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FA3-MS02-P03

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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In the vanadium-boron system the binary phases V_3B_2 , VB, V_5B_6 , V_2B_3 , V_3B_4 , and VB_2 have been reported so far. However, there is a lack of systematical and complete structure information. In most cases, crystal structures were not determined, but only the structure type was assigned and unit cell parameters were refined, except for V_2B_3 and V_3B_2 [1, 2]. Accounting for the similar environment of atoms, characteristic bond lengths in the boron substructure are expected (~ 1.75 Å). However, one of the published B-B bond distances in V_3B_4 is extraordinarily short (1.495 Å), although no crystal chemical reason is obvious [3]. The crystal structures of VB, VB, V_5B_6 , V_2B_3 and V_3B_4 were reinvestigated using high resolution single-crystal X-ray diffraction data. Topological aspects of the crystal structures as well as electron densities are analysed on basis of the precise crystallographic information.

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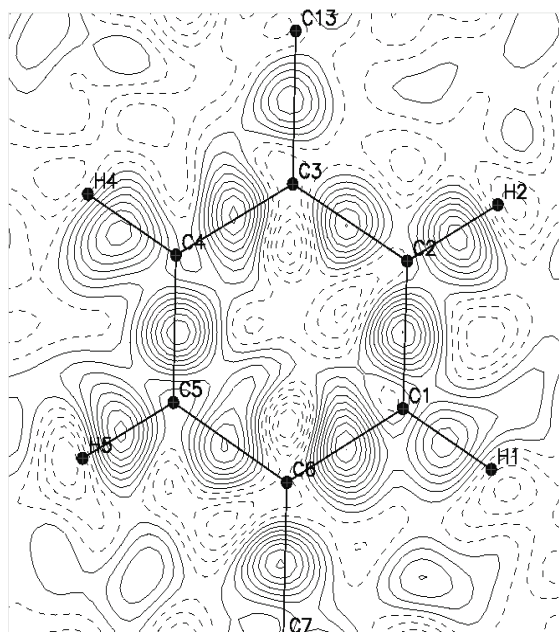
Keywords: vanadium borides; crystal structure; electron density

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Electron Charge Density Distribution in an Organic Compound : The 4,4 Dimethyl Cyano Biphenyl (DMACB). Naima Hamzaoui^a, Mokhtaria Drissi^a, Abdelkader Chouaih^a, Fodil Hamzaoui^a. ^aLaboratoire SEA2m-Facultés Des Sciences & Technologies - University of Mostaganem Algeria. Email: naimahamzaoui@yahoo.fr

At room temperature, the 4,4 dimethylamino-cyanobiphenyl (DMACB) appears in two polymorphic structures: orthorhombic and monoclinic forms. In the present work, we shall focus on the monoclinic form of this compound which has a centrosymmetric structure with the space group Cc. The molecular dipole moment has been estimated experimentally [1].

High resolution single crystal diffraction experiment was performed at low temperature with MoK α radiation. The crystal structure was refined using the multipolar model of Hansen and Coppens (1978) [2]. The molecular electron charge density distribution is described accurately. The study reveals the nature of inter-molecular interactions including charge transfer. The results could be analyzed in more detail, if they were complemented by a quantum chemistry calculation. The electronic structure of this molecule has been investigated theoretically by the Semi-empirical and Ab initio calculations. The agreement between the experimental and theoretical results such as: atomic net charge, molecular dipole moment, electrostatic potential and electron density was satisfactory. All these results will be presented in the meeting. The figure below gives the charge density distribution in the phenyl plane.



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