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Structures of the Lovozerite Type – a Quantitative Investigation

By Yu. A. Malinovsky

Institute of Crystallography, Leninsky pr. 59, 117333 Moscow, Russia

and H. Burzlaff and W. Rothammel

Lehrstuhl für Kristallographie, Institut für Angewandte Physik, Bismarckstr. 10, D-8520 Erlangen, Germany

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Abstract

The structure of lovozerite is derived from perovskite. For 24 members of the lovozerite family an aristotype is postulated. The method of quantitative comparison using the concept of mappings is applied to the lovozerite family using the aristotype as a 'structural unit'. The method is extended to relationships of symmetry-type II, *i.e.* the derived structure and the aristotype have only a common subgroup, the remaining non-common symmetry of the derived structure is used as 'distribution' symmetry for the structural unit. The numerical results are discussed in detail.

Introduction

Lovozerite is a silicate structure with the general composition $M1M2_2M3_3M4_3$ [Si_6O_{18}] where $M1$, $M2$, $M3$, $M4$ are different metals and Si_6O_{18} represents a chair-form ring silicate group. The compounds either occur as minerals or they may be synthetic. Details are given in Tables 3 and 4.

Recently one of the authors of the present work (Tamazyan & Malinovsky, 1990) showed that the structure of lovozerite can be regarded as a structural unit or motive which can be found in a series of different structures thus defining the lovozerite family. It was recognized that the structural unit will be repeated by translations, centres of symmetry, different screw and rotation axes and glide planes; the symmetry operations used for the repetition may be regarded as 'distribution' symmetry.

In addition, the other two authors (Burzlaff & Rothammel, 1992) proved that structural relations can be described by application of the concept of mappings: a pair of matrices (**A**, **S**) is used to map the lattices, the symmetry operations and the positions of the atoms of two related structures onto each other. This procedure gives rise to the introduction of 'figures of merit' that allow the degree of relationship to be characterized by numerical values. In the first step only those relations that use translations as distribution symmetry were discussed.

It is the intention of this paper to combine both ideas:

(i) the concept of mapping will be extended to structural relations with all types of distribution symmetry;

(ii) this procedure will be applied to structures of the lovozerite family.

Derivation of the lovozerite structure

The members of the lovozerite-type family which possess the highest symmetry occur in space group $R\bar{3}m$; it is convenient to use rhombohedral axes to describe the structure. The lovozerite structure may be derived from perovskite (*e.g.* $CaTiO_3$) with space group $Pm\bar{3}m$, Ca on 1(*a*) $m\bar{3}m$ (0, 0, 0), Ti on 1(*b*) $m\bar{3}m$ ($\frac{1}{2}$, $\frac{1}{2}$, $\frac{1}{2}$) and O on 3(*c*) $4/mm.m$ (0, $\frac{1}{2}$, $\frac{1}{2}$) (*cf.* Fig. 1*a*); eight unit cells of perovskite lead to a unit cell of lovozerite by doubling the lattice parameter of perovskite without any shift, small deviations from cubic metric occur with respect to the angles, α is

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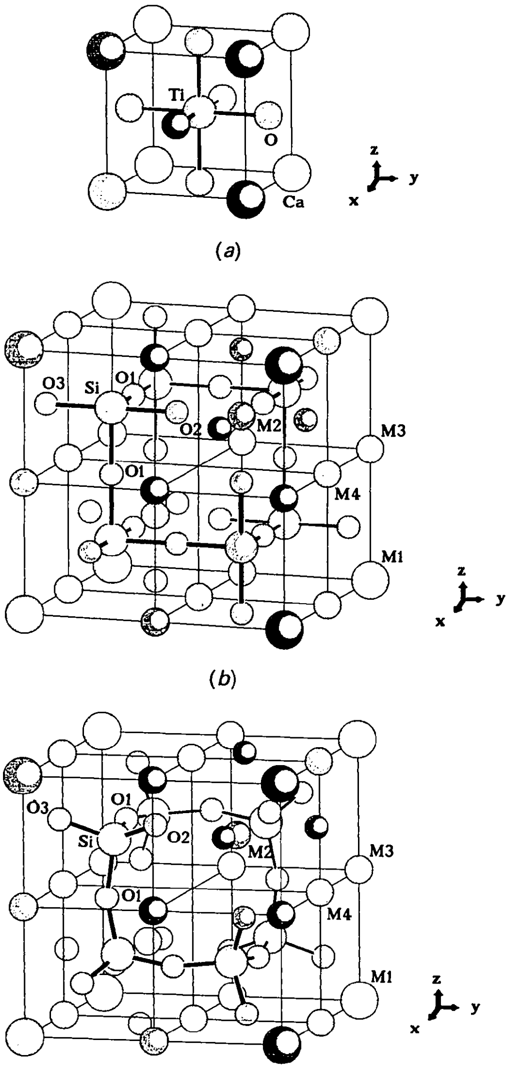
Table 1. *Derivation scheme for lovozerite from perovskite*

