ADDITIONAL INFORMATION

Computational Evidence Suggests that 1-Chloroethanol may be an Intermediate in the Thermal Decomposition of 2-Chloroethanol into Acetaldehyde and HCl

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1. Discussion of method and basis sets.
2. Optimum structures and energies of the five stable conformers of 2ClEtOH.
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1. Discussion of method and basis set

One of the reviewers objected to the method and basis set used in this work, suggesting that B3LYP with larger basis sets would be more appropriate.

The basis we used for production in the paper was cc-pVTZ. This in general is not considered to be a "fairly small" basis set as suggested by the referee. It is at least of the same quality than Pople´s 6-311++G(2df,2pd) basis set and, as we show in the table below, it gives lower total energies than the 6-311++G(3df,2pd) basis set.

B3LYP is a somehow dated method, superseded by newer methods like M06, MN15 or ωB97X-D. In fact, the need to include dispersion energy to obtain good geometries for non-covalent interactions and transition states is widely recognized in past years. In particular, a good reference is Mardirossian, N., & Head-Gordon, M. (2017). *Thirty years of density functional theory in computational chemistry: an overview and extensive assessment of 200 density functionals*. Molecular Physics, 115(19), 2315–2372 where hundreds of functionals are analyzed for different properties. Figure 17 in that reference, in particular, shows clearly that B3LYP "as is" gives some of the worst results, but improves markedly when dispersion is included.

To comply with the request of the referee, we show below geometry optimizations done with several basis sets (Pople and Dunning). Although it makes no sense to compare the total energy or enthalpy between functionals, the variational feature of the calculations imply that when using the same functional a more negative energy indicates that the basis set is better. This is seen both for B3LYP and ωB97X-D below.

Method	Basis Set	R(C-Cl) (Å)	R(C-C) (Å)	R(C-O) (Å)	R(OH) (Å)	R(Cl···H) (Å)	Enthalpy (H,298K)
B3LYP	6-31G(d)	1.8244	1.5225	1.4117	0.9715	2.7337	-614.553233
	6-31++G(d,p)	1.8245	1.5204	1.4173	0.9679	2.7744	-614.575987
	6-311++G(d,p)	1.8247	1.5176	1.4161	0.9644	2.7704	-614.641845
	6-311++G(2d,2p)	1.8244	1.5141	1.4159	0.9632	2.7376	-614.649758
	6-311++G(3df,2pd)	1.8122	1.5150	1.4127	0.9632	2.7339	-614.657609
	cc-pVTZ	1.8200	1.5145	1.4127	0.9640	2.7156	-614.661379
	aug-cc-pVTZ	1.8199	1.5139	1.4150	0.9640	2.7331	-614.666087
	cc-pVQZ	1.8156	1.5145	1.4124	0.9626	2.7280	-614.679654
	aug-cc-pVQZ	1.8153	1.5145	1.4134	0.9627	2.7336	-614.681250
ωB97X-D	6-31G(d)	1.8065	1.5206	1.4035	0.9662	2.7425	-614.488616
	6-31++G(d,p)	1.8064	1.5185	1.4075	0.9632	2.7673	-614.508442
	6-311++G(d,p)	1.8070	1.5157	1.4060	0.9601	2.7554	-614.571467
	6-311++G(2d,2p)	1.8054	1.5129	1.4058	0.9591	2.7217	-614.579634
	6-311++G(3df,2pd)	1.7956	1.5137	1.4029	0.9592	2.7202	-614.587844
	cc-pVTZ	1.8029	1.5133	1.4032	0.9597	2.7012	-614.592236
	aug-cc-pVTZ	1.8027	1.5129	1.4046	0.9597	2.7130	-614.596435
	cc-pVQZ	1.7986	1.5133	1.4025	0.9582	2.7105	-614.610650
	aug-cc-pVQZ	1.7984	1.5133	1.4031	0.9583	2.7155	-614.612175
Exp.	Microwave	1.801	1.519	1.413	1.063		
	Electron diffraction	1.789	1.519	1.411	1.008	2.609	

The one thing that is immediately obvious is that a large increase in the basis set chosen (i.e. going from the small 6-31G(d) basis (156 primitives/74 basis functions) to the large aug-cc-pVQZ one (823 primitives/554 symmetry adapted basis functions) makes a very modest difference in the bond

lengths (less than 0.01Å). There is no systematic reason to prefer B3LYP over the method chosen in this paper since, for instance, with B3LYP the R(CO) distance is nearer to experiment, but the R(CCl) distance is farther away. This does not imply that B3LYP is bad (see for instance Chong, D. P., *MP2 or B3LYP: computed bond distances compared with CCSD (T)/cc-pVQZ.*, Can. J. Chem. 2018, 96, 336-339).

One could ask whether B3LYP may show any advantage over ωB97X-D using the same cc-PVTZ basis set. To explore this point we performed geometry optimizations of some of the minima and TSs in this paper using the B3LYP method and compared the results. As it is seen in the table below, the numbers are reasonably similar, although certainly not equal.

	Δ(ET+ZPE)	
	B3LYP	**ωB97X-D**
1ClEtOH	0.0	0.0
2ClEtOH	6.1	5.8
Ethylene+HOCl	57.9	64.1
a-Vinyl alcohol + HCl	13.3	17.4
Oxirane + HCl	30.7	32.2
Ethylene glycol + HCl – H_2O	9.2	9.5
Acetaldehyde + HCl	1.4	4.9
TS1	25.1	29.0
TS2	36.1	39.3
TS4	66.4	71.2
TS7	59.1	63.6
TS8	63.6	69.4
Ts*as*	16.7	20.7

We feel therefore reasonably confident that the procedure used in this paper is appropriate.

