08.2-3 THE CRYSTAL STRUCTURE OF A NEW COBALT OXIDE SULFATE, $Bi_2CoO_3SO_4$. By I.A. Fanariotis and P.J.Rentzeperis, Applied Physics Laboratory, Aristotle University of Thessaloniki, Thessaloniki, Greece.

The crystal structure of $Bi_2CoO_3SO_4$ was determined within the framework of a systematic study of the various phases in the system $CoSO_4$-Bi_2O_3, prepared under different conditions.

The compound was synthesized in a crystalline form by heating a mixture of $CoSO_4$ and Bi_2O_3. The crystal structure has been determined from three-dimensional X-Ray diffraction data, collected on a computer-controlled Philips PW 1100 single crystal diffractometer (845 observed reflections). The crystals are orthorhombic, *Pbcm*, a = 7.123(2), b = 15.762(4), c = 5.416(2)Å, Z=4. The positional and thermal parameters were refined by full-matrix, least-squares calculations, to a final R=0.042. The structure in layered, with $[Bi_2CoO_3]_n$ layers normal to the a axis, interlinked by SO_4 groups (Fig. 1).

The Bi atoms, located by MULTAN, occupy two different positions and are seven coordinated, by four O atoms belonging to the layer and forming with them square pyramids (average distances : Bi(1)-O = 2.255 and Bi(2)-O=2.245Å) and three O atoms of the sulfate groups (average distances : Bi(1)-O=2.79 and Bi(2)-O=2.95Å). The Bi-O bonds to the latter may be considered as secondary bonds. The Co atom is six coordinated by four O atoms, again belonging to the layer, at the base of a square pyramid (average Co-O=2.07Å) and two further O atoms of the sulfate group at a distance 2.41Å. The six O atoms form a trigonal prism. The coordination of the O atoms in a layer is tetrahedral. Distances and angles are normal. The SO_4 tetrahedron is only slightly distorted with an average S-O=1.47Å. The layered structure explains very well the plate-like growth of the crystals normal to a.

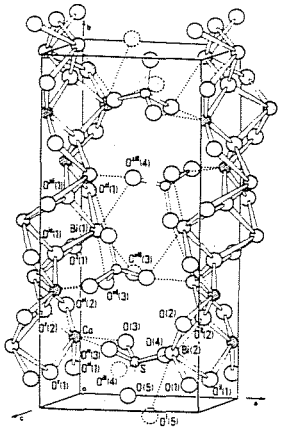

Fig. 1. Clinographic projection along the c axis.

08.2-4 CRYSTAL STRUCTURES OF SEVEN CADMIUM SELENITES. By J. Valkonen, University of Jyväskylä, Department of Chemistry, SF-40100 Jyväskylä, Finland.

Seven cadmium selenite compounds have been synthesized and their crystal structures have been solved using direct methods and least squares refinement. α-$CdSeO_3$ was found to be isomorphous with corresponding Mg, Mn, Co, Ni, Cu and Zn selenites (Kohn, Inoue, Horie and Akimoto, J. Solid State Chem. 1976, 18, 27).

Formula	a(Å)	b(Å)	c(Å)	β(°)	Z	SPGR
α-$CdSeO_3$	6.278	8.085	5.293		4	*Pnma*
β-$CdSeO_3$	5.708	12.828	8.585	101.21	8	$P2_1/c$
$CdSeO_3*\frac{3}{4}H_2O$	9.470	8.763	10.141	117.38	8	$P2_1$
$CdSe_2O_5$	8.024	11.319	6.020	119.38	4	$C2/c$
$Cd_3(HSeO_3)_2(SeO_3)_2$	9.405	9.147	7.284	112.62	2	$P2_1/c$
$(NH_4)_2Cd(SeO_3)_2$	5.714	5.714	20.033		3	$R\bar{3}$
$Cd(NH_3)SeO_3$	13.306	6.136	5.125		4	*Pnma*

Coordination number of cadmium is six in all compounds except $Cd_3(HSeO_3)_2(SeO_3)_2$. This has two different cadmium atoms with coordination numbers 6 and 7. Coordination polyhedron is octahedron for all six coordinated cadmium atoms except β-$CdSeO_3$, in which it is trigonal prism. Seven coordinated cadmium forms monocapped trigonal prism. Octahedra around cadmium atoms in $CdSeO_3*\frac{3}{4}H_2O$ are very distorted.

Formula	R(%)	N_{ref}	N_{as}	Cd-O(Å)	Se-O(Å)
α-$CdSeO_3$	2.1	730	1	2.33	1.71
β-$CdSeO_3$	4.4	2826	2	2.31	1.69
$CdSeO_3*\frac{3}{4}H_2O$	2.4	3652	4	2.30	1.70
$CdSe_2O_5$	2.8	1242	1	2.29	1.66
$Cd_3(HSeO_3)_2(SeO_3)_2$	3.4	2553	2	2.35	1.70
$(NH_4)_2Cd(SeO_3)_2$	1.2	293	1	2.32	1.69
$Cd(NH_3)SeO_3$	2.0	831	1	2.33	1.69

N_{ref} = number of refined reflections ($I>3*\sigma(I)$)
N_{as} = number of asymmetric Cd and Se atoms

Previous table shows average Cd-O and Se-O distances, but it does not contain diselenite Se-O(-Se) or hydrogenselenite Se-O(-H) distances, which are 1.80 and 1.75 Å, respectively.

All compounds form three-dimensional network. NH_3 group in $Cd(NH_3)SeO_3$ is coordinated to cadmium. Cd-N distance is 2.30 Å. NH_4 in $(NH_4)_2Cd(SeO_3)_2$ is not coordinated to cadmium.