die relativ hohe kontinuierliche Intensität zwischen Normalreflex und Zwillingsreflex, gemäss Fig. 1, während die Streifen auf den übrigen Teilstrecken der reziproken Gittergeraden geringere Intensität aufweisen.

Nach Formel (1) darf aber nur auf solchen Gittergeraden kontinuierliche Intensität auftreten, für die (in hexagonaler Indizierung) $h-k \not\equiv 0 \pmod 3$ ist. Für $h-k \equiv 0 \pmod 3$ verschwindet der kontinuierliche Anteil gemäss der Formel. Auf den Beugungsaufnahmen wird auch nur auf diesen Gittergeraden des reziproken Gitters das Auftreten von Streifen beobachtet.

Solche Streifen fand zuerst Cochrane (1936) bei Elektronenbeugungsaufnahmen von dünnen Nickelschichten, die er und später Kirchner & Rüdiger (1937) auf eine Flächengitterwirkung der 111-Ebenen im Kristall zurückführen. Diese Deutung ist aber nicht haltbar, da die 111-Ebenen zwar Spiegelungsebenen bei der Zwillingsbildung sind, aber vom beugungstheoretischen Standpunkt aus keine ausgezeichnete Rolle spielen. Die hier gegebene Deutung der Streifen durch Anwendung der Theorie von Jagodzinski gibt die Beobachtungen zwanglos wieder.

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The Crystal Structure of Baveno Bazzite

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The crystal structure of the silicate bazzite, of unknown quantitative composition, has been determined by using rotation and Weissenberg photographs (Fe $K\alpha$ radiation). Cell dimensions are: $a = 9\cdot51$ and $c = 9\cdot11$ Å; space group: $D_{6h}^2 - P6/mcc$. Bazzite has a beryl-type structure with two (Si_6O_{18}) rings at $z = 0$ and $\frac{1}{2}$ and with cations distributed at $z = \frac{1}{4}$ and $\frac{3}{4}$ in three special positions (a), (c) and (f) respectively on 6-, 3- and 2-fold axes. From the observed interatomic distances and the total electron content of special positions, corrected for series termination, the probable distribution of qualitatively recognized cations is discussed and an average weight percentage for each special position is evaluated.

Introduction and structure analysis

Bazzite is a very rare, light blue, natural silicate discovered by E. Bazzi in the geodes of Baveno granite (Italy) and containing (Artini, 1915; Bertolani, 1948) principally Sc, Fe, Na, Y, Yb beside other elements. Since, owing to the rarity of the mineral, no quantitative or even partial chemical analysis has ever been made, it seemed of interest, both from the point of view of general method and of the crystal- and geochemistry of rare earth elements, to establish its chemical constitution by the non-destructive X-ray analysis of a very small quantity of the substance.

Bazzite has a fascicular habitus resulting from the sub-parallel association of very small hexagonal prisms, 2 mm. long and some tenths of a millimetre thick. In order to obtain photographs without spurious spots, which might confuse the extinction conditions, a fragment of the mineral was carefully cut into a small, crystallographically homogeneous, specimen of about $0\cdot2 \times 0\cdot3 \times 0\cdot5$ mm. weighing less than $0\cdot1$ mg. [00.1], [01.0], and [11.0] were used as the principal directions for Laue and rotating crystal photographs, and $hki0$, $hki1$, $h0\bar{h}l$, $h,h,2\bar{h},l$ Weissenberg photographs (Fe $K\alpha$ radiation, $\lambda = 1\cdot9379$ Å)* were taken on this unique specimen and gave the following results:

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* Fe radiation was used as no other X-ray tube was available for this research. Some photographs taken with Cu $K\alpha$ and Mo $K\alpha$ radiation, using an old ion-discharge Seemann tube, did not give any further information except the intense reflexion (0,0,12).

Hexagonal diffraction symmetry D_{6h}–$6/mmm$.

$$a = 9\cdot51 \quad \text{and} \quad c = 9\cdot11\pm0\cdot01 \text{ Å} .$$

Conditions for non-extinction: $hkil$: no condition; $h0\bar{h}l$, $hh,\overline{2h},l$, $000l$ present with $l = 2n$, corresponding to the possible space groups $P6cc$ and $P6/mcc$.

