Acta Cryst. (1962). **15**, 219

A Modular Algebra for the Description of Crystal Structures*

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Received 15 *November* 1960 *and in revised form* 6 *April* 1961)

Anticuprite, cadmium iodide, perovskite, cesium chloride and many other structures can be considered as stacked, partially occupied hexagonal nets. Algorithms are presented for a mathematical description of such structures. Whereas previously only quarter-, half-, and three-quarter full nets were considered, one-twelfth, one-sixth, one-third, and two-thirds full nets are also described, and the results applied to quartz and corundum. Certain formalisms of mathematical logic are introduced. Rutile is described as a structure made up of closely packed anion pairs with cations occupying the interstices. Plastic modules have been constructed for implementing the mathematical descriptions.

1. Introduction

A description of the location and environment of crystal elements that is suitable for storage in computer and human memories and provides a physically meaningful system of classification of crystal structures has been the subject of two previous articles (Loeb, 1958; Morris & Loeb, 1960).

While those two articles were limited to structures containing closely packed ions and were concerned with the parity (modulo-2) value of coordinates, the present article extends the same approach to a larger group of structures. To this purpose modulo-3 and modulo-9 values of the coordinates are also used. For these reasons this third article in the series has been provided with a title different from the one used in the first two articles.

The following topics are discussed here:

(*a*) An application of the binary algebra to some structures containing closely packed ions, not covered in the earlier articles.
(*b*) An extension of the binary algebra to structures containing no closely packed ions.
(*c*) A modulo-9 algebra for corundum-like structures.
(*d*) A combination of the binary and modulo-9 algebras for quartz-like structures.
(*e*) Algorithms for the rutile structure, demonstrating the relation of this structure to the close-packed one.

The word 'algorithm' is here used in the sense of 'generating function', with the special connotation 'suitable for use in a computer program'.

2. Review of the previous articles

The importance of hexagonal nets has been pointed out by Wells (1954), Loeb & Goodenough (1957) and Iida (1957). Morris & Loeb (1960) considered a series of structures whose anions are either hexagonally or cubically close-packed, and whose cations occupy either octahedral or tetrahedral interstices, or both. Hexagonaly and cubically close-packed structures can both be considered to consist of stacked hexagonal nets; in hexagonal structures these nets are perpendicular to the six-(three-)fold axis, whereas in cubic structures they are perpendicular to a 111-axis. In order to describe the stacking of the hexagonal nets quantitatively, Morris & Loeb used a hexagonal coordinate system in which the h-axis is perpendicular to the stacked nets, and in which the v- and w-axis make an angle of 120° with each other in the plane of the nets. The origin is chosen on one of the closely packed ions, and in any h-plane lines of constant v and constant w connect closely packed ions to their nearest neighbors (see Morris & Loeb, 1960, Fig. 1; also see Fig. 1 of the present article).

The unit distance along the v- and w-directions is chosen such that adjacent lines of constant v and constant w differ by three units respectively in v and w. The unit length along the h-axis is chosen such that the shortest distance between adjacent nets containing close-packed anions equals two units in h.

The close-packed hexagonal nets are stacked in such a way that in any h-plane each net occupies one of three possible positions: in the D-position the v- and w-coordinates of all ions in the net equal integral multiples of three, while in the E- and F-positions these coordinates equal respectively one unit more and one unit less than a multiple of three. The well-known facts that closely-packed hexagonal structures are made up of hexagonal nets stacked in the sequence *DEDEDE*..., and that cubically close-

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* This work was supported in part by the U.S. Navy (Bureau of Ships); and in part by the U.S. Army (Signal Corps), and U.S. Air Force (Office of Scientific Research, Air Research and Development Command), and the U.S. Navy (Office of Naval Research).

packed structures contain nets stacked in the sequence *DEFDEF*..., are expressed by the following equations:

$$\left.\begin{aligned} v &= 3L + [f(h)]_{\mathrm{mod}\ 3} \\ w &= 3M + [f(h)]_{\mathrm{mod}\ 3} \end{aligned}\right\} \qquad (1)$$

where L and M are integers,

and

$$f(h) = 2h \text{ for cubic structures }, \qquad (2)$$

while

$$f(h) = 4 - 2|h_{\mathrm{mod}\ 4} - 2| \text{ for hexagonal structures.} \qquad (3)$$

All closely packed anions lie in planes having even values of h. All cations that occupy interstices surrounded octahedrally by anions lie in planes having odd values of h, and their positions within these planes are again given by equations (1), (2) and (3). All cations occupying tetrahedral sites between closely packed anions lie in planes with half-integer values of h; once more equations (1), (2) and (3) express their positions within these planes.

