present structure. Calculations based on data collected for the magnesium salt in this Laboratory (Montgomery & Lingafelter, to be published) and an independent structure determination by Margulis & Templeton (1962) show that the structure of this salt is essentially identical with the zinc compound.

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The Interpretation of Pseudo-Orthorhombic Diffraction Patterns

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Diffraction diagrams with pseudo-orthorhombic Laue symmetry may be produced by monoclinic crystals as a result of twinning. In such cases, the systematic absences often follow selection rules that are not characteristic of any orthorhombic space group. Various examples are discussed. In particular, it is shown that the absences may follow pseudo-selection rules. Monoclinic structures in which the projections down three mutually perpendicular axes have perfect rectangular symmetry constitute a special class of pseudo-orthorhombic structures and are said to be para-orthorhombic. The systematic absences and Laue symmetries of para-orthorhombic structures are discussed and examples are given.

Introduction

During the last few years, five crystals examined in the author's laboratory have been found to give X-ray photographs with *mmm* symmetry but with systematic absences that do not correspond to any orthorhombic space group. Crystallographic data are given in Table 1. More detailed examination has shown that each of these crystals is in fact monoclinic with all interaxial angles of a non-primitive unit cell exactly 90°. As we shall see, the unusual features of the X-ray diagrams are sometimes due simply to twinning, but it is sometimes necessary to invoke special 'para-orthorhombic' relationships between different sets of representative points in the monoclinic structures as well.

Table 1. *Crystallographic data for five pseudo-orthorhombic crystals*

I. 1-Anilino-4-chloropyromellitic acid diphenylimide,

$C_{24}H_{16}N_3O_4Cl$

$a = 14 \cdot 7$ Å	(1) $hkl = h+k = 2n$
$b = 12 \cdot 3$	(2) $hk0 : h = 2n \ (k = 2n)$
$c = 26 \cdot 6$	(3) hkl : if $h, k = 2n, h+k+2l = 4n$
$Z = 8$	

II. Cycloundecylamine hydrobromide, $C_{11}H_{21}NH_3{}^+Br^-$

$a = 65$ Å	(1) $hkl : h+k = 2n$
$b = 9 \cdot 75$	(2) $hk0 : h = 2n \ (k = 2n), h+k = 4n$
$c = 8 \cdot 15$	(3) $h0l : h = 4n$
	(4) $0kl : k = 4n, l = 2n$
$Z = 16$	(5) hkl : if $h, k = 2n, h+k = 4n$
	(6) All reflexions with h, k odd are weak

Table 1 (cont.)

III. Azacyclodecane hydrobromide, $C_9H_{22}N^+Br^-$

$a = 45.6$ Å (1) $hkl : h+k=2n$
$b = 23.4$ (2) $hk0 : h=2n, (k=2n), h+k=4n$
$c = 8.05$ (3) $h0l : h=4n, l=2n$
              (4) $0kl : k=4n, l=2n$
$Z = 32$ (5) $hkl :$ if $h, k=2n, h+k+2l=4n$
              (6) All reflexions with h, k odd are weak

IV. Nonactin, $(C_{10}H_{16}O_3)_4$

$a = 47.6$ Å (1) $hkl : h+k=2n$
$b = 31.5$ (2) $hk0 : h=2n, (k=2n)$
$c = 5.70$ (3) $h0l : h=4n$
              (4) $0kl : k=4n$
$Z = 8$

V. α-Cobalt dipyridine dichloride, $Co(C_5H_5N)_2Cl_2$

$a = 34.4$ Å (1) $hkl : h+k=2n$
$b = 17.4$ (2) $hk0 : h=2n, (k=2n)$
$c = 3.66$ (3) $h00 : h=4n$
   (4) $0k0 : k=4n$
$Z = 8$

Example I

We discuss first the case of 1-anilino-4-chloro-pyromellitic acid diphenylimide (Dunitz, Mez, Hopff & Manukian, 1960) in detail. The simplest ortho-rhombic space group that satisfies conditions (1) and (2) (Table 1, I) is $C2mb$ (No. 39) with the 8 general positions.

