

molecular mechanics calculation

Synonym: force-field calculation

An empirical calculational method intended to give estimates of structures and energies for conformations of molecules. The method is based on the assumption of 'natural' bond lengths and angles, deviation from which leads to strain, and the existence of torsional interactions and attractive and/or repulsive van der Waals and dipolar forces between non-bonded atoms. The method is also called '(empirical) force-field calculations'.

Source:

PAC, 1994, 66, 1077 (*Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994)*) on page 1142