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A study of the electronic structure and properties of the propargyl radical

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Abstract

© 2016, Pleiades Publishing, Ltd.By means of B3LYP/6-311++G(3df,3pd) the electron density distribution in the propargyl radical CH2CCH is obtained. Within the Quantum Theory of Atoms in Molecules the phenomenon of conjugation and the spin density distribution of the unpaired electron in CH2CCH are studied at the qualitative level. Characteristics of the electronic structure of CH2CCH and its parent molecules CH3–C≡CH and CH2=C=CH2 are compared. With the use of the rigid rotator-anharmonic oscillator model the thermodynamic properties of the propargyl radical and enthalpies of bond cleavage in propyne and allene are calculated in the temperature range 298-1500 K. The relationship between the electronic and thermodynamic properties of CH2CCH is considered and its conjugation energy is calculated.

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Keywords

conjugation, electron density, enthalpy of bond cleavage, enthalpy of formation, propargyl, quantum theory of atoms in molecules