

thites is virtually the same as in normal anorthite, differences being less than $20'$. As would be expected, the cell dimensions differ slightly.

The main reflections are thus virtually identical to those in anorthite. The intensity relations of the (*b*) subsidiary spots are greatly different in Ga-containing anorthite, Ge-containing anorthite, and normal anorthite. However, the general intensity relations of the Ga- and Ge-containing anorthite are much like those of normal anorthite. It is thus obvious that the (*b*) subsidiary reflections are controlled by Al and Si positions. The (*c*) type subsidiary reflections appear the same in all of the synthetic compounds, including normal anorthite. It is thus concluded that the Ca atoms are those influencing the (*c*) type subsidiary reflections.

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Variations in the anorthite structure: a note. By P. GAY and W. H. TAYLOR, *Crystallographic Laboratory, Cavendish Laboratory, Cambridge, England*

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The publication, in the preceding note by Laves & Goldsmith (1954), of abstracts (originally dated 1951) of their work on anorthite is very convenient. We still feel some regret that the authors have not yet published details of their work on this very complex problem.

We are glad to re-emphasize that our own findings are in no way in conflict with what we have gathered of the significance of the work of Laves & Goldsmith; this was made quite clear in our earlier publication (Gay & Taylor, 1953) where we refer three times to the 'similar observations' and 'similar ideas' of Laves & Goldsmith appearing in their publication, to which full and complete references were given by us.

Laves & Goldsmith quote the phrase 'not previously described' used by us in reference to the *D* pattern. Read in context in our paper, we hope it is clear that the phrase refers to the fact that whereas Cole, Sörum & Taylor (1951) discussed the *S* and *A* patterns, the *D* pattern was not previously described by them, for the remark appears in a section devoted to brief recapitulation of experimental

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The crystal structures of ZrBeSi and ZrBe₂. By J. W. NIELSEN and N. C. BAENZIGER, *Department of Chemistry, State University of Iowa, Iowa City, Iowa, U.S.A.*

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ZrBeSi

During an attempt to prepare a barium-beryllium alloy, reaction with a zirconium silicate crucible took place. The small cluster of crystals formed in the reaction product did not provide sufficient sample for quantitative chemical analysis. The composition of the crystals was determined primarily from X-ray diffraction data together

References

- COLE, W. F., SÖRUM, H. & TAYLOR, W. H. (1951). *Acta Cryst.* **4**, 20.
 GAY, P. & TAYLOR, W. H. (1953). *Acta Cryst.* **6**, 647.
 GOLDSMITH, J. R. & LAVES, F. (1951). A. C. A. Meeting, Chicago, October 1951. (Abstract, p. 11.)
 LAVES, F. & GOLDSMITH, J. R. (1951a). International Congress of Crystallography, Stockholm, June 1951. (Abstract.)
 LAVES, F. & GOLDSMITH, J. R. (1951b). A. C. A. Meeting, Chicago, October 1951. (Abstract, p. 10.)
 LAVES, F. & GOLDSMITH, J. R. (1951c). Mineralogical Society of America Meeting, Detroit, November 1951. (Abstract; also *Amer. Min.* (1952), **37**, 295.)

observations made in this laboratory, in a paragraph dealing with Gay's recent work, and in a sentence which compares this with the results of Cole *et al.*, mentioned in the line above. We realize, after reading the note by Laves & Goldsmith, that it is possible to misunderstand our wording at this place. We regret this, but would point out that if the whole paper is read, and that of Gay (1953) on which our discussion is based, it is abundantly clear that we have in no way underestimated the value of Laves & Goldsmith's researches.

References

- COLE, W. F., SÖRUM, H. & TAYLOR, W. H. (1951). *Acta Cryst.* **4**, 20.
 GAY, P. (1953). *Miner. Mag.* **30**, 169.
 GAY, P. & TAYLOR, W. H. (1953). *Acta Cryst.* **6**, 647.
 LAVES, F. & GOLDSMITH, J. R. (1954). *Acta Cryst.* **7**, 131.

with a few qualitative chemical tests. Synthesis of the compound further verified the composition as ZrBeSi.

