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On Miller-Bravais Indices and four-dimensional Vectors

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(*Received* 29 *June* 1964)

The Miller-Bravais and Weber symbols for planes and directions in hexagonal crystals can be interpreted as four-dimensional vectors, which are confined to a particular three-dimensional section of 4-space by the rule that the first three indices sum to zero. This is useful for the calculation of distances and angles in hexagonal crystals. The direction symbolized by $[uvtw]$ is that of the cartesian 4-vector $[u, v, t, \lambda w]$ and the normal to the plane $(hkil)$ is the cartesian vector $[h, k, i, l/\lambda]$, where $\lambda=(2/3)^{\frac{1}{2}}(c/a)$. The angle between two of these 4-vectors is given by the usual formula $\cos\alpha=(\mathbf{r}_1\cdot\mathbf{r}_2)/r_1r_2$, and other useful vector equations apply to these 4-vectors just as for the 3-vectors associated with Miller indices. Seeming inconsistencies in the naming of axes for the reciprocal lattice of a hexagonal structure are eliminated by regarding the direct lattice as the projection on to three dimensions and the reciprocal lattice as the three-dimensional section of four-dimensional lattices reciprocal to each other.

Introduction

The impetus to write this note came from discovering that a research student could work for some years with hexagonal crystals and still need a stereogram or a model to ascertain whether the direction $[10\bar{1}\bar{3}]$, for example, was parallel to the plane $(2\bar{1}\bar{1}1)$, and that though the author could tell him how, he could not easily explain why. In fact, though all who have to do with hexagonal crystals employ the Miller–Bravais notation, few exploit its capabilities to the full, the reason being that most students receive only an *ad hoc* exposition of the system in relation to its use in descriptive crystallography, which makes no attempt to relate it to any more general system of mathematics.

Three dimensions for the representation of two

It is a fairly familar device (not always explained in these terms) to use a three-dimensional coordinate system for a two-dimensional figure where that figure has threefold or sixfold symmetry, exploiting the redundant dimension to obtain a much more symmetrical algebraic representation, while still retaining the advantages of cartesian coordinates. Thus the equations for the sides of a regular hexagon, centred on the origin, when expressed in two-dimensional cartesian coordinates (x, y):

$$\begin{aligned} hx+ky &= \pm d \quad (1a, 1b)\\ -\tfrac{1}{2}(h+\sqrt{3}k)x+\tfrac{1}{2}(\sqrt{3}h-k)y &= \pm d \quad (1c, 1d)\\ -\tfrac{1}{2}(h-\sqrt{3}k)x-\tfrac{1}{2}(\sqrt{3}h+k)y &= \pm d \quad (1e, 1f)\end{aligned}$$

by no means reveal the symmetry instantaneously to the eye: whereas if we consider the figure to be described on the plane

$$x+y+z=0 \qquad (2)$$

of a three-dimensional cartesian system the equations:

$$\begin{aligned} hx+ky+iz &= \pm d \quad (3a, 3b)\\ kx+iy+hz &= \pm d \quad (3c, 3d)\\ ix+hy+kz &= \pm d \quad (3e, 3f)\end{aligned}$$

are simpler and more immediately revealing.

By themselves, of course, equations $(3a\ldots f)$ define planes in the three-dimensional space (x,y,z): but it is only the intersections of these planes with the (111) plane through the origin defined by (2) which we regard as significant. The normal from the origin to any one of the six planes $(3a\ldots f)$, say to the plane defined by $(3a)$, is simply expressed by the equations:

$$x/h=y/k=z/i\,, \qquad (4)$$

or, in equivalent terms, its direction is the vector with components $[h,k,i]$. We here employ square and round brackets for directions and planes respectively in accordance with crystallographic conventions. The

crystallographer's custom is also to employ other letters [*uvw*] or [*uvtw*], when symbolizing a direction, from those, (*hkl*) or (*hkil*), which he uses to symbolize a plane. This extravagance in letters of the alphabet would be inconvenient to follow systematically in this paper, and will not be followed: the shape of the brackets must generally suffice to distinguish planes from directions. Now, since it is not the planes (3*a*...*f*) to which we attach significance, but only the lines in which they intersect plane (2), it is convenient to arrange that this normal should lie in this plane and thus coincide with the normal to the appropriate line. That is to say, we impose the equation:

$$h+k+i=0\,. \tag{5}$$

We are free to do this, since, when equation (2) is satisfied, addition of any arbitrary constant to h, k and i is without effect on the validity of equations (3*a*...*f*). Geometrically, the effect of this is to make the planes (3*a*...*f*), which pass through the sides of our hexagon, stand perpendicular to plane (2).

