399582
O	0.540621	0.572612	1.450234
H	-0.010519	-0.009069	0.815046
C	2.145825	0.482482	-0.444434
O	2.790391	2.172860	2.553341
C	1.704245	0.845692	0.807987
O	3.848802	1.732227	0.579346
C	2.759922	1.640505	1.461167
O	4.420807	-1.095426	0.515767
H	3.490054	-1.388328	0.609649
O	6.828866	-1.051858	-0.692111
H	6.396960	-1.613622	-0.012839
C	3.578218	0.938412	-0.581103
H	3.732193	1.560805	-1.495293
C	4.528963	-0.278954	-0.645246
H	4.250349	-0.851007	-1.566733
C	6.007924	0.107214	-0.717720
H	6.209507	0.657727	-1.663056
H	6.219575	0.799789	0.134669
H	0.684891	-0.647781	-1.028200
O	-0.549659	-0.926552	-0.351644
C	-1.638880	-0.557382	-1.096878
H	-1.371563	-0.095889	-2.084095
C	-2.444759	-1.902731	-1.485677
C	-2.416387	0.492042	-0.251000
H	-1.654432	1.056070	0.315984
H	-3.162184	0.057979	0.436063

I	-3.510612	2.183494	-1.305789
O	-0.179112	-2.356508	2.485369
O	1.693395	-2.312699	1.065781
C	0.755157	-2.334580	1.777216
C	-1.631879	-2.623305	-2.612383
F	-1.747379	-1.945618	-3.783355
F	-0.322350	-2.718201	-2.339050
F	-2.088535	-3.884532	-2.830916
C	-2.534461	-2.852983	-0.242358
F	-2.828183	-2.177466	0.887627
F	-3.513708	-3.786844	-0.401798
F	-1.390366	-3.535465	-0.036924
C	-3.877555	-1.624713	-2.024160
F	-3.867586	-0.652528	-2.955897
F	-4.456405	-2.708619	-2.600173
F	-4.695909	-1.231805	-1.015328

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ACID-B SCF Done: -1899.29429126 A.U.

O	1.697956	-1.140124	-0.644601
O	0.738352	0.610825	1.811313
H	0.219349	-0.215030	1.504431
C	2.192903	-0.035585	-0.102895
O	2.753091	2.791346	1.893994
C	1.805702	0.724343	0.985991
O	3.726476	1.733439	0.121153
C	2.740307	1.859636	1.114349
O	4.797622	-0.807141	0.974305
H	3.905118	-0.743202	1.379711

O	7.058353	-0.833078	-0.513167
H	6.849694	-1.103826	0.405516
C	3.498152	0.527132	-0.620032
H	3.431208	0.771497	-1.706933
C	4.655809	-0.469271	-0.404346
H	4.407819	-1.379912	-1.007261
C	6.017396	0.078551	-0.839000
H	6.029497	0.232957	-1.940643
H	6.154304	1.074342	-0.349186
H	0.789835	-1.387859	-0.087467
O	-0.370927	-1.432620	0.657192
C	-1.445064	-1.247912	-0.175534
H	-1.166167	-1.245298	-1.261818
C	-2.413801	-2.530758	-0.012309
C	-2.090477	0.126538	0.175254
H	-1.279074	0.758592	0.579012
H	-2.924203	0.072896	0.895077
I	-2.880745	1.414933	-1.517681
C	-2.575350	-2.889939	1.503705
F	-2.765653	-1.787032	2.263179
F	-3.661915	-3.689323	1.707366
F	-1.514396	-3.552041	1.991999
C	-3.819294	-2.317110	-0.645863
F	-3.720342	-1.780806	-1.877484
F	-4.532799	-3.464006	-0.776321
F	-4.567016	-1.476733	0.115163
C	-1.728529	-3.731345	-0.746142
F	-0.432918	-3.874331	-0.434919
F	-2.341533	-4.910459	-0.458201

F	-1.799693	-3.560338	-2.092114
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ACID-CD SCF Done: -2087.74942005 A.U.

O	1.793521	-0.083793	-1.773769
O	1.979200	2.670769	-0.128504
H	1.121941	2.460130	-0.593995
C	2.721236	0.435067	-0.953591
O	4.596406	2.459016	1.188229
C	2.797440	1.601555	-0.231137
O	4.771388	0.420698	0.180453
C	4.100266	1.611076	0.476761
O	2.904127	-1.380469	1.392400
H	2.177905	-0.749303	1.220376
O	4.297144	-3.700927	1.271553
H	3.650993	-3.328042	1.908144
C	3.925399	-0.411681	-0.620960
H	4.475702	-0.711036	-1.545192
C	3.529559	-1.689887	0.152373
H	2.837872	-2.265904	-0.512051
C	4.722316	-2.573825	0.521343
H	5.220013	-2.941530	-0.402906
H	5.456523	-1.939328	1.077896
H	0.965472	0.497132	-1.745340
O	-0.167960	1.599568	-1.342862
C	-1.078553	1.207835	-0.574867
O	-1.490837	-0.111838	-0.745968
O	-1.672644	1.855375	0.336793
C	-3.242810	0.627115	0.706620

H	-3.749677	1.159015	-0.100658
H	-3.346797	0.979806	1.735584
C	-2.356695	-0.543821	0.308118
H	-2.978756	-1.343548	-0.134505
I	-5.832321	-0.469896	0.839124
C	-1.506099	-1.279240	1.439547
C	-2.488728	-1.990794	2.444581
F	-3.246536	-1.089519	3.095849
F	-3.295002	-2.838177	1.778413
F	-1.837408	-2.707389	3.386765
C	-0.554641	-0.341807	2.256661
F	-1.240175	0.607431	2.916013
F	0.160392	-1.039716	3.164842
F	0.350809	0.281102	1.455849
C	-0.639201	-2.390692	0.720130
F	0.361583	-1.859022	-0.003860
F	-0.083633	-3.247725	1.600196
F	-1.414393	-3.113847	-0.119246

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ACID-C SCF Done: -2087.75553906 A.U.

O	-2.943636	-0.302383	1.317802
O	-1.626088	1.185898	-1.247990
H	-0.937423	0.985536	-0.530481
C	-3.427035	0.438025	0.321616
O	-3.950795	2.436893	-2.502575
C	-2.881265	1.052052	-0.787872
O	-5.184487	1.495878	-0.833989
C	-3.981459	1.744499	-1.506045

O	-5.196183	-1.372853	-1.135448
H	-4.248926	-1.141701	-1.251366
O	-7.745926	-1.873623	-0.363052
H	-7.164763	-2.249066	-1.057278
C	-4.929202	0.619188	0.268711
H	-5.316236	1.085778	1.206310
C	-5.638889	-0.735303	0.060925
H	-5.394100	-1.361947	0.956075
C	-7.157777	-0.611570	-0.077161
H	-7.594824	-0.237774	0.875109
H	-7.365940	0.145767	-0.873072
H	-1.985041	-0.669854	1.142250
O	0.313740	0.652176	0.421445
C	0.301728	-0.520319	0.864230
O	-0.635243	-1.321564	1.059470
O	1.574401	-1.090223	1.204389
C	2.707115	-0.237649	1.075978
H	2.389790	0.824031	1.152501
C	3.624983	-0.558318	2.325810
C	3.174494	-0.542440	-0.363156
H	2.262948	-0.423430	-0.975505
H	3.572896	-1.566738	-0.464346
I	4.610095	0.777461	-1.488984
C	2.696239	-0.841610	3.577665
F	1.667985	0.025424	3.625940
F	2.214167	-2.093458	3.578501
F	3.393286	-0.691101	4.735536
C	4.529985	-1.802317	2.087636
F	5.094874	-2.250232	3.232580

F	3.830260	-2.824145	1.553781
F	5.535737	-1.505608	1.230004
C	4.510162	0.684537	2.676646
F	3.731129	1.684308	3.153776
F	5.447222	0.405076	3.611119
F	5.156554	1.161021	1.600903

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ACID-DminusI SCF Done: -2076.15391098 A.U.

O	1.818207	-0.322575	-1.699696
O	2.217414	2.761099	-0.823270
H	1.329494	2.516540	-1.171345
C	2.809889	0.344004	-1.068587
O	4.897772	2.755065	0.339717
C	2.973868	1.647930	-0.682802
O	4.925260	0.513178	-0.090681
C	4.332636	1.774127	-0.083738
O	3.155190	-0.731278	1.714015
H	2.643923	0.047768	1.416536
O	4.361008	-3.165101	2.078907
H	3.956424	-2.569124	2.741404
C	3.989868	-0.456953	-0.578965
H	4.456245	-1.033427	-1.411156
C	3.595480	-1.434238	0.555251
H	2.779823	-2.087769	0.154053
C	4.758756	-2.315617	1.017431
H	5.094578	-2.961518	0.177509
H	5.607417	-1.642622	1.295097
H	1.089608	0.301433	-1.933170

O	-0.207110	1.569671	-1.608032
C	-0.983978	1.136263	-0.778346
O	-1.570616	-0.082637	-0.881083
O	-1.363919	1.777689	0.334228
C	-2.288730	0.961077	1.082981
H	-3.295182	1.421839	1.033189
H	-1.952940	0.918566	2.132416
C	-2.252124	-0.405966	0.340791
H	-3.267500	-0.753733	0.069866
C	-1.553539	-1.613027	1.056425
C	-1.260805	-2.732481	-0.017733
F	-0.150152	-2.441717	-0.713411
F	-1.097282	-3.931617	0.568181
F	-2.293178	-2.825400	-0.883348
C	-0.207546	-1.219135	1.752773
F	-0.432435	-0.595229	2.933429
F	0.566859	-2.280080	1.980797
F	0.467507	-0.342410	0.963743
C	-2.562377	-2.164411	2.118283
F	-3.086107	-1.136847	2.838744
F	-3.594577	-2.780326	1.504158
F	-1.988431	-3.021904	2.968572

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ACID-D SCF Done: -2087.77588427 A.U.

O	2.008807	-0.100006	-1.861025
O	2.109435	2.652072	-0.171553
H	1.309418	2.491716	-0.729162
C	2.890374	0.420107	-0.986392

O	4.636965	2.416268	1.281758
C	2.928942	1.577066	-0.252083
O	4.880742	0.399419	0.245164
C	4.191374	1.578186	0.528281
O	2.997648	-1.425578	1.349561
H	2.203283	-0.895325	1.148158
O	4.408604	-3.743809	1.233508
H	3.745628	-3.388295	1.862553
C	4.081706	-0.425310	-0.610671
H	4.676953	-0.702103	-1.513252
C	3.662864	-1.718317	0.126434
H	2.997485	-2.289799	-0.567496
C	4.849648	-2.600300	0.521372
H	5.382012	-2.945443	-0.391840
H	5.559132	-1.970420	1.114209
H	1.210737	0.494931	-1.928207
O	-0.032400	1.639357	-1.568032
C	-0.918516	1.160116	-0.864580
O	-1.232406	-0.146081	-0.879647
O	-1.650679	1.854607	0.002390
C	-2.647009	0.975516	0.596202
H	-3.638748	1.180013	0.134215
H	-2.669310	1.158691	1.682141
C	-2.182482	-0.435361	0.170836
H	-3.054118	-0.972276	-0.291961
I	-5.466687	-0.657173	-1.470023
C	-1.514385	-1.365065	1.236358
C	-0.762392	-2.531178	0.491245
F	0.440581	-2.106644	0.036013

F	-0.538376	-3.575744	1.317213
F	-1.473743	-2.969253	-0.555526
C	-0.500268	-0.626580	2.163170
F	-1.131610	0.150674	3.071549
F	0.297021	-1.475783	2.834141
F	0.309955	0.194087	1.433049
C	-2.668378	-1.974368	2.107458
F	-3.530348	-1.003978	2.488552
F	-3.353455	-2.891471	1.411756
F	-2.190301	-2.557858	3.228956

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EPO SCF Done: -1203.34282930 A.U.

O	-3.063223	-1.158270	0.504334
C	-3.897252	-0.270932	-0.221818
C	-4.443855	-1.061862	0.899625
H	-3.711345	0.807420	-0.054182
H	-5.064741	-1.949949	0.693219
H	-4.633208	-0.548449	1.861667
C	-4.191770	-0.572183	-1.712095
C	-3.832308	-2.042477	-2.116631
F	-2.502682	-2.230230	-2.111954
F	-4.384602	-2.942789	-1.275390
F	-4.291894	-2.319889	-3.357132
C	-5.707728	-0.294073	-1.968222
F	-5.995954	-0.169083	-3.276218
F	-6.466325	-1.294841	-1.465807
F	-6.084598	0.846603	-1.346773
C	-3.317626	0.418082	-2.555347

F	-2.036543	0.381143	-2.136623
F	-3.340526	0.143086	-3.870568
F	-3.761401	1.687083	-2.384025

EPO-CH₂F

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ACID-AB SCF Done: -988.058230523 A.U.

O	-1.150545	-0.941977	0.219010
O	-1.065590	2.010092	-1.013465
H	-0.235612	1.446355	-1.048857
C	-2.030368	0.069899	0.222445
O	-3.676270	3.119698	-0.231142
C	-2.007645	1.332420	-0.322976
O	-4.068616	1.098735	0.750564
C	-3.285207	2.000212	0.022391
O	-4.353755	-0.985680	-1.221235
H	-3.569799	-0.478241	-1.521388
O	-6.281667	-2.461891	0.000249
H	-6.134084	-2.209114	-0.934733
C	-3.375880	-0.152148	0.865849
H	-3.259838	-0.407537	1.945712
C	-4.165776	-1.274384	0.162732
H	-3.570751	-2.214398	0.291961
C	-5.568750	-1.480670	0.739239
H	-5.496129	-1.832190	1.791832
H	-6.084407	-0.488684	0.741763
H	-0.270433	-0.593958	-0.170868

O	0.922283	0.326503	-0.623330
C	1.685509	0.812036	0.499707
H	1.798748	1.916395	0.505301
C	2.606524	0.051624	-0.342555
H	3.151181	0.547414	-1.154281
H	2.706302	-1.032965	-0.211528
I	5.240891	0.143015	1.135423
C	1.300434	0.286194	1.862578
H	1.097815	-0.807017	1.816569
H	2.136880	0.477717	2.571123
F	0.145966	0.936719	2.303009

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ACID-A+I SCF Done: -988.061835086 A.U.

O	-1.186599	-1.051794	-0.053820
O	-1.084759	2.016062	-1.024735
H	-0.269644	1.465379	-1.157526
C	-2.022640	-0.009246	0.100477
O	-3.590122	3.110375	0.028411
C	-1.992780	1.294042	-0.328196
O	-3.977310	1.026148	0.869485
C	-3.222873	1.963723	0.163537
O	-4.500140	-0.879393	-1.223513
H	-3.709999	-0.418101	-1.574093
O	-6.351779	-2.420930	0.048326
H	-6.289599	-2.100892	-0.875303
C	-3.320095	-0.248363	0.829990
H	-3.122026	-0.590514	1.872904
C	-4.201003	-1.288653	0.109396

H	-3.628145	-2.250978	0.110289
C	-5.554883	-1.509120	0.788782
H	-5.401019	-1.936897	1.803447
H	-6.042962	-0.510193	0.906358
H	-0.320688	-0.716382	-0.436941
O	0.955732	0.282800	-0.793160
C	1.656584	0.704972	0.439071
H	1.697533	1.805018	0.544005
C	1.314469	-0.032154	1.701622
H	1.161234	-1.114519	1.497487
H	2.163577	0.085375	2.412421
C	2.422612	0.072104	-0.635260
H	3.048783	0.692633	-1.295898
H	2.720517	-0.984875	-0.538736
I	5.297872	-0.239669	1.321449
F	0.143152	0.496041	2.252286

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ACID-A SCF Done: -976.448503051 A.U.

O	-0.921064	-1.388450	0.255496
O	-1.456858	1.697444	1.026164
H	-2.035225	1.026508	1.450415
C	-0.281554	-0.233398	-0.048609
O	0.722467	3.094788	-0.319976
C	-0.498033	1.072329	0.293719
O	1.395817	1.042219	-1.057576
C	0.561569	1.897263	-0.347323
O	2.400344	-0.491384	1.158603
H	1.602478	-0.530630	1.719157

O	4.400448	-1.874685	-0.142645
H	4.394238	-1.491571	0.758373
C	0.995098	-0.317739	-0.846357
H	0.820056	-0.803223	-1.835226
C	2.100817	-1.096368	-0.095093
H	1.732785	-2.145282	0.035001
C	3.428793	-1.135445	-0.857411
H	3.279377	-1.631670	-1.840467
H	3.740445	-0.079883	-1.052972
H	-1.778236	-1.174409	0.712260
O	-3.265640	-0.369766	1.132381
C	-3.999147	0.140765	-0.018059
C	-4.629031	-0.821180	0.908257
H	-4.268762	1.209890	0.071180
H	-4.717968	-1.882324	0.610973
H	-5.356790	-0.464792	1.658708
C	-3.477362	-0.284739	-1.376640
H	-2.635881	0.376537	-1.682777
H	-3.100548	-1.331183	-1.330611
F	-4.509766	-0.184903	-2.295912

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ACID-B+CO2 SCF Done: -1176.54543554 A.U.

