

The structure of slawsonite, a strontium analog of paracelsian

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Abstract

Slawsonite is a new mineral from the Triassic Martin Bridge Formation in Wallowa County, Oregon. Its composition ($\text{Sr}_{0.87}\text{Ca}_{0.13}\text{Al}_2\text{Si}_2\text{O}_8$), cell dimensions ($a = 8.888$, $b = 9.344$, $c = 8.326$ Å, $\beta = 90.33^\circ$), and $P2_1/a$ space group suggest it is isostructural with paracelsian, $\text{BaAl}_2\text{Si}_2\text{O}_8$. A structure refinement using 1617 twice-measured reflections with $|F_{\text{obs}}| > 3\hat{\sigma}$ was undertaken by conventional methods to $R = 0.048$. Like paracelsian, slawsonite has a completely ordered Al/Si distribution in its infinite 3-D framework of corner-sharing tetrahedra. The mean Al–O distances at $T10$ and $T2m$ are both 1.748 Å; mean Si–O distances are 1.623 and 1.624 Å for the $T1m$ and $T20$, respectively. The former are equal to those in paracelsian, while the latter are 0.004 Å longer on the average. The Sr atom is 7-coordinated; (Sr–O) = 2.630 Å. There is a high correlation among individual T –O distances, the mean intertetrahedral angle T –O– T , and the mean of the three O– T –O angles involved in the T –O bond.

Introduction

The structure of paracelsian ($\text{BaAl}_2\text{Si}_2\text{O}_8$, $P2_1/a$), originally solved by Smith (1953), was refined by Craig *et al.* (1973) who found it to have a completely ordered Al/Si distribution in its framework of corner-sharing tetrahedra. Recently structures of several paracelsian analogs have been reported, in particular hurlbutite ($\text{CaBe}_2\text{P}_2\text{O}_8$; Lindbloom *et al.*, 1974), and synthetic $\text{SrGa}_2\text{Si}_2\text{O}_8$ ² and $\text{SrGa}_2\text{Ge}_2\text{O}_8$ (Phillips *et al.*, 1975). Danburite ($\text{CaB}_2\text{Si}_2\text{O}_8$), which has paracelsian topology but a different T^{3+}/T^{4+} ordering scheme and space group ($Pnam$), was refined by Phillips *et al.* (1974). In addition, work is in progress on the paracelsian modifications of $\text{SrAl}_2\text{Ge}_2\text{O}_8$ (Kroll and Phillips, in preparation) and $\text{BaGa}_2\text{Ge}_2\text{O}_8$ (Calleri, personal communication). This study presents the structure of a new mineral, slawsonite ($\text{SrAl}_2\text{Si}_2\text{O}_8$), the Sr analog of paracelsian.

Barrer and Marshall (1964) synthesized pseudo-orthorhombic $\text{SrAl}_2\text{Si}_2\text{O}_8$ from gels in hydrothermal experiments. The lattice parameters determined by them are listed in Table 1. Erd *et al.* (1977) have

described natural slawsonite from metamorphosed limestones of the Triassic Martin Bridge Formation in Wallowa County, Oregon. Its cell dimensions and space group, $P2_1/a$, suggest that slawsonite is isostructural with paracelsian (Table 1).

Experimental procedures

The crystal used for this structure refinement came from the type locality (Wallowa County, Oregon) and was provided by Richard C. Erd of the U. S. Geological Survey. It is a clear, flat triangular prism 62 μm thick with sides measuring $140 \times 217 \times 155 \mu\text{m}$. The lattice parameters shown in Table 1 were determined by least-squares refinement of sixteen reflections measured with a fully automated four-circle Picker diffractometer using Zr-filtered $\text{MoK}\alpha$ radiation. Electron microprobe analysis gave an Al:Si ratio of 1:1, within the limits of error. The only other cations detected in significant concentrations were Sr and Ca, accounting for 0.82 and 0.12 atoms, respectively, in the formula unit. Because of some uncertainty about the Sr content of the "standard" used for microprobe analysis and because no substituents other than 0.04 weight percent Fe were detected, the values for Sr and Ca were scaled upward so that $\text{Sr} + \text{Ca} = 1.0$, giving an approximate formula of $\text{Sr}_{0.87}\text{Ca}_{0.13}\text{Al}_2\text{Si}_2\text{O}_8$.

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² $\text{SrGa}_2\text{Si}_2\text{O}_8$ has also been refined by Calleri and Gazzoni (*Periodico di Mineralogia*, XLIV, in press).

