1000 units (the scale of both the Patterson synthesis and the v.c.d. was relative). The sulphur atom reached 250; the rubidium 1400; the carbon, oxygen and nitrogen gave heights of about 50–100 units. Sixteen sections of Fourier space from $z=0$ to $z=15/60$ were used and these were viewed down the z-axis direction looking towards the origin. For the sake of compactness of representation, these sections were taken in four groups of four sections each, the contours for each of the four sections being drawn, superimposed on the other contours, on a single map. The resulting v.c.d. maps are reproduced in Fig. 1 (*a*)–(*d*).

To overcome the ambiguity referred to above, use was made of the Fourier projections which had been calculated by Crowfoot *et al.* (1949, p. 329, Figs. 9 (*a*) and (*b*)) based on signs derived from the contributions of rubidium at $x=0{\cdot}365$, $y=0{\cdot}55$, $z=0$, and sulphur at $x=0{\cdot}625$, $y=0{\cdot}375$, $z=0{\cdot}135$. Regions of the unit cell in which atoms were unlikely, as there were no peaks in the corresponding areas of projection, were marked out. Erasure of the vector convergence peaks in these regions gave the result shown in Fig. 2 (*a*)–(*d*).

Discussion of results

Fig. 3 gives, in projection down the z axis, the positions of the atoms in the quarter-volume of the unit cell of rubidium benzyl penicillin, as found by Crowfoot *et al.* The relevant atomic positions are also indicated in the various sections of Figs. 1 and 2; and in Fig. 1, their duplicates, generated by glide planes at $x=\frac{1}{4}$ and $\frac{3}{4}$, translation $=\frac{1}{2}b$, are also shown, using broken lines for the bond of the second set.

The diagrams show a fair measure of correlation between the structure found by Fourier and trial-and-error methods, and the results of the vector convergence method of Patterson function interpretation, especially as aided by Fourier projections.

How far this general agreement could have been utilized in the initial solution of the structure it is impossible to say. But it would seem that, given the presence of a heavy atom, suitable multiplicity in the space group, and the availability of three-dimensional intensity data, the vector convergence method is likely to be practicable as one further tool in structure determination. Generalization regarding the method is dangerous, considering that its applicability depends upon such a variety of factors. It can only be hoped that continued experiment will prove its real usefulness in crystallographic analysis.

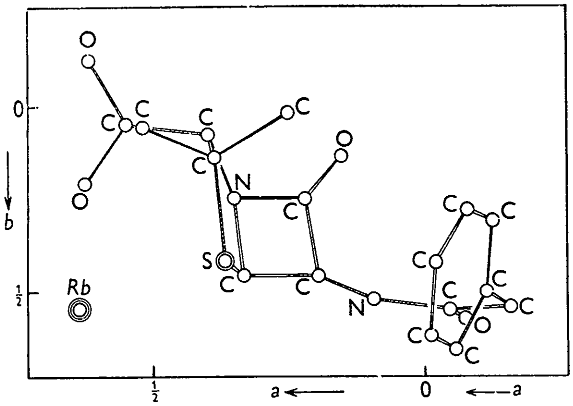

Fig. 3. Rubidium benzyl penicillin: projection down the c axis.

The author wishes to express his thanks to Dr C. A. Beevers, under whose guidance the vector convergence method was originally developed, to Mrs Dorothy Hodgkin, for her interest and encouragement, and to the Carnegie Trust for a scholarship which enabled the work to be carried out. He is also indebted to Mr Stern for a number of helpful suggestions.

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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.

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Confirmation of the structure of chromium boride, CrB.

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In a recent paper by Sindeband (1949) the preliminary findings of the structural analysis of CrB conducted by the present author were published. At the same time the structure of this material was being worked on by Dr R. Keissling, and the complete details of his structural analysis have subsequently appeared in print (1949). As there is no substantial difference in the results of these two investigations it will suffice to write a note on the difference in method and agreement of the results.

The two simplest crystals used were selected from a group of small intergrown prismatic crystals prepared by the American Electro-Metal Corporation by the electrolysis of fused borate baths. Precession and Weissenberg methods were used and intensities were visually estimated. The following cell dimensions were obtained:

$$a = 2{\cdot}96, \quad b = 7{\cdot}81 \quad \text{and} \quad c = 2{\cdot}94 \text{ A.},$$

which are within 0·6 % of those found by Dr Keissling. The diffraction symbol was determined as *mmmC–c–*. These dimensions and a density of 6·2 g.cm.$^{-3}$ require four CrB molecules per cell, and the symmetry necessitates that all the atoms fall on fourfold special positions with the x parameter fixed at 0 and perhaps the z parameter fixed at 0·25, but with the y parameter to be determined. Taking advantage of the fact that the chromium atoms will dominate the intensities, but accounting for the influence of the boron, the chromium y parameter was determined graphically from the (0k0) reflections of a Weissenberg picture taken with molybdenum radiation on a composite crystal having a common b axis but with the a axis in one part of the crystal coincident with the c axis in the other. In drawing curves representing change of intensity with change in chromium y parameter for each reflection (0k0), areas were plotted whose boundaries were determined by the maximum possible in-phase and out-of-phase scattering of boron for that reflection. The chromium y parameter was observed to be $0{\cdot}146 \pm 0{\cdot}007$, with 0·143 favored from a closer inspection of the relative intensities and from geometrical considerations.