Perovskite	(A, S)	Lovozerite $M1M2_2M3_3M4_3[Si_6O_{18}]$			
Ca: 1(*a*) $m\bar{3}m$	8 $m\bar{3}m$				
(0, 0, 0)	(0, 0, 0)	1(*a*) $\bar{3}m$	(0, 0, 0)		*M*1
	($\frac{1}{2}$, $\frac{1}{2}$, $\frac{1}{2}$)	1(*b*) $\bar{3}m$	($\frac{1}{2}$, $\frac{1}{2}$, $\frac{1}{2}$)		Not occupied
	($\frac{1}{2}$, 0, 0)	3(*d*) .2/*m*	($\frac{1}{2}$, 0, 0)		*M*3
	(0, $\frac{1}{2}$, $\frac{1}{2}$)	3(*e*) .2/*m*	(0, $\frac{1}{2}$, $\frac{1}{2}$)		*M*4
Ti: 1(*b*) $m\bar{3}m$	8 $m\bar{3}m$				
($\frac{1}{2}$, $\frac{1}{2}$, $\frac{1}{2}$)	± ($\frac{1}{4}$, $\frac{1}{4}$, $\frac{1}{4}$)	2(*c*) 3.	± (*x*, *x*, *x*)	$x \simeq 0.25$	*M*2
	± ($\frac{3}{4}$, $\frac{3}{4}$, $\frac{1}{4}$)	6(*h*) .*m*	± (*x*, *x*, *z*)	$x \simeq 0.75$ $z \simeq 0.25$	Si
O: 3(*c*) 4/*mm*.*m*	24 4/*mm*.*m*				
($\frac{1}{2}$, $\frac{1}{2}$, 0)	± ($\frac{1}{4}$, $\frac{1}{4}$, 0)	6(*h*) .*m*	± (*x*, *x*, *z*)	$x \simeq 0.75$ $z \simeq 0.50$	O
	± ($\frac{1}{4}$, $\frac{1}{4}$, $\frac{1}{2}$)	6(*h*) .*m*	± (*x*, *x*, *z*)	$x \simeq 0.75$ $z \simeq 0.00$	O
	± ($\frac{1}{4}$, $\frac{3}{4}$, 0)	6(*f*) .2	± (*x*, − *x*, 0)		Not occupied
	± ($\frac{1}{4}$, $\frac{3}{4}$, $\frac{1}{2}$)	6(*g*) .2	± (*x*, − *x*, $\frac{1}{2}$)	$x \simeq 0.25$	O



(*a*)

(*b*)

(*c*)

Fig. 1. (*a*) The perovskite structure. (*b*) Lovozerite derived from perovskite without local deviations. (*c*) Lovozerite A.

approximately 88°. The related mapping is given in Table 4, case 17. The result of the mapping may be followed by the aid of Table 1: an eighth of the Ca sites are not occupied in the enlarged cell, the Ti sites are occupied by two *M*2 and six Si atoms. A quarter of the oxygen positions are missing. Thus the Si position loses two neighbours from its octahedral environment (*cf.* Fig. 1*b*) and changes into a tetrahedral coordination polyhedron *via* small motions of all atoms [0.36 for Si, 0.05 for O1 in 6(*g*) and 0.56 or 0.81 Å for O2 and O3 respectively in position 6(*h*), *cf.* Fig. 1*c*]. The tetrahedra are vertex connected, they share O1 and form $[Si_6O_{18}]$ rings with the chair form.

The figure of deviation for lattice deformations is 0.037, the figure of displacement is 0.179, the figure of failure is 0.096; this leads to a total figure of misfit of 0.285 indicating a clear but not too strong relationship (*cf.* Table 4, case 17).

The aristotype problem

Derivation of the lovozerite type from a simple cubic structure leads to the suggestion that the lovozerite aristotype should be as close as possible to a cubic structure with respect to symmetry, metrical properties and atomic coordinates. An inspection, however, shows that this cannot be achieved:

(i) The chair form of the six-membered $[Si_6O_{18}]$ ring is not compatible with cubic symmetry in this cell. The same is true for the 2(*c*) position which is mostly occupied by metal ions.

(ii) Attempts to construct a structure with a cubic cell and ideal coordinates for Si lead to very unreasonable coordination polyhedra for all other metal ions with respect to distances and distortions.

(iii) On the other hand there are a lot of representatives of the lovozerite family with highest rhombohedral symmetry $R\bar{3}m$ which show very small deviations with respect to their metrical and positional parameters.

For these reasons the best solution for the determination of an aristotype seemed to be to average the free structural parameters of all members of the family determined at room temperature with highest symmetry $R\bar{3}m$. This structure will be called 'lovozerite A' (*cf.* Table 2). The following detailed description of the structure will make use of its data.

Description of the structure of lovozerite A

Whereas the global arrangement of the lovozerite structure is sufficiently described by comparison with the perovskite the local deviations of the atoms imply a remarkable change in the local surroundings. Thus it is necessary to discuss the coordination polyhedra for at least the metal positions. For this discussion the coordination polyhedra and Dirichlet

Table 2. *Aristotype–lovozerite A* (*average*)

$M1M2_2M3_3M4_3[Si_6O_{18}]$, space group $R\bar{3}m$.

