

transferability achievable with the use of different methods of molecular density partitioning.

Molecular densities (MDs) were calculated for natural amino acids and selected di- and tripeptides in geometries as observed in crystal structures. The MDs were obtained through Fourier space fitting of pseudoatom model to the electron densities computed *ab initio* at B3LYP/6-31G\*\* level. Such procedure was selected in order to be compatible with the idea of building a pseudoatom database [1-3] pursued in the charge density crystallography. Atomic multipole moments expressed in local coordination system were calculated (a) directly from pseudoatoms, (b) from atomic densities computed via stockholder partitioning and (c) from atomic basins derived via topological analysis. As a measure of transferability, standard deviations from averaging over multipole moment components of atoms that are considered equal in their chemical environments were calculated.

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**Keywords:** multipole moments, amino acids, transferability

#### FA4-MS37-P21

##### Polyhalogenated bipyridines: halogen interactions and building blocks.

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4,4'-Bipyridine skeleton represents an excellent building block in supramolecular chemistry [1] and biology [2] and is an important intermediate in the synthesis of viologens [3]. Recently, we developed a method to produce new polyhalogenated 4,4'-bipyridines [4], which can then be functionalized, potentially leading to new materials. Beside this use in synthesis, these halogenated molecules are also attractive to study the so-called halogen interactions. In the investigated compounds, which contain Cl, Br and I atoms at various positions on the pyridine rings, type-II halogen...halogen interactions [5] appear predominantly, along with halogen...Lewis base interactions. Interestingly, depending on the presence of one, two or three different halogen atoms on the same molecule, homo or hetero halogen...halogen interactions are observed in the crystal structures. Also, for substitutions at fixed positions on the pyridine ring, the nature of the halogen atom influences the crystal packing, leading to either isostructures or completely different packing schemes. These characteristics are also analyzed on the basis of intermolecular interaction energies by using the Pixel program [6]. Finally, new functionalized bipyridines will be presented together with recently obtained metal complexes, where very short M...halogen (M = Ag, halogen = Cl, Br) interatomic distances are obtained. Used for the building of metal organic frameworks, these M...halogen interactions show their influence on the crystal packing, tuning the porosity of the material.

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#### FA4-MS37-P22

##### Invariom refinement of two different modifications

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B. Anderson and D. Hodgkin [1] reported the first (but incomplete) monoclinic structure of thiostrepton exactly 40 years ago in 1970. The thiazole-containing antibiotic first isolated from *streptomyces azureus* exhibits activity against Gram-positive bacteria and *plasmodium falciparum*, the causal agent of malaria. Mechanistically, Thiostrepton binds to the GTPase centre of the large subunit 23s RNA [2]. Activity against breast-cancer cells through targeting the transcription factor forkhead box M1 has also been reported. Here the antibiotic selectively induces cell-cycle arrest and cell death in breast cancer cells through down-regulating FOXM1 expression [3]. We have reproduced the original monoclinic and the tetragonal crystal structure [4] to illustrate the benefits of high resolution in protein crystallography: it was e.g. possible to complete the originally published structural model of monoclinic thiostrepton with a missing flexible side chain. Complete and redundant Bragg data to 0.80 Å resolution measured with a CuK $\alpha$  rotating anode at 100K of the monoclinic form and 100 K / 5 K synchrotron data of the tetragonal form were evaluated with the independent atom model (IAM) and the non-spherical scattering factors of the invariom database [5], [6] which is based on the Hansen-Coppens multipole model [7]. Single-crystal diffraction data evaluated with invarioms provide not only detailed and accurate molecular geometries but also information on the electron-density distribution and on derived properties. With a view to biological and medical functionality of thiostrepton an analysis of the electrostatic potential and the molecular dipole moment is especially relevant, and both will be reported.

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