

observations many times greater than the maximum possible error. Furthermore, line 9 is sharp and not diffuse as required by Donohue's indexing.

The writer states without reservation that the orthorhombic structure for protactinium metal proposed in the preceding note must be rejected as incorrect because it does not fit the data.

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Crystal structures of $ZrBe_5$ and Zr_2Be_{17} .* By ALLAN ZALKIN, RAY G. BEDFORD and DONALD E. SANDS, Lawrence Radiation Laboratory, University of California, Livermore, California, U. S. A.

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An investigation of the Zr-Be system was undertaken to determine the number and compositions of the intermetallic compounds formed in this system. A variety of compositions of the elemental powders were weighed, mixed and heated to 1600 °C; these were crushed again and reheated. The resulting products were studied by X-ray diffraction powder methods using Debye-Scherrer techniques; both $Cu K\alpha$ ($\lambda = 1.5418$) and $Cr K\alpha$ ($\lambda = 2.2909$ Å) X-rays were used.

The resulting powder photographs showed four intermetallic phases. Two of these phases had been previously reported, $ZrBe_2$ (Nielsen & Baenziger, 1954) and $ZrBe_{13}$ (Baenziger & Rundle, 1949); two new phases hitherto unreported were found in the intermediate composition range, $ZrBe_5$ and Zr_2Be_{17} .

The structure of $ZrBe_5$ was determined from its powder pattern. The cell volume and the resulting intermetallic distances indicated the above formula. A powder pattern of a sample prepared using the above stoichiometry indicated a fairly pure $ZrBe_5$ phase. The Zr_2Be_{17} structure was determined from the close similarity of its powder patterns with those of Nb_2Be_{17} .

$ZrBe_5$

$ZrBe_5$ has a hexagonal cell with dimensions

$$a = 4.564 \pm 0.002, \quad c = 3.485 \pm 0.002 \text{ Å}.$$

There is one formula unit per unit cell. The X-ray density is 3.60 g.cm.⁻³. The structure has the $CaZn_5$ type structure (Haucke, 1940). The space group is D_{6h}^1-P6/mmm (*International Tables for X-ray Crystallography*, 1952). The atomic positions are:

1 Zr	(a)	0, 0, 0.
2 Be _I	(c)	$\frac{1}{3}, \frac{2}{3}, 0; \frac{2}{3}, \frac{1}{3}, 0.$
3 Be _{II}	(g)	$\frac{1}{2}, 0, \frac{1}{2}; 0, \frac{1}{2}, \frac{1}{2}; \frac{1}{2}, \frac{1}{2}, \frac{1}{2}.$

The interatomic distances are:

Zr- 6 Be	2.635 Å
-12 Be _{II}	2.871
Be _I - 3 Zr	2.635
- 6 Be _{II}	2.191
Be _{II} - 2 Zr	2.871
- 4 Be _I	2.191
- 4 Be _{II}	2.282

* This work was performed under the auspices of the U.S. Atomic Energy Commission.

Both of the original films are, of course, available on loan from the writer's collection.

Reference

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Zr_2Be_{17}

Zr_2Be_{17} has a rhombohedral cell with $a = 5.694 \pm 0.005$ Å and $\alpha = 83.02 \pm 0.02^\circ$. The triply primitive hexagonal cell has $a = 7.548 \pm 0.004$, $c = 10.997 \pm 0.010$ Å and $c/a = 1.457$. There are 3 formula units in the hexagonal cell. The X-ray density is 3.081 g.cm.⁻³. This structure is isomorphous with the Nb_2Be_{17} type structure (Zalkin, Sands & Krikorian, 1959). The space group is $R\bar{3}m$.

Table 1 shows the first 15 lines of powder patterns of these two structures. $Cr K\alpha$ radiation were used to obtain these patterns. In the case of Zr_2Be_{17} , the hexagonal indices are used.

Table 1. Powder patterns for $ZrBe_5$ and Zr_2Be_{17}

$ZrBe_5$			Zr_2Be_{17}		
<i>I</i>	<i>hkl</i>	<i>d</i> (Å)	<i>I</i>	<i>hkl</i>	<i>d</i> (Å)
<i>s</i> -	100	3.953	<i>m</i>	101	5.619
<i>m</i>	001	3.485	<i>m</i> -	102	4.208
<i>s</i> +	101	2.614	<i>s</i>	110	3.773
<i>m</i> +	110	2.282	<i>w</i> +	003	3.666
<i>m</i> +	200	1.976	<i>w</i> +	201	3.132
<i>s</i>	111	1.909	<i>w</i>	202	2.809
<i>w</i>	002	1.743	<i>s</i>	113	2.629
<i>m</i>	201	1.719	<i>w</i>	104	2.534
<i>m</i> -	102	1.594	<i>w</i> +	211	2.411
<i>m</i> -	210	1.494	<i>w</i>	212	2.253
<i>m</i>	112	1.385	<i>m</i> -	300	2.179
<i>m</i> +	211	1.373	<i>w</i>	204	2.104
<i>w</i> -	300	1.318	<i>w</i> -	105	2.085
<i>m</i>	202	1.307	<i>m</i> +	220	1.886
<i>m</i> +	301	1.232	<i>m</i> +	303	1.873

w = weak; *m* = medium; *s* = strong.

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