2. Optimum structures and energies of the five table conformers of 2ClEtOH (ωB97X-D/cc-pVTZ calculations)

a. Gg'

```
---------------------------------------------------------------------
Center     Atomic      Atomic             Coordinates (Angstroms)
Number     Number       Type              X           Y           Z
---------------------------------------------------------------------
     1          6           0       -0.946573   -0.148698   -0.071593
     2          6           0       -1.068244    1.352532    0.074967
     3         17           0        0.704342   -0.700977    0.397234
     4          8           0       -0.225566    2.059143   -0.796487
     5          1           0       -1.647447   -0.669570    0.575266
     6          1           0       -1.090042   -0.454992   -1.103778
     7          1           0       -2.090629    1.632532   -0.185699
     8          1           0       -0.899546    1.633977    1.120153
     9          1           0        0.679705    1.810053   -0.598062
---------------------------------------------------------------------
 Zero-point correction=                           0.072551
(Hartree/Particle)
 Thermal correction to Energy=                    0.077383
 Thermal correction to Enthalpy=                  0.078327
 Thermal correction to Gibbs Free Energy=         0.044496
 Sum of electronic and zero-point Energies=           -614.598015
 Sum of electronic and thermal Energies=              -614.593184
 Sum of electronic and thermal Enthalpies=            -614.592239
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Sum of electronic and thermal Free Energies= -614.626070

b. Tg

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.274751	-0.158700	0.206373
2	6	0	-3.380508	1.356979	0.209086
3	8	0	-4.720668	1.761325	0.037259
4	17	0	-1.563466	-0.669572	0.372471
5	1	0	-3.818985	-0.596352	1.040511
6	1	0	-3.651286	-0.570759	-0.725124
7	1	0	-2.944061	1.759578	1.127782
8	1	0	-2.819335	1.763990	-0.630657
9	1	0	-5.196939	1.613511	0.854300

Zero-point correction= 0.072373
(Hartree/Particle)
Thermal correction to Energy= 0.077436
Thermal correction to Enthalpy= 0.078380
Thermal correction to Gibbs Free Energy= 0.044122
Sum of electronic and zero-point Energies= -614.595479
Sum of electronic and thermal Energies= -614.590416
Sum of electronic and thermal Enthalpies= -614.589471
Sum of electronic and thermal Free Energies= -614.623730

c. Tt

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.329148	-0.076283	0.258756
2	6	0	-3.302472	1.436817	0.258776
3	8	0	-4.651471	1.855018	0.258787
4	17	0	-1.659147	-0.725100	0.258721
5	1	0	-3.827434	-0.455829	1.145759
6	1	0	-3.827462	-0.455805	-0.628242
7	1	0	-2.767568	1.791606	1.145350
8	1	0	-2.767578	1.791630	-0.627796
9	1	0	-4.678719	2.810947	0.258889

Zero-point correction= 0.072171
(Hartree/Particle)
Thermal correction to Energy= 0.077354
Thermal correction to Enthalpy= 0.078298
Thermal correction to Gibbs Free Energy= 0.043745
Sum of electronic and zero-point Energies= -614.595314
Sum of electronic and thermal Energies= -614.590131
Sum of electronic and thermal Enthalpies= -614.589187