The intensities were visually estimated by comparison with a time-exposure calibrated film strip and were corrected for Lorentz and polarization factors. An absorption correction was introduced in the last stage of the analysis, taking into account the resulting composition and the shape of the crystal. By plotting $\log |F_o|/|F_c|$ against $(\sin\theta/\lambda)^2$, the $|F_o|$'s were put on an absolute scale and were corrected for a temperature factor with $B = 3\cdot2$ Å^2. The density of the mineral (2·80 g.cm.$^{-3}$) given by Artini (1915) was checked on the specimen used for X-ray experiments by using the Thoulet solution and a calibrated Westphal balance. In order to establish the accuracy of the measurements, the density of several fragments of a very pure crystal of quartz was measured in the same conditions, giving an average value of 2·653±0·002 g.cm.$^{-3}$. Fragments of bazzite were carefully heated in the solution in order to remove air bubbles present on their surface and measurements were made at room temperature. A density of 2·819±0·002 g.cm.$^{-3}$ was obtained. From this density and the cell volume a cell atomic weight of 1211·5 is calculated.

Cell dimensions of bazzite are very close to those of beryl ($a = 9\cdot23$, $c = 9\cdot19$ Å; density = 2·65±0·05 g.cm.$^{-3}$; cell content 2 Be$_3$Al$_2$Si$_6$O$_{18}$; space group $P6/mcc$). The very intense (0008) reflexion shows that also in bazzite the atoms must be distributed in parallel planes at distances of about $c/8$ along the c axis. It was therefore likely to admit for bazzite a substituted beryl-type structure with hexasilicic rings (Si$_6$O$_6$O$_{12}$) distributed along the c axis. In the $P6cc$ group the 6 Si, 6 O$_I$ and 12 O$_{II}$ atoms should be all in the general position $12(x, y, z)$, that is the 24 O$_{II}$ atoms of the cell should be split into two crystallographically non-equivalent groups up and down the plane of the (Si–O$_I$)$_6$ ring. This unlikely crystallographic non-equivalence is excluded by the following analysis, and the space group of bazzite is, like that of beryl, D^2_{6h}–$P6/mcc$. In this space group two (Si–O$_I$)$_6$ rings are placed on the mirror planes at $z = 0$ and $\frac{1}{2}$, and therefore give a positive contribution to all the $000l$ reflexions. Their combined scattering power is greater than that of the 24 O$_{II}$ atoms and of the atoms at $z = \frac{1}{4}$ and $\frac{3}{4}$. The signs of the $000l$ reflexions must therefore be positive, as in the similar structures of beryl, benitoite and hexamethylcyclotrisiloxane.

A $\varrho_o(z)$ curve, calculated by assuming a positive sign for all the observed $000l$ reflexions, confirmed the postulated structure, and determined an approximate value of the z parameter for the external O$_{II}$ atoms bonded to the (Si–O$_I$)$_6$ ring. A Patterson projection $P(x, y)$ indicated the presence of heavy atoms in position $(\frac{2}{3}, \frac{1}{3})$. Assuming for the structure-factor cal-

culation the (Si$_6$O$_{18}$) rings and only scandium for position (c) $4(\frac{2}{3}, \frac{1}{3}, \frac{1}{4})$, the $000l$ structure factors gave already a fairly good absolute scale for intensities, and a factor $R_{hkio} = \Sigma||F_o|-|F_c|| \div \Sigma|F_o| = 0\cdot54$ was obtained. A $\varrho_o(x, y)$ synthesis showed clearly, besides the expected $(\frac{2}{3}, \frac{1}{3})$ maximum, two new very well defined maxima at $(0, 0)$ and $(\frac{1}{2}, 0)$. By calculating the electron content of the three maxima, introducing suitable atom form factors for them in the calculation of structure factors, and correcting the Si and O positions by successive $\varrho_o(x, y)$ syntheses, the factor R_{hkio} was improved to 0·31. The $h0\bar{h}l$ structure factors and $\varrho_o(x, \bar{x}, z)$ projections gave a final factor $R_{h0\bar{h}l} = 0\cdot31$ and established for the remaining cations the positions (a) $2(0, 0, \frac{1}{4})$ and (f) $6(\frac{1}{2}, 0, \frac{1}{4})$.*