For any vector we may define in this system, since only vectors in the plane (2) are to have significance, we shall likewise impose the condition, as in (5), that the sum of the components is zero.

Now, the intercepts of the plane (3*a*) on the axes *x*,*y*,*z* are inversely proportional to h, k, and i respectively (being d/h, d/k, d/i). Thus (h, k, i) are in the crystallographer's sense the 'indices' of this plane. Since these axes are equally inclined to the plane (2), and planes (3) are constrained by equation (5) to be normal to plane (2), the intercepts on the projections of these axes on (2), which are in the directions of the vectors [2,$\bar{1}$,$\bar{1}$], [$\bar{1}$,2,$\bar{1}$], and [$\bar{1}$,$\bar{1}$,2] respectively, are likewise inversely proportional to h, k, and i [being $(2/3)^{\frac{1}{2}}\,d/h$, $(2/3)^{\frac{1}{2}}\,d/k$, $(2/3)^{\frac{1}{2}}\,d/i$]. (h, k, i) may thus be taken as the indices of the line defined by (3*a*) and (2), and these indices can be read off as the reciprocals of intercepts on three lines in the plane.

Defining the normal vector to our line (*hki*) as

$$\mathbf{p}=[h,\,k,\,i] \tag{6}$$

and using the general position vector

$$\mathbf{r}=[x,\,y,\,z] \tag{7}$$

equation (3*a*) becomes the simple vector equation defining a plane in terms of its normal from the origin:

$$\mathbf{p}\,.\,\mathbf{r}=d\,. \tag{8}$$

It is thus that, when we can retain a cartesian reference system, the 'indices' of a plane and its normal correspond.

Four dimensions for the representation of three

Coming now to the case of a hexagonal crystal, we have need of a real, physical, dimension normal to the base plane while at the same time it remains advantageous for the representation of symmetry to use three dimensions, rather than two, in which to represent coordinates in the base plane. We can satisfy both of these requirements by representing the crystal in a certain three-dimensional section of a four-dimensional space. In this space the general position vector is

$$\mathbf{r}=[x,\,y,\,z,\,w] \tag{9}$$

The four axes x, y, z and w are all orthogonal to each other. The section we employ is parallel to w and equally inclined to x, y and z, satisfying equation (2). Thus the sum of the first three components of **r** is always zero. There are now *two* directions orthogonal to each other and both orthogonal to the base plane $x+y+z=0$, $w=$constant: these are the vectors [1,1,1,0] and [0,0,0,1] respectively. The first is physically empty, but usefully visualized for interpreting the basal coordinates of position: the second is physically occupied. It is unfortunately impossible to visualize both of these at once, together with the base plane, at least for the majority of people — but it is not difficult to visualize one or the other alternately.

We can now define a plane in our three-dimensional section of four-dimensional space by the equation

$$hx+ky+iz+lw/\lambda=d\,, \tag{10}$$

in conjunction with equation (2): the reason for introducing the factor $1/\lambda$ will emerge presently. We are free, as before, to impose equation (5), which causes the normal

$$\mathbf{p}=[h,\,k,\,i,\,l/\lambda] \tag{11}$$

to the hyperplane (10) to lie in our chosen three-dimensional section of the four-dimensional space, and coincide with that to the plane defined by (10) and (2). Equation (10) can be written as equation (8), with the difference of significance that the vectors now have four components instead of three.