O	1.580837	-0.160424	-1.604244
O	0.585772	1.250553	1.046498
H	-0.012568	0.624774	0.501153
C	2.208314	0.619949	-0.723343
O	3.043387	2.604140	2.037611

C	1.797353	1.222988	0.445682
O	4.070132	1.702039	0.209582
C	2.954878	1.922278	1.035051
O	4.142805	-1.150331	0.601674
H	3.171810	-1.249208	0.699782
O	6.548179	-1.714594	-0.460472
H	6.000866	-2.074032	0.271150
C	3.702701	0.796371	-0.836362
H	3.999099	1.233316	-1.820599
C	4.422635	-0.561095	-0.662140
H	4.069512	-1.215877	-1.499655
C	5.948229	-0.451914	-0.714300
H	6.269636	-0.107907	-1.722286
H	6.257761	0.324866	0.028706
H	0.616072	-0.375614	-1.212198
O	-0.569914	-0.538727	-0.408568
C	-1.855838	-0.525818	-0.950102
H	-1.902708	-0.039765	-1.961517
C	-2.287211	-1.992909	-1.108549
H	-1.457623	-2.518667	-1.634697
H	-2.408410	-2.450452	-0.098890
C	-2.668605	0.300695	0.052376
H	-2.221349	1.305843	0.165816
H	-2.722544	-0.204858	1.036435
I	-4.834900	0.756477	-0.496716
O	-0.859615	-1.767125	2.140584
O	1.280188	-1.875714	1.179631
C	0.177010	-1.755404	1.579726
F	-3.463826	-2.166329	-1.837210

ACID-B SCF Done: -988.073280858 A.U.

O	1.520766	-1.303875	0.009713
O	0.590815	1.399397	1.343556
H	0.093810	0.540653	1.477080
C	2.004222	-0.082811	-0.076807
O	2.791440	3.268815	0.615929
C	1.644370	1.111291	0.517731
O	3.669168	1.518258	-0.561075
C	2.679024	2.111210	0.252280
O	4.189403	-1.486399	0.736004
H	3.245186	-1.787392	0.748498
O	6.698623	-1.417855	-0.267087
H	6.242326	-1.888274	0.463998
C	3.274869	0.173562	-0.872657
H	3.067053	0.129363	-1.969673
C	4.353089	-0.897216	-0.554292
H	4.260537	-1.688273	-1.342887
C	5.788067	-0.370509	-0.582883
H	6.034763	0.023645	-1.592843
H	5.853022	0.483409	0.134066
H	0.372305	-1.246067	0.733524
O	-0.594820	-1.042468	1.231312
C	-1.565949	-1.074766	0.200663
H	-1.083422	-1.206664	-0.798626
C	-2.443036	-2.295808	0.505887
H	-1.773918	-3.184016	0.566161
H	-2.918757	-2.151527	1.505059

C	-2.274182	0.283422	0.253474
H	-1.522460	1.095756	0.231472
H	-2.906211	0.380315	1.159411
I	-3.652058	0.758779	-1.475445
F	-3.434894	-2.538402	-0.442066

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ACID-CD SCF Done: -1176.53318912 A.U.

O	2.283749	-0.891442	-0.399973
O	2.363082	2.115880	0.761676
H	1.527027	1.579011	0.900882
C	3.211175	0.074838	-0.407280
O	5.032987	3.035388	-0.030206
C	3.261660	1.352064	0.110220
O	5.318216	0.962278	-0.935652
C	4.581188	1.930574	-0.245200
O	5.437278	-0.995763	1.174186
H	4.651920	-0.467138	1.431418
O	7.307540	-2.658996	0.115134
H	7.138382	-2.343603	1.027240
C	4.563332	-0.254437	-0.993875
H	4.474294	-0.579631	-2.057713
C	5.268957	-1.368671	-0.191272
H	4.624746	-2.280770	-0.276783
C	6.673804	-1.689513	-0.706839
H	6.611922	-2.103362	-1.737330
H	7.245228	-0.729608	-0.754477
H	1.455368	-0.556298	0.088240
O	0.404592	0.338239	0.876151

C	-0.848456	0.358474	0.746368
O	-1.416489	-0.738301	0.148712
O	-1.639284	1.283237	1.108436
C	-3.371179	0.718805	0.190343
H	-3.123741	1.352879	-0.668086
H	-3.899406	1.175776	1.032481
C	-2.862955	-0.715132	0.236797
H	-3.201449	-1.292915	-0.644457
I	-5.852437	0.302537	-0.919579
C	-3.324109	-1.418320	1.511351
H	-4.435034	-1.372408	1.562511
H	-2.892215	-0.895493	2.395919
F	-2.912584	-2.742903	1.514160

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ACID-C SCF Done: -1176.54217918 A.U.

O	-2.630387	-1.009312	1.070002
O	-1.656224	1.689682	-0.439454
H	-0.885322	1.201058	0.014079
C	-3.246109	0.091327	0.646754
O	-4.146776	3.206839	-0.671394
C	-2.847609	1.233149	-0.021838
O	-5.156312	1.437521	0.349405
C	-4.042329	2.099302	-0.184428
O	-5.094973	-0.856702	-1.401037
H	-4.180337	-0.500862	-1.446285
O	-7.528652	-1.895367	-0.824832
H	-7.007144	-1.806598	-1.650093
C	-4.750769	0.144090	0.810188

H	-5.049304	0.024743	1.879562
C	-5.430682	-0.965428	-0.019128
H	-5.068922	-1.939419	0.398537
C	-6.959071	-0.919148	0.037832
H	-7.306087	-1.132210	1.073187
H	-7.277530	0.119772	-0.225998
H	-1.678970	-1.155630	0.646526
O	0.436033	0.540879	0.593258
C	0.533575	-0.688039	0.350478
O	-0.354975	-1.547573	0.139125
O	1.839281	-1.239664	0.314590
C	2.939345	-0.332086	0.455731
H	2.678721	0.659810	0.026677
C	4.049831	-1.016477	-0.342865
H	3.655195	-1.321700	-1.329695
H	4.466752	-1.897874	0.183662
I	5.823112	0.275063	-0.833093
C	3.186446	-0.184480	1.961889
H	2.268668	0.259396	2.405347
H	3.356025	-1.196148	2.400223
F	4.277944	0.628414	2.252704

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ACID-DminusI SCF Done: -1164.93720770 A.U.

O	2.836593	-1.320216	2.168917
O	1.715487	1.611110	1.654784
H	1.629568	1.231330	2.553361
C	2.874703	-0.524254	1.083239
O	1.930680	1.892179	-1.223500

C	2.393825	0.734853	0.862828
O	3.181647	-0.016841	-1.180967
C	2.463907	1.002343	-0.587774
O	5.661305	0.123590	0.265955
H	5.314780	0.412096	1.131928
O	7.137734	-1.683871	-1.204123
H	7.416587	-0.836303	-0.801010
C	3.531845	-1.002257	-0.187888
H	3.100138	-1.982181	-0.495583
C	5.066739	-1.126455	-0.065344
H	5.270175	-1.899670	0.717878
C	5.738626	-1.566555	-1.370260
H	5.347124	-2.561443	-1.673021
H	5.453873	-0.832391	-2.164272
H	1.946193	-1.203442	2.604567
O	0.226420	-0.682501	2.772570
C	-0.307336	-0.284493	1.750270
O	-0.146223	-0.864521	0.539868
O	-1.094419	0.806977	1.678365
C	-1.164323	1.218777	0.291450
H	-0.381419	1.986154	0.114753
H	-2.173621	1.628910	0.093566
C	-0.845652	-0.084188	-0.471048
H	-0.134983	0.082172	-1.305173
C	-2.075176	-0.838111	-0.956280
H	-2.635929	-0.185109	-1.665741
H	-2.738598	-1.076481	-0.092048
F	-1.706923	-2.005183	-1.593723

ACID-D SCF Done: -1176.55369089 A.U.

O	2.590676	-0.607659	-1.086836
O	2.516772	2.240307	0.450368
H	1.648325	1.786672	0.301139
C	3.537018	0.268957	-0.706454
O	5.340427	2.983505	0.549011
C	3.512604	1.466532	-0.032138
O	5.751133	1.015046	-0.526391
C	4.911639	1.957776	0.068197
O	5.199575	-1.172802	1.251884
H	4.364927	-0.676498	1.380144
O	7.169221	-2.892619	0.468851
H	6.801205	-2.682190	1.351816
C	4.976983	-0.114057	-0.949455
H	5.165912	-0.302242	-2.032814
C	5.373460	-1.373358	-0.147775
H	4.723248	-2.207086	-0.517123
C	6.842330	-1.764571	-0.326817
H	7.032668	-2.030902	-1.389489
H	7.464619	-0.869042	-0.079802
H	1.690554	-0.280347	-0.800276
O	0.417516	0.611297	-0.145744
C	-0.789793	0.413085	0.006360
O	-1.414893	-0.671654	-0.452094
O	-1.595487	1.261262	0.642279
C	-2.986203	0.792369	0.514976
H	-3.528700	1.442230	-0.197631
H	-3.475474	0.868368	1.503095

C	-2.817911	-0.654285	0.007805
H	-3.461562	-0.876827	-0.864182
I	-6.430839	0.074614	0.118798
C	-3.005968	-1.703861	1.090334
H	-4.070731	-1.654029	1.415080
H	-2.335494	-1.479359	1.954776
F	-2.707484	-2.965194	0.600496

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EPO SCF Done: -292.121983151 A.U.

O	-3.228114	-0.864379	0.847710
C	-3.940088	0.073133	0.030554
C	-4.662604	-0.867553	0.911028
H	-3.861353	1.136378	0.339709
H	-5.165193	-1.751043	0.468532
H	-5.104626	-0.497943	1.857009
C	-3.847660	-0.169562	-1.461422
H	-2.888042	0.232200	-1.861109
H	-3.878281	-1.265255	-1.660620
F	-4.903496	0.460474	-2.112220

EPO-CH₂Cl

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ACID-AB SCF Done: -1348.40556761 A.U.

O	-1.145428	-0.864408	0.237450
O	-1.126709	2.080071	-1.006903
H	-0.271247	1.558337	-0.993644

C	-2.059608	0.116311	0.214200
O	-3.783217	3.116377	-0.277106
C	-2.064311	1.376088	-0.337376
O	-4.132874	1.089182	0.707758
C	-3.364776	2.009047	-0.013756
O	-4.335191	-1.028707	-1.238567
H	-3.565756	-0.498032	-1.536274
O	-6.231030	-2.545248	-0.015808
H	-6.081537	-2.300440	-0.952607
C	-3.404105	-0.138959	0.845832
H	-3.287754	-0.375586	1.930040
C	-4.153002	-1.293313	0.151079
H	-3.531631	-2.213340	0.298853
C	-5.554890	-1.533821	0.716917
H	-5.482226	-1.869304	1.774724
H	-6.099682	-0.557639	0.701356
H	-0.270087	-0.484186	-0.132170
O	0.916819	0.450305	-0.565180
C	1.775779	0.832863	0.521030
H	2.017713	1.915756	0.530921
C	2.571364	-0.009863	-0.374147
H	3.131036	0.439813	-1.202721
H	2.559422	-1.100982	-0.260854
I	5.252885	-0.214928	1.003383
C	1.419829	0.314964	1.896088
H	1.077864	-0.737656	1.850542
H	2.303338	0.395912	2.560633
Cl	0.060421	1.285564	2.617403

ACID-A+I SCF Done: -1348.39892593 A.U.

O	-1.239589	-0.948937	0.415873
O	-1.141783	2.004067	-0.881234
H	-0.317805	1.449164	-0.937216
C	-2.136558	0.054143	0.327811
O	-3.812640	3.050735	-0.304541
C	-2.103152	1.303464	-0.241193
O	-4.226676	1.042977	0.694719
C	-3.422367	1.945656	-0.000628
O	-4.344005	-1.014860	-1.305987
H	-3.481932	-0.656749	-1.600274
O	-6.293371	-2.589684	-0.218461
H	-6.099759	-2.343509	-1.146480
C	-3.526768	-0.196863	0.857744
H	-3.503938	-0.464437	1.940685
C	-4.237749	-1.326470	0.079709
H	-3.633819	-2.256231	0.238337
C	-5.671980	-1.574800	0.552993
H	-5.663964	-1.909605	1.613170
H	-6.218881	-0.600788	0.504315
H	-0.371659	-0.649502	0.004745
O	0.889209	0.297636	-0.495230
C	1.747183	0.783331	0.589659
H	1.829701	1.886437	0.619693
C	1.452189	0.138021	1.926919
H	0.414832	0.374997	2.239906
H	1.567509	-0.962736	1.875830
C	2.376418	0.057814	-0.522702

H	2.908599	0.607310	-1.314984
H	2.664344	-0.998758	-0.396947
I	5.819467	-0.564829	-0.443822
Cl	2.571946	0.775008	3.190149

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ACID-A SCF Done: -1336.79551402 A.U.

O	-0.917103	-1.387565	0.275302
O	-1.449837	1.703215	1.022636
H	-2.023919	1.035799	1.457941
C	-0.276802	-0.236008	-0.039074
O	0.725204	3.090110	-0.342210
C	-0.492640	1.072549	0.292778
O	1.396241	1.031517	-1.065133
C	0.564608	1.892371	-0.358660
O	2.409623	-0.481876	1.160562
H	1.613258	-0.514289	1.723716
O	4.405315	-1.876606	-0.135474
H	4.402939	-1.485033	0.761912
C	0.996987	-0.326793	-0.840658
H	0.818657	-0.821011	-1.824607
C	2.105672	-1.098339	-0.086373
H	1.738281	-2.146100	0.054566
C	3.430823	-1.144092	-0.853243
H	3.277856	-1.649283	-1.831175
H	3.741471	-0.090281	-1.059571
H	-1.770796	-1.167602	0.737099
O	-3.254583	-0.369086	1.165659
C	-3.990536	0.137536	0.007789

C	-4.607631	-0.843421	0.920100
H	-4.277513	1.200924	0.104518
H	-4.674558	-1.902019	0.608423
H	-5.351320	-0.510531	1.665661
C	-3.443928	-0.262713	-1.341987
H	-2.622747	0.415712	-1.648048
H	-3.058710	-1.301245	-1.327282
Cl	-4.771449	-0.141121	-2.562136

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ACID-B+CO2 SCF Done: -1536.89055159 A.U.

O	1.576102	-0.131632	-1.620790
O	0.569218	1.213870	1.062299
H	-0.031824	0.610774	0.496453
C	2.199577	0.623847	-0.715444
O	3.023312	2.534091	2.100216
C	1.783578	1.198124	0.465875
O	4.057959	1.679122	0.254085
C	2.939445	1.879529	1.079459
O	4.128843	-1.180456	0.573778
H	3.157179	-1.272870	0.670336
O	6.538104	-1.719453	-0.496233
H	5.991543	-2.097008	0.226620
C	3.694698	0.801425	-0.816869
H	3.995541	1.263590	-1.788035
C	4.413177	-0.560564	-0.674318
H	4.062432	-1.194200	-1.528910
C	5.938946	-0.450696	-0.719139
H	6.263339	-0.081278	-1.717090

H	6.246489	0.306823	0.044287
H	0.607407	-0.349049	-1.247319
O	-0.590674	-0.522893	-0.452735
C	-1.878047	-0.521615	-0.988819
H	-1.931403	-0.069639	-2.014027
C	-2.288218	-2.005370	-1.084760
H	-1.432445	-2.545270	-1.534291
H	-2.479578	-2.419242	-0.073791
C	-2.668888	0.340457	0.005035
H	-2.182444	1.328774	0.099020
H	-2.725749	-0.147732	0.997381
I	-4.822784	0.894221	-0.498447
O	-0.875168	-1.740001	2.128867
O	1.260256	-1.891133	1.162622
C	0.164534	-1.753194	1.575289
Cl	-3.737767	-2.388234	-2.128764

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ACID-BC SCF Done: -1536.89055016 A.U.