Table 1. Crystallographic data for slawsonite

	Barrer and Marshall (1964)	Erd, Nolf, and Smith (pers. comm.)	This study
a (Å)	8.91 ₀	8.895(1)*	8.888(2)
b (Å)	9.34 ₃	9.359(1)	9.344(2)
c (Å)	8.34 ₅	8.333(1)	8.326(3)
β (°)	~90	90.24(1)	90.33(2)
Vol. (Å ³)	-	693.7(1)	691.5

* e.s.d.'s, given in parentheses, refer to last decimal place.

Computer programs used during this study, as listed in the *World List of Crystallographic Computer Programs* (Third Edition) were DATALIB, DATASORT, OR XFLS3, and OR FFE3. For the refinement of the structure, 4168 intensities were collected from two equivalent quadrants. A θ - 2θ scanning rate of 1°/min was used and intensities were measured in the range $0.12 < \sin\theta/\lambda < 1.22$. Observed intensities were corrected for Lorentz-polarization effects and for absorption ($\mu_L = 93.4 \text{ cm}^{-1}$), and converted to F_{obs}^2 with the program DATALIB. These were weighted according to $1/\hat{\sigma}^2$, and the weighted values for symmetry equivalent reflections were averaged using the program DATASORT, to give 1870 non-zero symmetry-independent observations.

The atomic coordinates of SrGa₂Si₂O₈ (Phillips *et al.*, 1975) were used as starting values in the least-

Table 3. Final atomic positional parameters

Atom	x	y	z
Sr	0.8902(1)*	0.4122(1)	0.2503(1)
T10	.2321(2)	.9249(2)	.9311(2)
T1m	.2405(2)	.9199(2)	.5605(2)
T20	.0595(2)	.2006(2)	.9440(2)
T2m	.0541(2)	.1944(2)	.5706(2)
O10	.1910(4)	.0934(4)	.0100(5)
O1m	.1875(4)	.0740(4)	.4937(5)
O20	.1192(4)	.3658(4)	.9458(5)
O2m	.1236(4)	.3699(4)	.5573(5)
O30	.9202(4)	.1919(4)	.0699(4)
O3m	.8979(4)	.1923(4)	.4399(5)
O4	.0092(5)	.1545(4)	.7662(5)
O5	.3139(4)	.9252(4)	.7407(5)

* e.s.d.'s, given in parentheses, refer to last decimal place.

Table 4. Isotropic and anisotropic temperature factors

Atom	B (Å ²)	Anisotropic temperature factors ($\times 10^4$)					
		β_{11}	β_{22}	β_{33}	β_{12}	β_{13}	β_{23}
Sr	0.66(1)*	30(1)	20(1)	29(1)	0(1)	0(1)	1(1)
T10	0.34(2)	9(2)	10(2)	12(2)	1(1)	0(1)	2(2)
T1m	0.31(2)	6(2)	9(1)	11(2)	0(1)	2(1)	0(1)
T20	0.27(2)	8(2)	6(1)	10(2)	-2(1)	0(1)	1(1)
T2m	0.30(2)	9(2)	7(2)	10(2)	-1(1)	1(1)	0(1)
O10	0.62(6)	21(4)	15(4)	22(5)	7(3)	3(4)	0(4)
O1m	0.67(6)	25(5)	10(4)	28(5)	8(4)	8(4)	5(4)
O20	0.48(6)	13(4)	7(4)	22(5)	-2(3)	-7(4)	3(3)
O2m	0.59(6)	17(5)	12(4)	20(5)	-1(3)	11(4)	-2(3)
O30	0.51(6)	13(4)	16(4)	15(5)	-2(3)	3(4)	-2(4)
O3m	0.63(6)	10(4)	16(4)	29(5)	0(3)	1(4)	4(4)
O4	0.89(6)	42(5)	27(4)	13(5)	-12(4)	0(4)	0(4)
O5	0.61(6)	12(4)	25(4)	17(5)	-6(4)	3(4)	2(4)

* e.s.d.'s, given in parentheses, refer to last decimal place.

squares refinement program OR XFLS3, and scattering factors for neutral atoms were employed (Doyle and Turner, 1968). Reflections for which $|F_{\text{obs}}|$ was less than $3\hat{\sigma}$ were omitted, and the remaining reflections were weighted according to $1/\hat{\sigma}^2$. An extinction correction was applied, and refinement with isotropic temperature factors yielded an unweighted residual of 0.050 ($wR = 0.055$) for 1617 reflections. With the introduction of anisotropic temperature factors, the refinement converged to $R = 0.048$ ($wR = 0.053$). No significant correlations were noted among the parameters. The final F_{obs} and F_{calc} values are listed in Table 2,³ and the fractional atomic coordinates are shown in Table 3. Table 4 gives the isotropic and anisotropic temperature factors. The important interatomic distances and bond angles (Table 5) were calculated with the computer program OR FFE3.