The effects of series termination on the Si and O positions and on the electron content of cation maxima

Table 1. *Comparison of F_o and F_c for $hki0$ and $h0\bar{h}l$ reflexions of bazzite*

$hki0$	F_o	F_c	$h0\bar{h}l$	F_o	F_c
$10\bar{1}0$	31·3	−56·2	$10\bar{1}0$	31·3	−56·2
$11\bar{2}0$	—	− 1·4	0002	63·9	82·5
$20\bar{2}0$	19·2	−14·4	$20\bar{2}0$	19·2	−14·4
$21\bar{3}0$	22·0	8·4	$10\bar{1}2$	50·0	54·4
$30\bar{3}0$	74·6	76·9	$20\bar{2}2$	48·5	−72·9
$22\bar{4}0$	57·8	64·1	$30\bar{3}0$	74·6	76·9
$31\bar{4}0$	30·3	37·5	$30\bar{3}2$	20·8	−24·2
$40\bar{4}0$	51·2	−50·0	0004	127·4	146·3
$32\bar{5}0$	26·6	−28·7	$10\bar{1}4$	37·8	39·5
$41\bar{5}0$	115·6	99·6	$40\bar{4}0$	51·2	−50·0
$50\bar{5}0$	109·6	−96·9	$20\bar{2}4$	58·8	−68·7
$33\bar{6}0$	26·7	− 3·0	$40\bar{4}2$	—	−17·2
$42\bar{6}0$	29·0	24·6	$30\bar{3}4$	96·5	122·8
$51\bar{6}0$	26·8	6·3	$50\bar{5}0$	109·6	−96·9
$60\bar{6}0$	46·6	54·5	$50\bar{5}2$	—	−28·0
$43\bar{7}0$	18·8	−13·3	$40\bar{4}4$	—	11·1
$52\bar{7}0$	100·0	97·2	0006	115·9	96·3
$61\bar{7}0$	26·0	−12·3	$10\bar{1}6$	—	11·1
$44\bar{8}0$	25·2	21·6	$20\bar{2}6$	—	−30·0
$70\bar{7}0$	42·6	−53·5	$60\bar{6}0$	46·6	54·5
$53\bar{8}0$	42·9	−34·2	$50\bar{5}4$	—	−26·5
$62\bar{8}0$	24·0	20·4	$30\bar{3}6$	—	−31·8
$71\bar{8}0$	32·3	33·1	$60\bar{6}2$	119·4	−119·9
$54\bar{9}0$	15·8	21·8	$40\bar{4}6$	—	−29·7
$63\bar{9}0$	34·8	36·1	$70\bar{7}0$	42·6	−53·5
$80\bar{8}0$	60·1	61·5	$60\bar{6}4$	—	− 6·1
			$70\bar{7}2$	—	− 9·7
			0008	204·2	199·2
			$10\bar{1}8$	—	−14·9
			$50\bar{5}6$	32·9	−34·6
			$20\bar{2}8$	—	−13·4
			$30\bar{3}8$	57·3	59·5
			$70\bar{7}4$	—	−15·9
			$80\bar{8}0$	60·1	61·5
			$60\bar{6}6$	52·7	−82·1
			$80\bar{8}2$	20·8	12·5
			$40\bar{4}8$	29·0	−21·7
			0,0,0,10	—	− 1·8
			0,0,0,12	75·6	93·8