O	1.575181	-0.118171	-1.619218
O	0.572012	1.202938	1.077224
H	-0.030201	0.606084	0.505933
C	2.200382	0.627598	-0.707128
O	3.028453	2.510833	2.125467
C	1.785978	1.191191	0.479949
O	4.060792	1.671461	0.270892
C	2.943078	1.865671	1.098867
O	4.128632	-1.190432	0.565046
H	3.156732	-1.277563	0.664499

O	6.535748	-1.723690	-0.512371
H	5.990069	-2.106301	0.208459
C	3.695693	0.804013	-0.807799
H	3.996610	1.274571	-1.774891
C	4.412220	-0.560248	-0.677998
H	4.059319	-1.185942	-1.537567
C	5.938106	-0.452287	-0.724023
H	6.261690	-0.075244	-1.719382
H	6.247810	0.298492	0.045171
H	0.606372	-0.337938	-1.246992
O	-0.591019	-0.517774	-0.453392
C	-1.878583	-0.509792	-0.988986
H	-1.932088	-0.046561	-2.009159
C	-2.289775	-1.992090	-1.101098
H	-1.434608	-2.527603	-1.556916
H	-2.481159	-2.416953	-0.094735
C	-2.668417	0.341831	0.014664
H	-2.181395	1.328830	0.118982
H	-2.724776	-0.157011	1.001724
I	-4.822351	0.902126	-0.481271
O	-0.876066	-1.760209	2.116378
O	1.258792	-1.904844	1.147856
C	0.163457	-1.769435	1.562397
Cl	-3.739999	-2.362432	-2.148741

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ACID-B SCF Done: -1348.41705773 A.U.

O	1.458908	-1.265565	0.374302
O	0.647244	1.711864	1.008162

H	0.106223	0.929140	1.329988
C	1.971597	-0.117924	-0.037080
O	2.864477	3.269121	-0.224924
C	1.657963	1.194969	0.252918
O	3.656287	1.253100	-0.949381
C	2.710953	2.062328	-0.284853
O	4.167703	-1.300364	1.065225
H	3.224434	-1.566231	1.201610
O	6.620909	-1.626869	-0.029851
H	6.193914	-1.856421	0.823831
C	3.219628	-0.113889	-0.901672
H	2.981868	-0.428186	-1.947527
C	4.279511	-1.100379	-0.344467
H	4.118023	-2.073464	-0.876324
C	5.726289	-0.667277	-0.581369
H	5.928169	-0.577802	-1.671091
H	5.856956	0.347097	-0.132541
H	0.318766	-0.980514	1.004589
O	-0.660166	-0.592383	1.397515
C	-1.561527	-0.576398	0.304971
H	-1.204982	0.068441	-0.537338
C	-1.656452	-2.030969	-0.188889
H	-0.617572	-2.382859	-0.344668
H	-2.149155	-2.667041	0.574850
C	-2.815166	0.031315	0.940620
H	-2.539247	0.987446	1.422381
H	-3.259250	-0.655048	1.688200
I	-4.523966	0.624614	-0.414924
Cl	-2.519191	-2.284300	-1.772786

ACID-CD SCF Done: -1536.87845116 A.U.

O	2.280572	-0.880369	-0.405594
O	2.369065	2.124685	0.763035
H	1.530529	1.591555	0.898912
C	3.211514	0.082726	-0.408715
O	5.043923	3.035214	-0.020886
C	3.265816	1.358536	0.111546
O	5.322898	0.963303	-0.930991
C	4.588407	1.932684	-0.239636
O	5.431706	-1.000017	1.173970
H	4.645647	-0.473608	1.433304
O	7.295840	-2.669466	0.113091
H	7.126535	-2.356402	1.025964
C	4.563498	-0.250365	-0.993558
H	4.475080	-0.572585	-2.058348
C	5.263420	-1.369283	-0.192456
H	4.615664	-2.278578	-0.280924
C	6.667634	-1.694710	-0.706811
H	6.605471	-2.105097	-1.738658
H	7.243300	-0.737155	-0.750672
H	1.452472	-0.543971	0.080846
O	0.400440	0.355494	0.867620
C	-0.851607	0.378987	0.737317
O	-1.421637	-0.713853	0.132596
O	-1.641978	1.303603	1.101511
C	-3.370144	0.742747	0.178232
H	-3.120408	1.370105	-0.685063

H	-3.900038	1.204061	1.016523
C	-2.864068	-0.694727	0.228285
H	-3.209579	-1.272553	-0.649603
I	-5.855294	0.311448	-0.921931
C	-3.335593	-1.371500	1.516794
H	-4.442671	-1.355523	1.551525
H	-2.926683	-0.834267	2.396389
Cl	-2.802621	-3.095849	1.619888

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ACID-C SCF Done: -1536.89183819 A.U.

O	-2.606646	-1.129551	0.892156
O	-1.651486	1.753361	-0.247402
H	-0.874166	1.207967	0.123848
C	-3.225933	0.018811	0.632894
O	-4.143433	3.285649	-0.227866
C	-2.836346	1.242498	0.122257
O	-5.139187	1.391255	0.553797
C	-4.032570	2.121340	0.099311
O	-5.111187	-0.639337	-1.496690
H	-4.194028	-0.287650	-1.510001
O	-7.535129	-1.751143	-1.027834
H	-7.025796	-1.550823	-1.841115
C	-4.727834	0.047174	0.825339
H	-5.009304	-0.218761	1.872804
C	-5.422720	-0.938263	-0.137502
H	-5.055028	-1.960121	0.135665
C	-6.949840	-0.902186	-0.048880
H	-7.279461	-1.255902	0.953147

H	-7.271397	0.162819	-0.161974
H	-1.653282	-1.214729	0.455504
O	0.448772	0.488105	0.614061
C	0.560525	-0.709511	0.242356
O	-0.320725	-1.542674	-0.073819
O	1.868677	-1.244625	0.171236
C	2.945335	-0.359263	0.451548
H	2.744223	0.655360	0.042486
C	4.220446	-0.960238	-0.117361
H	4.305389	-2.032674	0.144820
H	5.110252	-0.397970	0.221138
I	4.313582	-0.913389	-2.354315
C	3.050229	-0.232071	1.987416
H	2.094298	0.190287	2.350276
H	3.240583	-1.219261	2.454633
Cl	4.375629	0.901841	2.517682

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ACID-DminusI SCF Done: -1525.29374398 A.U.

O	2.486763	0.376410	-2.453763
O	2.495844	3.267220	-1.143892
H	1.577342	2.960174	-1.333200
C	3.237855	0.924892	-1.482504
O	4.641868	3.050005	0.903246
C	3.245060	2.165097	-0.904042
O	4.823320	0.867877	0.235268
C	4.271840	2.171314	0.161421
O	2.462176	-0.316905	1.065146
H	3.044459	0.345035	1.499031

O	3.323013	-2.837283	1.711659
H	2.878143	-2.179568	2.285078
C	4.133285	0.013989	-0.690431
H	4.874575	-0.525293	-1.322815
C	3.285884	-1.006087	0.108415
H	2.582729	-1.499840	-0.596902
C	4.130967	-2.061263	0.836288
H	4.586440	-2.754760	0.098459
H	4.964410	-1.548012	1.378110
H	1.636626	0.881981	-2.512069
O	0.300015	1.594528	-1.448750
C	-0.021471	0.759607	-0.616245
O	0.002859	-0.566979	-0.845896
O	-0.473088	1.053158	0.615789
C	-0.633959	-0.176393	1.360864
H	-1.571269	-0.117151	1.945090
H	0.244917	-0.295601	2.025974
C	-0.660994	-1.251123	0.251774
H	-1.697677	-1.467413	-0.090424
C	0.035958	-2.550017	0.613611
H	-0.525961	-3.036188	1.438054
H	1.082981	-2.399187	0.939084
Cl	0.068432	-3.688202	-0.784884

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ACID-D SCF Done: -1536.89917415 A.U.

O	2.586107	-0.594257	-1.089205
O	2.523171	2.251011	0.454264
H	1.652859	1.802611	0.301284

C	3.535815	0.277449	-0.705569
O	5.350102	2.980101	0.559606
C	3.516067	1.473594	-0.028818
O	5.753118	1.012685	-0.520586
C	4.917279	1.957633	0.075419
O	5.190349	-1.176339	1.251706
H	4.351553	-0.687781	1.381707
O	7.150843	-2.905469	0.465355
H	6.781255	-2.696923	1.348123
C	4.974322	-0.111698	-0.947459
H	5.163825	-0.298144	-2.031034
C	5.363837	-1.374832	-0.148288
H	4.709904	-2.204552	-0.520016
C	6.830860	-1.772984	-0.326735
H	7.021183	-2.036437	-1.390116
H	7.457410	-0.881509	-0.075787
H	1.687042	-0.263783	-0.803923
O	0.414875	0.635852	-0.151864
C	-0.792591	0.440110	-0.001065
O	-1.421031	-0.639674	-0.466697
O	-1.597216	1.287202	0.639045
C	-2.987494	0.824262	0.494596
H	-3.513537	1.464264	-0.239574
H	-3.494942	0.915966	1.471487
C	-2.818075	-0.631314	0.007908
H	-3.470654	-0.867945	-0.853081
I	-6.424745	0.042076	0.161028
C	-2.998979	-1.652648	1.119694
H	-4.070524	-1.637258	1.412542

H	-2.360559	-1.402947	1.992982
Cl	-2.571152	-3.324880	0.583465

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EPO SCF Done: -652.468527156 A.U.

O	-3.215275	-0.874926	0.896470
C	-3.910723	0.056570	0.056042
C	-4.652488	-0.874659	0.927733
H	-3.834787	1.122342	0.354502
H	-5.147801	-1.758703	0.478695
H	-5.115056	-0.498517	1.861031
C	-3.787726	-0.203374	-1.427790
H	-2.839288	0.203729	-1.832289
H	-3.828449	-1.291126	-1.636126
Cl	-5.147864	0.605113	-2.319098

EPO-CH₂Br

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ACID-AB SCF Done: -3462.42921788 A.U.

O	-1.159059	-0.829074	0.335048
O	-1.144953	2.092644	-0.963665
H	-0.288788	1.573100	-0.939702
C	-2.086158	0.137140	0.264941
O	-3.832250	3.106336	-0.324051
C	-2.092207	1.386137	-0.311099
O	-4.185223	1.090068	0.681790
C	-3.408687	2.007981	-0.033028

O	-4.300345	-1.047397	-1.249778
H	-3.526277	-0.513151	-1.528639
O	-6.216099	-2.576711	-0.074430
H	-6.039830	-2.338836	-1.008349
C	-3.447396	-0.128020	0.855843
H	-3.366334	-0.354672	1.945319
C	-4.159709	-1.297672	0.147131
H	-3.532484	-2.208700	0.323341
C	-5.576195	-1.550276	0.669730
H	-5.533777	-1.875043	1.732526
H	-6.131831	-0.581009	0.627206
H	-0.284963	-0.453454	-0.040189
O	0.903109	0.462255	-0.517350
C	1.824473	0.833424	0.519470
H	2.099789	1.908148	0.499973
C	2.548695	-0.042800	-0.405175
H	3.081201	0.380832	-1.265018
H	2.512473	-1.131591	-0.275619
I	5.276282	-0.302522	0.866478
C	1.527013	0.334895	1.913208
H	1.155637	-0.707728	1.905663
H	2.430684	0.418630	2.547617
Br	0.094617	1.421243	2.751905

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ACID-A+I SCF Done: -3462.42256651 A.U.

O	-1.226865	-0.987636	0.330351
O	-1.136233	2.001995	-0.879346
H	-0.319993	1.442542	-0.975265

C	-2.115724	0.024976	0.298972
O	-3.780475	3.053555	-0.198794
C	-2.086295	1.290863	-0.232654
O	-4.186568	1.019985	0.750507
C	-3.392419	1.936693	0.061907
O	-4.375276	-0.976404	-1.306094
H	-3.516384	-0.622562	-1.614236
O	-6.309391	-2.566698	-0.213754
H	-6.137581	-2.295209	-1.138998
C	-3.493820	-0.229882	0.858125
H	-3.444289	-0.529604	1.931681
C	-4.235342	-1.329974	0.066568
H	-3.636218	-2.269162	0.181671
C	-5.658892	-1.580024	0.570198
H	-5.626097	-1.945748	1.619606
H	-6.198011	-0.600507	0.564316
H	-0.359073	-0.672652	-0.070898
O	0.896872	0.286058	-0.551166
C	1.723192	0.794637	0.552504
H	1.816611	1.897029	0.549944
C	1.370394	0.186601	1.888836
H	0.366626	0.522236	2.216209
H	1.396216	-0.919190	1.853999
C	2.380001	0.030359	-0.516955
H	2.947992	0.551265	-1.303668
H	2.652790	-1.024549	-0.349502
I	5.826744	-0.551668	-0.342958
Br	2.650507	0.774678	3.261453

ACID-A SCF Done: -3450.81938520 A.U.

O	-0.908698	-1.390968	0.288948
O	-1.442523	1.698464	1.044263
H	-2.021928	1.029375	1.470158
C	-0.272738	-0.237451	-0.027351
O	0.724965	3.090344	-0.326781
C	-0.489172	1.070291	0.307586
O	1.395275	1.034098	-1.056866
C	0.565045	1.892522	-0.345821
O	2.417185	-0.485401	1.161817
H	1.624467	-0.526615	1.729475
O	4.410840	-1.871988	-0.145862
H	4.409771	-1.484279	0.753223
C	0.997861	-0.325072	-0.834301
H	0.816367	-0.816980	-1.818885
C	2.110192	-1.097670	-0.086527
H	1.745072	-2.146541	0.051714
C	3.432948	-1.138332	-0.857824
H	3.277679	-1.640004	-1.837208
H	3.741267	-0.083249	-1.061102
H	-1.765104	-1.173358	0.746311
O	-3.250144	-0.370466	1.167052
C	-3.982571	0.140637	0.004519
C	-4.609008	-0.826777	0.925436
H	-4.252574	1.208548	0.098357
H	-4.691584	-1.885936	0.619302
H	-5.348070	-0.479389	1.669000
C	-3.434975	-0.275722	-1.336569

H	-2.624394	0.402488	-1.665985
H	-3.055349	-1.314941	-1.317569
Br	-4.877238	-0.170911	-2.675477

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ACID-B+CO2 SCF Done: -3650.91452318 A.U.

O	1.575291	-0.120181	-1.617711
O	0.570765	1.184765	1.085994
H	-0.030169	0.589176	0.511982
C	2.198901	0.624094	-0.702953
O	3.023575	2.496831	2.137352
C	1.783907	1.181483	0.486530
O	4.056372	1.670987	0.276985
C	2.939464	1.856843	1.107520
O	4.136778	-1.192062	0.556642
H	3.165767	-1.288536	0.654884
O	6.545198	-1.708762	-0.528003
H	6.003111	-2.098353	0.191758
C	3.693213	0.807279	-0.805474
H	3.990314	1.284142	-1.770622
C	4.416076	-0.554207	-0.683526
H	4.065500	-1.177181	-1.545978
C	5.941426	-0.438888	-0.730641
H	6.261884	-0.053985	-1.723974
H	6.248628	0.308427	0.042892
H	0.607750	-0.342507	-1.248255
O	-0.594330	-0.524547	-0.454556
C	-1.882399	-0.503617	-0.989620
H	-1.931099	-0.034294	-2.006943

C	-2.277436	-1.989277	-1.096976
H	-1.432555	-2.522746	-1.570332
H	-2.464822	-2.420141	-0.093538
C	-2.668228	0.343030	0.022907
H	-2.153273	1.311773	0.157869
H	-2.752964	-0.176931	0.996944
I	-4.792625	0.986783	-0.486269
O	-0.862110	-1.747766	2.141882
O	1.267775	-1.907143	1.164327
C	0.177071	-1.767424	1.588623
Br	-3.860068	-2.443948	-2.227881

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ACID-BC SCF Done: -3650.91188450 A.U.

O	1.568745	-0.205846	-1.669598
O	0.631732	1.668945	0.702091
H	0.063406	0.888187	0.395318
C	2.229010	0.690745	-0.921852
O	3.141472	3.073858	1.466980
C	1.839795	1.493598	0.123362
O	4.133251	1.819977	-0.161516
C	3.028752	2.230774	0.599280
O	4.007584	-0.911188	0.760039
H	3.039876	-1.076900	0.813737
O	6.395371	-1.800454	-0.083864
H	5.792252	-1.982656	0.670599
C	3.729353	0.755111	-1.029627
H	4.073347	0.980287	-2.067803
C	4.356018	-0.587782	-0.577953

H	3.984734	-1.365866	-1.292674
C	5.887376	-0.577246	-0.595294
H	6.255392	-0.449916	-1.637575
H	6.227152	0.308015	-0.001537
H	0.647017	-0.356197	-1.237824
O	-0.554215	-0.459765	-0.266737
C	-1.887610	-0.402728	-0.699950
H	-1.996165	0.397696	-1.471312
C	-2.350922	-1.753028	-1.313165
H	-1.532817	-2.490465	-1.245257
H	-3.254556	-2.168112	-0.828815
C	-2.687481	0.005063	0.547254
H	-2.312206	0.965195	0.947457
H	-2.658941	-0.783097	1.323010
I	-4.890718	0.392882	0.176145
O	-0.924880	-2.538018	1.263050
O	1.218854	-1.638723	1.097323
C	0.056990	-1.901829	1.014488
Br	-2.799573	-1.626450	-3.246911

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ACID-B SCF Done: -3462.44069447 A.U.

