

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*.

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