Sum of electronic and thermal Free Energies= -614.623740

d. Gt

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.294405	-0.035981	0.203807
2	6	0	-3.200305	1.418915	-0.179540
3	8	0	-4.499068	1.933761	-0.348935
4	17	0	-3.931011	-0.262787	1.866692
5	1	0	-3.968531	-0.563073	-0.465857
6	1	0	-2.312955	-0.501275	0.176668
7	1	0	-2.642858	1.963304	0.588572
8	1	0	-2.629273	1.472459	-1.116301
9	1	0	-4.458596	2.888677	-0.354105

Zero-point correction= 0.072041
(Hartree/Particle)
Thermal correction to Energy= 0.077183
Thermal correction to Enthalpy= 0.078127
Thermal correction to Gibbs Free Energy= 0.043505
Sum of electronic and zero-point Energies= -614.594463
Sum of electronic and thermal Energies= -614.589321
Sum of electronic and thermal Enthalpies= -614.588377
Sum of electronic and thermal Free Energies= -614.622999

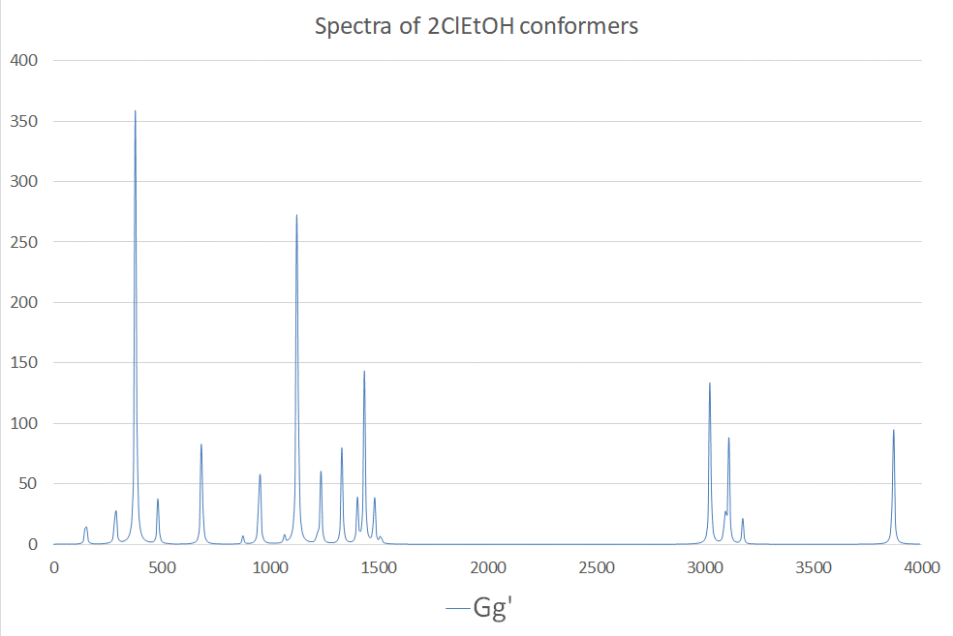
e. Gg

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.268123	-0.066375	0.211053
2	6	0	-3.214687	1.390161	-0.201817
3	8	0	-4.471488	2.002813	-0.325659
4	17	0	-3.993298	-0.295117	1.834628
5	1	0	-3.867833	-0.653075	-0.482933
6	1	0	-2.264851	-0.484390	0.248278
7	1	0	-2.667283	1.964105	0.544666
8	1	0	-2.647594	1.439154	-1.141406
9	1	0	-4.984844	1.534725	-0.984811

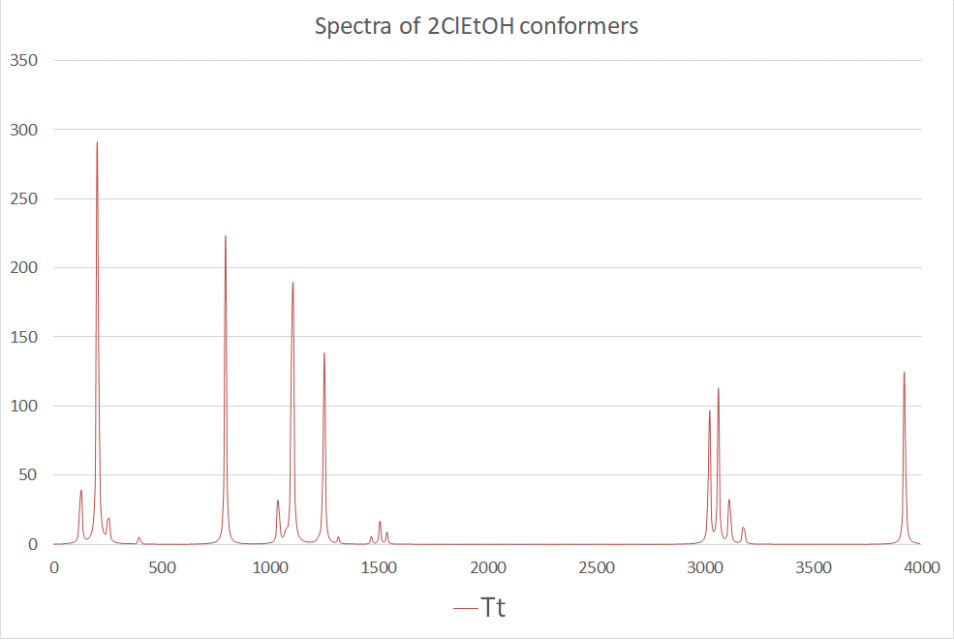
Zero-point correction= 0.072228
(Hartree/Particle)
Thermal correction to Energy= 0.077219
Thermal correction to Enthalpy= 0.078163
Thermal correction to Gibbs Free Energy= 0.043925
Sum of electronic and zero-point Energies= -614.594064
Sum of electronic and thermal Energies= -614.589074
Sum of electronic and thermal Enthalpies= -614.588129
Sum of electronic and thermal Free Energies= -614.622367

3. Spectra of the five stable conformers of 2ClEtOH

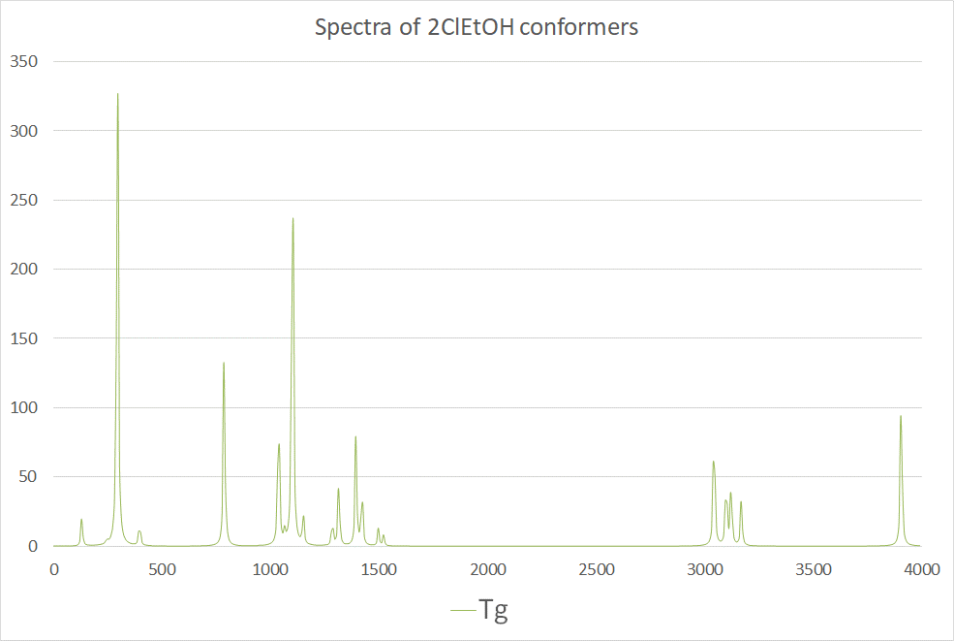
a. Gg’



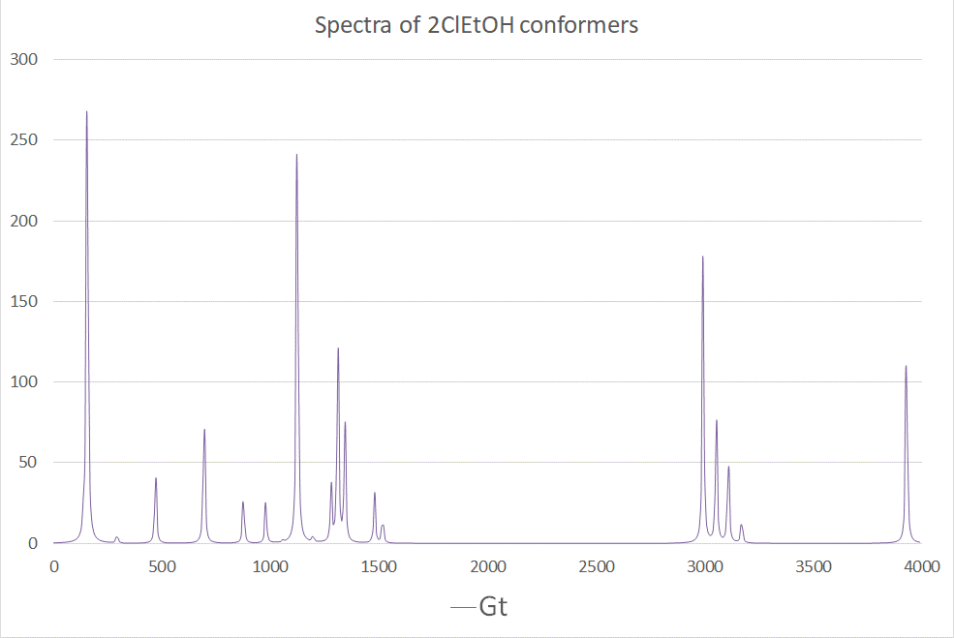
b. Tt



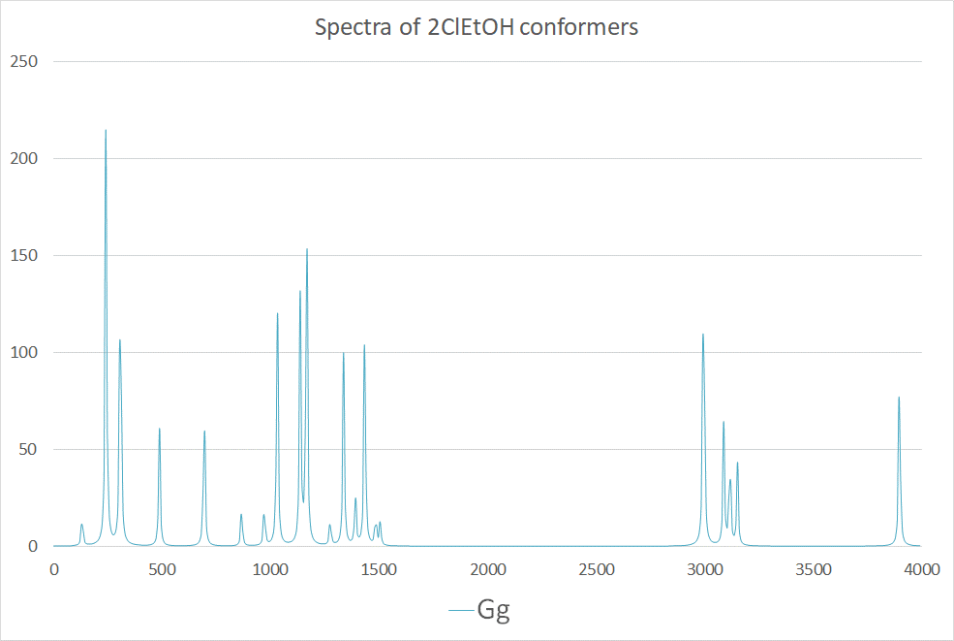
c. Tg


Spectra of 2ClEtOH conformers
350
300
250
200
150
100
50
0
0
500
1000
1500
2000
2500
3000
3500
4000
Tg

d. Gt


Spectra of 2ClEtOH conformers
300
250
200
150
100
50
0
0
500
1000
1500
2000
2500
3000
3500
4000
Gt

e. Gg



4. Full citation of the Gaussian 09 version used in this work

Gaussian 09, Revision D.01,
M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria,
M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci,
G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian,
A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada,
M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima,
Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr.,
J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers,
K. N. Kudin, V. N. Staroverov, T. Keith, R. Kobayashi, J. Normand,
K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi,
M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross,
V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann,
O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski,
R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth,
P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels,
O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski,
and D. J. Fox, Gaussian, Inc., Wallingford CT, 2013.

