

Marinellite, a new feldspathoid of the cancrinite-sodalite group

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Abstract: Marinellite, $[(\text{Na},\text{K})_{42}\text{Ca}_6](\text{Si}_{36}\text{Al}_{36}\text{O}_{144})(\text{SO}_4)_8\text{Cl}_2 \cdot 6\text{H}_2\text{O}$, cell parameters $a = 12.880(2)$ Å, $c = 31.761(6)$ Å, is a new feldspathoid belonging to the cancrinite-sodalite group. The crystal structure of a twinned crystal was preliminarily refined in space group $P31c$, but space group $P\bar{6}2c$ could also be possible. It was found near Sacrofano, Latium, Italy, associated with giuseppettite, sanidine, nepheline, h aüyne, biotite, and kalsilite. It is anhedral, transparent, colourless with vitreous lustre, white streak and Mohs' hardness of 5.5. The mineral does not fluoresce, is brittle, has conchoidal fracture, and presents poor cleavage on $\{001\}$. D_{meas} is $2.405(5)$ g/cm³, D_{calc} is 2.40 g/cm³. Optically, marinellite is uniaxial positive, non-pleochroic, $\omega = 1.495(1)$, $\epsilon = 1.497(1)$. The strongest five reflections in the X-ray powder diffraction pattern are $[d$ in Å (I) (hkl): 3.725 (100) (214), 3.513 (80) (215), 4.20 (42) (210), 3.089 (40) (217), 2.150 (40) (330)]. The electron microprobe analysis gives K_2O 7.94, Na_2O 14.95, CaO 5.14, Al_2O_3 27.80, SiO_2 32.73, SO_3 9.84, Cl 0.87, (H_2O 0.93), sum 100.20 wt %, less O = Cl 0.20, (total 100.00 wt %); H_2O calculated by difference. The corresponding empirical formula, based on 72 (Si + Al), is $(\text{Na}_{31.86}\text{K}_{11.13}\text{Ca}_{6.06})_{\Sigma=49.05}(\text{Si}_{35.98}\text{Al}_{36.02})_{\Sigma=72}\text{O}_{144.60}(\text{SO}_4)_{8.12}\text{Cl}_{1.62} \cdot 3.41\text{H}_2\text{O}$. The crystal structure of marinellite may be described as formed by the stacking along c of 12 layers containing six-membered rings of tetrahedra: the stacking sequence is ABCBCBACBCBC..., where A, B, and C represent the positions of the rings within the layers. Its structure consists of two liottite cages superimposed along $[0, 0, z]$ and of columns of cancrinite and sodalite cages along $[1/3, 2/3, z]$ and $[2/3, 1/3, z]$. Sulphate groups, surrounded by sodium, calcium and potassium cations, occupy the liottite cages. Chlorine anions and sulphate groups occupy the sodalite cages, whereas H_2O molecules are located within the cancrinite cages, bonded to Na cations. This structural model was refined in the space group $P31c$, conventional $R = 0.098$ for 2155 reflections. The structural relationships between marinellite and tounkite are discussed.

Key-words: marinellite, new mineral, Italy, cancrinite-sodalite group, crystal structure.

The cancrinite-sodalite group of minerals

The minerals of the cancrinite-sodalite group are characterised by layers of six-membered rings of tetrahedra, each ring being linked to three rings in a preceding layer and to three rings in a succeeding one, giving rise to a three-dimensional framework. Following the notation of the close-packed structures, the three possible positions of these rings within the layers may be labelled as A, B and C. Therefore, the members of the group are built up by the stacking of A, B and C layers, without repetition of identical layers as neighbours. Formally, they belong to the so-called ABC-6 family of crystal structures (Gies *et al.*, 1999); however, the condition that no repetition of identical layers occurs in the sequence differentiates these minerals from other members of the family, including offretite, erionite, levyne, gmelinite, chabazite, and several other synthetic zeolites.

