

Poster Sessions

atoms, *i.e.* adenine- thymine (AT), guanine- cytosine (GC)- hydrogen bonding, guanine- adenine (GA)- stacking, and a group of charged species. The energetic tendencies are very well preserved, however, the energy values differ between the two methods of about 5 kcal/mol on average.

The new version of databank has also been applied to the refinement of selected nucleic acid bases and their modifications as the source of aspherical atomic scattering factors (transferred aspherical atom refinement, TAAM). It significantly improved the final geometries of molecules in the crystal, R factors and ADPs. Several other calculations were performed for the aforementioned solved structures *i.e.* periodic calculations in CRYSTAL06 [7], energy calculations with PIXEL package [8]. The results were compared to the energy values obtained with the aid of a number of force fields in order to get an idea of the accuracy and limits of all the methods [9].

[1] P.M. Dominiak, A. Volkov, X. Li, M. Messerschmidt, P. Coppens, *J. Chem. Theory Comput.*, **2007**, 3, 232-247. [2] F.H. Allen, I. J. Bruno *Acta Cryst.*, **2010**, B66, 380-386. [3] *In preparation*. [4] A. Volkov, T. Koritsanszky, P. Coppens, *Chemical Physics Letters*, **2004**, 391, 170-175. [5] A. Volkov, H.F. King, P. Coppens, *J. Chem. Theory Comput.* **2006**, 2, 81-89. [6] Ż. Czyżnikowski, R. Zaleśny, P. Lipkowski, R.W. Góra, K.N. Jarzemska, P.M. Dominiak, J. Leszczyński, *J. Phys. Chem. B*, **2010**, 114, 9629-9644. [7] R. Dovesi, V.R. Saunders, C. Roetti, R. Orlando, C. M. Zicovich-Wilson, F. Pascale, B. Civalleri, K. Doll, N.M. Harrison, I.J. Bush, Ph. D'Arco, M. Llunell, *CRYSTAL06 2008 1.0 - v1_0_2 User's Manual*. [8] A. Gavezzotti *OPtX*, **2003**. [9] R.S. Paton, J.M. Goodman, *J. Chem. Inf. Model.*, **2009**, 49, 944-955.

Keywords: nucleic acids, aspherical pseudoatoms, electrostatic interaction energy

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Comparison of electrostatic energies between selected DNA-ZnF complexes

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Zinc Fingers (ZnF) are small protein domains widely present mostly in *Eucaryota*. Among other structural subgroups of ZnF, the most relevant is C2H2-like family, with zinc ion tetrahedrally coordinated by two cysteine and two histidine residues. Such ZnF domain consists of 24 aminoacids folded into two anti-parallel beta-strands and an alpha-helix and recognizes DNA via hydrogen bonding with outer side of helix. ZnF can be combined with an effector domain e.g. transcriptional activator, transcriptional repressor, methylation domain or nuclease. Especially ZFNs have the greatest role in molecular biology and medicine: their ability to recognize (ZnF) and cut DNA sequence (nuclease) is widely used in gene therapy.

Several structures of ZnF interacting with DNA were deposited in PDB databank. The structures with the best resolution were chosen for further studies and the UBDB databank [1] was extended with a set of new atom types.

The theoretical approach applied in this study is based on transferability of electron density parameters between atoms in chemically equivalent environments. It allows to reconstruct the unperturbed, static electron density of larger systems on the basis of experimentally obtained geometry. The electrostatic energy of interaction was calculated with EPMM method developed by Volkov [2] including Exact Potential for overlapping charge distributions and Buckingham-type multipole approximation for non-overlapping charge distributions. The quantitative characterization of particular electrostatic interactions for selected structures of interest will be presented and discussed.

[1] P.M. Dominiak, A. Volkov, X. Li, M. Messerschmidt, P. Coppens, *J. Chem. Theory Comput.* **2007**, 3, 232-247. [2] A. Volkov et al. *Chem. Phys. Lett.* **2004**, 391, 170; *J. Chem. Theory Comput.* **2006**, 2, 81

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Experimental charge density study and bond characterization on [Cu(I)(4-pytH)₂](HC₄O₄)

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The title compound, [Cu(I)(4-pytH)₂](HC₄O₄) (4-pyt = pyridine-4-thiolate), can be obtained by the in-situ generation of 4-pytH ligand obtained from the 4-dpds (4,4'-dipyridyldisulfide) precursor through the reductive cleavage of the disulfide bond of 4-dpds under solvothermal conditions. The structural analysis reveals that the tetrahedral Cu(I) ion is bonded to four sulfur atoms of the 4-Hpyt ligands forming a 1D cationic chain-like framework, [Cu(I)(4-pytH)₂]⁺, and further extended to a pseudo-3D supramolecular architecture via the intermolecular π - π interactions and the hydrogen bonds between cation and monohydrogensulfate. The Cu(I) ion is coordinated to sulfur atoms with four different Cu-S distances, 2.2458(2), 2.2793(1), 2.2983(1) and 2.8023(2) Å. A HC₄O₄⁻ dimer is formed through two strong O-H...O hydrogen bonds with the O...O distance of 2.500 Å. The experimental charge density distribution of [Cu(I)(4-pytH)₂](HC₄O₄) has been investigated in terms of a pseudo-atomic multipolar expansion (Hansen-Coppens' multipole model) using high resolution single-crystal X-ray diffraction data at 100(2) K with $\sin\theta/\lambda$ up to 1.0 and synchrotron data at 10(2) K with $\sin\theta/\lambda$ up to 1.3. The electron density will be presented in terms of deformation density as well as the Laplacian distribution. Bond characterizations are expressed in terms of topological properties associated with the bond critical points including the dative covalent Cu-S bonds and typical covalent character on N-N, N-C and C-C bonds. The detail comparison between in house and synchrotron data sets will be performed and the topological properties of those intra- and inter-molecule interactions will also be discussed in details.

Keywords: Cationic chain, Charge density analysis, Bond characterization

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MoProViewer: a molecular viewer for the MoPro charge density analysis program

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The MoPro program suite [1] is a crystal structure and charge density refinement package which includes two main modules: the MoPro least-squares refinement program and VMoPro, a tool dedicated to the computation of properties derived from the electron density. MoPro already possesses its own graphical user interface, but VMoPro was still a text-based program.