

Molecular Mechanics/Excel Problem Set

Conformations of Ethane

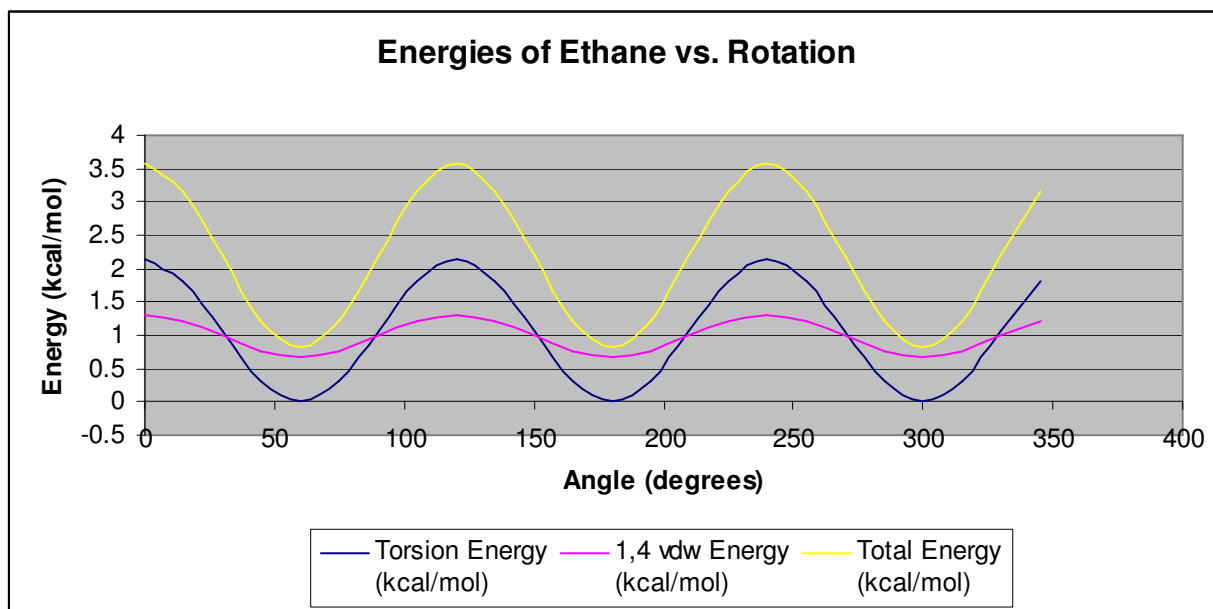
Ethane was made in Chem3D and then positioned in an eclipsed position. The energy was minimized with the energy minimizer under the MM2, Minimize Energy command. The Compute Steric Energy command calculated and the torsion energy, 1,4 vdw energy, and the total energy was recorded in an excel spreadsheet. The methyl was rotated by 15 degrees each time and the various energy was recorded.

The torsion energy, the 1,4 vdw energy, and the total energy was plotted as a function of rotational angle using EXCEL. The data is shown below in Table 1. The plotted chart is located below (Chart 1).

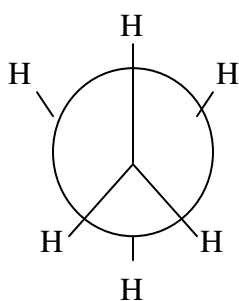
TABLE 1: Energy data for the rotation of Ethane

Number of Rotation	Degrees of Rotation of Ethane	Torsion Energy (kcal/mol)	1,4 vdw Energy (kcal/mol)	Total Energy (kcal/mol)
1	0	2.133	1.3058	3.5804
2	15	1.8206	1.2107	3.173
3	30	1.0665	0.9853	2.1935
4	45	0.3124	0.7657	1.2198
5	60	0	0.6764	0.8181
6	75	0.3134	0.7657	1.2198
7	90	1.0665	0.9853	2.1935
8	105	1.8206	1.2107	3.173
9	120	2.133	1.3058	3.5804
10	135	1.8206	1.2107	3.173
11	150	1.0665	0.9853	2.1935
12	165	0.3124	0.7657	1.2197
13	180	0	0.6764	0.8181
14	195	0.3124	0.7657	1.2197
15	210	1.0665	0.9853	2.1935
16	225	1.8206	1.2107	3.173
17	240	2.133	1.3058	3.5804
18	255	1.8206	1.2107	3.173
19	270	1.0665	0.9853	2.1935
20	285	0.3124	0.7657	1.2198
21	300	0	0.6764	0.8181
22	315	0.3124	0.7657	1.2198
23	330	1.0665	0.9853	2.1935
24	345	1.8206	1.2107	3.173
25	360	2.133	1.3058	3.5804

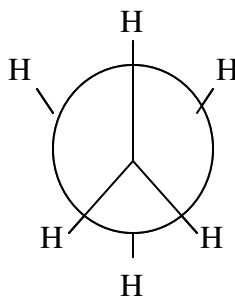
CHART 1: Energies for Ethane vs. Rotation.



