Single crystals of samples 1-3 have been grown from complex boron-containing hydrothermal solutions at range of temperatures of 400-750°C and pressures of up to 150 MPa in the IEM RAS [1]. Cu-bearing tourmaline (sample 4) has been synthesised in the Institute of Mineralogy and Petrography SB RAS [2]. X-ray experiment was carried out on four-circle single-crystal diffractometer Nicolett R3.

The content of 3d-elements in multicolor synthetic tourmalines can rise up to 24 wt. % (in oxide form) and in the case of Ni, Co, Cu-tourmalines it is significantly higher than that found in natural specimens. The total content of 3d-elements and the ratio of its' ionic radii are the reason for the unit cell parameters and octahedral dimensions variations. In all cases chromophore elements occupied Y (mainly) and Z octahedra (table 2).

Table 2. Characteristic of Y and Z octahedral.

| Smp | Y octahedron | | Z-octahedron | |
	Occupation, apfu	$\langle Y-O\rangle$, Å	Occupation, apfu	$\langle Z-O\rangle$, Å
1	$Al_{1.69}Ni_{0.81}Fe_{0.50}$	1.991	$Al_{5.40}Fe_{0.60}$	1.922
2	$Ni_{1.20}Cr_{0.96}Al_{0.63}\times Fe_{0.18}Mg_{0.03}$	2.008	$Al_{4.26}Ni_{1.20}\times Cr_{0.48}Ti_{0.06}$	1.937
3	$Al_{1.80}Co_{1.20}$	1.949	$Al_{5.28}Co_{0.66}\times Ti_{0.06}$	1.907
4	$Al_{1.86}Cu_{1.14}$	1.978	$Al_{5.88}Cu_{0.12}$	1.907

In the structure of samples 1, 3, 4 the main element in Y and Z sites is aluminium. The samples 3 and 4 (sodium in X site) are analogues of olenite mineral. The sample.1 (X site is mainly vacant) is an analogue of hypothetic oxyfoitite. Incorporation of bivalent 3d-elements (R^{2+}) in these tourmalines is described by equation: $Al^{3+}+O^{2-}=R^{2+}+OH^-$. There are no close analogues of sample 2 in nature.

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Keywords: crystallochemistry, silicate, X-ray.

MS54.P02

First Silicate Mineral with Triple Tetrahedral Layer
Sergey M. Aksenov,[a] Ramiza K. Rastsvetaeva,[a] Nikita V. Chukanov, [a]*Shubnikov Institute of Crystallography, RAS, Moscow (Russia).* [b]*Institute of Problems of Chemical Physics, RAS, Chernogolovka (Russia).* E-mail: rast@ns.crys.ras.ru

The crystal structure of a new silicate mineral from the Eifel paleovolcanic area, Rhineland-Palatinate, Germany was studied by X-ray single crystal diffraction (diffractometer Xcalibur Oxford Diffraction, CCD-detector). The orthorhombic unit-cell parameters are: a=6.528(1) Å, b=6.970(1) Å, c= 37.216(5) Å, V=1693.33(4) Å^3, space group $Pnm2_1$. The structure was solved by direct methods and refined to R=4.9%, 2706 $|F| > 3\sigma(F)$. Idealized crystal-chemical formula is: $(K,Ca,Ba)_2(Fe,Ca,Mg,Na)[(Si,Al)_{13}O_{25}(OH)_4]\cdot7H_2O$.

The mineral is representative of a new structure type. The most important specific feature of its structure is a block $[Si_{13}O_{29}]$ consisting of three connected single layers formed by four- and eight-membered rings of tetrahedra (T) centered by Si and Al. Two outer layers $[Si_4O_{10}]$

are topologically identical to that in some single-layer phyllosilicates (mountainite, shlykovite, cryptophyllite) and in double-layer silicates rhodesite, delhayelite, hydrodelhayelite, macdonaldite, monteregianite-(Y) and fivegite. The third (inner) layer $[Si_5O_{11}]$ is unique and contains an additional tetrahedron.

The triple tetrahedral blocks $[Si_{13}O_{29}]$ are connected to each other via the discrete polyhedra $(Fe,Ca)O_7$ to form 3D framework with channels filled by large cations (mainly K, as well as subordinate Ba, Ca) and H_2O molecules. Thus the new mineral is an intermediate between phyllosilicates and zeolites. One can outline polysomatic structures from single-layer via double-layer to triple-layer ones.

