Table 1. *Crystallographic data for the alkali salts of tetraphenyl boron*

	$NaB(C_6H_5)_4$	$KB(C_6H_5)_4$	$NH_4B(C_6H_5)_4$	$RbB(C_6H_5)_4$	$CsB(C_6H_5)_4$
a (Å)	11·45 ± 0·03	11·25 ± 0·02	11·24 ± 0·02	11·22 ± 0·03	11·27 ± 0·02
c (Å)	7·41 ± 0·02	7·91 ± 0·02	8·08 ± 0·02	8·07 ± 0·03	8·40 ± 0·02
U (Å^3)	971·5	1000·1	1020·8	1015·9	1066·9
Z	2	2	2	2	2
D_m (g.cm.$^{-3}$)	1·15	1·192	1·093	1·315	1·400
D_X (g.cm.$^{-3}$)	1·170	1·190	1·097	1·323	1·407
M.wt.	342·2	358·3	337·3	404·7	452·2

$I\bar{4}2m$–D_{2d}^{11}, and $I4/mmm$–D_{4h}^{17}. $I4$, $I\bar{4}$, $I4/m$ each require $|F(hkl)| \neq |F(\bar{h}kl)|$, which is contrary to observation. The diffraction conditions alone, therefore, allow the last five space groups in the list of eight above. Assuming the more than probable tetrahedral, not necessarily regular, distribution of phenyl groups about the boron atom, the space group is indeterminate only between $I\bar{4}m2$ and $I\bar{4}2m$. Both imply the same positions for the ions in the crystal and differ only in the orientation required of the phenyl groups with respect to the unit-cell vectors.

Caesium tetraphenyl boron was also recrystallized from methyl ethyl ketone, with which it forms a solvate, $CsB(C_6H_5)_4.CH_3COC_2H_5$, belonging to the orthorhombic system. The lattice constants of this solvate are

$$a = 16{\cdot}54 \pm 0{\cdot}02,\quad b = 14{\cdot}61 \pm 0{\cdot}02,\quad c = 10{\cdot}42 \pm 0{\cdot}02 \text{ Å}\,.$$

$$\text{Volume of cell} = 2517{\cdot}9 \text{ Å}^3,\ Z = 4,\ D_m = 1{\cdot}382 \text{ g.cm.}^{-3},\ D_X = 1{\cdot}382 \text{ g.cm.}^{-3}.$$

Reflexions are present in all orders except in $(h0l)$ when $h = 2n+1$ and in $(0kl)$ when $k+l = 2n+1$. The space group is hence either $Pnam$ or $Pna2_1$.

Attempts at preparing single crystals of the lithium salt of tetraphenyl boron, using several different solvents, were without success; powder photographs appeared to be more complex than those of the other alkali salts of tetraphenyl boron and were not unambiguously indexed, although it was clear that this salt was not isomorphous with those in Table 1.

Further work on these salts was suspended in 1956, when it was learned (private communication from Mrs M. S. Webster) that an independent investigation of the rubidium and ammonium salts had been completed elsewhere. The Fourier syntheses in this work (Webster, 1956) resolved the space-group ambiguity in favour of $I\bar{4}2m$–D_{2d}^{11}.

We thank L. Light and Company Limited for a gift of lithium, sodium and potassium salts of tetraphenyl boron. The remaining salts were prepared by double decomposition, using the sodium salt as starting material. We also thank Prof. J. Monteath Robertson for his interest.

References

Geilman, W. & Gebauhr, W. (1953). *Z. anal. Chem.* **139**, 161.

Webster, M. S. (1956). D. Phil. thesis, Oxford.

Acta Cryst. (1958). **11**, 450

Determination of the principal axes of the anisotropic temperature factor.

By William R. Busing and Henri A. Levy, *Chemistry Division, Oak Ridge National Laboratory,* Oak Ridge, Tennessee, U.S.A.*

(*Received* 27 *January* 1958 *and in revised form* 10 *March* 1958)

The following method for computing the principal axes of thermal motion from the anisotropic temperature-factor coefficients has recently been derived by Waser (1955). Let the expression for the temperature factor of an atom be $\exp(-\sum_{ij} B_{ij}h_ih_j)$ where the h_i are the indices of the reflection and the B_{ij} are the temperature-factor coefficients. Then the equations to be solved are

$$\sum_i [B_{ij}-\lambda(\mathbf{b}_i.\mathbf{b}_j)]q_i = 0,\quad j = 1, 2, 3\,, \qquad (1)$$

where the $\mathbf{b}_i$ are the reciprocal-lattice vectors and the q_i describe the vector $\mathbf{Q} = \sum_i q_i\mathbf{b}_i$. Solution of the secular determinant yields three roots, $\lambda^{(r)}$, corresponding to the three principal-axis directions, and substitution of each $\lambda^{(r)}$ in (1) gives a vector $\mathbf{Q}^{(r)} = \sum_i q_i^{(r)}\mathbf{b}_i$ which defines the direction of the rth principal axis. The mean-square atomic displacement along this axis is $\lambda^{(r)}/2\pi^2$.

The purpose of this note is to point out that equations (1) may be recast in two ways which offer computational advantage:

$$\sum_k \left[\sum_i (\mathbf{a}_k.\mathbf{a}_i)B_{ij}-\lambda\delta_{jk}\right] q_k = 0,\quad j = 1, 2, 3\,, \qquad (2)$$

and

$$\sum_k \left[\sum_j B_{ij}(\mathbf{a}_j.\mathbf{a}_k)-\lambda\delta_{ki}\right] p_k = 0,\quad i = 1, 2, 3\,. \qquad (3)$$

Here the $\mathbf{a}_i$ represent the direct-lattice vectors and the p_k are the components of $\mathbf{Q}$ in terms of these vectors:

$$\mathbf{Q} = \sum_k q_k\mathbf{b}_k = \sum_k p_k\mathbf{a}_k\,. \qquad (4)$$

In the determinants of equations (2) and (3) the unknown λ appears only in the diagonal elements, which simplifies the solution of the secular equation. (Note, however, that these determinants are no longer symmetric.)