Discussion

Lattice parameters of paracelsian analogs

The lattice parameters for five paracelsian analogs and danburite are listed in Table 6.⁴ Multiple linear regression analyses of the cell parameters as functions

³ To obtain a copy of this table, order Document AM-76-018 from the Business Office, Mineralogical Society of America, 1909 K Street, N.W., Washington, D.C. 20006. Please remit \$1.00 in advance for the microfiche.

⁴ Danburite is topologically identical to paracelsian, but topologically different: whereas paracelsian contains $T^{3+}-O-T^{4+}$ linkages but no $T^{3+}-O-T^{3+}$ or $T^{4+}-O-T^{4+}$ linkages, all three types occur in danburite (Phillips *et al.*, 1974). It is nonetheless valid to include it in a comparison of paracelsian-type structures, as demonstrated in the following discussion.

Table 5. Interatomic distances (Å) and angles (°)

	<i>T</i> - <i>O</i>	<i>O</i> ••• <i>O</i>	<i>O</i> - <i>T</i> - <i>O</i>
T10 tetrahedron			
T10-010	1.745(4)*	010-020	2.738(5)
-020	1.757(4)	-030	2.922(5)
-030	1.741(4)	-05	2.953(5)
-05	1.749(4)	020-030	2.914(6)
		-05	2.732(6)
		030-05	2.840(5)
Mean	1.748		2.850
			102.8(2)
			113.9(2)
			115.4(2)
			112.8(2)
			102.4(2)
			108.9(2)
Mean	1.623		2.649
			109.5
T20 tetrahedron			
T20-010	1.634(4)	010-020	2.678(5)
-020	1.631(4)	-030	2.628(5)
-030	1.628(4)	-04	2.649(6)
-04	1.602(4)	020-030	2.615(5)
		-04	2.659(6)
		030-04	2.675(5)
Mean	1.624		2.651
			110.2(2)
			107.4(2)
			109.9(2)
			106.8(2)
			110.6(2)
			111.8(2)
Mean	1.624		2.651
			109.5
T2m tetrahedron			
T2m-01m	1.756(4)	01m-02m	2.871(5)
-02m	1.757(4)	-03m	2.835(5)
-03m	1.758(4)	-04	2.873(6)
-04	1.720(4)	02m-03m	2.774(5)
		-04	2.853(6)
		03m-04	2.909(6)
Mean	1.748		2.853
			109.6(2)
			107.5(2)
			111.4(2)
			104.2(2)
			110.2(2)
			113.5(2)
Mean	1.748		2.853
			109.4
Sr-O distances		<i>T</i>-<i>O</i>-<i>T</i> angles	
Sr-010	2.662(4)	T10-010-T20	125.2(2)
-01m	2.723(4)	T1m-01m-T2m	130.0(2)
-020	2.641(4)	T10-020-T20	123.1(2)
-02m	2.594(4)	T1m-02m-T2m	124.6(2)
-030	2.562(4)	T10-030-T20	128.5(2)
-03m	2.591(4)	T1m-03m-T2m	127.3(2)
-05	2.635(4)	T20-04-T2m	138.7(3)
		T10-05-T1m	131.9(2)
Mean	2.630		128.7

*e.s.d's, given in parentheses, refer to last decimal place.

of mean *M*-*O* and grand mean *T*-*O* distances gave multiple correlation coefficients > 0.99 for *a*, *b*, *c*, and volume. Figure 1 shows plots of observed values versus values calculated from the various regression equations listed in the figure legend. An examination

