but which, for the same B ion, may vary with the lattice spacing in a fairly regular manner. The only quantity which seems likely to cause such effect is the presence of homopolar bonding between the B and oxygen ions. Such a suggestion has frequently been made (e.g. Eucken & Büchner, 1934; Megaw, 1947), but it has not been considered that the ferroelectricity depends primarily on the existence of such bonding, as these results suggest. The proportion of homopolar to ionic bonding would vary considerably for different ions, but if the A ion only is substituted in the structure a correlation between lattice spacing and change in Curie point might be expected. The experimental results require the ratio of change of Curie point with lattice parameter, to be positive, negative, and about zero in the titanates, tantalates, and niobates respectively.

On the other hand, the relation

$$\delta\theta \propto (1.5 - R_{\mathcal{A}}) \tag{2}$$

holds within about 20 % for all compounds in Table 2 with orthorhombic symmetry, and also for CaTiO<sub>3</sub>, which is not ferroelectric. Such a result has a reasonable interpretation if it is assumed that the internal stresses producing the shear in the different compounds are approximately the same, and are independent of temperature. The shear involves a change in the A-O, but not the B-O bond lengths, so that the restoring forces may be expected to be roughly of the form

$$1/{(A-O) - (R_A + R_O)},$$

reaching infinity when the ions are touching and t=1. This will lead to a relation of type (2).

The author wishes to express his thanks to Dr H. F. Kay for encouragement and advice throughout this work, to the Department of Scientific and Industrial Research for financial assistance, and to the Electrical and Allied Industries Research Association for financial assistance in the purchase of apparatus.

### References

- EUCKEN, A. & BÜCHNER, A. (1934). Z. phys. Chem. B, 27, 321.
- FORSBERGH, P. (1949). Phys. Rev. 76, 1187.
- GOLDSCHMIDT, V. M. (1926a). Skr. norske VidenskAkad., Matem.-Naturvid. Kl., no. 2.
- GOLDSCHMIDT, V. M. (1926b). Skr. norske VidenskAkad., Matem.-Naturvid. Kl., no. 8.
- HULM, J. K., MATTHIAS, B. T. & LONG, E. A. (1950). Phys. Rev. 79, 885.
- KAY, H. F. & VOUSDEN, P. (1949). Phil. Mag. 40, 1019.
- KEITH, H. D. (1950). Proc. Phys. Soc. Lond. B, 63, 208.
- MATTHIAS, B. T. (1949). Phys. Rev. 75, 1771.
- MEGAW, H. D. (1946). Trans. Faraday Soc. 42 (a), 224.
- MEGAW, H. D. (1947). Proc. Roy. Soc. A, 189, 261.
- ROBERTS, S. (1949). Phys. Rev. 76, 1215.
- RUSHMAN, D. F. & STRIVENS, M. A. (1946). Trans. Faraday Soc. 42, 231.
- VOUSDEN, P. (1951). Acta Cryst. 4, 68.

# Short Communications

Contributions intended for publication under this heading should be expressly so marked; they should not exceed about 500 words; they should be forwarded in the usual way to the appropriate Co-editor; they will be published as speedily as possible; and proofs will not generally be submitted to authors. Publication will be quicker if the contributions are without illustrations.

Acta Cryst. (1951). 4, 376

The crystal structure of salicylic acid. By W. COCHBAN,\* Crystallographic Laboratory, Cavendish Laboratory, Cambridge, England

(Received 8 March 1951)

Salicylic acid provides one of the best examples of a substance whose physical and chemical properties indicate hydrogen-bond formation between the hydroxyl group and an adjacent oxygen atom of the same molecule. The crystal structure of this compound has been determined from a study of the Patterson function projected on the (001) and (010) planes, and of the Fourier transform of a single molecule.

The optical and morphological properties of the crystals are described by Groth (1906–19, vol. 4, pp. 453, 493). X-ray measurements show

$$a = 11.5_2, b = 11.2_1, c = 4.90 \text{ A.}, \beta = 91^{\circ}.$$

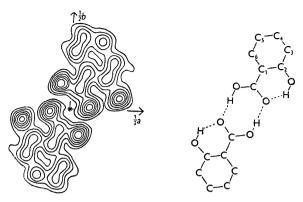
The space group is  $P2_1/a$ . Fig. 1 shows the electron density projected on the (001) plane. The corresponding F(hk0)'s were measured using a Geiger-counter spectrometer, and the value of  $\Sigma \mid F_o - F_c \mid \div \Sigma \mid F_o \mid$  is 0.12 at the present stage of refinement.

