

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

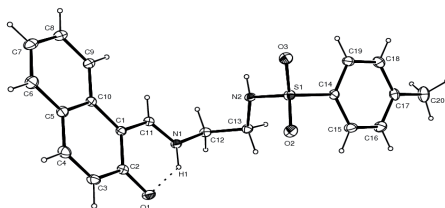
Ahmet Erdönmez,^a Gökhan Alpaslan,^a Mustafa Macit,^b Orhan Büyükgüngör,^a ^a*Ondokuz Mayıs Univ., Department of Physics, Samsun-Turkey.* ^b*Ondokuz Mayıs Univ., Department of Chemistry, Samsun-Turkey.* E-mail: erdonmez@omu.edu.tr

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

Sladjana B. Novaković,^a Goran A. Bogdanović,^a Bojana M. Francuski,^a Djenana Miodragović,^b Bernard Fraisse,^c ^a*“VINČA” Institute of Nuclear Sciences, Laboratory of Theoretical Physics and Condensed Matter Physics, P.O. Box 522, 11001 Belgrade, (Serbia).* ^b*Faculty of Chemistry, University of Belgrade, P.O. Box 158, Studentski trg 16, 11000, Belgrade, (Serbia).* ^c*Laboratoire SPMS, UMR CNRS 8580, Ecole Centrale Paris, Grande Voie des Vignes, 92295 Châtenay-Malabry, (France).* E-mail: snovak@vin.bg.ac.rs

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

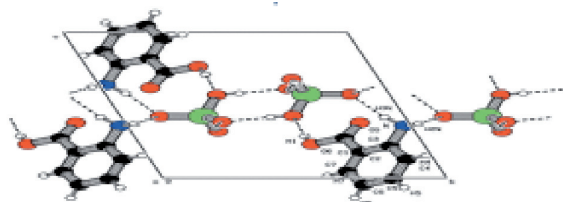
Fatima Allouche et Tahar.Benlecheb *Laboratoire des Structure, Propriétés et Interactions Inter Atomique (LASPIA), Centre Universitaire de Khenchela, 40000 Khenchela, (Algerie).* E-mail: allouche_f@yahoo.fr

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

electrical, magnetic and optical properties and the hydrogen bonding richness of these structures. This kind of hydrogen bonding appears in the active sites of several biological systems and is observed in similar previously studied hybrid compounds [1, 2, 3].

The combination of the matrix cation and the anion mineral anions allowed us to obtain original structures (hybrid compounds) [4, 5]. Presenting strong hydrogen bond, average and low. Several crystals were already isolated in this system. This study consists in studying the influences of hydrogen bond in the geometry of the crystal structures.

Our current domain of research involve the study of the hydrogen connections in a series of hybrids compound, to do it; we are going to use the potentialities which offer the ADF software (Amsterdam Density Functional) to study this type chap of compounds, under solid.



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Keywords: X-ray of diffraction, hybrid compounds, hydrogen bond.

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A charge density investigation into an Rh...C-C sigma interaction

Hazel A. Sparkes,^a Judith A. K. Howard,^a Simon K. Brayshaw,^b Andrew S. Weller,^c ^a*Department of Chemistry, University of Durham, University Science Laboratories, South Road, Durham, DH1 3LE, (UK).* ^b*Department of Chemistry, University of Bath, Claverton Down, Bath, BA2 7AY, (UK).* ^c*Inorganic Chemistry, University of Oxford, South Parks Road, Oxford, OX1 3QR, (UK).* E-mail: h.a.sparkes@durham.ac.uk

Developing an understanding of structure and bonding in transition metal complexes containing metal centres coordinated to saturated bonds (e.g. C-H, H-H, C-C) is of significant interest due to their potential catalysis applications. We have been investigating transition metal catalysed approaches for C-C bond activation: this process is both thermodynamically and kinetically unfavourable due to the strength of the C-C bond. One approach to overcome this is to use strained systems such as cyclopropanes, for which the reduction in strain is thought to provide the driving force to break the C-C bond [1]. The intermediates in this process are believed to involve M...C-C sigma interactions.

Experimental insight into the electron distribution within a system can be obtained through accurate, high resolution, charge density investigations [2]. The nature of the bonding and interactions can then be studied using powerful tools such as Bader's quantum theory of atoms in molecules (AIM) which classifies interactions on the basis of the topological properties of the electron density and its Laplacian at bond critical points (bcp) [3]. A large number of organic species have been successfully studied in this manner however the analysis of the

topological properties around heavy atoms is more challenging with bcp's often appearing in regions of charge depletion or missing where chemical intuition would expect them to be present.

We have previously reported experimental charge density studies for Rh(C₇H₈)(PR₃)Cl (R = PPh₃, P^tBu₃ and PCy₃) [4] these have served as precursors for our current study into [Rh(Binor-S)(PCy₃)]([HCB₁₁Me₁₁]) which contains a Rh...C-C sigma interaction. Particular attention will be paid to the nature of the interactions around the rhodium metal centre.

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Charge density measurements of the anomeric effect in disaccharides

Edwin D. Stevens,^a Michael K. Dowd,^b Alfred D. French,^b ^a*Department of Chemistry, University of New Orleans, New Orleans, LA 70148, (USA).* ^b*Southern Regional Research Center, ARS, USDA, New Orleans, LA 70124.* E-mail: estevens@uno.edu

The anomeric effect was first identified as the preference for pyranose rings to adopt the more hindered axial α -anomeric conformation in solution over the less hindered equatorial β -anomeric conformation. It is now recognized as a specific example of a 'generalized anomeric effect' in which systems with a R-Y-C-X linkage, where Y is an element with lone pairs and X is an electronegative element, show a preference for a *gauche* rather than a *trans* conformation. Several electronic models for the origin of the anomeric effect have been proposed, and it continues to be a topic of experimental and theoretical study and debate. In disaccharides, an additional complication exists because, in addition to the normal anomeric effect, the oxygen of the glycosidic linkage can give rise to an exo-anomeric effect which, depending on the torsion angles, may act with or against the normal effect.

Recently, an accurate experimental and theoretical determination of the charge density distribution of sucrose has been reported¹, and we have conducted similar charge density measurements of α,α -trehalose² and methyl- β -cellobioside. In addition to the determining the deformation density, the charge distribution has been analyzed using the *Atoms in Molecules*³ formalism. These studies allow the predictions of various electronic models for the anomeric effect to be compared with the actual charge density distribution.

The α -pyranose ring of sucrose shows variations in the total electron density at the bond critical points as well as variations in the bond lengths which are consistent with a model for the anomeric effect which involves a $n \rightarrow \sigma^*$ overlap between a lone pair orbital on the Y atom with the σ^* antibonding orbital of the C-X bond. In trehalose, the exo-anomeric effect is in competition with normal anomeric effect, resulting in less variation in the density at the bond critical points.

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Keywords: charge_density, anomeric_effect, topology