

## STRUCTURE REFINEMENT OF BAZZITE FROM PEGMATITIC AND MIAROLITIC OCCURRENCES

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### ABSTRACT

The crystal structure of two samples of bazzite, from the Baveno granite, in Piemonte, Italy (type locality, miarolitic occurrence) and from Tørdal, Norway (pegmatitic occurrence), has been refined. Compared to material from Alpine fissures, these specimens contain greater amounts of heavy alkali ions (Cs<sup>+</sup>, Rb<sup>+</sup>, and K<sup>+</sup>) in the channels and minor quantities of magnesium in the octahedral positions, in agreement with the results of electron-microprobe analyses. In the channels, the Na<sup>+</sup> ions lie at the center of the Si<sub>6</sub>O<sub>18</sub> rings, *i.e.*, in the Wyckoff position *b*, whereas H<sub>2</sub>O and the heavier alkali ions occupy the *a* position. The possibility of partial substitution of silicon by beryllium, which was inferred for bazzite by some authors on the grounds of chemical analysis, has not been confirmed.

*Keywords:* bazzite, miarolitic cavity, pegmatite, scandium, crystal-structure refinement, Baveno, Italy, Tørdal, Norway.

### SOMMAIRE

Nous avons affiné la structure cristalline de deux échantillons de bazzite, un provenant de la localité-type, le granite de Baveno, région de Piemonte, en Italie (miarole), et l'autre provenant de Tørdal, en Norvège (pegmatite). En comparaison avec la bazzite de fentes alpines, ces deux échantillons contiennent davantage d'alcalins lourds (Cs<sup>+</sup>, Rb<sup>+</sup>, et K<sup>+</sup>) dans les canaux, et des quantités mineures de magnésium dans les positions octaédriques, en accord avec les mesures faites avec un microsonde électronique. Dans les canaux, les ions Na<sup>+</sup> sont situés au centre des anneaux Si<sub>6</sub>O<sub>18</sub>, à la position *b* dans le système de Wyckoff, tandis que les molécules de H<sub>2</sub>O et les alcalins lourds occupent la position *a*. La possibilité d'une substitution partielle du béryllium au silicium, qui avait été évoquée dans la bazzite par certains auteurs à la lumière de résultats d'analyses chimiques, n'a pas été confirmée.

(Traduit par la Rédaction)

*Mots-clés:* bazzite, miarole, pegmatite, scandium, affinement de la structure cristalline, Baveno, Italie, Tørdal, Norvège.

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## INTRODUCTION

Artini (1915) made the original discovery of bazzite in the miaroles of the Baveno granite, then the second known scandium-rich mineral. A number of additional occurrences of the mineral have since been reported in Alpine fissures (Hänni 1980, and references therein), and in granitic pegmatites outside the Alps, as for instance in Kazakhstan (Chistyakova *et al.* 1966) and in Norway (Bergstøl & Juve 1988). In spite of the relative abundance of data concerning all these occurrences, the results of accurate crystal-structure refinements are scarce in the literature, the only notable exception being the recent study by Armbruster *et al.* (1995) on a specimen from an Alpine fissure in Furkabasistunnel, Switzerland.

Some differences have been noted between bazzite occurring in Alpine fissures and that from granitic pegmatites. For instance, the former contains significant amounts of magnesium, whereas the latter contains much less Mg but non-negligible amounts of heavy alkali metals, such as cesium, in the channels of the structure, as is common with beryl-group minerals (Gramaccioli *et al.* 2000). As different distributions of such ions (and H<sub>2</sub>O molecules) in the channels have been proposed for beryl by various authors (see below), additional crystallographic data for bazzite could well be useful to clarify the situation for all the minerals in the group.

The beryllium content of bazzite has been quantitatively determined by very few authors. Among these, Chistyakova *et al.* (1966) and Juve & Bergstøl (1990) studied specimens from Kazakhstan and Norway, respectively, and reported a chemical formula in which part of the silicon seems to be replaced by beryllium, corresponding to the proportions (Si<sub>5.9</sub>Be<sub>0.1</sub>) and (Si<sub>5.7</sub>Be<sub>0.3</sub>), respectively. No evidence for this replacement has ever been found in beryl (Aurischio *et al.* 1988, Artioli *et al.* 1993). If confirmed by new crystallographic information, this pattern of substitution in bazzite would represent an important departure from that established in beryl.

