

Notation for Felspar Structures

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(Received 22 July 1955)

A system is proposed for naming individual atomic sites and symmetry-related sets of sites in felspar structures, based on the original notation of Taylor for sanidine. It refers only to structures possessing a perfect lattice, but is applicable to all four known types, namely sanidine, albite, body-centred anorthite and primitive anorthite, and shows the relationship between them. This relationship is discussed from a geometrical standpoint. It is proposed that the notation should become standard.

Introduction

Work in progress on felspar structures suggests that it would be advisable to have a system of naming the atoms, or atomic sites, which could be transferred without confusion from one structure to another. A satisfactory system must fulfil several conditions: it must be based on the existing notation for sanidine (Taylor, 1933), which has been current for many years; it must introduce as few new conventions as possible, and avoid arbitrary numbering which would tax the memory; at the same time it must be comprehensive, so that it can be applied without ambiguity to the most complicated structure of the family. The modification of the sanidine notation used for albite (Taylor, Darbyshire & Strunz, 1934) is slightly clumsy and is not easily capable of further extension; its adaptation by Sörum (1953) for body-centred anorthite does not allow concise reference to independent atoms. The present note describes a system which it is hoped may become standard.

The proposed notation is limited to a description of the contents of the unit cell. It therefore applies in the first instance only to structures where the unit cell is the same throughout the crystal: that is, where there are no systematic differences in cell-dimensions or cell-content from place to place, such as would give rise to non-Bragg reflexions or very large apparent *c*-repeat distances. Such departures from a perfect lattice are characteristic of the intermediate plagioclases, which are thus outside the scope of this paper, except in so far as they can be described in terms of one or more structures with perfect lattices.

Four distinct structure types with a perfect lattice occur in the felspar family; each may be named after an important representative of the type. They are as follows:

- Monoclinic *C*-face-centred, with 7 Å *c*-repeat—sanidine type;
- Triclinic *C*-face-centred, with 7 Å *c*-repeat—albite type;
- Triclinic body-centred, with 14 Å *c*-repeat—body-centred anorthite type;

Triclinic primitive, with 14 Å *c*-repeat—primitive anorthite type.

Their characteristics are summarized in Table 1.

Structurally, the formula of a felspar may be written AB_4O_8 , where *A*, *B* and *O* refer to kinds of sites in a geometrical array. The sites *A* are normally occupied by a large cation *M* (which is commonly K, Na, or Ca), with high coordination by oxygen. The sites *B* are tetrahedrally coordinated, and are occupied by Si or Al. All the sites may be divided into symmetry-equivalent sets, in ways which will be discussed in detail later. Every site of a symmetry-equivalent set must either contain an atom of the same kind or have the same chance of containing an atom of a given kind; in the latter case we may think of every site as containing the same kind of 'statistically-averaged atom'. The first alternative, if it applies to all sets of sites in the structure, is the condition for perfect order. The second, which is merely a re-statement in physical terms of the geometrical postulate that the sites are symmetry-equivalent, specifies the kind of disorder which is permissible. Such disorder is of common occurrence in the felspars, and much experimental work is devoted to the search for detailed knowledge of it in particular cases. For example, the distinction between the monoclinic potassium felspars sanidine and orthoclase may be due to differences between the two structures in the amount of disorder in each of the several sets of sites (Chao, Hargreaves & Taylor, 1940; Cole, Sörum & Kennard, 1949). Any complete structure determination must answer the question how each set of symmetry-equivalent sites is occupied—whether by identical atoms or by statistically-averaged atoms, and of what kind—but the answer need not be known before the sites can be named. Indeed, the naming of the *sites* as distinct from their contents is likely to lead to less confusion in the early stages of a structure investigation, when the distribution of atoms between the sites is not known. It is, however, convenient and conventional to name the sites with some reference to the atoms commonly found in them; thus, the large cation sites will be called *M*, the tetrahedral

