

strain energy

The excess energy due to steric strain of a molecular entity or transition state structure, *i.e.* distortions relative to a reference (real or hypothetical) 'strainless' structure with the standard bond lengths, bond angles and dihedral angles. The strain energy components involve the following destabilizing terms: non-bonded repulsions, bond-angle distortions, bond stretch or compression, rotation around or twisting of double bonds, and electrostatic strain. In general, the contributions of these components are inseparable and interdependent. A quantitative assessment of strain and strain energies can be made by taking the difference between the heat of formation of the substance under consideration and that of a hypothetical strain-free model. Several approaches to the assessment of strain energies have been developed based on the use of energies of isodesmic and homodesmotic reactions and on the so-called 'strainless increments', *i.e.* heats of formation of certain groups (CH₃, CH₂, CH, C *etc.*).

Source:

PAC, 1999, 71, 1919 (*Glossary of terms used in theoretical organic chemistry*) on page 1964