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Data Analysis Exercises: Conformational Analysis Project

INTRODUCTION

Molecular structures can have various structures depending on its desire to minimize the overall energy. Chem3D is a program that can calculate the overall energy of bond angle strain, torsional strain, Vander-wall forces, etc. The following project will minimize the energy of cis-1,4-ditertbutylcyclohexane. Since the tert-butyl groups exist as a sigma bond, they may rotate to form the most stable conformer.

OBJECTIVE

The objective of this project is to take cis-1,4-ditertbutylcyclohexane and put it in the most stable conformation and minimize the energy using Chem3D.

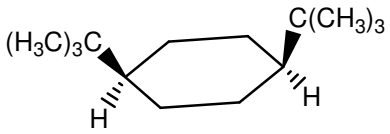
PROCEDURE

The first step in this procedure was to draw the molecule in ChemDraw using the wedge-dash notation (Picture 1). By using the wedge-dash notation, I could make sure that when the structure was copied into Chem3D, the conformer would remain a cis conformer. I copied the ChemDraw molecule and pasted it into Chem3D. Then, I made the molecular model to also make sure that I had the correct cis structure. Chem3D initially put the structure in the chair conformation and the tert-butyl groups were in the axial and equatorial positions. I selected "Run" in Chem3D and minimized the energy. A "twisted chair" structure (Picture 2) emerged with an energy of 27.9661 kcal/mol. I then realized that a boat conformer would place the large tert-butyl group in the equatorial position. I theorized that it was more important to minimize the steric hindrance of the tert-butyl groups rather than minimizing the ring strain in the boat conformation and minimizing the steric hindrance of the hydrogens on the 1^{st} and 4^{th} carbon. I selected "Run" in Chem3D and minimized energy. A "twisted boat" structure (Picture 3)

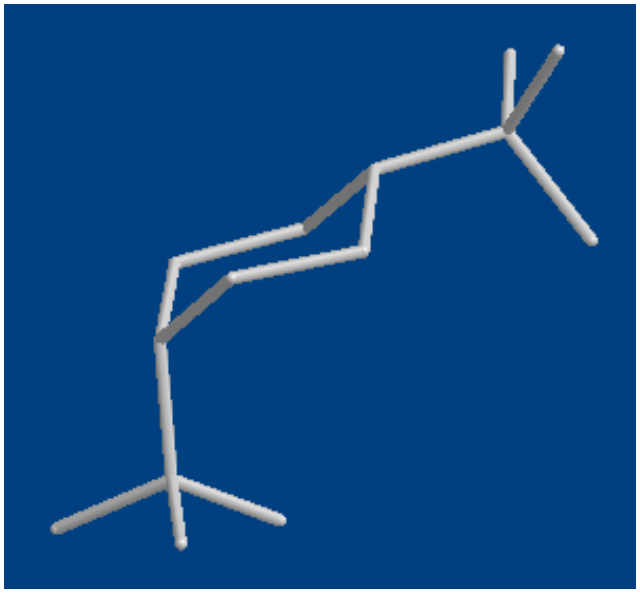
emerged with an energy of 27.4740 kcal/mol. The twisted boat had both tert-butyl groups equatorial, which had the least steric hindrance. I tried to move the tert-butyl groups but CHEM3D redirected the structure to form the "twisted boat" each time and I could not achive an energy lower that the initial 27.4740 kcal/mol.

DATA

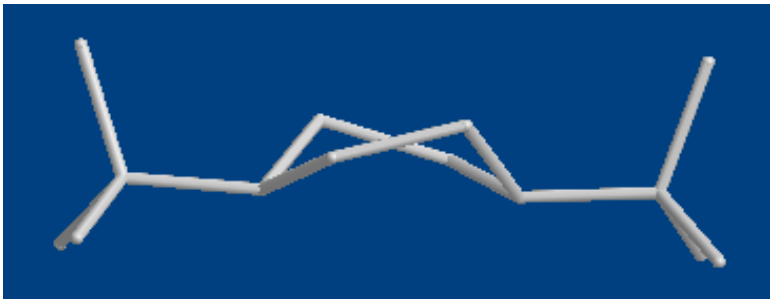
PICTURE 1: ChemDraw Picture



PICTURE 2: Twisted Chair



PICTURE 3: Twisted Boat



ANALYSIS OF RESULTS

I discovered that the most stable form of the cis-1,4-ditertbutylcyclohexane conformer was the “twisted boat” form. The minimization of the tert-butyl groups proved to be the most important aspect of minimizing the energy of the 6-membered ring. As seen in the Picture 3 above the tert-butyl groups are in the equatorial position and the hydrogens on carbons 1 and 4 are not eclipsed. The least amount of energy that the structures has was 27.4740 kcal/mol.