The intercepts of the hyperplane (10) on the axes x, y, z, w are of course d/h, d/k, d/i, $\lambda d/l$, respectively: but more valuable to us are the intercepts on four 'crystallographic axes' which lie in the physical section of the 4-space, namely on lines from the origin in the directions of vectors

$$[2,\,\bar{1},\,\bar{1},\,0]\,,\quad [\bar{1},\,2,\,\bar{1},\,0]\,,\quad [\bar{1},\,\bar{1},\,2,\,0] \quad\text{and}\quad [0,\,0,\,0,\,1]\,.$$

These intercepts are:

$$(2/3)^{\frac{1}{2}}d/h\,,\quad (2/3)^{\frac{1}{2}}d/k\,,\quad (2/3)^{\frac{1}{2}}d/i\,,\quad \text{and}\quad \lambda d/l\,.$$

Now, in the crystallographic application we have natural units of length (lattice parameters), a in the first three of these directions, and c in the fourth. Measured in terms of these units, the intercepts are

$$(2/3)^{\frac{1}{2}}d/ha\,,\quad (2/3)^{\frac{1}{2}}d/ka\,,\quad (2/3)^{\frac{1}{2}}d/ia\,,\quad \lambda d/lc\,.$$

If we now set

$$\lambda=(2/3)^{\frac{1}{2}}(c/a)\,, \tag{12}$$

the intercepts measured in natural units become

$$\lambda d/ch\,,\quad \lambda d/ck\,,\quad \lambda d/ci\,,\quad \lambda d/cl\,.$$

Crystallographic indices for the plane defined by (10) and (2) are thus (*hkil*).

There is one special axial ratio for a hexagonal crystal, $(c/a)=(3/2)^{\frac{1}{2}}$, for which the reference system becomes four-dimensionally cubic. The vector which is normal to the plane (*hkil*), given in general by (11), is in this case [*h*, *k*, *i*, *l*], showing the same correspondence between its components and the indices of the plane to which it is normal, as we have in the case of ordinary cubic crystals. The lattice with any other axial ratio, (c/a), may be thought of as derived from this special case by an affine deformation, an elongation by the factor λ along the *c* axis. The vector [*h*, *k*, *i*, *l*] thereby becomes [*h*, *k*, *i*, λl], according to the cartesian reference system, but its crystallographic direction-symbol remains [*hkil*]. The condition that a line lies in, or is parallel to, a plane is one that is retained under affine deformation. Thus the condition that a direction [*uvtw*] lies in or is parallel to a plane (*hkil*) (the zone law) is in four-dimensional notation, as in three, the zero scalar product relation:

$$uh+vk+ti+wl=0\,. \tag{13}$$

This was the basic fact which confirmed Weber (1922) in his choice of a four-index zone symbol.

We may now summarize the relation between Miller–Bravais indices and vectors as follows:

The normal to the plane crystallographically indexed as (*hkil*) is the cartesian 4-vector [*h*, *k*, *i*, l/λ]: the direction symbolized as [*uvtw*] is that of the cartesian 4-vector [*u*, *v*, *t*, λw].

Interconversion of coordinates

One of the easier ways to find the four-dimensional components of a vector from any three-dimensional representation is to consider its projection on to the crystallographic axes a_1, a_2, a_3, *c* which have the directions $[2\bar{1}\bar{1}0]$, $[\bar{1}2\bar{1}0]$, $[\bar{1}\bar{1}20]$ and [0001]. The vector being [*x*, *y*, *z*, *w*], these projections are

$$6^{-\frac{1}{2}}(2x-y-z)\,,\quad 6^{-\frac{1}{2}}(-x+2y-z)\,,$$
$$6^{-\frac{1}{2}}(-x-y+2z)\,,\quad w\text{:}$$

and thus by use of (2):

$$(3/2)^{\frac{1}{2}}x\,,\quad (3/2)^{\frac{1}{2}}y\,,\quad (3/2)^{\frac{1}{2}}z\,,\quad w\,. \tag{14}$$