In rocksalt, nickel arsenide, sphalerite, wurtzite and antifluorite all hexagonal nets are either completely occupied or completely empty. The distribution of ions is indicated for all of these structures in Table 1, where 1 indicates an occupied hexagonal net, while 0 indicates an empty one.

In structures such as spinel only part of all the available sites in some hexagonal nets is occupied. Morris & Loeb described the distribution of cations over such sites by subdividing each net into four subarrays, as shown in Fig. 1 by the letters *a*, *b*, *c* and *d*. The sites in different subarrays are distinguished from each other by the parities (modulo-2 values) of their v- and w-coordinates. One of the subarrays consists of those sites having even v and even w, the second of those having even v and odd w, the third of those having both v and w odd, while the fourth contains all sites having odd v and even w. The distribution of ions over available sites in spinel is shown in Table 2, with each row representing all sites having the same modulo-4 value of h, and each column representing all sites having the same parity-combination of v and w. The format of Table 2 is the one we shall continue to use in the present article; it differs from that used in the 1960 article in the explicit inclusion of the close-packed ions having even values of h. In the earlier article, which dealt exclusively with closely packed anions, such explicit exclusion was deemed redundant. Since the present article also deals with structures having no close-packed ions at all, explicit indication of close-packing is no longer superfluous.

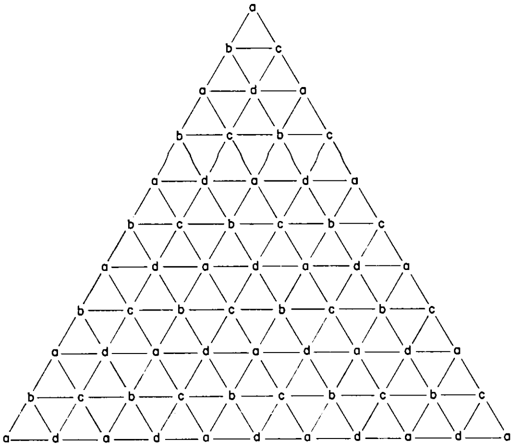


Fig. 1. Subdivision of a hexagonal net into four subarrays.

Table 1. *Distribution patterns for various cubic and hexagonal structures*

$h_{\mathrm{mod}\ 2}$ ↑ Cubic— Hexagonal—	Rocksalt NiAs	Sphalerite Wurtzite	Anti-fluorite
3/2	0	0 or 1	1
1	1	0	0
1/2	0	1 or 0	1
0	1	1	1

Table 2. *Distribution pattern of spinel*

$h_{\mathrm{mod}\ 4}$ ↑	($v_{\mathrm{mod}\ 2}$, $w_{\mathrm{mod}\ 2}$) →			
7/2	0	0	0	1
3	0	0	0	1
5/2	0	0	0	1
2	1	1	1	1
3/2	0	0	0	0
1	1	1	1	0
1/2	0	0	0	0
0	1	1	1	1

Table 2 can be slightly rearranged, as shown in Table 2(*a*), when it is remembered that $h_{\mathrm{mod}}\ 4$ is periodic in h with a period of four units. The purpose of this rearrangement is to point out the symmetry of the distribution pattern about the row $h = 1$. We say that the distribution pattern is an even function of $(h-1)$; it can be similarly observed that it is an even function of $(h-3)$. We shall see in the case of quartz (section 7) that the lack of such symmetry in the distribution pattern is an indication of optical isomerism.

Table 2(*a*). *Distribution pattern of spinel* (*rearranged*)

$h_{\mathrm{mod}\ 4}$ ↑	($v_{\mathrm{mod}\ 2}$, $w_{\mathrm{mod}\ 2}$) →			
3	0	0	0	1
5/2	0	0	0	1
2	1	1	1	1
3/2	0	0	0	0
1	1	1	1	0
1/2	0	0	0	0
0	1	1	1	1
7/2	0	0	0	1
3	0	0	0	1

3. Structures containing closely packed ions

To the structures discussed in the previous article (Morris & Loeb, 1960) should be added the cadmium iodide and the anticuprite structures. Cadmium iodide has hexagonally close-packed anions; the cations occupy half of all octahedral interstices. The distribution of cations over octahedral sites is such that alternate planes normal to the six-fold axis are completely occupied. The distribution pattern for cadmium iodide is therefore as given by Table 3; the distribution along the h-axis resembles that of octahedrally surrounded cations in spinel (see Table 2).

