Fig. 1 COORDINATION AROUND Hg IN



Hg (Br03)2 · 2H20

 $K_2H_9(BrO_3)_2(NO_3)_2$

There also exist analogous Cd compounds with the compositions Cd(BrO₃) $_2 \cdot 2H_2O$ (Murty & Murty, Z. Kristallogr. (1978) 148, 10) and K₂Cd(BrO₃) $_2$ (NO₃) $_2$. We have found that Cd(BrO₃) $_2 \cdot 2H_2O$ is isomorphous with Hg(BrO₃) $_2 \cdot 2H_2O$ and that K₂Cd(BrO₃) $_2$ (NO₃) $_2$ has most probably a structure very similar to that of the Hg-compound. The cell dimensions are close to those of K₂Hg(BrO₃) $_2$ (NO₃) $_2$ but the space group has changed from Pnnm to P2₁/n.

08.2-27 TRIPOTASSIUM cis-DIBROMO (HYDROGENDI-SULFITO) PLATINATE (II) MONOHYDRATE $K_3[Pt\{(SO_3)_2H\}Br_2] \cdot H_2O$ (I) AND ITS STRUCTURAL RELATIONSHIP TO $K_3[Pt\{(SO_3)_2H\}Cl_2]$ (II). D.K.Breitinger, G.Petrikowski and G.Bauer, Institut für Anorganische Chemie, Universität Erlangen-Nürnberg, Egerlandstr.1, D-8520 Erlangen, F.R.G. (I) crystallizes in P2 $_1$ /c with a = 8.764(4), b = 6.034(2) 2.721 544(9) 8 6.709 23(4) 9 7.4

(I) crystallizes in P2₁/c with <u>a</u> = 8.764(4), <u>b</u> = 6.934(2), <u>c</u> = 21.544(9) Å, ß = 99.32(4)°, Z = $\overline{4}$. The structure was solved by Patterson and Fourier methods using 1801 unique diffractometer data and refined to $R_{\rm W}=0.0288$. In the distorted square-planar anion Pt is surrounded by two S and two Br atoms in cis position. Short Pt-S and long Pt-Br bonds (averages 2.244 and 2.488 A, respectively) suggest a strong trans influence of the sulfite ligand. An extremely short intramolecular hydrogen bond [0.H.O distance 2.380(8) A] links the sulfite ligands to form a six-membered ring. The anions are arranged in layers, held together mainly by one kind of K+ ions and H₂O molecules. Linkage of the layers is performed by two further sets of K+ ions. In the anions of (II), Cmc21, Z = 4 (Kehr, W.G., Breitinger, D.K. and Bauer, G. (1980). Acta Cryst. B 36, 2545 - 2550) and of (I) the Pt-S and hydrogen bonds are very similar. For comparison of the structural arrangements (I) is transformed by 1,0,0;2,0,1;0,-1,0 (setting P2₁/b) and (II) by 1/2,1/2,0;0,1,0;0,0,1. Then $\underline{a}',\underline{c}'$ and χ' are almost the same in both structures, with $\underline{b}'(I)$ about 2.4 times that of (II). Building blocks common to both structures are pairs of anions correlated by 21 axes (IIc'); in (II) these pairs are the translational unit, whereas in (I) pairs of such pairs correlated by inversion centres constitute the translational unit in the layers.

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LixPt304, a member of the NaxPt304 structural family (Bergner and Kohlhaas, Z. Anorg. Allg. Chem. (1973) 401, 15), has been synthesized by solid state reaction of LiF, LiN03 and CPt02. Refinement of neutron powder diffraction data by profile analysis (Rietveld, J. Appl. Cryst. (1969) 2, 65) has determined that Li.65Pt304 is not isostructural with NaxPt304 (space group Pm3n), but belongs to the acentric subgroup P43n. Li.65Pt304, with unit cell dimension a=5.6242 A, contains Li in position 2a (0,0.0). Pt in position 6d (1/4,0,1/2) and 0 in position 8e (x,x,x) with x=0.2720(3). Equivalent isotropic temperature factors for Li, Pt and 0 are 2.8(4), 0.11(4) and 0.95(4), respectively. The structure is distinguished by distortion of the cubic coordination polyhedron about Li to two interpenetrating tetrahedra with Li-0 distances of 2.22 A and 2.65 A. Pt coordination remains square-planar with a slight tetrahedral distortion and a Pt-0 distance of 2.00 A. Refinement of scattering power on the Li site yields a Li occupancy of 0.67(5) atoms per formula unit, in close agreement with chemical analysis (0.64(11) by atomic absorption). Final discrepancy factors for this refinement are R₁=3.60, R₂=11.70 and R₃=15.94%.

Co_xNayPt₃O₄, with x-0.4 and y-0.1 as determined by atomic absorption, was synthesized by solid state reaction of CoF₂, NaF, Co(NO₃)2.6H₂O and & CPO₂. Neutron powder diffraction experiments have indicated the presence of reflections of the type hhl: 1\fo 2n, in violation of both space groups Pm3n and P43n. This reduction in symmetry is a result of ordering of Co and Na on distinguishable eight-coordinated sites. Co_xNayPt₃O₄ belongs to a subgroup of Pm3n, either the centric Pm3 or the acentric P23. Both these space groups are characterized by positions at 0,0,0 and 1/2,1/2,1/2 unrelated by symmetry, which is compatible with ordering of Co and Na.

08.2-29 PREPARATION, X-RAY STRUCTURE OF THE LINEAR CHAIN MIXED-VALENCE TETRAKIS (DITHIOACE-TATO) DIPLATINUM IODIDE: Pt₂(CH₂CS₂)₄I. By C.Bellitto, A.Flamini, L.Gastaldi and L.Scaramuzza, C.N.R., Istituto Teoria, Struttura Elettronica Composti di Coordinazione, Area della Ricerca, P.B. 10, Monterotondo Staz. (Roma) Italy.

In the past decade there has been a considerable interest in the chemical and physical properties of highly conducting 1-D systems. (See for ex. "Synthesis and properties of low-dimensional materials", Ann. N. York, Acad. Scie. 313 (1978)). In an attempt to synthesize new partially oxidized compounds, we studied the reaction of tetrakis(dithiocarboxylato)diplatinum(II)complexes with halogens (C.Bellitto , A.Flamini, unpublished results). Here we report the reaction of the tetrakis(dithioacetato)diplatinum(II) with iodine, and the crystal and molecular structure of Pt₂(CH₃CS₂)₄I .Direct reaction of equimolecular tetrakis(dithioacetato)diplatinum(II) with iodine, in toluene, gives a dark violet powder of $\text{Pt}_2(\text{CH}_3\text{CS}_2)_4^{\text{I}_2}$, while the same reaction carried out through a glass frit/polystyrol membrane, gives dark microcrystals of Pt $_2$ (CH CS $_2$) $_4$ I. The latter compound crystallises in the monoclinic C2/c space group with cell dimension : $\underline{a}=16.838(4),\underline{b}=$ 8.633(2), $\underline{c}=13.634(4)$ Å, $\beta=109.39(5)^{\circ}$, $\underline{Z}=8$. The structure was refined to R=0.06for 1206 significant reflections. The structu-