

FA3-MS02-P01

Experimental Charge Density Study of Co(III) Complex with Famotidine. Bojana M. Drašković^a, Sladjana B. Novaković^a, Goran A. Bogdanović^a, Bernard Fraisse^b. ^aVINČA Institute of Nuclear Sciences, Laboratory of Theoretical Physics and Condensed Matter Physics, Belgrade, Serbia. ^bLaboratoire „Structures Propriétés et Modélisation des Solides“, UMR 8580 du CNRS, Ecole Centrale Paris, 92295 Châtenay-Malabry, France.
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Famotidine belongs to a class of the stress-ulceration inhibitors, known to exhibit excellent histamine H2 blocking effect [1,2]. As a specific competitive histamine H2-receptor antagonist, famotidine inhibits the secretion of histamine-stimulated gastric fluids. Famotidine offers a set of potential coordination sites for metal ions and it is an efficient chelating agent. It has been shown that in coordination it involves the guanidine and thiazole nitrogen, as well as the thioether sulphur and amine group nitrogen [3, 4]. The experimental electron density distribution in (famotidine) (ethylenediamine) cobalt(III) chloride monohydrate has been determined from high-resolution X-ray diffraction data collected at a temperature of 100 K. After classical spherical refinement, the multipole refinement of the Co(III) complex was performed using the Hansen–Coppens model [5]. A great number of H-bonds as well as C–H... π and π ... π interactions were observed in the crystal packing of this compound. In order to determine quantitative parameters of the chemical bonds and nonbonded interactions in this compound we have carried out topological analysis of total electron density according to Bader's quantum theory of atoms in molecules [6].

Experimental details: The data were collected on a Bruker-SMART diffractometer equipped with a SMART 1000 CCD area detector using monochromated Mo $K\alpha$ X-ray radiation ($\lambda = 0.71073$ Å). Maximal resolution ($\sin\theta/\lambda$)_{max} = 1.10 Å⁻¹. The total number of the reflections collected was 86400. The data sorting and averaging led to a 19124 unique reflections with a final $R_{int} = 2.02$ %.

Crystallographic data: formula C₁₀H₂₃ClCoN₉O₃S₃, triclinic crystal system, space group P-1, $a = 9.0922(1)$, $b = 9.2850(1)$, $c = 12.3436(2)$ Å, $\alpha = 86.058(1)$, $\beta = 77.715(2)$, $\gamma = 73.977(1)^\circ$, $V = 978.59(8)$ Å³.

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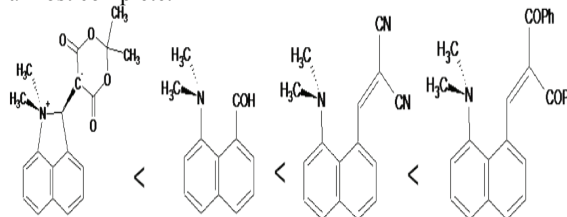
Keywords: Co(III) complex; charge density distribution; high-resolution X-ray diffraction experiment

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Probing Chemical Bonds: X-Ray Charge Density Studies on Bond Formation and Interactions in Peri-Substituted Naphthalenes. Mateusz Pitak^a, Simon J. Coles^a, John D. Wallis^b. ^aSchool of Chemistry, University of Southampton, UK. ^bDepartment of Chemistry and Physics, Nottingham Trent University, UK.
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Our present studies are focused on a solid state experimental characterisation of the correlation between the bond formation and bond breaking processes in the addition reaction of the nucleophilic Me₂N group and different electron deficient alkenes located in the *peri* positions of naphthalenes [1,2]. This type of reaction is significant in the organic area of synthesis and a full understanding of the mechanism is crucial for influencing the outcome of these reactions.

In our system, the two terminal groups can a) be splayed outwards with a Me₂N...C separation distance in the range of ~2.4–3.2 Å or b) arranged inward (~1.6 Å), where the nucleophilic addition of the Me₂N group to the alkene is almost complete.



The orientation of the dimethylamino group is such that a lone pair of electrons is directed towards the reacting adjacent carbonyl group. The strength of an interaction between a pair of atoms is considered to be an indicator of the formation and reactivity of a chemical bond and is defined by their separation. Greater insight into electronic structure of those compounds with emphasis put on attractive/repulsive interactions and reactivity can be obtained by analysis of the experimental charge density using Bader's 'Theory of Atoms in Molecules [3], in which bonding interactions are characterized by topology of the total electron density.