$$(0,0,0; \tfrac{1}{2}, \tfrac{1}{2}, 0)+ x, y, z; \ x, -y, -z;$$
$$x, \tfrac{1}{2}+y, -z; \ x, \tfrac{1}{2}-y, z$$

but to satisfy condition (3) a further set of 8 general positions is required. If these are assigned (Fig. 1) as

$$(000; \tfrac{1}{2}, \tfrac{1}{2}, 0)+\tfrac{1}{4}+x, \tfrac{1}{4}+y, \tfrac{1}{2}+z; \ \tfrac{1}{4}+x, \tfrac{3}{4}-y, \tfrac{1}{2}-z$$
$$\tfrac{1}{4}+x, \tfrac{3}{4}+y, \tfrac{1}{2}-z; \ \tfrac{1}{4}+x, \tfrac{1}{4}-y, \tfrac{1}{2}+z$$

condition (3) follows by substitution in the structure factor formula. It is not possible, however, to select 8 pairs out of these 16 general positions in such a way as to form 8 identical molecules; moreover, an alternative explanation in terms of 16 molecules is obviously excluded by the chemical constitution:
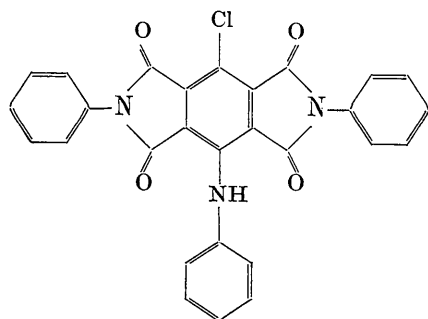
Orthorhombic space groups of higher symmetry than $C2mb$ can be excluded by similar arguments.
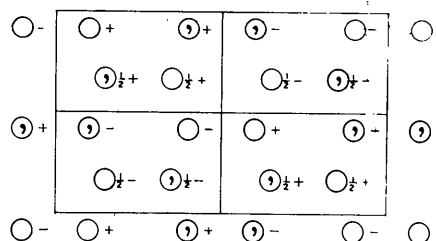

Fig. 1. Orthorhombic arrangement of 16 representative points (space group $C2mb$) that satisfies all selection rules of example I.

The only possible solution is to assume that the apparent Laue symmetry arises from twinning, the true symmetry of the crystal being only monoclinic. The extinction conditions can then all be explained if the 8 molecules occupy the 8 general positions

$$(0, 0, 0; \tfrac{1}{4}, \tfrac{1}{4}, \tfrac{1}{2}; \tfrac{1}{2}, \tfrac{1}{2}, 0; \tfrac{3}{4}, \tfrac{3}{4}, \tfrac{1}{2})+ x, y, z; \ x, \tfrac{1}{2}+y, -z.$$

This arrangement obviously satisfies conditions (1) and (2) and yields in addition the reflexion condition

$$hkl : h+k+2l=4n$$

which is more general than (3) but becomes equivalent when we take into account that, as a result of twinning, reflexions hkl and $\bar{h}kl$ are indistinguishable. For h, k odd, either $h+k+2l$ or $h-k+2l=4n$; for h, k even, $h\pm k+2l=4n$ (reflexion present) or $h\pm k+2l=4n+2$ (reflexion absent).

This arrangement (Fig. 2) corresponds to the space group Bb (No. 9, first setting, c axis unique), referred to the conventional end-centred cell. The higher space group $B2/b$ (No. 15) would require a molecular symmetry consisting either of a diad axis or of a centre of symmetry, but both of these possibilities are incompatible with the chemical constitution. The monoclinic, twinned nature of these crystals can thus be inferred indirectly from the X-ray diffraction pattern; it is confirmed by optical examination of the crystals between crossed Nicols.
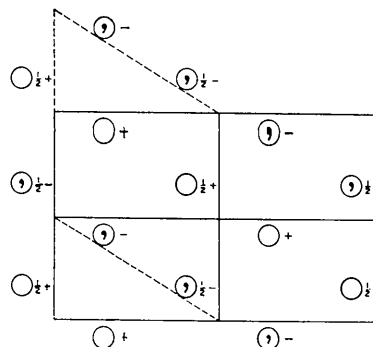

