Session Vb, Wednesday, June 24

L25

A SELF-ASSEMBLY OF COPPER(II) CARBOXYLATE THROUGH H-BONDS INTO SUPRAMOLECULAR STRUCTURE AND SUPRAMOLECULAR NETWORKS

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Coordination compounds connecting through hydrogen bonds are used as building block for construction of supramolecular networks. Some copper(II) carboxylate complexes have shown that the intermolecular H-bonds can modified their magnetic properties. We have recently published mononucler molecular complex [1] binuclear molecular complex [2] and more coordination polymers [3, 4] which exhibit similar magnetic properties. Very similar magnetic properties of mononuclear, binuclear as well as polymeric complexes could be explained by the presence of very similar H-bond supramolecular synthons that are pathway for antiferromagnetic interactions.

The lecture will present new supramolecular dimers $[Cu(3\text{-}NO_2bz)_2(ina)(H_2O)_2].H_2O$, $[Cu(3\text{-}NO_2bz)_2(ina)(H_2O)_2].2H_2O$, $[Cu(3,5\text{-}Cl_2bz)_2(H_2O)_3]$, $[Cu(3\text{-}Brbz)_2(dena)(H_2O)_2]$, $[Cu(3\text{-}Brbz)_2(dena)(H_2O)_2]$ (Figure 1), ($3\text{-}NO_2bz$ = 3-bromobenzoate, 3-Brbz = 3-bromobenzoate, $3,5\text{-}Cl_2bz$ = 3,5-dichlorobenzoate, dena = *N*,*N*-diethylnicotinamide, ina = isonicotinamide)

and series of 1D-coordination polymers $[Cu(3\text{-}Clbz)_2(\ \text{-dena})(H_2O)]_n$ (Figure 2), $[Cu(4\text{-}Clbz)_2(\ \text{-dena})(H_2O)]_n$, $[Cu(3,5\text{-}Cl_2bz)_2(\ \text{-dena})(H_2O)]_n$ (3-Clbz = 3-chlorobenzoate, 4-Clbz = 4-chlorobenzoate, $3,5\text{-}Cl_2bz$ = 3,5-dichlorobenzoate, and dena as bridging ligand) with similar system of hydrogen bonds and properties. Electronic structure from multipole refinement of polymeric complex $[Cu(4\text{-}Clbz)_2(\ \text{-dena})(H_2O)]_n$ will be also presented.

The hydrogen bonds described by $R_2^2(10)$ and $R_2^2(12)$ supramolecular synthons, formed by coordinated water molecule and two carboxylic group on each Cu^{2+} ions could create supramolecular dimer of two mononuclear complex molecules or 2D-supramolecular layers of 1D-coordination polymers.

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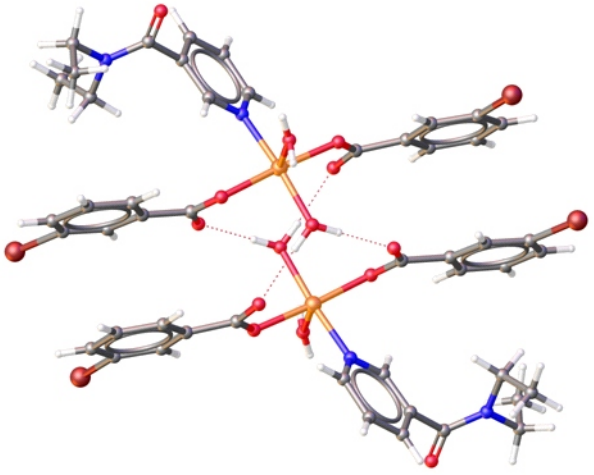

Figure 1 Structure of supramolecular dimmer of $[Cu(3\text{-}Brbz)_2(dena)(H_2O)_2]$.