O	1.459456	-1.265706	0.382432
O	0.648305	1.708172	1.028589
H	0.107252	0.924239	1.346266
C	1.969199	-0.116390	-0.029348
O	2.856980	3.271979	-0.211762
C	1.655557	1.194944	0.266139
O	3.647801	1.258888	-0.945269

C	2.704919	2.065294	-0.274428
O	4.178896	-1.283265	1.067366
H	3.239732	-1.555794	1.214212
O	6.621164	-1.621418	-0.050404
H	6.203137	-1.844925	0.809264
C	3.213917	-0.109008	-0.898153
H	2.973857	-0.422772	-1.943626
C	4.277408	-1.093149	-0.344908
H	4.108782	-2.069350	-0.868523
C	5.722439	-0.663884	-0.598584
H	5.913366	-0.581502	-1.690839
H	5.859100	0.353022	-0.157319
H	0.328417	-0.984868	1.009628
O	-0.659509	-0.600156	1.402630
C	-1.555237	-0.584786	0.304687
H	-1.179924	0.038015	-0.545733
C	-1.660821	-2.051748	-0.144777
H	-0.628582	-2.421798	-0.294653
H	-2.171666	-2.663922	0.624555
C	-2.802040	0.053340	0.926026
H	-2.501496	0.995483	1.420050
H	-3.276821	-0.625808	1.661070
I	-4.472176	0.718440	-0.441755
Br	-2.578260	-2.406016	-1.873355

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ACID-CD SCF Done: -3650.90208247 A.U.

O	2.279481	-0.878592	-0.402329
O	2.371588	2.128399	0.762186

H	1.532777	1.596690	0.899633
C	3.211068	0.083975	-0.407649
O	5.046196	3.035432	-0.025506
C	3.266910	1.360392	0.110721
O	5.322575	0.962157	-0.933285
C	4.589670	1.932983	-0.242446
O	5.432671	-0.998006	1.174201
H	4.645876	-0.473509	1.434992
O	7.293423	-2.671414	0.113235
H	7.125530	-2.357261	1.025991
C	4.562203	-0.251012	-0.993363
H	4.472414	-0.574666	-2.057597
C	5.262096	-1.369336	-0.191362
H	4.613424	-2.278189	-0.277584
C	6.665342	-1.696884	-0.706982
H	6.601478	-2.108334	-1.738296
H	7.241992	-0.740001	-0.752615
H	1.452015	-0.541207	0.083662
O	0.399125	0.361606	0.869349
C	-0.852143	0.386037	0.737320
O	-1.422518	-0.704939	0.127956
O	-1.643873	1.308963	1.103040
C	-3.368275	0.753706	0.175879
H	-3.119587	1.381799	-0.687370
H	-3.899946	1.212241	1.014400
C	-2.864170	-0.686206	0.222528
H	-3.209338	-1.257854	-0.659542
I	-5.856333	0.326157	-0.921225
C	-3.343834	-1.353389	1.511753

H	-4.450361	-1.357688	1.537018
H	-2.944810	-0.817754	2.395421
Br	-2.755554	-3.229024	1.661368

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ACID-C SCF Done: -3650.91036860 A.U.

O	-2.630434	-1.066762	0.993809
O	-1.659732	1.700052	-0.390898
H	-0.887015	1.189015	0.031785
C	-3.245081	0.057213	0.633682
O	-4.144724	3.238689	-0.516012
C	-2.848370	1.229066	0.018679
O	-5.151244	1.425479	0.427812
C	-4.040506	2.107882	-0.086146
O	-5.126786	-0.778803	-1.434769
H	-4.209786	-0.428939	-1.475852
O	-7.557565	-1.834841	-0.876092
H	-7.047909	-1.707734	-1.703722
C	-4.747159	0.108868	0.818728
H	-5.032730	-0.061822	1.884683
C	-5.443870	-0.954857	-0.055485
H	-5.081672	-1.950137	0.308139
C	-6.971072	-0.904560	0.025021
H	-7.304839	-1.166425	1.053503
H	-7.287670	0.147472	-0.183221
H	-1.684173	-1.193957	0.557170
O	0.436940	0.497928	0.578821
C	0.532345	-0.720647	0.283985
O	-0.356661	-1.566896	0.030268

O	1.837590	-1.272800	0.230072
C	2.935449	-0.372334	0.429844
H	2.696851	0.615364	-0.018942
C	4.142243	-1.057649	-0.233770
H	3.780528	-1.831572	-0.935032
H	4.849735	-1.494228	0.497784
I	5.427065	0.279490	-1.506412
C	3.068212	-0.209833	1.950159
H	2.162871	0.299747	2.327927
H	3.184970	-1.200835	2.431483
Br	4.616642	0.885692	2.522614

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ACID-DminusI SCF Done: -3639.31712976 A.U.

O	2.549686	0.422321	-2.431901
O	2.421197	3.296118	-1.089293
H	1.520429	2.960583	-1.312990
C	3.251721	0.984302	-1.431907
O	4.508247	3.123829	1.021840
C	3.199432	2.216696	-0.839418
O	4.783815	0.957461	0.334501
C	4.191443	2.243130	0.258202
O	2.447357	-0.309581	1.086176
H	3.004078	0.356998	1.546073
O	3.339985	-2.822843	1.702321
H	2.861278	-2.184357	2.270536
C	4.151169	0.093336	-0.621769
H	4.928601	-0.415032	-1.236063
C	3.309549	-0.961400	0.137653

H	2.635064	-1.455436	-0.594750
C	4.157036	-2.013424	0.866208
H	4.647031	-2.682181	0.127732
H	4.964143	-1.495144	1.442210
H	1.685094	0.899353	-2.512370
O	0.293506	1.556097	-1.485326
C	-0.025023	0.710610	-0.662408
O	0.032197	-0.614558	-0.896830
O	-0.503974	0.988984	0.562643
C	-0.646212	-0.247359	1.300605
H	-1.590746	-0.211628	1.874974
H	0.228780	-0.352316	1.972857
C	-0.640837	-1.316636	0.184568
H	-1.671270	-1.538699	-0.172858
C	0.064933	-2.606353	0.554344
H	-0.496576	-3.103808	1.370332
H	1.113662	-2.457103	0.873984
Br	0.118552	-3.867936	-0.953336

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ACID-D SCF Done: -3650.92277638 A.U.

O	2.585315	-0.591909	-1.087807
O	2.526373	2.255267	0.453198
H	1.655369	1.808445	0.300442
C	3.536029	0.279277	-0.705381
O	5.354001	2.980941	0.556518
C	3.518011	1.476057	-0.029807
O	5.754276	1.012080	-0.522007
C	4.919831	1.958582	0.073311

O	5.190174	-1.174361	1.252837
H	4.350469	-0.687562	1.383250
O	7.147919	-2.907040	0.466490
H	6.779225	-2.697613	1.349408
C	4.973978	-0.111845	-0.947411
H	5.162830	-0.299627	-2.030857
C	5.362425	-1.374598	-0.147062
H	4.707388	-2.204005	-0.517457
C	6.828906	-1.774569	-0.325954
H	7.018478	-2.038723	-1.389288
H	7.456535	-0.883678	-0.075679
H	1.686692	-0.260400	-0.803067
O	0.414483	0.643085	-0.152180
C	-0.792864	0.448745	-0.001608
O	-1.422680	-0.630352	-0.467935
O	-1.597341	1.296054	0.638576
C	-2.986898	0.834563	0.493445
H	-3.513289	1.473072	-0.242095
H	-3.495544	0.926254	1.469548
C	-2.818817	-0.623270	0.006525
H	-3.472533	-0.854387	-0.855179
I	-6.423072	0.049418	0.173850
C	-3.005707	-1.634127	1.124756
H	-4.078650	-1.628821	1.410260
H	-2.368382	-1.391916	1.999433
Br	-2.542655	-3.469595	0.569318

O	-3.214881	-0.889277	0.910709
C	-3.898620	0.050607	0.066973
C	-4.651608	-0.876140	0.934478
H	-3.813485	1.114574	0.368325
H	-5.152814	-1.755053	0.482036
H	-5.116258	-0.495551	1.864910
C	-3.761196	-0.214621	-1.412087
H	-2.824791	0.208760	-1.824268
H	-3.800470	-1.300254	-1.625276
Br	-5.245334	0.643405	-2.406629

EPO-Cycle

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ACID-AB SCF Done: -1005.56513512 A.U.

O	-1.420533	-0.847912	0.615973
O	-1.186665	2.016758	-0.763835
H	-0.368903	1.417024	-0.708375
C	-2.313451	0.127890	0.406209
O	-3.919216	3.099946	-0.498519
C	-2.222486	1.357904	-0.210555
O	-4.434957	1.119903	0.509411
C	-3.554094	2.005159	-0.125511
O	-4.293522	-1.023490	-1.416725
H	-3.470558	-0.514005	-1.578638
O	-6.386790	-2.520663	-0.543544
H	-6.062837	-2.291466	-1.439399
C	-3.752663	-0.108969	0.793100

H	-3.849289	-0.338014	1.881223
C	-4.368418	-1.270951	-0.015030
H	-3.787947	-2.189986	0.255496
C	-5.851257	-1.500507	0.287004
H	-5.975802	-1.821229	1.344711
H	-6.379012	-0.523225	0.158592
H	-0.502036	-0.531629	0.237355
O	0.663312	0.246798	-0.304053
C	1.705958	0.594340	0.625808
H	1.902065	1.686525	0.645709
C	1.557158	-0.009268	2.028987
H	2.062849	0.651046	2.762724
H	0.471042	0.003880	2.266859
C	2.478058	-0.153846	-0.384986
H	2.800730	0.386098	-1.284564
I	5.279776	0.601454	0.492028
C	2.119183	-1.441739	2.134184
H	3.221115	-1.381124	2.271258
H	1.703298	-1.944781	3.033523
C	2.534286	-1.658953	-0.356437
H	2.111477	-2.052939	-1.307004
H	3.609356	-1.935238	-0.356801
C	1.829728	-2.271383	0.871879
H	2.179171	-3.317420	1.006358
H	0.733084	-2.326173	0.699829

O	-1.572089	0.102322	1.737105
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O	-1.237578	2.516138	-0.349901
H	-0.420601	2.189749	0.117257
C	-2.410295	0.670174	0.855205
O	-3.900700	2.689791	-1.574493
C	-2.261508	1.684852	-0.061076
O	-4.458253	0.913468	-0.255695
C	-3.567354	1.873173	-0.744751
O	-2.943504	-1.467579	-1.039004
H	-2.311986	-0.717249	-1.058976
O	-4.915737	-3.320290	-0.640312
H	-4.242268	-3.236977	-1.346666
C	-3.784257	0.069501	0.688605
H	-4.353020	0.072039	1.648089
C	-3.691356	-1.382110	0.173056
H	-3.185343	-1.970310	0.979551
C	-5.057217	-2.005964	-0.126480
H	-5.654310	-2.070359	0.809776
H	-5.595230	-1.324111	-0.830566
H	-0.629890	0.416186	1.533793
O	0.660547	1.036509	0.800167
C	2.085265	0.618715	0.891970
H	2.784361	1.466504	0.785566
C	2.402193	-0.387957	1.970759
H	3.449407	-0.702058	1.761943
H	2.392576	0.115252	2.962773
C	1.302177	0.232581	-0.292457
H	1.436450	0.839233	-1.204426
I	4.849978	-0.627645	-1.196694
C	1.474061	-1.617218	1.942143

H	1.875130	-2.387460	2.634560
H	0.460712	-1.357016	2.322192
C	0.765706	-1.175644	-0.473659
H	-0.343139	-1.144964	-0.377375
H	0.982858	-1.487543	-1.515154
C	1.373582	-2.186242	0.517252
H	2.397717	-2.438707	0.163540
H	0.773815	-3.120968	0.509093

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ACID-A SCF Done: -993.969538543 A.U.

O	-0.636212	-1.438284	0.540418
O	-1.424170	1.668337	0.752670
H	-1.981113	1.017694	1.238462
C	-0.082300	-0.313518	0.031882
O	0.648309	2.984681	-0.836542
C	-0.408901	1.011143	0.137565
O	1.504309	0.897328	-1.183275
C	0.586839	1.792716	-0.643177
O	2.587929	-0.113695	1.276589
H	1.752061	-0.030298	1.774826
O	4.716619	-1.545668	0.273009
H	4.659468	-1.000234	1.084025
C	1.212791	-0.431476	-0.730789
H	1.100596	-1.101437	-1.615513
C	2.360567	-0.964441	0.158495
H	2.069149	-1.995742	0.483014
C	3.702197	-1.041773	-0.575655
H	3.612737	-1.730506	-1.443352

H	3.932397	-0.022054	-0.971762
H	-1.544629	-1.217022	0.892199
O	-3.054299	-0.482264	1.171897
C	-3.916048	-0.163315	0.018679
C	-4.400470	-1.042116	1.115033
H	-4.218806	0.899798	0.032317
H	-5.073857	-0.607157	1.878416
C	-3.480635	-0.728727	-1.323304
H	-3.912114	-0.096048	-2.126364
H	-2.378664	-0.599090	-1.397393
C	-3.878198	-2.205621	-1.518459
H	-4.959977	-2.262863	-1.777492
H	-3.327254	-2.627137	-2.384373
C	-4.482443	-2.541816	0.921093
H	-4.205619	-3.046714	1.872089
H	-5.554725	-2.783293	0.740900
C	-3.623441	-3.044358	-0.255786
H	-3.853382	-4.113247	-0.444586
H	-2.544485	-2.998495	0.005637

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ACID-B+CO2 SCF Done: -1194.04283869 A.U.

O	0.453039	0.788054	-2.865293
O	-0.460095	3.143098	-0.968176
H	-0.547771	2.211821	-0.623711
C	0.782577	2.092364	-2.838615
O	1.078749	5.469592	-2.003161
C	0.409481	3.112778	-2.003650
O	1.992869	3.985367	-3.475890

C	1.143565	4.329069	-2.415842
O	3.505736	2.214790	-1.797236
H	2.870151	1.723718	-1.211329
O	5.663596	1.820643	-3.316401
H	5.439457	1.865416	-2.358127
C	1.944775	2.566302	-3.665198
H	1.827237	2.347240	-4.753400
C	3.251729	1.900829	-3.151142
H	3.119683	0.798200	-3.298159
C	4.498496	2.366497	-3.913711
H	4.448184	2.030962	-4.974122
H	4.500921	3.485873	-3.909008
H	0.058220	0.568082	-1.957984
O	-0.412543	0.448189	-0.423471
C	-1.565501	-0.370439	-0.250492
H	-2.332555	0.090605	-0.912837
C	-1.351723	-1.844566	-0.746422
H	-2.196508	-2.111915	-1.420065
H	-0.436268	-1.848861	-1.372779
C	-2.111122	-0.379194	1.185838
H	-1.270562	-0.474291	1.898810
I	-2.966359	1.660284	1.717627
O	0.853755	-0.730166	1.228491
O	1.844886	0.832887	-0.126015
C	0.973004	0.120568	0.355984
C	-1.247009	-2.873538	0.387257
H	-1.065411	-3.887933	-0.029437
H	-0.361891	-2.605559	0.996766
C	-3.168703	-1.463641	1.372977

H	-3.947238	-1.338365	0.587788
H	-3.683376	-1.349520	2.348021
C	-2.518046	-2.875547	1.267165
H	-2.262891	-3.246331	2.283246
H	-3.277748	-3.579460	0.860562

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ACID-BC SCF Done: -1005.57268255 A.U.

O	1.700251	-1.373042	0.357413
O	0.678293	1.502869	1.164652
H	0.225660	0.660792	1.480748
C	2.091070	-0.171654	-0.022039
O	2.692294	3.285844	-0.112133
C	1.685972	1.101242	0.336028
O	3.608295	1.372398	-0.959381
C	2.633714	2.072791	-0.214541
O	4.404545	-1.266893	0.890681
H	3.479529	-1.596380	1.033544
O	6.839254	-1.269761	-0.277962
H	6.455630	-1.602892	0.562329
C	3.285672	-0.026157	-0.950990
H	3.012194	-0.314234	-1.995657
C	4.451521	-0.948374	-0.500037
H	4.366689	-1.889090	-1.103931
C	5.843395	-0.362037	-0.737251
H	6.004502	-0.174511	-1.821346
H	5.891792	0.624900	-0.216664
H	0.551642	-1.211679	1.072259
O	-0.409986	-0.898653	1.519299

C	-1.347579	-0.908442	0.448458
H	-0.938334	-0.364150	-0.436393
C	-1.718702	-2.353744	0.036893
H	-2.044521	-2.366647	-1.024667
H	-0.772182	-2.931463	0.084301
C	-2.531480	-0.130506	1.032374
H	-2.230657	0.915183	1.228428
I	-4.109355	0.241205	-0.628002
C	-2.814530	-2.977267	0.935874
H	-3.809985	-2.835043	0.459641
H	-2.665417	-4.075402	1.021795
C	-3.144266	-0.818952	2.266272
H	-4.236746	-0.630773	2.310873
H	-2.711909	-0.316169	3.158170
C	-2.839018	-2.334965	2.334176
H	-3.588545	-2.838116	2.983108
H	-1.841904	-2.470540	2.799990

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ACID-B SCF Done: -1005.57328446 A.U.

