

is known that this additional interaction can enhance the polymerization activity [3]. The link between the metal center and the neutral donor atom influences the coordination geometry and makes the ligand system eminently flexible. According to the HSAB principle the interaction between the soft donor atom (as part of the ligand system) and the Lewis acidic/electrophilic metal center is unbalanced. However, detailed knowledge about the nature of the bond character is scarce. Recently obtained high resolution X-ray diffraction data for a previously investigated compound [5] will help to clarify the nature of the mismatched interactions between the soft S atoms within the ligand and the hard titanium center. These systems will enable us to investigate the interaction in detail. Our results of the electron density studies [6,7] studies will enable us to investigate the mismatched interactions in detail. This work was supported by DFG, priority program 1178, Experimental Charge Density as the Key to Understand Chemical Interactions.

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Keywords: charge density, intramolecular interactions, bisphenolato metal complexes

FA4-MS37-P12

Electronic structure of Ni(II) complex of Schiff base and (S)-alanine. Marek Fronc^a, Jozef Kozisek^a, Alexander Popkov^b, Wolfgang Scherer^c, ^aSlovak Technical University Bratislava, Slovakia, ^bUniversity of South Bohemia, Czech republic, ^cUniversity of Augsburg, Germany
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One of the approaches to explore the mechanism of transition metal-based catalysts is the study of adequate model systems which allow an extrapolation of the results to real catalytical systems.

Our interest in structural research of Ni(II) complexes of Schiff bases of (S)-N-(2-benzoylphenyl)-1-benzylpyrrolidine-2-carboxamide (BPB) and α -amino acids is driven by growing number of successful applications of these chiral synthons of α -amino acids to achieve the preparation of carbon-11 and fluorine-18 labelled radiodiagnostics for positron emission tomography (PET). [1] Furthermore, we are intrigued with the structural similarity of our benchmark complexes with another family of transition metal-based catalysts for asymmetric transformations. [2]

The aim of this work is to study the distribution of the electron density in the Ni(II) complex of Schiff base of (S)-N-pentamethylbenzylproline (2-benzoylphenyl)amide and (S)-alanine.

An electronic structure analysis was performed with XD software package. The results of a detailed topological

analysis of electron density on the amplification of enantiomeric excess of a chiral molecule will be discussed.

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Keywords: charge density, nickel, chiral synthon

FA4-MS37-P13

The application of UBDB to description of Zinc Fingers' electrostatic. Anna Goral, Paulina Dominiak
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The UBDB (University at Buffalo Databank) [1] contains aspheric atomic electron density fragments represented by more than 100 atom types, which correspond to all atoms found in proteins, according to their first and second neighbors. This approach allows for a quantitative representation of electron density distribution - different from point charge force fields - and for analysis of the electrostatic properties of macromolecules, as well as the refinement of (macromolecular) X-ray data. The Zinc Fingers from CCHH family were chosen as a biological model to present the electrostatic characterization of the protein-metal interactions. Firstly, the statistical analysis was performed to find the average geometry around zinc atom. Then, the geometry of a simple tetra-coordinated zinc complex was optimized using theoretical calculations, because of a lack of suitable small molecule X-ray data. Next, the electron density distribution of the examined system was calculated and a set of new atom types was determined. The electrostatic properties with the use of the extended UBDB will be verified against ab initio calculations.

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Keywords: charge density, proteins, metals

FA4-MS37-P14

Experimental charge density study and topological analysis for metal barbiturates. Marlena Gryl, Anna Krawczuk-Pantula, Katarzyna Stadnicka, *Faculty of Chemistry, Jagiellonian University Cracow, Poland*
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Experimental charge density and its topological properties provide a means for the evaluation of intermolecular interactions in the context of understanding structure-property relationship and controlling the self assembly of the molecular building blocks. Barbituric acid molecule seems to be a valuable component in designing of new materials possessing prospective properties i.e NLO properties [1,2,3]. Organic materials modified with inorganic components are interesting from the viewpoint of their outstanding properties as NLO materials i.e. high SHG response, appropriate mechanical and optical resistance. Recently we have discovered the usage of barbituric acid and selected inorganic metal salts to form polar structures such as cadmium barbiturate dihydrate (Iba2) or copper barbiturate trihydrate (Fdd2) [4]. Moreover we have

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

FA4-MS37-P15

Electronic Structure of Mixed Valence Cu(I)-Cu(II) Complex, $[\text{Cu}_3(\text{en})_2(\text{CN})_4(\text{H}_2\text{O})]$. 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: $[\text{Cu}(1);\text{N}(1),\text{N}(2),\text{N}(3),\text{C}(4)]$ and $[\text{Cu}(2);\text{C}(1),\text{C}(2),\text{C}(3),\text{N}(4)]$.

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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Keywords: charge density, copper, mixed-valence compounds

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 N_2 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 ($\nabla^2\rho(\mathbf{r}_{\text{BCP}})$ and $H\rho(\mathbf{r}_{\text{BCP}})$) 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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Acknowledgements: The research leading to these results has received funding from the European Community's Seventh Framework Programme (FP7/2007-2013) under grant agreement No 226716.

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