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Conformational Analysis of Cis-1,4-Di-*tert-butyl*-Cyclohexane

The goal of this conformational analysis project is to find the lowest energy conformation for cis-1,4-di-tert-butyl-cyclohexane **(1)**. Normally cyclohexane molecules form the chair conformation because there are less stearic interactions between carbons 1 and 4. However, if substituents are rather bulky, it may be necessary to form a non-chair conformation to reduce stearic hindrance of the substituents. Substituents normally want to be found in the equatorial position on a ring because it reduces stearic hindrance with other substituents that would be in the axial position. However, if two substituents are found on carbons 1 and 4, they cannot both be equatorial if the ring is to keep the chair conformation.

Compound **1** was first built in ChemDraw 2005 in the cis-conformation (Fig. 1). This structure was copied and pasted into Chem3D to keep the cis-conformation.

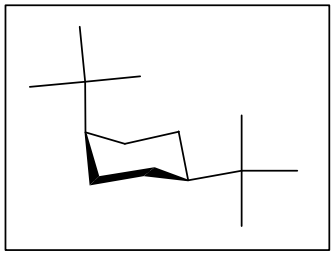
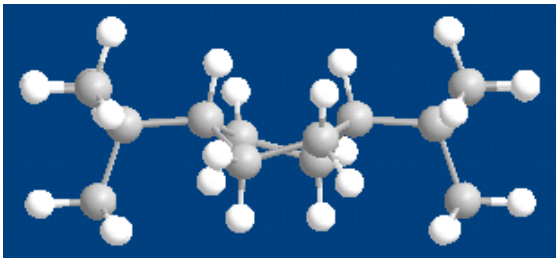


FIGURE 1 The ChemDraw 2005 structure for Compound **1.**

After many movements of the t-butyl groups and many movements of carbons 1 and 4, the minimum energy turned out to be 23.9834kcal/mol (Fig. 2). Since the t-butyl groups are so big,

it is more favorable for the t-butyl groups to be equatorial and the cyclohexane to be in the twist-boat conformation (Fig.3).



Stretch: 2.3219
Bend: 3.9318
Stretch-Bend: 0.4826
Torsion: 8.3714
Non-1,4 VDW: -2.1136
1,4 VDW: 10.9893
Total: 23.9834

FIGURE 3 The twist-boat conformation of Compound **1**.