Electron-topological, energetic and π-electron delocalization analysis of ketoenamine-enolimine tautomeric equilibrium.

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Streszczenie

The ketoenamine-enolimine tautometic equilibrium has been studied by the analysis of aromaticity and electron-topological parameters. The influence of substituents on the energy of the transition state and of the tautomeric forms has been investigated for different positions of chelate chain. The quantum theory of atoms in molecules method (QTAIM) has been applied to study changes in the electron-topological parameters of the molecule with respect to the tautomeric equilibrium in intramolecular hydrogen bond. Dependencies of the HOMA aromaticity index and electron density at the critical points defining aromaticity and electronic state of the chelate chain on the transition state (TS), OH and HN tautomeric forms have been obtained.

Słowa kluczowe

Aromaticity, Carbonylamine, Enolimine, intramolecular hydrogen bond, QTAIM, Tautomeric equilibrium, HOMA

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