If the vector is [*u*, *v*, *t*, λw] $(3/2)^{\frac{1}{2}}a$, then these projections are:

$$(3/2)ua\,,\quad (3/2)va\,,\quad (3/2)ta\,,\quad wc\,. \tag{15}$$

There are several different triaxial systems which are for various purposes convenient for the description of hexagonal crystals and interconversion between the four component system and any one of them may be required. The vector equation:

$$[h,\,k,\,i,\,\lambda l]\,(3/2)^{\frac{1}{2}}a=s\mathbf{a}'+t\mathbf{b}'+u\mathbf{c}' \tag{16}$$

readily gives the conversion formulae for direction symbols, once the expressions in the four-component system for the three triaxial basis vectors $\mathbf{a}'$, $\mathbf{b}'$, $\mathbf{c}'$ are known. The conversion formulae for planes are equally readily obtained from the equation $\mathbf{p}\,.\,\mathbf{r}=$constant, where $\mathbf{p}=[h,\,k,\,i,\,l/\lambda]$ is the normal to the plane (*hkil*), by putting $\mathbf{r}=\mathbf{a}'/s$, $\mathbf{b}'/t$, $\mathbf{c}'/u$ in turn (that is, by using the intercepts on the new axes to define Miller indices (*stu*) in the usual way). We thus obtain, apart from a constant multiplying factor of no importance:

$$s=\mathbf{p}\,.\,\mathbf{a}'\,,\quad t=\mathbf{p}\,.\,\mathbf{b}'\,,\quad u=\mathbf{p}\,.\,\mathbf{c}'\,, \tag{17}$$

these being four-component scalar products.

Thus for the conventional *hexagonal unit cell*, with the three basis vectors

$$\begin{aligned}\mathbf{a}_1&=[2,\,\bar{1},\,\bar{1},\,0]\,6^{-\frac{1}{2}}a\,,\\ \mathbf{a}_2&=[\bar{1},\,2,\,\bar{1},\,0]\,6^{-\frac{1}{2}}a\,,\\ \mathbf{c}\ &=[0,\,0,\,0,\,1]\ \mathrm{c}=[0,\,0,\,0,\,3\lambda]\,6^{-\frac{1}{2}}a\,,\end{aligned} \tag{18}$$

we obtain the correspondences for directions:

$$[hkil]\rightarrow[(h-i)\,(k-i)l]\,, \tag{19}$$
$$[stu]\rightarrow[(2s-t),\,(-s+2t),\,(-s-t),\,3u]\,, \tag{20}$$

and for planes:

$$(hkil)\rightarrow(hkl)\,, \tag{21}$$
$$(stu)\rightarrow[st(-s-t)u]\,. \tag{22}$$

For the *rhombohedral* reference system, with basis vectors

$$\begin{aligned}\mathbf{a}'&=[2,\,\bar{1},\,\bar{1},\,\lambda]\,6^{-\frac{1}{2}}a\,,\\ \mathbf{b}'&=[\bar{1},\,2,\,\bar{1},\,\lambda]\,6^{-\frac{1}{2}}a\,,\\ \mathbf{c}'&=[\bar{1},\,\bar{1},\,2,\,\lambda]\,6^{-\frac{1}{2}}a\,,\end{aligned} \tag{23}$$

we obtain

$$[hkil]\rightarrow[(h+l)\,(k+l)\,(i+l)] \tag{24}$$
$$[stu]\rightarrow[(2s-t-u)\,(-s+2t-u)\,(-s-t+2u)\,(s+t+u)] \tag{25}$$
$$(hkil)\rightarrow[(3h+l)\,(3k+l)\,(3i+l)] \tag{26}$$
$$(stu)\rightarrow[(3s-t-u)\,(-s+2t-u)\,(-s-t+2u)\,(3s+3t+3u)]\,, \tag{27}$$

and for the *orthorhombic* reference system, with basis vectors

$$\begin{aligned}\mathbf{a}''&=[2,\,\bar{1},\,\bar{1},\,0]\,6^{-\frac{1}{2}}a\,,\\ \mathbf{b}''&=[0,\,3,\,\bar{3},\,0]\,6^{-\frac{1}{2}}a\,,\\ \mathbf{c}''&=[0,\,0,\,0,\,3\lambda]\,6^{-\frac{1}{2}}a\,,\end{aligned} \tag{28}$$

we obtain

$$[hkil]\rightarrow(\tfrac{1}{2})\,[3h(k-i)\,2l]\,, \tag{29}$$
$$[stu]\rightarrow(\tfrac{1}{3})\,[2s(-s+3t)\,(-s-3t)\,3u]\,, \tag{30}$$
$$(hkil)\rightarrow[h(k-i)l]\,, \tag{31}$$
$$(stu)\rightarrow[2s(-s+t)\,(-s-t)\,2u]\,. \tag{32}$$

