

modification suggested by Pepinsky & Cochran (1951), should be useful. However, the amplitudes were so distributed that the latter modification failed entirely, and the equations relating the Fourier coefficients of the squared and unsquared density functions gave correct sign relationships only when the full set of coefficients was used in each equation. As a consequence, these methods were not useful at all in the early, critical stages.

The vector convergence density (VCD) method (Buerger, 1950; Beevers & Robertson, 1950) for interpretation of the Patterson diagram was first tried unsuccessfully. It was later discovered that a computational error (human, not machine!) was responsible for the failure. The  $a$ -axis projection was actually first solved by the very classical use of Bragg-Lipson charts and packing considerations. Subsequent application of the VCD method showed that this led directly to the correct projection on (100).

The  $a$ -axis projection is shown in Fig. 1, as photographed from X-RAC. The correctness ratio,  $R = \Sigma |F_o - F_c| / \Sigma |F_o|$ , for this projection is 0.20. The structural formula is shown in Fig. 2.

A projection on (010) was computed in order to determine the  $x$  coordinates. All coordinate assignments

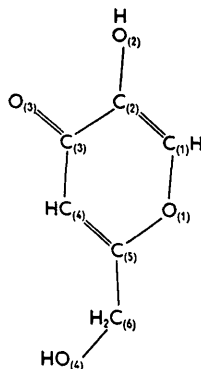


Fig. 2. Structural formula for kojic acid.

*Acta Cryst.* (1952). **5**, 286

**The crystal structure of artinite,  $Mg_2(OH)_2CO_3 \cdot 3H_2O$ .** By P. M. DE WOLFF, *Technisch Physische Dienst, T.N.O. T.H., Delft, Holland*

(Received 20 December 1951)

A trial structure of artinite has been derived from (a) unit-cell parameters (see below); (b) the presumed analogy to certain magnesium oxychlorides (de Wolff & Walter-Levy, to be published) involving infinite bands  $\parallel b$  with a brucite structure; (c) the outstanding strength of the (203) reflexion, indicating the azimuth of the bands; (d) Heritsch's (1948) conclusion (optical) that  $CO_3$  ions lie in planes  $\parallel b$ , and his value for their azimuth; (e) Fenoglio's (1942) conclusion from etching figures, that the space group is probably  $C2$ .

The value of  $F_c$  were compared with  $|F_o|$  values of the 34 ( $h0l$ ) reflexions with  $(\sin \theta)/\lambda < 0.32$ , obtained from the photometer record of a powder pattern (sample kindly submitted by Dr de Jong, with  $a = 16.56$ ,  $b = 3.15$ ,  $c = 6.22$  Å,  $\beta = 99^\circ 9'$ ) and completed for some coincident reflexions by using Heritsch's qualitative single-crystal data. Slight parameter changes led to a

Table 1. *Coordinates for kojic acid*

	$x$	$y$	$z$
C <sub>1</sub>	0.14	0.047	0.300
C <sub>2</sub>	0.00	0.099	0.393
C <sub>3</sub>	0.04	0.165	0.313
C <sub>4</sub>	0.22	0.170	0.159
C <sub>5</sub>	0.29	0.114	0.059
C <sub>6</sub>	0.26	0.091	0.902
O <sub>1</sub>	0.36	0.057	0.140
O <sub>2</sub>	0.12	0.091	0.545
O <sub>3</sub>	0.86	0.210	0.393
O <sub>4</sub>	0.16	0.162	0.799

to date are presented in Table 1. A full three-dimensional analysis is in progress and will be reported subsequently.

A projection on (010) is now in progress, to determine the  $x$  coordinates. Full details of the structure will be published upon completion of this phase of the analysis.

Computations on X-RAC were supported by Contract No. N6 onr-26916, T.O. 16, with the Office of Naval Research. The program on sugar structures has been aided by grants from the Research Corporation. The crystals were furnished by Charles Pfizer and Sons, Inc., of Brooklyn.

