Supporting Information

CO$_2$ Atmosphere Enables Efficient Catalytic Hydration of Ethylene Oxide by Ionic Liquids/Organic Bases at Low Water/Epoxide Ratios

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Experimental procedures

Cycloaddition of CO_2 with EO

EO (2.20 g, 50 mmol), VBImBr (0.116 g, 0.5 mmol), VIm (0.047 g, 0.5 mmol) and CO_2 (1.5 MPa) were added into the autoclave and heated to 100 °C for 3 h. After the completion of reaction, the autoclave was cooled to room temperature and slowly vented. The reaction mixture was analyzed by GC and biphenyl was used as the internal standard. The cycloaddition of CO_2 with VBImBr or VIm was performed following the same procedure.

Hydrolysis of EC

EC (4.40 g, 50 mmol), deionized water (1.35 g, 75 mmol), VBImBr (0.116 g, 0.5 mmol) and VIm (0.047 g, 0.5 mmol) were added into autoclave equipped with a magnetic stirrer. The reaction mixture was stirred at 100 °C for 3 h and the reaction pressure was held constant (1.5 MPa CO_2) using a backpressure valve. After completion of the reaction, the autoclave was cooled to room temperature and slowly vented. The products were analyzed using GC with biphenyl as an internal standard. The hydrolysis of EC with VBImBr or VIm as the catalyst was performed following the same procedure.

Reaction of EO and MEG

EO (2.20 g, 50 mmol) and MEG (3.10 g, 50 mmol), VBImBr (0.116 g, 0.5 mmol) and VIm (0.047 g, 0.5 mmol) were added into the autoclave. The autoclave was pressurized with N_2 (1.5 MPa) and heated to 100 °C. After 3 h, the autoclave was cooled to room temperature and vented. The products were analyzed using GC with biphenyl as an internal standard.

Reaction of EC and MEG

EC (4.40 g, 50 mmol), MEG (3.10 g, 50 mmol), VBImBr (0.116 g, 0.5 mmol), VIm (0.047 g, 0.5 mmol) and CO_2 (1.5 MPa) were added into a 30 mL stainless steel autoclave equipped with a magnetic stirrer. The reaction mixture was stirred at 100 °C for 3 h. After completion of the reaction, the autoclave was cooled and vented. The products were analyzed using GC with biphenyl as an internal standard.

Isotope labeling experiments

EO (0.44 g, 10 mmol), $H_2^{18}O$ (0.3 g, 15 mmol), VBImBr (0.023 g, 0.1 mmol) and VIm (0.009 g, 0.1 mmol) were added into the autoclave. The autoclave was pressurized with CO_2 or N_2 (1.5 MPa) and heated to 100 °C. After 3 h, the autoclave was cooled to room temperature and CO_2 or N_2 was vented in the air capture bag. The reaction mixture was analyzed by Shimadzu GCMS-QP2010 and the gas was analyzed by GC-MS (Agilent 5977B).

EC (0.88 g, 10 mmol), $H_2^{18}O$ (0.3 g, 15 mmol), VBImBr (0.023 g, 0.1 mmol) and VIm (0.009 g, 0.1 mmol) were added into a 30 mL stainless steel autoclave equipped with a magnetic stirrer. The reaction mixture was stirred at 100 °C for 3 h and the reaction pressure was held constant (1.5 MPa CO_2) using a backpressure valve. After completion of the reaction, the autoclave was cooled to room temperature and CO_2 was vented in the air capture bag. The products were analyzed using GC-MS (Shimadzu GCMS-QP2010, Agilent 5977B).

EO (0.44 g, 10 mmol), $H_2^{18}O$ (0.3 g, 15 mmol), VBImBr (0.023 g, 0.1 mmol) and VIm (0.009 g, 0.1 mmol) were added into the first autoclave. The autoclave was pressurized with CO_2 (1.5MPa). EO (0.44 g, 10 mmol) was added into the second autoclave. A vent tube was used to connect the two stainless steel autoclaves. After heated the first autoclave to 100 °C for 3 h, the autoclave valve was opened and CO_2 was vented to the second autoclave. The two autoclaves were still stirred at 100 °C for 3 h. After completion of the reaction, the autoclave was cooled to room temperature and CO_2 was vented. The products of the two autoclaves were analyzed by GC-MS (Shimadzu GCMS-QP2010, Agilent 5977B).

DFT calculations

The DFT calculations in this paper were all performed in Gaussian 09 software package.[2] M06-2X was chosen as the functional and 6-311+G* was selected to be the basis set, denoted as M06-2X/6-311+G*. The hybrid density functional M06-2X is believed to show an excellent performance in calculating thermodynamic properties of compounds made of main group elements.[3] The structures of intermediates and transition states were all optimized at first using M06-2X/6-311+G*, under the condition of 373 K in temperature and 1.5 MPa in pressure. The solvation effect of water was also included by using integral equation formalism polarizable continuum model

(IEFPCM).[4] The optimized structures were then treated with frequency analysis under the same computational level to prove their being a local minima or saddle point on the potential energy surface. The values of Gibbs free energies were also calculated in this step. All the relative energies reported in this paper are in the unit of kcal/mol.

Supported tables and figures

Table S1. Optimization of the reaction conditions.[a]

Entry	n(H$_2$O) /n(EO)	n(catalyst) /n(EO)	T (°C)	t (h)	P (MPa)	Yield /% MEG	EC	DEG	Selectivity of MEG / %
1			60	3	1.0	20	19	-	51
2			70			42	24	2	60
3	5:1	2	80			72	2	3	90
4			90			81	-	3	93
5			100			84	-	3	94
6			110			84	-	4	91
7					0.5	86	2	2	93
8	1:1	2	100	6	1.0	87	2	1	96
9					1.5	86	1	1	97
10					2.0	86	4	1	93
11	1:1					80	4	1	93
12	1.5:1	2	100	3	1.5	89	1	1	97
13	2:1					88	-	1	98
14	5:1					84	-	3	93
15		1				75	10	2	84
16	1.5:1	2	100	3	1.5	89	1	1	97
17		3				84	-	1	98
18		5				84	-	1	98

[a] Reaction conditions: EO (2.2 g, 50 mmol), n(VBImBr):n(VIm) = 1:1.

From Table S1, optimized reaction conditions of 100 °C, 3 h, 1.5 MPa, and 2 mol% catalysts, n(VBImBr):n(VIm) = 1:1 were obtained.

Table S2. Hydration of EO catalyzed by ionic liquids/organic bases under different atmospheres. [a]

Entry	n(H$_2$O) /n(EO)	Reaction atmosphere	Yield /% MEG	EC	DEG	TEG	Selectivity of MEG / %
1 [a]	1:1	CO_2	80	4	1	-	93
2 [b]	15:1	N_2	62	-	15	1.5	63