Lengths and angles: common planes and common directions

The recognition that Miller–Bravais indices are essentially 4-vectors can be put to good use in calculating, for example, the distance between two lattice points

(or two points within the unit cell) or the angle between two specified directions. The square of the length of the vector $\mathbf{r}=[x, y, z, w]$ is

$$r^2=x^2+y^2+z^2+w^2\,. \tag{33}$$

Here the sum of the first three terms is the square of the basal component of length, and the last term is the square of the axial component.

Given two vectors, $\mathbf{r}_1=[x_1, y_1, z_1, w_1]$ and $\mathbf{r}_2=[x_2, y_2, z_2, w_2]$, the square of the difference vector is

$$(\mathbf{r}_2-\mathbf{r}_1)^2=(x_2-x_1)^2+(y_2-y_1)^2+(z_2-z_1)^2 +(w_2-w_1)^2=\mathbf{r}_1^2+\mathbf{r}_2^2-2(\mathbf{r}_1\,.\,\mathbf{r}_2)\,. \tag{34}$$

But, by the usual trigonometric formula

$$(\mathbf{r}_2-\mathbf{r}_1)^2=r_1^2+r_2^2-2r_1\,.\,r_2\cos\alpha \tag{35}$$

where α is the angle between $\mathbf{r}_1$ and $\mathbf{r}_2$. Hence

$$\cos\alpha=(\mathbf{r}_1\,.\,\mathbf{r}_2)/r_1r_2\;; \tag{36}$$

i.e. we can calculate the angle between the two vectors from their scalar product and a normalizing factor in the four-component case exactly as in the three-component case. The angle between directions symbolized by $[h_1k_1i_1l_1]$ and $[h_2k_2i_2l_2]$ is thus given by:

$$\cos\alpha=\frac{h_1h_2+k_1k_2+i_1i_2+\lambda^2l_1l_2}{(h_1^2+k_1^2+i_1^2+\lambda^2l_1^2)^{\frac{1}{2}}\,(h_2^2+k_2^2+i_2^2+\lambda^2l_2^2)^{\frac{1}{2}}} \tag{37}$$

where $\lambda^2=2c^2/3a^2$.

To find the plane common to these two directions, when this cannot be done by inspection, it is easiest to convert to one of the three-axis systems, *e.g.* by (19), form the cross-product, and convert back, in this case by (22). For the inverse problem, of finding the direction common to two planes, there is some advantage, as already noted by Weber (1922), in making use of the duality between planes and directions (faces and zone axes) basically implied by equation (13), and thus making the conversions as though the planes were directions and the common direction a plane: in this way formally identical algorithms can be used for both problems.

For the angle between the direction $h_1k_1i_1l_1$ and the plane $(h_2k_2i_2l_2)$ we have

$$\sin\alpha=\frac{h_1h_2+k_1k_2+i_1i_2+l_1l_2}{(h_1^2+k_1^2+i_1^2+\lambda^2l_1^2)^{\frac{1}{2}}\,(h_2^2+k_2^2+i_2^2+l_2^2/\lambda^2)^{\frac{1}{2}}}\,. \tag{38}$$

The reciprocal lattice

The reciprocal lattice of a hexagonal lattice is a source of some confusion to students. It seems to be a rather puzzling accident that no contradiction arises from two alternative ways of defining the reciprocal lattice and the four-figure labelling of its points. By the first approach, the reciprocal lattice point *hkil* lies at a distance from the origin inversely as the spacings between (*hkil*) planes in the direct lattice, in a direction normal to these planes. This prescription yields a lattice, in which points are labelled as to position according to the four-index symbols for vectors. However, the axes, $\mathbf{a}_1^*$, $\mathbf{a}_2^*$, $\mathbf{a}_3^*$, $\mathbf{c}^*$, of the reference system according to which they have this labelling do not appear to be related to the direct crystallographic axes in the customary way. The directions coincide, $\mathbf{a}_i^*$ with $\mathbf{a}_i$ and $\mathbf{c}^*$ with $\mathbf{c}$: the length of $\mathbf{c}^*$ is c^{-1}; the length of each $\mathbf{a}_i^*$ is $3^{-\frac{1}{2}}$ times the distance from the origin to the nearest actual reciprocal lattice point, and thus equal to $(2/3)a^{-1}$.