Analysis of the Laplacian $\nabla^2\rho(r)$ and local kinetic (G^{CP}) and potential (V^{CP}) energy densities [4], calculated at the bond critical point (BCP) describes quantitatively how the nature of the Me₂N...C=C interaction changes from electrostatic (closed-shell) to covalent (shared) as a function of distance between interacting atoms [5].

This work aims to adopt a systematic approach to understanding and quantifying the electronic properties of the studied system and employ those properties to characterise the kinetics and mechanism of the bond formation/breaking process. Results obtained for different electronic models will be presented on this poster.

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Electronic Structure of Cu(III) Complex (P(Ph)₃CH₃)[Cu(bdt)₂]. Marek Fronc^a, Jiri Kamenicek^b, Peter Herich^b, Jan Moncol^c, Jozef Kozisek^a. ^a*Department of Physical Chemistry, Slovak Technical University, Bratislava, Slovakia.* ^b*Department of Inorganic and Physical Chemistry, Palacky University, Olomouc, Czech Republic.* ^c*Department of Inorganic Chemistry, Slovak Technical University, Bratislava, Slovakia.*
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For coordination compounds of copper the oxidation state Cu(III) is quite unusual. However, this oxidation state was found in the benzene-1,2-dithiole (bdt) complexes. Wide range of technical application (e.g. superconductors, resins) of the dithiolate complexes, as well as their biological activity makes them interesting subject for the research.

Set of several complexes of the general formula R[M(bdt)₂] with nickel, cobalt and copper as the central atom and various ammonium (phosphonium) derivatives as cations were prepared [1]. Aim of this work is to describe the distribution of the electron density in (P(Ph)₃CH₃)[Cu(benzene-1,2-dithiole)₂].

Two datasets of x-ray diffraction data from two single-crystals were collected at Gemini R diffractometer equipped with Oxford-Cryosystems low temperature device at 100 K to the resolution 0.58/0.39 Å for the first and the second set respectively. 132422/132770 reflections were measured from which 14475/15042 were unique.

Electronic structure study was performed with XD software package. The topological analysis of electron density will be discussed.

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Keywords: electronic structure; Cu(III); topological analysis

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Charge Density Study of (E)-4-(2,4-diisopropylphenyl)-4-oxo-2-Butenoic Acid. Sladjana B. Novaković^a, Goran A. Bogdanović^a, Branko J. Drakulić^b, Anne Spasojević-de Biré^c, Ivan O. Juranić^d. ^a*VINČA Institute of Nuclear Sciences, Laboratory of Theoretical Physics and Condensed Matter Physics, P.O. Box 522, 11001 Belgrade, Serbia.* ^b*Department of Chemistry, Institute of Chemistry, Technology and Metallurgy, University of Belgrade, Njegoševa 12,*

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4-Aryl-4-oxo-2-butenic acids (AAA) exert antibacterial and antineoplastic activity [1]. The (E)-4-(2,4-diisopropylphenyl)-4-oxo-2-butenic acid was a precursor of one of most active CSAB derivative [2] that selectively suppress proliferation of neoplastic HeLa cells in submicromolar concentration. The activity of AAA are ascribed to high affinity of their ketovinyl moieties (-C(O)-CH=CH-) toward octagonal thiol groups of biomolecules. Introduction of branched alkyl chains on phenyl ring significantly increases activities within the congeneric group of compounds. Here, we present the results of the experimental charge density study of the (E)-4-(2,4-diisopropylphenyl)-4-oxo-2-butenic acid. The Hansen-Coppens multipole model [3] was used to describe the electron density distribution within this compound. Subsequently, the topological analysis of the total electron density based on the Bader's quantum theory of Atoms in Molecules (AIM) [4] was performed to characterize the properties of the covalent bonds and interactions. The values of the electron density in the bond critical points corresponding to sixteen C-C bonds are ranging from 1.64-2.46 e.³. The highest value is found for the formally double bond of the ketovinyl moiety.

The analysis of the overall crystal packing showed the clear separation between the regions containing aryl and aliphatic parts of the molecule. The polar parts of the molecules form strong O-H...O hydrogen bond typical for carboxylic acids. On the other hand the non-polar aryl fragments with the branched isopropyl moieties accumulate in separate block giving the rise to a weak but abundant C-H...π local connectivity. The various types of non-covalent interactions present in this crystal structure are characterized in terms of the static deformation density, the topological analysis and the electrostatic potential.

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Keywords: charge density studies; carboxylic acids; biologically active small molecules

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Topological Analysis of Vanadium Borides from High Resolution Single-Crystal Diffraction Data. Bűrgehan Terlan^a, Horst Borrmann^a, Yuri Grin^a. ^a*Max-Planck-Institut für Chemische Physik fester Stoffe, Dresden, German.*

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