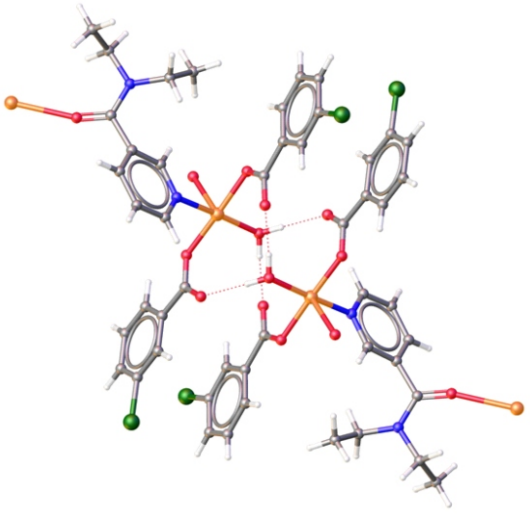

Figure 2. Structure of polymeric complex $[Cu(3\text{-}Clbz)_2(\ \text{-dena})(H_2O)]_n$.

L26

ISOPOLYOXOMETALATE FUNCTIONALISATION FACILITATED BY TRANSITION METAL COMPLEXES

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Polyoxometalates have a long record of interesting structures [1] and potentially exploitable properties in the area of nanotechnology, catalysis, magnetic properties [2]. Incorporation of paramagnetic, photochemically or photophysically active ions make them valuable components of materials. Antitumoral, antiviral and antibiotic properties of several POMs and specific POM–protein interactions were also studied [3].

In contrast with the relative high stability of hetero-POMs, the chemistry of isopolyoxometalates is more challenging. Vast majority of iso-POMs exists only in narrow pH and *c*(M) regions, often with the POM cores allowing to obtain several protonation modes. In solutions, there are complex protolytic (and eventually, redox) equilibria with many species present in reaction mixtures. The crystallisation of often marginally soluble products can be also tricky.

We studied several decavanadate-based systems (Fig. 1) based on transition metal ions (Cu^{II} [5, 8, 9], Mn^{II} [6, 7], Zn^{II} [7], Co^{II}) and proposed ligands (-alanine *bAla* [5, 7], 2-(2-hydroxyethyl)pyridine *hep* [6, 9], glycine *gly* [8], 2-(aminomethyl)pyridine *amp* [9]). Initially, we obtained one of the first compounds containing decavanadate as a bridging ligand (and first 1D coordination polymer), $(NH_4)_2[Cu_2(bAla)_4(V_{10}O_{28})]\cdot 10H_2O$ (**1**, Fig. 2). Coordination of the paddlewheel Cu(II) complex cation to the centrosymmetrically arranged G sites of the decavanadate core is assisted by strong hydrogen bonds. The attempts to prepare similar decavanadate complexes with *bAla* ligand lead to the preparation of the noncoordinated decavanadates

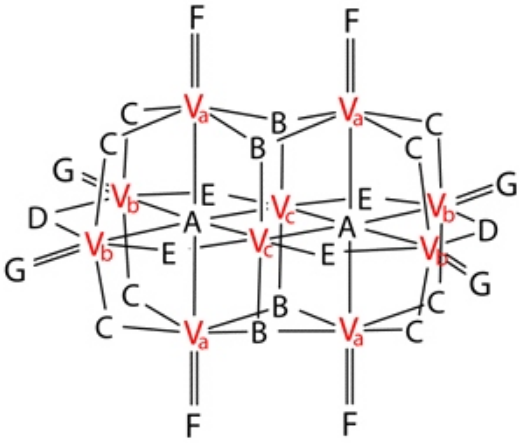

Figure 1. The scheme of the decavanadate anion with idealized D_{2h} point group geometry. A–G denote crystallographically non-equivalent O atoms and V_a–V_c denote crystallographically non-equivalent V atoms (based on [4]).