		Rhombohedral setting (a = 7.408 Å, α = 88.561°, Z = 1)					Hexagonal setting (a = 10.344, c = 13.149 Å, Z = 3)			
N	Atom	Wyckoff position	Symmetry position	*x*	*y*	*z*	Wyckoff position	*x*	*y*	*z*
1	*M*1	1(*a*)	$\bar{3}m$	0.0	0.0	0.0	3(*a*)	0.0	0.0	0.0
2	*M*2	2(*c*)	3*m*	0.24764	0.24764	0.24764	6(*c*)	0.0	0.0	0.24764
3	*M*3	3(*d*)	.2/*m*	0.0	0.0	0.5	9(*d*)	0.5	0.0	0.5
4	*M*4	3(*e*)	.2/*m*	0.5	0.5	0.0	9(*e*)	0.5	0.0	0.0
5	Si	6(*h*)	.*m*	0.71724	0.71724	0.26352	18(*h*)	0.15124	−0.15124	0.56600
6	O1	6(*g*)	.2	0.24556	0.75444	0.5	18(*g*)	−0.25444	0.0	0.5
7	O2	6(*h*)	.*m*	0.78844	0.78844	0.44640	18(*h*)	0.11401	−0.11401	0.67443
8	O3	6(*h*)	.*m*	0.80056	0.07942	0.80056	18(*h*)	0.24038	−0.24038	0.56018

Table 3. *Distances* (Å) *and angles* (°) *in the lovozerite A structure*

*M*1 octahedron			
*M*1—O3	6 × 2.1758	O3—*M*1—O3	83.04, 96.96, 180.0
*M*2 octahedron			
*M*2—O2	3 × 2.2853	O2—*M*2—O2	101.44
*M*2—O3	3 × 2.4937	O2—*M*2—O3	92.02, 158.54
		O3—*M*2—O3	70.67
*M*3 hexagonal dipyramid			
*M*3—O1	2 × 2.5401	O1—*M*3—O1	180.00
*M*3—O2	2 × 2.2926	O1—*M*3—O2	90.00
*M*3—O3	4 × 2.7098	O1—*M*3—O3	122.16, 57.84
		O2—*M*3—O2	180.00
		O2—*M*3—O3	86.51, 93.49
*M*4 distorted cube			
*M*4—O1	4 × 2.6522	O1—*M*4—O1	180.00, 59.50, 120.50
*M*4—O2	4 × 2.6457	O1—*M*4—O2	119.85, 99.54, 80.56, 60.15
		O2—*M*4—O2	180.00, 96.08, 83.82
Si tetrahedron			
Si—O1	2 × 1.6340	O1—Si—O1	107.29
Si—O2	× 1.5740	O1—Si—O2	111.68
Si—O3	× 1.5989	O1—Si—O3	103.75
		O2—Si—O3	117.81

domains of Fig. 2 and the values of distances and angles given in Table 3 are used.

The coordination polyhedron for *M*1 is shown in Fig. 2(*a*). It is a nearly ideal octahedron formed by O3 atoms; this is confirmed by the Dirichlet domain and by the values of distances and angles in Table 3, the octahedral angles varying from 83 to 97°. It should be emphasized that the position of *M*1 has cuboctahedral coordination in the perovskite structure.

Position *M*2 corresponds to a Ti position in perovskite; its octahedral coordination given by atoms O2 and O3 is mainly retained; the variations are stronger as for *M*1 (distances 2.29–2.49 Å, octahedral angles 70.7–101.4°). The Dirichlet domain, however, shows a significant change (*cf.* Fig. 2*b*), indicating contacts to metallic positions *M*3 and *M*4 by smaller triangles at the corners of the deformed cube. Their contribution to the total surface is nearly 12%.

Positions *M*3 and *M*4 have cuboctahedral surroundings in the perovskite structure. This is reduced to a hexagonal dipyramid for *M*3 (*cf.* Fig. 2*c*) with distances from 2.29 to 2.71 Å to atoms O1, O2 and O3 (*cf.* Table 3). The Dirichlet domain indicates only weak additional contacts to *M*2.

A very interesting situation occurs for *M*4: the coordination number is 8 with neighbours O1 and O2 and defines a deformed cube (*cf.* Fig. 2*d*). This is confirmed by the Dirichlet domain which is mainly an octahedron; two faces on top and bottom related to O3 show some influence of two additional oxygen neighbours with 6.3% of the total surface. The larger triangles belong to *M*2 distances (5% of the surface), the smaller ones to Si distances (2.5% of the surface for all).

The Si position (*cf.* Fig. 2*e*) stems from a Ti position in perovskite with octahedral coordination; this changes to a tetrahedral environment formed by O1, O2 and O3 with O1 being the bridging atom for the six-membered ring. The Dirichlet domain is influenced by two additional long-distance neighbours of O2 (3.84 Å), related to the small quadrangles. The influence of *M*4 is indicated by the small triangles. It should be emphasized that the discussed interaction among the metal atoms indicated by common faces in the Dirichlet domains may provide an explanation for the ionic conductivity reported for some representatives of the lovozerite type.

Extensions of the mapping procedure

In the previous paper (Burzlaff & Rothammel, 1992) it was proposed that for a valid structural relationship between a derived structure indexed by '*d*' and a basic structure indexed by '*b*', a mapping ($\mathbf{A}$, $\mathbf{S}$) should give rise to the following equations:

(i) The image of the basis is defined by $\dot{\mathbf{B}}_b = \mathbf{B}_b{\cdot}\mathbf{A}^{-1}$, $\mathbf{B}_b = (\mathbf{b}_1\mathbf{b}_2\mathbf{b}_3)_b$ and leads to $\dot{\mathbf{G}}_b = \mathbf{A}'{\cdot}\mathbf{G}_b{\cdot}\mathbf{A}$ with $\mathbf{G}_b = \mathbf{B}_b'{\cdot}\mathbf{B}_b$. $\mathbf{G}_b$, the image of the metric tensor, should be close to $\mathbf{G}_d$ after appropriate scaling and *vice versa*.