5. Energies of the species studied in this work

(Total energies are given in Hartrees; relative energies are given in kcal/mol)

ωB97X-D/6-31G(d)	No additional water		(Total					
	E	E+ZPE	H	G	ΔE	Δ (E+ZPE)	ΔH	ΔG
HCl	-460.777829	-460.771024	-460.767720	-460.788909				
H2O	-76.387070	-76.365400	-76.361622	-76.383050				
ClOH	-535.901836	-535.888397	-535.884523	-535.911345				
ethylene	-78.555873	-78.504168	-78.500193	-78.525037	74.6	69.9	71.2	59.8
Carbene Singlet	-78.432000	-78.385160	-78.381208	-78.407514	152.3	144.6	145.9	133.6
Carbene Triplet	-78.446140	-78.398271	-78.393693	-78.422208	143.5	136.3	138.0	124.4
1Cl1OH	-614.576596	-614.503944	-614.498174	-614.531734	0	0	0	0
2Cl1OH	-614.567579	-614.494338	-614.488616	-614.522353	5.7	6.0	6.0	5.9
anti-Vinyl Alcohol (aVA)	-153.749991	-153.692945	-153.688165	-153.717589	30.6	25.1	26.5	15.8
syn-Vinyl Alcohol (sVA)	-153.753505	-153.695989	-153.691460	-153.720412	28.4	23.2	24.5	14.1
Oxirane	-153.736880	-153.678469	-153.674407	-153.702532	38.8	34.2	35.2	25.3
Ethylene Glycol (EGly)	-230.171522	-230.084485	-230.078584	-230.111661	9.0	8.7	8.5	8.9
Acetaldehyde	-153.777687	-153.721349	-153.716500	-153.746352	13.2	7.3	8.8	-2.2
TS1	-614.524625	-614.455361	-614.449423	-614.484021	32.6	30.5	30.6	29.9
TS2	-614.503658	-614.436808	-614.430890	-614.465401	45.8	42.1	42.2	41.6
TS4	-153.660087	-153.608875	-153.604616	-153.633148	87.0	77.8	79.0	68.8
TS6	-614.388277	-614.322648	-614.315641	-614.353133	118.2	113.8	114.5	112.1
TS7	-614.461385	-614.396279	-614.390028	-614.425105	72.3	67.6	67.9	66.9
TS8	-614.460984	-614.391558	-614.385961	-614.419681	72.5	70.5	70.4	70.3
TS11	-614.466022	-614.398862	-614.392749	-614.427673	69.4	65.9	66.2	65.3
VA Tsas	-153.744154	-153.688027	-153.683736	-153.712368	34.3	28.2	29.3	19.1

ωB97X-D/cc-pVTZ No additional water

					w.r.t. 1ClEtOH				Complex w.r.t.Monomers			
	E	E+ZPE	H	G	ΔE	Δ(E+ZPE)	ΔH	ΔG	ΔE	Δ(E+ZPE)	ΔH	ΔG
HCl	-460.824946	-460.818143	-460.814839	-460.836022								
H2O	-76.434836	-76.413140	-76.409360	-76.430769								
ClOH	-535.981707	-535.968196	-535.964324	-535.991118								
Ethylene	-78.588246	-78.536914	-78.532940	-78.557771	68.6	64.1	65.4	54.1				
Carbene Triplet	-78.465455	-78.419093	-78.415130	-78.441429	145.6	138.1	139.3	127.1				
1Cl1OH	-614.679234	-614.607328	-614.601485	-614.635171	0	0	0	0				
2Cl1OH	-614.670566	-614.598011	-614.592236	-614.626063	5.4	5.8	5.8	5.7				
anti Vinyl Alcohol (aVA)	-153.818299	-153.761433	-153.756703	-153.786002	22.6	17.4	18.8	8.2				
aVA.HCl	-614.650442	-614.584784	-614.577164	-614.616557	18.1	14.1	15.3	11.7	-4.5	-3.3	-3.5	3.4
syn Vinyl Alcohol (sVA)	-153.820788	-153.763667	-153.759123	-153.788087	21.0	16.0	17.3	6.9				
sVA.HCl	-614.652400	-614.586417	-614.578959	-614.618269	16.8	13.1	14.1	10.6	-4.2	-2.9	-3.1	3.7
Oxirane	-153.795815	-153.737860	-153.733789	-153.761915	36.7	32.2	33.2	23.4				
Oxirane.HCl	-614.632940	-614.565378	-614.558903	-614.595184	29.1	26.3	26.7	25.1	-7.6	-5.9	-6.4	1.7
Ethylene Glycol (EGly)	-230.273584	-230.187178	-230.181180	-230.214450	9.8	9.5	9.3	9.7				
Egly.HCl	-691.111426	-691.015223	-691.006862	-691.047571	11.8	11.3	10.9	11.1	-8.1	-6.2	-6.8	1.8
Acetaldehyde	-153.837088	-153.781312	-153.776480	-153.806248	10.8	4.9	6.4	-4.5				
Acetaldehyde.HCl	-614.673402	-614.608088	-614.600737	-614.639017	3.7	-0.5	0.5	-2.4	-7.1	-5.4	-5.9	2.0
TS1	-614.629559	-614.561180	-614.555184	-614.589860	31.2	29.0	29.1	28.4				
TS2	-614.610936	-614.544679	-614.538716	-614.573252	42.9	39.3	39.4	38.9				
TS4	-153.726386	-153.675724	-153.671428	-153.700002	80.3	71.2	72.3	62.2				
TS4.HCl	-614.555606	-614.496465	-614.489057	-614.527979	77.6	69.6	70.5	67.3	-2.7	-1.6	-1.8	5.0
TS6	-614.491332	-614.426034	-614.418993	-614.456450	117.9	113.8	114.5	112.1				
TS7	-614.570892	-614.505942	-614.499710	-614.534704	68.0	63.6	63.9	63.0				
TS8	-614.565728	-614.496748	-614.491201	-614.524852	71.2	69.4	69.2	69.2				
TS11	-614.5638307	-614.497135	-614.491018	-614.525911	72.4	69.1	69.3	68.6				
TSas	-153.811986	-153.756136	-153.751843	-153.780466	26.5	20.7	21.8	11.7				
Tsas.HCl	-614.642405	-614.577956	-614.570536	-614.609899	23.1	18.4	19.4	15.9	-4.2	-2.9	-3.1	3.7

ωB97X-D/cc-pVTZ	Additional water							
	E	E+ZPE	H	G	ΔE	Δ(E+ZPE)	ΔH	ΔG
HCl	-460.824946	-460.818143	-460.814839	-460.836022				
H2O	-76.434836	-76.413140	-76.409360	-76.430769				
ClOH	-535.981707	-535.968196	-535.964324	-535.991118				