Keywords: X-ray analysis, mineral, silicate

MS54.P03

New members in sodium cadmium bisulfate: structure, property and thermal studies
Dipankar Saha,[a] Giridhar Madras,[b] Tayur N. Guru Row,[a] [a]*Solid State and Structural Chemistry Unit.* [b]*Department of Chemical Engineering, Indian Institute of Science, Bangalore 560 012 (India).* E-mail: s.dipankar@sscu.iisc.ernet.in

Bimetallic sulfates form an important constituent of the earth's crust and are recognized to provide essential link to mineral evolution. Depending on the level of hydration they form different class of minerals. The omnipresent water plays a decisive role in the formation of hydrates of complex inorganic materials generating complicated structural frameworks. These compounds exhibit properties like ionic conductivity, phase transitions in the context of electric, magnetic and elastic properties [1, 2] and believed to have played an important role in the formation of earth's atmosphere oxygen [3]. We have synthesized polymorphs of sodium cadmium bisulfate which differ in the extent of hydration and have studied their thermal properties and phase transition. $Na_2Cd_2(SO_4)_3.3H_2O$, $Na_2Cd(SO_4)_2.2H_2O$, $Na_2Cd(SO_4)_2.4H_2O$, were crystallized by slow evaporation method form water. $Na_2Cd_2(SO_4)_3.3H_2O$ crystallizes in a trigonal system with the space group $P3c$. It loses water completely after 250 °C and transforms to a dehydrated phase whose structure has been established using *abinitio* powder diffration. The dehydrated form crystallizes in the space group $I\bar{4}3d$. The phase transitions have been investigated using DSC, TGA and ionic conductivity studies. $\beta-Na_2Cd(SO_4)_2$, a polymorphic form of $\alpha-Na_2Cd(SO_4)_2$, has been isolated by quenching the parent compound $\alpha-Na_2Cd(SO_4)_2$ and characterised to belong to a monoclinic system, space group $P2_1/c$. $\beta-Na_2Cd(SO_4)_2$ takes up water from the atmosphere and gets converted to a Kröhnkite type mineral $Na_2Cd(SO_4)_2.2H_2O$. Upon heating, mineral loses water and gets converted to $\alpha-Na_2Cd(SO_4)_2$.

The phase transition analysis provides inputs for exploring the origin of Kröhnkite mineral. $Na_2Cd(SO_4)_2.4H_2O$ crystallizes in a monoclinic system with a space group $P2_1/c$. It is isostructural with the mineral Astrakhanite which is also known as Blödite [4]. This work describes a structure based analysis of phase transitions involved in these complexes, thus providing insights into their evolutionary aspects.
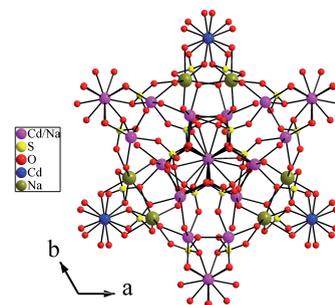
Figure 1. Repetitive unit of $Na_2Cd_2(SO_4)_3.3H_2O$

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Keywords: mineral, bimetallic sulfates, phase transition

MS54.P04

Structural analysis of new mineral phases

Marcin Stachowicz,[a] Jan Parafiniuk,[b] Boguslaw Baginski,[b] Raymond Macdonald,[b] Krzysztof Wozniak,[a] [a]*Chemistry Department, University of Warsaw.* [b]*Geology Department, University of Warsaw. (Poland).* E-mail: marcin.stachowicz@chem.uw.edu.pl

Redikortsevite, NH_4MgCl_3 x6H_2O, from the burned dumps of the Chelabinsk coal basin in Russia, described by Chesnokov et al. (1988), has not been submitted to IMA for approval and it is not recognized as a valid mineral species. The occurrence of this phase has also been noticed on burning waste dumps of one of the Upper Silesia coal mines in Poland. Redikortsevite forms there aggregates and fine crystals suitable for structural study. We have determined its 3D structure and performed chemical and mineralogical analysis necessary for the approval process.

Alumohydrocalcite is hydrated calcium and aluminium carbonate. It is ascribed to have chemical formula $CaAl_2(CO_3)_2(OH)_4$ x3H_2O and commonly forms compact fine-crystalline aggregates. This mineral still does not have reliable crystal structure although it has been known since 1926. The reason of such a situation is difficulty in finding single crystals of a good quality and adequate size. We have acquired a unique sample of this mineral from its classic occurrence site at Nowa Ruda, Sudetes Mts., Poland. It consists of spherulitic needle aggregates. Crystals are very well formed and large enough for X--ray structural investigations. They reach length even up to decimal parts of millimeter and are suitable for synchrotron sources rather than laboratory ones. For this mineral, powder diffraction and chemical analysis have been performed for the sake of its identification.