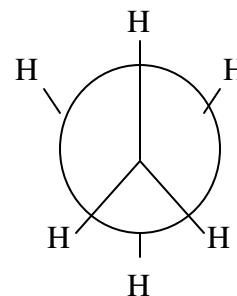
Newman Projections Minimum



60 °C

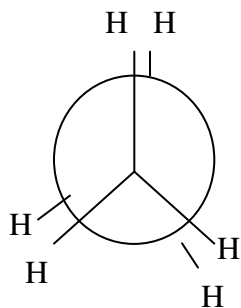


180 °C

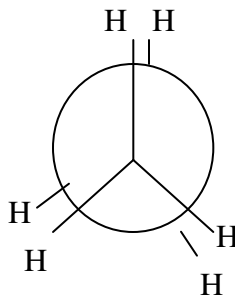


300 °C

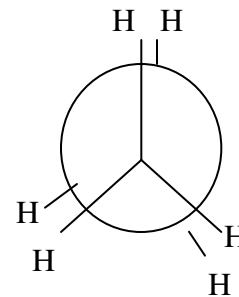
Newman Projections Maximum



0 °C & 360 °C



120 °C



240 °C

Conformations of Butane

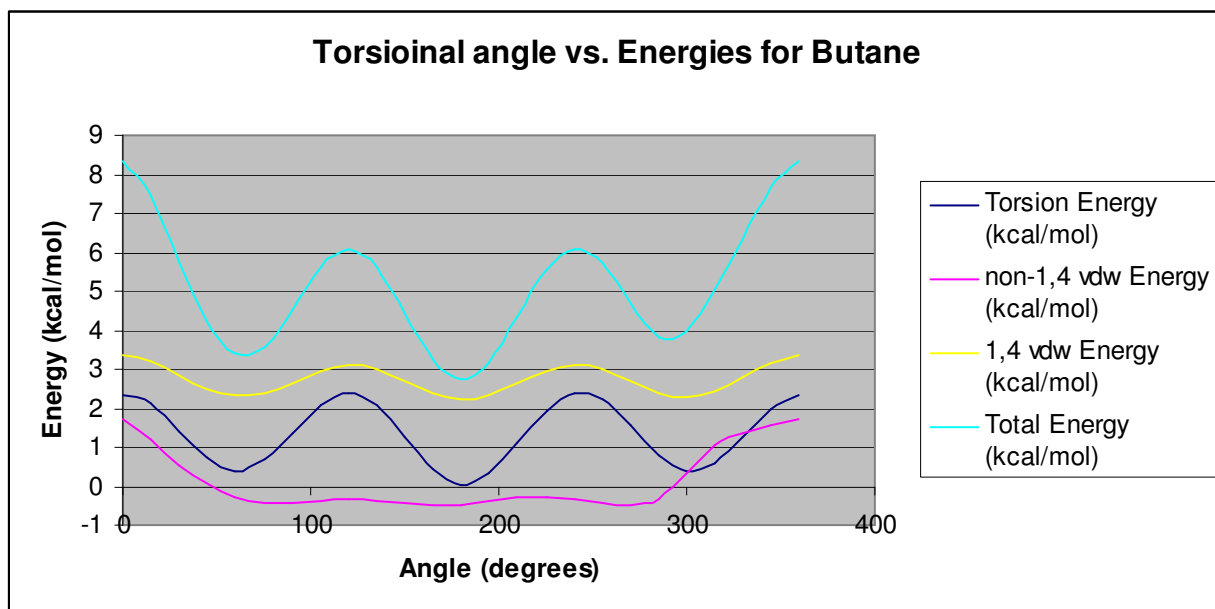
Butane was made in Chem3D and then positioned in the eclipsed position. The energy was minimized with the energy minimizer under the MM2, Minimize Energy command. The Compute Steric Energy command calculated and the torsion energy, 1,4 vdw energy, non-1,4 vdw energy and the total energy was recorded in an excel spreadsheet. The C₂-C₃ rotated by 15 degrees each time and the various energy was recorded.

