

molecular mechanics 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’.

1994, 66, 1142