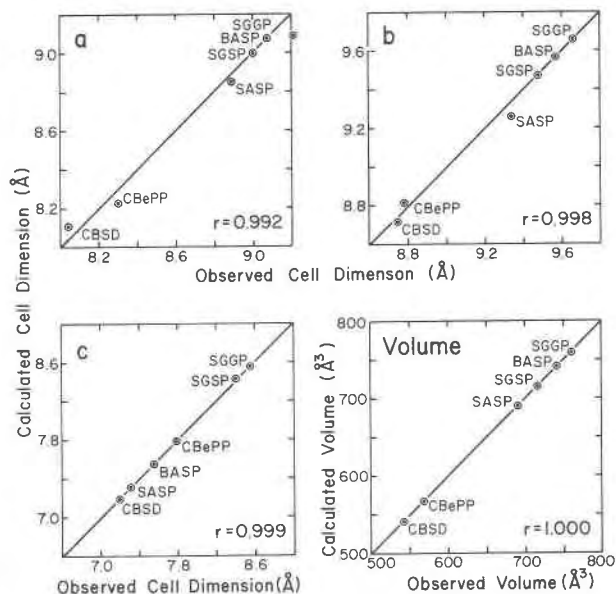


Fig. 1. Observed vs. calculated lattice parameters for five paracelsian-type structures and danburite. Lines are drawn at 45°; symbols and observed values are listed in Table 6. Correlation coefficients *r* are given in the figures. Calculated values *y* came from linear regressions equations of the type $y = a_0 + a_1 (M-O) + a_2 \langle\langle T-O \rangle\rangle$; the constants are listed below:

	\bar{a}_0	a_1	a_2
<i>a</i>	-0.9535	1.3246	3.7516
<i>b</i>	0.8823	1.2943	3.0072
<i>c</i>	0.1615	1.5119	2.4818
Volume	-1281.4	307.85	690.54

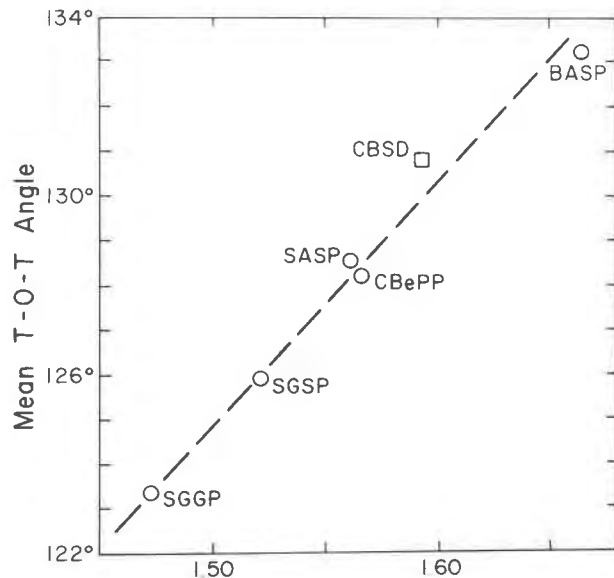


Fig. 2. Mean *T*-*O*-*T* angle as a function of mean *M*-*O* and grand mean *T*-*O* bond lengths for paracelsian-type structures and danburite. Symbols are listed in Table 6.

Table 6. Crystallographic data for five paracelsian analogs and danburite

	Paracelsian BaAl ₂ Si ₂ O ₈	Slawsonite SrAl ₂ Si ₂ O ₈	(Synthetic) SrGa ₂ Si ₂ O ₉	(Synthetic) SrGa ₂ Ge ₂ O ₈	Hurlbutite CaBe ₂ P ₂ O ₈	Danburite CaB ₂ Si ₂ O ₈
a (Å)	9.065(3)*	8.888(2)	9.001(1)	9.206(1)	8.299(1)	8.038(3)
b (Å)	9.568(1)	9.344(2)	9.484(1)	9.660(1)	8.782(2)	8.752(5)
c (Å)	8.574(5)	8.326(3)	8.399(1)	8.581(1)	7.798(3)	7.730(3)
β (°)	90.00(1)	90.33(2)	90.68(1)	90.43(1)	90.5	90.0
$\langle M^{VII}-O \rangle$ (Å)	2.801	2.630	2.626	2.630	2.469	2.461
$\langle T^{3+}-O \rangle$ (Å)	1.747	1.748	1.823	1.825	---	1.474
$\langle T^{4+}-O \rangle$ (Å)	1.619	1.624	1.628	1.748	---	1.617
$\langle \langle T-O \rangle \rangle$ (Å)	1.683	1.686	1.726	1.786	1.577	1.546
Symbol	BASP	SASP	SGSP	SGGP	CBePP	CBSD

* e. s. d. 's, given in parentheses, refer to last decimal place.