Table 3. *Distribution pattern of cadmium iodide*

$(h-2K_0)_{\text{mod } 4} \rightarrow$	
7/2	0
3	0
5/2	0
2	1
3/2	0
1	1
1/2	0
0	1

Table 4. *Distribution pattern of anticuprite*

$h_{\text{mod } 2} \rightarrow$	$(v_{\text{mod } 2}, w_{\text{mod } 2}) \rightarrow$			
3/2	1	0	0	0
1	0	0	0	0
1/2	1	0	0	0
0	1	1	1	1

Anticuprite has cubically close-packed anions, with one quarter of all tetrahedral sites occupied by cations. The distribution of cations over tetrahedral sites in anticuprite resembles that of cations over tetrahedral sites in spinel. The distribution pattern for anticuprite is given in Table 4; of course, it applies also to cuprite, with cations closely packed, and anions occupying one quarter of the tetrahedral interstices.

These two examples, cadmium iodide and anticuprite, illustrate the recurrence of the patterns of subdivision described in the 1960 article. In the next section we shall find that these patterns occur as well in structures containing no closely packed ions.

4. Structures containing no closely packed ions

The binary algebra is now extended to the perovskite and cesium chloride structures. Whereas these structures do not contain closely packed ions, they can nevertheless be derived from stacked hexagonal nets.

In perovskite ($CaTiO_3$), one type of cations (Ca) is sufficiently large to combine with the anions in forming a close-packed array, while the smaller cations (Ti) occupy octahedral interstices between the anions. From the chemical formula $CaTiO_3$ it follows that one-quarter of the close-packed array is occupied by cations; the subdivision of the close-packed array into quarters once more follows the pattern of spinel. In the case of perovskite we encounter for the first time h-planes occupied by two kinds of ions (Ca and O). In order to distinguish in distribution patterns between the symbol for an unoccupied site (0, zero) and that for a site occupied by an oxygen, we shall deviate from ordinary chemical usage, and denote oxygen in distribution patterns by the symbols Ox. In Table 5 it is shown that each hexagonal array having even h is one-quarter occupied by Ca, three-quarters occupied by Ox.

The small cations, Ti, in perovskite are octahedrally surrounded, hence occupy planes having odd values of h, as shown in Table 5. In these planes they fill one quarter of all available sites; to assign the Ti-ions the proper parity of v and w we recall from the description of spinel (Morris & Loeb, 1960) that the distance between ions in adjacent and next-adjacent planes is a maximum when the ions in *different* h-planes have the *same* v- and w-parity. Since maximum Ti–Ca-distance corresponds to minimum potential energy and hence greatest stability, the Ca- and Ti-ions have the same v- and w-parities, as shown in Table 5.

Table 5. *Distribution pattern of perovskite*

$h_{\text{mod } 2} \rightarrow$	$(v_{\text{mod } 2}, w_{\text{mod } 2}) \rightarrow$			
3/2	0	0	0	0
1	Ti	0	0	0
1/2	0	0	0	0
0	Ca	Ox	Ox	Ox

A structure closely related to perovskite is ReO_3. Here the oxygens occupy a three-quarters close-packed structure, with Re octahedrally surrounded by oxygens. The distribution pattern of ReO_3 is derived from that of perovskite by removing Ca and substituting Re for Ti (see Table 6). The close relationship between the distribution patterns of Tables 5 and 6 and the chemical formulas should be noted.

Table 6. *Distribution pattern for* ReO_3

$h_{\text{mod } 2} \rightarrow$	$(v_{\text{mod } 2}, w_{\text{mod } 2}) \rightarrow$			
3/2	0	0	0	0
1	Re	0	0	0
1/2	0	0	0	0
0	0	Ox	Ox	Ox

To this class of structures belongs also the cesium chloride structure. In this structure both the anions and the cations form separately primitive cubic structures. Since four interpenetrating primitive cubic structures form the cubically close-packed structure, the CsCl-structure is merely a one-quarter filled cubically close-packed structure, so that the distribution pattern for the cesium chloride structure is as shown in Table 7. There is a certain similarity between

Table 7. *Distribution pattern for the cesium chloride structure*

$h_{\text{mod } 2} \rightarrow$	$(v_{\text{mod } 2}, w_{\text{mod } 2}) \rightarrow$			
3/2	0	0	0	0
1	1	0	0	0
1/2	0	0	0	0
0	1	0	0	0

