Peculiarities of quasi-aromatic hydrogen bonding.

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Streszczenie

The analysis of the calculated topological and energetic characteristics is presented for the hydroxyaryl, alkyl Schiff and Mannich bases. The quantum theory of the atoms-in-molecules methodology has been used to explore the topology of the electron density at the bond and ring critical points in the studied compounds with intramolecular hydrogen bonding. The dependencies between the electron-topological, aromatic, and energetic parameters under tautomeric equilibrium have been analysed. The calculated non-adiabatic potential curves show the difference between the unconjugated and π-conjugated compounds. The calculated dependency between the binding energy of hydrogen bonding (ΔE_{HB}) and the aromaticity of the chelate chain (the HOMA aromaticity index) reveals a difference between the two types of compounds. The results obtained have made it possible to figure out a basic difference between unconjugated and π-conjugated compounds.

Adres publiczny

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