O	1.500068	-1.162843	0.488151
O	0.707760	1.887909	0.636946
H	0.183202	1.176524	1.116723
C	2.018680	-0.098926	-0.096110
O	2.935821	3.208110	-0.829764
C	1.714570	1.247166	-0.022717
O	3.711639	1.095827	-1.221650
C	2.772346	2.008237	-0.692823
O	4.173530	-1.177627	1.160223

H	3.215943	-1.396317	1.301882
O	6.654722	-1.597345	0.178788
H	6.202332	-1.727399	1.040530
C	3.263161	-0.241900	-0.956539
H	3.013031	-0.712716	-1.938915
C	4.318823	-1.143945	-0.259302
H	4.182512	-2.176024	-0.675449
C	5.767205	-0.724198	-0.511350
H	5.998758	-0.766442	-1.598061
H	5.876071	0.339224	-0.187781
H	0.335629	-0.765970	1.110842
O	-0.575346	-0.289280	1.496072
C	-1.609593	-0.417304	0.525299
H	-1.514207	0.382445	-0.248754
C	-1.609432	-1.802478	-0.168483
H	-2.059284	-1.702538	-1.178186
H	-0.542152	-2.069539	-0.316374
C	-2.864540	-0.177896	1.372656
H	-2.854696	0.844192	1.793600
I	-4.715683	0.028523	-0.024896
C	-2.353374	-2.893163	0.639105
H	-3.407600	-2.965538	0.290432
H	-1.894392	-3.887947	0.452717
C	-3.074618	-1.251879	2.456132
H	-4.158512	-1.419241	2.624247
H	-2.679363	-0.830217	3.405219
C	-2.352793	-2.584129	2.145758
H	-2.831755	-3.409299	2.716412
H	-1.301662	-2.506368	2.491729

ACID-CD SCF Done: -1194.03823803 A.U.

O	2.103701	0.499070	-1.959099
O	2.085524	2.912347	0.151054
H	1.298230	2.807226	-0.460557
C	2.888399	0.806406	-0.922904
O	4.441414	2.327625	1.816947
C	2.871959	1.824249	0.007183
O	4.705824	0.468204	0.521893
C	4.038683	1.639626	0.902647
O	2.525839	-1.349956	1.032662
H	2.054689	-0.496499	0.918886
O	3.877549	-3.714210	0.839958
H	3.164918	-3.414752	1.441501
C	3.983865	-0.161034	-0.544309
H	4.678497	-0.344663	-1.398079
C	3.397470	-1.514174	-0.085850
H	2.839190	-1.932545	-0.960605
C	4.465536	-2.512212	0.366338
H	5.123778	-2.771230	-0.491988
H	5.093890	-2.007477	1.141572
H	1.261374	1.086041	-1.908673
O	0.129542	2.057233	-1.431946
C	-0.747994	1.469629	-0.729000
O	-0.843802	0.109837	-0.907525
O	-1.532859	1.992234	0.110340
C	-2.849285	0.353294	0.474565
H	-3.444897	0.800653	-0.327418

C	-1.646266	-0.514347	0.118779
H	-1.989182	-1.463052	-0.335485
I	-5.020081	-1.585142	0.102771
C	-0.806687	-0.813202	1.368209
H	0.028032	-1.486679	1.088749
H	-0.356070	0.138521	1.729439
C	-3.138233	0.655160	1.920486
H	-4.175214	1.024405	2.033988
H	-2.469893	1.511552	2.160655
C	-1.697063	-1.440426	2.453312
H	-2.135811	-2.373804	2.038905
H	-1.073834	-1.744229	3.320151
C	-2.847044	-0.500987	2.910216
H	-3.772586	-1.097364	3.040746
H	-2.608695	-0.051101	3.897866

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ACID-C SCF Done: -1194.05502390 A.U.

O	-2.522996	-1.750879	1.765018
O	-2.009819	0.838662	-0.113232
H	-1.143186	0.460328	0.272960
C	-3.286823	-0.751153	1.336136
O	-4.635636	2.133080	-0.120712
C	-3.087945	0.341326	0.512516
O	-5.333158	0.408847	1.195461
C	-4.365773	1.093279	0.446224
O	-5.305322	-2.047557	-0.321699
H	-4.444416	-1.622820	-0.531693
O	-7.536537	-3.195892	0.693235

H	-7.139689	-3.155562	-0.202255
C	-4.753622	-0.794349	1.711489
H	-4.890353	-0.822216	2.819484
C	-5.438853	-2.033325	1.098328
H	-4.937922	-2.927487	1.549456
C	-6.943233	-2.095474	1.370936
H	-7.125852	-2.224874	2.460793
H	-7.385261	-1.116318	1.060690
H	-1.622843	-1.868030	1.224044
O	0.285627	-0.025606	0.728150
C	0.470771	-1.261697	0.591151
O	-0.358782	-2.205963	0.581664
O	1.798664	-1.706008	0.428540
C	2.827703	-0.698219	0.415926
H	2.458381	0.194637	-0.129782
C	3.221477	-0.314073	1.851724
H	3.975547	0.502034	1.807792
H	2.315249	0.100845	2.337204
C	3.958904	-1.404438	-0.351821
H	3.591406	-1.734844	-1.341700
I	5.557207	0.126238	-0.972554
C	3.783590	-1.519627	2.623036
H	2.975204	-2.274626	2.738709
H	4.088034	-1.214365	3.647496
C	4.580719	-2.548801	0.441982
H	3.770384	-3.314053	0.485585
H	5.428519	-3.006082	-0.109244
C	4.970738	-2.157242	1.877297
H	5.819719	-1.437456	1.840158

H	5.339789	-3.055223	2.418964
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ACID-DminusI SCF Done: -1182.46599725 A.U.

O	2.063566	0.184937	-1.866698
O	1.677429	2.999092	-0.330800
H	1.014924	2.786381	-1.034756
C	2.623152	0.727309	-0.763678
O	3.478392	2.727664	1.959344
C	2.454047	1.917510	-0.107723
O	4.054054	0.695030	1.086162
C	3.333662	1.908162	1.083516
O	2.167092	-1.238345	1.521100
H	2.580209	-0.575739	2.118088
O	3.684497	-3.557198	1.540200
H	2.946075	-3.244490	2.104035
C	3.653092	-0.099795	-0.042064
H	4.538914	-0.279271	-0.696322
C	3.123549	-1.451847	0.475271
H	2.574749	-1.960002	-0.347151
C	4.235727	-2.376802	0.991396
H	4.907075	-2.667439	0.154027
H	4.855952	-1.802843	1.728775
H	1.369995	0.795278	-2.227611
O	-0.095427	1.816666	-2.071772
C	-0.852194	1.153810	-1.367725
O	-1.392692	-0.016664	-1.746027
O	-1.202412	1.501421	-0.120594
C	-2.213913	0.545677	0.349708

H	-3.199216	0.971941	0.056025
C	-1.872721	-0.678515	-0.525019
H	-2.777817	-1.255694	-0.797231
C	-0.748415	-1.564325	0.028251
H	-0.699355	-2.502639	-0.560734
H	0.220028	-1.041187	-0.126144
C	-2.132805	0.353562	1.857575
H	-3.077519	-0.148458	2.165489
H	-2.138734	1.354576	2.337464
C	-0.903883	-1.828627	1.534329
H	-1.834825	-2.406402	1.739873
H	-0.048473	-2.444851	1.872608
C	-0.928049	-0.492983	2.292263
H	-0.964799	-0.655405	3.389225
H	0.016749	0.050093	2.076020

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ACID-D SCF Done: -1194.07494648 A.U.

O	2.323618	0.110489	-1.807373
O	2.297325	3.189496	-0.984860
H	1.466719	2.833630	-1.395462
C	3.011578	0.813879	-0.877284
O	4.300682	3.303788	1.194431
C	2.989408	2.131013	-0.507528
O	4.498002	1.048311	0.905243
C	3.957160	2.302132	0.607004
O	1.960811	0.043232	1.728181
H	1.334316	0.449265	1.088893
O	2.671689	-2.309015	2.906985

H	1.974140	-1.651220	3.113490
C	3.823338	0.050386	0.131489
H	4.577458	-0.621619	-0.340176
C	2.877943	-0.787643	1.031578
H	2.344876	-1.502488	0.353610
C	3.601462	-1.589715	2.114436
H	4.291122	-2.323348	1.643182
H	4.218694	-0.874929	2.713954
H	1.615381	0.699812	-2.173497
O	0.173583	1.736667	-1.953413
C	-0.563624	1.104639	-1.192876
O	-1.696076	0.524641	-1.579782
O	-0.305250	0.912641	0.115677
C	-1.541608	0.333875	0.735177
H	-2.169094	1.202179	1.030583
C	-2.153004	-0.362905	-0.486500
H	-3.260817	-0.323808	-0.439295
I	-5.280366	-0.399788	1.688230
C	-1.619849	-1.775090	-0.742314
H	-2.218312	-2.248938	-1.547326
H	-0.570493	-1.701032	-1.112116
C	-1.239656	-0.533881	1.944393
H	-2.215594	-0.611738	2.474574
H	-0.541541	0.009746	2.614561
C	-1.638984	-2.604128	0.553950
H	-2.681763	-2.665084	0.939122
H	-1.301753	-3.639925	0.337239
C	-0.734677	-1.944494	1.606297
H	-0.706253	-2.551222	2.535638

H	0.312981	-1.905637	1.238515
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EPO SCF Done: -309.636476804 A.U.

O	-3.042092	-0.513476	1.140908
C	-3.895112	-0.161251	0.030251
C	-4.376831	-1.044210	1.124781
H	-4.216994	0.900796	0.040008
H	-5.053094	-0.609910	1.891598
C	-3.488182	-0.724313	-1.327740
H	-3.935390	-0.102551	-2.132713
H	-2.385361	-0.602419	-1.415108
C	-3.877293	-2.205024	-1.515055
H	-4.960354	-2.270762	-1.769217
H	-3.328956	-2.630773	-2.382157
C	-4.501619	-2.542927	0.914050
H	-4.243367	-3.066813	1.860876
H	-5.572295	-2.772753	0.707562
C	-3.619908	-3.036061	-0.247156
H	-3.816734	-4.111977	-0.438154
H	-2.550837	-2.948040	0.045570

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ASCORBICACID SCF Done: -684.308898051 A.U.

O	0.788824	2.365763	-0.531135
O	3.051740	0.547158	0.663432
H	3.472152	-0.311448	0.899972
C	0.903876	1.019200	-0.439504
O	2.043997	-2.167290	0.315044

C	1.866856	0.221555	0.093239
O	0.202319	-1.204373	-0.663329
C	1.430112	-1.179207	-0.041965
O	-1.307852	0.250372	1.330132
H	-0.787710	1.010001	1.651897
O	-3.839965	-0.226718	0.325516
H	-3.538809	-0.192649	1.256742
C	-0.248026	0.149752	-0.880765
H	-0.467437	0.277320	-1.965985
C	-1.534889	0.418617	-0.066870
H	-1.861321	1.461457	-0.304143
C	-2.679067	-0.538747	-0.418237
H	-2.928324	-0.442503	-1.496743
H	-2.317202	-1.582272	-0.246145
H	1.608404	2.767583	-0.177394

3

CO2 SCF Done: -188.454651986 A.U.

O	-0.000000	0.000000	1.175478
C	0.000000	-0.000000	-0.000000
O	-0.000000	0.000000	-1.175478

KI

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ACID-A+I SCF Done: -1488.81019900 A.U.

O	-5.627846	-0.393882	-1.371850
O	-7.800675	-1.542408	-3.480854

H	-7.111651	-0.951577	-3.908970
C	-6.842540	-0.949477	-1.234717
O	-9.967391	-2.375844	-1.815924
C	-7.752373	-1.446875	-2.129683
O	-8.681473	-1.776259	-0.029104
C	-8.915665	-1.926947	-1.369260
O	-6.325160	-3.444319	0.212469
H	-5.723343	-3.292849	-0.540112
O	-6.159782	-3.485979	2.973399
H	-5.980499	-4.201636	2.329338
C	-7.360793	-1.221415	0.158159
H	-7.458957	-0.282716	0.749987
C	-6.466984	-2.219680	0.928023
H	-5.478895	-1.719789	1.080325
C	-7.033969	-2.603636	2.299369
H	-7.148439	-1.692184	2.924454
H	-8.053089	-3.035204	2.140814
H	-5.456999	-0.226985	-2.346549
O	-5.799834	0.125488	-3.954600
C	-6.092542	1.542537	-4.255863
H	-7.125745	1.660642	-4.640406
C	-5.605186	2.530310	-3.230163
H	-5.655502	3.556612	-3.649358
H	-6.246350	2.501434	-2.325478
H	-4.558796	2.324106	-2.926139
C	-5.186157	0.760064	-5.118684
H	-5.578761	0.377833	-6.079593
H	-4.093020	0.894789	-5.026354
I	-8.678368	0.034588	-6.724350

K	-10.256895	-2.032439	-4.575250
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ACID-AB SCF Done: -1488.79495126 A.U.

O	-3.928596	0.076730	-0.202581
O	-4.594749	-1.207575	-3.043121
H	-3.662111	-1.327847	-2.622198
C	-5.075283	-0.074642	-0.874531
O	-7.514644	-1.138909	-3.125253
C	-5.368230	-0.612568	-2.106156
O	-7.403076	-0.027364	-1.142138
C	-6.831726	-0.619712	-2.246407
O	-6.635546	-2.241563	0.296856
H	-6.083404	-2.896495	0.787848
O	-8.044435	-1.764998	2.710010
H	-8.115700	-2.605128	2.214904
C	-6.376401	0.137676	-0.145649
H	-6.468496	1.145390	0.315093
C	-6.581402	-0.952310	0.940899
H	-5.706979	-0.908032	1.628919
C	-7.874540	-0.749217	1.741246
H	-7.825366	0.219664	2.283313
H	-8.724107	-0.688402	1.017109
H	-3.208042	-0.448322	-0.663015
O	-2.490848	-1.695266	-1.623598
C	-2.461867	-3.130365	-1.656319
H	-2.926727	-3.546043	-2.580285
C	-1.120348	-3.763739	-1.356246
H	-1.245363	-4.855181	-1.202734

H	-0.419921	-3.597347	-2.199262
H	-0.680178	-3.319888	-0.440531
C	-3.394720	-2.879258	-0.552509
H	-4.428093	-2.572491	-0.736974
H	-2.990126	-2.714084	0.456551
I	-4.761836	-5.304560	0.281501
K	-6.705638	-3.573715	-2.270412

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ACID-B SCF Done: -1488.81924012 A.U.

O	-3.514991	0.318877	-0.249050
O	-4.730765	-1.891533	1.641113
H	-4.220099	-2.160960	0.809147
C	-4.085977	0.417382	0.886184
O	-5.696513	-0.254977	3.974602
C	-4.614851	-0.547293	1.781172
O	-4.978607	1.532822	2.774489
C	-5.160924	0.127790	2.925719
O	-2.049607	1.230031	2.745315
H	-2.442955	0.363132	2.484940
O	-2.935834	2.986028	4.352207
H	-2.424708	2.133939	4.295124
C	-4.165699	1.764563	1.612340
H	-4.647179	2.538982	0.975295
C	-2.764406	2.249871	2.036368
H	-2.231807	2.518030	1.093739
C	-2.783471	3.459020	3.008863
H	-1.832737	4.034312	2.910439
H	-3.621544	4.146140	2.764979

H	-3.391764	-1.195114	-0.649331
O	-3.504002	-2.219435	-0.679477
C	-4.439280	-2.557599	-1.712557
H	-4.015383	-2.272499	-2.706187
C	-4.651138	-4.067416	-1.660609
H	-5.324138	-4.414538	-2.469007
H	-3.673532	-4.578951	-1.764716
H	-5.090640	-4.357201	-0.682736
C	-5.704075	-1.723603	-1.452804
H	-5.464044	-0.643900	-1.436418
H	-6.191160	-2.014475	-0.500972
I	-7.285463	-1.917047	-3.035870
K	-5.282013	1.978749	5.326978

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ACID-C SCF Done: -1677.27773980 A.U.