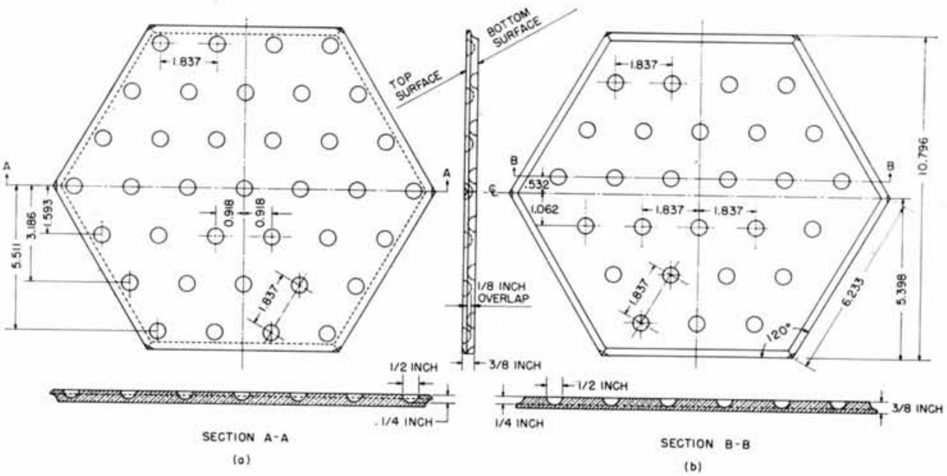


Fig. 2. Plastic sheet modules. (*a*) Plan of top surface. (*b*) Plan of bottom surface.

the CsCl and ReO_3 structures: The empty sites surrounding the Re are just the filled ones surrounding the Cs, while the empty sites surrounding the Cs are just the filled ones surrounding the Re.

5. Modules for displaying crystal structures

Morris & Loeb (1960) have described four modules, two tetrahedral and two octahedral, for constructing crystal models with the use of distribution patterns. These modules are particularly suitable for construction models of crystals containing closely packed ions. While these modules could be adapted for wider applicability, the resulting modules would be far clumsier for use with close-packed arrays than were the original ones. Because of the importance of structures having closely packed ions, it has been decided to leave the original modules unchanged, and a different set of modules has been built to construct models of any crystal that can be derived from hexagonal nets. Some of the mathematics underlying these modules has been discussed by Morris & Loeb (1960, section 2 and Tables 2(*a*) and 2(*b*)). These modules consist of plastic sheets, with hemispherical cavities on both sides. These cavities form an hexagonal array on each side of the sheet; the relative positions of the two arrays are just those of D- and E-arrays, or of E- and F-arrays. In other words, if the v- and w-coordinates of the centers of the cavities all equal an integral multiple of three on one side of a plastic module, then they equal one more or one less than an integer multiple of three on the other side. (See Fig. 2). According to equations (1), (2) and (3) proper stacking of such modules with proper distribution of colored spheres over the cavities can produce a large variety of cubic and hexagonal structures. The thickness of the sheets has, of course, been chosen such that properly close-packed structures with correct tetrahedral and octahedral interstices are obtained. It should be emphasized that the colored spheres represent *centers* of ions; these are *not* packing models.

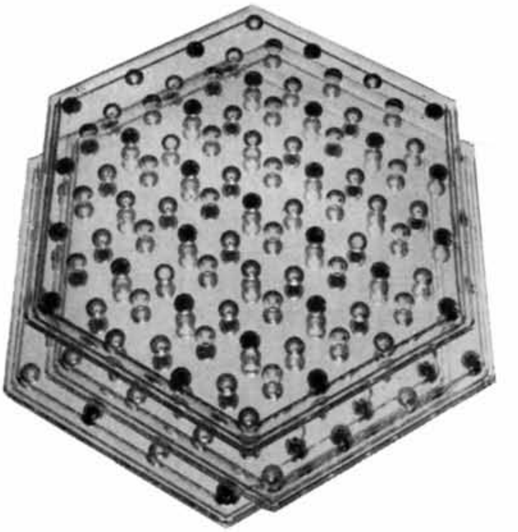


Fig. 3. Model of ReO_3, constructed with plastic sheet modules.

Fig. 3 shows the ReO_3 structure, as constructed from these modules. The perovskite structure is built just as easily, but on a black and white photograph it would be difficult to distinguish the three types of ions. It should be noted that each Re-ion is at the center of an octahedron having oxygens at the corners.

6. Corundum

Corundum, one of the Al_2O_3 structures, has hexagonally close-packed anions, with 2/3 of the octahedral interstices occupied by cations. It is easy to subdivide the hexagonal net into three subarrays (Iida, 1957); it is interesting to note that whereas cubically symmetrical structures are easily subdivided into *four* equivalent subarrays while preserving cubic symmetry, it appears impossible to subdivide cubically symmetrical structures into *three* equivalent subarrays without loss of symmetry.