(ii) The image of a symmetry operation ($\mathbf{R}_b$, $\mathbf{T}_b$) is defined by $\dot{\mathbf{R}}_b = \mathbf{A}{\cdot}\mathbf{R}_b{\cdot}\mathbf{A}^{-1}$ and $\dot{\mathbf{T}}_b = \mathbf{A}{\cdot}(\mathbf{T}_b + \mathbf{L}_b) + (\mathbf{E} - \dot{\mathbf{R}}_b){\cdot}\mathbf{S}$; $\mathbf{L}_b$ designates the lattice translations of the basic structure. A similar relation is valid for the opposite direction of the mapping. Two cases are distinguished: (*a*) The operations ($\mathbf{R}_d$, $\mathbf{T}_d$) form a subgroup of $\{(\dot{\mathbf{R}}_b, \dot{\mathbf{T}}_b)\}$; this case is called symmetry-type I ('Bärnighausen' relation). (*b*) $\{(\dot{\mathbf{R}}_b, \dot{\mathbf{T}}_b)\}$ and $\{(\mathbf{R}_d, \mathbf{T}_d)\}$ have only a common subgroup; this case is called symmetry-type II.

(iii) The image of an atom of the basic structure with the coordinates $\mathbf{X}_b$ is defined by $\dot{\mathbf{X}}_b = \mathbf{A}\cdot(\mathbf{X}_b + \mathbf{L}_b) + \mathbf{S}$; a similar relation is valid for the opposite direction of mapping.

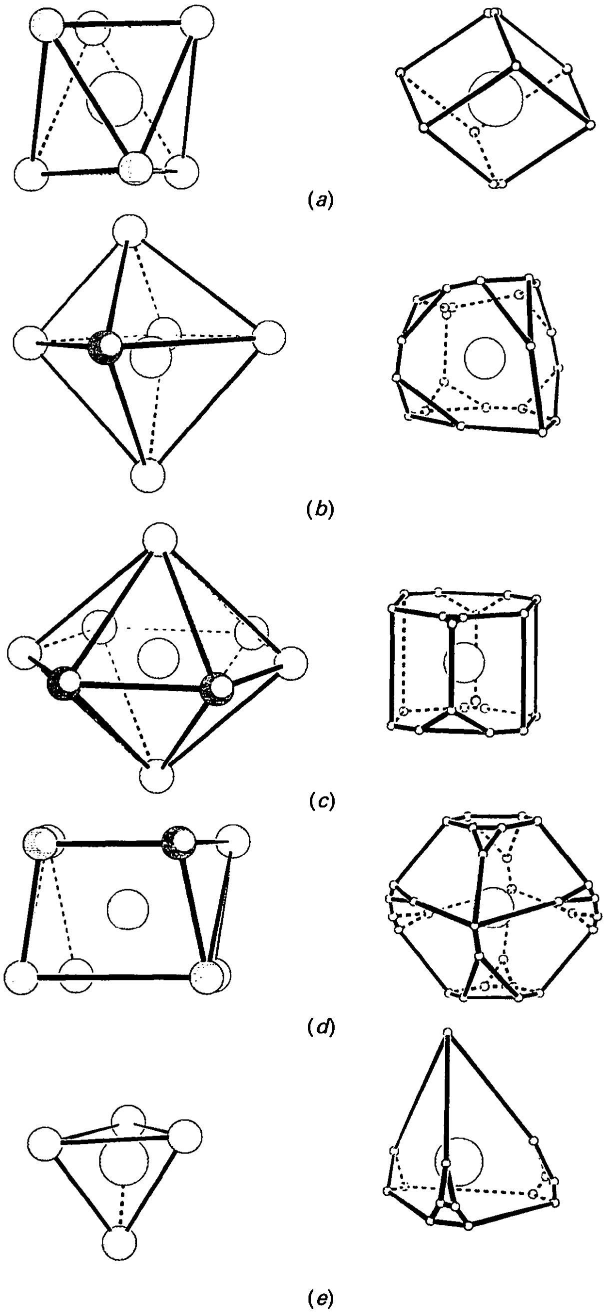


Fig. 2. Coordination polyhedra and Dirichlet domains for *M*1–*M*4 and Si. (*a*) *M*1. (*b*) *M*2. (*c*) *M*3. (*d*) *M*4. (*e*) Si.

In the previous paper only those pairs of structures of symmetry-type II were compared that could be mapped to each other without the use of symmetry operations ($\mathbf{R}_d$, $\mathbf{T}_d$) not belonging to the common subgroup. The application to more complicated relationships requires changes and extensions of the previous procedure.