Ethylene	-78.588246	-78.536914	-78.532940	-78.557771	78.7	72.1	73.8	53.7
1Cl1OH_W	-691.130198	-691.033195	-691.024295	-691.065290	0	0	0	0
2Cl1OH_W	-691.118310	-691.021038	-691.012020	-691.053921	7.5	7.6	7.7	7.1
VA.HCl.H2O_s	-691.106450	-691.014462	-691.004736	-691.048518	14.9	11.8	12.3	10.5
VA.HCl.H2O_a	-691.101517	-691.010261	-690.999915	-691.046650	18.0	14.4	15.3	11.7
Ox.HCl.H2O	-691.083625	-690.990787	-690.981485	-691.025331	29.2	26.6	26.9	25.1
Egly.HCl	-691.111426	-691.015223	-691.006862	-691.047571	11.8	11.3	10.9	11.1
Acetaldehyde.HCl.H2O	-691.124370	-691.033681	-691.023522	-691.069575	3.7	-0.3	0.5	-2.7
TS1_W	-691.105020	-691.014029	-691.005957	-691.045739	15.8	12.0	11.5	12.3
TS2_W	-691.084785	-690.993693	-690.985574	-691.025155	28.5	24.8	24.3	25.2
TS4_W	-691.094180	-691.003090	-690.995244	-691.034282	22.6	18.9	18.2	19.5
TS6_W	-690.968288	-690.876950	-690.866944	-690.911474	101.6	98.0	98.7	96.5
TS7_W	-691.035515	-690.943471	-690.934956	-690.975513	59.4	56.3	56.1	56.3
TS8_W	-691.017269	-690.922400	-690.914194	-690.954086	70.9	69.5	69.1	69.8
TS9_W	-691.002736	-690.908894	-690.900785	-690.940524	80.0	78.0	77.5	78.3
TS10_W	-691.036191	-690.943957	-690.936040	-690.975224	59.0	56.0	55.4	56.5
Tsas_W	-691.098320	-691.007537	-690.998148	-691.041641	20.0	16.1	16.4	14.8
TS12_W	-691.024199	-690.930122	-690.922133	-690.961399	66.5	64.7	64.1	65.2

6. Structures of the species studied in this work (ωB97X-D/cc-pVTZ calculations).

a. HCl

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	17	0	0.000000	0.000000	0.210107
2	1	0	0.000000	0.000000	1.489893

b. H2O

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	0.000000	0.757212	-0.468040
2	8	0	0.000000	0.000000	0.117010
3	1	0	0.000000	-0.757212	-0.468040

c. HOCl

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	0.087679	0.000000	0.103949
2	8	0	-0.144039	0.000000	1.037746
3	17	0	1.355397	0.000000	1.808305

d. Ethylene

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.000000	0.039365
2	6	0	0.000000	0.000000	1.360635
3	1	0	0.921725	0.000000	1.928298
4	1	0	-0.921725	0.000000	1.928298
5	1	0	-0.921725	0.000000	-0.528298
6	1	0	0.921725	0.000000	-0.528298

e. Carbene (triplet)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.140738	0.000000	-0.157488
2	6	0	0.000289	0.000000	1.298112
3	1	0	1.053360	0.000000	1.588723
4	1	0	-0.460883	0.884710	1.754362
5	1	0	-0.460883	-0.884710	1.754362
6	1	0	-0.988083	0.000000	-0.828576

f. 1ClEtOH

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.216241	-1.099165	-0.097913
2	6	0	0.321444	0.082219	0.162156
3	8	0	1.004557	1.240306	-0.128030
4	17	0	-0.216187	0.072930	1.924380
5	1	0	0.703993	-2.027446	0.141990
6	1	0	1.495083	-1.104132	-1.151652
7	1	0	2.118116	-1.019666	0.505959
8	1	0	-0.623249	0.010797	-0.376187
9	1	0	0.419285	1.991450	-0.016998

g. 1ClEtOH_W

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.882518	-1.887849	0.603375
2	1	0	1.217899	-2.332705	1.540910
3	1	0	1.454225	-2.325898	-0.214064
4	6	0	1.118585	-0.397746	0.676706
5	17	0	0.433042	0.358311	-0.903940
6	1	0	-0.172095	-2.110253	0.458990
7	8	0	2.413539	-0.030978	0.854637
8	1	0	2.952449	-0.449956	0.162272
9	8	0	3.347132	-0.975067	-1.605614
10	1	0	4.077378	-0.519987	-2.025729
11	1	0	2.550050	-0.548980	-1.940739
12	1	0	0.519278	0.086108	1.441195

h. 2ClEtOH (Gg’)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.946573	-0.148698	-0.071593
2	6	0	-1.068244	1.352532	0.074967
3	17	0	0.704342	-0.700977	0.397234
4	8	0	-0.225566	2.059143	-0.796487
5	1	0	-1.647447	-0.669570	0.575266
6	1	0	-1.090042	-0.454992	-1.103778
7	1	0	-2.090629	1.632532	-0.185699
8	1	0	-0.899546	1.633977	1.120153
9	1	0	0.679705	1.810053	-0.598062

i. 2ClEtOH_W

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.346981	-0.225838	-0.004771
2	1	0	-1.837803	-0.490731	-0.936393
3	1	0	-1.938438	-0.564414	0.842013
4	17	0	0.176528	-1.202584	0.047634
5	6	0	-1.096709	1.268550	0.060664
6	1	0	-2.072576	1.734227	0.228438
7	1	0	-0.473755	1.497727	0.932703
8	8	0	-0.575377	1.803110	-1.117680
9	1	0	0.389161	1.722968	-1.099557
10	8	0	2.175346	1.291183	-0.779075
11	1	0	1.962996	0.383684	-0.538327
12	1	0	2.568606	1.676117	0.004350

j. Anti Vinyl Alcohol (aVA)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.051095	0.000000	-0.044984
2	6	0	-0.000309	0.000000	1.276199
3	1	0	0.956511	0.000000	1.773652
4	1	0	-0.900914	0.000000	1.873521
5	1	0	0.850681	0.000000	-0.648939
6	8	0	-1.223174	0.000000	-0.730976
7	1	0	-1.046494	0.000000	-1.670065