The cations in corundum occupy planes having odd values of h. When h is odd, $h_{\mathrm{mod}\ 4}$ in equation (3) is either 1 or 3, hence $|h_{\mathrm{mod}\ 4}-2|$ equals unity, and $f(h)=2$. Thus all cations occupy sites having $v=3L+2$, $w=3M+2$, hence occupy F-arrays. Two thirds of each hexagonal net having odd values of h are occupied in corundum, with the empty sites staggered so that they never lie directly above each other. We shall first describe an idealized corundum structure, and then show how the actual structure is easily inferred from the distribution pattern of the idealized structure.

The idealized structure requires for its distribution pattern subdivision of the hexagonal net into three subarrays, as shown in Fig. 4. This subdivision is coded mathematically in terms of a function of the v- and w-coordinates of the individual sites. Whereas subdivision of the hexagonal net into four subarrays was done on the basis of the parities of v and w, the subdivision into three subarrays is described by the modulo-9 value of the difference between v and w. From equation (1) it follows that the function $(v-w)$ always equals an integral multiple of 3, i.e. 0, 3, 6, 9, 12, etc. Therefore $(v-w)_{\mathrm{mod}\ 9}$ equals 0, 3 or 6; inspection of Fig. 4 shows that the sites labeled p, q and r are distinguished from each other by the value of $(v-w)_{\mathrm{mod}\ 9}$ for each site. It should be noted that, as was the case with the a, b, c and d arrays, the labels p, q and r can be permuted at will between the three possible values of $(v-w)_{\mathrm{mod}\ 9}$ by a suitable choice of the origin; the important fact is that all sites bearing the same label have the same value of $(v-w)_{\mathrm{mod}\ 9}$.

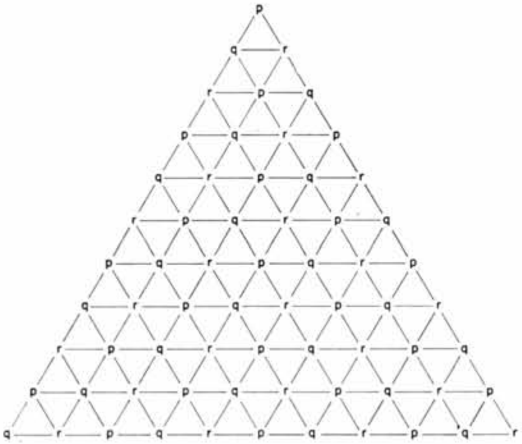


Fig. 4. Subdivision of a hexagonal net into three subarrays.

Table 8 contains the distribution pattern of the idealized corundum structure; the planes having even values of h contain the hexagonally close-packed anions, while each of the planes having odd values of h is two-thirds occupied by cations. With increasing value of h it is alternately the p, the q and the r arrays that are empty; therefore the distribution pattern has a period of six units in h.

Table 8. *Distribution pattern of corundum*

$h_{\mathrm{mod}\ 6} \rightarrow$	$(v-w)_{\mathrm{mod}\ 9} \rightarrow$		
11/2	0	0	0
5	1↓	0	1↑
9/2	0	0	0
4	1	1	1
7/2	0	0	0
3	0	1↑	1↓
5/2	0	0	0
2	1	1	1
3/2	0	0	0
1	1↑	1↓	0
1/2	0	0	0
0	1	1	1

When it is recalled that all hexagonal nets having odd values of h are stacked in the F position, the distortion from the idealized corundum structure follows directly from the distribution pattern. It is observed that, in a direction parallel to the h-axis, cations occur in pairs, with empty sites between the pairs. A stabilizing distortion therefore occurs in the h-direction, with each cation being displaced away from its companion, in the direction of an empty site. The real corundum structure therefore contains puckered hexagonal cation nets instead of plane ones. For convenience arrows are drawn in Table 8 from each cation in the direction of an empty site; these arrows are, of course, not really a part of the distribution pattern. In Fig. 5 we show the idealized corundum structure as constructed out of octahedral modules.

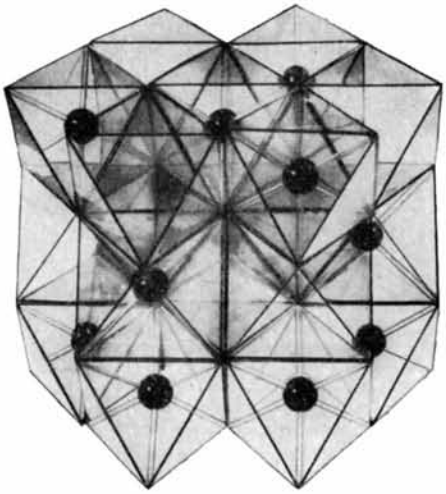


Fig. 5. Model of corundum,
constructed with octahedral modules.

7. Quartz

The somewhat idealized structure of high-temperature quartz as given by Wyckoff (1948) can be derived from stacked hexagonal nets. R. Newnham and the author have constructed this quartz structure out of the modules described in section 4.

