Table 2 (*cont.*)

hkl	*d*(*hkl*)	$10^4 \sin^2\theta_o$	$10^4 \sin^2\theta_c$	I_o
310 } 221 }	2·716	804	802	59
302	2·705	810	808	100
222	2·442	994	991	31
213	2·432	1002	999	33
004	2·421	1011	1009	31
312	2·370	1056	1053	4
104	2·350	1074	1071	24
320	2·235	1188	1170	2
114	2·225	1198	1194	5
321	2·189	1238	1233	9
204	2·172	1257	1256	4
410	2·140	1295	1293	6
223	2·128	1310	1307	13
313	2·080	1371	1368	10
322	2·040	1425	1422	10
304	1·945	1568	1563	4
323	1·846	1741	1737	5
421 } 502 }	1·818	1794	1787 1791	9
314	1·809	1813	1810	5
413	1·784	1864	1861	5
510	1·759	1916	1908	12
404	1·723	1998	1994	5
215	1·716	2008	2013	26
600	1·635	2218	2216	15
414	1.603	2309	2303	9
315	1·577	2384	2377	19
520	1·570	2404	2401	5

Numerous additional observed lines less than 1·57 Å.

The density was measured by the double pycnometer method of Collett (1954), using carbon tetrachloride.

No further structural work on this substance is contemplated.

References

COLLETT, C. T. (1954). *J. Res. NBS*, **52**, 4, 201.

MURTHY, M. K. & AGUAYO, J. (1964). *J. Amer. Ceram. Soc.* **47**, 444.

NOWOTNY, H. & WITTMANN, A. (1954). *Mh. Chem.* **85**, 558.

SCHWARZ, R. & HEINRICH, F. (1932). *Z. Anorg. u. Allgem. Chem.* **205**, 43.

TRESVYATS'KII, S. G. (1958). *Dopovidi Akad. Nauk Ukr. RSR*, **3**, 295.

SHAW, A. A., CORWIN, A. A. & EDWARDS, A. A. (1958). *J. Amer. Chem. Soc.* **80**, 1536.

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Crystallography of zinc selenite dihydrate.

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(*Received* 27 *November* 1967)

$ZnSeO_3 . 2H_2O$ has 2/*m* symmetry and grows as small and well developed colorless crystals (0·1 – 5 mm) of pseudo-rhomboedral habit. The main observed interfacial angles are: (110) ∧ (102) = 63° 50′ and (110) ∧ (1$\bar{1}$0) = 80° 10′, and the observed optical constants $X=\alpha=1{\cdot}660$, $Y=\beta=1{\cdot}710$, $Z=\gamma=1{\cdot}750$; $(\gamma-\alpha)=0{\cdot}090$ and $2V_{calc}=82°$. The unit cell parameters determined in the precession photographs and refined by the powder method are $a_0=7{\cdot}68$, $b_0=8{\cdot}80$, $c_0=6{\cdot}49$ Å, $\beta=81°\ 34'$ and $a_0:b_0:c_0=0{\cdot}87:1:0{\cdot}74$. Space group $P2_1/n$. The observed specific gravity 3·52 g.cm^{-3} suggests 4 formulae per unit cell.

Selenites of several metals, such as Ni, Co, Mn, Cu and Zn, have been recently prepared by the Chemistry Department of the University of São Paulo, Brazil, and later investigated from the crystallographic point of view by various authors.

$ZnSeO_3.2H_2O$ precipitates as monoclinic crystals, with 2/*m* symmetry, the individuals being approximately equidimensional and of size of the order of a millimetre, resembling a pseudo-rhombohedral habit. Some fibrous radiated aggregates may however be formed occasionally. Most of the crystals are colourless, although a few may exhibit a white colour.

The crystal morphology is very simple, showing only the two crystallographic forms {110} and {102}, as determined by the following interfacial angles measured in the two-circle goniometer:

$$(110) \wedge (102) = 63°\,50'$$
$$(110) \wedge (1\bar{1}0) = 80°\,10'.$$

The axial ratio $a_0:b_0:c_0=0{\cdot}87:1:0{\cdot}74$, has been calculated from the unit-cell dimensions obtained by X-ray diffraction. The compound is biaxial (–), $2V=82°$, and has the following indices of refraction:

$$X=\alpha=1{\cdot}660\pm0{\cdot}005$$
$$Y=\beta=1{\cdot}710\pm0{\cdot}005$$
$$Z=\gamma=1{\cdot}750\pm0{\cdot}005.$$

The unit cell has been determined by precession methods with Mo $K\alpha$, by using photographs of the reciprocal level *h*0*l* and 0*kl*. The parameters have been refined by the powder method with Cu $K\alpha$, for greater accuracy, giving

$$a_0=7{\cdot}68, \quad b_0=8{\cdot}80, \quad c_0=6{\cdot}49\ \text{Å},$$
$$\beta=81°34'.$$

The main reflexions of the powder diagram are listed in Table 1.