[a] Reaction conditions: EO (2.2 g, 50 mmol), H$_2$O (0.9 g, 50 mmol), VBImBr (0.5 mmol, 1mol%)/VIm (0.5 mmol, 1mol%), 100 °C, 3 h, 1.5 MPa;
[b] Reaction conditions: EO (2.2 g, 50 mmol), H$_2$O (13.5 g, 750 mmol), VBImBr (0.5 mmol, 1mol%)/VIm (0.5 mmol, 1mol%), 100 °C, 3 h, 1.5 MPa.
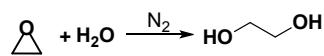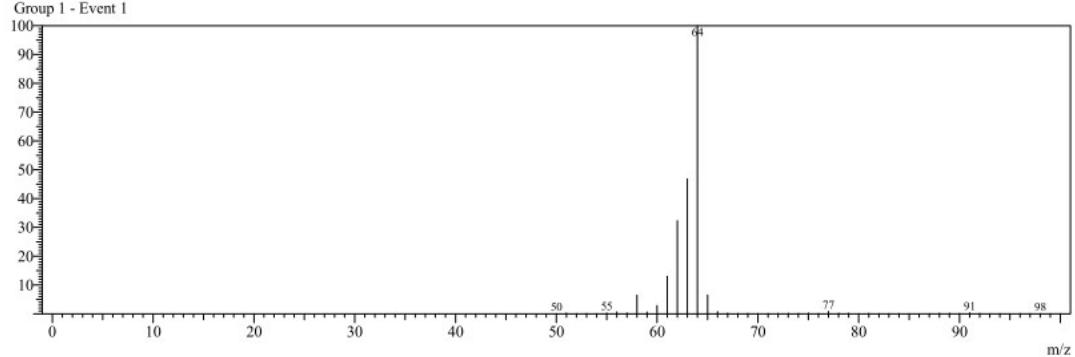
Fig. S1 Typical GC-MS spectrum of the crude product in the hydration of EO under N_2 atmosphere.
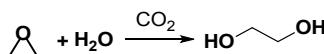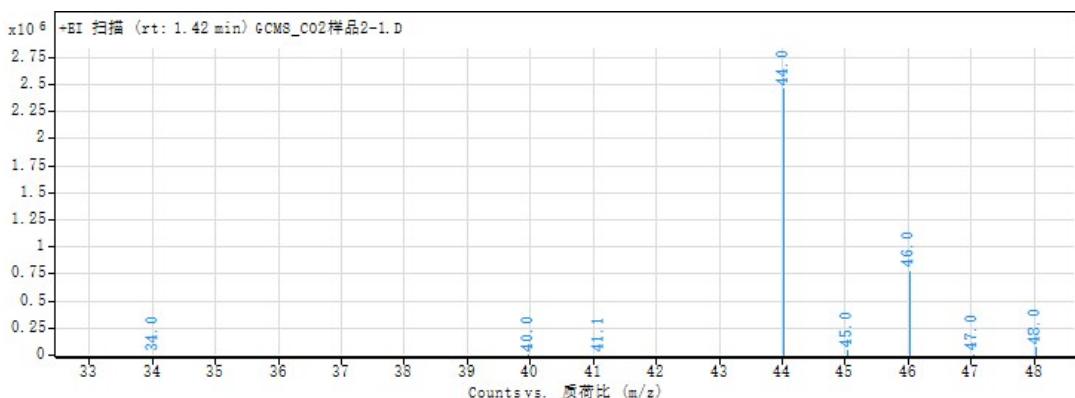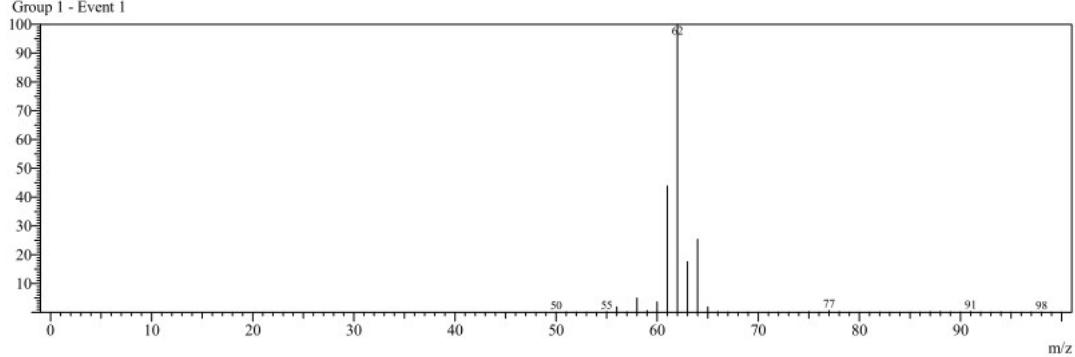
Fig. S2 Typical GC-MS spectra of the crude product in the hydration of EO under CO_2 atmosphere.
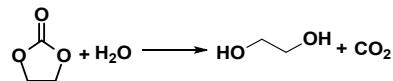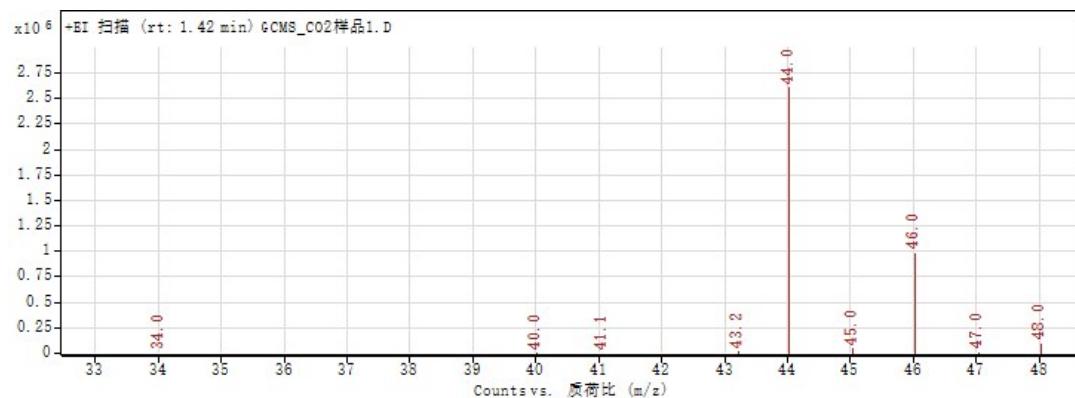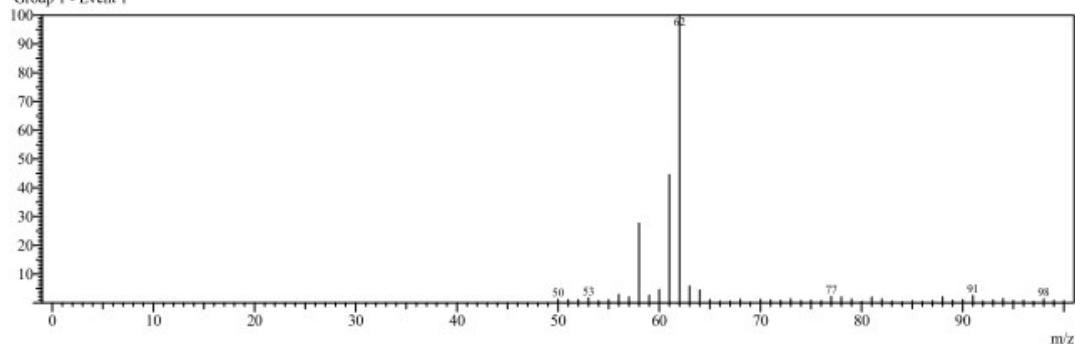
Fig. S3 Typical GC-MS spectra of the crude product in the hydrolysis of EC.
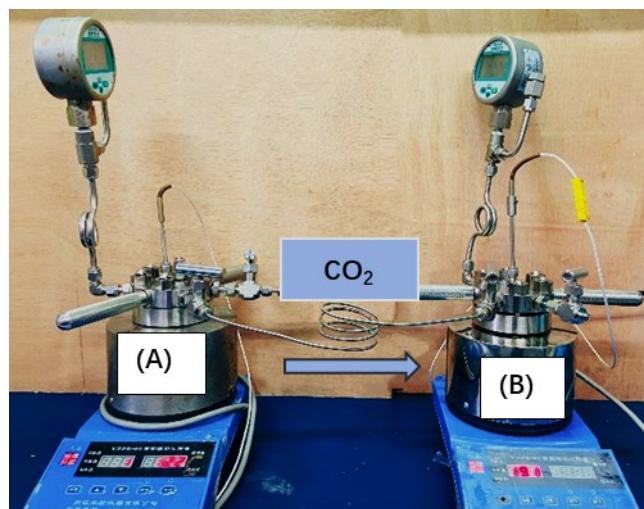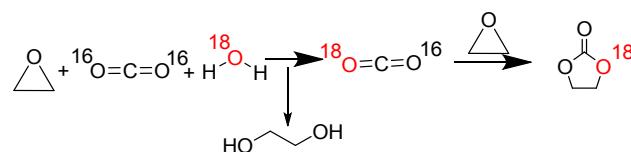
Fig. S4 Cascade reactors in which Hydration of EO with $H_2^{18}O$ under CO_2 atmosphere occurs in reactor A, and cycloaddition of EO with the released CO_2 vented from reactor A takes place in reactor B. Reaction conditions: (A) EO (0.44 g, 10 mmol), $H_2^{18}O$ (0.3 g, 15 mmol), VBImBr (0.023 g, 0.1 mmol)/VIm (0.009 g, 0.1 mmol), CO_2 (1.5 MPa), 100 °C, 6 h; (B) EO (0.44 g, 10 mmol), 100 °C, 3 h.
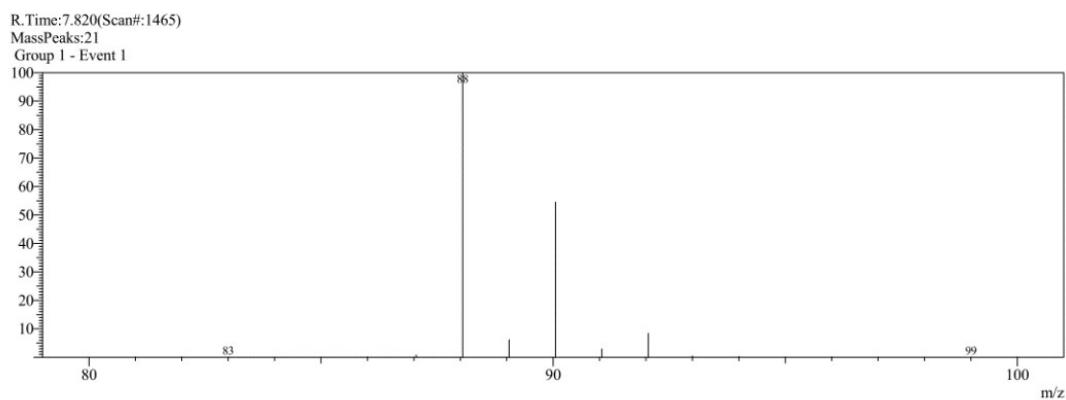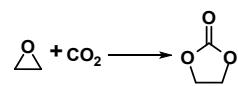
Fig. S5 Typical GC-MS spectrum of the crude product in the cycloaddition of EO.
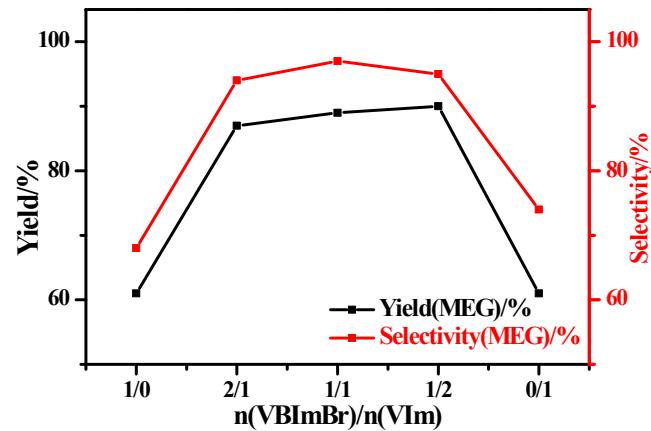
Fig. S6 Effect of the ratio of VBImBr and VIm for hydration of EO. Reaction conditions: EO (2.2 g, 50 mmol), H_2O (1.35 g, 75 mmol), CO_2 (1.5 MPa), catalysts: VBImBr+VIm (1 mmol, 2 mol%), 100 °C, 3 h.
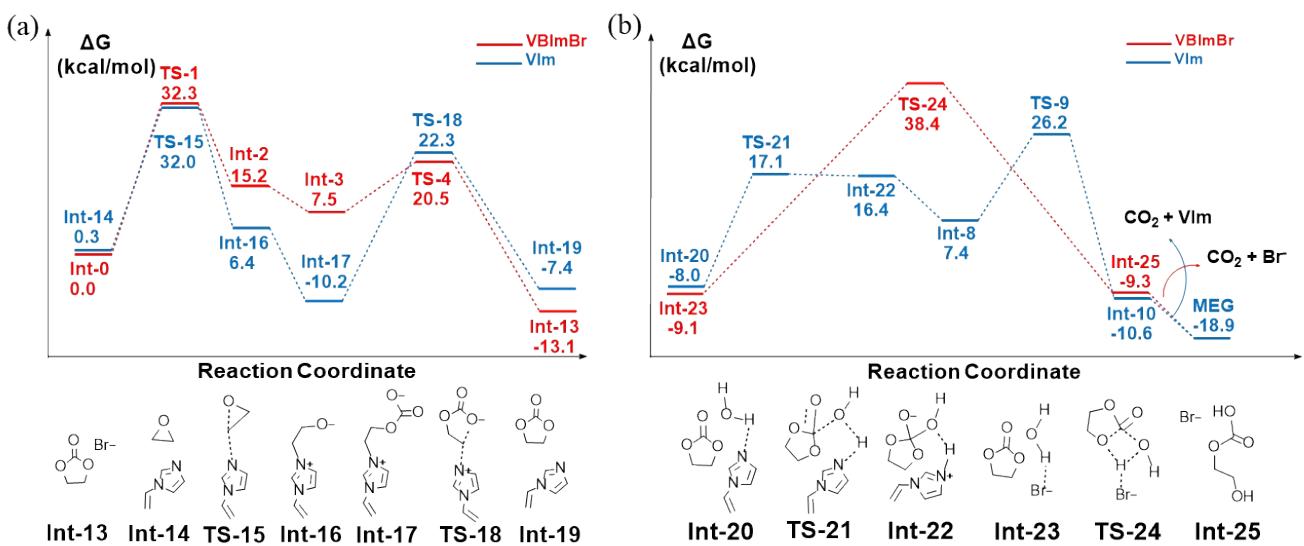
Fig. S7 Calculated free energy profiles of cycloaddition of EO (a) and hydrolysis of EC (b) catalyzed by VBImBr or VIm. Optimized structures of intermediates and transition states are shown below.

