

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
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 $\frac{1}{2}$ H <sub>2</sub> 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 CaAl<sub>2</sub>Si<sub>2</sub>O<sub>8</sub>.** By GABRIELLE DONNAY, *Geophysical Laboratory, Carnegie Institution of Washington, 2801 Upton Street, Washington 8, D.C., U.S.A.*

(Received 11 October 1951)

CaAl<sub>2</sub>Si<sub>2</sub>O<sub>8</sub>, 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

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

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 BaAl<sub>2</sub>Si<sub>2</sub>O<sub>8</sub>. 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*, CaO.Al<sub>2</sub>O<sub>3</sub>.2SiO<sub>2</sub>. 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).*

### *Acta Crystallographica*: important notice

The Executive Committee has decided to entrust the publication of this journal to Messrs Ejnar Munksgaard of Copenhagen as from 1 January 1952. The subscription price per volume is now 100 Danish crowns post free, or its equivalent in other currencies. (At the present rates

of exchange American and British subscriptions will be accepted at \$15 and £5 respectively.) Orders should be placed direct with the publisher (Ejnar Munksgaard, Nørregade 6, Copenhagen, Denmark) or with any bookseller. Advance orders for complete volumes from subscribers in the United States of America, its territories and

possessions, in Canada and in Mexico may alternatively be placed through the American Institute of Physics, 57 E 55th Street, New York 22, N.Y., U.S.A. at a price of \$15 post free.

Orders already placed with the Cambridge University Press will be forwarded to the new publishers and no further action on the part of subscribers is necessary.

As already announced, it is proposed to make arrangements whereby bona fide crystallographers may obtain the journal for their private use at a reduced price. Such subscriptions, at a rate of 60 Danish crowns or \$9 post free, can be accepted *only if placed direct* with Messrs Ejnar Munksgaard or with the American Institute of Physics, and *must be accompanied by a declaration* that the journal will be used solely for the personal purposes of the subscriber. Unless such a declaration is given, correspondence and delay will be involved. Proposals are still awaited from some of the Adhering Bodies and at present it is possible to offer this concession only as follows:

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The Crystallographic Society of Japan.

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Det Kgl. Norske Videnskabers Selskab, Norsk Geologisk Forening, Norsk Kjemisk Selskap.

The Chemical Society, the Institute of Metals, the Institute of Physics, the Iron and Steel Institute, the Physical Society, the Royal Society.

The American Crystallographic Association.

*In placing their orders, subscribers in these countries should state of which society they are members.*

Further announcements will be made as soon as it is possible to give details of arrangements in other countries.

### Commission on Solid-State Physics

The International Union of Pure and Applied Physics has established a Commission on Solid-State Physics and has invited certain other Unions to appoint representatives. The Executive Committee of the International Union of Crystallography has nominated as its representatives P. P. Ewald (U.S.A.), A. Guinier (France) and W. H. Taylor (U.K.). Crystallographers interested in the work of this Commission are invited to communicate with its Secretary (P. P. Ewald, Polytechnic Institute of Brooklyn, 99 Livingston Street, Brooklyn 2, N.Y., U.S.A.).

### Book Reviews

*Works intended for notice in this column should be sent direct to the Editor (P. P. Ewald, Polytechnic Institute of Brooklyn, 99 Livingston Street, Brooklyn 2, N.Y., U.S.A.). As far as practicable books will be reviewed in a country different from that of publication.*

#### Structure of Molecules and the Chemical Bond.

By Y. K. SYRKIN and M. E. DYATKINA, translated and revised by M. A. PARTRIDGE and D. O. JORDAN. Pp. ix + 509, with 87 figs. and 174 tables. New York: Interscience Publishers; London: Butterworth's Scientific Publications. 1950. Price \$8.75; 63s.

Like many young and rapidly growing subjects, theoretical chemistry is difficult to present as a coherent whole. The subject has, moreover, its own peculiar weaknesses, which often lead the experimental chemist to doubt its value as an independent discipline. It is a commonplace that all the facts of molecular structure could in principle be derived from the wave equation; it is equally well known that this equation cannot be solved explicitly if more than one electron is present. Progress therefore depends entirely upon the shrewd choice of assumptions and approximations in solving the wave equation; and many of the most important con-

cepts, such as 'resonance', 'bond order', 'electronegativity', 'molecular orbital', 'hybridization' and 'ionic character', only have meaning in terms of some particular framework of approximations.

One's immediate questions about a new book such as this are: First, does it make clear the basic assumptions on which the theory rests? Secondly, are the secondary concepts properly defined, and their range of application and limitations fully discussed? And thirdly, how useful will the book be to research workers and students in enabling them to interpret, correlate, and even predict, new experimental facts?

Judged by the third of these criteria, *The Structure of Molecules* is a good book. The qualitative discussion of various molecular properties, particularly in Chapters 8-16, is clear and readable, and packed with interesting examples and useful tables. The chapter on the chemical bond in crystals, which is perhaps of special interest to readers of this journal, is authoritative and well docu-