O	-2.947710	1.294619	3.347998
O	-1.833062	4.045058	4.442967
H	-0.981673	3.489032	4.279525
C	-3.279371	2.013669	4.401915
O	-3.038794	4.163144	7.121827
C	-2.799055	3.202826	4.904495
O	-4.386930	2.460276	6.429847
C	-3.389692	3.380782	6.233993
O	-6.021757	3.096496	4.152510
H	-5.331531	3.353404	3.511141
O	-8.208257	1.521519	4.708134
H	-8.158778	2.417385	4.315507
C	-4.442270	1.591588	5.274315

H	-4.325807	0.540586	5.622235
C	-5.796606	1.746981	4.546056
H	-5.768346	1.060611	3.663041
C	-6.996983	1.372189	5.421808
H	-6.913125	0.308756	5.733319
H	-6.955789	2.001961	6.345306
H	-1.954664	1.485935	3.077257
O	0.316818	2.725947	4.597862
C	0.417914	1.842899	3.671333
O	-0.467220	1.474458	2.870808
O	1.636153	1.223349	3.506830
C	2.734819	1.609575	4.363652
H	2.655609	2.697110	4.580358
C	2.681870	0.806510	5.662371
H	3.520293	1.068846	6.338340
H	1.726118	1.016517	6.182587
H	2.726648	-0.280344	5.444139
C	3.958766	1.345023	3.483300
H	3.859964	1.865109	2.512250
H	4.124614	0.263173	3.313713
I	5.853890	2.117996	4.376220
K	-0.374800	4.268703	6.709123

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ACID-CD SCF Done: -1677.26287482 A.U.

O	2.443202	-1.154088	1.600246
O	1.486407	1.675792	0.476825
H	1.193130	1.371487	1.383965
C	2.681587	-0.530049	0.458506

O	2.588554	1.713749	-2.213083
C	2.287952	0.689340	-0.037431
O	3.609349	-0.251894	-1.684220
C	2.816803	0.822740	-1.389260
O	5.566432	-0.040820	0.473211
H	5.148360	0.156038	1.332398
O	7.351037	-1.928447	-0.468740
H	7.518366	-1.078892	-0.010751
C	3.627575	-1.144989	-0.547165
H	3.258676	-2.140045	-0.884726
C	5.060754	-1.290351	0.006816
H	5.011496	-2.041994	0.832165
C	6.067046	-1.780841	-1.040321
H	5.748714	-2.771787	-1.429258
H	6.051003	-1.060908	-1.895717
H	1.666564	-0.664085	2.086102
O	0.517015	0.232219	2.574605
C	-0.579285	0.151386	1.940030
O	-0.524723	-0.500168	0.731448
O	-1.686389	0.676600	2.254722
C	-2.385037	0.968317	0.339926
H	-1.760242	1.865583	0.377190
H	-3.419047	1.064587	0.691321
C	-1.776814	-0.387080	0.001591
H	-1.465116	-0.426098	-1.059834
I	-3.129837	1.888728	-2.129440
C	-2.711482	-1.549138	0.322699
H	-3.616708	-1.494072	-0.315358
H	-2.199054	-2.511383	0.128659

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ACID-D SCF Done: -1677.30101588 A.U.

H	-3.016907	-1.509922	1.387251
K	0.334391	2.960866	-1.859933

O	1.130198	1.868994	-2.506793
O	0.258588	4.568873	-4.036322
H	-0.479345	3.958946	-3.763583
C	1.822239	2.818183	-3.142896
O	2.758082	5.569883	-5.062823
C	1.457158	3.974241	-3.781819
O	3.766976	3.861980	-3.942944
C	2.672688	4.586337	-4.330154
O	3.486380	4.050796	-1.061572
H	2.543991	3.953100	-0.828990
O	5.926031	2.965941	-0.357934
H	5.425304	3.701549	0.051229
C	3.330785	2.747777	-3.135007
H	3.692972	1.809264	-3.613226
C	3.915116	2.855296	-1.709360
H	3.577772	1.946759	-1.152202
C	5.446874	2.900082	-1.686292
H	5.854372	1.977189	-2.151843
H	5.774266	3.767517	-2.311193
H	0.149662	2.009949	-2.687447
O	-1.335667	2.552370	-3.223886
C	-2.010111	1.914971	-4.041855
O	-1.621991	0.757289	-4.568826
O	-3.224876	2.296181	-4.426656

C	-3.738140	1.360365	-5.407971
H	-3.919912	1.920358	-6.346667
H	-4.681342	0.934043	-5.007198
C	-2.607357	0.308029	-5.559043
H	-2.108248	0.416927	-6.544788
I	-1.339236	3.295117	-7.493876
C	-3.005227	-1.127397	-5.270024
H	-3.737984	-1.468145	-6.030382
H	-2.123523	-1.796261	-5.319452
H	-3.468842	-1.219956	-4.266055
K	0.490949	5.920814	-6.481984

TBAI

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ACID-A+I SCF Done: -1574.50402186 A.U.

O	-5.554635	-0.559554	-1.417337
O	-7.608430	-2.203928	-3.263408
H	-7.004850	-1.565312	-3.734504
C	-6.651191	-1.283561	-1.142933
O	-9.560715	-3.192760	-1.349299
C	-7.518013	-2.002700	-1.925772
O	-8.294076	-2.190956	0.255620
C	-8.562964	-2.557583	-1.045569
O	-5.759156	-3.524535	0.562850
H	-5.286484	-3.412381	-0.283296
O	-5.433718	-3.174981	3.284863
H	-5.208232	-3.946505	2.725506

C	-7.053744	-1.458412	0.299296
H	-7.247338	-0.473235	0.782223
C	-6.001060	-2.236393	1.120258
H	-5.072581	-1.613459	1.132163
C	-6.438669	-2.487908	2.567111
H	-6.618311	-1.516448	3.075730
H	-7.410222	-3.040825	2.539007
H	-5.508377	-0.396989	-2.406088
O	-6.064065	-0.163306	-3.986307
C	-6.859596	1.096404	-4.120083
H	-7.889002	0.916272	-4.490657
C	-6.747519	2.082381	-2.995062
H	-7.246805	3.019986	-3.316849
H	-7.293367	1.710498	-2.105767
H	-5.694138	2.285246	-2.716087
C	-5.752028	0.794484	-5.042803
H	-5.971530	0.432871	-6.063000
H	-4.779225	1.302384	-4.911153
I	-10.165518	2.716406	-5.063553
N	-11.569993	-1.200804	-3.452556
C	-12.467757	-0.308808	-4.303222
C	-13.340855	0.680068	-3.540946
C	-14.168657	1.523756	-4.526292
C	-15.029130	2.574986	-3.817173
C	-10.539178	-0.336664	-2.689011
C	-10.827460	0.015144	-1.231748
C	-9.696719	0.918009	-0.705093
C	-9.759775	1.123552	0.811485
C	-12.373604	-2.058123	-2.479260

C	-13.462619	-2.941368	-3.087830
C	-14.179447	-3.741379	-1.984343
C	-15.287888	-4.647010	-2.533843
C	-10.783027	-2.140461	-4.374037
C	-9.845640	-1.468095	-5.374194
C	-9.050630	-2.527667	-6.155729
H	-13.077202	-0.985098	-4.935937
H	-11.786397	0.271390	-4.959586
H	-14.018178	0.165600	-2.822714
H	-12.690904	1.369428	-2.961056
H	-8.942240	1.785051	1.165977
H	-9.672272	0.152039	1.343692
H	-10.720184	1.589113	1.119144
H	-16.065884	-4.057515	-3.064332
H	-15.789972	-5.211206	-1.721611
H	-8.722149	0.452973	-0.973855
H	-9.724545	1.891648	-1.241071
H	-9.743446	-3.121175	-6.794342
H	-8.594732	-3.242531	-5.436454
H	-10.396157	-0.810389	-6.078077
H	-9.132690	-0.809424	-4.840984
H	-11.531644	-2.754769	-4.911432
H	-10.207032	-2.796354	-3.689337
H	-14.813115	0.852977	-5.140015
H	-13.466000	2.026326	-5.227509
H	-13.036965	-3.654374	-3.825649
H	-14.211785	-2.326220	-3.632035
H	-9.598030	-0.908718	-2.731053
H	-10.400180	0.583876	-3.300104

H	-11.797704	0.542864	-1.117040
H	-15.620568	3.168848	-4.543699
H	-15.742040	2.108788	-3.102453
H	-14.393345	3.284258	-3.246499
H	-13.431103	-4.350841	-1.430417
C	-7.949715	-1.901010	-7.019055
H	-7.408366	-2.665193	-7.613519
H	-8.360382	-1.145548	-7.721321
H	-7.202711	-1.385399	-6.378380
H	-10.867851	-0.901054	-0.606175
H	-14.606793	-3.034325	-1.237732
H	-14.882440	-5.387774	-3.255581
H	-11.625933	-2.664939	-1.931167
H	-12.837165	-1.361613	-1.758153

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ACID-B SCF Done: -1574.51543745 A.U.

O	-3.742630	0.268651	-0.205317
O	-5.624980	-1.718238	1.344497
H	-4.915014	-2.093186	0.729842
C	-4.450908	0.443792	0.854453
O	-6.761976	0.006412	3.484645
C	-5.280387	-0.408936	1.593443
O	-5.416029	1.645380	2.660087
C	-5.889535	0.336799	2.675095
O	-2.692307	0.922159	3.189247
H	-2.872434	0.066098	2.751391
O	-1.615463	3.389806	3.656761
H	-1.444083	2.517825	4.068678

C	-4.403511	1.752956	1.639615
H	-4.644240	2.620837	0.985724
C	-3.013157	1.963177	2.270171
H	-2.287312	1.990356	1.418030
C	-2.900280	3.260532	3.074064
H	-3.058877	4.131463	2.401366
H	-3.721070	3.261136	3.834338
H	-3.608946	-1.184304	-0.432118
O	-3.720636	-2.235729	-0.469505
C	-4.221272	-2.586108	-1.758542
H	-3.522864	-2.231101	-2.554858
C	-4.344828	-4.104249	-1.827958
H	-4.712663	-4.440985	-2.817300
H	-3.353419	-4.561116	-1.638345
H	-5.043870	-4.465711	-1.045575
C	-5.545034	-1.818501	-1.874582
H	-5.367407	-0.727082	-1.839598
H	-6.215854	-2.110175	-1.047830
I	-6.757753	-2.139634	-3.740614
N	-9.534390	-1.282875	0.745390
C	-10.046798	-1.687785	2.134392
C	-8.968268	-2.166468	3.106920
C	-9.422307	-2.036106	4.570744
C	-8.312366	-2.457603	5.541325
C	-8.809775	0.061834	0.899503
C	-8.036231	0.550999	-0.320204
C	-7.562594	2.002278	-0.120084
C	-6.583197	2.441931	-1.215646
C	-8.551855	-2.318645	0.204665

C	-9.050778	-3.760158	0.121912
C	-7.891472	-4.676832	-0.310562
C	-8.303137	-6.147501	-0.430724
C	-10.699650	-1.171387	-0.230862
C	-11.735615	-0.084460	0.051140
C	-12.906170	-0.175785	-0.945385
H	-10.830133	-2.455556	1.970189
H	-10.547989	-0.785316	2.536390
H	-8.694553	-3.221082	2.891396
H	-8.037665	-1.566730	3.003811
H	-6.274552	3.498516	-1.077790
H	-7.037479	2.354333	-2.225967
H	-5.663355	1.819174	-1.202413
H	-8.679251	-6.544012	0.536586
H	-7.446221	-6.778882	-0.741671
H	-8.447250	2.679167	-0.096577
H	-7.079384	2.095035	0.876631
H	-13.384997	-1.177431	-0.859982
H	-12.508898	-0.117135	-1.983812
H	-12.131235	-0.173552	1.085957
H	-11.273592	0.922479	-0.028570
H	-11.186085	-2.166381	-0.238239
H	-10.249671	-1.022535	-1.232690
H	-10.348266	-2.631458	4.748432
H	-9.690473	-0.972935	4.764323
H	-9.881646	-3.858829	-0.610552
H	-9.441767	-4.110724	1.100724
H	-9.588222	0.789869	1.198843
H	-8.130757	-0.052214	1.765538

H	-7.142287	-0.085570	-0.468862
H	-8.633924	-2.349363	6.597419
H	-8.019406	-3.517793	5.384139
H	-7.413431	-1.827120	5.381931
H	-7.489072	-4.318757	-1.283851
C	-13.954185	0.922009	-0.727731
H	-14.787679	0.834055	-1.453742
H	-14.389663	0.867826	0.292606
H	-13.510080	1.932903	-0.847032
H	-8.645921	0.489304	-1.249437
H	-7.060159	-4.571336	0.421418
H	-9.108674	-6.281863	-1.183828
H	-8.283906	-1.971403	-0.811673
H	-7.636009	-2.235386	0.826973

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ACID-C SCF Done: -1762.98622137 A.U.

O	-2.809919	1.127324	3.984659
O	-1.768430	4.068149	4.687903
H	-0.936078	3.471991	4.592373
C	-3.256996	2.070836	4.793679
O	-3.619778	4.900871	6.808663
C	-2.824681	3.344913	5.104606
O	-4.723743	2.945685	6.408346
C	-3.713057	3.874316	6.152265
O	-5.885258	2.945952	3.782194
H	-5.055023	3.098831	3.289751
O	-8.150490	1.470937	4.283743
H	-8.008279	2.238839	3.692485

C	-4.562362	1.827147	5.516084
H	-4.527100	0.890601	6.121684
C	-5.749609	1.743703	4.530482
H	-5.550557	0.866270	3.865271
C	-7.098712	1.544320	5.226695
H	-7.086192	0.590782	5.798276
H	-7.230514	2.379805	5.958913
H	-1.857383	1.326097	3.554959
O	0.344195	2.627095	4.651000
C	0.420257	1.766651	3.718185
O	-0.514546	1.296671	3.020595
O	1.661610	1.238157	3.423236
C	2.794109	1.717801	4.183409
H	2.659469	2.802423	4.384475
C	2.884411	0.953320	5.503943
H	3.757996	1.275733	6.104925
H	1.961972	1.148794	6.085358
H	2.959964	-0.137449	5.314143
C	3.960650	1.497023	3.218318
H	3.762431	1.994725	2.250738
H	4.164887	0.421303	3.051138
I	5.882113	2.372366	3.948943
N	-0.834791	2.270338	8.675423
C	-2.344204	2.273577	8.923975
C	-2.936918	3.524577	9.561434
C	-4.453855	3.347960	9.764683
C	-5.134627	4.666010	10.148924
C	-0.455507	3.327607	7.609391
C	-0.121280	4.741921	8.081552

C	-0.037201	5.684797	6.865180
C	0.380369	7.104278	7.261014
C	-0.054445	2.523235	9.957089
C	-0.334528	1.584724	11.131013
C	0.507987	1.984215	12.356689
C	0.258234	1.076287	13.566702
C	-0.444105	0.889707	8.134644
C	-1.052037	0.468477	6.798469
C	-0.526690	-0.925971	6.404595
H	-2.559233	1.372523	9.534100
H	-2.806716	2.117786	7.931735
H	-2.453797	3.755678	10.536649
H	-2.785553	4.388866	8.885546
H	0.422301	7.769133	6.374336
H	1.382740	7.123227	7.742132
H	-0.342564	7.551346	7.976949
H	-0.806521	1.107221	13.881195
H	0.873882	1.383973	14.436043
H	0.675545	5.263033	6.122322
H	-1.024693	5.689462	6.358671
H	-0.780720	-1.652542	7.211380
H	0.585561	-0.895478	6.362727
H	-2.159256	0.430885	6.861421
H	-0.802156	1.200889	6.005996
H	-0.717205	0.159298	8.921376
H	0.663175	0.904879	8.061951
H	-4.640289	2.566227	10.536909
H	-4.896599	2.979413	8.814856
H	-0.108876	0.529528	10.867437

H	-1.410352	1.622031	11.406909
H	0.394207	2.909787	7.036482
H	-1.308934	3.358971	6.913450
H	-0.895520	5.131003	8.774302
H	-6.219367	4.521949	10.329937
H	-4.693705	5.105312	11.070016
H	-5.020711	5.400013	9.324468
H	1.587268	1.962093	12.084289
C	-1.075665	-1.420259	5.061201
H	-0.728554	-2.452376	4.849665
H	-2.184972	-1.417501	5.053438
H	-0.750036	-0.767176	4.227630
H	0.846319	4.758729	8.630581
H	0.284683	3.041199	12.625871
H	0.507259	0.018650	13.336365
H	1.016301	2.486251	9.669317
H	-0.273360	3.562695	10.258896

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ACID-D SCF Done: -1762.99643180 A.U.

