



[1] J. Zyss, I. Ledoux, A. Jutand & C. Amator. *Chem. Phys.*, 150 (1991) 117-123 [2] N.K.Hansen & P.Coppens, (1978).*Acta Cryst.*, A34, 909.

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FA4-MS37-P10

The electron density of isoindole derivatives from synchrotron diffraction data. Lilianna Chęcińska^a, Magdalena Malecka^a Agnieszka Rybarczyk-Pirek^a, Carsten Paulmann^{b,c}, Simon Grabowsky^d, Peter Luger^d
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The isoindolin-1-ones are the important structural units found in natural products, biologically active substances and synthetic intermediates [1], [2]. Here, the electron density of two isoindole derivatives is considered: 3-hydroxy-2-phenyl-2,3-dihydro-isoindol-1-one (I) and 5-hydroxy-6-phenyl-5,6-dihydro-pyrrolo[3,4-*b*]pyridin-7-one (II).

The high-resolution synchrotron-diffraction data sets were collected at beamline F1 at Hasylab/DESY (Hamburg, Germany). The *XDS* [3] was used for an integration of frames and data reduction. Initial spherical refinements were performed with *SHELXL97* [4] providing starting values for subsequent aspherical-atom least-squares refinements with *XDLSM* of *XD2006* program package [5].

Two analyzed molecular structures of I/II consist of isoindol-1-one/aza-isoindol-1-one moiety substituted by phenyl and hydroxyl groups at position 2 and 3, respectively. The geometry of the investigated molecules is similar but not

identical, but their arrangement in the crystal structures is different.

In I, the molecules are linked by intermolecular hydrogen bond O-H...O ($\frac{1}{2}-x, \frac{1}{2}+y, z$) forming an infinite chain along [010] direction. In the aza-isoindole derivative (II) additional nitrogen atom is an accepting centre of hydrogen bonding, instead of oxygen atom, and O-H...N ($x, \frac{1}{2}-y, \frac{1}{2}+z$) is observed. This interaction generates an infinite chain along [001] direction.

The qualitative and quantitative analysis of the electron density distribution within isoindole moieties and hydrogen bonding areas will be presented in the poster.

[1] Neumann H., Strobing D., Lalk M., Hubner S., Spannenberg A., Lindequist U., Beller M., *Org. Biomol. Chem.* 2006, 4, 1365. [2] Sun C., Xu B., *J. Org. Chem.* 73, 2008, 7361 and references cited therein. [3] Kabsch W., *J. Appl. Cryst.* 1993, 26, 795. [4] Sheldrick G.M., *Acta Cryst.* 2008, A64, 112. [5] Volkov A., Macchi P., Farrugia L.J., Gatti C., Mallinson P.R., Richter T., Koritsanszky T., 2006, *XD2006*: A computer program package for multipole refinement, topological analysis of charge densities and evaluation of intermolecular energies from experimental or theoretical structure factors.

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Keywords: structure and charge-density analysis, synchrotron X-ray diffraction, isoindole derivatives

FA4-MS37-P11

Mismatched interactions in bis(phenolato) metal complexes Thomas S. Dols^{a,b}, Thomas P. Spaniol^a, Jun Okuda^a, Christian W. Lehmann^b, ^a*Institut für anorganische Chemie, RWTH Aachen University, Germany*, ^b*MPI für Kohlenforschung, Mülheim, Germany*
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Three-dimensional crystal structures have become an indispensable tool in modern catalyst research. To improve the product properties, the structural changes of homogeneous catalysts and their precatalysts are correlated with their impact on polymerization. We are investigating transition metal complexes with bridged bisphenolato ligands that are used in olefin-polymerization. The molecular structure of the ligand has a strong influence on the stereochemistry of the resulting polymer[1,2]. For this reason, the bis(phenolate) ligands have been tuned by different substituents on the aromatic rings as well as by modifying the bridging unit. S atoms as part of the bridge can improve the catalytic activity, obviously as a result of hemilabile interactions between the soft donor S atom and the hard metal center [3].

In several S-C-C-S-bridged bis(phenolato)titanium complexes, the M...S interactions lead to a stereorigid O,S,S,O-tetradentate coordination in solution [4]. Such a system has made it possible to polymerize styrene in homogeneous phase to give isotactic polystyrene for the first time [1]. The results prove the high conformational stability of the metal complexes under the conditions of polymerization.

The focus of our investigations is on metal complexes where, according to the HSAB principle, the hard metal centers are interacting with the sulfur atom of the bisphenolato ligand. It

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.

[1] Capacchione, C., Proto, A., Ebeling, H., Mülhaupt, R., Möller, K., Manivannan, R., Spaniol, T. P., Okuda, J., *J. Mol. Catal. A*, 2004, 213, 137–140. [2] Beckerle, K., Manivannan, R., Lian, B., Meppelder, G.-J. M., Raabe, G., Spaniol, T. P., Ebeling, H., Pelascini, F., Mülhaupt, R., Okuda, J., *Angew. Chem. Int. Ed.* 2007, 46, 4790–4793. [3] Froese, R. D. J., Musaev, D. G., Morokuma, K., *Organometallics*, 1999, 18, 373–379. [4] Capacchione, C., Manivannan, R., Barone, M., Beckerle, K., Centore, R. Oliva, L., Proto, A., Tuzi, A. Spaniol, T. P., Okuda, J., *Organometallics*, 2005, 24, 2971–2982. [5] Dols, T. S., Spaniol, T. P., Okuda, J. *Acta Crystallogr. Sect. C*, 2009, m443–m446. [6] Volkov A., Macchi, P., Farrugia L. J., Gatti C., Mallison P. R., Richter T., Koritsanszky T., *XD2006*. University of New York at Buffalo, USA 2006. [7] Hansen N. K., Coppens P., *Acta Crystallogr. Sect. A*, 1978, 34, 909.

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.

[1] Krasikova R. N., O. F. Kuznetsova O. F., Fedorova O. S., Maleev V. I., Saveleva T. F., Belokon Y. N., *Bioorganic & Medicinal Chemistry*, 2008, 16, 4994 [2] Belokon Y. N., Fuentes J., North M., Steed J. W., *Tetrahedron*, 2004, 60, 3191

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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.

[1] Dominiak PM, Volkov A, Li X, Messerschmidt M, Coppens P: *Journal of Chemical Theory and Computation* 2007, 3:232-247.

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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