The cycloaddition of CO_2 catalyzed by VBImBr (the red curve in Fig. S7a) has been discussed in Fig. 3. The rate-determining step is the EO ring-opening, with a barrier of 32.3 kcal/mol. In the CO_2 cycloaddition catalyzed by VIm (the blue curve in Fig. S7a), the alkaline N atom of VIm attacks the EO ring through **TS-15** and needs to overcome a barrier of 32.0 kcal/mol. The ring-opening product **Int-16** adds with a CO_2 to yield a stable intermediate **Int-17**. The EC ring in **Int-17** forms via **TS-18** to yield **Int-19**, overcoming a barrier of 32.5 kcal/mol. It is found that the rate-determining of the VBImBr-catalyzed pathway is 0.3 kcal/mol lower than that catalyzed by VIm. Moreover, we notice that another high barrier exists in the Vim-catalyzed pathway (**TS-15**, 31.7 kcal/mol) via **TS-18**. The **Int-17** is too stable so that it might be kinetically unfavorable in catalysis. The calculated results suggest the VIm catalyst is less favorable than VBImBr and support that ionic liquids mainly catalyzed the cycloaddition of CO_2.

In the hydrolysis of EC catalyzed by VIm (the blue curve in Fig. S7b), starting from **Int-20**, the water molecule attacks carbonic C while one of H atoms is transferred to VIm in **TS-21**, with a barrier of 25.1 kcal/mol. The generated **Int-22** is simialar to **Int-8** and the following reaction steps has already been discussed in Fig. 3. The rate-determining step is the penta-ring opening, with a barrier of 34.2 kcal/mol. In the hydrolysis of EC catalyzed by VBImBr (the red curve in Fig. S7b), starting from **Int-23**, a water molecule stabilizes Br^- with EC. One of H atoms of water is transferred to the O atom of EC ring with the help of Br^-. At the same time, the penta-ring is broken, via a four-atom ring transition state **TS-24** with a 47.5 kcal/mol barrier. The formed **Int-25** then releases a CO_2 to generate the MEG. The rate-determining step here is the ring-opening, which is extremely endothermic with an energy of 47.5 kcal/mol. Such reaction is impossible to take place under experimental condition. The reaction catalyzed by VIm has a much lower barrier than VBImBr in the EC hydrolysis, indicating that the organic bases play an importance role in catalyzing the hydrolysis of EC.

Cartesian coordinates of geometric structures in DFT calculations

Int-0

Charge = 0   Multiplicity = 1

C	0.4553922723	0.8993412533	-0.8911081602
C	0.6847919473	2.7446334549	0.2977036668
C	-0.6361599197	2.5481173559	0.0685633222
N	-0.7543705417	1.3966303543	-0.6862263443
H	0.707012018	-0.008463171	-1.4193875808
H	1.193380306	3.5246341196	0.8358457571
H	-1.4957508706	3.1259991833	0.36345775
N	1.3553009608	1.7050307595	-0.3207243488
C	-2.0142576947	0.7687443555	-1.1051236384
C	-2.7490664337	0.1616097154	0.0841617834
H	-1.7516738571	0.0140177471	-1.8459970651
H	-2.6142036402	1.5344448371	-1.6008563893
C	-4.0831095921	-0.461584139	-0.3274367545
H	-2.1006355496	-0.5879748838	0.548677303
H	-2.9227176316	0.9414869022	0.8319927938
H	-4.5825686129	-0.8187302962	0.5769572586
H	-4.732763189	0.3113258052	-0.7521395246
C	-3.9362709237	-1.6171065686	-1.316673487
H	-4.8910326217	-2.1237072173	-1.4688084739
H	-3.5917138492	-1.2776666433	-2.2963262078
H	-3.2198722093	-2.3571033617	-0.9483041265
Br	0.6804971217	-0.934971896	1.8548672088
C	1.3122906203	-2.724735837	-1.4495269433
C	2.6781013618	-2.4935629977	-0.9750698274
O	2.0427435874	-1.5638883578	-1.8550965062
H	1.1334873737	-3.4407259319	-2.2438785987
H	3.4993391857	-3.0420978857	-1.4227739658
H	2.8163483662	-2.1253560662	0.0359625532
H	0.4904977249	-2.5176956627	-0.7707987407
C	2.7468425295	1.4180892898	-0.3143536745
H	2.9721032535	0.4769737309	-0.801449482
C	3.6610579365	2.2068204032	0.2269413665
H	3.4257991594	3.1469056916	0.7103660733
H	4.6999464917	1.9085335767	0.1912543534

TS-1

Charge = 0   Multiplicity = 1

Br	-0.6599511701	-2.8852221552	-0.1311215049
C	-1.032212973	0.2520254127	0.480790678
C	-0.5852540053	-0.9191713587	1.2381061416
O	-0.7524651174	0.9723032995	1.6317714599
H	-0.4050586058	0.4927936977	-0.3938340032
H	0.4731484751	-1.0185951633	1.4316575265