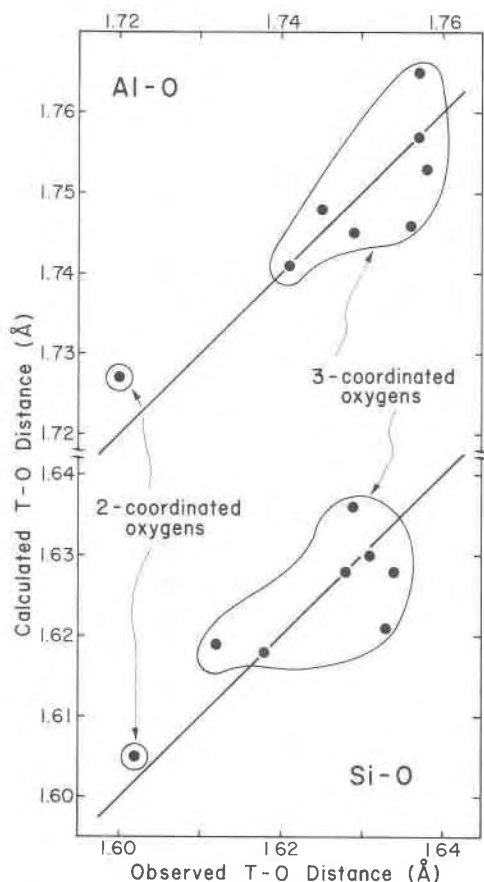


Fig. 3. Least-squares regression lines showing the relationship between the calculated and observed Al-O and Si-O distances in slawsonite. Calculated values came from these multiple linear regression equations:

$$(Al-O)_{calc} = 2.354 - 0.0055 (O-T-O)_3 - 0.0010 (T-O-T)$$

$$(Si-O)_{calc} = 2.239 - 0.0029 (O-T-O)_3 - 0.0013 (T-O-T)$$

of the regression coefficients indicates that the cell parameters are approximately twice as dependent on $\langle \langle T-O \rangle \rangle$ as they are on $\langle M-O \rangle$.

The Sr atom

As in the other paracelsian structures and danburite, the *M* cation in slawsonite may be considered seven-coordinated. Phillips *et al.* (1975) have established the sympathetic relationship between mean *T-O-T* angles and $\langle M-O \rangle / \langle \langle T-O \rangle \rangle$ for paracelsian analogs and danburite (Fig. 2). By examining changes in individual *T-O-T* angles Phillips and Kroll (in preparation) have shown that the tetrahedral framework collapses (*i.e.*, individual *T-O-T* angles decrease) with decreasing $\langle M-O \rangle$ and with increasing $\langle \langle T-O \rangle \rangle$, thus providing a physical interpretation for the parameter $\langle M-O \rangle / \langle \langle T-O \rangle \rangle$. In light of this it is interesting to note that the mean Sr-O distances for the three Sr paracelsian analogs are statistically identical despite the increase in framework size in the order SrAl₂Si₂O₈ < SrGa₂Si₂O₈ < SrGa₂Ge₂O₈. The range in individual Sr-O distances, however, increases in the same order, suggesting that the collapse of the framework about the Sr atom causes some Sr-O distances to increase while others decrease, leaving the mean essentially unchanged. The same is true for the Ca-O distances in danburite and hurlbutite, where the framework size increases for CaB₂Si₂O₈ to CaBe₂P₂O₈.

Al/Si order in the tetrahedral framework

The mean Si-O and Al-O distances in fully-ordered anorthite have been generally used as standards

for the estimation of order in framework aluminosilicates. The mean Al–O distances in slawsonite, paracelsian and anorthite are statistically identical (1.748Å, 1.747Å, and 1.747Å, respectively), whereas the mean Si–O distances are 1.624Å, 1.619Å, and 1.614Å, respectively. Phillips *et al.* (1975) found a mean Si–O distance of 1.628Å in SrGa₂Si₂O₈, and they attributed this increase over ⟨Si–O⟩ in BaAl₂Si₂O₈ to inductive effects of the much larger Ga atoms. Because silicon and gallium possess quite different X-ray scattering characteristics, they were able to determine by site refinement techniques that SrGa₂Si₂O₈ is completely ordered. Since the mean Si–O distance in this paracelsian analog is 0.004Å larger than that in slawsonite, it may be concluded with some confidence that slawsonite is also fully-ordered. Thus the significantly larger mean Si–O bond length in SrAl₂Si₂O₈ relative to BaAl₂Si₂O₈ suggests that the *M* cation may also be influential in determining the sizes of the tetrahedral sites.