Structural units

As shown by Tamazyan & Malinovsky (1990) in the case of symmetry-type II a suitable volume of the basic structure is regarded as a *structural unit* that may be distributed by translations, but also by other symmetry operations stemming from the derived structure. To permit this procedure in the mapping relation $\dot{\mathbf{X}}_b = \mathbf{A}\cdot(\mathbf{X}_b + \mathbf{L}_b) + \mathbf{S}$, $\mathbf{L}_b$ has to be restricted to only those translations that lead to images within the structural unit. The structural unit must cover at least one unit cell of the basic structure and simultaneously at least an asymmetric unit of the derived structure; it is convenient to use only structural units that are parallelepipeds.

Symmetry of the structural unit and distribution symmetry

In the next step all symmetry operations of the derived structure that map the structural unit onto itself are selected. These operations form a subgroup of the common subgroup of both structures. This subgroup is the *minimum symmetry group of the structural unit* in the relationship. It is used to decompose the space group of the derived structure into cosets. The first element of each coset is regarded as the representative of the coset. The set of representatives is defined as the *distribution symmetry* of the structural relationship. Each representative leads to an image of the structural unit. The structural unit itself is represented by the unit operation.

Boundaries

Since the boundaries of the structural unit may be symmetrically nonequivalent in the derived structure, a separate investigation for atoms in the boundary region is necessary to decide which of the allowed images due to the distribution symmetry operations is valid. Special treatment is necessary for the case of a boundary position which is mapped onto a special position of the derived structure. In the case of symmetry-type I, one unit cell of the basic structure is used as a structural unit, its lattice translations act as distribution symmetry.

Changes for the calculation of lattice deviations

In the previous paper comparison of the lattices was performed on the basis of Delaunay parameters for the sake of homogeneity. It turned out, however, that this set of parameters is not necessarily invariant under the distribution symmetry. For this reason the lattice deviations here are calculated on the base of the length of the six face diagonal vectors of the unit cell. If the face diagonals are designated by $d_{ik} = |\mathbf{b}_i + \mathbf{b}_k|$ and $f_{ik} = |\mathbf{b}_i - \mathbf{b}_k|$ then the elements g_{ik} of the metric tensor can be expressed by:

$$g_{11} = \tfrac{1}{4}(d_{12}^2 + f_{12}^2 + d_{13}^2 + f_{13}^2 - d_{23}^2 - f_{23}^2), \qquad g_{23} = \tfrac{1}{4}(d_{23}^2 - f_{23}^2),$$

$$g_{22} = \tfrac{1}{4}(d_{12}^2 + f_{12}^2 - d_{13}^2 - f_{13}^2 + d_{23}^2 + f_{23}^2), \qquad g_{13} = \tfrac{1}{4}(d_{13}^2 - f_{13}^2),$$

$$g_{33} = \tfrac{1}{4}(-d_{12}^2 - f_{12}^2 + d_{13}^2 + f_{13}^2 + d_{23}^2 + f_{23}^2), \qquad g_{12} = \tfrac{1}{4}(d_{12}^2 - f_{12}^2).$$

The figure of deviation is defined by $f_{\mathrm{dev}} = 1 - (1 - \Delta_{12})(1 - \Delta_{13})(1 - \Delta_{23})$ with $\Delta_{ik} = (|\dot{d}_{ik} - d_{ik}| + |\dot{f}_{ik} - f_{ik}|)/(d_{ik} + f_{ik})$.

Displacements and failures

For determination of the figure of displacement and the figure of failure the unit cell of the derived structure is filled with images $\dot{\mathbf{X}}_b$ by application of the distribution symmetry to all atoms in the structural unit. A displacement is measured by the distance $d_i = |\dot{\mathbf{x}}_b - \mathbf{x}_d|$ between an atom and the related image with $\mathbf{x} = \mathbf{B}_d \cdot \mathbf{X}$. A figure of local displacement is defined by $f_{\mathrm{dis}} = (\sum d_i)/(\sum d_{i\mathrm{coor}})$ were $d_{i\mathrm{coor}}$ designates the shortest coordination distance for the ith atom. The sum runs over all atoms of the unit cell of the derived structure if $d_i \leq 0.5 d_{i\mathrm{coor}}$. In the case $d_i > 0.5 d_{i\mathrm{coor}}$ the mapping is regarded as a failure and an integer n_i is set from 0 to 1. The influence of failures is taken into account by $f_{\mathrm{fail}} = (\sum n_d + \sum \dot{n}_b)/(N_d + \dot{N}_b)$. The first sum takes care of missing atoms and runs over all N_d atoms of the derived structure, the second sum takes care of interstitial images and runs over all $\dot{N}_b$ images of the basic structure. The three figures may be combined to give a figure of misfit:

$$f_{\mathrm{mis}} = 1 - (1 - f_{\mathrm{dev}})(1 - f_{\mathrm{dis}})(1 - f_{\mathrm{fail}}).$$

General remarks about the tables

Tables 4 and 5 contain the results of a quantitative comparison between an aristotype and a derived structure. With the exception of case 17 in Table 4 the aristotype is always lovozerite A. In case 17 lovozerite A is regarded as being derived from the perovskite. Since this discussion deals with the geometrical properties of a structure for all Wyckhoff positions used the occupation factors are regarded to be 1.0 even if the structure determination procedure indicates partial occupation. For the same reason split positions were treated as separate atomic positions as long as their distance was not equal to zero.