Fig. 2. Monoclinic arrangement of 8 representative points (space group Bb) that satisfies all selection rules of example I if twinning is assumed.
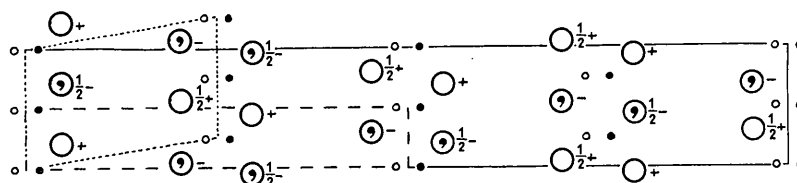
Fig. 3. Arrangement of representative points in crystals of cycloundecylamine hydrobromide (example II). The orthorhombic sub-cell of bromine atoms at $z = \frac{1}{4}$ (small black circles) and $z = \frac{3}{4}$ (small open circles) is outlined by the dashed line; the primitive monoclinic cell (space group $P2_1/b$) is outlined by the dotted line.

Pseudo-selection rules

The reflexion condition, $h + k + 2l = 4n$ if h, k even is an example of a pseudo-selection rule (Niggli, 1959). A pseudo-selection rule differs from an ordinary selection rule in that it applies only to a regularly chosen sub-set of general, zonal or axial reflexions — in this case to half of the general reflexions permitted by the ordinary selection rule, $h + k = 2n$. Niggli has shown that pseudo-selection rules may arise from pseudo-translations which, in contrast to the space group operations, do not form a group in the usual mathematical sense; such a pseudo-translation $(\frac{1}{4}, \frac{1}{4}, \frac{1}{2})$ would occur in the orthorhombic structure described above and rejected as being incompatible with the chemical evidence. We have shown that pseudo-selection rules may also arise as a result of twinning of a monoclinic crystal to give a pseudo-orthorhombic X-ray diagram, provided that the pseudo-orthorhombic cell has a multiplicity of 4. Any multiplicity greater than 2 can be shown to lead to a pseudo-selection rule by twinning, e.g. the selection rule $h + k = 3n$ would lead to the pseudo-selection rule: if $h = 3n$, then $k = 3n$.

Example II

The case of cycloundecylamine hydrobromide will be considered next. The observation (6) that all reflexions with h, k odd are weak suggests that the heavy Br atoms lie in special positions such that they contribute only to reflexions with $h = 2n$, $k = 2n$, $h + k = 4n$. This together with (4) would mean that the Br atoms can be referred to an end-centred cell with $a' = a/2$, $b' = b/2$, space group $Ccmm$ (No. 63). From general intensity considerations it was clear that they occupy the fourfold positions $4c(mm)$, x', 0, $\frac{1}{4}$ etc., with $x' = a'/36 = a/72$. In order to explain the weak reflexions with h, k odd, two possibilities are open. Either the organic cations are distributed over two sets of eightfold general positions of $Cc2a$ (No. 41) in x, y, z, etc., $\frac{1}{4} + x, \frac{1}{4} + y, z$, etc., or the structure is actually monoclinic. Here the orthorhombic possibility requires no molecular symmetry and hence it cannot be excluded a priori, as in the previous example.

In order to try to distinguish between these possibilities, X-ray photographs were made of a large number of crystals, and finally one that displayed

a clear breakdown of orthorhombic symmetry was found. The symmetry of the X-ray diagram of this untwinned crystal was only $2/m$, c axis unique, and the condition $h + k = 4n$ was seen to be a general one, arising from the non-primitive nature of the orthogonal cell which has lattice points at $0, 0, 0$; $\frac{1}{4}, \frac{1}{4}, 0$; $\frac{1}{2}, \frac{1}{2}, 0$; $\frac{3}{4}, \frac{3}{4}, 0$. The apparent mmm Laue symmetry of most specimens arises from twinning such that reflexions hkl and $h\bar{k}l$ coincide. For when h, k are both odd either $h + k$ or $h - k = 4n$ and when h, k are both even, $h \pm k = 4n$ or $4n + 2$; hence in a twinned crystal, the condition $h + k = 4n$ appears only as the pseudo-selection rule (5).