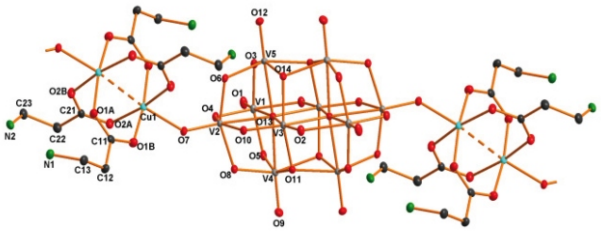

Figure 2. The 1D chain motif in the structure of **1**.

$(NH_4)_2[M(H_2O)_5(NH_3CH_2CH_2COO)]_2V_{10}O_{28}\cdot nH_2O$ (M = Zn^{II}, n = 4; M = Mn^{II}, n = 2). Although both containing $[M(H_2O)_5(NH_3CH_2CH_2COO)]^{2+}$ cation, these cations are structurally different.

In attempt to prepare *hep* based complexes, in the system with Mn^{II}, *hep* is acting only as a counterion *hep*H^+ to the pendant complex with the $[Mn(H_2O)_5]^{2+}$ complex unit coordinated to the centrosymmetrically arranged F sites of the bridging decavanadate anion in the $(hepH)_2[\{Mn(H_2O)_5\}_2V_{10}O_{28}]\cdot 4H_2O$ (**2**, Fig. 3). Complex anions forms the supramolecular chains *via* the hydrogen bonding network consisting of aqua ligands.

From the reaction system containing Cu^{II} and *hep*, the complex with bridging decavanadate ligand coordinated at the centrosymmetricaly arranged C sites by the two $[Cu(H_2O)_2(O,N\text{-}hep)]^{2+}$ units,
$(hepH^+)_2[\{Cu(H_2O)_2(O,N\text{-}hep)\}_2V_{10}O_{28}]\cdot 6H_2O$ (**3**, Fig. 4), was prepared.

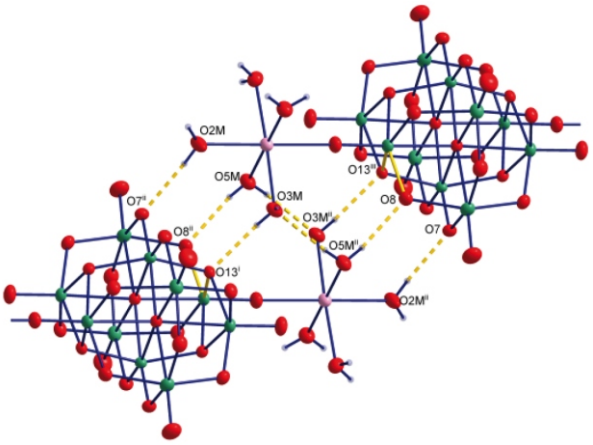

Figure 3. Supramolecular anionic chains in the structure of **2**.