Relationships of type I among members of the lovozerite family are tabulated in Table 4, those of type II in Table 5. Column 1 of these tables gives the sequence number, the next column contains the chemical composition, the chemical or the mineral name and the literature reference. The third column gives the lattice parameters; for derived rhombohedral structures the rhombohedral setting was always used. Column 4 contains the space group, the setting used for the aristotype and the final R value in the structure determination. The following three columns give information on the mapping (**A**, **S**) and the index of the common subgroup. Column 8 contains the figure of lattice deviation, the figure of displacement and the figure of failure; the last column gives the combined figure of misfit.

Relationships of symmetry-type I

The first five structures of Table 4 were used for the definition of the aristotype lovozerite A. So the related figures of misfit show the 'allowed' variations for deviation and displacement; the combined figures of misfit vary from 0.024 to 0.043. The subgroup index is 1 for all cases.

The next two structures (cases 6 and 7) also show good relationships in all figures of merit.

The next eight cases (8–15) refer to structures with equal or nearly equal chemical composition collected under the mineral name combeite. They are cement-like phases and may be separated into the low-temperature group (structure determination between room temperature and $T = 738$ K, cases 8–12) and the high-temperature group ($T \geq 773$ K, cases 13–15). All representatives from the low-temperature group occur with space group $P3_121$ and show rather high figures of misfit. With the exception of case 8 a systematic behaviour can be recognized: the figure of misfit decreases with increasing temperature; if the high-temperature group is reached the symmetry changes to $R\bar{3}m$ and the figure of misfit is lowered to very satisfactory values of between 0.054 and 0.058. Case 16 is a special case. In the related paper it is suggested that H atoms occupy metallic positions of the lovozerite M structure; however, this suggestion was not proved. In addition to the formula presented in Table 4 an amount of 0.5 NaOH per formula unit is assumed. The authors of the paper believe that it is located at one of the unoccupied metal positions. Taking data from the literature two different calculations are given in Table 4: (i) case 16 leaving out the assumed hydrogen positions and (ii) case 16′ including H atoms on the ideal metallic positions. In the latter case the figure of failure is zero, the figure of misfit is diminished remarkably from 0.226 to 0.137. A closer inspection of the figure of deviation showed that a much better agreement can be achieved if instead of β, $180° - \beta$ is used. The related values are reported under cases 16″ and 16‴. This problem can only be solved by an experimental reinvestigation.

Case 17 deals with the derivation of lovozerite A from perovskite.