Table I. *Structure types in the felspar family (MSi₄O₈)*

(1)	(2)	(3)	(4)	(5)
Structure type	Sanidine	Albite	Body-centred anorthite	Primitive anorthite
Approximate <i>c</i> -repeat (Å)	7	7	14	14
Lattice	<i>C</i>	<i>C</i>	<i>I</i>	<i>P</i>
Symmetry	Monoclinic	Triclinic	Triclinic	Triclinic
No. of formula-units per cell	4	4	8	8
Multiplicity of general position	8	4	4	2
No. of independent formula-units	$\frac{1}{2}$	1	2	4
Atoms in special positions	<i>M</i> , O _{A1} , O _{A2}	—	—	—
Atoms in general positions	Si ₁ , Si ₂ O _B , O _C , O _D	<i>M</i> , O _{A1} , O _{A2} , 2Si ₁ , 2Si ₂ 2O _B , 2O _C , 2O _D	2 <i>M</i> , 2O _{A1} , 2O _{A2} , 4Si ₁ , 4Si ₂ , 4O _B , 4O _C , 4O _D	4 <i>M</i> , 4O _{A1} , 4O _{A2} , 8Si ₁ , 8Si ₂ , 8O _B , 8O _C , 8O _D
Total no. of independent atoms	8	13	26	52
Total no. of atoms	52	52	104	104

sites Si (following the precedent of the sanidine usage), the oxygen sites O.

The proposed notation gives a name to each atomic site in the structure. This consists of two parts, (i) a symbol naming the set of sites in sanidine (the simplest of the felspar structures), (ii) a symbol describing the derivation of the individual site from the prototype site of a set which in sanidine is symmetry-equivalent.

The first symbol is taken direct from the notation for sanidine introduced by Taylor (1933). The list of symbols is given in Table 1, column (2), and in Table 3, column (1). In sanidine, atoms *M*, O_{A1} and O_{A2} are in special positions, the rest in general positions.

The second symbol is the new feature of the notation. It will be dealt with in the sections that follow. A way of modifying the complete symbol to allow reference to symmetry-equivalent sets instead of individual atomic sites will also be explained.

Notation for a set of atomic sites in general positions in sanidine

Sanidine has the space group *C2/m*, and the general position is eightfold; each atomic site is derived from its prototype by the application of one or more operations of symmetry or translation. If these operations are arranged in a standard order, a symbol using positional notation may be devised in which each position is occupied by either zero or a letter indicating the particular operation; the symbol then specifies the site by specifying its derivation from the prototype.

The operations used in sanidine are (i) a mirror plane at *y* = 0, (ii) face-centring on *C*, (iii) a centre of symmetry at (0, 0, 0). Neither this particular choice of operations nor the order of performing them is unique; it is proposed, however, that the set in this order should be taken as standard. Sites derived from the prototype by these three operations are distinguished by the letters *m*, *i*, *c*, respectively (*m* serving as a

reminder of the mirror plane, *c* of the centre of symmetry, *i* of the body-centring which, in the 14 Å structures, replaces *C*-face-centring in the 7 Å structures). Another operation is needed in the 14 Å structures (see below), and it is convenient that it should stand in the second place. Thus a four-figure symbol is needed, the second figure in sanidine being always zero.

This four-figure symbol is added to the symbol specifying the particular set of symmetry-related sites in sanidine, and specifies the individual site within the set. For example, we may have Si₁(0000), Si₁(00*ic*), Si₂(*m0i0*), O_B(*m000*), O_C(000*c*). (If preferred, the new symbol may be written as a subscript, e.g. O_{B*m000*}, but this has typographical disadvantages.)

Atomic sites in special positions in sanidine

The sites in special positions need separate consideration. Of these, *M* and O_{A2} lie on the mirror plane, and the operation of the plane creates nothing new. O_{A1} lies on a diad axis, and the operation of the plane therefore gives rise to the same site as the operation of the symmetry centre. Hence there is no need to reserve the first place in the symbol for the mirror plane. For the cation it is either filled by zero permanently or dropped altogether to leave a 3-figure symbol. For the two oxygens it conveniently accommodates the digit 1 or 2 which distinguishes them from each other, e.g. O_A(10*ic*), O_A(2000).

Extension to other structures

In the other structures, certain of the operations of symmetry or translation found in sanidine have disappeared. Nevertheless the actual sites are recognizably near those which would be given by such operations; hence the same nomenclature can be used.

