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

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Electronic structure of Ni(II) complex of Schiff base and (S)-alanine. Marek Fronc[a], Jozef Kozisek[a], Alexander Popkov[b], Wolfgang Scherer[c], [a]*Slovak Technical University Bratislava, Slovakia,* [b]*University of South Bohemia, Czech republic,* [c]*University 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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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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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 possesing 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 responce, 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