Conformational Analysis of 3-methylpentane

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ABSTRACT:

This report explores the conformations of 3-methylpentane, a branched alkane, and assess their stability through Jmol application. Through Newman projections diagrams, six stable conformations were identified, 3 staggered and 3 gauche. Staggered conformations, with lower torsional strain and energy levels between 3.4 and 3.8 kJ/mol, indicates greater stability. Eclipsed conformations suffer from increased repulsion. Their energy levels are from 18 to 21 kJ/mol, pointing to less stability. The results confirm that staggered conformations are energetically favourable. Understanding these conformations aids in predicting molecular behaviour and their reactivity crucial for various chemical applications. In this report the 3D model of 3-methylpentane was created using Jmol application. Using bond rotation option we have created various possible 3D models of the conformers, which gave us an insight about the torsional strain and stability in a broader perspective. which made this concept very easy to understand.

Keywords:

Jmol, conformational isomerism, Conformations, 3-methylpentane, stereochemistry, 3D models