The silicons and the oxygens are stacked alternately in planes perpendicular to the six-fold axis; the distance between adjacent oxygen-planes is taken as two units in h. The hexagonal nets used in the description of quartz are stacked neither cubically nor hexagonally, but vertically above each other, just like, for instance, the F-arrays containing the cations in corundum.

The oxygens occupy 1/6 of their hexagonal nets, the silicons 1/12 of their nets; each silicon is surrounded by four oxygens at corners of a tetrahedron. As is observed from Wyckoff's diagram, this tetrahedron is not a regular one, but one distorted in such a way that opposite edges perpendicular to the h-axis make an angle more nearly 120° than 90° with each other. In fact, the four oxygens surrounding a silicon more nearly occupy four of the six corners of a regular octahedron around the silicon.

For a mathematical description of quartz the hexagonal net must be divided into twelve equivalent subarrays. To this purpose the division into four (a, b, c, d) and the division into three (p, q, r) subarrays are combined. By superposition of Figs. 1 and 4, Fig. 6 results; the twelve combinations of a, b, c and d with p, q and r produce twelve equivalent subarrays, each denoted by a combination of two letters. In order to avoid distribution patterns with twelve columns, we use the following notation common in mathematical logic.

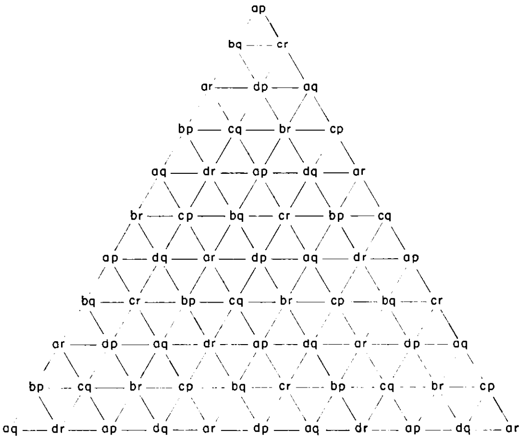


Fig. 6. Subdivision of a hexagonal net into 12 subarrays.

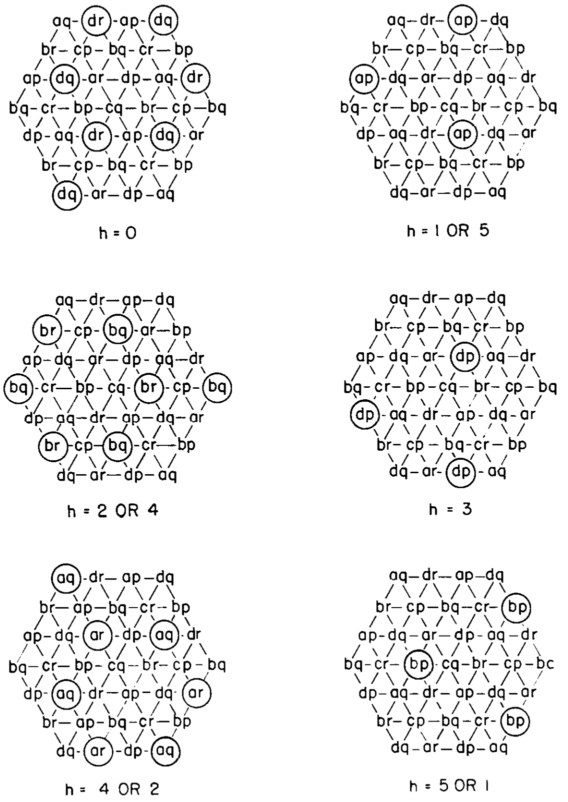
If a symbol a denotes all sites belonging to the subarray a (Fig. 1), and the symbol p denotes all sites belonging to subarray p (Fig. 4), then the symbol ap is interpreted as the 'logical product' of a and p, namely all sites belonging to both subarray a and subarray p. In addition, the notation $(p \oplus q)$ indicates 'all sites belonging to either the p or the q array.' Accordingly, $a(p \oplus q)$ means 'all sites belonging to the a-array and to either the p- or the q-array.'

