Bikitaite has an H-bonded H_2O chain along [010] termed 'one-dimensional ice'. The molecules are ordered, whereby one H atom per molecule is unbonded and the other is H-bonded. With increasing temperature, the H-bonding weakens continuously until the chain 'breaks' and isolated H_2O molecules are present.

Melanophlogite has quasi-free N_2, CO_2 and CH_4 molecules, but no H_2O, which partition between the [5^{12}] and [$5^{12}6^2$] cages. The molecules are orientationally disordered in the cavities and they have only weak dispersion interactions with the SiO_2-crystal framework. However, the incorporation of molecules is necessary to allow the SiO_2 framework to condense.

Cordierite and beryl contain quasi-free CO_2 molecules, as well as H_2O, in small cavities. The CO_2 molecules are orientated parallel to the crystallographic *x*-axis. The H_2O molecules have their H-H vector parallel to the *z*-axis in alkali-free crystals and are dynamically disordered about the *z*-axis. They show weak H-bonding with their frameworks.

Keywords: nanopores, H-bonding, vibrational spectroscopy

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TEM and XPS Evidences of O/F Ordering in NbO_2F

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NbO_2F is a member of a relatively small group of $MO_{3-x}F_x$ (M = Nb, Ta, Ti, Mo, W) oxyfluorides with the cubic ReO_3 structure type. They have been of interest in recent years as host compounds for Li-insertion in battery electrolytes [1] and also because of a pressure-induced phase transition from cubic (*Pm*3*m*) to rhombohedral (*R*3*c*) [2]. The average structure consists of corner-sharing $M(O,F)_6$ octahedra, as in undistorted ABO_3 perovskite, with the *A* sites being empty. Oxyfluorides are reported to exhibit a statistical distribution of O and F, generally attributed to their similar ionic radii (1.35 and 1.285Å, respectively). Bond-length/bond-strength calculations, however, suggest there should be a strong driving force for ordering. Evidence for one-dimensional O/F ordered columns along ⟨*001*⟩, but with no lateral correlation from one column to the next has already been recognized from transmission electron diffraction [4]. In the present work, coupled HRTEM and electron diffraction revealed the presence of characteristic transverse planes of diffuse intensity running through G±⟨*hk*⅓⟩* regions (*i.e.* existence of O/F-ordering), and XPS confirmed the existence of two distinct atomic positions for O and F and just one for Nb. These data are consistent with three-dimensional O/F ordering within NbO_2F structure.

[1] Permér L., Lundberg M., *J. Solid State Chem.*, 1989, **81**, 21. [2] Carlson S., et al., *Acta Cryst. B*, 2000, **56**, 189. [3] Vogt T., et al., *J. Solid State Chem.*, 1999, **144**, 228. [4] Brink F.J., et al., *J. Solid State Chem.*, 2002, **166**, 73.

Keywords: O/F ordering, electron diffraction, XPS

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Crystal Structures and Topology of New and Rare Arsenates

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The crystal chemical phenomena (e.g. polyhedral stacking variations, microtwinning etc.) which accompany the formation of real structures are considered on the basis of the results of structural study of a large group of new and rare natural arsenates (pushcharovskite, tillmannsite, zdenekite and mahnertite). The use of synchrotron radiation allowed to perform the crystal structure investigation of these four new and rare minerals and to reveal their structural peculiarities and topology.

The structure of pushcharovskite is characterized by some structural disorder and contains heteropolyhedral sheets formed by Cu-polyhedra and As -tetrahedra and linked by hydrogen bonds.

The main peculiarity of tillmannsite structure is connected with unique tetrahedral clusters $(Ag_3Hg)^{3+}$ revealed in this mineral in which mercury is characterized by the low-valence state.

Mahnertite and zdenekite have close chemical composition but different symmetry. These minerals contain a new type of mixed polyhedral sheets, which are characterized by the different mode of stacking.

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Keywords: arsenates, crystal structures, topology

MS08 MEMBRANEPROTEIN STRUCTURE AND FUNCTION

Chairpersons: Jacqueline M. Gulbis, Michael R. Garavito

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Does the Crystal Structure of Ammonium Transporter Tell us its Function?

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Ammonium is one of the most important nitrogen sources for bacteria, fungi and plants but it is toxic to animals. The ammonium transport proteins (Mep/Amt/Rh) are present in all domains of life, but the chemical identity of their substrate was uncertain. We have solved the structure of wild type AmtB from *E. coli* in two crystal forms at 1.8 and 2.1 Å resolution, respectively. Substrate transport occurs through a narrow, mainly hydrophobic pore located at the centre of each monomer of the trimeric AmtB. At the periplasmic entry, a binding site for NH_4^+ is observed. Two phenylalanine side chains (F107 and F215) block access into the pore from the periplasmic side. Further into the pore, the side chains of two highly conserved histidine residues (H168 and H318) bridged by a H-bond, lie adjacent with their edges pointing into the cavity. These histidine residues may facilitate the deprotonation of an ammonium ion entering the pore. Adiabatic free energy calculations support that an electrostatic barrier between H168 and H318 hinders the permeation of cations but not that of the uncharged NH_3. The structural data and energetic considerations strongly indicate that the Mep/Amt/Rh proteins are ammonia gas channels [1]. Interestingly at the cytoplasmic exit of the pore, two different conformational states are observed which might be related to the inactivation mechanism by its regulatory partner.

[1] Zheng L., Kostrewa D., Berneche S., Winkler F.K., Li X.D., *Proc. Natl. Acad. Sci. USA*, 2004, **101**,17090.

Keywords: ammonia transport, conformational change, X-ray structure

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Two OMPs: Autotranslocation and LPS-Deacylation

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The outer membrane proteins (OMPs) of Gram-negative bacteria are often involved in pathogenesis. Their exposure to the extracellular environment make them potential targets for antimicrobial treatments. We present recent crystal structures of two outer membrane proteins, NalP [1] and PagL.

NalP belongs to the autotransporter family. Autotransporters secrete their own N-terminal passenger domain with their C-terminal translocator domain. The crystal structure of the translocator domain of NalP from *Neisseria meningitidis* reveals an N-terminal helix inside