Comprehensive Empirical Model of Substitution—Influence on Hydrogen Bonding in Aromatic Schiff Bases

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Streszczenie

In this work, over 500 structures of tri-ring aromatic Schiff bases with different substitution patterns were investigated to develop a unified description of the substituent effect on the intramolecular hydrogen bridge. Both proximal and distal effects were examined using Density Functional Theory (DFT) in the gas phase and with solvent reaction field (Polarizable Continuum Model (PCM) and water as the solvent). In order to investigate and characterize the non-covalent interactions, a topological analysis was performed using the Quantum Theory of Atoms In Molecules (QTAIM) theory and Non-Covalent Interactions (NCI) index. The obtained results were summarized as the generalized, empirical model of the composite substituent effect, assessed using an additional group of simple ring-based Schiff bases. The composite substituent effect has been divided into separate increments describing the different interactions of the hydrogen bridge and the substituent: the classical substituent effect, involving resonance and induction mediated through the ring, steric increment based on substituent proximity to the bridge elements, and distal increment, derived from substitution on the distal ring.

Słowa kluczowe

density functional theory, polarizable continnum model, quantum theory of atoms in molecules, non-covalent interactions, hydrogen bond, proton transfer, schiff base, salen-type ligand

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