The torsion energy, the 1,4 vdw energy, the non-1,4 vdw energy and the total energy was plotted as a function of torsional angle using EXCEL. The data is shown below in Table 2. The plotted chart is located below (Chart 2).

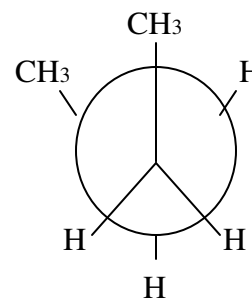
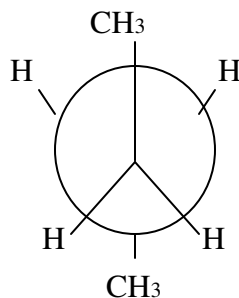
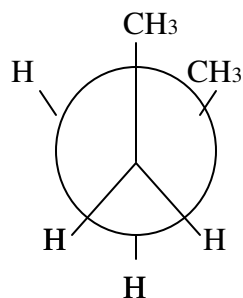
TABLE 2: Energy data for the rotation of Butane

Number of Rotation	Degrees of Rotation of butane (torsion angle)	Torsion Energy (kcal/mol)	non-1,4 vdw Energy (kcal/mol)	1,4 vdw Energy (kcal/mol)	Total Energy (kcal/mol)
1	0	2.3353	1.6938	3.3448	8.3151
2	15	2.1065	1.2128	3.2184	7.4788
3	30	1.4338	0.5133	2.8678	5.7561
4	45	0.722	0.0656	2.5042	4.2329
5	60	0.4012	-0.264	2.3195	3.3979
6	75	0.67	-0.4596	2.3918	3.5433
7	90	1.3743	-0.4511	2.665	4.5292
8	105	2.0937	-0.3776	2.9736	5.6309
9	120	2.3878	-0.3585	3.1216	6.092
10	135	2.0561	-0.3923	3.007	5.6119
11	150	1.2606	-0.4493	2.6986	4.4511
12	165	0.4378	-0.501	2.3823	3.2603
13	180	0.0487	-0.4962	2.2344	2.728
14	195	0.3137	-0.4102	2.3307	3.1753
15	210	1.0852	-0.304	2.6189	4.3412
16	225	1.932	-0.2711	2.9371	5.5391
17	240	2.3878	-0.3312	3.0927	6.0904
18	255	2.2178	-0.4339	2.9888	5.7138
19	270	1.5497	-0.4961	2.6983	4.6931
20	285	0.7941	-0.3189	2.4082	3.8245
21	300	0.4012	0.312	2.2961	3.9505
22	315	0.5979	1.0486	2.4412	5.0289
23	330	1.2584	1.349	2.7897	6.3382
24	345	1.9824	1.5587	3.1641	7.6463
25	360	2.3353	1.6938	3.3448	8.3151

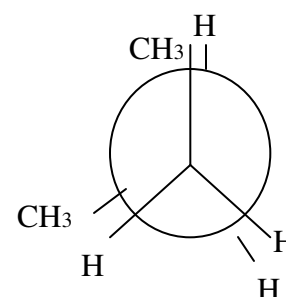
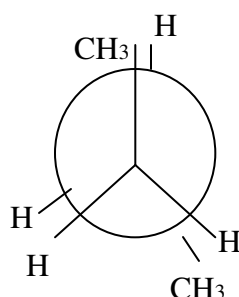
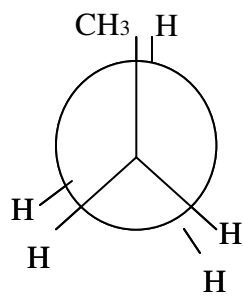
CHART 2: Torsional Angle vs Energies for Butane



Newman Projections Minimum



Newman Projections Maximum



Comparison of Ethane and Butane

When comparing the plots of the energies of Ethane and the energies of Butane, there are similarities and differences. The torsion energy vales for both compounds are nearly identical. The 1,4-vdw energies are similar in their wave-like nature, but the butane has higher energy values and has higher “highs” and lower “lows”. The same is true for the total energy. Because of the 1,4-vdw energies being so high, the total energy of butane is higher overall than ethane. The similar wave-like line is just higher in energy, as seen in Chart 1 and Chart 2.