

To verify and support these findings, the Quantum Theory of Atoms In Molecules (QTAIM), [8] has been applied to two observables, the electron density, ρ , and its Laplacian, $\nabla^2\rho$. This allowed us to analyze the charge transfer, the nature of bonding interactions and the valence anisotropy of iron directly from the topology of these observables. Independently from the adopted partitioning scheme, a mainly covalent rather than a fully ionic description emerges for the bonding interactions in the two systems. In accordance with the atomic electronegativities, a higher degree of covalency is found for the Fe-P interaction.

Besides supporting and confirming the orbital-based view, the topological analysis and the examination of the Valence Shell Charge Concentration (VSCC) regions provides a rigorous link among such a view, the VSEPR theory and the structural modifications (namely the compression along the *c* crystallographic axis) that occurs when substituting S with P in the marcasite structure.

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Keywords: quantum theory of atoms in molecules, marcasite

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Structural analysis and DFT calculations of (*Z*)-4-methyl-*N*-(2-((2-oxonaphthalen-1(2*H*)-ylidene)-methylamino)ethyl)benzenesulfonamide

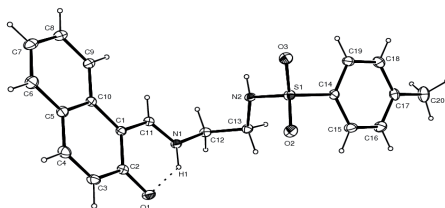
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The molecular and crystal structure of the title compound, C₂₀H₂₀N₂O₃S, has been determined by X-ray single crystal diffraction technique. The compound crystallizes in the monoclinic, space group *Pc* with unit cell dimensions

$a=13.2967(7)$ Å, $b=6.9654(5)$ Å, $c=9.9714(6)$ Å, $\beta=99.907(4)^\circ$, $V=909.75(10)$ Å³, $Z=2$, $R_1=0.042$ and $wR_2=0.109$. The molecule adopts a keto-amine form, stabilized by an intramolecular N-H...O type hydrogen bond.

Molecular geometry of the title compound in the ground state have been calculated using the density functional method (DFT) with 6-31G(d,p) basis set and compared with the experimental data. The calculated results show that the optimized geometry can well reproduce the crystal structure.

In addition, DFT calculations of the compound, total energy, molecular electrostatic potential (MEP) and non-linear optical (NLO) properties were performed at B3LYP/6-31G(d,p) level of theory.



Keywords: X-ray, tautomerism, NLO

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Electronic properties of noncovalent interactions in [Co(fam)en]Cl complex

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It has been found that the cobalt(III) complex with the well-known antiulcer drug famotidine (fam) and ethylenediamine (en) shows higher antimicrobial activity and higher selectivity in comparison to the metal free drug [1]. The electronic structure of this complex was described by Hansen-Coppens multipole model [2] using the data collected in a single-crystal X-ray diffraction experiment at 100 K. As the complex is abundant in atoms, which can be involved in hydrogen bond formation either as hydrogen acceptors or hydrogen donors, the crystal structure is stabilized by numerous interactions of this type. In addition, the extended π -systems give rise to variety of interactions such as C–H... π , N–H... π and π ... π . Our present study is focused on a qualitative and quantitative characterization of the hydrogen bonds and other noncovalent interactions from the aspects of the experimental electron density distribution, electrostatic complementarities [3], and topological analysis (Bader's quantum theory of atoms in molecules, QTAIM) [4]. Energy densities at bond critical points are calculated according to Abramov and virial theorem [5]. The geometrical, topological and energetic properties of 32 noncovalent interactions are analyzed and related with the effects they produce on the deformation density of the interacting atoms. A particular attention has been paid on the sensitivity of the valence electron densities of the various hydrogen bonding acceptors, O, N, S, Cl, to their crystal environment.

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Keywords: cobalt (III) complex, charge density, noncovalent interactions

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The original crystal structures of hybrid materials and the influences of hydrogen bonds

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The crystal organic-inorganic hybrid materials have been extensively investigated due to their interest in the filed of new materials, and the number of reported structures is rapidly growing owing to their applications in medicine, material science and their