k. aVA.HCl

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.136399	1.223702	-0.037414
2	6	0	1.290588	0.006015	0.467436
3	8	0	1.613443	-1.058235	-0.298074
4	17	0	-2.267188	0.213104	-0.333291
5	1	0	1.280262	1.416512	-1.091201
6	1	0	-1.011897	0.519594	-0.218899
7	1	0	0.903620	2.047275	0.619014
8	1	0	1.158373	-0.188887	1.526918
9	1	0	1.604154	-1.856693	0.228182

l. aVA.HCl_W

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.395607	-0.053474	0.101028
2	6	0	-1.073570	1.230216	0.155376
3	1	0	-1.847584	1.961392	0.328652
4	1	0	-0.045759	1.554171	0.056751
5	1	0	-2.418039	-0.401089	0.197970
6	8	0	-0.459762	-1.025200	-0.076810
7	1	0	-0.878522	-1.864489	-0.263342
8	8	0	2.175556	0.325684	-0.216699
9	1	0	2.393283	0.283474	0.714290
10	1	0	1.440827	-0.286600	-0.314892
11	17	0	-1.632822	0.646892	-3.400486
12	1	0	-1.406733	0.891388	-2.150207

m. Syn Vinyl Alcohol (sVA)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.028685	0.494923	0.002650
2	6	0	0.899249	0.341373	0.935654
3	1	0	1.858123	0.822615	0.825862
4	1	0	0.731693	-0.259129	1.821478
5	1	0	0.134937	1.093997	-0.883643
6	8	0	-1.270515	-0.039374	-0.004446
7	1	0	-1.393615	-0.565333	0.788636

n. sVA.HCl

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.125733	1.307168	-0.109510
2	6	0	1.569549	0.168351	0.415096
3	8	0	1.812137	-0.982253	-0.235739
4	17	0	-2.017993	-0.251168	-0.360516
5	1	0	0.945927	1.420200	-1.171648
6	1	0	-0.897647	0.314079	-0.035454
7	1	0	0.981689	2.167963	0.524196
8	1	0	1.773571	0.064041	1.472866
9	1	0	1.604242	-0.880988	-1.167939

o. sVA.HCl_W

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.420850	-0.272632	-0.046782
2	6	0	1.389038	1.064442	-0.057466
3	1	0	2.312518	1.618904	0.002172
4	1	0	0.470658	1.611728	-0.222450
5	1	0	2.359755	-0.805280	0.054070
6	8	0	0.390641	-1.109123	-0.133869
7	1	0	-0.454503	-0.621096	-0.108185
8	8	0	-1.929994	0.248701	0.434993
9	1	0	-2.307817	1.010354	-0.004551
10	1	0	-1.705435	0.542180	1.325187
11	17	0	-0.014954	1.121173	3.009578
12	1	0	0.729457	1.003313	1.934229

p. Oxirane

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.079104	-0.127199	-0.041903
2	6	0	0.083823	0.296648	1.354187
3	1	0	1.028060	0.393400	1.879134
4	1	0	-0.780425	0.091844	1.976798
5	1	0	1.019890	-0.340392	-0.537871
6	1	0	-0.788595	-0.641948	-0.440207
7	8	0	-0.127813	1.227647	0.309863

q. Oxirane.HCl

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.056282	0.912709	-0.581891
2	6	0	1.536751	0.029203	0.472915
3	17	0	-2.051544	-0.631606	0.547113
4	8	0	0.768359	-0.484001	-0.613782
5	1	0	0.199122	1.547249	-0.388437
6	1	0	1.735961	1.247476	-1.355251
7	1	0	2.571547	-0.289036	0.479169
8	1	0	1.027225	0.024503	1.429551
9	1	0	-0.883990	-0.707544	-0.048363

r. Oxirane.HCl_W

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.589614	-0.909945	-0.671953
2	1	0	-2.401859	-1.350815	-1.236088
3	1	0	-0.592829	-1.042079	-1.075758
4	17	0	2.055956	-0.523933	0.551427
5	6	0	-1.740908	-0.684653	0.759108
6	1	0	-2.665395	-0.959844	1.251261
7	1	0	-0.851479	-0.657657	1.377513
8	8	0	-1.866535	0.396454	-0.165731
9	1	0	-0.455264	1.473044	-0.236666
10	8	0	0.437572	1.867431	-0.243018
11	1	0	1.416938	0.587142	0.195826
12	1	0	0.425604	2.567597	0.409843

s. Ethylene Glycol (EGly)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.127226	-0.078377	0.138801
2	6	0	0.035138	0.247456	1.606216
3	1	0	1.004927	0.728284	1.776182
4	1	0	-0.758908	0.935277	1.913458
5	8	0	-0.060073	-0.980717	2.310885
6	1	0	-1.481916	-1.383119	0.498810
7	1	0	0.691629	-0.738061	-0.172924
8	1	0	-0.065484	0.837571	-0.449093
9	8	0	-1.379880	-0.662883	-0.127218
10	1	0	-0.185198	-0.801241	3.241164

t. EGly.HCl

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.569423	0.804948	0.306599
2	1	0	2.507502	0.962043	-0.231448
3	1	0	1.614481	1.355178	1.245172
4	17	0	-2.160623	-0.027400	0.160156
5	6	0	1.351287	-0.677467	0.560962
6	1	0	2.255012	-1.108340	0.997052
7	1	0	0.533216	-0.819960	1.269915
8	8	0	1.077268	-1.336657	-0.662388
9	1	0	0.532744	0.937400	-1.311987
10	8	0	0.495861	1.359335	-0.448722
11	1	0	0.141938	-1.541914	-0.689233
12	1	0	-1.079543	0.708298	-0.007417

u. Acetaldehyde (Ac)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.050078	0.000000	-0.042633
2	6	0	0.020546	0.000000	1.456227
3	1	0	1.029285	0.000000	1.861092
4	1	0	-0.526819	0.876754	1.808684
5	1	0	-0.526819	-0.876754	1.808684
6	8	0	1.049824	0.000000	-0.705341
7	1	0	-0.945346	0.000000	-0.532483

v. Ac.HCl