The possibility of dealing with a crystal structure different, in some details at least, with respect to that of beryl might also account for the existence of a compositional gap between the two minerals in nature (Hänni 1980). Thanks to Mr. Roy Kristiansen from Seldebakk, Norway, we obtained a crystal of bazzite from a granitic pegmatite (Tørdal, Norway) that has provided X-ray data of very good quality; similarly, in the mineral collection of the Dipartimento di Scienze della Terra of the University of Milan, one of the cotype specimens from the original find at Baveno (miarolitic occurrence) and belonging to Mr. Bazzi's own collection (see Artini 1915), also was available. For these reasons, we had the possibility of carrying out accurate crystal-structure refinements of bazzite from two different types of environments, including material from the type locality.

## EXPERIMENTAL

*X-ray data collection and structure refinement*

Crystal data for the two samples here studied are reported in Table 1. For the sample from Baveno, a fragment measuring approximately 0.10 × 0.12 × 0.02 mm was selected from a homogeneous portion of a crystal also used for electron-microprobe analysis (Gramaccioli *et al.* 2000); this fragment was mounted on a Siemens P4 single-crystal diffractometer using graphite-monochromatized MoK $\alpha$  radiation. The orientation matrix for data collection and the unit-cell dimensions were obtained from least-squares refinement, using the setting angles of 36 reflections with 11.6 <  $\theta$  < 15.6°.

For bazzite from Tørdal, a fragment measuring about 0.15 × 0.10 × 0.18 mm was mounted on a CAD4 single-crystal diffractometer (graphite-monochromatized MoK $\alpha$  radiation); the unit-cell dimensions were obtained using 25 reflections with 9.6 <  $\theta$  < 20.4°.

Intensity data for the Baveno and Tørdal samples were collected at room temperature with a variable scan-rate using the omega-scan technique up to  $\theta = 30^\circ$  for the former and  $\theta = 40^\circ$  for the latter; the different strategy in collecting such data from the two samples was selected in order to take advantage of the better quality of the Norwegian crystal. The  $\omega$ -scan rate varied from 1 to 20°/min. Data reduction, including background and Lorentz and polarization corrections, was carried out using the Personal SDP software [Frenz 1992]. An absorption correction was performed as described in Demartin *et al.* (1992). The structure was refined

TABLE 1. BAZZITE: CRYSTAL DATA

	Baveno	Tørdal
Crystal system		Hexagonal
Space group		<i>P6/mcc</i> (#192)
<i>a</i> (Å)	9.549(2)	9.555(3)
<i>c</i> (Å)	9.163(3)	9.160(2)
<i>V</i> (Å <sup>3</sup> )	723.6(3)	732.1(3)
<i>Z</i>		2
Radiation used		MoK $\alpha$ (0.71073 Å)
Measured reflections	4359	4543
	473 unique	937 unique
Diffractometer	Siemens P4	Enraf-Nonius CAD4
Transmission factors	0.930 – 1.100	0.937 – 1.074
$R_{int}$ <sup>(1)</sup>	0.028	0.027
Max $2\theta$	60	80
Observed reflections { <i>I</i> > 2 $\sigma$ ( <i>I</i> )}	325	545
Refined parameters	36	39
<i>R</i> <sup>(2)</sup>	0.018	0.019
<i>wR</i> <sup>(3)</sup>	0.063	0.067
Min./max $\Delta\rho$ (e / Å <sup>3</sup> )	-0.36/0.37	-0.38/0.53

(1)  $R_{int} = \{ [\sum F_o^2 - F_c^2 (ave.)] / [\sum F_o^2] \}$ .(2)  $R = \{ [\sum (F_o - F_c)] / [\sum F_o] \}$ .(3)  $wR^2 = \{ \sum [w(F_o^2 - F_c^2)^2] / \sum [w(F_o^2)^2] \}^{1/2}$ .

