

Table 1 (cont.)

<i>hkl</i>	<i>d</i> _{calc}	<i>d</i> _{obs}	<i>I</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
303	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 *h0l* the absences are for *h+l*=odd, in the *0kl* level for *00l*, *l*=odd, and for *0k0*, *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: ZnSeO₃·2H₂O, CoSeO₃·2H₂O and NiSeO₃·2H₂O (see Palache, 1937; Berman, Frondel & Palache, 1951; Goñi & Guillemin, 1953; Sindeeva, 1964; Camargo, Giesbrecht & Leite, 1964; Camargo, 1965; Camargo & Leite, 1966; Camargo & Svisero, 1967).

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A note on the structure of YCd₂.* By ROBERT ELMENDORF and EARLE RYBA, *Department of Materials Science, The Pennsylvania State University, University Park, Pennsylvania, U.S.A.*

(Received 9 October 1967)

Crystal structure data, including the results of a least-squares refinement based on single-crystal intensities, for YCd₂ (CdI₂ type structure) are presented.

Bruzzone & Ruggiero (1962) reported that the compound YCd₂ exhibits the CdI₂ (*C6*) type structure, space group *P3m1*, 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 planimetry of the recorded peaks. No absorption correction was applied. The results are as follows:

$$\begin{aligned}
 &a = 4\cdot882 \pm 1, \quad c = 3\cdot501 \pm 3 \text{ \AA} \\
 &(\text{Cu } K\alpha_1 \text{ radiation; } \lambda = 1\cdot54051 \text{ \AA}) \\
 &\text{Y: } 1(a)000; \quad B = 1\cdot00 \pm 16 \text{ \AA}^2 \\
 &\text{Cd: } 2(d)\frac{1}{2}\frac{1}{2}z; \quad z = 0\cdot4783 \pm 14 \\
 &\quad \quad \quad B = 1\cdot06 \pm 8 \text{ \AA}^2 \\
 &\quad \quad \quad R = 9\cdot0\% .
 \end{aligned}$$

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

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
<i>a</i> ₀ (Å)	7·68	7·58	7·55
<i>b</i> ₀ (Å)	8·80	8·73	8·75
<i>c</i> ₀ (Å)	6·49	6·59	6·43
β	81° 34'	81° 30'	81°
Space group	<i>P2</i> ₁ / <i>n</i>	<i>P2</i> ₁ / <i>n</i>	<i>P2</i> ₁ / <i>n</i>
Unit cell volume (Å ³)	434	431	420
<i>Z</i>	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.

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

Table 1. *Observed and calculated structure factors for YCd₂*

<i>hkl</i>	$ F_o $	F_c	<i>hkl</i>	$ F_o $	F_c
001	109	-100	01 $\bar{2}$	15	14
002	177	173	01 $\bar{3}$	44	37
003	52	-49	12 $\bar{1}$	69	71
004	85	83	12 $\bar{2}$	17	11
110	201	210	12 $\bar{3}$	14	31
220	133	136	12 $\bar{4}$	21	18
330	89	83	23 $\bar{1}$	58	46
111	89	-81	23 $\bar{3}$	21	22
221	51	-55	020	20	-10
331	39	-35	101	96	84
112	159	150	021	77	70
222	99	107	102	17	12
332	65	69	022	16	11
113	46	-44	103	29	32
223	37	-33	023	35	28
114	74	76	104	26	18
224	60	59	131	34	47
11 $\bar{1}$	86	-82	132	17	8
011	130	130	133	26	21
012	30	-32	242	11	5
013	98	88	10 $\bar{1}$	106	109
210	15	-11	10 $\bar{2}$	25	-27
121	82	93	10 $\bar{3}$	70	75

Table 1 (cont.)

<i>hkl</i>	$ F_o $	F_c	<i>hkl</i>	$ F_o $	F_c
123	71	72	10 $\bar{4}$	19	-22
124	19	-22	02 $\bar{1}$	83	91
231	47	60	02 $\bar{3}$	75	67
233	51	51	24 $\bar{1}$	34	39
01 $\bar{1}$	111	99	24 $\bar{2}$	12	-11
			13 $\bar{1}$	63	62

Table 2. *Interatomic distances for YCd₂*

Y-6Y	4.882 ± 1 Å	Cd-3Y	3.279 ± 3 Å
Y-2Y	3.501 ± 3	Cd-3Y	3.359 ± 3
Y-6Cd	3.279 ± 3	Cd-3Cd	2.823 ± 1
Y-6Cd	3.359 ± 3		

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Acta Cryst. (1968). **B24**, 463

The structure of the *M'*-phase of YTaO₄, a third fergusonite polymorph. By G. M. WOLTEN, *Aerospace Corporation, Laboratories Division, El Segundo, California, U.S.A.*

(Received 1 January 1968).

A correction to *Acta Cryst.* (1967), **23**, 939.

An error in a computer program has caused erroneous values of the bond angles to be given in Table 3 of the article under the above title (Wolten, 1967). The numbers should read, in the order given, 133.8, 91.3, 116.6, 92.7, 96.3, 130.4. The distances of Table 3 are correct.

Reference

- WOLTEN, G. M. (1967). *Acta Cryst.* **23**, 939.

Acta Cryst. (1968). **B24**, 463

Lattice parameters and space groups of some aromatic Schiff bases. By H. B. BÜRGI, J. D. DUNITZ and C. ZÜST, *Organic Chemistry Laboratory, Swiss Federal Institute of Technology, 8006 Zürich, Switzerland*

(Received 27 November 1967)

Lattice parameters and space groups of some aromatic Schiff bases are recorded.

In the course of our structural investigations of Schiff bases, we have prepared the compounds listed in column 1 of Table 1. The compounds were obtained by heating a 1:1 mixture of the corresponding aniline and benzaldehyde to about 100°C (with or without solvent). The solvent for recrystallization is indicated in column 2, Table 1.

Lattice parameters were derived from measurements on 30° precession photographs (Cu K α , $\lambda = 1.542$ Å). The stan-

dard deviations are approximately 0.2% of the values in columns 3–6, Table 1. The space groups (column 7, Table 1) are determined from systematic absences, in some cases backed by structural considerations. Measured densities, tabulated in column 9, were obtained by flotation in aqueous potassium iodide solutions.

Detailed structural investigations of I, X and XII are in progress.