---

* Operated for the U.S. Atomic Energy Commission by Union Carbide Corporation.

Moreover, solution of linear equations (3) yields the direct-lattice components $p_k^{(r)}$ of the principal-axis vectors. These will sometimes be preferred to the components $q_k^{(r)}$.

Derivation of equations (2) and (3) is most convenient in matrix notation. Equations (1) may be written

$$(\mathbf{B}-\lambda\mathbf{g})\mathbf{q} = 0, \quad \mathbf{g} = [\mathbf{b}_i.\mathbf{b}_j]\,. \tag{1a}$$

Taking the scalar product of (4) with $\mathbf{b}_j$, and noting that $\mathbf{a}_i.\mathbf{b}_j = \delta_{ij}$, yields $\mathbf{p} = \mathbf{g}\mathbf{q}$. A similar product of (4) with $\mathbf{a}_j$ shows that $\mathbf{g}^{-1} = [\mathbf{a}_i.\mathbf{a}_j]$, since $\mathbf{q} = \mathbf{g}^{-1}\mathbf{p}$.

Premultiplying (1*a*) by $\mathbf{g}^{-1}$ gives

$$(\mathbf{g}^{-1}\mathbf{B}-\mathbf{g}^{-1}\lambda\mathbf{g})\mathbf{q} = (\mathbf{g}^{-1}\mathbf{B}-\lambda\mathbf{1})\mathbf{q} = 0\,. \tag{2a}$$

Substituting $\mathbf{q} = \mathbf{g}^{-1}\mathbf{p}$ into (1*a*) yields

$$(\mathbf{B}-\lambda\mathbf{g})\mathbf{g}^{-1}\mathbf{p} = (\mathbf{B}\mathbf{g}^{-1}-\lambda\mathbf{1})\mathbf{p} = 0\,. \tag{3a}$$

These are the matrix equivalents of equations (2) and (3).

Criticism and suggestions from Prof. J. Waser and Prof. V. Schomaker are gratefully acknowledged.

Reference

Waser, J. (1955). *Acta Cryst.* 8, 731.

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 direcct to the Editor (P. P. Ewald, Polytechnic Institute of Brooklyn, 333 Jay Street, Brooklyn 1, N.Y., U.S.A.) or to the Technical Editor (R. W. Asmussen, Chemical Laboratory B of the Technical University of Denmark, Sølvgade 83, Copenhagen K, Denmark)

The X-ray Powder Data File

Upon the resignation of Dr G. W. Brindley, Dr J. V. Smith has been appointed acting Editor to the X-ray Powder Data File. New data and information concerning errors in the published data are always welcome and correspondence should be addressed to Dr J. V. Smith, Mineral Science Building, The Pennsylvania State University, University Park, Pennsylvania, 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, 333, Jay Street, Brooklyn 1, N.Y., U.S.A.). As far as practicable books will be reviewed in a country different from that of publication.

Solid State Physics. Advances in Research and Applications. Volume 4. Edited by F. Seitz and D. Turnbull. Pp. xiv+540 with many figs. New York: Academic Press; London: Academic Books. 1957. Price $12·00; £4·16.0.

This volume contains five articles, of which two, 'Ferroelectrics and antiferroelectrics' by W. Känzig (197 pages) and 'Techniques of zone melting and crystal growing' by W. G. Pfann (100 pages) are reviewed here. The others are 'Theory of mobility of electrons in solids' by F. J. Blatt (168 pages), 'The orthogonalized plane-wave method' by T. O. Woodruff (45 pages), and a 'Bibliography of atomic wave-functions' by R. S. Knox (9 pages).

Ferroelectricity is the existence of reversible spontaneous polarization in a dielectric; antiferroelectricity, less easy to define macroscopically, has its origin in permanent dipole moments associated with symmetry-equivalent parts of the structure, whose resultant moment is zero. The technological importance of ferroelectrics has inspired a large amount of fundamental work, but the results are scattered through the literature, so that it is not easy for anyone who wants an up-to-date picture to assemble it for himself. Dr Känzig's monograph therefore meets a real need. It is comprehensive, authoritative, and written with a sense of order and attention to detail which make it a valuable work of reference. It includes a long and important section on the physical properties of single crystals; an account (perhaps too short for clarity) of the phenomenological theories; discussion of domain effects; descriptions of crystal structures, as known from X-ray and neutron diffraction, infra-red and Raman spectroscopy, and nuclear magnetic resonance; brief notes on solid solutions; and a summary of the various model theories. New ferroelectrics discovered up to 1957 are included. Full references are given (though, regrettably, as footnotes). The article is no mere compilation of results and theories. Trouble has been taken to sort them into logical order, to express them in forms which allow comparison, to assess their reliability and interpret their significance. This of course enhances their value. Indeed, not the least valuable parts of the article are some of these interpretations (though it is sometimes not clear from the text just how much is due to Dr Känzig rather than to the original author).

The article is likely to be of most value to those who already have some knowledge of ferroelectricity and want to extend it. It cannot be recommended without reserve as an introduction to the subject, partly because explanations are kept short, and partly because of limitations inherent in the conventional solid-state approach. Solid-state physics, generally concerned with very simple structures where the atoms are all in special positions,