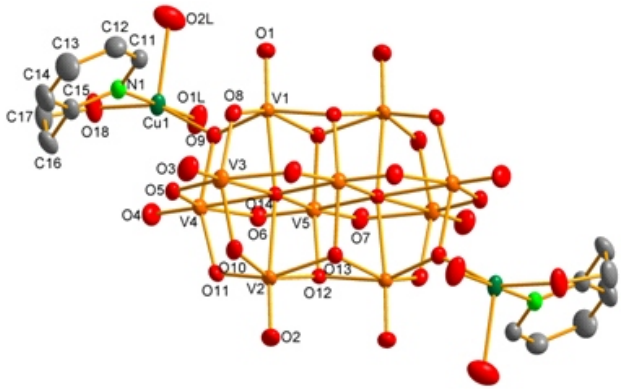

Figure 4. The anionic unit of **3.**

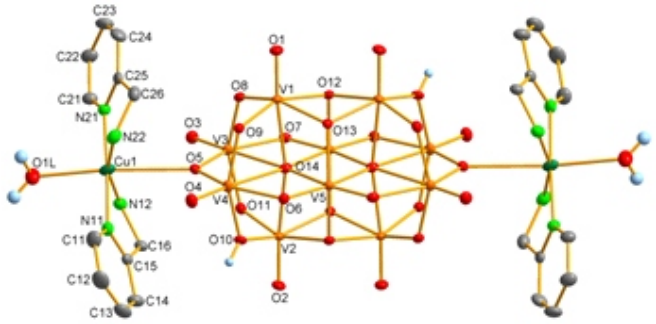

Figure 5. The structure of the neutral complex **4.**

To illustrate coordination possibilities of the decavanadate core, from the same system with the *amp* used instead of *hep*, the $[\{Cu(amp)_2(H_2O)\}_2H_2V_{10}O_{28}]\cdot 4H_2O$ (**4**, Fig. 5) was prepared. If in the **3** we had shortest (V–)O–*M* bond ever found (1.9563(16) Å), in the **4** it is the longest one (2.665(2) Å). It is due to coordination of the cationic unit to the centrosymmetrically arranged D sites of the anion, which are hard to access.

From the system with Cu(II) and glycine, $(NH_4)_2[Cu_2(H_2O)_4(gly)_2\ (gly^-)_2]H_2V_{10}O_{28}\cdot 6H_2O$ was prepared. The compound contains dinuclear copper complex with bridging water ligands along the dihydrogendecavanadate anion. The interesting feature of the cation is that it contains both O-coordinated glycine a N,O-coordinated glycinato ligands.

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L27

"FINE STRUCTURE" OF DOUBLE HELICAL DNA

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Double helical DNA became an emblematic symbol of fast-growing field of molecular biology soon after formulation of its architecture. The antiparallel double helix with the ladder of hydrogen-bonded bases four of which are able to code for all living creatures on Earth is not only esthetically appealing and intellectually satisfying but also conceptually very simple. Deceivingly simple, as has become evident in the later years when several new and unexpected conformations of DNA emerged. An important stimulus for renewed interest in detailed investigation of DNA conformations can be expected in connection with the need to understand fine-tuning of storing and decoding of genetic information, sequence preferences for packing into histones, conformational behavior of regions with repetitive sequences, and structural implications of DNA modifications such as cytosine or adenine methylation crucial in epigenetics.

In our effort to understand structural details of double helical architecture, we have taken advantage of vast volume of information accumulated by crystallographers. Based on the available crystal data, we classified conformations of dinucleotide steps into about twenty classes (Svozil *et al*. ***Nucleic Acids Research* 36**, 3690 (2008)), developed technique of automatic assignment of these step conformational classes to any DNA structure (Čech *et al*. ***BMC Bioinformatics* 14**, 205 (2013)), and recently improved both these steps significantly (Černý *et al*. to be published (2015)). In the talk, we present our latest results, in which we correlate conformation classes of two dinucleotides forming the base-paired counterparts of the DNA duplex. We analyze separately the correlations for dinucleotides joined in the duplex by Watson-Crick pairing of both pairs and dinucleotides in which one or both pairs are non-canonical. The crystal data provided enough information to analyze sequence dependencies for the Watson-Crick paired steps; the non-canonical parts of duplexes can be discussed only qualitatively. Some of the more interesting results will be discussed in the talk. Even the preliminary results demonstrate that the classes of dinucleotide steps represent a powerful tool to describe details of the double helical architecture. The main conclusion of our research is that combination of correlations between the dinucleotide classes and base pair types provides sufficient structural characterization of the related step.

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L28

LUCOAMYLASES FROM *SACCHAROMYCOPSIS FIBULIGERA* - STRUCTURE AND STABILITY

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Two glucoamylases Glu and Gla produced by variant strains of yeast *Saccharomycopsis fibuligera*, HUT 7212 and KZ, respectively. The mature enzymes consist of 492 amino acid residues. An alignment of their amino acid sequences revealed a high homology, with seven amino acid residue alterations causing differences in the specific activity and thermal stability between both enzymes. Previous biochemical tests indicated that a significant part of both, Glu and Gla, renewed their catalytic activity after thermal denaturation. Glucoamylase Gla, in contrast with glucoamylase Glu, has lower catalytic activity but higher stability and better ability to re-nature [1].

