08.2-12 THE CRYSTAL STRUCTURE OF NH₄La₅P₄O₁₂.

During our studies on lanthanum phosphates' phase relations the apparently new compound was obtained in the pure, crystalline form. Both preparative procedures and X-ray powder data based on literature reports suggested it to be lanthanum oxophosphate. Single-crystal X-ray analysis, however, proved that the compound is NH₄La₅P₄O₁₂ which is surprisingly stable at elevated temperatures. Preliminary X-ray data are: system monoclinic, space group C2/c with \(a = 7.941(1), b = 12.645(15), c = 10.702(5) \, \text{Å}\). Diffractometer collected data were reduced in a standard way the absorption correction being allowed for using program DIFABS by N. Walker and D. Stuart (1983). 1366 reflections with \(I > 1.96(F)\) were used for structure solution (Patterson) and refinement. H-atoms were partly resolved in a difference Fourier synthesis. The refinement led to \(R1 = 0.037\) and \(R2 = 0.045\). The structure consists of PO₄ tetrahedra linked together to form tetracycles, LaO₃ dodecahedra and ammonium tetrahedra. The La-O bond lengths vary between 2.475(5) and 2.516(5) Å. Distances vary from 2.829(5) to 1.923 Å. A planar complex of CuII and shows two Mo₆ tetrahedra, acting as monodentate oxygen-donor ligands, and two Ni²⁺ in a twin configuration. Bond distances in the copper plane are 1.953 and 2.071 Å (Cu-N) and 1.662 and 2.000 Å (Cu-O), while in the tetrahedra they range from 1.677 to 1.840 Å. The crystal structures with space group \(P_{2}1\) and the following cell dimensions:

- \(a = 6.155(3)\), \(b = 7.148(3), c = 7.516(4)\, \text{Å}\)
- \(\beta = 108.5210(\), \(\gamma = 93.906(6), \tau = 113.72(4)^{\circ}\)

The structure was solved by Patterson and Fourier methods using 1071 unique reflections (Four-circle diffractometer, MoKα radiation, 0–20 scan), and refined to \(R=0.036\). The \([\text{Cu(NH}_3]_2\text{MoO}_4] \cdot \text{H}_2\text{O}\) anion is a planar complex of CuII and shows two Mo₆ tetrahedra, acting as monodentate oxygen-donor ligands, and two Ni²⁺ in a twin configuration. Bond distances in the copper plane are 1.953 and 2.071 Å (Cu-N) and 1.662 and 2.000 Å (Cu-O), while in the tetrahedra they range from 1.677 to 1.840 Å.

08.2-13 A DEFENDER OF KY₂P₀₁₄.
By T. Ozeki, H. Ichida & Y. Sasaki, Department of Chemistry, Faculty of Science, The University of Tokyo, Japan.

KY₂P₀₁₄, Mr=196.0, trigonal, P₃₃m, \(a=8.5909(4), c=4.9973(3)\, \text{Å}\), \(U=326.88(8)\, \text{Å}^3\), \(Z=1, K=0.031\) for 793 unique reflections (2<Ω<40, F>3σ(F)). The structure, which was first determined by Byström & Evans (Acta Chem. Scand. 12(1959)377-378), was refined. It contains two independent V atoms, one (A site) and refinement. H-atoms were partly resolved in a difference Fourier synthesis. The refinement led to \(R1 = 0.037\) and \(R2 = 0.045\). The structure consists of PO₄ tetrahedra linked together to form tetracycles, LaO₃ dodecahedra and ammonium tetrahedra. The La-O bond lengths vary between 2.475(5) and 2.516(5) Å. The figure resembling that found in LaP₃O₉ (J. Matuszewski, J. Kropiwnicka and T. Szamierowska, 1986). The crystals of NH₄La₅P₄O₁₂ are isomorphous with those of NH₄Pr₅P₄O₁₂ (Nasse R. et al., 1977).

08.2-14 THE CRYSTAL AND MOLECULAR STRUCTURE OF \([\text{Cu(NH}_3]_2\text{MoO}_4] \cdot \text{H}_2\text{O}\).
By W. Degmeyer, Institut für Kristallographie, Universität, D-7500 Karlsruhe, Federal Republic of Germany.

Our research program on aluminosilicates of general composition \(M[\text{Al}_2\text{O}_5](\text{XO})\cdot(N\text{H}_4,\text{Sr}, \ldots, \text{X}=\text{Sr,Cr,Mo,W}, \ldots)\) has been continued. These compounds are interesting for several reasons, the most important ones being: i) The occurrence of ferroic phase transitions; ferroelectric and ferroelastic species have been found. ii) Strong repulsive host-guest interactions lead to important structural strains (bond length and angular). iii) Complicated superstructures occur which in some cases are best described as commensurate modulations; iv) The possible existence of tricritical points. The actual investigations focused on:

a) The phase sequence of \(\text{Ca}_8[\text{Al}_{12}\text{O}_{24}](\text{NO}_3)_2\) with its two phase transitions at 614 and 66 K.

b) The phase sequence of \(\text{Sr}_8[\text{Al}_{12}\text{O}_{24}](\text{CrO}_4)_2\) with temperatures of transition near room temperature (-291 K and -297 K).

c) The room temperature phase of \(\text{Sr}_8[\text{Al}_{12}\text{O}_{24}](\text{MoO}_4)_2\). Its distribution of superstructure reflections suggests that it might be regarded as commensurately modulated.

d) The room temperature phase of \(\text{Sr}_8[\text{Al}_{12}\text{O}_{24}](\text{WO}_4)_2\). Latest results will be presented.