O	1.229292	1.958312	-2.515504
O	0.320244	4.830575	-3.600562
H	-0.394965	4.177659	-3.393233
C	1.916850	3.022508	-2.955048
O	2.831027	6.013003	-4.492019
C	1.536064	4.256533	-3.409674
O	3.842184	4.154321	-3.650962
C	2.741733	4.949425	-3.903048
O	3.661318	4.054706	-0.792756

H	2.689030	4.071883	-0.704253
O	6.062977	2.820190	-0.229541
H	5.606842	3.540886	0.251283
C	3.422489	2.956333	-2.971789
H	3.773041	2.073831	-3.554810
C	4.026461	2.906025	-1.549218
H	3.655471	1.964295	-1.071827
C	5.558328	2.884920	-1.548665
H	5.918220	1.986562	-2.094944
H	5.911547	3.787115	-2.107057
H	0.254159	2.089812	-2.696422
O	-1.286497	2.636671	-3.227188
C	-2.024055	2.073394	-4.041548
O	-1.766150	0.888158	-4.587800
O	-3.170093	2.610325	-4.471263
C	-3.852564	1.651529	-5.332481
H	-4.220158	2.180240	-6.236423
H	-4.689984	1.209308	-4.751636
C	-2.744586	0.644432	-5.675285
H	-2.249877	0.956011	-6.623748
I	-3.188712	2.497476	-9.042729
C	-3.143501	-0.811687	-5.715339
H	-3.863010	-0.958351	-6.546626
H	-2.261873	-1.452660	-5.911830
H	-3.618267	-1.128638	-4.764196
N	-0.158698	5.520099	-7.757261
C	-1.614452	5.602012	-7.266726
C	-1.849815	5.467985	-5.765820
C	-3.309163	5.799760	-5.410612

C	-3.541769	5.833175	-3.895003
C	0.527754	6.884617	-7.687784
C	0.638368	7.539525	-6.312000
C	1.654632	8.694794	-6.333249
C	1.796823	9.353551	-4.956178
C	0.673778	4.526515	-6.942444
C	0.333252	3.050489	-7.141392
C	1.002598	2.185881	-6.060479
C	0.978331	0.689974	-6.387182
C	-0.174752	5.054104	-9.219028
C	-0.978467	5.896587	-10.207128
C	-0.979062	5.212302	-11.587485
H	-2.169622	4.798859	-7.801262
H	-1.991979	6.576842	-7.633320
H	-1.635676	4.429153	-5.444023
H	-1.174259	6.115603	-5.176916
H	2.533351	10.182743	-4.977623
H	2.140369	8.606111	-4.211848
H	0.828928	9.771037	-4.604547
H	-0.051909	0.342229	-6.603882
H	1.364341	0.090379	-5.538122
H	2.642794	8.290815	-6.647611
H	1.363675	9.450063	-7.099644
H	-1.404053	4.190606	-11.469927
H	0.070086	5.083749	-11.939668
H	-2.031808	5.978553	-9.866235
H	-0.574126	6.928368	-10.302624
H	-0.617954	4.038412	-9.205983
H	0.889479	4.979932	-9.526336

H	-3.981749	5.056816	-5.892933
H	-3.580056	6.787100	-5.849949
H	0.667115	2.705230	-8.142066
H	-0.767898	2.889686	-7.131340
H	1.539510	6.721254	-8.114471
H	-0.021949	7.542332	-8.388408
H	-0.353457	7.925273	-5.993225
H	-4.602397	6.050168	-3.652429
H	-3.282093	4.860603	-3.430927
H	-2.917492	6.615018	-3.411874
H	2.054517	2.518728	-5.906826
C	-1.788188	5.993707	-12.628464
H	-1.777486	5.482085	-13.612445
H	-2.849039	6.090634	-12.314963
H	-1.384945	7.018925	-12.777001
H	0.980194	6.815165	-5.545419
H	0.497159	2.365937	-5.091242
H	1.595617	0.462258	-7.281691
H	1.730653	4.724277	-7.215260
H	0.562827	4.816645	-5.883039

Br-

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ACID-AB SCF Done: -890.836396907 A.U.

O	-1.262357	-0.893823	0.520440
O	-1.150883	2.001416	-0.852934
H	-0.317826	1.433633	-0.842405

C	-2.170492	0.080226	0.372778
O	-3.866828	3.038038	-0.402725
C	-2.135816	1.315744	-0.237253
O	-4.293936	1.044470	0.619491
C	-3.467569	1.944920	-0.061879
O	-4.260364	-1.073763	-1.332521
H	-3.440200	-0.583445	-1.553356
O	-6.264331	-2.616623	-0.332063
H	-6.007024	-2.377803	-1.246729
C	-3.580318	-0.177984	0.846665
H	-3.603554	-0.418250	1.936200
C	-4.233596	-1.339579	0.067491
H	-3.624438	-2.253649	0.286371
C	-5.689076	-1.593560	0.467086
H	-5.736525	-1.922462	1.528437
H	-6.238586	-0.623539	0.381897
H	-0.368775	-0.565475	0.130430
O	0.795789	0.301628	-0.418990
C	1.742493	0.735992	0.600085
H	1.908755	1.832841	0.576729
C	1.548146	0.181159	1.990402
H	2.482506	0.346091	2.565144
H	0.699140	0.679793	2.501753
H	1.349340	-0.909111	1.954936
C	2.447824	-0.030462	-0.422357
H	2.890344	0.466409	-1.293933
H	2.559074	-1.116655	-0.313299
Br	5.088258	-0.014631	0.576472

ACID-A+Br SCF Done: -890.837913898 A.U.

O	-1.308900	-0.839501	0.575722
O	-1.209881	2.031005	-0.880817
H	-0.366423	1.496349	-0.839088
C	-2.222948	0.125071	0.380364
O	-3.941062	3.032756	-0.516286
C	-2.192016	1.341304	-0.262830
O	-4.361258	1.067430	0.561561
C	-3.537029	1.956715	-0.132350
O	-4.279949	-1.103786	-1.323761
H	-3.446047	-0.645976	-1.559066
O	-6.267119	-2.657098	-0.292939
H	-6.010253	-2.446435	-1.214453
C	-3.637165	-0.138434	0.837433
H	-3.675274	-0.345679	1.933145
C	-4.263703	-1.331064	0.082862
H	-3.645165	-2.230168	0.334687
C	-5.719814	-1.595361	0.473474
H	-5.774665	-1.885504	1.545566
H	-6.284334	-0.638646	0.346246
H	-0.422111	-0.533168	0.192076
O	0.796213	0.356460	-0.374379
C	1.809334	0.743819	0.645103
H	1.989101	1.835143	0.645762
C	1.704270	0.092132	1.994463
H	2.712742	0.142540	2.457831
H	0.959177	0.602544	2.638642
H	1.427279	-0.976796	1.897195

C	2.257209	0.010912	-0.535127
H	2.753334	0.542736	-1.361445
H	2.468668	-1.066595	-0.449731
Br	5.199236	-0.096198	0.626173

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ACID-B SCF Done: -890.856429982 A.U.

O	1.475389	-1.270573	0.375609
O	0.655875	1.712420	1.002645
H	0.132002	0.927892	1.353066
C	1.976331	-0.124856	-0.041560
O	2.851550	3.267801	-0.272536
C	1.661306	1.192241	0.240127
O	3.643462	1.249064	-0.991044
C	2.701258	2.058768	-0.317779
O	4.142206	-1.386841	0.996922
H	3.183037	-1.625699	1.100103
O	6.628299	-1.582919	-0.031254
H	6.175597	-1.865913	0.793007
C	3.210598	-0.118346	-0.929911
H	2.949566	-0.433936	-1.969812
C	4.284553	-1.107331	-0.395191
H	4.168463	-2.055540	-0.982388
C	5.724477	-0.622956	-0.568411
H	5.957487	-0.476849	-1.645778
H	5.812502	0.372547	-0.069808
H	0.306746	-0.979813	1.076602
O	-0.626625	-0.579861	1.476416
C	-1.536413	-0.587896	0.387673

H	-1.175110	0.067897	-0.446239
C	-1.741756	-2.006700	-0.151809
H	-2.446504	-2.025718	-1.008320
H	-0.757482	-2.398265	-0.479964
H	-2.131160	-2.665949	0.653617
C	-2.785821	0.051063	0.990965
H	-2.571614	1.076404	1.345716
H	-3.202243	-0.567661	1.809640
Br	-4.326369	0.280947	-0.348540

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ACID-B+CO2 SCF Done: -1079.32882467 A.U.

O	1.526778	-0.233776	-1.618182
O	0.662704	1.721468	0.710689
H	0.091608	0.920206	0.472671
C	2.215690	0.678357	-0.916016
O	3.203989	3.122411	1.379116
C	1.857294	1.514937	0.113396
O	4.148686	1.801717	-0.224289
C	3.064069	2.251379	0.543199
O	3.976169	-0.889747	0.805948
H	3.012146	-1.086778	0.869548
O	6.334535	-1.857931	-0.014762
H	5.722548	-1.994424	0.743299
C	3.714808	0.711378	-1.045110
H	4.053329	0.888185	-2.094479
C	4.317429	-0.626818	-0.545254
H	3.921773	-1.423272	-1.225757
C	5.849105	-0.649149	-0.578928

H	6.209057	-0.577340	-1.629579
H	6.213832	0.255028	-0.029822
H	0.641745	-0.398163	-1.116238
O	-0.521950	-0.478734	-0.107056
C	-1.844218	-0.449521	-0.615915
H	-1.912045	0.396968	-1.344958
C	-2.213474	-1.752326	-1.334177
H	-3.231118	-1.697176	-1.772093
H	-1.485889	-1.937645	-2.150771
H	-2.170032	-2.601987	-0.624499
C	-2.735720	-0.111478	0.584021
H	-2.414773	0.832628	1.062346
H	-2.765178	-0.938207	1.316830
Br	-4.700652	0.227910	0.063464
O	-0.894238	-2.441013	1.491202
O	1.256423	-1.652273	1.123698
C	0.067172	-1.830609	1.107230

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ACID-CD SCF Done: -1079.31705014 A.U.

O	2.264919	-0.848805	-0.432769
O	2.380866	2.152863	0.734046
H	1.535382	1.626521	0.866111
C	3.209017	0.099825	-0.427681
O	5.076060	3.029561	-0.025958
C	3.275167	1.375688	0.093287
O	5.337922	0.951872	-0.928089
C	4.607806	1.932508	-0.246267
O	5.391035	-1.011684	1.182209

H	4.621379	-0.451656	1.421074
O	7.252843	-2.698865	0.150468
H	7.075003	-2.378732	1.059320
C	4.562949	-0.251574	-0.997311
H	4.482395	-0.574478	-2.062572
C	5.238417	-1.378527	-0.186826
H	4.580424	-2.279605	-0.283882
C	6.645502	-1.721159	-0.682030
H	6.592438	-2.135613	-1.712822
H	7.231992	-0.770072	-0.722430
H	1.436478	-0.496377	0.051523
O	0.409392	0.399861	0.835012
C	-0.847349	0.408856	0.708107
O	-1.401181	-0.675520	0.085855
O	-1.643694	1.317064	1.095876
C	-3.375626	0.745924	0.231786
H	-3.184522	1.421882	-0.609642
H	-3.896197	1.143555	1.107635
C	-2.854433	-0.686336	0.191457
H	-3.193087	-1.174918	-0.741961
Br	-5.664460	0.276094	-0.720661
C	-3.275039	-1.498717	1.413075
H	-4.379700	-1.583804	1.438780
H	-2.829338	-2.512155	1.371899
H	-2.929283	-0.993870	2.339257

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ACID-C SCF Done: -1079.32760981 A.U.

O	-2.653311	-1.064746	1.028979
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O	-1.660775	1.680577	-0.378067
H	-0.891990	1.162113	0.051726
C	-3.260534	0.055229	0.651394
O	-4.139398	3.229191	-0.538515
C	-2.854999	1.219305	0.024808
O	-5.160847	1.429021	0.414307
C	-4.041979	2.101583	-0.097167
O	-5.121743	-0.795075	-1.425923
H	-4.206573	-0.438369	-1.457531
O	-7.563765	-1.830293	-0.889884
H	-7.038885	-1.713201	-1.709558
C	-4.764554	0.115017	0.821906
H	-5.060845	-0.044559	1.886720
C	-5.456206	-0.954931	-0.048527
H	-5.101861	-1.947618	0.329556
C	-6.984000	-0.897145	0.013154
H	-7.331759	-1.150926	1.039099
H	-7.293153	0.154949	-0.205809
H	-1.697911	-1.206426	0.596069
O	0.412578	0.472140	0.596850
C	0.505449	-0.748940	0.309146
O	-0.397274	-1.591881	0.074469
O	1.798028	-1.303300	0.236748
C	2.902425	-0.411512	0.447305
H	2.672806	0.580009	-0.001773
C	3.183447	-0.240544	1.939170
H	4.066590	0.407522	2.111985
H	2.296695	0.229550	2.406869
H	3.362719	-1.229421	2.411883

C	4.013001	-1.101559	-0.344314
H	3.720370	-1.235864	-1.401904
H	4.301104	-2.073448	0.101189
Br	5.738458	-0.007962	-0.399777

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ACID-D SCF Done: -1079.33470371 A.U.

O	2.542392	-0.371175	-1.355039
O	2.495018	2.398489	0.313851
H	1.618490	2.011643	0.052261
C	3.498922	0.406283	-0.819885
O	5.336201	2.913522	0.773801
C	3.482423	1.570887	-0.088305
O	5.725167	0.965704	-0.346281
C	4.891743	1.945854	0.196032
O	4.801613	-1.246598	1.239737
H	4.008049	-0.674622	1.295441
O	6.720414	-3.079440	0.607443
H	6.263605	-2.876255	1.449772
C	4.925430	-0.079003	-0.913850
H	5.228150	-0.235631	-1.976288
C	5.128467	-1.399146	-0.138364
H	4.467309	-2.161379	-0.624510
C	6.575273	-1.897903	-0.164543
H	6.871673	-2.135563	-1.209664
H	7.227742	-1.065081	0.197337
H	1.639582	0.013451	-1.144781
O	0.388329	0.939358	-0.560218
C	-0.766885	0.624291	-0.246075

O	-1.343433	-0.505653	-0.641365
O	-1.546926	1.388402	0.511524
C	-2.902614	0.795606	0.545656
H	-3.567857	1.388530	-0.110222
H	-3.281839	0.843928	1.581024
C	-2.665575	-0.639655	0.036442
H	-3.405567	-0.916525	-0.736750
Br	-5.969437	-0.354874	0.603440
C	-2.566842	-1.699985	1.116402
H	-3.581581	-1.816617	1.550666
H	-2.238297	-2.667473	0.687130
H	-1.852404	-1.394695	1.910513

Cl-

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ACID-A+I SCF Done: -1337.66618528 A.U.

O	-1.033793	-0.868964	0.051845
O	-1.241832	2.233884	-0.470537
H	-0.442200	1.706141	-0.769849
C	-1.977838	-0.023656	0.320952
O	-3.859875	2.929863	0.755444
C	-2.125465	1.343802	0.074317
O	-4.066851	0.695657	1.192956
C	-3.378555	1.813115	0.665479
O	-4.277746	-0.763360	-1.299102
H	-3.636183	-0.017205	-1.351324
O	-6.126771	-2.564796	-0.553681

H	-5.963690	-2.023248	-1.355516
C	-3.298736	-0.486621	0.930399
H	-3.124943	-1.035755	1.886322
C	-4.044007	-1.413555	-0.048061
H	-3.385991	-2.306839	-0.198998
C	-5.419690	-1.857188	0.458753
H	-5.304185	-2.532901	1.335642
H	-5.967378	-0.942547	0.796703
H	0.021611	-0.158792	-0.580898
O	0.782893	0.510008	-0.956028
C	1.764556	0.623842	0.063548
H	2.544978	1.338674	-0.292364
C	1.194586	1.119006	1.399690
H	1.997359	1.250560	2.153891
H	0.666419	2.080910	1.243425
H	0.452430	0.388741	1.782969
C	2.401223	-0.768364	0.156199
H	2.762333	-1.097601	-0.836525
H	1.677630	-1.501681	0.566888
Cl	3.921162	-0.824624	1.303492

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ACID-B+CO2 SCF Done: -1526.13539423 A.U.

O	1.528221	-0.181678	-1.683093
O	0.676548	1.786072	0.637067
H	0.127147	0.964769	0.458917
C	2.228110	0.721788	-0.975885
O	3.231034	3.162737	1.313653
C	1.874652	1.564302	0.047247

O	4.170307	1.814777	-0.270410
C	3.088406	2.286000	0.484540
O	3.907101	-0.832214	0.827859
H	2.942922	-1.059273	0.878428
O	6.248211	-1.890512	0.094972
H	5.607478	-1.977474	0.837790
C	3.728410	0.715443	-1.075908
H	4.097682	0.857059	-2.119686
C	4.279313	-0.626764	-0.521360
H	3.869829	-1.430959	-1.184337
C	5.811305	-0.694713	-0.530877
H	6.189469	-0.679588	-1.577815
H	6.195289	0.221702	-0.015593
H	0.673729	-0.371288	-1.164655
O	-0.489196	-0.505047	-0.076893
C	-1.840770	-0.478982	-0.545023
H	-1.909333	0.414404	-1.210735
C	-2.202603	-1.732845	-1.345224
H	-3.238008	-1.660272	-1.736055
H	-1.505572	-1.842179	-2.201080
H	-2.117243	-2.628220	-0.699228
C	-2.744321	-0.220088	0.667413
H	-2.399960	0.671444	1.225867
H	-2.795886	-1.101925	1.331377
Cl	-4.522268	0.168311	0.132708
O	-0.857012	-2.423065	1.376524
O	1.263414	-1.588213	1.048854
C	0.055192	-1.729302	0.969415

ACID-B SCF Done: -1337.66340670 A.U.