Quite different axes are obtained by an equally regular approach, according to which the primitive cell edges $\mathbf{e}_i^*$ of the reciprocal lattice are related to those, $\mathbf{e}_j$, of the direct lattice by:

$$\mathbf{e}_i^*\,.\,\mathbf{e}_j=\delta_{ij}\equiv\left\{\begin{array}{l}1,\ i=j\\0,\ i\neq j\end{array}\right\}\ i,j,=1,2,3\,. \tag{39}$$

Identifying $\mathbf{e}_1$ with $\mathbf{a}_1$, $\mathbf{e}_2$ with $\mathbf{a}_2$, $\mathbf{e}_3$ with $\mathbf{c}$ (discarding $\mathbf{a}_3$) we obtain an $\mathbf{e}_3^*$ identical with $\mathbf{c}^*$ above, but a pair of axes $\mathbf{e}_1^*$ and $\mathbf{e}_2^*$ in the base plane making an angle of 60° with each other. These axes put the reciprocal lattice points $hk\,.\,l$ in the same positions as the former approach, when no account is taken of the third index, and one may proceed blindly to restore this third index by using the rule $h+k+i=0$: but as they do not describe a conventional hexagonal cell, and do not provide a symmetrical third position for a third basal axis, the geometrical significance of the restoration of the third index is in this case a complete change of the basal axes, from $\mathbf{e}_1^*$ and $\mathbf{e}_2^*$, 60° apart, to

$$\begin{aligned}\mathbf{a}_1^*&=\tfrac{2}{3}\mathbf{e}_1^*-\tfrac{1}{3}\mathbf{e}_2^*\,,\\ \mathbf{a}_2^*&=-\tfrac{1}{3}\mathbf{e}_1^*+\tfrac{2}{3}\mathbf{e}_2^*\,,\\ \text{and}\quad \mathbf{a}_3^*&=-\tfrac{1}{3}\mathbf{e}_1^*-\tfrac{1}{3}\mathbf{e}_2^*\,,\end{aligned} \tag{40}$$

120° apart.

This untidiness is removed when we appreciate that the four-index system brings in an auxiliary dimension. To explain the matter in visualizable terms, let us consider how we generate the two-dimensional reciprocal lattice of a two-dimensional hexagonal direct lattice: the subsequent extension in the $\mathbf{c}$ or $\mathbf{c}^*$ dimension is entirely straightforward (by way of equation (39), with $i, j=1, 2, 3, 4$).

Let the two-dimensional hexagonal lattice D_{h2} (of lattice parameter a) be regarded as the projection on the plane $x+y+z=0$ of a simple cubic lattice D_{c3}, having a lattice parameter $a_c=(3/2)^{\frac{1}{2}}\,a$, and its axes along x, y, z. The reciprocal lattice R_{c3} of the latter is another simple cubic lattice, similarly oriented, with lattice parameter $a_c^*=(2/3)^{\frac{1}{2}}a^{-1}$. Those of its points which lie in the plane $x+y+z=0$ form the required two-dimensional lattice R_{h2} which is the reciprocal lattice of D_{h2}, since these points correspond to those planes of D_{c3} which are parallel to the projection axis [111] and appear as lattice rows in D_{h2}. R_{h2} is a hexagonal lattice of lattice parameter $2^{\frac{1}{2}}a_c^*=(4/3)^{\frac{1}{2}}a^{-1}$, differing in orientation by 30° from D_{h2}. The reference axes $\mathbf{a}_1^*$, $\mathbf{a}_2^*$, $\mathbf{a}_3^*$ of length $(2/3)a^{-1}$ which appeared above are now seen to be the projections on $x+y+z=0$ of the cubic reciprocal lattice axes $\mathbf{a}_c^*$.