The y parameter of the boron was determined graphically to be $0{\cdot}45 \pm 0{\cdot}03$ from curves showing the variation of boron y parameter with intensity for each reflection (0k0) assuming 1·43 to be the correct chromium parameter. To equate the length of the bonds to the nearest chromium atoms which form a co-planar triangle 0·43 seems the best boron y parameter.

From the intensities of the (0kl) reflections from a zero-level a-axis precession photograph of a crystal twinned with (110) as the twin law, and accounting for the fact that the (04l) and (08l) reflections were superimposed with the (13l) and (26l) reflections respectively, the z parameters for both the chromium and the boron atoms were confirmed to be 0·25, thus placing both the boron and chromium atom in the 4(c) special position of space group *Cmcm*–D_{2h}^{17} (nomenclature that of the *Internationale Tabellen*) with the y parameters as determined above. These parameters are within 2·3 % of those determined by Dr Keissling.

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The space group of calcium peroxide octahydrate.*

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Compounds in which eight molecules of water are co-ordinated about a central ion have been studied, but in no instance has an analysis been reported which can be accepted as representing the correct structure.

Natta (1928, 1932) examined the octahydrate of strontium hydroxide† by Laue, rotation and powder methods, and the octahydrate of strontium peroxide‡ by the powder method alone. He proposed structures for these substances in which the water was cubically co-ordinated about the strontium ion. On the basis of powder data, Miller & King (1936) arrived at a similar conclusion for $CaO_2.8H_2O$, $SrO_2.8H_2O$ and $BaO_2.8H_2O$.§ In all cases the system was found to be tetragonal with a primitive cell containing a single molecule.

Mellor (1938) reinvestigated $Sr(OH)_2.8H_2O$ by single-crystal methods, but he was unsuccessful in determining the atomic positions. He reported the space group to be D_{2h}^{4}–*P*4/*mmc*, with a cell having the dimensions $a = 8{\cdot}97$, $c = 11{\cdot}55$ A. which contained four molecules instead of one as reported by Natta (1928).

The alkaline earth metal peroxide octahydrates are quite insoluble in water, hence previous investigations of their structures have been limited to the powder method.

By slow diffusion of NH_3 into a very cold solution containing a mixture of $Ca(NO_3)_2$ and H_2O_2, crystals of $CaO_2.8H_2O$ suitable for single-crystal studies have been obtained. The data presented below represent the preliminary results of a reinvestigation of this compound.

Optical and Laue studies confirmed the tetragonal character of the crystal. Oscillation patterns taken about the a and c axes gave the cell dimensions $a = 6{\cdot}21$, $c = 11{\cdot}00$ A. The density, 1·672 g.cm.$^{-3}$, obtained by the flotation method, required a cell containing two molecules instead of one, as previously reported. Systematic extinctions occurred only for ($h0l$), (00l) and (hhl) with l odd, hence the space group is either D_{h}^{2}–*P*4/*mcc* or C_{4v}^{5}–*P*4*cc*. The latter was ruled out as improbable on the basis of the equivalent positions available for the atoms of two molecules of $CaO_2.8H_2O$.

A preliminary attempt to establish the positions of the atoms by trial methods led to inconclusive results, but indicated that the water molecules probably occupy the sixteen general positions of the space group with approxi-

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[*] Abstract from a thesis presented in partial fulfilment of the requirements for the degree of M.S., Syracuse University, 1950.

[†] $Sr(OH)_2.8H_2O$. Tetragonal. $a = 6{\cdot}41$, $c = 5{\cdot}807$ A. Sr^{++} at 0, 0, 0. (OH)′ at ½, 0, 0; 0, ½, 0. H_2O at x, x, z; $x, x, \bar{z}$; $\bar{x}, x, z$; $\bar{x}, x, \bar{z}$; $x, \bar{x}, z$; $x, \bar{x}, \bar{z}$; $\bar{x}, \bar{x}, z$; $\bar{x}, \bar{x}, \bar{z}$; with $x = 0{\cdot}29$–$0{\cdot}30$; $z = 0{\cdot}25$.

[‡] $SrO_2.8H_2O$. Tetragonal. $a = 6{\cdot}32$; $c = 5{\cdot}56$ A. Sr^{++} at 0, 0, 0. O′ at ½, ½, $\pm z$; with $z = 0{\cdot}10$. H_2O at x, x, z; $x, x, \bar{z}$; $\bar{x}, x, z$; $\bar{x}, x, \bar{z}$; $x, \bar{x}, z$; $x, \bar{x}, \bar{z}$; $\bar{x}, \bar{x}, z$; $\bar{x}, \bar{x}, \bar{z}$; with $x = 0{\cdot}20$; $z = 0{\cdot}25$.

§	a (A.)	c (A.)	w	x	y	z
$CaO_2.8H_2O$	6·20	5·50	0·12	0·32	0·11	0·25
$SrO_2.8H_2O$	6·32	5·55	0·11	0·32	0·13	0·26
$BaO_2.8H_2O$	6·51	5·75	0·10	0·32	0·12	0·27

Sr^{++} at 0, 0, 0. O′ at ½, ½, $\pm w$. H_2O at x, y, z; $\bar{x}, \bar{y}, z$; $x, y, \bar{z}$; $\bar{x}, \bar{y}, \bar{z}$; $\bar{y}, x, z$; $y, \bar{x}, z$; $\bar{y}, x, \bar{z}$; $y, \bar{x}, \bar{z}$.