The chevkinite group of minerals are found as accessory phases in a wide variety of parageneses, including igneous rocks ranging from gabbros to peralkaline granites, fenites, ore deposits, granulite facies gneisses and metacarbonates [1]. The composition of the majority of occurrences closely approaches the ideal formula $A_4BC_2D_2Si_4O_{22}$, where A = REE, Ca, Sr, Th; B = Fe^{2+};
C = Ti, Al, Fe^{2+}, Fe^{3+}, Mn, Mg, Zr, Nb; and D = Ti, but there is a wide range of compositionally different species. The geochemical importance of chevkinite group is that they are strong REE-concentrators; total REE_2O_3 contents are up to 50 wt%. They can be the dominant REE-bearing phase in any given rock. The REE are being increasingly used in a host of green technologies, such as the production of novel wind turbines, low-energy light bulbs also mobile phones. Additionally neodymium, one of the most common REE, is a key part of neodymium-iron-boron magnets used in hyperefficient motors and generators. Published work has shown that compositional variations in the group are mirrored in the structure but there is still no consensus as to how. Further, several species within the group have not been structurally determined. We are attempting to define the complete composition-structure relationships in the group.

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Keywords: minerals, structure, diffraction

MS54.P05

The crystal structure of huemulite

Fernando Colombo,[a] Ricardo Baggio,[b] Anthony R. Kampf,[c] [a]*Facultad de Ciencias Exactas, Físicas y Naturales, Universidad Nacional de Córdoba, Córdoba (Argentina).*[b]*Departamento de Física (Lab. TANDAR), Comisión Nacional de Energía Atómica. San Martín, Buenos Aires (Argentina).* [c]*Natural History Museum of Los Angeles County, Los Angeles, California (USA).* E-mail: fosfatos@yahoo.com.ar

The crystal structures of natural (from the West Sunday Mine, Utah, USA) and synthetic huemulite, $Na_4Mg(V_{10}O_{28})\cdot24H_2O$, have been solved and refined to $R_1 = 0.0313$ (for 3535 unique $F_o > 4\sigma F$ reflections) and 0.0246 (for 3672 unique $F_o >$ _ $4\sigma F$ reflections), respectively. Huemulite is triclinic, space group $P\overline{1}$, with Z = 1; unit-cell dimensions of the natural sample are a 9.0453(2), b 11.3337(3), c 11.7372(8) Å, α 105.223(7), β 97.383(7), γ 100.790(7)°, V 1120.30(9) Å³, whereas those of the synthetic sample are a 9.0425(2), b 11.3303(2), c 11.7353 (8) Å, α 105.222 (7), β 97.377 (7), γ 100.791 (7)°, V 1119.47(8) Å³. The structure consists of decavanadate oxyanions $(V_{10}O_{28})^{6-}$ linked via an interstitial complex composed of isolated $[Mg(H_2O)_6]^{2+}$ octahedra and an $[Na_4(H_2O)_{14}]^{4+}$ cationic group (defining an infinite zig-zag chain). There are also four isolated H_2O groups, two of them positionally disordered. All except 4 H atoms have been located, showing a network of H-bonds that further links the interstitial complex and the structural unit, stabilizing the atomic arrangement. The Lewis acidity of the interstitial complex (0.18) is almost coincident with the upper limit of basicity of the structural unit (0.17), thus showing that the valence-matching principle is maintained in this structure.

It is probable that the X-ray pattern and the unit-cell dimensions informed in the original description of huemulite [1] were measured using a mixture that included fully hydrated and partially dehydrated material.

Huemulite is closely related to a synthetic family of general formula $Na_4M^{2+}(V_{10}O_{28})\cdot23H_2O$ (M=Ni,Mg) [2] [3], the main difference (in addition to having $\approx$ 23 H_2O molecules instead of $\approx$ 24) being that the latter compounds have a unit cell with doubled volume. Unit cell and atomic positions of huemulite are related to those of the synthetic family by the transformation matrix M = [1 0 0 / 0 1 1 / 0 $\underline{1}$ -1]. After the transformation, the space group of huemulite becomes $A\overline{1}$. Some of the symmetry restrictions (inversion centers, cell centering, etc.) present in huemulite are relaxed, with the consequence that fewer atoms are symmetry-related in the synthetic family.

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Keywords: mineralogy, vanadium, valence-matching principle

MS54.P06

Structural Investigations of Synthetic Analogues of Murataite

Anna S. Pakhomova,[a] Sergey V. Krivovichev,[a] Sergey V. Stefanovsky,[b] Sergey V. Yudintsev,[c] [a]*Departament of Crystallography, Saint-Petersburg State University, Saint-Petersburg.* [b]*MosNPO Radon, Moscow.* [c]*Institute of Geology of Ore deposits, Petrograghy, Mineralogy and Geochemistry, Moscow (Russia).* E-mail: a.s.pakhomova@mail.ru

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