MS18-04 **Electronic structure of Tetrakis(μ_2-Acetato)-diaqua-di-chromium (II) complex, [$C_8H_{16}Cr_2O_{10}$].** Jozef Kozisek, Peter Herich, Marek Fronc and Marian Gall *Slovak University of Technology in Bratislava, Faculty of Chemical and Food Technology, Radlinskeho 9, 812 37 Bratislava 1, Slovak Republic*
E-mail: jozef.kozisek@stuba.sk

Experimental electronic structure of *3d*-complexes is still a challenge, particularly in the sense of determination the *d*-orbital population. In order to compare very accurate point-detector Picker four-circle diffractometer data [1] with the Oxford Diffraction CCD GEMINI R ones, a good quality single crystal of Tetrakis(μ_2-Acetato)-diaqua-di-chromium (II) complex was prepared. The GEMINI R data at 100K will be used for electronic structure study. Data collection strategy was as follows: 70 runs, 154487 diffractions, resolution till 0.41 $Å^{-1}$. Data reduction was done by CrysAlis171.35.19 and an average redundancy of 13.8 gives R_{int} 0.022 and R(σ) 0.003. The final refinement of crystal structure data at 100 K with a resolution of d = 0.41 $Å^{-1}$ by SHELXL gives a R1-factor of 0.0158 for 10194 Fo > 4sig(Fo) which undoubtedly indicate the correctness of the model. After the multipole refinement R-values were: R(F)=0.0229 and Rall(F)= 0.0267 for all 132180 diffractions. The topological analysis was performed using XD package. Theoretical calculation was done using CRYSTAL06 and TOPOND software. Comparison of experimental and theoretical results will be disscussed.

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MS18-05 **Topological analysis of hydrogen-bonds and weak interactions in protein helices.** Dorothee Liebschner,[a] Christian Jelsch,[b] Enrique Espinosa,[b] Claude Lecomte,[b] Eric Chabričre[c] and Benoît Guillot,[b] [a]*Synchrotron Radiation Research Section, MCL, National Cancer Institute, ANL, Argonne, USA,* [b]*Résonance Magnétique et Modélisations, CNRS UMR 7036, Nancy-Université, Nancy, France,* [c]*Unité de Recherche sur les Maladies Infectieuses et Tropicales Emergentes, CNRS UMR 6236, Université de la Méditerranée, Marseille, France*
E-mail: dliebschner@anl.gov

Helices represent the most abundant secondary structure motif in proteins and are often involved in various functional roles. They are stabilized by a network of hydrogen bonds between main chain carbonyl and amide groups. Several surveys scrutinized these hydrogen bonds, mostly based on the geometry of the interaction [1-3]. Alternatively, the topological analysis of the electron density provides a powerful technique to investigate these interactions. For the first time, transferred experimental charge density parameters from the ELMAM database [4] were used to carry out a topological analysis of the electron density in protein helices [5]. New geometrical parameters (involving the position of the oxygen lone pairs) have been defined to characterize hydrogen bonds. Bonding contacts between the amide N and carbonyl O atoms (N···O) of helices (Figure 1), poorly addressed in the literature so far, were characterized from topological, geometrical and local energetic analyses. Particularly, a geometrical criterion, based on the donor-acceptor N-H···O angle, has been elaborated allowing for the discrimination between hydrogen bonds and N···O contacts. Furthermore, hydrogen bonds in helices show the same topological features as those observed in intermolecular regions of small molecules and N···O contacts exhibit the same topological characteristics as weak hydrogen bonds.

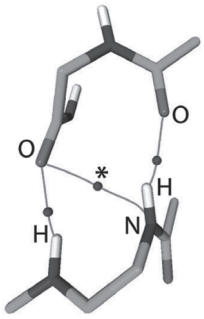

Figure 1: Hydrogen bonds and N···O contact in a helix fragment

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