Table 4. *Structural relations with the symmetry-relationship type* I

No.	Compound	Lattice parameters (Å, °)	Space-group setting of aristotype $R(hkl)$	Mapping A			S	Index	Figures of relative merit f_{dev} f_{dis} f_{fail}	f_{mis}
1	$TiMnNa_6[Si_6O_{18}]$	$a = 10.174$	$R\bar{3}m$	1	0	0	0	1	0.012	0.043
	Kazakovite	$c = 13.053$	r	0	1	0	0		0.032	
	Sov. Phys. Dokl. **24**, 132 (1979)		0.054	0	0	1	0		0.000	
2	$SnNa_8[Si_6O_{18}]$	$a = 10.189$	$R\bar{3}m$	1	0	0	0	1	0.019	0.041
	Na-Sn-Lovozerite-1	$c = 13.186$	r	0	1	0	0		0.023	
	Sov. Phys. Dokl. **25**, 962 (1980)		0.025	0	0	1	0		0.000	
3	$Na_6Ca_3[Si_6O_{18}]$	$a = 10.500$	$R\bar{3}m$	1	0	0	0	1	0.013	0.035
	Na6-Ca3-Lovozerite	$c = 13.184$	r	0	1	0	0		0.023	
	Acta Cryst. **C41**, 1575 (1985)		0.042	0	0	1	0		0.000	
4	$Na_5Ca_3(Fe,Mn)_{0.6}[Si_6O_{18}]$	$a = 10.429$	$R\bar{3}m$	1	0	0	0	1	0.008	0.025
	HT-Combeite	$c = 13.149$	r	0	1	0	0		0.017	
	Acta Cryst. **C43**, 1852 (1987)		0.042	0	0	1	0		0.000	
5	$Na_4Ca_4[Si_6O_{18}]$	$a = 10.429$	$R\bar{3}m$	1	0	0	0	1	0.008	0.024
	Combeite from Zaire	$c = 13.149$	r	0	1	0	0		0.016	
	Neues Jahrb. Mineral. Monatsh. **2**, 49 (1983)		0.041	0	0	1	0		0.000	
6	$SnNa_8[Si_6O_{18}]$	$a = 7.340$	$A2/m$	$-\frac{1}{2}$	$-\frac{1}{2}$	0	$\frac{1}{2}$	3	0.012	0.034
	Na-Sn-Lovozerite-2	$b = 10.576$	h	$\frac{1}{2}$	$-\frac{1}{2}$	0	$\frac{1}{2}$		0.022	
	Sov. Phys. Dokl. **25**, 669 (1980)	$c = 10.251$	0.038	0	0	1	0		0.000	
7	$ZrCaNa_6[Si_6O_{18}]$	$a = 10.290$	$R\bar{3}c$	$-\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$	0	2	0.008	0.063
	Zirsinalite	$c = 26.310$	r	$\frac{1}{2}$	$-\frac{1}{2}$	$\frac{1}{2}$	0		0.056	
	Sov. Phys. Dokl. **25**, 69 (1980)		0.087	$\frac{1}{2}$	$\frac{1}{2}$	$-\frac{1}{2}$	0		0.000	
8	$Na_{4.4}Ca_{3.8}[Si_6O_{18}]$	$a = 10.464$	$P3_121$	1	0	0	$\frac{1}{3}$	6	0.008	0.137
	LT-Combeite	$c = 13.176$	h	0	1	0	0		0.130	
	Acta Cryst. **C43**, 1852 (1987)		0.050	0	0	1	$\frac{1}{3}$		0.000	
9	$Na_4Ca_4[Si_6O_{18}]$	$a = 10.464$	$P3_121$	1	0	0	$\frac{1}{3}$	6	0.009	0.187
	Na4-Ca4-Lovozerite	$c = 13.168$	h	0	1	0	0		0.167	
	Acta Cryst. **C42**, 934 (1986)		0.031	1	0	1	$\frac{1}{3}$		0.015	
10	$Na_4Ca_4[Si_6O_{18}]$	$a = 10.494$	$P3_121$	1	0	0	$\frac{1}{3}$	6	0.010	0.174
	LT-Combeite, $T = 523$ K	$c = 13.189$	h	0	1	0	0		0.152	
	Acta Cryst. **B46**, 125 (1990)		0.036	0	0	1	$\frac{1}{3}$		0.015	
11	$Na_4Ca_4[Si_6O_{18}]$	$a = 10.513$	$P3_121$	1	0	0	$\frac{1}{3}$	6	0.011	0.165
	LT-Combeite, $T = 643$ K	$c = 13.195$	h	0	1	0	0		0.142	
	Acta Cryst. **B46**, 125 (1990)		0.040	0	0	1	$\frac{1}{3}$		0.015	
12	$Na_4Ca_4[Si_6O_{18}]$	$a = 10.530$	$P3_121$	1	0	0	$\frac{1}{3}$	6	0.012	0.155
	LT-Combeite, $T = 738$ K	$c = 13.203$	h	0	1	0	0		0.132	
	Acta Cryst. **B46**, 125 (1990)		0.046	0	0	1	$\frac{1}{3}$		0.015	
13	$Na_4Ca_4[Si_6O_{18}]$	$a = 10.561$	$R\bar{3}m$	1	0	0	0	1	0.017	0.054
	HT-Combeite, $T = 773$ K	$c = 13.199$	r	0	1	0	0		0.037	
	Acta Cryst. **B46**, 125 (1990)		0.048	0	0	1	0		0.000	
14	$Na_4Ca_4[Si_6O_{18}]$	$a = 10.574$	$R\bar{3}m$	1	0	0	0	1	0.018	0.057
	HT-Combeite, $T = 888$ K	$c = 13.209$	r	0	1	0	0		0.040	
	Acta Cryst. **B46**, 125 (1990)		0.051	0	0	1	0		0.000	
15	$Na_4Ca_4[Si_6O_{18}]$	$a = 10.588$	$R\bar{3}m$	1	0	0	0	1	0.018	0.058
	HT-Combeite, $T = 993$ K	$c = 13.222$	r	0	1	0	0		0.041	
	Acta Cryst. **B46**, 125 (1990)		0.052	0	0	1	0		0.000	
16	$ZrNa_2H_6[Si_6O_{18}]$	$a = 10.48$	$C2$	$\frac{1}{2}$	$\frac{1}{2}$	0	0	6	0.056	0.241
	Lovozerite M without H atoms	$b = 10.20$	h	$-\frac{1}{2}$	$\frac{1}{2}$	0	0		0.123	
	Sov. Phys. Crystallogr. **5**, 186	$c = 7.33$	0.180	0	0	1	0		0.082	
	(1960)	$\beta = 92.50$								
16′	$ZrNa_2H_6[Si_6O_{18}]$	$a = 10.48$	$C2$	$\frac{1}{2}$	$\frac{1}{2}$	0	0	6	0.038	0.137
	Lovozerite M with H atoms	$b = 10.20$	h	$-\frac{1}{2}$	$\frac{1}{2}$	0	0		0.103	
	Sov. Phys. Crystallogr. **5**, 186	$c = 7.33$	0.180	0	0	1	0		0.000	
	(1960)	$\beta = 92.50$								
16″	$ZrNa_2H_6[Si_6O_{18}]$	$a = 10.48$	$C2$	$\frac{1}{2}$	$\frac{1}{2}$	0	0	6	0.005	0.198
	Lovozerite M without H atoms	$b = 10.20$	h	$-\frac{1}{2}$	$\frac{1}{2}$	0	0		0.122	
	Sov. Phys. Crystallogr. **5**, 186	$c = 7.33$	0.180	0	0	1	0		0.082	
	(1960)	$\beta = 92.50$								
16‴	$ZrNa_2H_6[Si_6O_{18}]$	$a = 10.48$	$C2$	$\frac{1}{2}$	$\frac{1}{2}$	0	0	6	0.005	0.106
	Lovozerite M with H atoms	$b = 10.20$	h	$-\frac{1}{2}$	$\frac{1}{2}$	0	0		0.101	
	Sov. Phys. Crystallogr. **5**, 186	$c = 7.33$	0.180	0	0	1	0		0.000	
	(1960)	$\beta = 92.50$								

