

*Synthesis, crystal structure and theoretical study of a new carbohydrazone*Rafael Mendoza Meroño<sup>1</sup>, Ruben Soria Martinez<sup>1</sup>, Klaus Merz<sup>2</sup>, Santiago García Granda<sup>1</sup><sup>1</sup>Faculty Of Chemistry. University Of Oviedo, Oviedo, Spain, <sup>2</sup>Lehrstuhl für Anorganische Chemie I. Ruhr-Universität Bochum, Bochum, Germany

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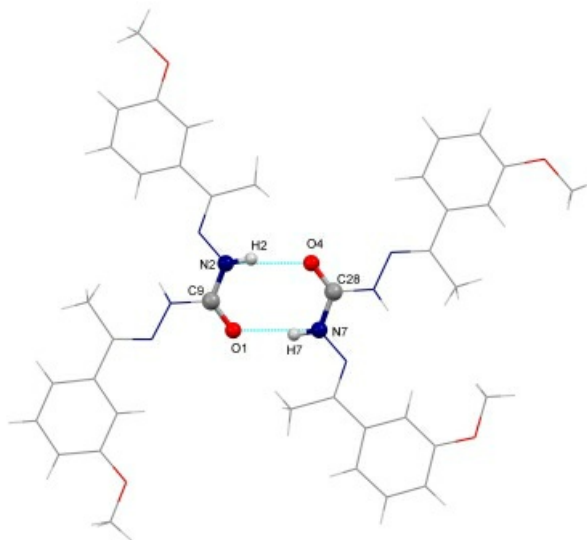
Hydrazone Schiff bases derived from an amino and carbonyl compound are an important class of ligands due to their fascinating chemical and biological behavior [1]. Coordination versatility is a structural important aspect for these kinds of compounds, which is the result of the tautomeric equilibrium between keto and enol forms like in hydrazones and semicarbazones, coordinating for many complexes the iminic-N to the metal. Carbohydrazone Schiff derivatives has not been studied as much as others homologous hydrazones (thiosemicarbazones and semicarbazones); however the interest for these ligands is increasingly due to the use for the targeted construction of extended metal-organic architectures, and also as an important class of components for the self-assembly of supramolecular structures [2]. In this work, the experimental and theoretical studies of new carbohydrazone are reported. The new carbohydrazone was synthesized and characterized by FT-IR, and NMR, the crystal structure was determined by X-ray single-crystal diffraction. The molecular conformation in the molecular crystals is determined by the interactions and weak interactions present in the packing, such as hydrogen bonding,  $\pi$ - $\pi$  stacking, or Van der Waals interactions between layers. These interactions play an important role in a wide range of chemical and biological fields, and also in the stability of the crystals, providing an important tool for crystal engineering. Computational studies have been performed in order to achieve a better description of the interactions established between these molecules in the crystal packing. The molecular geometry was optimized with a WB97XD functional level of theory, using as input the previously conformation obtained from single crystal X ray diffraction studies. The computed, natural bond orbital analysis, global and local reactivity descriptors have been done in gas phase. Dimer interactions energies, noncovalent interaction study (NCI approach) complemented with Quantum Theory of Atoms in Molecules (QTAIM) have been performed [3].

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