The space group of the primitive monoclinic cell is $P2_1/b$ (No. 14), $Z = 4$, but the Br atoms, as mentioned above, are distributed in a perfectly orthorhombic arrangement (Fig. 3). This means that the reflexions of the untwinned crystal with h, k even display very nearly perfect mmm Laue symmetry, deviations being apparent only in the case of weak reflexions where the Br contribution is very small.

Very few $0kl$ reflexions (with $k = 4n$) are observable and condition (4) should not be regarded as inconsistent with the structure shown in Fig. 3. The apparent c glide is obeyed by the bromine atoms, which do not contribute to $0kl$ reflexions with l odd; these reflexions are therefore predicted to be very weak rather than formally absent.

Example III

The next case, that of azacyclodecane hydrobromide, has ostensible similarities to the previous example, but there are some very important differences. Once again, all reflexions with h, k odd are weak, but now, from (5) and (6) the Br atoms must be referred to a body-centred cell with $a' = a/2$, $b' = b/2$, space group $Ibam$ (No. 72). From general intensity considerations they must occupy the eightfold special positions $8j(m)$, x', y', 0 with $x' = 0.117$, $y' = 0.167$. In order to explain the weak reflexions with h, k odd, there are again two apparent possibilities. Either the organic cations are distributed over two sets of sixteenfold general positions of $Ccca$ (No. 68) in x, y, z, etc. and $\frac{1}{4} + x, \frac{1}{4} + y, \frac{1}{2} + z$, etc. as shown in Fig. 4, or the structure is monoclinic with lattice points at $0, 0, 0$; $\frac{1}{4}, \frac{1}{4}, \frac{1}{2}$; $\frac{1}{2}, \frac{1}{2}, 0$; $\frac{3}{4}, \frac{3}{4}, \frac{1}{2}$, corresponding to a selection
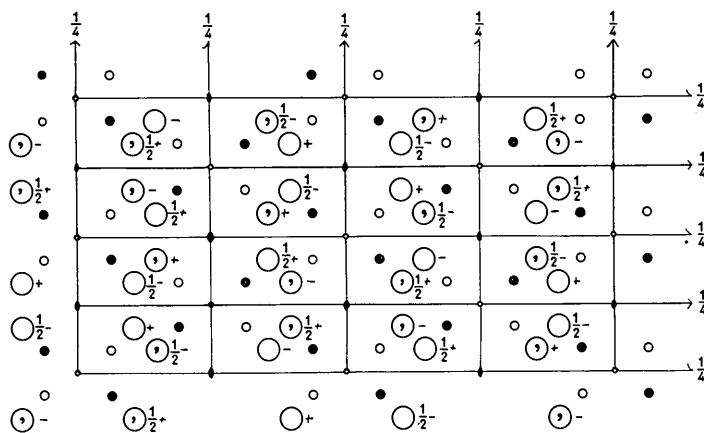
Fig. 4. Possible orthorhombic arrangement of representative points (space group $Ccca$) in crystals of azacyclodecane hydrobromide (example III). Bromine atoms are at $z=0$ (small open circles) and $z=\frac{1}{4}$ (small black circles).

rule $h+k+2l=4n$. The apparent translations $a/2$ and $b/2$ relating the bromine tetrads cannot be lattice translations of the cell as a whole; otherwise reflexions with h, k odd would be absent, whereas they are only weak.

Some X-ray photographs do in fact show slight differences between the intensities of hkl and $h\bar{k}l$ reflexions with h, k odd, indicating that the monoclinic possibility is the correct one; and careful scrutiny of the differences indicates that the stronger of the pair corresponds always to the condition $h+k+2l=4n$, the weaker to $h+k+2l=4n+2$. In these crystals, the twins are present in unequal proportion and presumably an untwinned crystal would yield an X-ray diagram in which reflexions with $h+k+2l=4n+2$ were entirely absent. The standard monoclinic cell, space group $B2/b$ (No. 15), has eightfold general positions and covers only half of the orthogonal

pseudo-cell. This pseudo-cell contains 32 molecules, which must be distributed over two sets of general positions. One distribution that accounts for all the reflexion conditions and at the same time corresponds to equivalence of the two sets of organic cations with respect to the orthorhombic arrangement of bromine ions (but not to each other) is to place one set at x, y, z; etc., the other at $\frac{1}{4}+x, \frac{1}{4}-y, -z$; etc. This distribution is shown in Fig. 5. Note that although it is monoclinic, the projection down the unique axis has perfect rectangular symmetry, pmm; $a'=a/2$, $b'=b/2$.