* Results at this stage of the analysis were presented at the Third International Congress of Crystallography in Paris, on 22 July 1954, and a short summary has been published (Peyronel, 1954). The synopsis included in the report of the Congress was a first summary, given at the very early stage of this work.
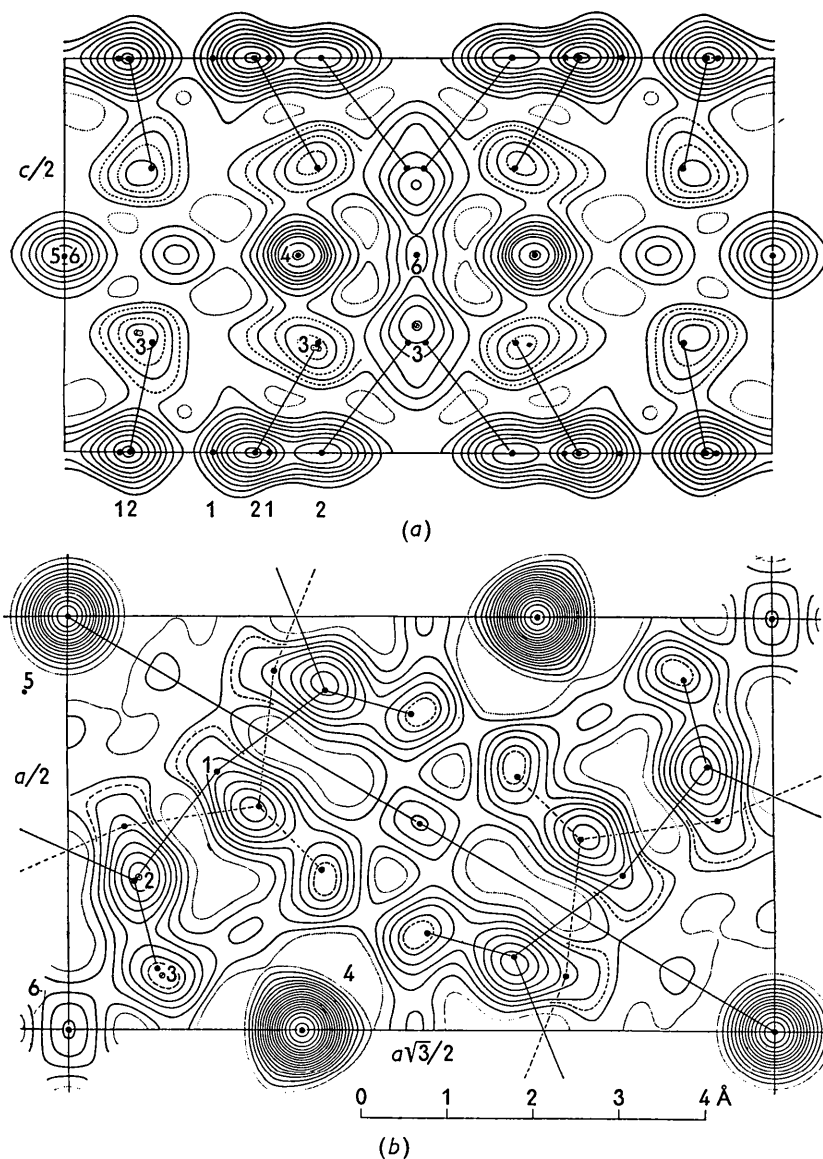
Fig. 1. Electron-density projection (a) $\varrho_0(x, \bar{x}, z)$ and (b) $\varrho_0(x, y)$. Dotted lines at zero electron level. Full lines at intervals of 4 e.Å^{-2}. Broken lines at intervals of 2 e.Å^{-2} from full lines. Final positions of atoms (•), ϱ_0 maxima (⊙) and ϱ_c maxima (⊖) are indicated. 1 = O_I, 2 = Si, 3 = O_{II}, 4 = (c), 5 = (a), 6 = (f) positions.