Correlations between T–O distances and T–O–T and O–T–O angles

The T–O bond length variations in the feldspars correlate with the angles within and between the tetrahedral ions of the framework, shorter bonds tending to involve wider angles (Ribbe *et al.*, 1974; Gibbs *et al.*, 1974). The same correlation can be made for the tetrahedral bond lengths in slawsonite as evinced by Figure 3 where observed T–O bond lengths are plotted against bond lengths calculated as a function of the intertetrahedral angle T–O–T and the mean of the three O–T–O angles common to the T–O bond. As expected, the shortest Al–O and Si–O bonds in slawsonite are both to the only 2-coordinated oxygen (O4) and are involved in the widest T–O–T and ⟨O–T–O⟩₃ angles.

Acknowledgments

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Vibrational spectra of the alkaline earth double carbonates

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Abstract

Raman spectra and mid-range and far infrared spectra have been measured on polycrystalline norsethite [BaMg(CO₃)₂], barytocalcite [BaCa(CO₃)₂], the high-temperature modification of barytocalcite, huntite [CaMg₃(CO₃)₄], benstonite [Ca₇Ba₆(CO₃)₁₃], and alstonite [CaBa(CO₃)₂]. Factor-group calculations permit the assignment of the internal modes of the known structures. Effects of ordering in these derivative structures appear mainly in the IR spectra. A degree of translational disorder in the high-temperature modification of barytocalcite and in alstonite appears as a line broadening of the symmetric stretching mode in the Raman spectra.

Introduction

Seven known minerals containing alkaline-earth cations possess derivative or superstructures based on the calcite or aragonite structures (Table 1).

Two distinct types of ordering occur in the double carbonates. The first type represents an ordering of cation layers, while the second type is based on a superstructure of calcite with an ordering of cations within the layers. The high-temperature barytocalcite, barytocalcite, norsethite, and dolomite belong to the first type, and benstonite and huntite belong to the second type.

Barytocalcite (Dickens and Bowen, 1971) has a monoclinic cell, with space group $P2_1/m$ and $Z = 2$, that is related to the rhombohedral cell of calcite. If one considers Ca and Ba as identical, then a pseudocell can be constructed along the monoclinic $\{10\bar{1}\}_{\text{mono}} = a_{\text{pc}}$; $\{010\}_{\text{mono}} = b_{\text{pc}}$; and $\{101\}_{\text{mono}} = c_{\text{pc}}$. The pseudocell matches well with the orthohexagonal cell of calcite. The barytocalcite cell possesses alternating layers of Ca and Ba ions and two non-equivalent carbonate ions, one associated with the Ba ion and one with the Ca ion. The carbonate groups are non-planar and rotated 30° about “3-fold axis” with respect to the calcite carbonate groups. In addition, the carbonate group related to the calcium layer is tilted by 20° with respect to (101). Perpendicular to the layering, barytocalcite possesses a three-layer repeat similar to calcite, but because of the 30° rotation of the carbonate groups, the structure in this respect is similar to aragonite.

Prior to the structural determination of Dickens and Bowen (1971), Alm (1960) had investigated the structure and determined the space group to be $P2_1$. A second-harmonic generation test performed on a specimen verified the centrosymmetric cell and supports Dickens and Bowen’s assignment of space group $P2_1/m$.

Norsethite (Lippmann, 1973) has a cell (space group $R32$) similar to dolomite, with alternating Mg–CO₃–Ba–CO₃ layers. In norsethite, however, the planar carbonate groups are rotated by 17.5° about the “3-fold axis” with respect to calcite, and the carbonate ions follow a fundamentally different stacking pattern than in dolomite. The carbonate groups in norsethite are related by two fold axes, while in dolomite they are related by a center of symmetry.

The second type of ordering includes ordered cation sites within the cation layers. Of the two examples studied, only the structure of huntite is known in detail (Graf and Bradley, 1962). Huntite is related to calcite by $a_{\text{hex}} = 9.505 = 2 \times 4.752$; $c_{\text{hex}} = 7.821 = 15.642/2$. The relationship to calcite arises from the ordering of the cations on the expanded cation layer (Fig. 1). Two crystallographically distinct carbonate groups are present—one in the basal plane of the cell and three symmetry-related CO₃²⁻ canted to the basal plane.

No detailed structural data are available for benstonite, which possesses a superstructure of calcite, or for alstonite, an aragonite-related, polymorphic