Experimental charge density study of salicylaldehyde thiosemicarbazone

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Thiosemicarbazones and their metal complexes are studied due to their wide biological activities spectrum, analytical applications and specific chemical and structural properties [1]. Up to date almost a thousand thiosemicarbazide based crystal structures have been reported, among them over one hundred were structures containing salicylaldehyde thiosemicarbazone (Sal-TSC) structural fragment. Sal-TSC and its derivates have been recently reported as a potential thrombopoetin mimic agents [2], and two thiosemicarbazone based molecules are in clinical phase I due to to their inhibitor activity against ribonucleotide reductase [3]. Here, we present an experimental charge density study of one of the most simple compound [4] of this family, in order to characterize the electronic and electrostatic properties of this potent pharmacophore fragment.

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