Since the array a occupies one quarter of a hexagonal net and the array p one third of such a net, ap occupies one twelfth, $a(p \oplus q)$ one sixth of the net. In Table 9 we show the distribution pattern of quartz in terms of this notation. In the left-most column we denote $h_{\bmod 6}$, in analogy with the preceeding distribution patterns, and the middle column represents in the short hand of mathematical logic the twelve columns of the binary distribution pattern. This distribution pattern does not have the property that we observed for spinel and that is common to all distribution patterns considered so far, namely invariance to reversal in direction of the h-axis. For convenience the row $h = 0$ is shown explicitly at both the bottom and the top of Table 9, and the right hand column of that table shows the effect of reversing the direction of the h-axis. It is observed that this reversal produces a new pattern that cannot be turned into

Table 9. *Distribution pattern of quartz*

$h_{\bmod 6}$ ↑		$h_{\bmod 6}$ ↓
0*	$d(q \oplus r)$	0*
5	bp	1
4	$a(q \oplus r)$	2
3	dp	3
2	$b(q \oplus r)$	4
1	ap	5
0*	$d(q \oplus r)$	0*

* The row $h = 0$ has been repeated for the reason explained in the text.


h = 0

h = 1 OR 5

h = 2 OR 4

h = 3

h = 4 OR 2

h = 5 OR 1

Fig. 7. Hexagonal-net occupancy for quartz.

the original one, because the reversal of the axis reverses the order in which the symbols *d*, *a* and *b* occur in the center column.

The original and the new model are therefore each other's mirror images; they represent the two optical isomers of quartz. One of these isomers is characterized by the sequence *dab* in the center column of Table 9, the other by the sequence *dba*.

As an example of the construction of a model with the aid of the models described in section 4, Fig. 7 contains the layout of the hexagonal nets that are to be stacked according to the instructions of Table 9; one isomer results when the values of *h* are taken from the left hand column while the other isomer results when the right hand column is consulted.

It should be observed that no subarray containing the letter *c* is occupied (see Table 9). Yet the *c*-arrays play an important role in the quartz structures, for the *cq* and *cr* subarrays in each hexagonal net represent the locations at which those axes intersect the *h*-planes, around which the silicons and oxygens together form the well-known spirals. Inspection of Fig. 7 will confirm the fact that in the two isomers the spirals wind in opposite directions.

8. The rutile structure

With the rutile structure we reach a structure that does not appear to be built of stacked hexagonal nets. Yet we shall show that this structure is very simply related to the close-packed one.

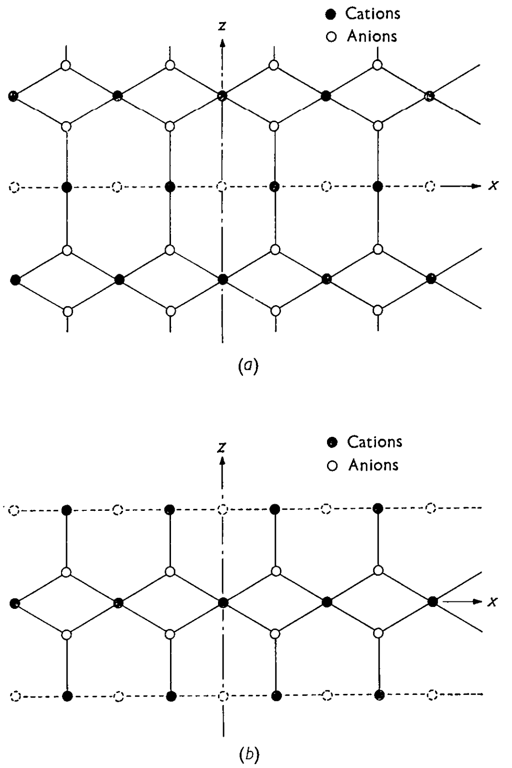


Fig. 8. Arrangement of ions in the rutile structure; cross sections are parallel to XZ-plane.

In rutile the anions are surrounded by only three cations instead of four, as is the case for instance, in sphalerite and wurtzite. These three cations are coplanar with the anion. The cations are octahedrally surrounded by anions; the octahedron is not regular, but distorted so that two anion–cation–anion straight lines make angles of 60° with each other. The third anion–cation–anion straight line is perpendicular to the first two. All cation–anion bonds are equally long. These are the constraints upon which our idealized model for rutile is built; this model is drawn in Fig. 8. In this figure a Cartesian coordinate system is used for reference.

The X-axis is chosen in such a way that it bisects the angle of 60° made by some of the anion–cation bonds. The Y- and Z-axes bisect the 120° angle between such bonds. The origin is chosen half way between two neighboring anions. The unit distance is chosen such that the shortest anion–cation distance equals two units; this is also the shortest anion–anion distance. Fig. 8 shows sections made normal to the Y-axis along alternate planes containing cations. Half of the anions lie in these same planes, but the other half lies out of the planes with the bonds connecting them to their nearest cations making angles of 30° with these planes. All bonds and anions lying outside the planes containing the cations are shown dotted. The two planes shown Fig. 8 are identical, except for a translation in the Z-direction; sections made normal to the Z-axis are again identical with these two. Inspection of Fig. 8 shows that the constraints of trigonal environment of the anions and the special octahedral environment of the cations postulated above are indeed satisfied. The distance between adjacent cation-planes is three units.