O	1.543391	-1.325448	0.110924
O	0.602457	1.455798	1.261808
H	0.119434	0.600809	1.465165
C	2.011342	-0.112144	-0.069616
O	2.762618	3.295444	0.349879
C	1.645066	1.121532	0.438288
O	3.644890	1.471343	-0.706985
C	2.659043	2.110745	0.079410
O	4.184107	-1.506342	0.752006
H	3.226868	-1.778732	0.765550
O	6.713888	-1.373097	-0.165483
H	6.242471	-1.840969	0.558000
C	3.263404	0.102222	-0.909550
H	3.029934	-0.023486	-1.994907
C	4.365711	-0.932733	-0.541618
H	4.324382	-1.739699	-1.319290
C	5.784223	-0.361103	-0.537972
H	6.053285	0.017243	-1.548273
H	5.799888	0.510878	0.159709
H	0.348668	-1.228901	0.882929
O	-0.586771	-0.978891	1.349184
C	-1.545853	-1.022239	0.302752
H	-1.027872	-1.055742	-0.687547
C	-2.441939	-2.256649	0.446074
H	-3.222455	-2.293053	-0.342039
H	-1.821840	-3.173976	0.382437
H	-2.936356	-2.246069	1.441239

C	-2.310748	0.303371	0.389546
H	-1.617119	1.161231	0.291512
H	-2.875739	0.377562	1.341018
Cl	-3.598774	0.494520	-0.992385

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ACID-CD SCF Done: -1526.11727131 A.U.

O	2.275323	-0.878663	-0.393404
O	2.372790	2.156440	0.685674
H	1.532582	1.627665	0.837631
C	3.210171	0.078780	-0.424491
O	5.052754	3.035802	-0.122971
C	3.268637	1.369554	0.058949
O	5.326088	0.936035	-0.968795
C	4.592958	1.928754	-0.308181
O	5.418163	-0.967436	1.194379
H	4.643635	-0.411481	1.426692
O	7.285277	-2.666348	0.191026
H	7.113038	-2.323477	1.092627
C	4.561947	-0.275952	-0.997091
H	4.474377	-0.629062	-2.052172
C	5.255713	-1.373672	-0.162331
H	4.605452	-2.283162	-0.227937
C	6.661153	-1.717030	-0.661630
H	6.602136	-2.159723	-1.680282
H	7.238459	-0.762182	-0.733433
H	1.447582	-0.520238	0.086371
O	0.413060	0.391412	0.847935
C	-0.840467	0.393536	0.702782

O	-1.399034	-0.698983	0.119996
O	-1.636422	1.326301	1.051658
C	-3.317887	0.787819	0.304551
H	-3.229781	1.462124	-0.554578
H	-3.863594	1.145935	1.182294
C	-2.861963	-0.663148	0.186765
H	-3.205509	-1.071825	-0.782022
Cl	-5.558807	0.274962	-0.545909
C	-3.336153	-1.531731	1.346560
H	-4.443701	-1.558341	1.333781
H	-2.934352	-2.560028	1.250576
H	-2.990148	-1.103031	2.310856

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ACID-C SCF Done: -1526.13449672 A.U.

O	-2.650303	-1.063600	1.032405
O	-1.658379	1.682857	-0.371838
H	-0.889298	1.162966	0.057264
C	-3.258003	0.055639	0.654819
O	-4.138188	3.230091	-0.533631
C	-2.852785	1.220567	0.029062
O	-5.159362	1.428187	0.416227
C	-4.040137	2.102030	-0.093285
O	-5.114799	-0.794271	-1.426011
H	-4.200793	-0.434154	-1.455197
O	-7.556913	-1.831073	-0.896434
H	-7.029662	-1.712479	-1.714396
C	-4.762415	0.114181	0.823185
H	-5.060184	-0.046742	1.887397

C	-5.451697	-0.955587	-0.049330
H	-5.097007	-1.948260	0.328462
C	-6.979648	-0.899150	0.009581
H	-7.329216	-1.155105	1.034386
H	-7.289241	0.153087	-0.208086
H	-1.692623	-1.205285	0.599723
O	0.413793	0.473682	0.599121
C	0.507717	-0.747507	0.310824
O	-0.396732	-1.590551	0.079554
O	1.798491	-1.299838	0.230000
C	2.903554	-0.409997	0.440583
H	2.677922	0.581303	-0.011632
C	3.189260	-0.232956	1.930996
H	4.084253	0.401806	2.092254
H	2.311496	0.253073	2.399424
H	3.356139	-1.221117	2.409947
C	4.022591	-1.094487	-0.346177
H	3.732809	-1.222992	-1.406226
H	4.292077	-2.075460	0.093545
Cl	5.608591	-0.070369	-0.351938

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ACID-D SCF Done: -1526.12676934 A.U.

O	2.532194	-0.380683	-1.343483
O	2.484509	2.395241	0.311233
H	1.607308	2.001317	0.053997
C	3.488780	0.401102	-0.817784
O	5.328530	2.921737	0.753590

C	3.472823	1.569713	-0.090890
O	5.716524	0.968748	-0.357546
C	4.882140	1.949869	0.183606
O	4.802536	-1.238602	1.242983
H	4.010640	-0.663815	1.297638
O	6.725441	-3.066006	0.618135
H	6.264305	-2.858603	1.457184
C	4.916393	-0.080421	-0.916097
H	5.214584	-0.241869	-1.979211
C	5.125951	-1.396309	-0.135461
H	4.465140	-2.162387	-0.615997
C	6.574060	-1.890914	-0.163077
H	6.867728	-2.135741	-1.207383
H	7.225267	-1.053461	0.190351
H	1.627148	0.005152	-1.128112
O	0.398856	0.930687	-0.553226
C	-0.760398	0.617044	-0.234763
O	-1.328581	-0.517160	-0.621134
O	-1.537084	1.389427	0.510295
C	-2.907195	0.788684	0.556701
H	-3.581647	1.383873	-0.085289
H	-3.272476	0.832404	1.596329
C	-2.673746	-0.640337	0.035182
H	-3.408083	-0.894422	-0.750604
Cl	-5.681410	-0.299082	0.608094
C	-2.606976	-1.718085	1.100034
H	-3.638570	-1.806825	1.502858
H	-2.286649	-2.685528	0.663285
H	-1.901304	-1.436076	1.910895

F-

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ACID-AB SCF Done: -977.215432837 A.U.

O	-1.299032	-0.844063	0.543816
O	-1.236832	2.037381	-0.864649
H	-0.387922	1.491071	-0.823049
C	-2.223515	0.107681	0.375667
O	-3.981221	3.016764	-0.453242
C	-2.212328	1.337002	-0.250852
O	-4.373424	1.025281	0.586475
C	-3.558861	1.936668	-0.096068
O	-4.262682	-1.113211	-1.340921
H	-3.452386	-0.602683	-1.553664
O	-6.247240	-2.683777	-0.357416
H	-5.970066	-2.449236	-1.267542
C	-3.633318	-0.176957	0.836179
H	-3.663570	-0.405568	1.928075
C	-4.249286	-1.362315	0.062823
H	-3.621857	-2.259091	0.300083
C	-5.704308	-1.644503	0.444360
H	-5.759665	-1.968100	1.507040
H	-6.272882	-0.686798	0.345303
H	-0.399953	-0.498470	0.172143
O	0.733159	0.391446	-0.372632
C	1.724979	0.849638	0.623137
H	1.835651	1.953219	0.591252

C	1.720512	0.232879	2.002785
H	2.785370	-0.068726	2.166298
H	1.324399	0.912212	2.785430
H	1.120234	-0.699487	1.999996
C	2.300450	0.063713	-0.463026
H	2.742668	0.577417	-1.331986
H	2.670303	-0.955735	-0.198572
F	4.140554	-0.853854	0.678669

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ACID-A+F SCF Done: -977.302118026 A.U.

O	-1.018707	-0.882108	0.036884
O	-1.231817	2.221921	-0.480323
H	-0.428382	1.696396	-0.777279
C	-1.959566	-0.037865	0.314224
O	-3.839155	2.915312	0.770907
C	-2.110328	1.331042	0.070611
O	-4.042794	0.679955	1.204623
C	-3.357767	1.798798	0.673657
O	-4.269757	-0.771998	-1.290859
H	-3.632279	-0.021795	-1.340952
O	-6.118087	-2.569145	-0.540055
H	-5.955770	-2.024545	-1.340120
C	-3.276722	-0.501464	0.933074
H	-3.095957	-1.053645	1.886032
C	-4.029220	-1.425383	-0.042577
H	-3.372908	-2.318775	-0.200096
C	-5.402361	-1.868600	0.471541
H	-5.282543	-2.549096	1.344218

H	-5.945686	-0.954445	0.817766
H	0.047754	-0.157752	-0.609266
O	0.798653	0.515454	-0.969760
C	1.772714	0.619448	0.057625
H	2.575194	1.307841	-0.304165
C	1.210773	1.160214	1.379682
H	2.014317	1.252562	2.139741
H	0.733679	2.147115	1.214980
H	0.428857	0.471714	1.761831
C	2.397585	-0.770946	0.227464
H	2.782205	-1.136859	-0.749892
H	1.630045	-1.479261	0.613815
F	3.489477	-0.747583	1.152702

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ACID-B SCF Done: -977.310570936 A.U.

O	1.675104	-1.315916	0.049354
O	0.823176	1.599143	0.923480
H	0.380942	0.778219	1.294391
C	2.112193	-0.135848	-0.325275
O	2.762848	3.311519	-0.558534
C	1.776257	1.156251	0.045762
O	3.590994	1.356909	-1.411453
C	2.683568	2.095556	-0.610912
O	4.043918	-2.247757	-0.726942
H	3.114697	-2.175963	-0.339471
O	6.003071	-1.424109	0.912899
H	5.534121	-2.249338	0.642593
C	3.264455	-0.032323	-1.312204

H	2.941170	-0.407917	-2.313402
C	4.467024	-0.886337	-0.862800
H	5.261502	-0.864234	-1.645536
C	5.093656	-0.426347	0.467506
H	5.635745	0.533573	0.329256
H	4.273627	-0.242742	1.208639
H	0.529525	-1.123904	0.954755
O	-0.340290	-0.775884	1.442026
C	-1.358605	-0.821493	0.451494
H	-0.915073	-0.683142	-0.566023
C	-2.107041	-2.157005	0.485851
H	-2.944546	-2.165471	-0.242666
H	-1.408782	-2.983950	0.242995
H	-2.513634	-2.334342	1.504800
C	-2.274585	0.373820	0.725531
H	-1.703633	1.320136	0.607474
H	-2.684255	0.308681	1.759800
F	-3.377542	0.393640	-0.181625

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ACID-B+CO2 SCF Done: -1165.77202279 A.U.

O	1.510789	-0.176373	-1.683510
O	0.679520	1.815451	0.622381
H	0.130336	0.990452	0.466607
C	2.219296	0.728246	-0.986612
O	3.244999	3.183216	1.277763
C	1.874639	1.581591	0.030396
O	4.170734	1.814052	-0.295983
C	3.094295	2.299210	0.457696

O	3.885918	-0.815039	0.835790
H	2.920500	-1.042697	0.890353
O	6.215576	-1.902902	0.118909
H	5.570884	-1.971967	0.860594
C	3.719261	0.708659	-1.087955
H	4.089723	0.834132	-2.133327
C	4.258020	-0.631710	-0.515821
H	3.839397	-1.440364	-1.167632
C	5.789568	-0.714153	-0.527339
H	6.165929	-0.720605	-1.575127
H	6.183341	0.207336	-0.028569
H	0.662657	-0.362841	-1.154050
O	-0.489577	-0.492288	-0.052430
C	-1.841497	-0.471669	-0.518368
H	-1.920743	0.441856	-1.155524
C	-2.193116	-1.699933	-1.360505
H	-3.242446	-1.629239	-1.714332
H	-1.523123	-1.764488	-2.242345
H	-2.074034	-2.617049	-0.750785
C	-2.796960	-0.258528	0.663086
H	-2.456964	0.606287	1.274219
H	-2.859150	-1.166496	1.295699
F	-4.104309	0.039604	0.163015
O	-0.857355	-2.412814	1.365360
O	1.258068	-1.563475	1.061415
C	0.047422	-1.701251	0.965704

O	2.301692	-0.891748	-0.445684
O	2.395351	2.148774	0.627822
H	1.552544	1.627619	0.772317
C	3.239414	0.064613	-0.466459
O	5.086484	3.015991	-0.147159
C	3.295397	1.355697	0.013802
O	5.363590	0.914436	-0.987220
C	4.626551	1.910114	-0.337108
O	5.429927	-0.983228	1.179690
H	4.646041	-0.440647	1.410799
O	7.296977	-2.696825	0.196468
H	7.119406	-2.353655	1.096856
C	4.596736	-0.295580	-1.022016
H	4.520288	-0.650487	-2.077297
C	5.277966	-1.393415	-0.176874
H	4.625308	-2.300904	-0.246250
C	6.686769	-1.743722	-0.661568
H	6.635806	-2.185402	-1.681037
H	7.269589	-0.791757	-0.726961
H	1.471159	-0.535423	0.020770
O	0.412297	0.386831	0.777170
C	-0.836179	0.369135	0.655423
O	-1.452814	-0.682611	0.124035
O	-1.611497	1.347587	1.032527
C	-3.125330	0.971609	0.616536
H	-3.354298	1.682252	-0.188465
H	-3.694238	1.166062	1.534969
C	-2.948368	-0.486472	0.207712
H	-3.339649	-0.649106	-0.810642

F	-5.167393	0.432795	0.054891
C	-3.507036	-1.500646	1.189824
H	-4.601711	-1.323482	1.178115
H	-3.261341	-2.536975	0.879873
H	-3.097364	-1.327459	2.208531

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ACID-C SCF Done: -1165.77198510 A.U.

O	-2.634615	-1.068401	1.022769
O	-1.654881	1.690088	-0.363991
H	-0.883643	1.168035	0.060436
C	-3.246938	0.050562	0.654440
O	-4.140630	3.231114	-0.508779
C	-2.847297	1.221485	0.035493
O	-5.153827	1.418534	0.429335
C	-4.037454	2.099891	-0.077328
O	-5.103524	-0.791047	-1.428904
H	-4.192362	-0.423297	-1.455946
O	-7.541930	-1.837392	-0.905460
H	-7.014551	-1.710959	-1.722208
C	-4.751415	0.103027	0.826006
H	-5.046628	-0.066743	1.889580
C	-5.438485	-0.962803	-0.052939
H	-5.080045	-1.956904	0.317461
C	-6.966543	-0.911458	0.008030
H	-7.314381	-1.177087	1.030986
H	-7.279507	0.141629	-0.200541
H	-1.674290	-1.205597	0.586683
O	0.418247	0.479102	0.595067

C	0.518422	-0.739787	0.296555
O	-0.386153	-1.584043	0.063990
O	1.807734	-1.283720	0.200570
C	2.908037	-0.394541	0.421837
H	2.693382	0.594935	-0.041099
C	3.185832	-0.199230	1.911394
H	4.100908	0.410624	2.058314
H	2.322889	0.320065	2.371444
H	3.325373	-1.183350	2.407562
C	4.062496	-1.063622	-0.324294
H	3.814031	-1.172912	-1.402336
H	4.276160	-2.068641	0.105003
F	5.246896	-0.279069	-0.214548

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ACID-D SCF Done: -1165.72377725 A.U.

O	2.483256	-0.295139	-1.444179
O	2.440173	2.469094	0.218246
H	1.563238	2.090530	-0.080709
C	3.437267	0.450766	-0.870290
O	5.280084	2.909546	0.796578
C	3.422821	1.617471	-0.136677
O	5.658226	0.946835	-0.300469
C	4.827812	1.953148	0.203800
O	4.591078	-1.234648	1.244002
H	3.824579	-0.623304	1.259017
O	6.487243	-3.114231	0.721423
H	5.979422	-2.890728	1.529014
C	4.852695	-0.074577	-0.900937

H	5.197315	-0.243900	-1.948931
C	4.981113	-1.398320	-0.116553
H	4.321692	-2.141409	-0.633738
C	6.412414	-1.937905	-0.070138
H	6.751075	-2.195606	-1.097742
H	7.070735	-1.119975	0.314578
H	1.575764	0.122051	-1.257126
O	0.393349	1.063566	-0.735170
C	-0.737508	0.706098	-0.328688
O	-1.247268	-0.472145	-0.665896
O	-1.495071	1.451558	0.433341
C	-2.890210	0.710829	0.621177
H	-3.606705	1.322919	0.056402
H	-3.073274	0.748282	1.703542
C	-2.579789	-0.662010	0.034136
H	-3.308347	-0.921215	-0.751910
F	-4.818402	-0.358948	0.861541
C	-2.426679	-1.779805	1.048855
H	-3.437674	-1.883604	1.493554
H	-2.099345	-2.721768	0.563166
H	-1.684346	-1.504783	1.829113