

re consists of chains of $--Pt_2(CH_3CS_2)_4--I--Pt_2(CH_3CS_2)_4--I--$, with an intradimeric Pt-Pt distance of 2.677(2) Å and the Pt-I distances of 2.975(2) and 2.981(3) Å. The Pt and I atoms lie along the twofold axes of the unit cell. Each platinum is surrounded by four sulphur atoms in a square planar arrangement with an average Pt-S distance of 2.324 Å. The two $[Pt-S_4]$ units are rotated by 21° from the eclipsed structure. The full structure with some relevant physical properties will be discussed.

08.2-30 THE DISORDER STRUCTURE OF BENZYLURANOCENE, $(C_6H_4C_8H_8)_2U$. Allen Zalkin, Robert Kluttz and David H. Templeton, Materials and Molecular Research Division, Lawrence Berkeley Laboratory and Department of Chemistry, University of California, Berkeley, California 94720 U.S.A.

Benzyl uranocene crystallizes in the monoclinic system, space group $P2_1/c$ with cell dimensions, $a = 9.524(4)$ Å, $b = 8.558(4)$ Å, $c = 11.758(6)$ Å, $\beta = 113.52(4)^\circ$. For $Z=2$ $d_x = 2.065$ g/cm³. The uranium-phased Fourier showed severe disorder and did not reveal the molecular structure. The structure was solved by recognizing the nature of the disorder and then refining the structure by least-squares using distance restraints on the geometry of the ligands. The conventional R factor was 0.056. In each molecule the two octagonal rings are intermediate between eclipsed and staggered configurations, with the hexagonal rings about 20° from being eclipsed. Thus the external shape is somewhat symmetrical, but the uranium atom, which is sandwiched by the octagonal rings, is not in the center of the molecule. The disorder consists of a mixture of this structure and its inverse, located at the centers of symmetry of the space group in such a way that the carbon atoms of the two kinds of rings are intermingled.

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08.2-31 CRYSTAL DATA OF $NH_3(MoO_3)_3$. By J. Garin and Johnny Blanc. Departamento de Metalurgia, Universidad Técnica del Estado. Santiago, Chile.

Many compounds are formed in the system $MoO_3-NH_3-H_2O$. Several new ones have been prepared by direct synthesis from the component chemicals, and powder and single crystal data have been collected.

The crystal data for $NH_3(MoO_3)_3$ has been determined by recording three dimensional data on Weissenberg and precession photographs, using Ni-filtered $Cu K\alpha$ radiation. The compound crystallizes in the hexagonal system with space group $P6_3/m$. The unit cell dimensions are:

$$a = 10.568 \pm 0.003 \text{ \AA}, \quad c = 3.726 \pm 0.001 \text{ \AA}$$

The density calculated assuming two formula units in the unit cell is 4.137 g cm⁻³; the measured value is 4.100 g cm⁻³. The chemical composition of the crystal, calculated from data given by usual analysis techniques, was found to be very close to stoichiometry.

Studies to determine the precise crystal structure are being continued.

08.2-32 THE CRYSTAL STRUCTURE OF A SODIUM DODECAMOLYBDOMONOPHOSPHATE. By B. Hedman, Department of Inorganic Chemistry, University of Umeå, S-901 87 Umeå Sweden.

Aqueous equilibrium studies of the $H^+-MoO_4^{2-}-HPO_4^{2-}$ system have shown that complexes $(H^+)_p(MoO_4^{2-})_q(HPO_4^{2-})_r$ are formed (Pettersson, L., Chem. Scr. (1975) 7, 145). In solutions with Mo/P ratios ~2.5 complexes (p,5,2) with p=8, 9 and 10 dominate, while for Mo/P ratios 9 complexes (p,9,1) with p=14,15,16 and 17 are formed. In the most acidic range weak indications of an additional complex was found and it was assumed to be a (23,12,1) complex. Numerous solid phases with an Mo/P ratio of 12 have been reported (Gmelin, 8. Aufl., 53, (1935), 347), and the pure acid $H_3Mo_{12}P_{40} \cdot 29-30H_2O$ has been structurally investigated (Strandberg, R., Acta Chem. Scand. (1975) A29, 359). However, apart from the present phase, no single crystal investigation of a sodium salt has been reported.

By slow evaporation of extremely acidic solutions (pH<0) with a slight excess of P (Mo/P=12/1.33) bright yellow crystals were obtained. They are triclinic, $P\bar{1}$, $a=14.100(2)$, $b=15.514(2)$, $c=20.385(3)$ Å, $\alpha=85.39(1)^\circ$, $\beta=83.68(1)^\circ$, $\gamma=81.23^\circ$, $V=4370.9$ Å³, $D_m=3.20$ Mg m⁻³. A total of 22601 unique reflexions within $2\theta < 58^\circ$ were measured (4-circle diffractometer, $MoK\alpha$ -radiation, θ - 2θ scan). The unit cell contains four $Mo_{12}P_{40}^{3-}$ anions with the Keggin structure (Keggin, J.F., Proc. Roy. Soc. London (1934) A144, 75). Sodium ions and water molecules connect the anions in a three-dimensional framework. Raman spectra (Lyhamn, L. and Pettersson, L.) and ³¹P NMR spectra of solutions prepared from the solid phase as well as of the corresponding equilibrium solutions will be discussed. In addition, structural relationships between this anion and other molybdophosphate anions will be described.