

## QUANTUM CHEMICAL INVESTIGATION OF INTRAMOLECULAR HYDROGEN BONDS IN OXYGENATED AROMATIC MOLECULES: INFLUENCE OF RING SIZE, DONOR/ACCEPTOR GROUPS AND SUBSTITUTANTS

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Hydrogen bonds (HBs) are important for a broad range of applications and play a fundamental role in structural chemistry and biology. HB interactions, dynamics and their directionality are discussed for almost one century and there is still a need for further experiments and theoretical investigations to fully encompass this complex interaction. Especially the experimental investigation of weak intramolecular HBs of isolated molecules in the gas phase remains challenging. Quantum chemical tools are needed to support high resolution THz and IR spectroscopies which can reveal the influence of intramolecular HBs on the rovibrational dynamics<sup>1</sup>.

In this work we focus on intramolecular HBs of oxygenated aromatic molecules. They are investigated through a combination of quantum theory of atoms in molecules QTAIM<sup>2</sup>, non-covalent interactions NCI<sup>3</sup>, natural bond orbitals NBO<sup>4</sup>, and topological data analysis TDA<sup>5</sup>. We studied the influence of the substituents, of the donor or acceptor groups and of the number of atoms included in the ring formed by the HB. We relate our findings with recent rovibrational measurements in catechol (1,2-dihydroxybenzene) and guaiacol. We provide an overview of the problems arising while studying weak intramolecular HBs stabilizing oxygenated aromatic compounds and we discuss the performance of the different quantum chemical tools.

<sup>1</sup> J. Bruckhuisen, *Molecules*, **2021**, 26, 3645; <sup>2</sup> R. Bader, *International series of monographs on chemistry*, **1994**, 22; <sup>3</sup> C. Narth, *Challenges and advances in computational chemistry and physics*, **2016**, 491-527; <sup>4</sup> E. Glendening, *NBO 6.0*, **2013**; <sup>5</sup> N. Otter, *EPJ Data Sci.*, **2017**, 6, 17.