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**Keywords: Ribonucleotide reductase, furanone derivatives, model**

**P.30.01.5 Poster Session: 25 August, Board: 227**

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**Structure and Properties of Aminoacid Adducts with 3d Metals**

Leonore Wiehl[a*], Jürgen Schreuer[a], Eiken Haussühl[a], Katarina Removic-Langer[b], [a]*Institut für Mineralogie / Kristallographie.* [b]*Physikalisches Institut, Universität Frankfurt am Main, Germany.* E-mail: L.wiehl@kristall.uni-frankfurt.de

Compounds with low-dimensional magnetic interactions can be designed by combining spin bearing metals with organic molecules. The metal ions are connected e.g. to amino groups or carboxylate groups of the organic ligand and two different metal ions may be bridged via the organic molecule, thus allowing for an electron transfer between the metals. Depending on size and geometry of the organic molecules and the amount of metal salt, many different arrangements are realized, e.g. dimers, trimers, chains [1] or even 2-dimensional sheets [2]. The different metal-metal distances and the chemical surroundings characterize the type and strength of magnetic interaction.

In adducts with betaine the carboxylate group can bridge two different metal ions. With aminoacids like histidine or glycine, the nitrogen atoms of the amino groups present additional bridging options.

Crystals of betaine and aminoacid adducts with $MeX_2$ (Me = Cu, Mn; X = Cl, Br) were grown from aqueous solution. The crystal structures will be presented together with magnetic susceptibilities, showing low-dimensional interactions and/or antiferromagnetic ordering at low temperature.

[1] Schreuer J., Haussühl S., Z. Krist., 1993, **205,** 313. [2] Lu J.Y., Lawandy M.A., Li J., Inorg. Chem., 1999, **38**, 2695.

**Keywords: structure determination, betaine, magnetic ordering**

**P.30.01.6 Poster Session: 26 August, Board: 201**

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**Structure Discovery Using an Integrated Microfluidic Crystallization System**

Andy May, Shelley Godley, Kathy Yokobata, Kyle Self, Kevin Farrell, Paul Wyatt, *Fluidigm Corporation, 7100 Shoreline Court, South San Francisco, CA 94080.*

Use of the three-dimensional structures of biological macromolecules is now a key component of many research programs. Identifying conditions for the growth of diffraction quality crystals of target proteins remains one of the main bottlenecks in structure determination. The TOPAZ™ system provides a rapid and efficient path to structure through the use of *integrated fluidic circuits* (IFCs), which enable the routine setup of sub-nanoliter crystallization experiments. IFCs are miniaturized fluidic devices that control the precise metering of fluid through the use of integrated valves controlling the flow between interconnected channels and chambers. Crystallization in TOPAZ IFCs is effected through microfluidic free-interface diffusion (μFID). μFID provides a complementary approach to crystallization by traditional methods, such as vapor diffusion.

Data will be presented describing evaluation studies carried out at academic and pharmaceutical customer sites. These studies include comparisons of screening experiments carried out using the TOPAZ system and vapor diffusion on a variety of samples. Results from screening experiments demonstrate the highly reproducible reagent distribution and crystallization behavior within experiments conducted using TOPAZ IFCs. Paths for successful translation of sub-nanoliter crystallization hits to larger-scale diffraction-quality crystals will also be discussed, including examples from experiments carried out at Fluidigm and independently at customer sites.

The presentation will also discuss ongoing product development at Fluidigm, highlighting paths for future additions and improvements to the TOPAZ system.

**P.30.01.7 Poster Session: 29 August, Board: 223**

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**EM and X-ray Studies of HupR, A Response Regulator from the NtrC Family**

Karen Davies, Louise Johnson, Catherine Vénien-Bryan, *Lab of Molecular Biophysics, Department of Biochemistry, University of Oxford, Oxford, UK*. E-mail:karen@biop.ox.ac.uk

HupR, a member of the NtrC response regulator family, enhances transcription of a membrane-bound hydrogenase in response to environmental change. It is a 53kDa protein composed of 3 domains: An N-terminal receiver domain, a central putative AAA+ ATPase domain, and C-terminal DNA binding domain. Regulation of transcription occurs via a two-component signalling pathway resulting in the phosphorylation of the receiver domain. In most NtrC-like proteins, phosphorylation causes the oligomerisation of the central domain, which activates ATP hydrolysis and promotes interaction with the $\sigma^{54}$ RNA polymerase (RNAP). Transcription is initiated using the energy released from ATP hydrolysis.