Para-orthorhombic structures

Monoclinic structures in which the projections down three mutually perpendicular directions have perfect rectangular symmetry appear to occur fairly frequently, two other examples having been discovered in the author's laboratory during the last few years, and it is interesting to study their characteristics in a little more detail. The essential features can be derived from examining the distribution shown in Fig. 6, based on the space group $P2/b$ (No. 13). This distribution has the following characteristics:

1. The non-primitive cell centred on the oblique C face is orthogonal (for simplicity we shall refer to the corresponding orthogonal axial system rather than to monoclinic axes).
2. There are two sets of equivalent points, related to one another *in projection* by the operation of the plane group pgg. In Fig. 6, one set of equivalent points has coordinates x, y, z, etc., the other has coordinates $\frac{1}{4}+x, \frac{1}{4}-y, z$, etc. referred to the orthogonal axial system.
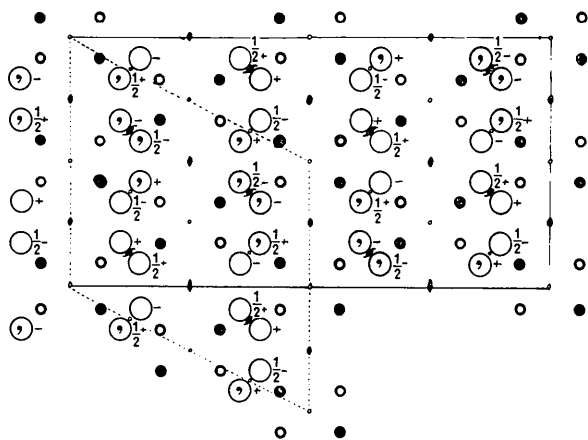

Fig. 5. Monoclinic (para-orthorhombic) arrangement of representative points (space group $B2/b$) in crystals of azacyclodecane hydrobromide (example III). The standard monoclinic cell is outlined by a dotted line. The arrangement of bromine atoms is the same as in the orthorhombic arrangement shown in Fig. 4.

Although all three projections have rectangular symmetry, the structure as a whole is only monoclinic. The representative point A at x, y, z is con-
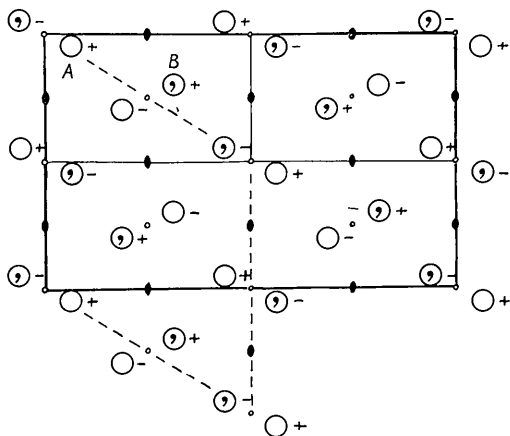
Fig. 6. A para-orthorhombic arrangement of representative points based on the monoclinic space group $P2/b$. This arrangement is found in crystals of nonactin (example IV).

verted into the point B at $\frac{1}{4}+x$, $\frac{1}{4}-y$, z by reflexion across the plane $y=0$ followed by translation $\frac{1}{4}$, $\frac{1}{4}$, 0. The same operations applied to the point B, however, do not lead to a member of the A set; they would lead to a point at $\frac{1}{2}+x$, y, z and would thus produce the non-existent lattice translation $a/2$. In other words, the operation that converts point A into point B is not a symmetry operation of the arrangement as a whole, which belongs to the monoclinic space group $P2/b$.