In the 14 Å structures, the *c* axial length is doubled. If the sanidine structure were described with reference

Table 2. *Parameters and symbols of atomic sites*

Parameters				
Sanidine	Albite	Body-centred anorthite*	Primitive anorthite*	Symbol
x, y, z	x_1, y_1, z_1	x_{11}, y_{11}, z'_{11}	$x_{111}, y_{111}, z'_{111}$	0000
$\bar{x}, \bar{y}, \bar{z}$	$\bar{x}_1, \bar{y}_1, \bar{z}_1$	$\bar{x}_{11}, \bar{y}_{11}, \bar{z}'_{11}$	$\bar{x}_{111}, \bar{y}_{111}, \bar{z}'_{111}$	000c
$\frac{1}{2}+x, \frac{1}{2}+y, z$	$\frac{1}{2}+x_1, \frac{1}{2}+y_1, z_1$	$\frac{1}{2}+x_{11}, \frac{1}{2}+y_{11}, \frac{1}{2}+z'_{11}$	$\frac{1}{2}+x_{112}, \frac{1}{2}+y_{112}, \frac{1}{2}+z'_{112}$	00i0
$\frac{1}{2}-x, \frac{1}{2}-y, \bar{z}$	$\frac{1}{2}-x_1, \frac{1}{2}-y_1, \bar{z}_1$	$\frac{1}{2}-x_{11}, \frac{1}{2}-y_{11}, \frac{1}{2}-z'_{11}$	$\frac{1}{2}-x_{112}, \frac{1}{2}-y_{112}, \frac{1}{2}-z'_{112}$	00ic
—	—	$x_{12}, y_{12}, \frac{1}{2}+z'_{12}$	$x_{121}, y_{121}, \frac{1}{2}+z'_{121}$	0z00
—	—	$\bar{x}_{12}, \bar{y}_{12}, \frac{1}{2}-z'_{12}$	$\bar{x}_{121}, \bar{y}_{121}, \frac{1}{2}-z'_{121}$	0z0c
—	—	$\frac{1}{2}+x_{12}, \frac{1}{2}+y_{12}, z'_{12}$	$\frac{1}{2}+x_{122}, \frac{1}{2}+y_{122}, z'_{122}$	0zi0
—	—	$\frac{1}{2}-x_{12}, \frac{1}{2}-y_{12}, \bar{z}'_{12}$	$\frac{1}{2}-x_{122}, \frac{1}{2}-y_{122}, \bar{z}'_{122}$	0zic
x, \bar{y}, z	x_2, \bar{y}_2, z_2	$x_{21}, \bar{y}_{21}, z'_{21}$	$x_{211}, \bar{y}_{211}, z'_{211}$	m000
\bar{x}, y, \bar{z}	$\bar{x}_2, y_2, \bar{z}_2$	$\bar{x}_{21}, y_{21}, \bar{z}'_{21}$	$\bar{x}_{211}, y_{211}, \bar{z}'_{211}$	m00c
$\frac{1}{2}+x, \frac{1}{2}-y, z$	$\frac{1}{2}+x_2, \frac{1}{2}-y_2, z_2$	$\frac{1}{2}+x_{21}, \frac{1}{2}-y_{21}, \frac{1}{2}+z'_{21}$	$\frac{1}{2}+x_{212}, \frac{1}{2}-y_{212}, \frac{1}{2}+z'_{212}$	m0i0
$\frac{1}{2}-x, \frac{1}{2}+y, \bar{z}$	$\frac{1}{2}-x_2, \frac{1}{2}+y_2, \bar{z}_2$	$\frac{1}{2}-x_{21}, \frac{1}{2}+y_{21}, \frac{1}{2}-z'_{21}$	$\frac{1}{2}-x_{212}, \frac{1}{2}+y_{212}, \frac{1}{2}-z'_{212}$	m0ic
—	—	$x_{22}, \bar{y}_{22}, \frac{1}{2}+z'_{22}$	$x_{221}, \bar{y}_{221}, \frac{1}{2}+z'_{221}$	mz00
—	—	$\bar{x}_{22}, y_{22}, \frac{1}{2}-z'_{22}$	$\bar{x}_{221}, y_{221}, \frac{1}{2}-z'_{221}$	mz0c
—	—	$\frac{1}{2}+x_{22}, \frac{1}{2}-y_{22}, z'_{22}$	$\frac{1}{2}+x_{222}, \frac{1}{2}-y_{222}, z'_{222}$	mzi0
—	—	$\frac{1}{2}-x_{22}, \frac{1}{2}+y_{22}, \bar{z}'_{22}$	$\frac{1}{2}-x_{222}, \frac{1}{2}+y_{222}, \bar{z}'_{222}$	mzic

