Assessing parameter suitability for the strength evaluation of intramolecular resonance assisted hydrogen bonding in O-carbonyl hydroquinones

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© 2019 by the authors. Intramolecular hydrogen bond (IMHB) interactions have attracted considerable attention due to their central role in molecular structure, chemical reactivity, and interactions of biologically active molecules. Precise correlations of the strength of IMHBs with experimental parameters are a key goal in order to model compounds for drug discovery. In this work, we carry out an experimental (NMR) and theoretical (DFT) study of the IMHB in a series of structurally similar o-carbonyl hydroquinones. Geometrical parameters, as well as Natural Bond Orbital (NBO) and Quantum Theory of Atoms in Molecules (QTAIM) parameters for IMHB were compared with experimental NMR data. Three DFT functionals were employed to calculated theoretical parameters: B3LYP, M06-2X, and ?B97XD. O . . . H distance is the most suitable geometrical parameter to distinguish among similar IMHBs. Second order stabilization energies ?Eij(2) from NBO analysis and hydrogen bond energy (EHB) obtained from