It is not even necessary that the z coordinates of the two points A and B be equal. Restrictions are only introduced in case that the sixteen general positions of the orthogonal cell are occupied by eight centrosymmetric molecules. In this case, $z_B = \pm z_A$ or $z_B = \frac{1}{2} \pm z_A$ if the molecules are to be identical; on the other hand, eight identical molecules with a diad axis parallel to c can be constructed with arbitrary values of z_A and z_B.

We can derive the Laue symmetry and systematic absences of the above structure (with $z_B = z_A$) by substitution in the structure factor expression for $P2/b$.

Reflexion condition	Symmetry relationship
(1) hkl : $h+k=2n$	$I(hkl) \neq I(h\bar{k}l)$ h, k odd
(2) $hk0$: $h=2n$ $(k=2n)$	$I(hkl) = I(h\bar{k}l)$ h, k even
(3) $h0l$: $h=4n$	
(4) $0kl$: $k=4n$	

For this special case we see that all the axial and zonal reflexions, and half of the general reflexions, have mmm Laue symmetry. The same is true if $z_B = z_A + \frac{1}{2}$, the only difference being in the reflexion conditions for $h0l$ and $0kl$ which now become $h+2l=4n$ and $k+2l=4n$ respectively. If z_A and z_B are unrelated, then the general reflexions have only $2/m$ Laue symmetry and conditions (3) and (4) reduce to $h00$: $h=4n$ and $0k0$: $k=4n$. Twinning could, of course, lead to apparent mmm Laue symmetry in all of these cases but the systematic absences would still not be

characteristic of any orthorhombic space group. It seems appropriate to refer to such structures as para-orthorhombic since certain regularly chosen subsets of reflexions exhibit perfect mmm symmetry.

A para-orthorhombic monoclinic structure is to be distinguished from a nearly orthorhombic one. In the latter case, the structure represents a distortion of an orthorhombic arrangement; the interaxial angles need not be exactly 90° and the structure can be made orthorhombic by introducing small displacements of some or all of the atoms. Manganite MnO(OH) (Buerger, 1936) is a good example. On the other hand, the interaxial angles in a para-orthorhombic structure are exactly 90° and it is not, in general, possible to convert the arrangement into an orthorhombic one by small displacements of the atoms. Some crystals, e.g. stilbene, tolane and trans-azobenzene (Robertson, Prasad & Woodward, 1936) can be described as nearly para-orthorhombic.

Going back to Figs. 5 and 6, we see that a para-orthorhombic structure can be regarded as a pair of interlaced structures related to one another by a kind of twinning; in Fig. 6, every member of the A set of representative points is related to one of the B set by reflexion across the plane $y=0$ followed by translation $\frac{1}{4}$, $\frac{1}{4}$, 0. In ordinary twinning, even of the polysynthetic type, relationships of this kind may occur between crystal domains of greater or smaller extension, but there is no special phase-relationship between molecules in different domains. In a para-orthorhombic structure, on the other hand, definite phase-relationships between the two interlacing sets of molecules do occur, leading to abnormal selection rules and diffraction symmetries.

From the nature of para-orthorhombic crystals, it would be expected that such crystals would show a strong tendency to twin and thus to simulate full orthorhombic symmetry. This indeed proves to be the case but, nevertheless, as the previous and the following two examples show, it is sometimes possible to identify para-orthorhombic crystals quite unambiguously.

Example IV

Nonactin is a colourless, crystalline, optically inactive metabolite obtained from cultures of several *Actinomyces* strains; it was known from chemical studies to be the macrocyclic trilactone, $C_{30}H_{48}O_9$, or tetralactone, $C_{40}H_{64}O_{12}$, of nonactic acid, $C_{10}H_{18}O_4$, and the X-ray investigation (Dominguez, Dunitz, Gerlach & Prelog, 1962) was undertaken in order to try to distinguish between these alternatives.

The systematic absences, shown in Table 1, and Laue symmetry are just those derived above for the arrangement shown in Fig. 6. Reflexions with h, k even appear to have perfect mmm symmetry, while there are marked differences in the intensities of hkl and $h\bar{k}l$ reflexions with h, k odd. The crystals are

thus monoclinic, c axis unique, and the 32 formula units of $C_{10}H_{16}O_3$ in the C-centred para-orthorhombic cell are distributed over 2 sets of eightfold general positions.

