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A Computational Study of N–H…O Hydrogen Bonding to Investigate Cooperative Effects

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Abstract : In this study, nuclear magnetic resonance spectroscopy and nuclear quadrupole resonance spectroscopy parameters of 14N (Nitrogen in imidazole ring) in N–H…O hydrogen bonding for Histidine hydrochloride monohydrate were calculated via density functional theory. We considered a five-molecule model system of Histidine hydrochloride monohydrate. Also, we examined the trends of environmental effect on hydrogen bonds as well as cooperativity. The functional used in this research is M06-2X which is a good functional and the obtained results have shown good agreement with experimental data. This functional was applied to calculate the NMR and NQR parameters. Some correlations among NBO parameters, NMR, and NQR parameters have been studied which have shown the existence of strong correlations among them. Furthermore, the geometry optimization has been performed using M062X/6-31++G(d,p) method. In addition, in order to study cooperativity and changes in structural parameters, along with increase in cluster size, natural bond orbitals have been employed.

Keywords : hydrogen bonding, density functional theory (DFT), natural bond orbitals (NBO), cooperativity effect
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