H	-1.2533013069	-1.3090109947	1.9914604306
C	1.6530502513	2.001739989	0.4192632002
C	2.2621867158	3.4872161883	-1.103440056
C	3.2134661168	2.5226116764	-1.046093606
N	2.8149772561	1.6114102272	-0.087959377
H	1.0331275934	1.5018590001	1.1676310346
H	2.1944500492	4.3698770378	-1.7145468819
H	4.1316585885	2.4027405591	-1.5962872602
N	1.2912324673	3.1414228757	-0.1805241247
C	3.4725128181	0.3339790232	0.2212279531
C	2.9398588363	-0.7770485572	-0.6793426939
H	3.2926689535	0.1330089903	1.2769699373
H	4.5445829936	0.481282629	0.0855106723
C	3.6138788919	-2.121457015	-0.4063983
H	1.857032847	-0.8745144796	-0.5320173637
H	3.0943145362	-0.4856253722	-1.7225361951
H	3.242344146	-2.8397270583	-1.1422284789
H	4.6916850981	-2.0323834461	-0.5794206882
C	3.3497514964	-2.6586567035	0.9991364595
H	3.7524524161	-3.6670009398	1.1119768012
H	3.8096671354	-2.0384947238	1.7720811635
H	2.27487169	-2.7075221467	1.196158973
H	-2.0854340788	0.2323641663	0.1793460304
C	0.0702357599	3.8080123092	0.1289919828
H	-0.5564593291	3.2092928858	0.7825285905
C	-0.2509605719	5.0035740985	-0.3374400119
H	0.3951020932	5.5843145513	-0.984214326
H	-1.2041742671	5.4347758171	-0.0635856134

Int-2

Charge = 0   Multiplicity = 1

C	1.7188030025	-0.4781870364	-1.4803113967
C	3.4299822969	-1.8059521112	-0.7548604645
C	3.7748855214	-0.5235481526	-0.5052593801
N	2.726549122	0.2566847009	-0.9672678473
H	-0.0319763577	0.1149076765	-1.128561382
H	3.9549610268	-2.7305808901	-0.5790921142
H	4.6629268929	-0.1017927028	-0.0630896207
N	2.1810558565	-1.7589915027	-1.3585844639
C	2.6653240409	1.7078902755	-0.8113718834
C	2.2094607473	2.1128521367	0.5869736064
H	1.9775718788	2.0729421149	-1.5739837196
H	3.6563915853	2.1150339673	-1.0302413665
C	2.2943258466	3.6220512562	0.8122042823
H	1.1807819333	1.7656483375	0.7322522435

H	2.8259921427	1.5902818751	1.3255079144
H	1.9914341026	3.8366385123	1.8409243542
H	3.3378233605	3.9450280254	0.7257436926
C	1.423522405	4.4276452324	-0.1513402701
H	1.4100674389	5.4848725678	0.1211123896
H	1.7863076622	4.3613011478	-1.1797332227
H	0.3911684361	4.0656057495	-0.1388870924
Br	0.6899450179	-1.1710223323	1.7505579137
C	-1.515933242	-0.632095417	-0.0584750034
C	-1.1666947711	-0.60497434	1.4163914093
O	-0.9191943323	0.4050713497	-0.7955724855
H	-1.2747354843	-1.614267462	-0.4798924498
H	-1.7854041364	-1.2936420558	1.9872813629
H	-1.2439557022	0.3998032543	1.8256350857
H	-2.6016811441	-0.5006426432	-0.1225804769
C	1.4687395286	-2.9177033317	-1.7420274291
H	1.9497779194	-3.8348113928	-1.4214285544
C	0.3279565961	-2.9193443256	-2.4203259596
H	-0.1463635563	-2.0028040887	-2.7495175002
H	-0.1491134044	-3.8614190751	-2.6552889716

Int-3

Charge = 0   Multiplicity = 1

C	-2.497729	-0.135866	-0.119641
C	-4.629152	0.405545	-0.371466
C	-3.943844	1.527451	-0.038816
N	-2.621328	1.164536	0.113218
H	-1.577716	-0.711675	-0.064238
H	-5.673479	0.244271	-0.577299
H	-4.274438	2.542394	0.100339
N	-3.708553	-0.624872	-0.416665
C	-1.50794	2.055866	0.482998
C	-0.357883	1.942142	-0.509123
H	-1.190074	1.771519	1.484861
H	-1.917149	3.066594	0.502391
C	0.769461	2.92408	-0.190666
H	0.04	0.921932	-0.482757
H	-0.741005	2.121722	-1.518522
H	1.524098	2.835306	-0.976737
H	0.388657	3.950072	-0.242834
C	1.423107	2.671821	1.166922
H	2.318289	3.286078	1.28737
H	0.750408	2.908949	1.994881
H	1.711049	1.621796	1.264004
Br	2.976838	0.043072	-1.156582
C	2.64271	-1.986074	0.868607
C	3.712509	-1.122971	0.243724

O	1.749949	-1.199091	1.630979
H	2.102944	-2.559213	0.116734
H	4.477915	-1.725139	-0.239561
H	4.164695	-0.452256	0.970273
C	0.407751	-1.116901	1.247394
O	0.042958	-1.768604	0.248289
O	-0.265078	-0.37877	1.979675
H	3.142673	-2.679808	1.553121
C	-4.01127	-1.985088	-0.717584
H	-5.032609	-2.11981	-1.048279
C	-3.134475	-2.970465	-0.605561
H	-2.113743	-2.818906	-0.267063
H	-3.442774	-3.97449	-0.86447

TS-4

Charge = -1   Multiplicity = 1

Br	2.5096569849	-1.4606345096	-1.1674619767
C	-0.2225163452	-1.9913547547	-0.0601553522
C	1.0201370181	-1.5326148098	0.6799057949
O	-1.3979452986	-1.531719434	0.5953307751
H	-0.2587333611	-1.5787449751	-1.0631300131
H	1.1651562294	-0.4822935833	0.8771173463
H	1.6797232621	-2.2323946196	1.1593486282
C	-1.2634511389	-1.472757713	1.9681543905
O	-0.0765920341	-1.6581043003	2.3676047056
O	-2.274165424	-1.2402752505	2.6166989843
H	-0.2318448927	-3.0827540499	-0.1159222829

Int-5

Charge = 0   Multiplicity = 1

H	2.0034659834	-1.5330992635	1.0545478735
O	2.3975925038	-0.6505558738	1.1575029998
C	0.9709235528	1.4562914914	2.6592822052
C	2.2818690653	2.1220901916	2.2155565321
H	1.1353957305	0.4824181926	3.1139678866
H	3.157080189	1.5392003127	2.488108528
H	2.3783290366	3.1511417441	2.5542141097
O	2.1877136749	2.136687763	0.7815613965
O	0.2678626419	1.2556172529	1.4212551933
C	1.0623805334	1.5589904305	0.3884430755
O	0.7519436826	1.3767877956	-0.7573405728
H	3.0669155714	-0.5667031711	0.4581170933
C	-0.4327870497	-1.9428644167	1.2195997848
C	-1.4678410628	-3.8806767762	1.1072558417
C	-0.1257962571	-4.0441894692	0.9218318589
N	0.5111279836	-2.8251799795	0.990981738
H	-0.2798331847	-0.8783545757	1.3244478006

H	-2.291899808	-4.575106862	1.1246494616
H	0.4152412737	-4.9584650748	0.7359578161
N	-1.6591397231	-2.5279990463	1.3060665172
C	-2.8966245521	-1.8957924786	1.5657756378
H	-3.7513479409	-2.5216377317	1.3367879817
C	-3.0216734416	-0.6587518175	2.0303294142
H	-2.1706876399	-0.0359518102	2.28506773
H	-4.010371542	-0.2416004963	2.1700241953
H	0.3557633229	2.0876871937	3.2957474498
C	-1.9445527958	-0.0355886286	-1.0806762816
N	-2.8943922499	0.846990211	-0.7975251956
N	-2.5237978072	-1.1504706146	-1.5366740874
C	-4.1223214761	0.2920998989	-1.0798519368
C	-2.6315769725	2.1878608115	-0.2499149319
C	-3.8928937505	-0.9647674011	-1.5391186337
C	-1.8587029414	-2.3529893928	-1.922333423
H	-5.0411332122	0.8287717311	-0.9154030206
C	-2.1505782028	3.1506304675	-1.329739112
H	-1.8927231564	2.0622992392	0.5418843825
H	-3.5621897611	2.5289135901	0.2046986353
H	-4.5685229873	-1.7370451309	-1.8654243102
H	-2.5366064511	-3.1919253999	-2.0079197453
C	-0.5551667354	-2.4340218676	-2.1320643816
C	-1.8121099258	4.5246378185	-0.748304901
H	-1.2644119757	2.7273457512	-1.8137410294
H	-2.929721336	3.2437319005	-2.091379011
H	0.1172223454	-1.5870590766	-2.0555379305
H	-0.1235288515	-3.3922959819	-2.3869279812
H	-1.630533443	5.2110238714	-1.5792688824
H	-2.6804054085	4.9190876221	-0.2097353503
C	-0.5883370069	4.5122854393	0.1678957594
H	-0.3459221288	5.5213810259	0.5060302206
H	-0.7478391229	3.9032819912	1.0619442162
H	0.2849739692	4.1197687562	-0.3602554588
H	-0.8853506514	0.1491298938	-0.9618412361
Br	4.6197454915	-0.4655100502	-1.3755009217

TS-6

Charge = 0   Multiplicity = 1

H	-1.0343745232	2.560984598	0.288593731
O	0.0621817923	3.0184304783	0.4004312157
C	1.1309389611	2.1633133877	-2.0137307624
C	2.1959935245	3.0305334428	-1.3027952075
H	0.3092302763	2.7691013314	-2.4006689598
H	1.8814877267	4.0730201523	-1.236090602
H	3.1770164498	2.9738647326	-1.7724659354
O	2.2884868941	2.4638668386	-0.0033467073