* This set of parameters assumes that the symmetry centre remains at (0, 0, 0). Since the anorthite structures are referred to a 14 Å c-axis, $z' \simeq \frac{1}{2}z$.

to this axis, sites at (x_1, y_1, z_1) and $(x_2, y_2, \frac{1}{2}+z_2)$, with x_1, y_1, z_1 equal to x_2, y_2, z_2 respectively, would be crystallographically identical. In the 14 Å structures this identity disappears. The second site of such a pair is distinguished in the proposed notation by writing z in the second place of the symbol, for example $O_D(0z0c)$.

Coordinates of sites in the different structures, and the corresponding symbols, are given in Table 2.

Necessity for a standard set of atomic positions

If this notation is to be used to full advantage, it is essential that the same set of prototype sites should be used by all workers.

For sanidine-type structures, it is proposed that the sites listed in Table 3, column (2), should be taken as prototypes and given the symbol 0000. This choice follows that of Taylor (1933) and of all subsequent workers on structures of this type.

For the other structures, the choice of prototype sites will be considered below, when the structures are discussed in detail.

In all cases it is recommended that sites whose positions are recorded should lie within the unit cell; that is, their coordinates should be between 0 and 1 cycles. For convenience, coordinates should be expressed as decimal fractions of a cycle (i.e. decimal fractions of the cell edge) rather than in degrees.

Choice of origin in the 14 Å structures

A certain ambiguity arises in the derivation of the 14 Å structures from the 7 Å structures. If a 7 Å structure is described in terms of a 14 Å repeat, the points (0, 0, 0)

and $(0, 0, \frac{1}{2})$ are identical; there will be no difference in the coordinates if the origin is moved from one to the other. For a true 14 Å structure this is not the case; a choice must be made between two possible origins giving slightly different values to the coordinates. It is proposed that the choice should be such that, if $M(0000)$ is (x_1, y_1, z_1) and $M(0z00)$ is $(x_2, y_2, \frac{1}{2}+z_2), z_1 > z_2$ (this follows the choice made by Sörum (1953)).

Relation of origin and symmetry centres

It does not necessarily follow that the origin is a centre of symmetry. In the sanidine and albite structures there are 16 symmetry centres in the small unit cell, which may be divided into four sets with representative points $(0, 0, 0)$, $(0, 0, \frac{1}{2})$, $(\frac{1}{4}, \frac{1}{4}, 0)$, $(\frac{1}{4}, \frac{1}{4}, \frac{1}{2})$. In the 14 Å structure these points become $(0, 0, 0)$, $(0, 0, \frac{1}{4})$, $(\frac{1}{4}, \frac{1}{4}, 0)$ and $(\frac{1}{4}, \frac{1}{4}, \frac{1}{4})$; the body-centred anorthite structure can retain two only of them as symmetry centres, the primitive anorthite structure one only. Which sets are in fact retained is a matter for experimental determination. There are arguments suggesting that they include $(0, 0, 0)$ in both cases (Sörum, 1951; Goldsmith & Laves, 1955). Should these findings be confirmed, the use of the proposed notation is straightforward and simple. Should it turn out that the symmetry centre lies elsewhere, it is nevertheless proposed that the origin should be kept in its former position for the purpose of specifying atomic positions, because only so can the comparison between different structures be made clear. A second set of coordinates referred to the centre of symmetry as origin may usefully be given *in addition*.

