

Aronsson (1961) noted that the occurrence of the FeB structure usually depends on a favourable radius ratio $r_X/r_M \simeq 0.7$ and the ratio $r_{Pa}/r_{Th} = 0.77$ is in general agreement with this observation. It is of interest to note that in several systems where compounds of the FeB type occur, compounds of the $CuAl_2$ (C16) type have also been observed, e.g. Hf-Si, Zr-Si, Mn-B, Co-B and Th-Pd.

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The structure of $SrZn_2$. By B. G. BERGMAN* and P. J. SHLICHTA†, *Gates and Crellin Laboratories of Chemistry‡, California Institute of Technology, Pasadena, California, U.S.A.*

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An investigation of the strontium-zinc system (Bergman & Shlichta, to be published) disclosed a phase, in slowly cooled alloys of 40 to 60% wt. zinc, characterized by prismatic crystals embedded in a eutectic matrix. Both crystals and matrix had to be stored under hexane to prevent reaction with air.

A chemical analysis of 50 mg of crystals, selected from an alloy containing 40% wt. zinc, indicated a composition of 55.6% wt. zinc. An alloy of 55% wt. zinc gave an X-ray powder pattern almost identical with that of the pulverized crystals; the density of this sample was 4.71 g.cm^{-3} .

Laue photographs from a single crystal, 0.2 mm long, indicated orthorhombic symmetry. The unit-cell edges, as determined by rotation and Weissenberg photographs, were $a = 4.78 \text{ \AA}$, and $b \simeq c = 7.80 \text{ \AA}$. The refined values, obtained from extreme high-angle reflections recorded on films asymmetrically mounted in a precision rotation camera, were

$$a = 4.779 \pm 0.002, \quad b = 7.795 \pm 0.001, \quad c = 7.820 \pm 0.001 \text{ \AA};$$

the precision was estimated from the differences between the $Cu K\alpha_1$ ($\lambda = 1.5405 \text{ \AA}$) and $Cu K\alpha_2$ ($\lambda = 1.5443 \text{ \AA}$) reflections. All of the 180 Weissenberg reflections observed on the layers $h = 0, 1, 2, 3$, and 4 were of the kind $h + k + l = 2n$ and $h = 2n, k = 2n, l = 0$. These indicated a body-centered unit cell with a glide plane perpendicular

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to the c axis. Hence, the probable space groups were $Imma$ (D_{2h}^{28}) and $Im2a$ (C_{2v}^{22}) both having a minimum multiplicity of four.

The measured density, chemical analysis, and unit-cell volume correspond to a unit cell content of $Sr_{4.14}Zn_{7.00}$, but, because of the fourfold multiplicity, the only permissible unit cell content for an ordered structure is Sr_4Zn_8 ; i.e. 59.8% wt. zinc with $\rho = 4.98 \text{ g.cm}^{-3}$.

Layer lines with alternate values of h had closely similar intensity distributions, indicating that the structure consisted of planar layers, perpendicular to the a axis, with a spacing of $a/2$. The only permissible positions for the four strontium atoms, compatible with their large size and the layering and symmetry requirements, are $4(e)$ of $Imma$ (D_{2h}^{28}), namely $(0, 0, 0; \frac{1}{2}, \frac{1}{2}, \frac{1}{2}) + 0, \frac{1}{4}, z; 0, \frac{3}{4}, \bar{z}$, where $z < 0.10$. This arrangement leaves holes appropriate for the accommodation of eight zinc atoms at $8(h)$: $(0, 0, 0; \frac{1}{2}, \frac{1}{2}, \frac{1}{2}) + 0, y, z; 0, \bar{y}, \bar{z}; 0, (\frac{1}{2} + y), \bar{z}; 0, (\frac{1}{2} - y), z$, where $y > 0.90$ and $z \simeq 0.33$. Equalization of the Sr-Sr and of the Zn-Zn contact distances yields $z = 0.051$ for Sr and $y = 0.95, z = 0.325$ for Zn. Trial and error adjustment, to obtain the best qualitative agreement with the $0k0$ and $00l$ reflections, resulted in $z = 0.049$ for Sr and $y = 0.941, z = 0.338$ for Zn. The intensities calculated from these parameters gave good

Table 1. *Refinement of parameters*

		Trial and error	Least squares 1st	2nd
4 Sr in 4(e)	x	0	0	0
	y	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$
	z	0.049	0.051	0.052
8 Zn in 8(h)	x	0	0	0
	y	0.941	0.939	0.939
	z	0.338	0.335	0.335
	B_y	0.238	1.086	0.006
	B_z			1.019
	R	23.1%	17.9%	17.6%

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qualitative agreement with those observed in 35 out of the 40 $0kl$ reflections used; four of the remaining five were at high θ values and therefore sensitive to slight variations of the positional parameters.