O	0.6579090535	1.2896422936	-0.9938686671
C	1.0749413054	1.813763227	0.2612809514
O	1.0212659316	1.0412047214	1.2408502452
H	0.1733019152	3.408510259	1.2949668244
C	-2.4117005235	1.0164135403	-0.7213340037
C	-4.2768205448	1.327815049	0.4105890702
C	-3.3343148526	2.2057062312	0.8472050886
N	-2.179961823	1.9946414508	0.1288191993
H	-1.6904916013	0.6256903649	-1.4210557606
H	-5.2979690907	1.158156169	0.7087534987
H	-3.3968412644	2.9577717727	1.6162206728
N	-3.6808637991	0.5777620324	-0.5849381164
C	-4.3131635444	-0.4851317032	-1.28242743
H	-5.3109468568	-0.6867194064	-0.9145645352
C	-3.7596152012	-1.1716999202	-2.2705644975
H	-2.7643480347	-0.9740067934	-2.651040719
H	-4.3187049511	-1.9740897355	-2.7325068407
H	1.5452498315	1.557752406	-2.8199852371
C	-0.2628361236	-1.4151916095	0.1055139353
N	0.1985720542	-2.0881824752	-0.9416344199
N	-1.4354876261	-1.9550540007	0.4643656926
C	-0.6899857295	-3.0941925971	-1.262369781
C	1.4597884772	-1.7814592976	-1.6381816659
C	-1.7168663973	-3.0126347504	-0.380139485
C	-2.2668757982	-1.5157745465	1.5378629865
H	-0.5141860482	-3.768347821	-2.082994422
C	2.6116922589	-1.6424869674	-0.6510880764
H	1.2997963054	-0.8636300621	-2.2037615401
H	1.6331654861	-2.5999018087	-2.3376336201
H	-2.6138058164	-3.5992320719	-0.2767058447
H	-3.1589625397	-2.1190496432	1.6456143676
C	-1.9765322069	-0.4796300196	2.3099613064
C	3.9471962519	-1.414186918	-1.3582334209
H	2.4095409395	-0.8002425535	0.0197406977
H	2.6583290882	-2.549041417	-0.040283109
H	-1.0823047335	0.1246487419	2.1838161177
H	-2.6641171512	-0.2113519476	3.1008245354
H	4.7359535888	-1.4260517709	-0.6014274398
H	4.1566798564	-2.2495672345	-2.0346072196
C	3.9990049874	-0.0913040158	-2.1199545199
H	5.0053427389	0.1098325413	-2.4921415586
H	3.3280696117	-0.0888166216	-2.9825688692
H	3.7106747943	0.733331618	-1.4619495445
H	0.2250447283	-0.5646104942	0.5805431687
Br	0.209214733	4.4232109126	3.3561990432

Int-7

Charge = 0   Multiplicity = 1

H	0.8670080988	-2.0614479041	0.0924175203
O	-0.4373602953	-2.8611374569	0.902350199
C	-1.8005253702	-1.6899559821	-1.2505007921
C	-2.7572382412	-2.6626551397	-0.5246718582
H	-1.0840736778	-2.2207990143	-1.8836831363
H	-2.4324542774	-3.699515264	-0.6386354702
H	-3.7911313458	-2.5712938152	-0.8570420817
O	-2.6800411498	-2.265219072	0.8310735327
O	-1.1279373312	-1.0093762493	-0.1989068962
C	-1.3746024655	-1.7306852908	1.0340649382
O	-1.2167027749	-1.0644391924	2.0999518598
H	-0.280405017	-3.1824210631	1.7976688206
C	1.8725932394	-0.5403893439	-0.9675817543
C	3.9024281246	-1.2166532369	-0.3905122501
C	3.0029303384	-2.0730234291	0.1519669707
N	1.7569703601	-1.6300145735	-0.2220730099
H	4.9779757393	-1.1906799893	-0.3505463374
H	3.1372311799	-2.9428155425	0.7714532605
N	3.1809523795	-0.2638458531	-1.0896864676
C	3.7914959171	0.8012037557	-1.8181131534
H	4.8407535568	0.908943944	-1.5763222511
C	3.1538995431	1.572167192	-2.6832759858
H	2.1031979171	1.4506137474	-2.9308440163
H	3.7044722964	2.364176058	-3.1744195865
H	-2.32177103	-0.9525722772	-1.8610736104
H	-0.5439048942	0.6457823624	1.5606847727
C	-0.0410827127	1.4078405042	0.9672923832
N	-0.5822037263	2.1122832325	-0.0178227545
N	1.2554595727	1.7383878331	1.0522546927
C	0.3841240763	2.9153478168	-0.5870043925
C	-1.9769967938	1.9983049096	-0.474116454
C	1.5389840366	2.6883319447	0.0870305927
C	2.2151860185	1.1484905827	1.9260917054
H	0.1621553283	3.569954988	-1.4120856586
C	-2.930386637	1.7188853607	0.6773788709
H	-1.9883244105	1.2097084873	-1.2253796685
H	-2.2169845947	2.943550999	-0.9648094847
H	2.5244572674	3.1070609462	-0.0262008388
H	3.1426368335	1.7053383028	1.9655456898
C	1.9888501643	0.0327515516	2.6031393776
C	-4.3844578235	1.6930348988	0.2049605787
H	-2.6824361044	0.7527614929	1.1283941585
H	-2.7998326786	2.4888579753	1.4447650445
H	1.0518037346	-0.5161718063	2.5377396551
H	2.7661664882	-0.3494119937	3.2517298031
H	-5.0248110455	1.5746567321	1.0832362484

H	-4.6476454619	2.6580958225	-0.2414254918
C	-4.6686096295	0.5615188695	-0.7813489061
H	-5.7377909563	0.4740347467	-0.9844227256
H	-4.1671850292	0.7175954069	-1.7401622114
H	-4.3218609653	-0.3912664546	-0.3712644318
H	1.0525904288	0.0093882012	-1.4181354788
Br	-0.4351870399	0.8647776092	-3.6051329106

Int-8

Charge = 0   Multiplicity = 1

C	1.4839097199	0.834463013	1.5807374181
C	1.8826021107	-0.5744851082	1.1600994029
H	1.706154845	1.0662072975	2.6196521877
H	1.9184597591	1.5933023688	0.9244148769
H	1.8259301059	-1.2770629462	1.9946403796
O	0.8859669068	-0.9089593712	0.1941877302
O	0.0717379485	0.7924827563	1.4170430482
C	-0.1646784823	0.0184099238	0.2748435647
O	-0.1184915108	0.7704346358	-0.8859655099
H	-1.8584563236	-0.6478092547	-0.4037808397
H	-0.8675236257	1.4044628854	-0.8754598941
H	-2.9012194042	0.675268752	-1.7125669611
O	-2.8472800407	-0.2892887677	-1.8119566016
H	-3.7457683319	-0.6258321035	-1.8821610614
H	2.8666148747	-0.6283357182	0.6967746675
O	-1.3788354965	-0.590438549	0.4498913524
N	-2.4678103243	2.3733681337	-0.6851459346
C	-2.7330029624	3.5787520128	-1.1386397917
C	-3.0816327187	2.2862984555	0.5493989728
H	-2.4239348812	3.9766120096	-2.092447752
N	-3.4900224919	4.2812833217	-0.2594386459
C	-3.7235553981	3.4557948355	0.8236312432
H	-3.0110379799	1.3895106759	1.1448385416
C	-3.9576723858	5.6132416499	-0.3842850183
H	-4.3058002652	3.7873460764	1.66761054
H	-4.8039728834	5.8250974155	0.2572397668
C	-3.4287611839	6.5186189208	-1.1948053298
H	-2.5650074435	6.3200395962	-1.8179120517
H	-3.8685580463	7.5055452926	-1.244702871

TS-9

Charge = 0   Multiplicity = 1

C	-0.4090803406	-0.1577243358	1.4221683958
C	-1.5915739222	0.1751553739	0.5038551278
H	-0.0680841013	0.7607256427	1.9225529947
H	-0.7255400255	-0.8672509874	2.1995292644
H	-2.2491548037	0.9551619792	0.8836645325

O	-0.9755243116	0.6791593688	-0.6757201993
O	0.5774246373	-0.6753558178	0.5922235564
C	-0.0907158869	-0.2350002545	-1.1832595068
O	-0.4384843013	-1.31210684	-1.6637288536
H	1.4139923447	-0.1432115707	-2.3158677986
H	0.1226223714	-3.2057866296	-0.6572078076
O	0.6376595134	-3.1770316106	0.1583965671
H	0.5505413264	-2.1991746312	0.4365515555
H	-2.1751209971	-0.7174720381	0.2596763625
O	0.9678911307	0.4506313102	-1.699115903
N	3.1640431752	-2.6190977487	-0.4327704691
C	4.2445968993	-3.2468433503	-0.8635670262
C	3.4335129523	-1.2737763922	-0.3069682867
H	4.3254353537	-4.2980019865	-1.0839721872
N	5.2232412479	-2.3466200695	-1.0169615424
C	4.7276791557	-1.0982952649	-0.6789385713
H	2.6651721573	-0.5935672153	0.0351896902
C	6.5577564681	-2.6101630274	-1.4476008083
H	5.3460503741	-0.2182843375	-0.7246499824
H	6.9973248784	-1.7861921931	-1.9942715245
C	7.1825751025	-3.7494999816	-1.2003995243
H	6.7365892973	-4.548839574	-0.6201971205
H	8.182629921	-3.8999772753	-1.5838117035
H	2.2121314035	-3.032793433	-0.2356689215