(SHELX-93) by full-matrix least-squares starting from the atomic coordinates reported by Armbruster *et al.* (1995). Scattering factors of neutral atoms were used, and anomalous dispersion effects were included in Fc; furthermore, a correction for secondary extinction according to Zachariasen (1963) also was applied. Occupancies of the octahedral and channel sites were refined (*vide infra*) and are reported in Table 2, together with the final atomic coordinates and equivalent displacement parameters. The anisotropic displacement parameters are given in Table 3. All sites were labeled according to the convention of Armbruster *et al.* (1995), together with Wyckoff's notation. Selected interatomic distances are reported in Table 4. Structure factors may be obtained from The Depository of Unpublished Data, CISTI, National Research Council, Ottawa, Ontario K1A 0S2, Canada.

## RESULTS AND DISCUSSION

The  $AO_6$  octahedron

For the sample from Baveno, which contains only minor amounts of Mg, Al, and Zr (the total content being less than 0.05 atoms per formula unit), the scattering at the octahedral site was accounted for by refining [Sc, Fe] coupled occupancies, starting from the values obtained from the results of the chemical analysis. For the sample from Tørdal, the constrained occupancies of Sc, Fe and Al were instead refined; here the presence of significant amounts of Mn and Mg is modeled by Fe and Al, respectively, because of the similarity of the corresponding scattering-factors. The refinement con-

TABLE 2. POSITIONAL PARAMETERS AND EQUIVALENT DISPLACEMENT PARAMETERS ( $\text{\AA}^2$ ) FOR BAZZITE FROM BAVENO AND FROM TØRDAL

Site*	$x/a$	$y/b$	$z/c$	$B_{eq}$ ( $\text{\AA}^2$ )
<i>A</i> ( <i>c</i> )	2/3	1/3	1/4	0.47(2)
	2/3	1/3	1/4	0.52(1)
<i>Si</i> ( <i>l</i> )	0.37412(6)	0.09916(7)	0	0.40(1)
	0.37370(4)	0.09899(4)	0	0.38(1)
<i>W</i> ( <i>a</i> )	0	0	1/4	2.69(8)
	0	0	1/4	2.45(4)
<i>Na</i> ( <i>b</i> )	0	0	0	1.72(15)
	0	0	0	1.76(11)
<i>O1</i> ( <i>l</i> )	0.3006(2)	0.2192(2)	0	0.84(4)
	0.2998(1)	0.2186(1)	0	0.92(3)
<i>O2</i> ( <i>m</i> )	0.4819(1)	0.1288(1)	0.1447(1)	0.70(3)
	0.4813(1)	0.1286(1)	0.1445(1)	0.79(2)
<i>Be</i> ( <i>f</i> )	1/2	1/2	1/4	0.53(8)
	1/2	1/2	1/4	0.66(5)

First row: bazzite from Baveno; second row: bazzite from Tørdal.

$$B_{eq} = 8\pi^2/3 \sum_i U_{ij} a_i a_j$$

\* For clarity, Wyckoff's notation of the site follows between parentheses.

Refined occupancies for the sample from Baveno: site *A* [Sc 0.76(3), Fe 0.24(3)]; site *Na* [Na 0.44(2)]; site *W* [Cs 0.10(1), H<sub>2</sub>O 0.90(1)].

Refined occupancies for the sample from Tørdal: site *A* [Sc 0.68(4), Fe 0.26(3), Al 0.06(3)]; site *Na* [Na 0.36(2)]; site *W* [Cs 0.14(1), H<sub>2</sub>O 0.87(1)].