The asymmetric unit corresponds then to $C_{20}H_{32}O_6$ and the nonactin molecule can be identified as the tetralactone $C_{40}H_{64}O_{12}$. It is not possible without a more detailed analysis to say whether the molecules occupy the two sets of symmetry centres $(0, 0, 0;$ $\frac{1}{4}, \frac{1}{4}, 0,$ etc.$)$ or are located on the two sets of diad axes $(\frac{1}{4}, 0, z;$ $0, \frac{1}{4}, z,$ etc.$)$. In the latter case the z coordinates of the two independent sets of molecules must be equal, because of the symmetry relationship $I(hkl) = I(h\bar{k}l)$ for h, k even.

Example V

The systematic absences (Table 1) and diffraction symmetry $(I(hkl) \neq I(h\bar{k}l)$ for all non-zero l) show that α-cobalt dipyridine dichloride is another para-orthorhombic crystal, based on the plane group pgg but with z_A and z_B unrelated. This means, of course, that the eight molecules must occupy the two independent sets of diad axes, as has been confirmed by a more detailed analysis (Dunitz, 1957) which leads to $z_A = 0.15$, $z_B = -0.44$.

Most crystals of α-cobalt dipyridine dichloride show perfect mmm diffraction symmetry, due to twinning. Only after a systematic search was a crystal found that showed deviations from mmm symmetry in the sense mentioned above.

Conclusions

The results of this study, summarized in Table 2, lead to the following conclusions.

Crystals should not be classified as orthorhombic simply on the basis of the apparent Laue symmetry of their diffraction patterns. Special caution is called for if the selection rules are uncharacteristic of any orthorhombic space group, of if pseudo-selection rules are observed, for such features may be caused by twinning or may be due to the para-orthorhombic nature of the crystals. It is especially dangerous to assign crystals to the orthorhombic system from considerations of the zonal reflexions alone, since these do not distinguish orthorhombic from para-orthorhombic crystals.

Although no systematic search of the literature has been made, there are probably many crystals described on the evidence of their diffraction symmetry as orthorhombic that are really monoclinic. Thus, the apparent mmm Laue symmetry of 2,4,6-trinitrotoluene (Hultgren, 1936) is probably due to twinning,

Table 2. *Summary of results for the five pseudo-orthorhombic crystals listed in Table* 1

Orthorhombic axes are here designated with subscript O

I. Monoclinic
Bb $a_O = 2a - b$
$Z = 4$ $b_O = b$

II. Monoclinic
$P2_1/b$ $a_O = 4a - b$
$Z = 4$ $b_O = b$

III. Monoclinic
$B2/b$ $a_O = 2a - b$
$Z = 16$ $b_O = b$

Para-orthorhombic $(pmm$: $a' = a_O/2,$ $b' = b_O/2)$. Two sets of representative points at $x_O, y_O, z,$ etc.; $\frac{1}{2} + x_O, \frac{1}{2} - y_O, -z,$ etc.

IV. Monoclinic
$P2/b$ $a_O = 2a - b$ Molecular symmetry, $\bar{1}$ or 2
$Z = 4$ $b_O = b$

Para-orthorhombic $(pgg$: $a' = a_O/2,$ $b' = b_O/2)$. Two sets of representative points at $x_O, y_O, z,$ etc.; $\frac{1}{2} + x_O, \frac{1}{2} - y_O, z,$ etc.

V. Monoclinic
$P2/b$ $a_O = 2a - b$ Molecular symmetry, 2
$Z = 4$ $b_O = b$

Para-orthorhombic $(pgg$: $a' = a_O/2, b' = b_O/2)$. Two sets of representative points at $x_O, y_O, z_1,$ etc.; $\frac{1}{2} + x_O, \frac{1}{2} - y_O, z_2,$ etc.

for the abnormal selection rules previously reported for this crystal (Hertel & Römer, 1930) suggest strongly that it corresponds to a para-orthorhombic arrangement, based on the space group $P2_1/b$ (C_{2h}^5).

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