Int-10

Charge = 0   Multiplicity = 1

C	-1.3760611205	-1.2462011329	2.0606162732
C	-0.7586477885	-1.5576495659	0.7142112241
H	-1.3163298959	-0.1724483298	2.2648561945
H	-1.2669465535	-1.0281141762	-0.0903083202
H	-0.7841153482	-2.6300915227	0.5251904074
O	0.6441879602	-1.2303149465	0.7184452645
O	-0.7665542369	-1.9929917757	3.1002285562
C	1.0357427959	0.0334501763	0.5022230808
O	2.2142809475	0.3107105787	0.5239216439
H	0.1642357594	-1.7475644054	3.1560712674
H	0.4411892979	1.8195858545	0.1118099228
N	1.1144830191	3.2193171709	-0.1296337193
C	2.4216737608	3.3528450732	-0.1369619828
C	0.5905614458	4.4665230596	-0.3907010994
H	3.1239344873	2.5493763299	0.0170012705
N	2.7761215327	4.6369657379	-0.3910197241
C	1.6083519074	5.355758385	-0.5597849773
H	-0.4723317099	4.6379887028	-0.4415137981
C	4.0834547636	5.1781015711	-0.4686099059
H	1.622869072	6.4120551117	-0.7716334784

H	4.1127739933	6.1373958709	-0.9702731036
C	5.1691309454	4.5888992394	0.011687052
H	5.1443331577	3.6405600429	0.5348179253
H	6.1308660464	5.0665832774	-0.1175400863
O	0.0562066769	0.8728202752	0.2765393851
H	-2.4280546661	-1.5345274527	2.0438843079

TS-11

Charge = -1   Multiplicity = 1

Br	2.1984329433	-1.5017742686	-1.1760152284
C	1.4773745592	-2.0177784209	1.7140686493
C	1.1127079729	-0.8627360498	0.7848151492
O	0.4288052326	-2.3048034867	2.6050487079
H	1.6742306794	-2.9152228753	1.1308853072
H	0.138752258	-0.8660277796	0.3205834354
H	1.6530873885	0.064246584	0.8050209332
O	0.144868021	0.1465443213	2.456579126
H	2.3990846632	-1.7483225047	2.2464531485
H	0.0829707826	-1.383030765	2.8132663972
H	-0.6541585007	0.5318842454	2.0827223744

TS-12

Charge = -1   Multiplicity = 1

Br	4.7889129249	-0.0306006689	-0.3699219202
C	2.1554714055	-1.3268606211	0.4539768292
C	2.514163607	0.0825087807	0.0088672517
O	1.0165553372	-1.7820505386	-0.2353871571
H	2.9658237481	-2.0234313235	0.2486814778
H	2.287818749	0.3632449354	-1.0067906901
H	2.6411573118	0.8765405718	0.7243392522
C	0.2003497069	1.0807837844	1.589110345
O	0.4208356227	0.6296450752	0.306844245
H	1.1159092317	1.0230991836	2.2179293807
H	-0.1046018516	2.1446155675	1.6099693206
C	-0.8754611907	0.309705333	2.3376739268
H	-1.0994460813	0.8057297783	3.2917471587
H	-1.7910947482	0.2854528437	1.7346356882
O	-0.4077973628	-1.0166934796	2.5730062774
H	-1.131583613	-1.5514435029	2.9137459828
H	1.971707101	-1.3057661597	1.5348415214
H	0.385439102	-1.0393255593	-0.0693758901

Int-13

Charge = -1   Multiplicity = 1

C	-1.0541384828	1.2721138324	-0.1619308224
C	-0.9546350145	0.3804737389	1.0850063227
H	-1.1566806406	2.3297552666	0.0709404981

H	-1.0014220973	0.9371744569	2.0184124764
H	-0.0809186753	-0.2665528951	1.0624677258
O	-2.123498749	-0.4465229555	1.0010033895
O	-2.2666462949	0.8354361788	-0.7915023756
C	-2.8016123421	-0.1851822041	-0.1183195577
O	-3.7916574211	-0.7677330507	-0.4558826574
H	-0.2341132129	1.1054161141	-0.8564110494
Br	-0.2009323941	-1.9054902571	-1.5561659465

Int-14

Charge = 0   Multiplicity = 1

C	-1.6160472866	0.2637864784	1.2012822712
C	-1.5887791959	-1.028399373	0.5148590958
O	-2.4754319454	-0.7981235274	1.6069332431
H	-0.8263059265	0.5048552557	1.9064712757
H	-0.7833623956	-1.7247179185	0.7278280768
H	-2.0692580295	-1.1293882358	-0.452541919
H	-2.1182452942	1.1043307476	0.7349558924
N	0.0754178749	0.2222731952	-2.323162056
C	0.8029291808	-0.407299	-1.4346442321
C	-0.0494301198	1.5109773763	-1.8498856073
H	1.1149938111	-1.4390343691	-1.4925088668
N	1.1651131784	0.4079054728	-0.4008621415
C	0.6182967887	1.6463529335	-0.6678253208
H	-0.6073528016	2.2614203296	-2.387824654
C	1.8898307103	0.0774594014	0.7638723531
H	0.7522636828	2.4777844342	0.0051242841
H	2.1890611899	0.9489694223	1.334031432
C	2.1841767937	-1.1567708774	1.1535408363
H	1.8837200614	-2.0402099885	0.6032881617
H	2.7592037231	-1.3014367572	2.0579638754

TS-15

Charge = 0   Multiplicity = 1

C	0.7878463148	-2.0254878697	1.4795655409
C	0.7884250695	-1.765975444	0.0429132762
O	-0.5275034006	-2.389797788	1.2264580825
H	1.4522926842	-2.834012107	1.8107117954
H	0.8166010182	-2.6193783401	-0.6178755995
H	0.2769020598	-0.8804687962	-0.3029357865
H	0.9247222144	-1.1422192891	2.1167848576
N	2.5386007734	-1.1030726847	-0.5565667533
C	3.5692617727	-1.8386304442	-0.9031796044
C	2.9775719915	0.1961716057	-0.4709227076
H	3.5571504961	-2.9035397366	-1.0762801899
N	4.6728491041	-1.0670995745	-1.055765629
C	4.3021842914	0.2357129961	-0.7885157687

Int-16

Charge = 0   Multiplicity = 1

H	2.3155336539	1.0012802926	-0.1943216743
C	5.9794355466	-1.4903853359	-1.4141580404
H	5.0117293841	1.0449596601	-0.8401558604
H	6.5686075003	-0.706095622	-1.8728545345
C	6.4379230273	-2.7176222188	-1.2183779706
H	5.8562542921	-3.4919992871	-0.7324819809
H	7.4357112964	-2.9708021565	-1.5503832826

Int-16

Charge = 0   Multiplicity = 1

C	-0.2268135956	-2.0682625589	1.1164276676
C	-1.368924712	-2.5454024448	0.1860818898
O	0.9806198857	-2.0992261329	0.5054632703
H	-0.5295225104	-1.0566341091	1.4714398233
H	-2.3581256638	-2.4727759104	0.6398691661
H	-1.1885532942	-3.5742683194	-0.1284859776
H	-0.3162756108	-2.7285006632	2.0069044082
N	-1.3809697236	-1.7092926416	-1.0177656306
C	-0.3737665617	-1.6481990367	-1.8778782345
C	-2.3237958881	-0.7626429437	-1.3636082518
H	0.498909486	-2.2751322872	-1.8430620486
N	-0.6432763154	-0.693408473	-2.7808181081
C	-1.8688508416	-0.128709714	-2.4720623209
H	-3.2290702603	-0.6302013783	-0.7961181623
C	0.1881865064	-0.3015623602	-3.8682360885
H	-2.2928713052	0.6642055198	-3.0638241092
H	-0.3668267654	0.1290994915	-4.6914126214
C	1.5027530256	-0.4538583818	-3.8671991302
H	2.0459394717	-0.8583491296	-3.0209790318
H	2.0708925527	-0.1636437265	-4.7404360498

Int-17

Charge = 0   Multiplicity = 1

C	2.6851693293	-2.0869756341	0.7702369634
C	3.7912847534	-1.1281954565	0.341752499
O	1.5831117617	-1.3798012018	1.2935807996
H	2.3778865283	-2.7098152619	-0.0702981341
H	4.6396772677	-1.6679906897	-0.0787623836
H	4.1390476948	-0.5297727542	1.1829179657
C	0.5016018215	-1.0782896669	0.4218700726
O	0.5996634807	-1.4636772896	-0.7516923241
O	-0.3986336512	-0.4539417074	0.9951485225
H	3.0777009288	-2.7240051769	1.5650381995
N	3.2893821093	-0.1920652476	-0.6690257612
C	3.1442852749	-0.4719130862	-1.9568885006
C	2.6626620374	1.0064226182	-0.4006007242
H	3.4793269089	-1.3718700179	-2.4457232812