TABLE 3. ANISOTROPIC DISPLACEMENT PARAMETERS FOR BAZZITE FROM BAVENO AND FROM TØRDAL

Site	U(1,1)	U(2,2)	U(3,3)	U(1,2)	U(1,3)	U(2,3)
<i>A</i>	0.0055(2)	U(1,1)	0.0070(3)	U(1,1)/2	0	0
	0.0065(2)	U(1,1)	0.0068(2)	U(1,1)/2	0	0
<i>Si</i>	0.0052(3)	0.0044(3)	0.0056(3)	0.0024(2)	0	0
	0.0051(2)	0.0045(2)	0.0048(2)	0.0024(1)	0	0
<i>W</i>	0.0384(12)	U(1,1)	0.0255(12)	U(1,1)/2	0	0
	0.0344(7)	U(1,1)	0.0242(8)	U(1,1)/2	0	0
<i>Na</i>	0.0157(21)	U(1,1)	0.0339(37)	U(1,1)/2	0	0
	0.0176(16)	U(1,1)	0.0317(30)	U(1,1)/2	0	0
<i>O1</i>	0.0117(7)	0.0095(7)	0.0134(8)	0.0073(6)	0	0
	0.0136(4)	0.0100(4)	0.0151(4)	0.0087(4)	0	0
<i>O2</i>	0.0111(5)	0.0085(5)	0.0077(5)	0.0054(4)	-0.0038(4)	-0.0012(4)
	0.0125(3)	0.0098(3)	0.0084(3)	0.0059(2)	-0.0042(2)	-0.0013(2)
<i>Be</i>	0.0066(10)	U(1,1)	0.0060(14)	0.0025(12)	0	0
	0.0091(7)	U(1,1)	0.0079(9)	0.0053(7)	0	0

Notes: First row: bazzite from Baveno; second row: bazzite from Tørdal.

The displacement parameters are of the form:  $\exp[-2\pi^2(U(1,1)h^2a^{*2} + U(2,2)k^2b^{*2} + U(3,3)l^2c^{*2} + 2U(1,2)hka^*b^* + 2U(1,3)hla^*c^* + 2U(2,3)kib^*c^*)]$ .

TABLE 4. INTERATOMIC DISTANCES ( $\text{\AA}$ ) AND ANGLES ( $^\circ$ ), BAZZITE AND BERYL

	Baveno	Tørdal	Furka-tunnel <sup>a</sup>	beryl <sup>§</sup>
SiO <sub>4</sub> tetrahedron				
Si-O1	1.616(2)	1.616(1)	1.616(1)	1.592(1)
Si-O1	1.616(1)	1.615(1)	1.613(1)	1.594(1)
Si-O2 (2 $\times$ )	1.614(1)	1.612(1)	1.612(1)	1.620(1)
O1-O1	2.572(2)	2.566(2)	2.558(1)	2.582(1)
O2-O1 (2 $\times$ )	2.643(2)	2.644(2)	2.645(1)	2.607(1)
O2-O1 (2 $\times$ )	2.654(3)	2.653(2)	2.650(1)	2.638(1)
O2-O2	2.651(2)	2.648(1)	2.652(1)	2.668(1)
O1-Si-O1	105.44(9)	105.12(6)	104.81(5)	108.24(3)
O2-Si-O1 (2 $\times$ )	110.53(5)	110.59(4)	110.52(4)	108.42(3)
O2-Si-O1 (2 $\times$ )	109.87(5)	109.99(4)	110.08(3)	110.40(2)
O2-Si-O2	110.47(6)	110.43(4)	110.68(3)	110.88(2)
Si-O1-Si	165.4(1)	165.12(8)	164.81(7)	168.24(3)
BeO <sub>4</sub> tetrahedron				
Be-O2	1.640(1)	1.641(1)	1.642(1)	1.653(1)
O2-O2 (2 $\times$ )	2.493(2)	2.500(1)	2.483(1)	2.335(1)
O2-O2 (2 $\times$ )	2.651(2)	2.648(1)	2.650(1)	2.688(1)
O2-O2 (2 $\times$ )	2.876(2)	2.874(1)	2.893(1)	3.012(1)
O2-Be-O2 (2 $\times$ )	98.93(5)	99.19(4)	98.28(2)	90.90(2)
O2-Be-O2 (2 $\times$ )	122.50(5)	122.21(4)	123.45(2)	131.40(2)
O2-Be-O2 (2 $\times$ )	107.91(5)	107.89(4)	107.66(2)	108.85(2)
Si-O2-Be	130.44(7)	130.59(5)	130.20(2)	127.05(2)
AO <sub>6</sub> octahedron				
A-O2 (6 $\times$ )	2.101(1)	2.105(1)	2.080(1)	1.904(1)
O2-O2 (3 $\times$ )	2.493(2)	2.500(1)	2.483(1)	2.335(1)
O2-O2 (3 $\times$ )	2.882(3)	2.884(1)	2.868(1)	2.712(1)
O2-O2 (6 $\times$ )	3.237(3)	3.242(2)	3.188(1)	2.847(1)
O2-A-O2 (3 $\times$ )	72.81(4)	72.83(3)	73.29(1)	76.40(1)
O2-A-O2 (3 $\times$ )	86.61(4)	86.46(3)	87.15(1)	90.79(1)
O2-A-O2 (6 $\times$ )	100.56(4)	100.62(3)	100.06(1)	96.76(1)
O2-A-O2 (3 $\times$ )	171.15(4)	171.27(3)	171.07(1)	170.40(1)
Structural channel				
Na-W (2 $\times$ )	2.291(1)	2.290(1)	2.295	
Na-O1 (6 $\times$ )	2.572(2)	2.566(1)	2.558(1)	