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satisfactory agreement. The final projection (Fig. 1, Table 1) shows the bands consisting of two rows of

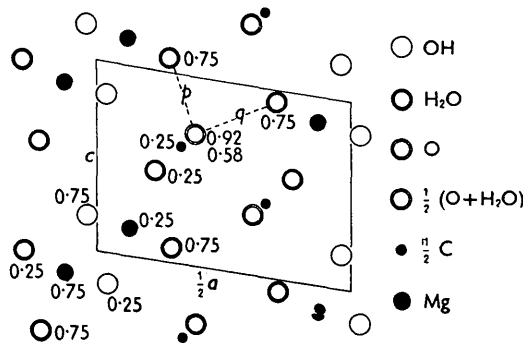


Fig. 1. (010) projection.

octahedra, sharing with  $\text{CO}_3$  ions those oxygen atoms which have only one magnesium neighbour. The anions

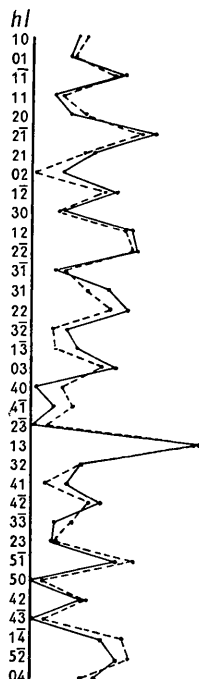


Fig. 2. Observed (full line) and calculated (broken line) values of  $|F(h0l)|$ .

must have a repeat distance of  $2b$ , but the resulting reflexions with non-integral  $k$  are diffuse (Heritsch). This can now be understood as a consequence of the extremely weak correlation between the rows of anions; disorder within any single row seems improbable. The  $y$  coordinates in Table 1 refer to the averaged structure

Table 1. Atomic positions in fractional coordinates

	$x$	$y$	$z$
Mg	0.064	0.250	0.139
OH	-0.019	0.750	0.175
$\text{H}_2\text{O}_{\text{II}}$	0.146	0.750	0.067
$\frac{1}{2}(\text{O}_{\text{I}} + \text{H}_2\text{O}_{\text{I}})$	0.114	0.250	0.466
$\frac{1}{2}\text{O}_{\text{II}}$	0.194	0.583	0.689
$\frac{1}{2}\text{O}_{\text{II}}$	0.194	-0.083	0.689
$\frac{1}{2}\text{C}$	0.167	0.250	0.611

(space group  $C2/m$ ), assuming minimum distortion of the octahedra and assuming right angles between the direction  $\text{C}-\text{O}_{\text{I}}$  and  $[010]$ . The corresponding  $F_c$  values of 25 ( $hll$ ) reflexions agree reasonably with Heritsch's qualitative estimates. Further refinement has not been attempted because of the difficulties ensuing from overlapping in the averaged structure. The length of  $q$  (2.88 Å) as compared with  $p$  (2.65 Å) (Fig. 1) explains the perfect cleavage along (100) observed by Heritsch.

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*Acta Cryst.* (1952). **5**, 287

**Physical constants of isotropic solids.** By T. VENKATARAYUDU and T. S. G. KRISHNAMURTY, *Andhra University, Waltair, South India*

(Received 7 December 1951)

Bhagavantam & Suryanarayana (1949) obtained the number  $n_i$  of physical constants for properties such as photo-elasticity, elasticity, piezo-electricity etc. in each of the 32 crystal classes. Jahn (1949) derived the same numbers by a different method and extended the results to isotropic solids and solids having complete rotational symmetry\*. Jahn's results can be derived from group characters using the formula

$$n_i = \frac{1}{2\pi} \int_0^{2\pi} (\chi'_+ \chi_- + \chi_- \chi'_+) d\varphi,$$

where  $\chi'_\pm$  stands for the character of the physical property and  $\chi_\pm = 1 \pm \cos \varphi$ , the upper sign holding for rotations, and the lower sign for rotation reflexions.

For example, in the case of elasticity,

$$\chi'_\pm = 16 \cos^4 \varphi \pm 8 \cos^3 \varphi - 4 \cos^2 \varphi + 1,$$

and

$$n_i = 2.$$

Similarly, other constants for isotropic solids can be evaluated.

In the case of solids possessing only symmetry  $R_\infty$ , the formula takes the form

$$n_i = \frac{1}{\pi} \int_0^\pi \chi'_+ \chi_- d\varphi.$$

The results thus obtained agree in all cases with those of Jahn (1949, Table 1). The above formulae follow directly (Wigner, 1931, p. 167) from the orthogonality relations between the characters of the irreducible representations of the symmetry groups  $R_\infty^i$  and  $R_\infty$ .

Our thanks are due to Dr H. Juretschke for his helpful suggestions on this paper.

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\* The last heading  $R_\infty^i$  of Table 1 of Jahn's paper should be replaced by  $R_\infty$ .