

Ca(ReO₄)₂.Urea.H₂O: triclinic, P $\bar{1}$, $a = 7.322(3)$, $b = 9.088(5)$, $c = 9.175(3)$ Å, $\alpha = 111.67(2)$, $\beta = 91.26(2)$, $\gamma = 104.89(3)^\circ$, $Z = 2$, $D_x = 3.67$ g.cm⁻³, $R = 0.030$ for 2104 3 σ -reflections.

Pb(ReO₄)₂.Urea.H₂O: monoclinic, P 2₁/c, $a = 10.283(2)$, $b = 7.389(6)$, $c = 14.402(8)$ Å, $\beta = 99.72(1)^\circ$, $Z = 4$, $D_x = 4.727$ g.cm⁻³, $R = 0.042$ for 1951 3 σ -reflections.

The CaO₈ environment consists of five apices of the ReO₄ tetrahedra [2.43(1)-2.52(2)Å], O atoms of two urea and one water molecules at distances 2 x 2.41(1) and 2.39(1)Å. Ca atoms are chained by alternating double Ca-O-Ca bridges of urea [Ca...Ca 3.92(1)Å] and fourfold Ca-(OReO)-Ca bridges [Ca...Ca 5.49(3)Å]. Adjacent chains are linked by pairs of Re(1)O₄ tetrahedra [Ca...Ca 6.85(2)Å] and arranged in layers parallel to the *ab*-plane. The layers are packed by H-bonds only.

The Pb atom has a nine-fold coordination of six ReO₄ apices (Pb...O 2.55(2)-2.76(1)Å), two urea molecules [2.61(1), 2.86(1)Å], and a water molecule at 2.47(1)Å. The structure consists of layers parallel to the *bc*-plane in which the Re(1)O₄ tetrahedra form double bridges between Pb atoms (Pb...Pb 4.12(2), 6.64(2), 2 x 6.85(2)Å). The shortening of the first Pb...Pb distance is due to the complementary Pb-O-Pb urea double bridge. The layers are held together by double bridges of Re(2)O₄ tetrahedra [Pb...Pb 7.45(4)Å] and a system of H-bonds.

PS-08.01.34 NEW MEMBERS OF TRIPLE MOLYBDATE FAMILY: COMPOSITIONS, CRYSTAL STRUCTURES, THERMAL STABILITY. By R.F.Klevtsova*, L.A.Glinskaya, N.M.Kozhevnikova, Zh.G.Bazarova, P.V.Klevtsov. Institute of Inorganic Chemistry, Russian Academy of Sciences, Siberian Branch, Russia.

Triple molybdates were synthesized by solid state reactions and the complicated character of chemical interactions in the systems was established. Products of the synthesis were investigated by X-ray and DTA methods. Single crystals were obtained by spontaneous flux crystallization. The compositions are: I-Li₃Ba₂Im₃(MoO₄)₈, Im=Gd,Tm; II-NaMg₃In(MoO₄)₅, III-K₁₀MgZr₃(MoO₄)₁₂. Their crystallographic characteristics are given in the Table.

	Sp.gr.	a, Å	b, Å	c, Å	Z	N	R
I-Gd	C2/c	5.2380	12.758	19.151	2	2453	0.042
		-	91.126	-			
II	P $\bar{1}$	7.0476	17.935	6.9849	2	4503	0.047
		87.650	100.96	92.510			
III	R3c	10.576	-	37.511	3	1166	0.026

The crystal structures were solved using single crystal data (KUMA and CAD-4, Mo K α radiation). The characteristic features of the structures are statistically distributed atoms of bi- and trivalent metals. Structural peculiarities (size, shape, site occupancy and stacking of the coordination polyhedra) are used for interpretation of physical properties. The comparative crystal chemistry analysis of known triple molybdates has been carried out. The compounds studied melt incongruently, polymorphism was not found.

PS-08.01.35 STRUCTURAL CHEMISTRY OF BaAl₄/ThCr₂Si₂ TYPE COMPOUNDS. By G.Just and P.Paufler, Institute of Crystallography and Solid State Physics, University of Technology, Dresden, Federal Republic of Germany.

Lattice ratios *c/a* and structural parameters x_3 of about 180 representatives of the BaAl₄ type of structure (space group I 4/mmm) have been critically reviewed taking binary and multicomponent phases into account. Leaving out data of minor reliability a considerable scatter of experimental values in a x_3 -*c/a* plane remains, which is classified according to the concepts of equal interatomic spacing and coordination polyhedra. Lines of equal spacings *d* were calculated for all atom positions in the unit cell up to $d = 1.9$ Å. Moreover, the coordination of all atom positions is given. Several points in the x_3 -*c/a* plane were found to represent special structural features like coordination polyhedra with coordination numbers of 16, 18 or 20 for the barium position with characteristic packing of distorted tetrahedra. Individual space requirements of atoms are met with different spacing conditions between Al(1) and Al(2) positions. Subdivision of representatives into families behaving similarly from a point of view of crystal chemistry is discussed.

PS-08.01.36 NON-STOICHIOMETRIC V-Mo OXIDE COMPOUNDS WITH V₂O₅ STRUCTURE TYPE. By L. M. Plyasova, L. P. Solovyeva*, G. N. Kryukova, S. V. Tsybulya and T. V. Andrushkevich.

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The V-Mo oxide system was studied by X-ray analysis because such oxides serve as catalysts for oxidation of acrolein to acrylic acid. Thermal treatment of products from reaction between para-molybdate and meta-vanadate resulted in the formation of V-Mo compounds of varying composition (V₆Mo₄O₂₅, (V⁵⁺, V⁴⁺)MoO₅, VMo₃O₁₁, etc.). The structures of these compounds appear to depend on the degree of vanadium reduction and on V/Mo ratio. V_{0.95}Mo_{0.97}O₅ (V⁴⁺/V=0.6) was selected for structural investigations. Crystal structure analysis and refinement using Rietveld method ($R_1 = 0.072$, $R_p = 0.11$) were carried out using X-ray powder diffraction data. Layers of edge-sharing octahedra of two types (Mo+V⁴⁺) and (Mo+V⁵⁺) are connected by corners. Structurally the compound is similar to the V₂O₅ type. Our results indicate that for compounds of V₂O₅ structure