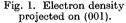
The association of two molecules through their carboxyl groups can be clearly seen from this projection. It is known that salicylic acid forms dimers in solvents such as benzene.  $(F_o - F_c)$  syntheses lead to the following conclusions. The hydrogen atoms in the 3, 4, 5 and 6 positions are represented by electron-density maxima<sup>†</sup> of about 0.8 e.A.<sup>-2</sup>; the position of a similar maximum close to the oxygen of the hydroxyl group is consistent with an O-H

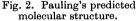
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<sup>†</sup> These maxima cannot be distinguished in the projection reproduced in Fig. 1.

bond length of  $1.0 \pm 0.1$  A., and a C-O-H bond angle of  $120 \pm 10^{\circ}$ . However, no comparable maximum occurs in the region between adjacent carboxyl groups. It is







possible, although improbable, that a real maximum has been obscured by the assumption of incorrect temperature-factor parameters for adjacent oxygen atoms. This possibility will be investigated by extending the range of measurement to higher values of  $\sin \theta / \lambda$ .

The above results provide confirmation of Pauling's prediction of the molecular structure shown in Fig. 2 (Pauling, 1945).

A number of the Fourier syntheses used in the course of this work were evaluated on XRAC, the automatic computer designed by Prof. R. Pepinsky and constructed in his laboratory. I am indebted to Prof. Pepinsky for making this possible, and to the Rockefeller Foundation for a grant which has enabled me to work at State College.

#### References

GROTH, P. (1906-19). Chemische Krystallographie. Leipzig: Engelmann.

PAULING, L. (1945). The Nature of the Chemical Bond. Ithaca: Cornell University Press.

### Acta Cryst. (1951). 4, 377

The crystal structure of tetragonal barium titanate. By Howard T. Evans, Jr., Philips Laboratories, Inc., Irvington-on-Hudson, N.Y., U.S.A.

(Received 21 March 1951)

A detailed crystal structure study of tetragonal barium titanate has been carried out with diffraction intensities measured at room temperature. Integrated intensities have been measured on a single untwinned crystal  $0.16 \times 0.19 \times 0.07$  mm., using a Weissenberg camera on which has been mounted a Geiger counter. Ninety-nine reflections (h0l) have been measured using Mo  $K\alpha$  radiation. Intensities have been corrected by analytical methods for absorption and secondary extinction. The best fit of calculated and observed intensities was obtained with the following structure:

Space group:	P4mm	
Ba in $(a)$ :	0, 0, 0.	
Ti in (b):	$\frac{1}{2}, \frac{1}{2}, (\frac{1}{2}+z_{\rm Ti}),$	$z_{\rm Ti} = 0.015.$
$O_I$ in $(b)$ :	$\frac{1}{2}, \frac{1}{2}, z_{0_{\rm I}},$	$z_{0_1} = -0.024.$
$2O_{II}$ in (c):	$\frac{1}{2}$ , 0, $(\frac{1}{2} + z_{0_{\Pi}})$ ;	
	$0, \frac{1}{2}, (\frac{1}{2} + z_{0_{II}}),$	$z_{0_{\rm II}} = -0.020.$

This structure gave a ratio of sum of absolute deviations of calculated and observed structure factors to sum

## of calculated structure factors of 5.71 %. A temperature correction was applied to the calculated values for which the coefficient $B = 0.30 \times 10^{-16}$ cm.<sup>2</sup>. The structure given above is in approximate agreement with the partial solution of the structure given by Kaenzig (1950).

Interatomic distances are as follows:

$Ti-O_{I}$ above	1·860A.	$Ba-4O_I$	2·826A.
$O_I$ below	2.174	-40 <sub>11</sub> above	2.782
$4O_{II}$	2.002	$-4O_{II}$ below	<b>2·896</b>
$O_I - 4O_{II}$ above	2.850	$O_{I} - O_{I}$	2.824
$4O_{II}$ below	2.827		

A shift of 0.005A. of any atom makes the agreement between calculated and observed structure factors significantly poorer.

A detailed description of the work leading to these results will be published shortly.

### Reference

KAENZIG, W. (1950). Phys. Rev. 80, 94.

#### Acta Cryst. (1951). 4, 377

A cubic structure for the phase Pt<sub>3</sub>Cu.\* By YOU-CHI TANG, Gates and Crellin Chemical Laboratories, Pasadena, California, U.S.A. (Received 13 February 1951 and in revised form 1 April 1951)

Schneider & Esch (1944) proposed for the intermetallic phase with composition about Pt<sub>c</sub>Cu an orthorhombic structure which is derived from a face-centered cubic arrangement. They found that this structure gave satisfactory agreement with X-ray intensities on their powder photographs, and that no other well-defined arrangement of the atoms gave as good agreement. However, the proposed structure for Pt<sub>3</sub>Cu may well not be the right one. inasmuch as an orthorhombic structure such as this would very probably distort the cubic lattice perceptibly: yet no splitting of the diffraction lines was observed.

<sup>\*</sup> Contribution no. 1527 from the Gates and Crellin Laboratories of Chemistry, California Institute of Technology.