oriented along the axis of the model; (*c*) represents the surface of the oxygen atom, showing the poles of the magnet. Fig. 2 shows the construction of the hydrogen bonds in an adenine–thymine pair corresponding to the Watson–Crick structure for nucleic acid (Watson & Crick, 1953; Crick & Watson, 1954). The formation of the N–H · · · O hydrogen bonds in this model requires that the magnet be inclined at about 60° to the axis of the oxygen atom.

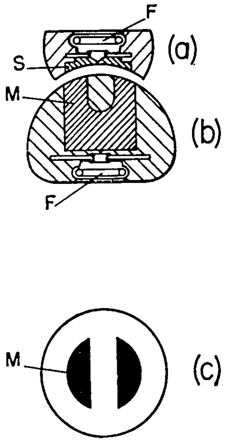

Fig. 1. A cross-sectional view of a typical hydrogen atom (*a*) and oxygen atom (*b*). Covalent bonds are made by means of the snap fasteners, *F*; hydrogen bonds by means of the steel insert *S* and the cylindrical permanent horseshoe magnet *M*. The appearance of the poles of the magnet on the surface of the oxygen atom is shown in (*c*).

One valuable feature of these magnetic models is that the angle of the hydrogen bond (the angle between the N–H and H · · · O vectors in N–H · · · O bonds, for example) can be varied continuously over a wide range. Hydrogen and oxygen atoms of the general type shown in Fig. 1 are held firmly together even when the H · · · O vector makes an angle of as much as 30° with the axis of the oxygen atom. For special structures, such as that shown in Fig. 2, it may be desirable to cast an oxygen atom in which the magnet is given special orientation.

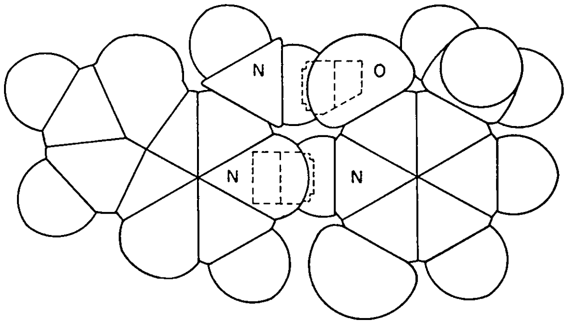

Fig. 2. A drawing showing the use of magnetic N–H · · · O and N–H · · · N hydrogen bonds in a model of the adenine–thymine pair of the Watson–Crick nucleic acid structure. Note that in the N–H · · · O bond the magnet is inclined at about 60° from the axis of the oxygen atom.

These magnetic hydrogen bonds permit the construction of three-dimensional models of the crystal structures of amino acids and peptides and of typical configurations of the polypeptide and polynucleotide chains in proteins and nucleic acids.

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The lattice constants of the alkali salts of tetraphenyl boron.

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The solubility behaviour of the alkali salts of tetraphenyl boron exhibits an interesting discontinuity. The lithium and sodium salts are very water-soluble, whereas the potassium, ammonium, rubidium and caesium salts are very insoluble. Geilman & Gebauhr (1953) report the solubility product of $KB(C_6H_5)_4$ in water at 20° C. to be $2{\cdot}25 \times 10^{-8}$. The present investigation was undertaken partly to determine whether a corresponding change in crystal symmetry accompanies the abrupt change in solubility, and partly in an effort to determine the detailed structure of the $[B(C_6H_5)_4]^-$ ion.

Sodium, potassium, ammonium, rubidium, and caesium tetraphenyl boron all crystallize from acetone (in the case of sodium water was used) as prismatic needles, in the tetragonal system. For each salt precession photographs with Mo $K\alpha$ radiation ($\lambda = 0{\cdot}7107$ Å) were used to obtain the crystallographic data presented in Table 1. In all cases (hkl) was present only for $h+k+l = 2n$: hence also ($hk0$) only when $h+k = 2n$, etc. These systematic absences are compatible with all of the space groups $I4\text{–}C_4^5$, $I\bar{4}\text{–}S_4^2$, $I4/m\text{–}C_{4h}^5$, $I422\text{–}D_4^9$, $I4mm\text{–}C_{4v}^9$, $I\bar{4}m2\text{–}D_{2d}^9$,

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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

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

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

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.

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Determination of the principal axes of the anisotropic temperature factor.

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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

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

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:

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

and

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

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:

$$\mathbf{Q} = \sum_k q_k\mathbf{b}_k = \sum_k p_k\mathbf{a}_k\ . \tag{4}$$

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.)

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