

diffracting qualities usually preclude their practical use.

One such crystal which appears to overcome these difficulties, however, is dioctadecyl adipate,



Excellent single crystals can be grown in benzene.

Small crystals were subjected to X-ray analysis and the unit-cell dimensions were determined from Weissenberg and precession photographs with Cu  $K\alpha$  radiation. The cell is monoclinic with

$$a = 44.45, b = 7.414, c = 94.76 \text{ \AA}, \beta = 107^\circ 20'.$$

Systematic absences and optical examination show that it belongs to space group  $A2/a$  or  $Aa$ . The density was measured by the flotation method in a mixture of water and methanol and found to be  $0.883 \text{ g.cm}^{-3}$ . This density corresponds to 24 molecules per cell. The melting point is  $64^\circ \text{C}$ .

The maximum usable  $2d$  spacing of the crystal is  $90.55 \text{ \AA}$  (002 plane) and the reflections are fairly strong. Fortunately, the crystals grow in platelet form with the large face parallel to the  $90 \text{ \AA}$  spacing.

Dioctadecyl adipate gives a rather poor powder pattern and the large cell dimensions make it quite difficult to assign all possible indices to each powder line. There were, however, about twenty spots on the single-crystal photographs which were much more intense than the rest of

the spots and these were used to index the powder pattern as is shown in Table 1. The pattern was taken with a 2-radian Debye-Scherrer camera and Cu  $K\alpha$  radiation.

Table 1. Indexed powder pattern for  $\text{C}_{42}\text{H}_{82}\text{O}_4$

$d$	$I/I_1$	$hkl$
14.9 Å	1	006
11.3	< 1	008
9.06	< 1	0,0,10
4.13	100	717
3.70	30	020
3.23	1	0,0,28
2.48	5	14,0,14
2.22	5	18,0,30
1.99	10	4,0,42
1.72	5	25,1,23

The generosity of Dr Warren Ruderman of Isomet Corporation for supplying the single crystals is gratefully acknowledged.

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### Gadolinium and dysprosium intermetallic phases. III. The structures of $\text{Gd}_3\text{Al}_2$ , $\text{Dy}_3\text{Al}_2$ , $\text{Gd}_5\text{Ge}_3$ , $\text{Dy}_5\text{Ge}_3$ and $\text{DyAl}_3$ . By N. C. BAENZIGER and J. J. HEGENBARTH, *Department of Chemistry, State University of Iowa, Iowa City, Iowa, U.S.A.*

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The structures of  $\text{Dy}_3\text{Al}_{12}$  and  $\text{Gd}_3\text{Al}_2$  were determined by single-crystal X-ray diffraction techniques. Single-crystal chips from arc-melted alloys (for preparation, see Baenziger & Moriarty, 1961) were mounted and aligned on Buerger precession cameras. The tetragonal cell constants are for  $\text{Gd}_3\text{Al}_2$ :

$$a = 8.344 \pm 0.004, c = 7.656 \pm 0.006 \text{ \AA}, Z = 4;$$

for  $\text{Dy}_3\text{Al}_2$ :

$$a = 8.164 \pm 0.005, c = 7.560 \pm 0.007 \text{ \AA}, Z = 4.$$

Possible space groups are  $P4_2nm$ ,  $P\bar{4}n2$ ,  $P4_2/mnm$ .

Since the smallest and most perfect alloy fragment found was from a  $\text{Gd}_3\text{Al}_2$  alloy, the intensity data were collected from this crystal. Precession data ( $0kl$  to  $3kl$ ) and Weissenberg ( $hkl$ ) were collected and estimated by visual comparison with a calibrated intensity strip. The data were corrected by Lorentz and polarization factors, but not for absorption. Patterson maps calculated from the ( $hkl$ ) and ( $0kl$ ) data suggested that the structure was similar to that reported by Edshammar (1962) for  $\text{Hf}_3\text{Al}_2$ . (Edshammar determined this structure from powder data but did not report any parameters, only a projection of the structure.) Trial structures in space groups  $P\bar{4}n2$  and  $P4_2/mnm$  using the Patterson parameters for Gd did not refine below  $R = 39\%$ . The trial structure in

$P4_2nm$  refined in five cycles of least-squares to  $R = 12.2\%$  including absent reflections ( $R = 10.6\%$  for present reflections only).

The final atomic positions are:

4 Gd(1) in (c):

$$x, x, z; \bar{x}, \bar{x}, z; \frac{1}{2} + x, \frac{1}{2} - x, \frac{1}{2} + z; \\ \frac{1}{2} - x, \frac{1}{2} + x, \frac{1}{2} + z; \text{ with } x = 0.152 \pm 0.0006, \\ z = 0.268 \pm 0.0008, B = 1.55 \text{ \AA}^2.$$

4 Gd(2) in (c):

$$\text{with } x = 0.205 \pm 0.0006, z = 0.742 \pm 0.0008, \\ B = 1.65 \text{ \AA}^2.$$

4 Gd(3) in (b):

$$0, \frac{1}{2}, z; \frac{1}{2}, 0, z; 0, \frac{1}{2}, \frac{1}{2} + z; \frac{1}{2}, 0, \frac{1}{2} + z; \text{ with } \\ z = 0.517 \pm 0.0008, B = 1.75 \text{ \AA}^2.$$

4 Al(1) in (c):

$$\text{with } x = 0.377 \pm 0.001, z = 0.048 \pm 0.002, B = 1.97 \text{ \AA}^2.$$

4 Al(2) in (c):

$$\text{with } x = 0.396 \pm 0.001, z = 0.456 \pm 0.002, B = 1.97 \text{ \AA}^2.$$

The interatomic distances based on these positions are:

Gd(1) has

$$1 \text{ Al(1) at } 3.14 \text{ \AA}, 2 \text{ Al(1) at } 3.15, 1 \text{ Al(2) at } 3.22, \\ 1 \text{ Al(2) at } 3.23, 1 \text{ Gd(1) at } 3.58, \text{ and } 1 \text{ Gd(2) at } \\ 3.69 \text{ \AA}.$$

Gd(2) has

1 Al(1) at 3·10, 1 Al(2) at 3·14, 2 Gd(3) at 3·46,  
2 Gd(3) at 3·66, and 1 Gd(1) at 3·69 Å.

Gd(3) has

2 Al(1) at 3·32, 2 Gd(2) at 3·46, 2 Gd(2) at 3·66, and  
2 Gd(3) at 3·84 Å.

Al(1) has

1 Al(1) at 2·90, 1 Gd(2) at 3·10, 1 Gd(1) at 3·14,  
2 Gd(1) at 3·15, and 2 Gd(3) at 3·32 Å<sup>2</sup>.

Al(2) has

1 Al(2) at 2·45, 1 Gd(2) at 3·14, 1 Gd(1) at 3·22,  
1 Gd(1) at 3·23, and 2 Gd(3) at 3·45 Å<sup>2</sup>.

Estimated standard deviations in the Gd–Gd and Gd–Al distances are 0·01 Å; in Al–Al distances, 0·015 Å.

Peterson & Rinn (1961) reported cell parameters and a possible space group for Zr<sub>3</sub>Zn<sub>2</sub> based on diffractometer data. Intensities of 35 indexed lines of this phase calculated using the Gd<sub>3</sub>Al<sub>2</sub> parameters give a discrepancy factor of 17%. Hence, Zr<sub>3</sub>Zn<sub>2</sub> is isostructural with Gd<sub>3</sub>Al<sub>2</sub>.

The structures of Gd<sub>5</sub>Ge<sub>3</sub> and Dy<sub>5</sub>Ge<sub>3</sub> were determined by a combination of single-crystal and powder diffraction methods. The hexagonal cell dimensions

(Dy<sub>5</sub>Ge<sub>3</sub>:  $a = 8.438 \pm 0.007$ ,  $c = 6.336 \pm 0.005$  Å;  
Gd<sub>5</sub>Ge<sub>3</sub>:  $a = 8.546 \pm 0.002$ ,  $c = 6.410 \pm 0.002$  Å)

indicated on *hk0* and *hkl* precession films were confirmed by indexing the powder diagrams. The agreement of calculated intensities based on the Mn<sub>5</sub>Si<sub>3</sub> structure type (*Strukturbericht*, 4, 24) and those observed for Dy<sub>5</sub>Ge<sub>3</sub> and Gd<sub>5</sub>Ge<sub>3</sub> confirmed the isostructural nature of these phases.

Powder diagrams of DyAl<sub>3</sub> were indexed with a hexagonal unit cell:  $a = 6.097 \pm 0.009$ ,  $c = 9.534 \pm 0.008$  Å,  $Z = 4$ . Intensities calculated on the basis of Ni<sub>3</sub>Ti parameters (*Strukturbericht*, 7, 14) gave good agreement with the observed values.

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## Notes and News

*Announcements and other items of crystallographic interest will be published under this heading at the discretion of the Editorial Board. The notes (in duplicate) should be sent to the General Secretary of the International Union of Crystallography (D. W. Smits, Rekencentrum der Rijksuniversiteit, Grote Appelstraat 11, Groningen, The Netherlands). Publication of an item in a particular issue cannot be guaranteed unless the draft is received 8 weeks before the date of publication.*

### International Union of Crystallography Change of Address of General Secretary

The General Secretary of the Union, Dr D. W. Smits, has recently been appointed Head of the new Computing Center of the State University of Groningen. As from 1 April his new address is:

Rekencentrum der Rijksuniversiteit  
Grote Appelstraat 11  
Groningen, The Netherlands.

### International Conference on Electron Diffraction and Crystal Defects, Melbourne, 1965

The Australian Academy of Science is cooperating with the International Union of Crystallography and the International Union of Pure and Applied Physics in arrangements for an International Conference to be held in Melbourne, 16–21 August 1965.

The scientific programme will consist of two simultaneous symposia:

- (i) A symposium on 'Electron Diffraction', and
- (ii) A symposium on 'The Nature of Defects in Crystals'.

In the first symposium the emphasis will be on developments in the theory and techniques for electron scattering rather than on applications of established

techniques to particular problems. Similarly, in the second symposium, the emphasis will be on the nature of defects in crystalline solids and the evidence for their existence rather than on their influence on the properties of solids.

The First Circular for the Conference is now available and copies may be obtained on request from Secretaries of National Committees of Crystallography and National Committees of Pure and Applied Physics, or from the Chairman of the Conference Organizing Committee, Dr R. I. Garrod, Aeronautical Research Laboratories, Box 4331, G.P.O., Melbourne, Victoria, Australia.

### International Colloquium on Semi-Metal Compounds

A 'Colloque International sur les Dérives Semi-Métalliques' will be held in Paris from 27 September to 2 October 1965, under the sponsorship of the Centre National de la Recherche Scientifique. The subjects of the Colloquium will be the structural, physical, thermodynamic, and chemical properties, and the nature of the bonding, in combinations of elements 22–28, 40–46, 57–78, and  $\geq 89$  with one or more of the following elements: H-B-S, Se, Te-N, P, As, Sb, Bi-C, Si, Ge, Sn. Further information may be obtained from André Michel or Pierre Lecocq at Centre d'Orsay, Faculté des Sciences de Paris, Orsay, Seine et Oise, France.