were then corrected by successive F_c syntheses until the positions of Si and O_{II} maxima, in the F_o and F_c syntheses, coincided within the graphical errors by analysing every peak along several sections according to the method of Megaw (1954), and until the ϱ_o and ϱ_c curves of the three cation maxima, considered in two orthogonal directions, were practically coincident. The position of O_I, the maximum of which cannot be resolved in either of the two projections, was established by resolving the common maximum with silicon in the $\varrho_o(x, y)$ projections and refining the coordinates by $(F_o - F_c)$ syntheses. In calculating the $\varrho_o(x, y)$ and $\varrho_o(x, \bar{x}, z)$ syntheses of Fig. 1 the value $F(0000) = 600$ was assumed from the knowledge of the final composi-

tion; because of the difficulties of measuring the intensity of (10$\bar{1}$0) the lowest calculated value, $F_c(10\bar{1}0) = -55$ (resulting from several combinations of x, y, z parameters for silicon and oxygen and of cation form factors) was used instead of the experimental value. This substitution does not affect the positions of the maxima but only the general background of the Fourier syntheses. Final reliability factors, for F_o and F_c as given in Table 1, are:

Without (10$\bar{1}$0): $R_{hki0} = 0.17$, $R_{h0\bar{h}l} = 0.15$.

Including (10$\bar{1}$0): $R_{hki0} = 0.19$, $R_{h0\bar{h}l} = 0.16$.

$R_{h0\bar{h}l}$ factors refer only to observed reflexions, owing to the fact that the level of observation for the inten-
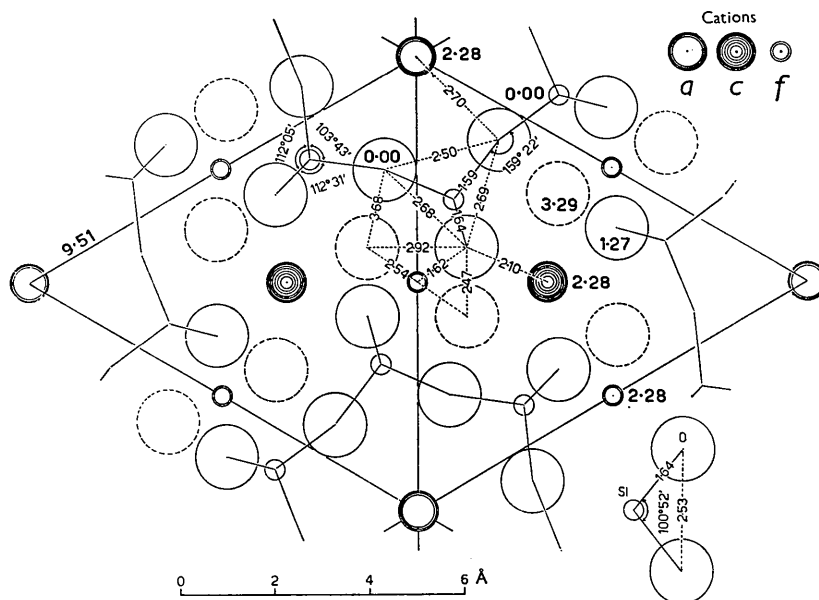
Fig. 2. Interatomic distances (in Å) and angles for bazzite. The z parameters (in Å) are written in larger type.
O_{II} atoms, drawn with broken lines, belong to upper (Si_6O_{18}) rings.

sities of this zone was higher than for the other. Both R factors are of the same order as, or lower than, many of those recently obtained for other silicate structures of known composition.

Discussion of results

Final positions of silicon and oxygen atoms (Table 3) and the corresponding positions of distinct maxima, for Si and O_{II}, in the ϱ_o and ϱ_c syntheses, are given in Fig. 1. The positions of the maxima of ϱ_o and ϱ_c coincide exactly for O_{II} and almost exactly (within 0·02 Å) for Si in $\varrho(x, y)$ syntheses. In the $\varrho(x, \bar{x}, z)$ syntheses the z component of their displacement relative to the atomic positions is the same for the two syntheses, indicating that the z parameter of O_{II} is substantially correct; the small discrepancy in the $x, \bar{x}$ direction was not taken into account because in this direction lie also the biggest deformations of these syntheses: $(F_o - F_c)$ syntheses clearly showed that spurious maxima, especially in the $\varrho(x, \bar{x}, z)$ projections, are diffraction effects. The $\varrho_o(x, y)$ synthesis is more accurate than that of $\varrho_o(x, \bar{x}, z)$, not only because it was calculated with all the reflexions obtainable with iron radiation, but also because the $hki0$ reflexions, being referred only to two axes (x, y) instead of three (x, y, i) in the Fourier calculations, are split in several groups of distinct frequencies $hk0$; e.g. for ortho-hexagonal axes the reciprocal-lattice points are so shared:

$$h0\bar{h}0 \text{ and } h,h,\overline{2h},0 \quad 6 \rightarrow 2+4$$
$$hki0 \quad\quad\quad\quad 12 \rightarrow 4+4+4 \ .$$

The 25 intensities (amplitudes) used for the $\varrho_o(x, y)$ syntheses correspond therefore, in this case, to 64

distinct frequencies $hk0$ in the Fourier calculations. An evaluation of the standard deviations $\sigma(x) = \sigma(y)$ for the Si and O_{II} positions was made by Cruickshank's (1949) method, using, for the calculation of p the electron-density curves of Si and O_{II} obtained by averaging the electron density at the same distances from the centre of their maxima, in several directions not affected by neighbouring maxima. The projection area A, instead of the volume V, was used in calculating

$$\sigma(A_h) = \frac{2\pi}{aA} \{\Sigma_2 h^2 \Delta F^2\}^{\frac{1}{2}} = 5 \cdot 50 \text{ Å}^3 \ .$$

The following results were obtained:

	p	A_{hh}	$\sigma(x) = \sigma(y)$
Si	4·51	$-273 \cdot 7$ Å^{-4}	0·02 Å
O_{II}	3·95	$-189 \cdot 2$	0·03

The interatomic distances and angles are given in Fig. 2. All are quite normal, except the O_{II}–O_{II} distance of 2·47 Å, which will be discussed later.

The atom form factors given by Halla & Mark (1937) for silicon and oxygen in silicate structures were used in calculating the final structure factors. For the (c), (a) and (f) positions, occupied by unknown fractions of several possible cations qualitatively recognized in the mineral, a very good agreement between ϱ_o and ϱ_c curves of maxima in the $\varrho(x, y)$ projections was obtained by using the values given by the f_a curves of Table 2, multiplied by a suitable multiplicity factor (m), which substitutes the multiplicity factor of each position. From the extrapolated values at $\sin \theta/\lambda = 0$ (the ionic effective numbers) the total electron contents (i.e. m times the ionic effective numbers) associated

Table 2

Position	f_a curve	Source	Ionic effective number	m	Total electron contents
(c)	Sc^{3+}	*Internationale Tabellen* (1935)	18	4·277	77·00
(a)	Fe^{2+}	Halla & Mark (1937)	24	1·054	25·31
(f)	Si	Halla & Mark (1937)	13	1·678	21·80

with each special position can be evaluated. To a good approximation this can be considered as the effective electron contents of the site, because these numbers are corrected for series termination.

The effective ionic number 13 for silicon is that generally accepted for silicates. The heights for the five distinct maxima of the observed and calculated $\varrho(x, y)$ projections are:

	(c)	(a)	(f)	Si	2 O$_{II}$	
ϱ_o	70·45	53·00	15·54	30·60	23·72	e.Å^{-2}
ϱ_c	70·61	53·29	15·65	27·58	23·62	e.Å^{-2}

Some information about cation distribution can be obtained from the observed interatomic distances (Fig. 2) and the above electron contents of special positions. Artini (1915) concluded, after repeated, very accurate, qualitative microanalysis, that Baveno bazzite contains principally Sc, appreciable quantities of Fe, small quantities of Na and of other rare earth elements; that flame reaction of B and microchemical reactions of Be and Al were 'always absolutely negative' and that H$_2$O$_2$ 'does not give any trace of Ti reaction'. Bertolani (1948) found spectrographically the following elements: Al, Be, B, Ca, Fe, K, Li, Mg, Mn, Na, Sc, Si, Sn, Ti, Y, Yb, but no evaluation was made of their relative abundance, except for Sc (lines of considerable intensity), Y and Yb (lines of good intensity), whilst lines of the remaining rare earths are very weak or negligible. As the analysed bazzite was accompanied by muscovite, intimately mixed to it, the presence of Al, Ca, K, Mg, Li, Na, can be influenced by this impurity.