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.315407	-0.654810	-0.055648
2	6	0	-0.888778	-0.244085	0.080780
3	8	0	-0.374714	0.637128	-0.564048
4	17	0	2.527604	0.657482	0.485100
5	1	0	-2.812377	-0.550206	0.910990
6	1	0	-2.822648	-0.057266	-0.807989
7	1	0	-2.359841	-1.713758	-0.318259
8	1	0	-0.288876	-0.797910	0.825817
9	1	0	1.346702	0.782353	-0.067772

w. Ac.HCl_W

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.138199	-1.351814	-0.067276
2	6	0	-2.986571	-0.405265	-0.082116
3	8	0	-3.098530	0.785970	-0.257612
4	1	0	-5.077151	-0.829492	-0.229242
5	1	0	-3.986503	-2.109416	-0.838932
6	1	0	-4.155341	-1.879811	0.888355
7	1	0	-1.987832	-0.847132	0.078734
8	1	0	-1.524262	1.659223	-0.262151
9	8	0	-0.592709	1.942320	-0.200563
10	1	0	-0.558439	2.576267	0.516282
11	1	0	0.251721	0.553368	0.175961
12	17	0	0.794818	-0.620218	0.493560

x. TS1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.805001	-0.665288	-0.172985
2	6	0	0.700582	0.207199	0.232716
3	8	0	0.205861	1.021915	-0.606249
4	17	0	-1.829793	-0.358693	0.619953

5	1	0	1.461657	-1.691790	-0.019189
6	1	0	2.078646	-0.518646	-1.213249
7	1	0	2.657763	-0.518708	0.491725
8	1	0	0.373464	0.243628	1.262516
9	1	0	-0.730343	1.171559	-0.264687

y. TS1_W

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.750209	-1.325100	0.956399
2	1	0	1.049242	-2.374596	0.853357
3	1	0	-0.174660	-1.282864	1.525979
4	6	0	0.572014	-0.809820	-0.426487
5	17	0	0.297630	1.651989	0.391719
6	1	0	1.536076	-0.783944	1.472391
7	8	0	-0.489159	-0.930797	-1.068291
8	1	0	-1.444429	-0.527019	-0.419994
9	8	0	-2.124001	0.197726	0.226832
10	1	0	-2.772028	0.633048	-0.333225
11	1	0	-1.371657	0.894470	0.419062
12	1	0	1.470161	-0.561387	-0.993039

z. TS2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.942160	1.291194	-0.054751
2	6	0	-1.131880	-0.044900	0.318457
3	8	0	-1.167250	-0.384737	1.561365
4	17	0	1.589211	-0.294863	-0.316523
5	1	0	-1.035995	2.033494	0.727484
6	1	0	0.234959	1.005764	-0.222715
7	1	0	-1.307127	1.559801	-1.038122
8	1	0	-1.160340	-0.829757	-0.428710
9	1	0	-1.023933	-1.331443	1.672100

aa. TS2_W

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.226414	1.617181	0.101570
2	1	0	1.342895	2.294770	0.936480
3	1	0	-0.016938	1.367386	0.036735
4	6	0	1.355067	0.257904	0.362982
5	17	0	-1.663261	0.597837	-0.018258
6	1	0	1.517101	1.973198	-0.878640
7	8	0	1.496733	-0.608955	-0.563896
8	1	0	0.985849	-1.443835	-0.303405
9	8	0	-0.309324	-2.181447	0.235423
10	1	0	-0.704055	-2.892641	-0.269102
11	1	0	-0.934818	-1.420118	0.180113

12	1	0	1.126067	-0.113158	1.361657

bb. TS4

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.221379	1.190801	-0.281602
2	6	0	1.629061	0.106235	0.525917
3	8	0	2.740389	-0.349964	0.123026
4	17	0	-2.126238	-0.200095	0.088155
5	1	0	1.014240	0.893639	-1.309042
6	1	0	-0.988509	0.333096	-0.203084
7	1	0	0.616368	2.007171	0.092461
8	1	0	1.155809	-0.332379	1.404924
9	1	0	2.604642	0.739012	-0.542570

cc. TS4_W

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.546660	-0.781764	-0.258605
2	6	0	0.780031	-1.110715	0.865846
3	1	0	0.745448	-0.364659	1.653541
4	1	0	0.879963	-2.132054	1.208703
5	1	0	1.999224	-1.559404	-0.870108
6	8	0	1.703558	0.387527	-0.734620
7	1	0	1.127786	1.093108	-0.257570
8	8	0	0.014069	2.000412	0.208936
9	1	0	-0.022073	2.395774	1.079775
10	1	0	-0.782952	1.417869	0.128087
11	17	0	-1.938126	-0.274590	-0.029503
12	1	0	-0.380788	-0.937461	0.420332

dd. TS6

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.078274	1.148489	0.006290
2	6	0	1.423954	0.795860	0.003126
3	17	0	-0.570063	-1.715617	-0.011862
4	8	0	1.327920	-0.933673	-0.008343
5	1	0	-0.448836	1.315463	0.933008
6	1	0	-0.450025	1.327519	-0.917495
7	1	0	1.981388	0.955749	-0.911592
8	1	0	1.982530	0.943658	0.919178
9	1	0	2.134052	-1.494651	-0.012331

ee. TS6_W

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.069920	-1.001663	0.004517
2	6	0	1.807814	0.063616	0.462027
3	17	0	-2.336444	0.703342	0.194913
4	8	0	-0.244780	0.217578	0.263488
5	1	0	1.041465	-1.236263	-1.050827
6	1	0	0.685709	-1.759468	0.673786
7	1	0	1.938209	0.232824	1.519713
8	1	0	2.287965	0.750730	-0.220836
9	1	0	-0.199365	0.750013	-0.544180
10	8	0	-1.453366	-2.327157	1.309137
11	1	0	-1.852376	-1.522057	0.954098
12	1	0	-1.844610	-2.422683	2.176712

ff. TS7

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.155412	1.143129	0.003766
2	6	0	1.111644	0.205601	0.374382
3	17	0	-1.794417	-0.408446	-0.370316
4	8	0	2.042616	-0.170380	-0.560923
5	1	0	-0.445424	1.634954	0.750880