If the centre of symmetry is not at $(0, 0, 0)$, atomic sites whose symbols differ only by c in the last place

Table 3. *Parameters of atoms in sanidine*
(From Cole *et al.* (1949) quoted to two-figure accuracy)

(1) Symbol	(2) 0000*	(3) 000c	(4) 00i0	(5) 00ic	(6) m000	(7) m00c	(8) m0i0	(9) m0ic
K	0.29 0	0.71 0	0.79 0.50 0.14	0.21 0.50 0.86	—	—	—	—
Si ₁	0.01 0.19 0.22	0.99 0.81 0.78	0.51 0.69 0.22	0.49 0.31 0.78	0.01 0.81 0.22	0.99 0.19 0.78	0.51 0.31 0.22	0.49 0.69 0.78
Si ₂	0.71 0.12 0.35	0.29 0.88 0.65	0.21 0.62 0.35	0.79 0.38 0.65	0.71 0.88 0.35	0.29 0.12 0.65	0.21 0.38 0.35	0.79 0.62 0.65
O ₄₁ †	0 0.15 0	0 0.85 0	0.50 0.65 0	0.50 0.35 0	—	—	—	—
O ₄₂ †	0.64 0 0.29	0.36 0 0.71	0.14 0.50 0.29	0.86 0.50 0.71	—	—	—	—
O _B	0.83 0.15 0.22	0.17 0.85 0.78	0.33 0.65 0.22	0.67 0.35 0.78	0.83 0.85 0.22	0.17 0.15 0.78	0.33 0.35 0.22	0.67 0.65 0.78
O _C	0.03 0.31 0.26	0.97 0.69 0.74	0.53 0.81 0.26	0.47 0.19 0.74	0.03 0.69 0.26	0.97 0.31 0.74	0.53 0.19 0.26	0.47 0.81 0.74
O _D	0.18 0.13 0.40	0.82 0.87 0.60	0.68 0.63 0.40	0.32 0.37 0.60	0.18 0.87 0.40	0.82 0.13 0.60	0.68 0.37 0.40	0.32 0.63 0.60

* Prototype.

† The symbols of these two atoms have 1 or 2 respectively replacing the first zero.

will not be symmetry-equivalent, but every site with *c* in the last place will be equivalent to *some* site with 0 in the last place. For example, if the symmetry centre is at $(0, 0, \frac{1}{2})$, site 000*c* is equivalent to site 0z00.

Application to the different structures

Albite

The plane of symmetry occurring in orthoclase is no longer present in albite. Atomic sites which were related by it, that is, sites whose symbols differ by *m*, are now independent; thus it is necessary to quote separately the coordinates of atoms such as 0000 and *m*000. The fourfold sets of which these are representative may be specified by dropping the last three figures of the complete symbol; thus for example instead of Si₁ we have Si₁(0) and Si₁(*m*).

The recommendation that the prototype sites should be 0000 and *m*000 is not in accordance with existing usage; for albite, Taylor *et al.* (1934) recorded the coordinates of atoms 0000 and *m*0*i*0, and other authors have followed them. The convenience of the present notation is considered to justify a change. Transference from one system to the other is easy, since it merely involves addition of ± 0.5 to all *x* and *y* coordinates of atoms which are not prototypes in the sanidine structure.

Body-centred anorthite

Referred to a 14 Å axis, albite had a repeat distance of *c*/2; this identity has disappeared in anorthite. It is now necessary to quote separately the coordinates of 0000 and 0z00 as well as *m*000 and *mz*00. The fourfold symmetry-related sets of which these are representative may be specified by dropping the last two figures of the complete symbol; for example, Si₁(00), Si₁(0z), Si₁(*m*0), Si₁(*mz*) are the crystallographically distinct sets.

The only published work giving coordinates for body-centred anorthite is that of Sörum (1951, 1953). There is no easily-recognized principle in his selection of prototype atoms, and the present proposals should make for greater clarity.

Primitive anorthite

In this the body-centring translation has disappeared. The atoms whose coordinates must be separately quoted are 0000, 00*i*0, 0z00, 0z*i*0, *m*000, *m*0*i*0, *mz*00, *mz**i*0. The pairs of symmetry-related atoms may be specified by dropping the last figure of the complete symbol, for example Si₁(*m*0*i*).

No detailed coordinates have yet been published for this structure type.

Coordinates in the different structure types

Table 2 gives lists of atomic coordinates in each of the four structure types. The subscripts distinguish values

of (x, y, z) which are strictly independent though approximately equal. It must be remembered that the z coordinate referred to the 14 Å axis is half that referred to the 7 Å axis.

