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Original Research Article

Study of the Formation, Energetics, Specific Interaction, Charge Transfer and Nature of Hydrogen Bonds in Dimerization of the 2PY (C_5H_4X N (O) Derivatives (X= F, Cl, and Br): DFT, AIM and NBO analyses

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ABSTRACT

The hydrogen bonding interaction plays an important role in determining the shape, the structure and stability, physical properties and functions of molecules. In current research, two intermolecular interactions, i.e., (1) hydrogen bonds and (2) substituent effects, were analyzed and compared. For this purpose, the geometries of 2-pyridone and its substituted dimers (C_5H_4X N (O) X = F, Cl and Br) were optimized by means of B_3LYP/6-311 + +G (d, p) method. The dependence between the strength of hydrogen bonding and the H···Y distance is discussed for the hydrogen bonds N-H…O (X=N; Y=O) system. The N-H…O angle is another geometrical characteristic of hydrogen bonding. To further investigation of nature and strength of hydrogen bond interactions in these systems the structural and electronic parameters were analyzed by using the quantum theory of atoms in molecule (QTAIM) and natural bond orbital (NBO) analyses. Natural bond orbital (NBO) analysis was performed to reveal the origin of the interaction.

Keywords: Density function theory, Hydrogen bond, Quantum Theory of atoms in molecule (QTAIM), NBO *analysis, Bond critical points, Interaction energy removal*

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