

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.*).

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