Extension to hypothetical structures of the feldspar family

It must be borne in mind that future work on the feldspars may yet reveal examples of new structure types. If a feldspar structure is defined as a structure in which displacements of atomic sites from their positions in any of the hitherto-determined feldspars are small, and if the possibility of a larger unit cell is excluded for the moment, the number of structure types is strictly limited. (Here, as throughout this paper, only structures with a perfect lattice come into consideration.) The possible structures can all be defined by different combinations of one or more of the symmetry operations (including lattice translations) already considered, namely m, z, i, c . For example, there might be a type with triclinic primitive lattice and 7 Å c -repeat, or one with triclinic C -face-centred lattice and 14 Å c -repeat. These can all be described by the proposed notation. The individual symbols for sites of a symmetry-related set would not show up their relationship at a glance (as they do for the existing structures, because the particular choice of order for the symmetry operations, *mzic*, was designed to secure that); but they would remain unambiguous and self-consistent, as would the shortened symbols referring to the sets as a whole. (The loss of elegance is of the same kind as would occur for either of the existing 14 Å structures if the origin were not at a centre of symmetry—a question discussed above.)

If a structure with a larger unit cell should be found—for example, one with a doubled a -edge—the notation could be extended by using a five-position symbol.

Distribution of atoms in the sites

The discussion so far has been wholly geometrical and has strictly referred to atomic sites without regard to their contents. If, however, it is desired to modify the notation so that the kind of atom occupying the site can be specified, this is very easy. The second part of the symbol remains unchanged; only the chemical symbol for the atom is altered. Thus, Sörum's results for body-centred anorthite might be expressed by saying that the symmetry-related sets of 4-coordinated atoms are $(\text{Si}, \text{Al})_1(00)$, $(\text{Si}, \text{Al})_1(0z)$, $(\text{Si}, \text{Al})_1(m0)$, $(\text{Si}, \text{Al})_1(mz)$, $\text{Si}_2(00)$, $\text{Si}_2(0z)$, $\text{Si}_2(m0)$, $\text{Si}_2(mz)$. Similarly, for microcline (Bailey & Taylor, 1955) the symmetry related sets are approximately $(\text{Si}_{0.75}\text{Al}_{0.25})_1(0)$, $(\text{Si}_{0.50}\text{Al}_{0.50})_1(m)$, $\text{Si}_2(0)$ and $\text{Si}_2(m)$. A distribution of M cations in the various sets of sites can be described in the same way.

Summary of proposals

(1) The atomic sites chosen by Taylor (1933) are kept as prototype sites in the sanidine structure and their symbols for these sites are used (see Table 3).

(2) The axes of reference define a unit cell double that of sanidine (i.e. a cell with a 14 Å repeat). Each individual atomic site of a set which in sanidine is symmetry-related has a four-figure symbol specifying its derivation from the prototype. This derivation is made by the following operations, in the order stated: (i) mirror plane, m ; (ii) $c/2$ translation, z ; (iii) body-centring, i ; (iv) centre of symmetry at $(0, 0, 0)$, c . (Referred to the 7 Å axis, (ii) is not used and (iii) is a C -face-centring, but the symbols are unaltered.) Oxygen sites in special positions use the first place in the symbol for the digit 1 or 2 which distinguishes the prototypes; for the large cation it is omitted, or marked with a zero.

(3) The complete symbol for any individual site consists of the two parts considered in (1) and (2).

(4) In structures of lower symmetry, each site has the same symbol as the site to which it corresponds in the doubled sanidine cell. Sets of symmetry-equivalent sites are indicated by dropping one or more figures from the complete symbol.

(5) The standard origin of coordinates is that of the sanidine structure (whether or not this remains a centre of symmetry). For choosing between the two possible origins in the 14 Å structure, the following rule is used: if, in body-centred anorthite, $\text{Ca}(0000)$ is at (x_1, y_1, z_1) and $\text{Ca}(0z00)$ at $(x_2, y_2, \frac{1}{2}+z_2)$, then $z_1 > z_2$.

(6) Tables of coordinates refer to atoms lying within the unit cell; i.e. all coordinates lie between 0 and 1 cycles. Coordinates are expressed in decimal fractions of a cycle rather than in degrees.

I wish to express my thanks to Dr W. H. Taylor for helpful discussions during the preparation of this paper, and to Dr S. W. Bailey, Dr R. B. Ferguson and Dr R. J. Traill for useful comments.

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