

Comparison of resonance assisted and charge assisted effects in strengthening of hydrogen bonds in dipyrins.

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Streszczenie

This paper deals with the study of two types of hydrogen bonding: a quasi-aromatic hydrogen bonding in dipyrromethene and the ionic one in dipyrromethane. The study focuses on two phenomena—the proton transfer process and tautomeric equilibrium. Metric parameters and spectroscopic assignments have been calculated; this allowed a further comparison of spectral features calculated with four methods (Car–Parrinello molecular dynamics (CPMD), ab initio, density functional theory (DFT), and numerical calculation of anharmonic vibrational levels via a solution of the corresponding 1D Schrödinger equation). A significant dynamics of the bridged proton and bent vibration of pyrrole fragments in dipyrromethane have been exposed by the CPMD calculations. The prevailing of the ionic effect over the π -electronic coupling in the strengthening of the hydrogen bonding has been shown on the basis of the calculated structural, electron-topological, and spectral data as well as potential energy surface (PES). The analysis of the aromaticity and electronic state of pyrrole and chelate moieties depending on the tautomeric equilibrium by the quantum theory of atoms in molecules (QTAIM) method was conducted. The principle divergence in the behavior of aromaticity of the chelate chains in the analyzed compounds was demonstrated.

Adres publiczny

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<https://www.acs.org/content/acs/en.html>