filtered iron radiation. Extinctions observed were (hkl) with ($h+k$) odd and ($h0l$) with l odd. The Weissenberg photographs indicated an end-centered orthorhombic cell. These criteria led to possible space groups *Cmcm* or *Cmc*. Tests for pyroelectric effect were negative and therefore suggested the centrosymmetrical space group. The crystals (approximately 20 microns diameter) were too small for piezoelectric tests. An additional basis for trying the space group *Cmcm* was the possible isomorphism of aluminum titanate with pseudo-brookite, Fe_2TiO_5 (Pauling, 1930).

The chosen point positions in space group *Cmcm* are 4(c) for titanium, 8(f) for aluminum, 4(c) for one set of four oxygen atoms, and 8(f) for two sets of eight oxygen atoms. Approximate atomic parameters were selected from atomic-radii and coordination considerations. These were refined by comparison of calculated and observed structure factors. The final parameters are given in Table 1.

Table 1. *Atomic parameters for* Al_2TiO_5

Atom	Position	X	Y*	Z*
Ti	4(c)	0	0·190	0·250
Al	8(f)	0	0·145	0·560
O_1	4(c)	0	0·760	0·250
O_2	8(f)	0	0·040	0·120
O_3	8(f)	0	0·320	0·090

* ±0·003.

An acceptable agreement between observed intensities and those computed from the structure was obtained. Atomic-scattering-factor data from the *Internationale Tabellen*, vol. 2, were used. The calculated intensities were corrected for absorption, Lorentz and polarization factors. Table 2 gives interatomic distances.

Table 2. *Interatomic distances in* Al_2TiO_5

Atom	Neighbor	Number	Distance (Å)
Ti	O_{I}	2	1·90
Ti	O_{II}	2	1·90
Ti	O_{III}	2	2·00
Al	O_{I}	1	2·05
Al	O_{II}	1	2·14
Al	O_{II}	1	1·96
Al	O_{II}	1	1·86
Al	O_{III}	2	1·84
O_{I}	O_{II}	4	2·99
O_{I}	O_{III}	4	2·45
O_{II}	O_{II}	1	2·52
O_{II}	O_{II}	1	2·45
O_{II}	O_{III}	2	2·77
O_{II}	O_{III}	2	2·99
O_{II}	O_{III}	1	2·64
O_{III}	O_{III}	1	3·08
O_{III}	O_{III}	2	2·79

Powder X-ray diffraction patterns were obtained for determination of the lattice constants. The values obtained were

$$a_0 = 3\cdot557\pm0\cdot002,\quad b_0 = 9\cdot436\pm0\cdot005,\quad \text{and}\quad c_0 = 9\cdot648\pm0\cdot005\ \text{Å}\,,$$

(Fe $K\alpha_1$ radiation, $\lambda = 1\cdot93597$ Å). The measured density was 3·67 g.cm.$^{-3}$. The calculated density, assuming 4 molecules per unit cell, was 3·71 g.cm.$^{-3}$.

Aluminum titanate, Al_2TiO_5, is isomorphous with pseudo-brookite, Fe_2TiO_5. There is some shift of position parameters. Because of this shift, the aluminum atoms tend toward tetrahedral coordination more than do the iron atoms in pseudo-brookite, although both do maintain distorted octahedral coordination.

Reference

Pauling, L. (1930). *Z. Krystallogr.* **73**, 97.

Acta Cryst. (1953). **6**, 813

A computational procedure for determining lattice parameters from powder photographs.

By G. D. Archard,* *The University, Reading, England*

(*Received* 2 *April* 1953 *and in revised form* 12 *June* 1953)

Cohen (1935) has given a method for computing lattice parameters of hexagonal crystals. Three summations are involved. In the expression for the parameters, these nearly cancel, so that a large number of significant figures must be carried throughout.