N	2.4728464062	0.5240002881	-2.5372588398
C	2.1504918561	1.4590769764	-1.571504332
H	2.6422108151	1.4222073652	0.5924651602
C	2.1361340015	0.6218381515	-3.920813819
H	1.6105473419	2.3584318824	-1.8129469395
H	1.203335737	1.142350134	-4.0932320458
C	2.8938830293	0.1189146023	-4.8809628741
H	3.8423576309	-0.3675041469	-4.6846507638
H	2.5674066065	0.1934893595	-5.9093197695

TS-18

Charge = 0   Multiplicity = 1

C	-0.2765741494	-1.9856566857	0.0868963803
C	0.9167661932	-1.4596782331	0.8749611829
O	-1.483420962	-1.801119466	0.8125025459
H	-0.3942812867	-1.4468724678	-0.8495676664
H	1.0232355614	-0.4016680585	1.0607343758
H	1.6562365758	-2.1221278906	1.2921014776
C	-1.2832913742	-1.7113753549	2.1695821503
O	-0.0530741506	-1.6557755325	2.4890867456
O	-2.2658547409	-1.6837383642	2.8902802195
H	-0.1376485413	-3.0482438031	-0.1249127035
N	2.0503764636	-1.2891933937	-0.71213991
C	3.0441256642	-2.0925655271	-1.0183634461
C	2.0157382827	-0.2990301769	-1.6659045203
H	3.3233296426	-2.9875481054	-0.4840929619
N	3.666047728	-1.6647718295	-2.1407757361
C	3.0129247657	-0.5250026687	-2.5654555956
H	1.28648468	0.4951750459	-1.6387567264
C	4.7900719517	-2.2534201363	-2.7803890529
H	3.3295384598	0.0130504805	-3.4435938387
H	4.8398802979	-2.0323390292	-3.8390950402
C	5.685510425	-3.0001893333	-2.1524903096
H	5.646956505	-3.1910784542	-1.0865373269
H	6.4966814285	-3.4417875957	-2.7153259331

Int-19

Charge = 0   Multiplicity = 1

C	-0.8204763733	0.0446377066	-1.5747696969
C	-2.1124828087	0.8347281414	-1.3604264154
H	-0.259832764	0.3611105197	-2.4499656814
H	-2.446838838	1.3521689797	-2.2589063426
H	-2.0629867005	1.5219480489	-0.5202248713
O	-3.0667715886	-0.1937776299	-1.0537903614
O	-1.2994975769	-1.2893534578	-1.8013559641
C	-2.5726073398	-1.3884050809	-1.3997150577
O	-3.1968796987	-2.4074094817	-1.3833691502

H	-0.1773714705	0.0363976789	-0.6949091693
C	-0.1433978552	-1.6159906882	1.3753394153
C	-0.3843751294	0.4600294757	2.0663842153
C	-1.5972742251	-0.0986919499	1.7827004577
N	-1.435157123	-1.3974600842	1.3521298483
H	0.3462181865	-2.5419577032	1.1152630791
H	-0.0928397703	1.4361762593	2.4188671797
H	-2.5743720395	0.3526802074	1.8610966894
N	0.5511071505	-0.5188197901	1.7967507624
C	1.951483892	-0.3637112258	1.9210476508
H	2.2286390407	0.4953079423	2.5200666944
C	2.8518649916	-1.168757395	1.3729816381
H	2.5867400115	-2.0172238705	0.7537566328
H	3.9031174986	-0.9809140124	1.5450679571

Int-20

Charge = 0   Multiplicity = 1

H	-0.8397609824	-1.6260780338	-0.1889647793
O	-1.813479783	-1.7411126042	-0.2039946954
C	-1.6483727025	1.0785688346	-1.0324686977
C	-3.1302091908	0.6974552998	-1.1684343458
H	-0.9833395888	0.3665061147	-1.5168819934
H	-3.2675137992	-0.2463272193	-1.6879423956
H	-3.7363906487	1.4818575431	-1.6157072816
O	-3.5585250055	0.5239994323	0.1886216706
O	-1.4134184765	1.0152170028	0.3808502971
C	-2.5189074478	0.6166134693	1.0178014647
O	-2.5767901667	0.4192393678	2.1972559281
H	-2.0318766324	-2.4208372504	0.439670241
C	1.5063193591	-0.0772839615	0.1301222856
C	3.1439372244	-1.2300746612	-0.7851566171
C	1.967679331	-1.9116888602	-0.8890374162
N	0.9516602246	-1.1822388978	-0.3100143659
H	0.9955335207	0.7109278672	0.6608461157
H	4.147365518	-1.4524485471	-1.1095917107
H	1.7891873034	-2.876043619	-1.33794722
N	2.8404155195	-0.0502833933	-0.1355142417
C	3.7651505221	0.9767745697	0.1694379739
H	4.7925739674	0.633828098	0.1766446279
C	3.4301809373	2.233549354	0.4271326643
H	2.4066561915	2.5875964737	0.3947972357
H	4.2020042697	2.9472499942	0.6814171549
H	-1.4300264643	2.0910566265	-1.3657618995

TS-21

Charge = 0   Multiplicity = 1

H	-0.3461591233	1.7582434696	-0.1850529256

O	-1.1416668233	1.1104196774	-0.9681975467
C	-1.3895928387	-1.0137210665	0.7974003989
C	-2.3478224333	-1.3090471159	-0.3782870255
H	-1.7334190248	-0.1676282611	1.3958071442
H	-3.1647908136	-0.5879812538	-0.4196901445
H	-2.7489599942	-2.3211582583	-0.3564818406
O	-1.5288285064	-1.1793392454	-1.5310837027
O	-0.1564516848	-0.6919362595	0.1651943308
C	-0.41399859	-0.4158591836	-1.1876278159
O	0.5252835051	-0.327437736	-1.9754637719
H	-1.1668684753	1.5037005822	-1.847796978
C	1.2669674334	1.6728080689	1.3610238526
C	1.549368792	3.8360969455	1.6922081217
C	0.5639367355	3.6521402659	0.7741124262
N	0.4055572452	2.298725697	0.5828192504
H	1.3969376835	0.6041565417	1.4056689858
H	1.9756059664	4.7262609857	2.1229291408
H	-0.0310950027	4.37604844	0.2434518715
N	1.9801702082	2.5751947306	2.0604102184
C	2.9944541035	2.3054646583	3.0210231687
H	3.7200084767	3.1043005815	3.1069753146
C	3.0478686434	1.19122233	3.7336407509
H	2.2972787849	0.4127168469	3.6617538146
H	3.8679281207	1.0404035206	4.4224329837
H	-1.2274834282	-1.8757703718	1.4432876976

Int-22

Charge = 0   Multiplicity = 1

H	-0.1505069312	-1.1937879033	-0.1403327013
O	-1.807515401	-1.3842242556	-0.0260575454
C	-1.7288322916	1.2525285822	-0.9748727456
C	-3.1647712903	0.709359153	-1.165400079
H	-1.0446002281	0.8514505882	-1.7290868733
H	-3.1904738724	-0.0821502814	-1.9187672055
H	-3.8798859992	1.4864892664	-1.4336054929
O	-3.5072982595	0.1971503683	0.105634989
O	-1.3569956775	0.8142385874	0.3219303243
C	-2.2930154047	-0.2078063204	0.7488817615
O	-2.3717395276	-0.4115655015	1.984811335
H	-2.136461712	-2.1594556278	0.4423559727
C	1.4705974581	0.1055527944	0.150854566
C	3.0318453227	-1.2911538186	-0.5548551957
C	1.829123759	-1.9107768024	-0.6580626255
N	0.879185396	-1.0202462061	-0.2144435077
H	0.9657682569	0.9625890744	0.5637315841
H	4.027972048	-1.6188738288	-0.7979779862
H	1.5718924343	-2.8967819156	-1.0034958023

N	2.7869405561	-0.0252221739	-0.0517627609
C	3.7846625853	0.9652512716	0.1939888075
H	4.7451608628	0.5421823309	0.457533511
C	3.5467123156	2.263378579	0.1076271461
H	2.5850323682	2.6640939418	-0.1914065373
H	4.3374441476	2.964208371	0.3383170814
H	-1.6839759157	2.3422677267	-0.9989690201

Int-23

Charge = -1   Multiplicity = 1

O	4.5390092827	1.8478573404	-4.2830477903
C	2.3867047431	2.4290344829	-2.279290499
C	3.7039991049	2.9106049837	-1.6547755513
H	2.4153208131	1.3842350295	-2.5824857045
H	1.5190239723	2.6204602274	-1.650174374
H	4.4936141154	2.1678970123	-1.7285179661
H	3.5929844752	3.2582935259	-0.6304391345
O	4.0682772362	4.0317726665	-2.469871572
O	2.2630037346	3.2327735787	-3.4613794306
C	3.2730533901	4.1014062433	-3.5397602482
O	3.4180761335	4.8845705439	-4.4339096871
Br	2.4561668265	-0.7230769917	-4.7457124254
H	5.4482841854	1.5357781311	-4.3138709653
H	3.973408787	1.0820906161	-4.483102122

