

alanine by preparing mixtures containing equal quantities of the pure optical isomers and crystallizing these mixtures from various solvents. With dialanine two types of triclinic crystals were obtained from water-methylcellosolve and water-dioxane solutions respectively. The crystals from the former mixture were anhydrous, while those from the latter contained one-half molecule of water for each molecule of peptide. The Weissenberg photographs of both forms revealed no symmetry elements or systematic absences, consequently the space groups of both crystals were either  $P\bar{1}$  or  $P1$ . Unfortunately, we

were unable to obtain data which would serve to distinguish between these two space groups, and since resolution could easily have taken place during crystallization, it was uncertain whether these were crystals of racemates or of pure optical isomers. Data for these crystals are listed in Table 1. Mixtures of the trialanines yielded only very poor crystals which were unsatisfactory for X-ray examination.

We wish to thank Dr Robert B. Corey, who suggested this investigation, for helpful advice and discussion.

Table 1. *Crystallographic data*

Peptide	Crystal system	Space group	General positions in unit cell	Molecules in unit cell	Unit-cell dimensions			Density (g.cm. <sup>-3</sup> )
					$a$ (Å)	$b$ (Å)	$c$ (Å)	
D,D-Dialanine	Tetragonal	$I4$	8	8.05	18.00	18.00	5.16	1.280
L,L,L-Trialanine	Monoclinic	$P2_1$	2	4.01	9.86	10.04	11.88	1.333
$\beta = 101^\circ$								
Dialanine (D,D- or racemate)	Triclinic	$P1$	1	8.00	14.10	12.02	10.51	1.261
		or $P\bar{1}$	2		$\alpha = 105^\circ$	$\beta = 101^\circ$	$\gamma = 90^\circ$	
Dialanine $\frac{1}{2}\text{H}_2\text{O}$ (D,D- or racemate)	Triclinic	$P1$	1	2.00	5.15	13.34	13.47	1.277
		or $P\bar{1}$	2		$\alpha = 102^\circ$	$\beta = 96^\circ$	$\gamma = 101^\circ$	

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**Hexagonal  $\text{CaAl}_2\text{Si}_2\text{O}_8$ .** By GABRIELLE DONNAY, *Geophysical Laboratory, Carnegie Institution of Washington, 2801 Upton Street, Washington 8, D.C., U.S.A.*

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$\text{CaAl}_2\text{Si}_2\text{O}_8$ , which in nature is triclinic (anorthite), has been synthesized recently in two polymorphic forms (Davis & Tuttle, 1951). Dr N. L. Bowen kindly supplied a sample of one of the forms for single-crystal work. Equi-inclination Weissenberg photographs show the crystals to be hexagonal with diffraction symbol  $6/mmm$   $C-/-$ . The cell dimensions are

$$a = 5.10 \pm 0.01, \quad c = 2 \times 7.36 \pm 0.01 \text{ Å.}$$

Reflections with  $l$  odd are few and very weak, many of them barely discernible, indicating marked pseudo-halving of  $c$ . With two formula units per cell,

$$d_{\text{calc.}} = 2.78 \text{ g.cm.}^{-3}$$

as compared with

$$d_{\text{meas.}} = 2.7 \pm 0.1 \text{ g.cm.}^{-3}.$$

W. L. Bond (Bell Telephone Laboratories) kindly performed pyroelectric and piezoelectric tests, and could not rule out a center of symmetry. The most probable space group is therefore  $C6/mmm$ .

Ito (1950) has proposed a structure for  $\alpha$ -celsian, the high-temperature modification of  $\text{BaAl}_2\text{Si}_2\text{O}_8$ . Because this barium compound and the new calcium compound have similar physical properties and cell dimensions, and because they belong to the same space group, they were suspected of being isostructural. Structure-factor calculations, however, have disproved this hypothesis.

Perfect cleavage on  $(00.1)$  indicates a layer structure. The  $a$ -axis Weissenberg photographs of the odd (1st and 3rd) levels (taken by Mr K. Güler) show streaks along the festoons representing reciprocal-lattice rows parallel to  $[00.1]^*$ . Mistakes in the stacking of the layers may therefore be expected. The structure determination will be attempted.

## References

- DAVIS, G. L. & TUTTLE, O. F. (1951). *Two New Crystal-line Phases of the Anorthite Composition*,  $\text{CaO} \cdot \text{Al}_2\text{O}_3 \cdot 2\text{SiO}_2$ . In preparation.
- ITO, T. (1950). *X-Ray Studies on Polymorphism*. Tokyo: Maruzen.

## Notes and News

*Announcements and other items of crystallographic interest will be published under this heading at the discretion of the Editorial Board. Copy should be sent direct to the British Co-editor (R. C. Evans, Crystallographic Laboratory, Cavendish Laboratory, Cambridge, England).*

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