Inspection of Fig. 8 shows another important relationship, namely that rutile might be considered constructed out of equilateral TiO_2 triangles, half of them oriented normal to the Z-axis, the other half normal to the Y-axis. When we consider the cations in rutile, then we observe that these form a close-packed array that is tetragonally compressed along the X-axis. The centers of mass of the O_2-pairs also form a tetragonally distorted close-packed array congruent with that formed by the cations. Accordingly, we find that the anions form a close-packed array of *anion pairs*, half of these pairs being oriented parallel to the Y-axis is due to the parallel to the Z-axis. The compression along the X-axis is due to the fact that the anion pairs are not spherical in shape, but elongated.

In view of this interpretation we might re-interpret the cation environment. Along the X-axis one finds one anion pair in the positive and one anion pair in the negative X-sense; both of these pairs are normal to the X-axis. Along the other two axes there are four more anion pairs, two parallel, the other two normal to the respective axes. Altogether, therefore, each cation is surrounded by six anion pairs, one along each coordinate direction and sense.

Our interpretation of the rutile structure is easily put in mathematical form. Since each cation–anion bond is two units long, the height of each TiO_2 triangle is $\sqrt{3}$ units. The coordinates of the cations therefore obey equation (6).

$$\sqrt{3}x+y+z=6K+3\ , \tag{6}$$

where K is an integer.

The centers of mass of the anion pairs have coordinates that obey equation (7).

$$\sqrt{3}x+y+z=6K\ . \tag{7}$$

Since each anion is just one unit away from such a center of mass, the coordinates of the anions themselves obey equation (8).

$$\sqrt{3}x+y+z=6K\pm1\ . \tag{8}$$

Equation (8) does not give information regarding the orientation of each oxygen pair. This information is given as follows:

$$x=L\sqrt{3}\ , \tag{9}$$

$$y=3M\pm(L+1)_{\mathrm{mod}\ 2}\ , \tag{10}$$

where L and M are integers.

From equation (9) we learn that the x-coordinates of all anions are integral multiples of $\sqrt{3}$. From equation (10) it follows that if x is an odd multiple of $\sqrt{3}$, then y is a multiple of 3, so that the anion is coplanar with the cations. On the other hand, if x is an even multiple of $\sqrt{3}$, then y is not a multiple of 3, so that the anion is not coplanar with the cations (dotted in Fig. 8).

By combining equations (8), (9) and (10), we find:

$$\begin{aligned} z&=6K\pm1-3L-3M\mp(L+1)_{\mathrm{mod}\ 2}\\ &=3(2K-L-M)\mp L_{\mathrm{mod}\ 2}\ . \end{aligned}$$

If we define $N\equiv 2K-L-M$, this becomes:

$$z=3N\mp L_{\mathrm{mod}\ 2}\ . \tag{11}$$

Equation (11) is, of course dependent on equations (8), (9) and (10), and therefore yields no new information. In summary, the following equations are most convenient in describing the locations of all ions in the rutile structure.

$$\left.\begin{array}{lr} x=L\sqrt{3} & (9)\\ y=3M\pm(L+1)_{\mathrm{mod}\ 2} & (10)\\ z=3N\mp L_{\mathrm{mod}\ 2} & (11)\\ L+M+N=2K & (12) \end{array}\right\}\ \text{(anion locations)}$$

$$\sqrt{3}x+y+z=6K+3 \qquad (6) \qquad \text{(cation locations)}$$

Equations (6), (9), (10), (11) and (12) represent the algorithms for the rutile structure.

9. Conclusions

The binary algebra developed initially (Loeb, 1958; Morris & Loeb, 1960) for structures containing closely packed ions has been shown to have wider applicability, and new modules have been developed for building crystal models with the use of the mathematical expressions presented here. The power of this modular algebra for representing complex three-dimensional structures and concepts is demonstrated particularly in the case of high-temperature quartz, whose optical activity is not easily predicted from two-dimensional projections of the structure, but follows directly from the distribution pattern. Finally the various unit-cell representations of rutile have been reconciled by means of algorithms showing this structure to consist of closely packed oxygen pairs with titanium in the octahedral interstices.

The author is indebted to Prof. Robert E. Newnham of the Electrical Engineering Department at M.I.T. for his collaboration in constructing the quartz model, and to Dr E. W. Gorter of the Philips Laboratories at Eindhoven for calling to his attention the independent parallel work by Iida. Special thanks are due the two referees whose comments on the first draft of this article were very helpful in improving the presentation of the material.

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