TS-24

Charge = -1   Multiplicity = 1

H	3.0285646709	0.9755737108	-4.3257002597
O	4.5582788701	2.3049619636	-4.1877405764
C	2.2221734939	2.4866083548	-2.1824241611
C	3.6021171893	2.7303113074	-1.5766028942
H	1.8666662585	1.462745939	-2.0415153104
H	1.4808737804	3.1848360073	-1.7809141155
H	4.2213194254	1.8272146476	-1.627188223
H	3.5715350483	3.0969820264	-0.5512315885
O	4.1217237588	3.7368007026	-2.4179277728
O	2.4239405624	2.7441528117	-3.560964438
C	3.7239585623	3.4161739492	-3.7659405456
O	3.7204882106	4.3930112728	-4.564459306
Br	2.6606636762	-0.4322375121	-4.4525501674
H	5.1388061728	2.6684424588	-4.8650612313

Int-25

Charge = -1   Multiplicity = 1

C	-4.185335766	0.6648341227	0.6199218376
C	-3.7978191909	0.2153802883	-0.7723260797
H	-3.3065862284	1.0340603406	1.1578958519

H	-3.3670858908	1.0303332962	-1.3518456434
H	-4.6630995142	-0.1917790147	-1.2932531365
O	-2.873897232	-0.8905833692	-0.703604306
O	-4.8253944802	-0.3711580974	1.3450323843
C	-1.5696621863	-0.6691917882	-0.5188559281
O	-0.7916900752	-1.5863611563	-0.44726469
H	-4.2018078018	-1.0947610288	1.4747385766
H	-0.2852656033	0.7330772637	-0.3070957524
O	-1.2617461151	0.6131809903	-0.4328144944
H	-4.9048552989	1.4808141597	0.5401806675
Br	1.832371783	1.2981677229	-0.0397667975

Br-

Charge = -1   Multiplicity = 1

Br	0.	0.	0.

CO2

Charge = 0   Multiplicity = 1

C	-3.68990686	4.46782155	3.69695739
O	-4.8448987016	4.46782155	3.69695739
O	-2.5349150184	4.46782155	3.69695739

DEG

Charge = 0   Multiplicity = 1

C	0.8605737112	3.1432081848	-0.8677738206
C	0.4375984953	2.9578291758	-2.3069790673
H	1.8488386425	2.696537565	-0.7002639821
H	1.1605818036	3.4271984057	-2.9744844734
H	-0.5388388846	3.4299687023	-2.4649292824
H	0.9049607739	4.2085343517	-0.6098466072
O	-0.1036945721	2.4815844202	-0.069207426
C	0.220617539	2.4633230087	1.3091088365
H	0.3904626014	3.48821506	1.6626490491
H	1.1300460012	1.8742181167	1.4803158619
C	-0.9587310867	1.8486927596	2.0274065395
H	-1.1006649127	0.8181728672	1.6821856118
O	-2.1376777581	2.6086516152	1.817856934
H	-2.2523048375	2.7122017086	0.8653278968
H	-0.7765560408	1.8312502194	3.1021547923
O	0.3851721893	1.5830702485	-2.6514396383
H	-0.1773116649	1.1414525907	-2.0035512243

EC

Charge = 0   Multiplicity = 1

C	-2.6919011983	-0.6602459204	-1.5644240108
C	-2.740607169	0.7839048359	-1.0753072506
H	-2.9439510881	-0.7770338793	-2.6142336944

H	-3.3900490001	1.4139480444	-1.6823893753
H	-1.7626884559	1.2420629268	-0.9611358582
O	-3.3366273221	0.6462187918	0.2261379158
O	-3.7182112801	-1.2855295286	-0.7746997781
C	-3.973394212	-0.5293944682	0.3005775194
O	-4.676909021	-0.8602526973	1.20740221
H	-1.7445505332	-1.1501841851	-1.3413432676

EO

Charge = 0   Multiplicity = 1

C	-2.474267928	-2.2597104713	-0.3701354903
C	-1.5049860288	-2.8095874047	0.5807368022
O	-1.0982186122	-2.3802316877	-0.7142546996
H	-3.1368307278	-2.9330523762	-0.9028985592
H	-1.4635469634	-3.881896539	0.7377381473
H	-1.1504783774	-2.1898323746	1.3970940122
H	-2.8237079123	-1.2408544764	-0.2434847426

H2O

Charge = 0   Multiplicity = 1

O	-8.8053193793	4.6114412245	0.
H	-7.8435063441	4.6379867119	0.
H	-9.1013562919	5.5269471633	0.

MEG

Charge = 0   Multiplicity = 1

O	-8.7840237085	4.5818253007	-0.0635310986
H	-9.1221632945	5.4814931369	-0.0131225323
C	-7.3658538872	4.6103551488	0.0141402461
H	-7.0377660282	5.1172064094	0.9285194769
H	-6.942259576	5.1385408604	-0.8471117683
C	-6.8539093296	3.1940046598	0.0169034127
H	-7.283053492	2.6507167482	-0.8323912055
H	-5.7643711093	3.2108875557	-0.0960626411
O	-7.2209470985	2.5794644865	1.2439675855
H	-6.9418945762	1.6584504435	1.2329397946

VBIm+

Charge = 1   Multiplicity = 1

C	-1.2177826716	-0.374560571	-0.2923235375
C	-2.5436083603	-2.1152452873	-0.0088014899
C	-1.2829171656	-2.5728783269	-0.2082451882
N	-0.4747736024	-1.4689114704	-0.3861922884
H	-0.8651361797	0.6363988416	-0.4148693889
H	-3.470847545	-2.6332424514	0.166534982
H	-0.8932338638	-3.5757594075	-0.2526988966
N	-2.4825441847	-0.7356831482	-0.0567118888

C	0.979747471	-1.5009811265	-0.6049091453
C	1.7196265216	-1.8653630718	0.6773702679
H	1.2621445078	-0.5153873677	-0.972532331
H	1.1714199123	-2.2263578646	-1.3972521856
C	3.2274939946	-1.9839530047	0.4515476102
H	1.5118765341	-1.1034999691	1.4357566834
H	1.3307573107	-2.814668356	1.0568215885
H	3.6828566413	-2.3099948046	1.3900672901
H	3.4239312347	-2.776620373	-0.2778605488
C	3.8812868895	-0.6811159785	-0.0053858587
H	4.9682846283	-0.7771799501	-0.0236494691
H	3.5658549805	-0.3927701341	-1.0108444402
H	3.6299102875	0.1401185406	0.6717667255
C	-3.5967729566	0.1410142808	0.1189703773
H	-4.5312271669	-0.2950013305	-0.2083199464
C	-3.4814768119	1.355968909	0.6277039456
H	-2.5391120735	1.7586810679	0.9802139904
H	-4.3594443325	1.982650354	0.7056591425

VBImBr

Charge = 0   Multiplicity = 1

C	1.4582041806	-0.2150637735	-0.2377825815
C	3.2288165184	1.0574973801	0.1186947981
C	2.1704253362	1.8683354465	-0.1292283381
N	1.0810293998	1.050283083	-0.3511660799
H	0.7974269661	-1.0665221388	-0.3605019091
H	4.2600384402	1.2788429445	0.3354745951
H	2.0961722054	2.9416188882	-0.1767893617
N	2.7633798559	-0.2433232295	0.0524880259
C	-0.2991061276	1.4876004106	-0.6085153596
C	-0.9737139453	1.9509537714	0.6777070229
H	-0.8145420683	0.6342891235	-1.0493782945
H	-0.2538463294	2.2877588008	-1.3490732721
C	-2.3780305945	2.4978074305	0.4194310651
H	-1.0213025558	1.1066993797	1.3743264133
H	-0.3569065062	2.7237164963	1.1459316315
H	-2.7613932692	2.9052384371	1.3585664965
H	-2.3156309184	3.3400072117	-0.2780371274
C	-3.3532588595	1.4494477944	-0.1129017434
H	-4.3607438057	1.862153779	-0.1933852526
H	-3.0713526083	1.0875468843	-1.1046347774
H	-3.3987494173	0.5850249441	0.5552617141
Br	-1.2662882158	-2.469720012	-0.3439536424
C	3.5522193466	-1.410998135	0.2725546837
H	4.6144529875	-1.2112970872	0.2289210696
C	3.0337698789	-2.6062056781	0.5026642581
H	1.965364811	-2.7875018876	0.5585672218

H	3.6963486747	-3.4495550041	0.6415769638

VIm

Charge = 0   Multiplicity = 1

C	1.4306798768	-0.1483251841	-0.2220219645
C	3.2549173645	1.0598153853	0.0072439685
C	2.1826105896	1.8546030892	-0.2733998596
N	1.045658516	1.087983597	-0.4175031999
H	0.7972826097	-1.0205142204	-0.2713487616
H	4.2959157651	1.273300095	0.1867307129
H	2.1606727347	2.9276177514	-0.3831299999
N	2.7672885434	-0.2310173633	0.0436153346
C	3.5404552283	-1.3819891972	0.3133041391
H	4.6050500125	-1.1811369754	0.3086177469
C	3.0510836773	-2.5924070203	0.5486400677
H	1.9900229561	-2.8085133549	0.5727784359
H	3.7338545058	-3.4116103422	0.7282915998

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