

strain

Strain is present in a molecular entity or transition structure if the energy is enhanced because of unfavourable bond lengths, bond angles or dihedral angles ('torsional strain') relative to a standard. It is quantitatively defined as the standard enthalpy of a structure relative to a strainless structure (real or hypothetical) made up from the same atoms with the same types of bonding. (The enthalpy of formation of cyclopropane is 53.6 kJ mol^{-1} , whereas the enthalpy of formation based on three 'normal' methylene groups, from acyclic models, is -62 kJ mol^{-1} . On this basis cyclopropane is destabilized by *ca.* 115 kJ mol^{-1} of strain energy.)

See: molecular mechanics calculation

Source:

PAC, 1994, 66, 1077 (*Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994)*) on page 1168