6	1	0	0.056767	1.453388	-1.025122
7	1	0	1.374137	0.103061	1.424217
8	1	0	0.019333	-0.393468	0.236183
9	1	0	2.261352	-1.095770	-0.444171

gg. TS7_W

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.680187	0.739342	-0.582102
2	1	0	-0.197181	0.221147	-1.395617
3	1	0	-1.742248	0.917860	-0.651443
4	17	0	-1.146255	-1.740521	0.018955
5	6	0	0.027279	1.247109	0.513455
6	1	0	-0.437849	2.019166	1.117231
7	1	0	-0.533656	0.228626	0.865267
8	8	0	1.366024	1.174946	0.648082
9	1	0	1.694564	0.359385	0.201129
10	8	0	1.808735	-1.173094	-0.559499
11	1	0	0.949095	-1.607972	-0.374320
12	1	0	2.487423	-1.795207	-0.299808

hh. TS8

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.415769	0.916359	-0.650888
2	6	0	1.381236	0.392775	0.300552
3	17	0	-1.716854	-0.524550	0.358328

4	8	0	1.017149	-0.894088	-0.191554
5	1	0	-0.519903	1.367650	-0.368251
6	1	0	0.664515	0.822078	-1.697918
7	1	0	2.428193	0.580560	0.083968
8	1	0	1.135177	0.543543	1.347620
9	1	0	0.070215	-1.068207	0.127157

ii. TS8_W

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.964280	0.853604	0.472355
2	1	0	-1.763981	0.908563	-0.247916
3	1	0	-0.863759	-0.059926	1.031293
4	17	0	-0.280988	-1.362386	-0.877206
5	6	0	-0.165185	2.035853	0.753165
6	1	0	-0.647676	3.001308	0.637145
7	1	0	0.456348	2.000017	1.644808
8	8	0	0.522155	1.678130	-0.442413
9	1	0	1.268986	1.033816	-0.236824
10	8	0	2.303660	-0.138071	-0.081310
11	1	0	1.631800	-0.789910	-0.399418
12	1	0	2.625521	-0.474531	0.754583

jj. TS9

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.508836	0.562234	0.666772
2	1	0	2.462649	0.989004	0.379453
3	1	0	0.609617	1.166127	0.844883
4	17	0	-1.526767	0.956217	1.256305
5	6	0	1.453855	-0.886988	0.802303
6	1	0	2.225459	-1.312302	1.441788
7	1	0	0.461358	-1.240311	1.081154
8	8	0	1.790939	-1.120512	-0.558203
9	1	0	-0.213922	1.207348	-1.817842
10	8	0	-0.158436	0.447689	-1.237818
11	1	0	1.036997	-0.774298	-1.083152
12	1	0	-0.819860	0.602198	-0.488513

kk. TS10

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.508836	0.562234	0.666772
2	1	0	2.462649	0.989004	0.379453
3	1	0	0.609617	1.166127	0.844883
4	17	0	-1.526767	0.956217	1.256305
5	6	0	1.453855	-0.886988	0.802303
6	1	0	2.225459	-1.312302	1.441788
7	1	0	0.461358	-1.240311	1.081154
8	8	0	1.790939	-1.120512	-0.558203

9	1	0	-0.213922	1.207348	-1.817842
10	8	0	-0.158436	0.447689	-1.237818
11	1	0	1.036997	-0.774298	-1.083152
12	1	0	-0.819860	0.602198	-0.488513

ll. TS11

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.244678	-1.007765	-0.070080
2	6	0	0.769948	-0.222379	0.455251
3	8	0	1.617127	0.395198	-0.324893
4	17	0	-1.882714	0.885043	-0.302105
5	1	0	-0.994845	-1.393817	0.598213
6	1	0	-0.324931	-1.148933	-1.135630
7	1	0	0.808546	-1.683754	0.300277
8	1	0	0.820491	-0.062670	1.526809
9	1	0	2.293970	0.852546	0.179567

mm. TS12

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.435436	-0.515921	0.926202
2	6	0	1.327429	-0.866964	-0.171032
3	1	0	0.802637	0.122067	1.715391
4	1	0	-0.426231	-1.134782	1.121643
5	1	0	1.738318	-1.840902	0.153065
6	1	0	0.734028	-1.087057	-1.065619
7	8	0	2.385923	0.003154	-0.386450
8	1	0	1.989161	0.863563	-0.563214
9	17	0	-2.105639	-0.223951	-0.193693
10	8	0	0.122035	1.534244	0.018755
11	1	0	-0.757153	1.135312	-0.244070
12	1	0	-0.088526	2.206212	0.671155

nn. TSas

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.053270	0.431344	0.010765
2	6	0	1.203045	-0.216756	0.002506
3	1	0	2.134143	0.327925	0.057330
4	1	0	1.237517	-1.295518	-0.069451
5	1	0	0.005480	1.515998	0.058012
6	8	0	-1.168527	-0.186369	-0.108168
7	1	0	-1.478698	-0.454773	0.756907

oo. TSas.HCl

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	6	0	1.145871	1.220350	-0.208854
2	6	0	1.564332	0.141599	0.433652
3	8	0	1.957468	-1.008369	-0.197959
4	17	0	-2.202333	-0.155338	0.001377
5	1	0	1.138413	1.261009	-1.289823
6	1	0	-0.940271	0.115510	-0.011867
7	1	0	0.810263	2.084664	0.345552
8	1	0	1.563191	0.085744	1.519093
9	1	0	2.891791	-0.967641	-0.404531

pp.TSas.HCl_W

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.101450	-0.561215	0.112304
2	6	0	1.242812	-1.554903	0.228662
3	1	0	1.597472	-2.564978	0.368890
4	1	0	0.175399	-1.382831	0.198320
5	1	0	3.175555	-0.709270	0.147637
6	8	0	1.716214	0.742460	-0.123003
7	1	0	1.603225	1.204648	0.716442
8	8	0	-0.945278	1.326792	-0.727008
9	1	0	-1.493942	0.592666	-1.003397
10	1	0	-0.024561	1.031852	-0.817432
11	17	0	-0.376391	1.880963	2.183311
12	1	0	-0.816489	1.664687	0.953172