Table 4 (*cont.*)

No.	Compound	Lattice parameters (Å, °)	Space-group setting of aristotype $R(hkl)$	Mapping				Index	Figures of relative merit	
					A		S		f_{dev} f_{dis} f_{fail}	f_{mis}
17	Lovozerite A compared with perovskite	$a = 7.408$	$R\bar{3}m$	$\frac{1}{2}$	0	0	0	32	0.037	0.285
		$\alpha = 88.561$		0	$\frac{1}{2}$	0	0		0.179	
	Strukturbericht, **1**, 300 (1931)			0	0	$\frac{1}{2}$	0		0.096	

Table 5. *Structural relations with the symmetry-relationship type* II

No.	Compound	Lattice parameters (Å, °)	Space-group setting of aristotype $R(hkl)$	Mapping				Index	Figures of relative merit	
					A		S		f_{dev} f_{dis} f_{fail}	f_{mis}
1	(Fe,Ti)(Ca,Mn)$Na_6[Si_6O_{18}]$	$a = 10.179$	*Pmnb*	$\frac{1}{2}$	$-\frac{1}{2}$	0	$\frac{3}{4}$	12	0.013	0.095
	Koashvite	$b = 20.899$	*h*	$\frac{1}{4}$	0	$-\frac{1}{4}$	$-\frac{1}{8}$		0.083	
	Mineral. Zh. **2**, 40 (1980)	$c = 7.335$	0.108	0	0	1	0		0.000	
2	$FeCa_{1.5}Na_6[Si_6O_{18}]$	$a = 10.331$	*Pmnn*	$\frac{1}{2}$	$-\frac{1}{2}$	0	$\frac{1}{2}$	6	0.020	0.064
	Imandrite	$b = 10.546$	*h*	$\frac{1}{2}$	$\frac{1}{2}$	0	$-\frac{1}{2}$		0.045	
	Sov. Phys. Dokl. **25**, 337 (1980)	$c = 7.426$	0.085	0	0	1	0		0.000	
3	$Cd_3Na_6[Si_6O_{18}]$	$a = 10.40$	$Pm2_1n$	$\frac{1}{2}$	$-\frac{1}{2}$	0	$\frac{1}{2}$	12	0.029	0.169
	Na-Cd-Lovozerite	$b = 10.40$	*h*	$\frac{1}{2}$	$\frac{1}{2}$	0	$-\frac{1}{4}$		0.144	
	Sov. Phys. Dokl. **12**, 662 (1968)	$c = 7.45$	0.115	0	0	1	$\frac{1}{4}$		0.000	
4	Mn(Na,Mn)$_3Na_5[Si_6O_{18}]$	$a = 10.259$	$Pmn2_1$	$\frac{1}{2}$	$-\frac{1}{2}$	0	$\frac{1}{2}$	12	0.026	0.087
	Na-Mn-Lovozerite 1	$b = 7.378$	*h*	0	0	1	$\frac{1}{4}$		0.063	
	Sov. Phys. Dokl. **18**, 100 (1973)	$c = 10.355$	0.059	$\frac{1}{2}$	$\frac{1}{2}$	0	$-\frac{1}{4}$		0.000	
5	$NdCa_2Na_7[Si_6O_{18}]$	$a = 7.501$	$P2_1/b$	1	0	0	0	12	0.025	0.093
	Na-Nd-Lovozerite	$b = 14.926$	*h*	0	0	$-\frac{1}{2}$	$\frac{1}{4}$		0.070	
	Sov. Phys. Crystallogr. **34**, 181 (1989)	$c = 7.446$	0.041	0	1	1	0		0.000	
		$\gamma = 91.79$								
6	$Mn_3Na_6[Si_6O_{18}]$	$a = 10.354$	*Pnnm*	$-\frac{1}{2}$	$-\frac{1}{2}$	0	$\frac{1}{2}$	6	0.026	0.078
	Na-Mn-Lovozerite 2	$b = 7.374$	*h*	0	0	1	0		0.054	
	Sov. Phys. Dokl. **21**, 365 (1976)	$c = 10.251$	0.105	$-\frac{1}{2}$	$\frac{1}{2}$	0	$\frac{1}{2}$		0.000	
7	$Ca_9(Al_6O_{18})$	$a = 15.263$	*Pa*3	0	$-\frac{1}{2}$	0	$\frac{5}{8}$	32	0.037	0.214
	Tricalcium aluminate		*r*	$\frac{1}{2}$	0	0	$\frac{3}{8}$		0.183	
	Acta Cryst. **B31**, 689 (1975)		0.051	0	0	$\frac{1}{2}$	$-\frac{1}{8}$		0.000	

Relationships of symmetry-type II

The structures with symmetry-relationship type II show in all cases figures of misfit in the same range as structures of symmetry-type I. All figures of failure are zero, all figures of displacement are small with the exceptions of case 3 and case 7. In spite of these two cases the result confirms the idea that structures related to each other by symmetry-type II belong to the same family. Any attempt to apply only translation symmetry as distribution symmetry leads to very unreasonable results.

An inspection of those cases with high figures of misfit (mostly due to high figures of displacement) showed that in the common subgroup the center of symmetry is missing even if the space group of the derived structure is centrosymmetric (*cf.* Table 5, case 7).

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