HupR is an unusual member of the NtrC family, as phosphorylation inhibits HupR-dependent transcription. We have calculated a low-resolution structure of the full-length protein using electron crystallography. This model shows HupR crystallised as a dimer. The volume is half that expected suggesting only part of the protein was imaged. We believe this part is the central domain. In addition, 3D crystals of the receiver domain ±$BeF_3^-$ have been obtained. Preliminary results show the domain has the classic receiver fold with an extended α5. The protein forms a weak dimer which is strengthened by $BeF_3^-$. The dimer interface involves β5 & α5.

**Keywords: electron crystallography, response regulators, NtrC**

**P.30.01.8 Poster Session: 26 August, Board: 202**

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**Crystal and Molecular Structure of 2, 5 – bis(butoxy) 1,4-bis (biphengthethynyl) benzene and 2, 5-bis (Octyloxy) 1, 4-bis (biphenyl ethynyl) benzene**

S. A. Chawdhury[1], Paul R . Raithby[2], Muhammad Younus[3], [1]*Sylhet International University, Sylhet, Bangladesh.* [2]*University of Bath, U. K.* [3]*Shahjalal University of Science and Technology, Sylhet, Bangladesh.*

Conjugated organic polymers are semiconductors which are used in wide range of devices such as light emitting diodes and photocells. Conjugated organic polymers have two major emissive states – singlets and triplets Radiative emission from triplet series is spin forbidden, so that only emission from the singlet state occurs. Recently the synthesis and investigation of spectrospic properties have been undertaken in Department of Chemistry, Shahjalal University of Science and Technology, Sylhet, Bangladesh and Department of Chemistry, University of Bath, U. K. The monomeric precursors have been structurally characterized by the single crystal X-ray crystallography. X-ray analysis of the two monomers (a) 2,5 – (butoxy) 1,4 – bis(biphenylethynyl)benzene, $C_{42}$ $H_{36}$ $O_2$ (b) 2,5 – bis(octyloxy) 1,4 – bis(biphenylethynyl) benzene, $C_{50}$ $H_{34}$ $O_2$ have been carried out to find the linear arrangements of the monomeric units in the polymers derived from them.

Crystal data of the compound (a) $C_{42}$ $H_{36}$ $O_2$, Triclinic, P1 with a = 9.2290 (3) $A^0$, b = 9.5120 (4) $A^0$, C = 19.2850(7) $A^0$ α = 99.206 (2) $^0$. β = 100.980 (2)$^0$ γ = 105.393 (2)$^0$, Z=2, $\rho_0$ = 1.222 $Mg/m^3$, absorption coefficient 0.923 m $m^{-1}$, F (000) 612, crystal size 0.50 x 040 x 0.10 $mm^3$, teta range for data collection 2.98 to 27.60 ; final R = 0.0609 for 7130 independent reflections (b) $C_{50}$ $H_{36}$ $O_2$ is controsymmetric, monoclinic $P2_1/C$ with a = 16.8910(8) $A^0$, b, = 5.4580 (3) $A^0$, C = 22.6030 (13)$A^0$, β = 106.490, ($2^0$), Z=2, ρ=1.142 $Mg/m^3$, absorption coefficient o.667 $nm^{-1}$, F (000)=740, crystal size 0.45 x 0.15 x 0.03 mm, teta range for data collection 3.71 to 24.44 degrees. Final R indices 0.0577 for 3252 independent reflections.

Both structures were solved by direct methods and refined by full matrix least squares methods.

**Keywords: X-ray, crystal structure, semiconductors**