# Data from Armbruster *et al.* (1995); § data from Morosin (1972).

verged to values for the site populations in good agreement with the composition established by analysis (Tables 2, 5). As is well known, bazzite can be considered as the scandium-dominant analogue of beryl, in which most of the  $Al^{3+}$  in the octahedral *A* sites is replaced by  $Sc^{3+}$ , together with a number of other cations, either trivalent or divalent, e.g.,  $Fe^{3+}$ ,  $Fe^{2+}$ , or  $Mg^{2+}$ , with widely different radii. Since  $Al^{3+}$  is the smallest of all these cations, the observed *A*–O2 distance in bazzite (average 2.103 Å for our data: see Table 4) is larger than the corresponding one in beryl, whose average is 1.904 Å only; as a consequence, the octahedron also becomes considerably larger in size than that occurring for beryl, besides being strongly compressed along *c* and distorted. Such a flattening is responsible for the greater value of the unit-cell parameter *a* with respect to that of beryl [9.209 Å for the pure synthetic beryl, according to Morosin (1972)]. The *A*–O2 distances observed in the two samples are statistically identical (Table 4), and are significantly longer than those of bazzite from Furkabasistunnel, this feature most likely depending on the higher content of Mg for the material from Alpine fissures.

#### The $BeO_4$ tetrahedron

The  $BeO_4$  tetrahedron shares two edges with two adjacent  $AO_6$  octahedra and two vertices with two different  $Si_6O_{18}$  rings. Because the  $Si_6O_{18}$  ring is almost invariable in size, and its flexibility is limited by symmetry constraints, the lengthening of the *A*–O2 bonds described above, which takes place on passing from beryl to bazzite and, consequently, that of the O2–O2 edges of the octahedra, imply a modification of the geometry of the adjacent  $BeO_4$  tetrahedron (Table 4). As a consequence, this tetrahedron in bazzite becomes less distorted than in beryl, and the Be–O distances are subject to significant shortening (average 1.641 versus 1.653 Å in beryl).

#### Channel sites

In the open channels of the beryl structure, the metal ions and the  $H_2O$  molecules are located in the 0,0,1/4 (*a*) and 0,0,0 (*b*) positions of the *P6/mcc* space group, using Wyckoff's labels. According to most authors, for instance, Hawthorne & Černý (1977),  $H_2O$  and the larger alkali ions ( $Cs^+$ ,  $Rb^+$ , and  $K^+$ ) should occupy the *a* position, whereas the  $Na^+$  ions should instead lie at *b*, i.e., at the center of the  $Si_6O_{18}$  rings. On considering the case of a unique natural example of beryl containing no  $H_2O$ , and on grounds of reliable crystallographic data, Aurisicchio *et al.* (1988) inferred that in this anhydrous sample,  $Na^+$  occupies instead the *a* site exclusively, together with all the heavier alkali ions; similarly, for a series of  $H_2O$ -containing natural samples of beryl, the same authors have noticed that the residual electron-density maxima in the *a* and *b* positions can be ac-