Table 1. *Interplanar spacings for* $ZnSeO_3.2H_2O$

hkl	d_{calc}	d_{obs}	I_{rel}
110	5·744 Å	5·754 Å	10
10$\bar{1}$	5·314	5·322	2
11$\bar{1}$, 101	4·545	4·540	2
020	4·402	4·393	2
111	4·061	4·047	5
200, 120	3·795	3·795	5
210	3·485	3·480	6
21$\bar{1}$	3·256	3·253	2

Table 1 (*cont.*)

hkl	d_{calc}	d_{obs}	I_{rel}
121	3·173	3·167	2
012	3·019	3·015	6
11$\bar{2}$	2·950	2·953	2
130	2·737	2·732	5
031	2·670	2·666	3
12$\bar{2}$	2·552	2·556	2
221	2·520	2·516	2
31$\bar{1}$	2·390	2·390	4
230	2·322	2·321	1
202	2·291	2·287	1
23$\bar{1}$, 301	2·243	2·247	2
040	2·201	2·199	2
032	2·167	2·168	2
013, 041	2·082	2·083	1
222, 14$\bar{1}$	2·032	2·034	1
141	1·984	1·985	1
32$\bar{2}$	1·932	1·933	1
400, 33$\bar{1}$	1·898	1·897	1
30$\bar{3}$	1·770	1·772	1
420	1·743	1·741	2
150	1·715	1·715	1
241	1·695	1·694	1

In the reciprocal level *h*0*l* the absences are for $h+l=$ odd, in the 0*kl* level for 00*l*, $l=$ odd, and for 0*k*0, $k=$ odd, indicating the space group $P2_1/n$. The observed specific gravity of 3·52 g.cm^{-3}, gives 4 formulae per unit cell.

The data of the compound as compared in Table 2 with the data of other selenites published in previous papers by Camargo and others show that the following substances are isostructural: $ZnSeO_3.2H_2O$, $CoSeO_3.2H_2O$ and $NiSeO_3.2H_2O$ (see Palache, 1937; Berman, Frondel & Palache, 1951; Goñi & Guillemin, 1953; Sindeeva, 1964; Camargo, Giesbrecht & Leite, 1964; Camargo, 1965; Camargo & Leite, 1966; Camargo & Svisero, 1967).

Table 2. *Crystallographic data of selenites of* Zn, Co *and* Ni

Selenites of	Zn^{2+}	Co^{2+}	Ni^{2+}
Ionic radius (Å)	0·74	0·72	0·69
a_0 (Å)	7·68	7·58	7·55
b_0 (Å)	8·80	8·73	8·75
c_0 (Å)	6·49	6·59	6·43
β	81°34′	81°30′	81°
Space group	$P2_1/n$	$P2_1/n$	$P2_1/n$
Unit cell volume (Å^3)	434	431	420
Z	4	4	4

The authors express their gratitude to Professor Ernesto Giesbrecht of the Chemistry Department of the University of São Paulo, who was responsible for the synthesis of the material kindly offered for crystallographic study.

References

BERMAN, H., FRONDEL, C. & PALACHE, C. (1951). *The System of Mineralogy*, Vol. II. New York: John Wiley.
CAMARGO, W. G. R. (1965). *Amer. Min.* **50**, 296.
CAMARGO, W. G. R., GIESBRECHT, A. M. & LEITE, C. R. (1964). *Ciência e Cultura*, **16**, 104.
CAMARGO, W. G. R. & LEITE, C. R. (1966). *An. Acad. Bras. Cienc.* **38**, 273.
CAMARGO, W. G. R. & SVISERO, D. P. (1967). *Ciência e Cultura*, **19**, 252.
GOÑI, J. & GUILLEMIN, C. (1953). *Bull. Soc. franç. Minér. Crist.* **76**, 442.
PALACHE, C. (1937). *Amer. Min.* **22**, 790.
SINDEEVA, N. D. (1964). *Mineralogy and Types of Deposits of Selenium and Tellurium*. New York: John Wiley.

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A note on the structure of YCd_2.*

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(*Received* 9 *October* 1967)

Crystal structure data, including the results of a least-squares refinement based on single-crystal intensities, for YCd_2 (CdI_2 type structure) are presented.

Bruzzone & Ruggiero (1962) reported that the compound YCd_2 exhibits the CdI_2 ($C6$) type structure, space group $P\bar{3}m1$, with $a=4·879$, $c=3·500$ Å. Y and Cd atoms are located in equipoints 1(*a*) and 2(*d*) with $z=0·470$. However, since no details or supporting data for this work were given, we made an independent determination of the lattice and positional parameters following the procedure outlined by Michel & Ryba (1965). The alloy sample was a portion of the thermal analysis sample used in the determination of the Y–Cd phase diagram (Ryba, Kejriwal & Elmendorf, 1967). The single crystals used in the determination were coated with an acrylic plastic to retard the very rapid oxidation. The intensities of 57 *hkl* ($h=0,1,2$) reflections from a roughly cylindrical single crystal 0·03 mm in diameter × 0·29 mm in length were measured by planimetering the recorded peaks. No absorption correction was applied. The results are as follows:

$a=4·882\pm1$, $c=3·501\pm3$ Å
(Cu $K\alpha_1$ radiation; $\lambda=1·54051$ Å)
Y: 1(*a*)000; $B=1·00\pm16$ Å^2
Cd: 2(*d*)$\frac{1}{3}\frac{2}{3}z$; $z=0·4783\pm14$
$B=1·06\pm8$ Å^2
$R=9·0\%$.

The structure factors and interatomic distances are given in Tables 1 and 2, respectively.

* This investigation was supported by the Army Research Office (Durham) under Contract DA-31-124-ARO(D)-129.