

chemical properties of the nitramine [2].

In the communication will be shown results of structure determination together with a charge density analysis of N-phenyl-N-methylnitramine together with 1-nitroindoline. Topological properties associated with the bond critical points (BCP), molecular geometry, crystal packing and topological properties of those compounds will also be presented.

[1] Daszkiewicz Z., Zaleski J., Nowakowska E., Kyzioł J., *Pol. J. Chem.*, 2002, 76, 1113. [2] Anulewicz R., Krygowski T., Gawinecki R., Rasała D., *J. Phys. Org. Chem.*, 1993, 6, 257.

Keywords: charge density, nitramines, topological analysis

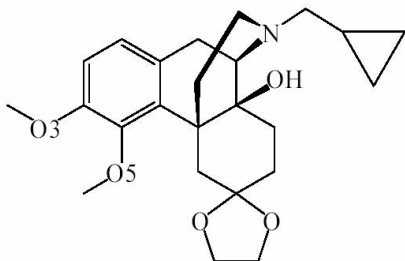
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Rapid Charge Density Data Collection

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A charge density study has been completed on 17-Cyclopropylmethyl-4,14-dihydroxy-3-methoxymorphinan-6-ethylene ketal, a member of an important class of opioid compounds. The two methoxy groups of this compound exhibit unexpected chemical reactivity. Addition reactions strongly favor the more sterically hindered O5 position rather than the O3 position.



Data were collected on an R-Axis Rapid Curved Image Plate. The statistical analysis of the data set as well as the complete results of the multipole refinement will be presented. This will include topological analysis as well as an analysis of the electrostatic potential.

Keywords: electron density distribution, charge density, chemical reactivity and structure

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Experimental Electron Density of [Cu(phen)₂Cl](NO₃)(H₂O)

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The electron density of the title complex was obtained from a high resolution (0.55Å) X-ray diffraction experiment at 100 K, with a KappaCCD diffractometer. Experimental data were collected with MoK α radiation. 11199 independent reflections were used in the refinements. The charge density model was obtained from the Hansen-Coppens formalism. R(F)=0.0368, wR(F)=0.0406.

The copper ion presents coordination between trigonal bipyramidal and square pyramidal. The chlorine atom and one phenantroline nitrogen are in the equatorial plane. Deformation density maps around the copper ion and its d-orbital occupations can be explained in terms of crystal field theory and the π -donating effect of chlorine. Two hydrogen bonds with the water oxygen stabilize the crystalline complex: [Cl \cdots H1–O(w) and O(w)–H2 \cdots O(nitrate)].

Bader's¹ topological analysis of the electron density was performed. (3,-1) critical points were found in all chemical bonds. This analysis shows that the Cu–N and Cu–Cl bonds are ionic, and that the hydrogen bonds are electrostatic. The C–C, C–N and C–H

bonds, on the other hand, are covalent. (3,+1) critical points are present approximately in the center of each phenantroline ring, as well as in the center of the rings containing the copper atom.

[1] Bader R. F. W., *Atoms in Molecules – A Quantum Theory*, Oxford University Press, Oxford, 1994.

Keywords: copper compounds, crystal field theory, multipole refinements

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Phase Transition and Charge Density Study of the m-carboxy-phenyl ammonium phosphite

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Hybrid materials resulting from the association of amino acids with phosphorous acid have a great importance in industry (frequency doubling; can be used as infrared detector and pyroelectric devices). The structure determination, thermal behaviour and the charge density of a new hybrid material of this family (m-carboxy phenyl ammonium monohydrogenphosphite C₇H₈NO₂⁺, H₂PO₃⁻ (m-CPAMP) at low and high temperature phases (LTP) and (HTP) respectively will be presented and discussed. This study will improve the understanding of the phase transition mechanism

Crystals of m-CPAMP, space group P2₁/c, grown from aqueous solution undergo a reversible phase transition as evidenced by the behaviour of the unit-cell parameters versus temperature and by DSC measurements at about T_c = 246 \pm 2 K. The reported phase transition appears to be first order type according to the thermal hysteresis, 3.6 K, and the observed abrupt jumps of the unit-cell parameters.

Using accurate X-ray single crystal investigations between 100 and 320 K, we were able to describe the transition by the rotation of both cations and anions by ca 4.6° around the crystallographic b axis induced by their translation along the b direction. We also will show how the precise description of the electron charge density and its topology modelled from high resolution X-ray diffraction helps in the description of the phase transition.

Keywords: hybrid materials, phase transitions, charge density

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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 derivatives have been recently reported as a potential thrombopoietin mimic agents [2], and two thiosemicarbazone based molecules are in clinical phase I due 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.

[1] Casas J.S., *et al*, *Coord. Chem. Rev.*, 2000, 209, 197. [2] Duffy K. J., *et al*, *J. Med. Chem.*, 2002, 45, 3573. [3] Finch R. *et al*, *Advan. Enzyme regul.*, 1999,