THE CRYSTAL STRUCTURE OF NH₄LaP₄O₁₂.


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 oxypophosphate. Single-crystal X-ray analysis, however, proved that the compound is NH₄LaP₄O₁₂ which is surprisingly stable at elevated temperatures. Preliminary X-ray data are: system monoclinic, space group C2/c with a = 7.941(4), b = 12.645(15), c = 10.702(5) Å, β = 110.00(5)°. Diffractionometer collected data were reduced in a standard way the absorption correction being allowed for using program DIFABS by N. Walker and D. Stuart (1983). 1566 reflections with 0 > 1.96(1) 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 = 0.046. The structure consists of PO₄ tetrahedra linked together to form tetracycles, LaO₆ dodecahedra and ammonium tetrahedra. The La-O bonds lengths vary between 2.475(5) and 2.516(5) Å. The figure resembling that found in LaP₃0₉ (J. Matuszewski, Y.Sasaki, Department of Chemistry, Tokyo, Japan. Acta Cryst., C32(1976) 1467-1469). The crystals of NH₄LaP₄O₁₂ are isomorphous with those of NH₄PrP₄O₁₂ (Maase R. et al., 1977).

THE CRYSTAL AND MOLECULAR STRUCTURE OF [Cu(NH₃)₂(MoO₄)₂](NH₄)₂.

By J. Kropiwnicka and T. Znamierowska, (1986). The room temperature phase of [Cu(NH₃)₂(MoO₄)₂](NH₄)₂ is planar complex of Cu(II) and shows two MoO₄ tetrahedra, acting as monodentate oxygen-donor ligands, and two NH₄ in a trans configuration. Bond distances in the copper plane are 1.955 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.

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08.2-12

THE CRYSTAL STRUCTURE OF NH₄LaP₄O₁₂.


08.2-13

A DEFICIENCY OF K₂V₅O₁₄.

By T.Ozeki, H.Ichida and Y.Sasaki, Department of Chemistry, Faculty of Science, The University of Tokyo, Japan.

K₂V₅O₁₄. Mr=2266.0, trigonal, P31m, a=8.6609(4), c=4.9973(3) Å, V=328.88(4) Å³, Z=1, R=0.031 for 793 unique reflections (2θ<40, F>3σ(F)). The structure, which was first determined by Byström & Evans (Acta Chem. Scand. 13(1959)377-378), was refined. It contains two independent V atoms (in a Vo and an ammnonium tetrahedra). The La-O bond lengths vary between 2.475(5) and 2.516(5) Å. The crystals of NH₄LaP₄O₁₂ are isomorphous with those of NH₄PrP₄O₁₂ (Maase R. et al., 1977).

08.2-14

STRUCTURAL STUDIES ON ALUMINATE SODALITES.

By W. Depmeier, Institut für Kristallographie, Universität, D-7500 Karlsruhe, Federal Republic of Germany.

08.2-15

Our research program on aluminates is evaluated. The compounds are interesting for several reasons, the most important ones being: 1) The occurrence of ferroic phase transitions, ferroelectric and ferroelastic species have been found. 2) Strong repulsive host-guest interactions lead to important structural strains (bond length and angular). 3) Complicated superstructures occur which in some cases are best described as commensurate modulations; 4) The possibility of existence of tricritical points. The actual investigations focused on:

a) The phase sequence of Ca₈[Al₁₂O₃₆](WO₄)₂ with its two phase transitions at 614 and 656 K.

b) The phase sequence of Sr₆[Al₁₂O₃₆](CRO₄)₂ with temperatures of transition near room temperature (-291 K and -297 K).

c) The room temperature phase of Sr₆[Al₁₂O₃₆](MoO₄)₂. Its distribution of superstructure reflections suggests that it might be regarded as commensurately modulated.

d) The room temperature phase of Sr₆[Al₁₂O₃₆](WO₄)₂.

Latest results will be presented.