Previous stability studies are complemented now by the study of thermal denaturation and determination of melting point using a method of dynamic light scattering. The method is based on the measurement of light scattered on the protein particles in the solution and determination of particle size. Melting point was defined as the temperature at which the size of the molecules rapidly increased due to thermal unfolding. DLS measurements revealed different behaviour of Gla and Glu enzymes during thermal denaturation.

Up to now, only tertiary structure of glucoamylase Glu in the complex with its inhibitors acarbose (PDB code 2F6D) or TRIS was determined (PDB code 1AYX, 2FBA) [2, 3]. In spite of the fact, that Gla and Glu are very similar, structure determination of glucoamylase Gla was not successful for a long time due to crystal twinning and/or low crystal quality. Finally, after further optimization of crystallization conditions, a diffraction quality crystal of Gla was obtained. A complete data set to 1.77Å resolution was collected using synchrotron radiation at the X-13 beamline

at EMBL, DORIS storage ring, DESY, Hamburg. The crystal was monoclinic with $P2_1$ space group and unit cell dimensions a = 66.5, b = 81.5, c = 83.4 Å, ß = 109.94 °. There are two protein molecules in the asymmetric unit. For comparison, crystals of Glu prepared at very similar conditions, were orthorhombic with $P2_12_12_1$ space group, and only one protein molecule in the asymmetric unit. The two molecules in Gla structure are arranged in head to tail manner with active sites on the opposite sides. Five of seven altered amino acid residues are located on the surface of the molecule and participate also in intermolecular contact formation. Intermolecular contacts between A and B molecule in the asymmetric unit as well as crystal contacts are analysed and compared with those in Glu structure. As expected, the presented tertiary structure of glucoamylase Gla is very close to that of Glu, however, the small changes on the molecular surface can be used for explanation of different physico-chemical properties of the two enzymes.

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L29

ACTINOPHAGE ENDOLYSINS: BIOINFORMATIC ANALYSIS OF DOMAINS AND THEIR INTERACTIONS WITH SUBSTRATE

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Phage endolysins, the specific peptidoglycan hydrolases, have antimicrobial properties while bacterial resistance against them is excluded. Consequently, they could become a replacement for antibiotics against multi-drug resistant bacteria. Bioinformatics and proteomics studies are likely to lead to new opportunities for domain swapping, construction of chimeras and the production of specifically engineered tailor-made endolysins.

The aim of this work was (i) to study their presence within the actinophage genomes available in sequence databases, (ii) to analyse endolysin sequence organisations, and (iii) to model the protein-substrate interactions of these enzymes with peptidoglycan, by *in silico* methods.

Based on results of *in silico* analysis, in the set of studied sequences was confirmed modular structure of actinophage endolysins. There were predicted conserved domains with catalytic properties (Ami2, Ami6, PGRP and NlpC / P60), and those with binding activity, namely LysM, PG_biding binding_1. Within the domain with unknown function, NlpC / P60, was identified the same amino acid residues in the active site as in CHAP domain. Thus this domain may also be responsible for the amidase activity. Evolution analysis of obtained endolysin sequences revealed in recognition of clearly defined clusters depending on catalytic domains presence. The study of protein-substrate interactions required tertiary models of all here identified endolysins, that lead us to prediction of catalytic residues and requisite residues for reliable peptidoglycan hydrolysing activity.

The results obtained in this work will be used to subsequent preparation of recombinant, mutant and chimeric endolysins with enhanced antibacterial spectrum.