The same accuracy can be attained by the following method; this involves only one summation, and, after the plane spacings d_{hkl} have been deduced from the Bragg angles, three-figure working suffices. Consider

$$a = \{(\tfrac{4}{3})(h^2+k^2+hk)+l^2/C^2\}^{\frac{1}{2}}.d_{hkl} = f(hkl).d_{hkl}\,. \qquad (1)$$

Guess the axial ratio C ($= c/a$) and plot the values of a against $x = \frac{1}{2}$ ($\cos^2\theta/\sin\theta+\cos^2\theta/\theta$) (Nelson & Riley, 1945), obtaining a best straight line of slope m. Then the 'residuals' of the plot are given by

$$\Delta = a'-mx'\,,$$

where

$$\left.\begin{aligned} a' &= a-\Sigma a/n\,,\\ x' &= x-\Sigma x/n\,,\end{aligned}\right\} \qquad (2)$$
$$n = \text{number of reflexions } hkl.$$

If the guessed value of C is varied, it is reasonable to accept as optimum that value which makes the variance $\Sigma\Delta^2$ of the best straight line a minimum. This is easily shown to be

$$C_{\text{opt.}} = C_{\text{guessed}}-\Sigma\Delta A_m/a\Sigma A_m^2\,, \qquad (3)$$

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* Now at Associated Electrical Industries Ltd, Aldermaston, Berkshire, England.

in which

$$A_m = A - \Sigma A/n - x'\Sigma x'A/\Sigma x'^2\,, \quad (4)$$

$$aA = da/dC = -al^2/C^3f^2\,. \quad (5)$$

The value of a, corrected for absorption, is then given by the Nelson–Riley extrapolation with $C = C_{\text{opt.}}$.

For a typical photograph with ten diffraction lines, the factors A_m can be deduced in half an hour, and are then always available for the same crystal. A similar procedure applies to tetragonal crystals; for orthorhombic crystals, in which *two* axial ratios are unknown, the process is slightly more complex.

Hess (1951) pointed out that Cohen's method effectively weighted the a's deduced from various reflexions by a factor $\sin^2\theta$. The method here given assigns all reflexions equal weight. A group of eight photographs was computed by both methods, and also by a modification which weighted reflexions by a further factor of $\tan\theta$. All the methods agreed for both parameters to within 1 part in 50,000, but Cohen's method gave values of axial ratio consistently a little low.

I wish to thank the Department of Scientific and Industrial Research for a Maintenance Grant.

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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. Copy should be sent direct to the British Co-editor (R. C. Evans, Crystallographic Laboratory, Cavendish Laboratory, Cambridge, England).

Acta Crystallographica: Important Notices

1. The Executive Committee regrets that the continually growing size of this journal makes an increase in price unavoidable. As from the beginning of Volume 7, to be published in January 1954, the subscription price per volume will be 180 Danish crowns (or $ 25 or £ 9), post free; the preferential rate for personal subscribers (see *Acta Cryst.* (1953), **6**, 108) will be 100 Danish crowns (or $ 14 or £ 5), post free.

2. Messrs Ejnar Munksgaard now have a banking account in the U.S.A. Subscribers (at the full rate or at the preferential rate) who place their orders direct with the publishers may pay their subscription either to Messrs Munksgaard in Copenhagen or to Messrs Munksgaard's account at the Chase National Bank, New York 15, N.Y., U.S.A. Payment for reprints may also be made to either account.

3. Parts 11 and 12 of the current volume will be published together as a single issue on 10 November 1953. To ensure continuity of supply, orders for Volume 7, with remittance, should be placed through the usual channels as soon as possible, and in any case in time to reach the publishers in Copenhagen not later than 31 December 1953. Part 1 of Volume 7 will be sent only to subscribers whose subscriptions have been renewed.

4. The arrangement whereby advance orders for complete volumes from subscribers in the U.S.A., Canada and Mexico may be placed with the American Institute of Physics has been discontinued; instead, subscriptions for future volumes (at either the full or the preferential rate) may be placed with the Polycrystal Book Service (84 Livingston Street, Brooklyn 1, N.Y., U.S.A.). Orders from these countries may alternatively be placed direct with the publishers.