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Ring strain energy and its influence on dissociation energy of C–H-bond in cycloalkanes, cycloalkenes, cycloaromatic hydrocarbons and O-H-bond in cyclocarboxylic acids

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Abstract

Empirical research of influence of ring stain energy (E_{rsc}) on dissociation energy of C–H-bond ($D_{C–H}$) in cycloalkanes, cycloalkenes and cycloaromatic hydrocarbons (indane, tetraline) is conducted. It is shown that for all cyclic compounds, except cyclopropane, the simple relation is carried out: $D_{C–H} = D_{C–H}(\Delta E_{rsc} = 0) + \Delta E_{rsc}$, где ΔE_{rsc} represents a difference of energies of ring strain energy of the formed radical and an initial molecule. Values $D_{C–H}(\Delta E_{rsc} = 0)$ are close to $D_{C–H}$ of linear hydrocarbons (paraffins, olefins). For cyclocarboxylic acids linear correlation between dissociation energy of O–H-bond and its electronegativity is established.