Cation–oxygen ionic radius sums for Sc^{3+} (2·21 Å), Fe^{2+} (2·15 Å), Al^{3+} (1·90 Å), Mg^{2+} (2·10 Å, obs.), Mn^{2+} (2·20 Å), Ti^{4+} (2·08 Å), Sn^{4+} (2·11 Å) (Pauling, 1948) are close enough to the cation–oxygen distance of 2·10 Å observed for position (c). The isomorphic substitution of these cations in this octahedral position is quite normal (Rankama & Sahama, 1950). Iron has to be assumed in the ferrous state owing to the light blue color of the mineral and to its acid composition. A small amount of Al has to be admitted in order to explain the short cation–oxygen distance (2·10 Å) of the most abundant cations, Sc and Fe.

The cation–oxygen ionic radius sums (coordination number 6) for Y^{3+} (2·33 Å), Yb^{3+} (2·40 Å), Na$^+$ (2·35 Å), Ca^{2+} (2·39 Å), K$^+$ (2·73 Å), are much greater than the observed distance for position (c). Normally Y and lanthanides cannot replace Mg and Fe^{2+} in

mineral structures. Y and Yb substitute Sc in thorveitite, but it is doubtful whether this can happen (except for traces) in position (c) of bazzite, which is occupied by appreciable amounts of Fe and by the other smaller cations mentioned above. On the other hand Y, Yb, Na, Ca, K have a cation/oxygen radius ratio favourable to a coordination number greater than 6; Na and Y can replace Ca, whilst Sc cannot extensively replace Ca (Rankama & Sahama, 1950). These cations, and perhaps also water molecules, would therefore more likely be located, as in beryl, in the holes of position (a), having a coordination number 12. The cation–oxygen distances calculated for this coordination number (Pauling, 1948) Y^{3+} (2·57 Å), Yb^{3+} (2·63 Å), Na$^+$ (2·64 Å), Ca^{2+} (2·65 Å), K$^+$ (3·02 Å), are close enough to the observed (a)–oxygen distance of 2·70 Å. Owing to the 50% ionic character of the Si–O bond there should be, also for trivalent cations in position (a), a sufficient amount of negative charge ($\frac{1}{4}$ from each oxygen is required) to saturate their positive valencies. Their location in this position is, however, very exceptional and questionable.

The tetrahedral position (f) has a cation–oxygen distance of 1·62 Å, which agrees well with the more accurately observed Si–O distance of 1·60 Å (Smith, 1954), but is much lower than the ionic radius sum (Pauling, 1948), which in turn is the same as the more accurately observed Al–O distance of 1·78 Å (Smith, 1954) and much higher than the distance B–O = 1·44–1·47 Å observed by Ito & Mori (1953) in datolite. The Be–O ionic radius sum is 1·59 Å; its observed distance is 1·73 Å for beryl (Bragg, 1932) and 1·64–1·65 Å for BeO (Wyckoff, 1948). Whilst it is possible to exclude Al and B, at least in appreciable amounts, from position (f), it is very difficult to say anything about the presence of Be from interatomic distances only.

If, according to the very accurate observations of Artini (1915), Be is absent, or present only in very small amounts, neighbouring (Si$_6$O$_{18}$) rings of bazzite should be considered as linked together through some SiO$_4$ tetrahedra, as in milarite (Ito, Morimoto & Sadanaga, 1952), and there would be less than the 24 positive charges required to saturate those of the hexasilicic rings. In that case it would be necessary to admit the presence of SiOH groups corresponding to the empty (f) positions, with O$_{II}$–H · · · O$_{II}$ bridges between superposed hexasilicic rings, as seems to be indicated by the short distance O$_{II}$–O$_{II}$ = 2·47 Å observed in this structure, which is shorter than the O–H · · · O distance of 2·49–2·56 Å or more observed in afwillite by Megaw (1952). The presence, besides water molecules in the (a) position, of acid hydrogen in this structure could also agree with the fact that bazzite has a pneumatolitic-hydrothermal origin, and by heating becomes opaque without melting.

