This work has been supported by Slovak Grant Agency APVV (APVV-0202-10) and VEGA (1/0679/11).

[1] Mrkvova K., Kamenıcek J., Sindelar Z., Kvıtek L.; *Transition Metal Chemistry* 29: p. 238–244(2004)
[2] Fronc, M., Kamenicek, J., Herich, P., Moncol, J., Kozisek, J.: *Acta Crystallographica*, A65, p. 226 (2009)

Keywords: substituted dithiolate, Cu(III), electron density

L.A.21

Acta Cryst. (2011) A**67,** C818

The crystal structures of two new synthetic compounds $CsNaCu(P_2O_7)$ and $Rb_2Cu(P_2O_7)$

A.P. Chernyatieva, D.V. Spiridonova, S.V. Krivovichev
Faculty of Geology, St. Petersburg State University, University Emb. 7/9, 199034 St. Petersburg (Russia)
E-mail: university_spsu@mail.ru

Two new compounds, $CsNaCu(P_2O_7)$ (**1**) and $Rb_2Cu(P_2O_7)$ (**2**), have been obtained by high-temperature solid state reaction of $CsNO_3$, $Cu(NO_3)_2$, NaOH and $(NH_4)_4P_2O_7$. The chemical reagents were mixed in agate mortar in ratios of Cs:Na:Cu:P 1:1:3:4 (**1**) and Rb:Cu:P 1:3:3 (**2**). The mixtures were heated up to 650°C and kept at this temperature for 8 h in air, followed by cooling to 25 °C at a cooling rate of 25 °C/h. The product consisted of blue platy crystals of **1** and **2**.

The structures of synthetic compounds were solved using single crystal X-ray diffraction.

$CsNaCu(P_2O_7)$ (**1**) is orthorhombic, space group $Pmn2_1$, a = 5.147(8), b = 15.126(2), c = 9.717(2) Å, V = 756.20 Å^3, R_1 = 0.0660 for 1221 unique reflections [$I > 2\sigma(I)$]. The structure is based upon 2-D layers of Cu square pyramids and P_2O_7 groups. $Rb_2Cu(P_2O_7)$ (**2**) is orthorhombic as well, space group *Pmcn*, a = 5.183(8), b = 10.096(1), c = 15.146(3) Å, V = 793.55 Å^3, R_1 = 0.0632 for 1326 unique reflections [$I > 2\sigma(I)$]. The structure is based upon the same 2-D layers as in the structure of (**1**), but the adjacent layers are rotated relative to each other by 180^o in comparison with their mutual position in (**2**). It is noteworthy that the layers are non-centrosymmetric. The arrangement of layers in the structure of (**1**) is non-centrosymmetric (the sequence of layers is ...AAAA..., whereas it is centrosymmetric in (**2**) (the sequence of layers is ...ABAB... (A and B are two opposite orientations of the same layer).

Keywords: Phosphates-1, X-ray -2, synthesis -3

L.A.22

Acta Cryst. (2011) A**67,** C818

Structure and functional characterisation of utrophin and dystrophin N-terminal first spectrin repeats.

Muralidharan Muthu, Andrew J Sutherland-Smith, *Centre for Structural Biology, Institute of Molecular Biosciences, Massey University, Palmerston North, New Zealand.* E-mail: M.A.Muthu@massey.ac.nz

Duchenne and Becker muscular dystrophies (DMD & BMD) are muscle-wasting disorders caused by mutations in the X-linked dystrophin gene. Utrophin is a widely expressed protein with high sequence similarity to dystrophin that has been shown to functionally compensate for dystrophin in cultured muscle cells and in the muscular dystrophy *(mdx)* mice model. Replacement of utrophin for dystrophin in DMD and BMD patients is a potential therapeutic strategy [1].

Dystrophin and utrophin are large cytoskeletal proteins, belonging to the spectrin superfamily, that link intracellular F-actin and the extracellular matrix via a membrane-associated protein complex. Utrophin and dystrophin are characterized by N-terminal actin binding domains and C-terminal variable domains separated by 22 or 24 spectrin-like repeats respectively. Certain utrophin and dystrophin spectrin repeats can bind F-actin, and were hypothesized to act as a shock absorbers or molecular springs. These multiple spectrin repeat proteins contribute to the stability of the membrane cell. The aim of this research is a structural determination and biochemical comparison of utrophin and dystrophin N-terminal spectrin repeats. The crystal structure of the N-terminal repeats from utrophin and dystrophin have been determined to 1.95 Å and 2.3 Å, and exhibit the characteristic triple-helix structure folded into a left-handed coiled-coil [2]. Studies have shown that spectrin repeats of utrophin are required for a higher affinity interaction of the actin binding domain with F-actin. It is unclear whether the N-terminal repeats have an intrinsic affinity for F-actin and in the current study we are determining the actin-binding properties of these spectrin repeats.

[1] Tinsley JM, Deconinck N, Fisher R, Kahn D, Phelps S, Gillis JM and Davies KE. Expression of full-length utrophin prevents muscular dystrophy in *mdx* mice. *Nat. Med.* **4** (1998), 1441-1444.
[2] Parry DA, Dixon TW and Cohen C. Analysis of the three-α-helix motif in the spectrin superfamily of proteins. *Biophys. J.* **61** (1992) 858–867

Keywords: coiled-coil, spectrin repeat, molecular shock absorbers

L.A.24

Acta Cryst. (2011) A**67,** C818

Interaction of Saturated Fatty acids with Apoferritin

Weiming Bu, David Liang, Renyu Liu,Patrick Loll, Ivan Dmochowski, Roderic Eckenhoff, Department of Anesthesiology & Critical Care, University of Pennsylvania School of Medicine, 3620 Hamilton Walk, Philadelphia, PA 17104 Email:buw@uphs.upenn.edu

Apoferritin has been an attractive model for the study of anesthetic-protein interactions because it binds a wide range of general anesthetics at high affinity ($Ka\sim 10^5$ M^{-1}) in a single interhelical cavity located at a dimer interface [1,2]. The in vivo function of this interfacial cavity is not clear; apoferritin isolated from tissues such as the horse spleen do not reveal an occupant when crystallized. Because of its tunnel-like "U" shaped geometry, and positively charged "gatekeeper" arginine residues, we hypothesized that ferritin may be an intracellular fatty acid binding protein.

Fatty acids have physiological, behavioral and toxicologic activities. They are known to bind with a variety of small fatty acid-binding proteins as their normal endogenous ligands. A connection to iron metabolism has not been established but would make physiological sense. To evaluate binding interactions between fatty acids and apoferritin, we present the x-ray structural data of apoferritin complexed to caprylic (C8) and myristic (C14) acid, together with the calorimetric data. Using competition assays, we provide evidence that fatty acids share the same binding site as the anesthetic, suggesting that anesthesia could modulate intracellular FA concentrations, and whatever function is subserved by the interaction between FA and ferritin.

Figure 1. Different density map shows C14 Bound to the interface of dimers as U shape

Reference:
1. Vedula LS, Brannigan G, Economou NJ, Xi J, Hall MA, et al. A unitary anesthetic-binding site at high resolution. *J Biol Chem* 2009,24176-24184.
2. Liu R, Loll PJ, Eckenhoff RG. Structural basis for high-affinity volatile anesthetic binding in a natural 4-helix bundle protein. *FASEB J.* 2005;19:567–576.

Key words: ferrtin, fatty acid binding protein.