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L30

ENGINEERING OF ACCESS TUNNEL IN HALOALKANE DEHALOGENASE TO MINIMISE STABILITY-FUNCTION TRADE-OFF

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Haloalkane dehalogenases (HLDs, EC 3.8.1.5) are bacterial enzymes with / -hydrolase fold, which catalyse hydrolytic conversion of a broad range of halogenated aliphatic hydrocarbons into three reaction products: an alcohol, a halide anion and a proton. HLDs catalyse the reactions of great environmental and biotechnological significance with potential application in bioremediation, biosensing, decontamination of warfare agents, synthesis of optically pure compounds, cellular imaging and protein tagging [1]. However, their use in these applications is limited by their low stability and activity under the harsh conditions. Recently constructed variant of haloalkane dehalogenase DhaA exhibited 4000-fold improved kinetic stability in 40 % (v/v) DMSO, enhanced thermostability by 16.4 °C, but 100-fold lower catalytic activity with 1,2-dibromoethane in pure buffer compared to the wild type enzyme. Enzyme stabilisation was achieved by introduction of four bulkier and mostly hydrophobic residues into the enzyme access tunnel. Introduced residues improved a contact with other residues of the access tunnel, enhanced packing of hydrophobic core and prevented entry of DMSO into the active-site cavity [2].

Herein presented study aimed to improve catalytic activity of the highly stable DhaA in buffer, with minimum loss of its stability. Systematic mutagenesis of two of the four originally modified tunnel residues (F176 and V172) resulted in a single point variant F176G possessing 32- and 10-times improved catalytic activity in buffer and in 40 % (v/v) DMSO, respectively. Thermostability of the mutant was lowered by 4 °C only. Moreover, the newly evolved variant exhibited enhanced activity towards 26 out of 30 tested halogenated compounds similarly to wild-type enzyme. Structural analysis and molecular dynamics revealed that newly introduced mutation F176G reopened previously closed tunnel in stable DhaA and increase the mobility of the two -helices lining the tunnel, thus restoring the enzyme activity, while remaining tunnel mutations maintained its stability. Fine-tuning of amino acid residues lining the access tunnels thus represents generally-applicable strategy for minimisation of stability-function trade-off of enzymes with buried active sites [3].

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L31

STRUCTURE-FUNCTIONAL STUDIES OF HALOALKANE DEHALOGENASES

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Haloalkane dehalogenases (EC 3.8.1.5) are bacterial enzymes cleaving a carbon-halogen bond by a hydrolytic mechanism in a broad range of halogenated aliphatic compounds [1]. The enzymes can be potentially applied in bioremediation, biosensing, biosynthesis, cellular imaging and protein immobilization [2]. Structurally haloalkane dehalogenases belong to the /ß-hydrolase superfamily with two domain organization: an /ß-hydrolase core domain and -helical cap domain, which lies on the top of the core domain. Active site residues are located in a hydrophobic cavity at the interface between the two domains and are connected to the protein surface by several tunnels. Nowadays more than 20 proteins and their mutant variants from haloalkane dehalogenases family are systematically studied. The main target is focused on research of proteins such as DhaA from *Rhodococcus rhodochrous* NCIMB 13064, DbeA of *Bradyrhizobium elkanii* USDA94, LinB of *Sphingobium japonicum* UT26 or noval haloalkane dehalogenases DpcA from *Psychrobacter cryohalolentis* K5 and DmxA from *Marynobacter sp.* ELB 17, etc.

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16th International Conference on the Crystallization of Biological Macromolecules
se uskuteční od 2. 7. do 8. 7. 2016 v hotelu Pyramida v Praze. Jedná se o již 16. konferenci o krystalizaci biologických makromolekul. Konference je pořádána každé dva roky. Kromě Krystalografické společnosti jsou pořadateli Mezinárodní organizace biologické krystalizace (International organization for biological crystallization - IOBCr), Jihočeská univerzita v Českých Budějovicích a Akademie věd ČR. Předsedkyní konference je Ivana Kutá Smatanová, t. č. také prezidentka IOBCr a místopředsedkyní Pavlína Řezáčová. www.iccbm16.org