The intensities of the $0kl$ Weissenberg reflections were estimated visually by the method of de Lange, Robertson & Woodward (1939). The intensity strips were calibrated against each other and were found to have a relative precision of one exposure interval or better. The structure was refined by the method of least squares (Hughes, 1941). The weighting factors were $W = 1/(\sigma_F \cdot F^2)$, where σ_F

Table 2. Observed and calculated structure factors

hkl	F_o	F_c	wt.	hkl	F_o	F_c	wt.
000	—	—	—	051	63	83	28
002	15	5	66	053	76	-68	23
004	68	-59	13	055	176	-170	6
006	109	92	5	057	7	16	1
008	84	-105	14				
				060	137	-170	7
011	27	25	12	062	26	-28	16
013	106	-91	13	064	20	18	91
015	155	-139	25	066	35	-34	28
017	24	-26	45				
019	11	-10	113				
				071	40	66	30
020	8	16	95	073	64	64	21
022	131	-155	6	075	49	36	42
024	95	-84	11	077	43	75	11
026	113	118	10				
028	34	34	56	080	13	-22	23
031	142	174	5	082	90	102	7
033	100	88	10	084	54	64	18
035	19	-17	85				
037	125	134	9	091	54	-45	40
039	14	20	63	093	56	-55	22
040	84	107	6				
042	90	75	19				
044	33	21	36				
046	37	-27	26				
048	44	-60	12				

was the standard deviation (in intensity strip units) of the measurements of each reflection. The atomic scattering factors for Zn were taken from Berghuis, Haanappel, Potters, Loopstra, MacGillavry & Veenendaal (1955). No scattering factors of comparable precision were available for Sr, but the values given by Berghuis for Zn correspond closely to the arithmetic mean of the Thomas-Fermi and Pauling-Sherman values. Such an average was therefore used for f_{Sr} . A plot of $\log F_o/F_c$ versus $\sin^2 \theta$ indicated after the first cycle anisotropy in the temperature factor, probably due to absorption. This term was therefore split into two directional parts, the parameters of which are B_y and B_z given in Table 1.

Table 3. Interatomic distances in $SrZn_2$

Zn-2 Zn	2.73 Å	Sr-2 Sr	3.91 Å
-1 Zn	2.75	-2 Sr	3.98
-1 Zn	2.95	-4 Zn	3.28
-2 Sr	3.28	-2 Zn	3.28
-1 Sr	3.28	-2 Zn	3.37
-1 Sr	3.37	-4 Zn	3.52
-2 Sr	3.52		

The results of the least-squares refinements are given in Table 1, the final structure factors are listed in Table 2, and the interatomic distances in Table 3.

The structure is of the same type as that of $CeCu_2$ reported by Larson & Cromer (1961); the positional parameters as well as the ratios between the cell edges are nearly the same in both structures.

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Paramètres cristallins et groupe de symétrie de position du sulfite de magnésium trihydraté, $MgSO_3 \cdot 3H_2O$. Par JEAN-PAUL WENDLING et RAYMOND WEISS, Laboratoire de Chimie Minérale Structurale, Institut de Chimie de l'Université de Strasbourg, B.P. 296, Strasbourg (Bas-Rhin), France

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Le sulfite de magnésium trihydraté $MgSO_3 \cdot 3H_2O$ cristallise par évaporation d'une solution aqueuse de sulfite acide de magnésium portée à une température voisine de 90 °C, en atmosphère inerte.

Les cristaux appartiennent au système orthorhombique; la classe de symétrie d'orientation est $mm2$. Ils sont faiblement piézoélectriques. Les formes observées sont:

$\frac{1}{2}\{111\}$, $\frac{1}{2}\{11\bar{1}\}$ et $\{120\}$ avec $a:b:c=1,06:1:0,59$.

Des clichés de cristal tournant autour des axes $[100]$, $[010]$ et $[001]$, des rétigrammes contenant les nœuds $0kl$, $1kl$, $2kl$, $3kl$, $h0l$, $h1l$, $hk0$ et $hk1$ et un diffractogramme ont conduit à;

$$a = 9,54 \pm 0,02, \quad b = 9,36 \pm 0,02, \quad c = 5,51 \pm 0,01 \text{ \AA};$$

$$a : b : c = 1,019 : 1 : 0,588;$$

$$Z = 3,98 \pm 4 \text{ avec } d_{mes.} = 2,13;$$

$$\lambda \text{ Cu } K\alpha = 1,5418 \text{ \AA}.$$

Les rétigrammes ne comportent pas d'extinctions systématiques des nœuds hkl ; le mode de réseau est primitif.

Les nœuds $0kl$ sont systématiquement éteints lorsque la somme $k+l$ est égale à $2n+1$; les nœuds $h0l$ sont systématiquement éteints lorsque l'indice h est égal à $2n+1$.

Le groupe de symétrie de position compatible avec les extinctions relevées et l'effet piézoélectrique observé est; $Pna2_1 (C_{2v}^9)$.

Une étude détaillée de la structure est en cours.