Zero- to fourth-layer Weissenberg diagrams, using Cu *K* radiation, were obtained from one of the crystals, and the dimensions of the hexagonal cell were determined from a powder diagram. Final intensity comparisons were made on the basis of the powder diagrams. The unit cell dimensions are

Table 2. Intensity comparisons for ZrBeSi

(<i>hkl</i>)	<i>I_c</i>	<i>I_o</i>	(<i>hkl</i>)	<i>I_c</i>	<i>I_o</i>	(<i>hkl</i>)	<i>I_c</i>	<i>I_o</i>
00.1	0		21.1	7	}	31.0	36	<i>w</i>
00.2	145	<i>m</i>	20.4	47		31.1	4	
10.0	355	<i>s</i>	00.6	5	}	31.2	165	}
10.1	58	<i>w</i>	21.2	185		22.3	0	
00.3	0	}	11.5	0	20.7	2	}	
10.2	1227		<i>vs</i>	10.6	84	10.8		39
10.3	16	<i>vw</i>	21.3	5	30.5	0		
11.0	305	<i>ms</i>	30.0	54	}	21.6	172	<i>s</i>
11.1	0	}	20.5	2		31.3	5	
00.4	93		<i>mw</i>	30.1	0	22.4	141	<i>ms</i>
11.2	85	<i>mw</i>	30.2	20	}	11.8	152	<i>ms</i>
20.0	65	<i>w+</i>	00.7	0		40.0	31	
20.1	9	}	21.4	67	00.9	0		
10.4	119		<i>mw</i>	11.6	20	30.6	42	}
20.2	207	}	30.3	0	31.4	134	}	
11.3	0		<i>ms</i>	10.7	0	40.1		3
00.5	0		20.6	73	20.8	96	}	
20.3	7		21.5	4	31.7	10		}
10.5	6		22.0	49	40.2	194		
11.4	181	<i>ms</i>	22.1	0	}	22.5	0	}
21.0	108	<i>mw</i>	30.4	99		10.9	8	
			22.2	22				
			00.8	17				
			11.7	0				

$$a = 3.71 \text{ \AA}, c = 7.19 \text{ \AA}, U = 85.8 \text{ \AA}^3, Z = 2, \\ D_x = 4.95 \text{ g.cm.}^{-3}.$$

The structure is the 'filled' nickel arsenide structure with the atoms located as follows:

$$\begin{aligned} 2 \text{ Zr at } & 0, 0, 0; 0, 0, \frac{1}{2}; \\ 2 \text{ Be at } & \frac{1}{3}, \frac{2}{3}, \frac{1}{4}; \frac{2}{3}, \frac{1}{3}, \frac{3}{4}; \\ 2 \text{ Si at } & \frac{2}{3}, \frac{1}{3}, \frac{1}{4}; \frac{1}{3}, \frac{2}{3}, \frac{3}{4}. \end{aligned}$$

The ideal structure has a rather short Si-Be distance (2.14 Å) so that structures deviating from the ideal arrangement were investigated. Owing to the low relative scattering powers of Si and Be compared to Zr, their positions cannot be fixed precisely. Comparisons of the intensities of suitable neighboring sets of lines on the powder diagram indicate limits in the parameter variation. The observed order of the nearly equal reflections (00.4) > (11.2) > (20.0) would be altered for a change of the Si parameter greater than 0.02 from its value of 0.25.

Table 1. Interatomic distances in ZrBeSi

Atom	Number of neighbors	Distance (Å)
Zr	2 Zr	3.60
	6 Zr	3.71
	6 Si	2.80
	6 Be	2.80
Si	6 Zr	2.80
	3 Be	2.14
	6 Si	3.71
Be	6 Zr	2.80
	3 Si	2.14
	6 Be	3.71

Comparisons of (21.6), (22.4), (11.8) and (31.4), (30.6), (40.1) also support this conclusion. Beryllium atoms can be placed almost anywhere without affecting the intensities. Making the maximum possible variation of Si and Be positions consistent with the observed intensities and also reasonable Zr-Be distances enables the Si-Be distance to be increased by only 0.01 Å. It is likely that a change from the ideal structure is not justified.

The interatomic distances are given in Table 1. The comparison of calculated and observed intensities is given in Table 2.

ZrBe₂

The compound ZrBe₂ has been prepared and found from powder diagrams to have the aluminum boride structure. The unit cell dimensions are

$$a = 3.82 \text{ \AA}, c = 3.24 \text{ \AA}, U = 41.9 \text{ \AA}^3, Z = 1, \\ D_x = 4.32 \text{ g.cm.}^{-3}.$$

The interatomic distances are shown in Table 3.

Table 3. Interatomic distances in ZrBe₂

Atom	Number of neighbors	Distance (Å)
Zr	12 Be	2.74
	2 Zr	3.24
	Be	3 Be
2 Be		3.24
6 Zr		2.74

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