

obtained centrosymmetric structure of silver barbiturate hydrate (P2(1)/m), which can be further modified to obtain the polar structure. For those three structures experimental charge density study and its topological properties were analyzed using XD2006 package [5]. The studies revealed different topological features for the three oxygen atoms of the barbituric acid. Molecular recognition and the formation of specific hydrogen patterns in all of the examined structures seems to have origin in the resonance structures of the barbituric acid molecule.

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Keywords: crystal engineering, experimental charge densities, nonlinear optics

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Electronic Structure of Mixed Valence Cu(I)-Cu(II) Complex, [Cu₃(en)₂(CN)₄(H₂O)]. Jozef Kozisek, Marek Fronc, and Martin Breza, *Technical University Bratislava, Slovakia*
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The mixed valence Cu(I)-Cu(II) complex [1] was chosen for a detailed study of $3d^{10}$ and $3d^9$ copper atom configurations in the same experiment. As shown in our previous study [2] there was a disorder of two cyano groups in 3D Cu(I) framework. By a specific method of crystallization we have obtained the rod-shaped single crystals with a different morphology compared to the previous work. The final refinement of crystal structure data at 100 K with a resolution of $d = 0.41$ by SHELXL gives a R1-factor of 0.0297 for 11934 $F_o > 4\sigma(F_o)$ and Flack x equal 0.011(5) which undoubtedly indicate the correctness of the model: there is no disorder. Surprisingly, the crystal structure framework consists of different Cu(I) chromophores: [Cu(1);N(1),N(2),N(3),C(4)] and [Cu(2);C(1),C(2),C(3),N(4)].

The GEMINI R data at 100K will be used for electronic structure study. As the monoclinic space group *Cc* is a non-centrosymmetric one, the constrained refinement with phases calculated by a quantum-chemical software will be performed. The results of topological analysis both experimental and theoretical will be discussed. This work has been supported by Slovak Grant Agency APVV and VEGA (APVV-0093-07 and 1/0817/08).

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FA4-MS37-P16

Charge density studies on hydrogen bonds in chromone derivatives. Magdalena Matecka^a, Lilianna Chęcińska^a, Agnieszka Rybarczyk-Pirek^a, Carsten Paulmann^{b,c}, Wolfgang Morgenroth^d, ^a*Department of Crystallography and Crystal Chemistry University of Łódź, Tamka 12, 91-403 Łódź, Poland, b/c/o DESY/HASYLAB, Notkestr. 85, D-22603 Hamburg, Germany, c*Mineralogisch-Petrographisches Institut, Universität Hamburg, Grindelallee 48, D-20146 Hamburg, Germany, ^d*Goethe Universität, Department of Geosciences, Altenhöferallee 1, D-60438 Frankfurt, Germany*

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The charge density of two chromone derivatives has been studied using very high precision single-crystal synchrotron-radiation diffraction data collected at beamline F1 at Hasylab/DESY. The data collection was performed in low temperature using liquid N₂ for the measurement in 100K (F1). The data sets were collected on MAR165-CCD area detector. The XDS software was applied for integration of the images [1]. Spherical refinement was performed with SHELXL [2] and the obtained model was used as the input for aspherical atom multipole formalism [3] using the XD package program [4]. Results of model densities were analyzed quantitatively in terms of AIM theory [5] especially in the formation of hydrogen bonds.

The geometrical and topological analysis shows that the intramolecular N-H...O hydrogen bonds are of medium strength while the other intermolecular C-H...O bonds are rather weak. According to Rozas's approach [6], based on Laplacians of the electron density and the total energy density ($\nabla^2\rho(\mathbf{r}_{BCP})$ and $H\rho(\mathbf{r}_{BCP})$) a partially covalent character can be indicated only for one intramolecular hydrogen (N-H...O) bond in structure I. The energy of hydrogen bonds calculated due to the QTAIM theory points out the intramolecular hydrogen bonds to be of medium strength with partially covalent character in both examined structures.

It was found that a π -electron delocalization exists within the hydrogen bonded ring containing the conjugated system of single and double bonds. The π -bonding density within the chelate ring can be confirmed by bond lengths as well as high values of bonds ellipticity.

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Keywords: structure and charge-density analysis, hydrogen bonding, chromones