Since the generation of a reciprocal lattice is a genuinely reciprocal process we could, as an equally valid alternative, have employed *selection* of points on the plane $x+y+z=0$ from a simple cubic lattice to represent D_{h2} and would then have found that *projection* on this plane of the simple cubic reciprocal lattice reproduced R_{h2}: the imaginary simple cubic lattices used for these two alternative representations have different orientations with respect to the direct hexagonal lattice.

Since selection of the points on one plane is equivalent to multiplication by a plane delta function, since the generation of a reciprocal lattice is equivalent to Fourier transformation, and since the Fourier transform of a plane delta-function is a rod delta-function normal to that plane, the whole representation (in either alternative) is an application of Parseval's theorem, namely that the Fourier transform of the operation 'multiply by' is 'fold with': folding a [111] rod delta-function with the simple cubic lattice points is equivalent, after discarding the superfluous dimension, to projection on the (111) plane.

Of the two alternative representations (the first, in which D_{h2} is a projection, R_{h2} a section, of a cubic lattice, and the second, in which D_{h2} is a section, R_{h2} a projection of a cubic lattice in another orientation) the first is to be preferred: it is only in this representation that names of points in D_{h2} or R_{h2}, according to customary conventions, correspond directly (save for scale factors) with their names in the cubic reference system. Now an inconsistency seems to have emerged, since in the earlier sections of this paper, while lattices were not under discussion, the re-lowering of dimensionality after introducing an auxiliary dimension was considered to be performed by taking a section. This was the effect of equation (2). However, the procedure in that part of the paper, which related to the descriptive crystallography of macroscopic bodies, clearly ought to correspond to the procedure employed for the representation of the direct, rather than that of the reciprocal lattice, namely a lowering of dimensionality by projection. The inconsistency is only apparent, since we also imposed equation (5); the projections and sections on plane (or hyperplane) (2) of all planes conforming to (5) are identical with each other. Projection for real space, section for reciprocal space is thus the representation applying consistently throughout.

The author expresses his thanks to Dr A. R. Lang for several discussions on these topics.

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Acta Cryst. (1965). **18**, 866

The Crystal Structure of Orthorhombic Acetamide*

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(*Received* 4 *June* 1964 *and in revised form* 13 *August* 1964)

The metastable form of acetamide has been studied by X-ray diffraction. The crystals are orthorhombic, space group *Pccn*, $a=7{\cdot}76$, $b=19{\cdot}00$, $c=9{\cdot}51$ Å, $Z=16$. There are two molecules in the asymmetric unit. These are bound in two-molecule units by a pair of hydrogen bonds. Further hydrogen bonds link these dimers together in columns parallel to **c**. The average bond lengths in the planar molecules are C–C, $1{\cdot}505\pm0{\cdot}013$; C–N, $1{\cdot}334\pm0{\cdot}017$; C–O, $1{\cdot}260\pm0{\cdot}011$, in good agreement with those in the stable (trigonal) solid phase, the vapor, and in similar compounds.

Introduction

Acetamide, $CH_3CO–NH_2$, exists in two crystalline modifications. The structure of the stable (trigonal) form has been reported by Senti & Harker (1940)†. The metastable (orthorhombic) form at room temperature is obtained on cooling from the melt. The two forms differ markedly in their behavior when irradiated by γ rays (Rao, 1960). The principal products obtained from the irradiated crystals are acetonitrile (CH_3CN) and water. The yields per 100 eV of deposited energy are considerably greater for the trigonal form than for the orthorhombic. Since one would presume that the molecular structure is the same in both compounds, it must be details of the intermolecular interaction which are responsible for the differences in the radiation chemistry. In particular, one might expect the hydrogen bond-

* Research performed under the auspices of the U.S. Atomic Energy Commission.

† A reinvestigation of this structure is presently being carried out by Mills, Harris & Harker (1964). The original investigation, carried out long before the age of the modern digital computer, is noteworthy for being the first example of the use of a Fourier refinement in an acentric structure.