TABLE 5. CHEMICAL COMPOSITION\* OF BAZZITE FROM BAVENO AND TØRDAL

	Baveno		Tørdal		Baveno		Tørdal	
	(1)	(2)	A	B	A	B	A	B
MgO wt%	0.13	0.10	Mg <i>apfu</i>	0.019		0.014		
$Al_2O_3$	0.14	0.80	Al	0.016		0.090	0.12	
MnO	0.10	1.43	Mn	0.009		0.112		
$Fe_2O_3$	6.62	5.70	Fe	0.496	0.48	0.399	0.52	
$Sc_2O_3$	16.24	14.50	Sc	1.409	1.52	1.182	1.46	
$ZrO_2$	0.30		Zr	0.014				
			$\Sigma A$	1.963		1.797		
$Na_2O$	2.13	1.60	Na	0.412	0.44	0.292	0.36	
$K_2O$	0.00	0.13	K	0.000		0.017		
$Rb_2O$	0.00	0.25	Rb	0.000		0.015		
$Cs_2O$	2.30	2.93	Cs	0.096	0.10	0.116	0.14	
CaO	0.00		Ca	0.000				
			$\Sigma B$	0.508		0.440		
$SiO_2$	58.18	58.00	Si	6.000		5.431		
BeO	<sup>§</sup> 12.11	14.50	Be	<sup>§</sup> 0.000		0.569		
			$\Sigma C$	6.000		6.000		
			Be	3.000		2.909		
$Li_2O$		0.24	Li			0.091		
			$\Sigma D$	3.000		3.000		
$H_2O$	<sup>¶</sup> 2.72	1.10	H		1.80	0.699	1.94	
total	100.97	101.28						

\* Normalized to 9 (Si + Be) atoms per formula unit (*apfu*).

A: determined by chemical analysis; B: determined from the crystal-structure refinement. <sup>§</sup> Obtained by assuming Be/Si = 0.5.

<sup>¶</sup> Calculated on the basis of the crystal-structure refinement.

Samples: (1) Cotype specimen from the collection of the Dipartimento di Scienze della Terra, Università di Milano (Gramaccioli *et al.* 2000). (2) From Juve & Bergstøl (1990).

counted for almost exactly by locating  $Na^+$  and all the other alkali ions noted in the results of the electron-microprobe analyses in *a*, and the  $H_2O$  molecules in *b*, in contrast to the model of Hawthorne and Černý (1977). However, in general, there is no reason why the  $H_2O$  molecules should not occupy the *a* as well the *b* position, and such a possibility could account for the presence of two types of  $H_2O$  in the infrared spectra (Wood & Nassau 1967, Polupanova *et al.* 1985).

On the basis of the refined occupancies in the case of the bazzite from Furkabasistunnel, Armbruster *et al.* (1995) suggested that the *a* position essentially contains  $H_2O$  molecules, whereas the cations ( $Na^+$  and  $Ca^{2+}$ ) are located instead in *b*, the occupancy in this position corresponding to 0.46 Na *pfu*. However, since the amount of Na + Ca determined by electron-microprobe analysis corresponds to an occupancy of 0.32 Na *pfu* only, the possibility that this site also contains small amounts of heavy elements or  $H_2O$  (or both) cannot be ruled out.

In the present study, the refined occupancies of the *b* site for our samples from Baveno and Tørdal can be reproduced very well by locating in this position an amount of Na corresponding to the chemical composition as determined by electron-microprobe analysis; the remaining alkali atoms can be placed instead in the *a*

site, together with most of the H<sub>2</sub>O molecules, thereby confirming the validity of the proposal of Hawthorne & Černý (1977) also for bazzite.