Recent investigations (Huttenlacher, Hügi & Nowacki, 1954) on bazzite of Val Strem (Switzerland)

Table 3. *Positions and weight percentages of constituents*

Hexasilicic rings						W (%)	
	$12(l)$	$(x, y, 0)$	12 Si	$x = 0.367, y = 0.095$.		27.81	
	$12(l)$	$(x, y, 0)$	12 O_I	$x = 0.294, y = 0.214$.		47.54	
	$24(m)$	(x, y, z)	24 O_{II}	$x = 0.489, y = 0.128, z = 0.139$.			
Cations							
	$4(c)$	$(\frac{2}{3}, \frac{1}{3}, \frac{1}{4})$	Sc, Fe, Al, Mg, Mn, (Ti, Sn)–(Y, Yb)			15.70–15.96	(16.00)
	$2(a)$	$(0, 0, \frac{1}{4})$	(Y, Yb)–Na, Ca, K, H_2O			4.72	(4.34)
	$6(f)$	$(\frac{1}{2}, 0, \frac{1}{4})$	Si, (Be)			3.88–4.17	
						99.65–100.20	

Density (obs.) = 2.819 ± 0.002 g.cm.$^{-3}$; density (calc.) = 2.809–2.825 g.cm.$^{-3}$.

give the following spectrographic results: very strong: Be, Si, Al, Mg, Sc (3%); strong: Fe, Na, Ba; medium: Ca, Sr; weak: Cu; very weak: Ga, V, Sn, Yb, Y, Ag. It is noteworthy that the Val Strem bazzite has the same a dimension (9.50 Å) as the Baveno bazzite, but the same c dimension (9.18 Å) as beryl. It is possible that the a dimension of this structure is principally determined by the substituents of Al in the (c) position, whilst the c dimension is more influenced by the substituents of Be in the (f) position and perhaps also, in the Baveno bazzite, by the postulated hydrogen bonds between superposed hexasilicic rings. The shortening of the c axis from 9.19 Å (beryl) to 9.11 Å (Baveno bazzite) should be related in this case to the short observed distance O_{II}–O_{II} = 2.47 Å.

A rough evaluation of the weight percentage (W) of substituents in the three positions (c), (a) and (f), referred to the observed cell atomic weight of 1211.5, can be obtained by their total electron contents, corrected for series termination (Table 2), multiplied by the average atomic weight associated to one electron for each position, according to the postulated cation distribution (Table 3). For position (c) the W value 15.96% includes also the cations Ti and Sn, which can be considered as less abundant or less probable. The value 16.00% corresponds to the transfer of Y and Yb from position (a) to position (c). For position (f) the value 3.88% corresponds to the maximum possible amount of 1.68 Si atoms; the average value 4.17% includes also the maximum possible amount of 6 Be atoms. The average W's for special positions do not change very much (on the average within 1% of the total composition) with other combinations of substituents, so that the values given can be considered as a fairly good approximation. Because of the lack of a complete analytical evaluation of the relative abundance of constituents, and of the multiple pos-

sibilities of isomorphous substitutions, it is very difficult to get reliable informations of the W's of individual cations within the average of each position. To account for the high electron content, 77, of position (c), the presence of Al and perhaps of Mg, with a low ionic number 10, must be compensated by appreciable amounts of Fe (ionic number = 24) or by other cations with higher ionic number, so that the amount of Sc (ionic number = 18) must be substantially reduced. As much as 1% of scandium was found in beryl (Rankama & Sahama, 1950) and about 3% in Val Strem bazzite; it should not be less in Baveno bazzite.

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