#### The Si<sub>6</sub>O<sub>18</sub> ring

The pattern of bond distances and angles observed for the SiO<sub>4</sub> tetrahedra is identical to that observed in bazzite from Furkabisstunnel (Armbruster *et al.* 1995), and is similar to what has been found for samples of Na-rich beryl (Aurischio *et al.* 1988). On introducing Na<sup>+</sup> at the center of the Si<sub>6</sub>O<sub>18</sub> rings, as invariably happens in bazzite (see above), in order to satisfy the bond-valence requirements of oxygen, the Si–O1 distances should become longer than those occurring for alkali-free beryl; however, at the same time, the Si–O2 distances should be shortened to maintain an acceptable bond-valence sum for silicon (Table 4). The average Si–O distance is 1.615 and 1.614 Å, respectively, for our samples, and is 1.613 Å for bazzite from Furkabisstunnel; these values are only slightly but significantly larger than the corresponding values for beryl (average 1.609 Å, according to Aurischio *et al.* 1988). Rather than an inferred partial substitution of Si by Be (see below), such an increase is much more likely to be due to the strain occurring in the Si<sub>6</sub>O<sub>18</sub> ring as a consequence of having replaced Al<sup>3+</sup> in the octahedral sites with larger cations (see above).

As we have seen, the chemical composition of two specimens reported by Chistyakova *et al.* (1966) and Juve & Bergstøl (1990) was interpreted to show partial substitution of Si by Be. The sample from Tørdal is presumably similar to our material from that locality, showing the more marked degree of substitution. Therefore, after completion of the crystal-structure refinement independently for both our samples, we have considered the possibility of carrying out a further stage by also allowing the occupancy of the Si sites to vary. The final result can be considered to be at least partially dependent upon the number of electrons assigned to the Be, Si, and O atoms, as well as upon the range of sin θ/λ considered, since the scattering curves are not strictly proportional to the number of electrons. There are also problems if corrections for extinction are inadequate. The results are reported in Table 6; the various attempts

differ because the form factors of neutral atoms or ions have been alternatively considered, or because a maximum value of sin θ/λ for the reflections has been introduced in some cases.

On examining these results, a deviation from the theoretical value of the occupancy (1.00) can be noticed for bazzite in all cases. The deviation seems significant on the basis of the estimated standard deviations obtained from the final cycles of the least squares; however, the possible presence of systematic errors should be seriously considered. In the case of beryl, there is general and well-grounded agreement about the absence of such substitution of Si by Be (Aurischio *et al.* 1988, Artioli *et al.* 1993); the absence of significant Be-for-Si substitution in beryl has also been proved by our lattice-dynamics calculations (Pilati *et al.* 1997), since our theoretical estimates of the atomic displacement parameters (ADP) of the Si atoms almost match the corresponding experimental values, whereas the replacement of some Si by Be would lead to considerably higher values of the ADP.

As a test, we have refined the structure of a sample of beryl under the same conditions, and the data were collected and processed using the same equipment and routines. These data, also reported in Table 6, might constitute a good standard for comparison. An examination of these results and a comparison with the corresponding data for bazzite reveal no significant difference between the two minerals in this respect. Therefore, no clear evidence has been obtained in favor of the possibility of Be-for-Si substitution. Furthermore, on examining the results of the different models tested for bazzite, the values of the occupancy are clearly ambiguous because, even for the same sample, they can be either higher or lower than 1.00; therefore, we conclude that their actual uncertainty is much greater than the corresponding estimated standard deviation, owing to the presence of systematic errors in the collected data (including their treatment) and to the inadequacy of the scattering curves used.

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TABLE 6. REFINED VALUES OF THE OCCUPANCY OF THE Si SITE\*

	bazzite, Baveno	bazzite, Tørdal	beryl
Neutral atoms	0.948	0.960	0.986
Ions	0.968	0.974	0.978
sinθ/λ > 0.4 neutral atoms	1.010	1.038	1.034
sinθ/λ > 0.4 ions	0.966	1.016	1.014

\* The estimated standard deviation for all the cases shown above is 0.001.

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