According to the stacking sequence, three "subgroups" of minerals may be recognised. Several phases occur with the simplest sequences AB... and ABC..., corresponding to the subgroups known as "cancrinite group" and "sodalite group", respectively, whereas the third subgroup includes

trigonal or hexagonal phases showing more complex stacking sequences of layers (Table 1). The known minerals with complex sequences have 4, 6, 8, 10, 12, 16, and 28 layers for c translation; moreover, domains showing 14, 18 and 24 layer sequences were observed in TEM images (Rinaldi & Wenk, 1979; Rinaldi, 1982). All these phases with complex sequences were originally named "cancrinite-like" minerals by Leoni *et al.* (1979), and later on, they were usually grouped together within the "cancrinite group". Such grouping is probably misleading, even because the minerals really belonging to the "cancrinite group" (*i.e.* with AB-AB... stacking sequence) may display themselves supercells, as due to ordering of cations and/or anions within the framework. As a consequence of this somewhat ambiguous classification, minerals with complex stacking sequences such as afghanite, bystrite, franzinite, liottite, and giuseppettite, have been recently described (Gaines *et al.*, 1997) as having a constant aluminosilicate framework and differing "only in the ordering of the cations outside the tetrahedral framework, which leads to the appearance of satellite reflections" (Gaines *et al.*, 1997). The scheme reported in Table 1 should clarify the relationships, as well as the differences,

Table 1. Minerals of the cancrinite-sodalite group.

Sequence AB... (Cancrinite group)	Space group	<i>a</i> (Å)	<i>c</i> (Å)	Chemical formula
cancrinite	<i>P6₃</i>	12.615	5.127	[(Ca,Na) ₆ (CO ₃) _{1-1.7}][Na ₂ (H ₂ O) ₂](Si ₆ Al ₆ O ₂₄)
vishnevite	<i>P6₃</i>	12.685	5.179	[(Na ₆ (SO ₄))[Na ₂ (H ₂ O) ₂](Si ₆ Al ₆ O ₂₄)
hydroxycancrinite	<i>P3</i>	12.740	5.182	[Na ₆ (OH) ₂][Na ₂ (H ₂ O) ₂](Si ₆ Al ₆ O ₂₄)
cancrisilite	<i>P6₃mc</i>	12.575	5.105	Na ₇ Al ₅ Si ₇ O ₂₄ (CO ₃) · 3H ₂ O
pitiglianoite	<i>P6₃</i>	22.121	5.221	[(Na ₄ K ₂)(SO ₄)][Na ₂ (H ₂ O) ₂](Si ₆ Al ₆ O ₂₄)
davyne	<i>P6₃/m</i> or <i>P6₃</i>	12.705	5.368	[(Na,K) ₆ (SO ₄) _{0.5-1} Cl ₁₋₀](Ca ₂ Cl ₂)(Si ₆ Al ₆ O ₂₄)
microsommitte	<i>P6₃</i>	22.142	5.345	[Na ₄ K ₂ (SO ₄)](Ca ₂ Cl ₂)(Si ₆ Al ₆ O ₂₄)
quadridavyne	<i>P6₃/m</i>	25.771	5.371	[(Na,K) ₆ Cl ₂](Ca ₂ Cl ₂)(Si ₆ Al ₆ O ₂₄)
tiptopite	<i>P6₃</i>	11.655	4.692	[(Li _{2.9} Na _{1.7} Ca _{0.7})(OH) ₂ (H ₂ O) _{1.3}](K ₂)(Be ₆ P ₆ O ₂₄)
Sequence ABC... (Sodalite group)	Space group	<i>a</i> (Å)		Chemical formula
sodalite	<i>P4̄3n</i>	8.882		(Na ₈ Cl ₂)(Si ₆ Al ₆ O ₂₄)
häüyne	<i>P4̄3n</i>	9.082		[Na ₆ Ca ₂ (SO ₄) ₂](Si ₆ Al ₆ O ₂₄)
nosean	<i>P4̄3n</i> (<i>P23</i>)	9.090		[Na ₈ (SO ₄)(H ₂ O)](Si ₆ Al ₆ O ₂₄)
lazurite	<i>P4̄3n</i>	9.074		{(Na,Ca) ₈ [(SO ₄),S,Cl,(OH)] ₂ }(Si ₆ Al ₆ O ₂₄)
helvite	<i>P4̄3n</i>	8.291		(Mn ₈ S ₂)(Be ₆ Si ₆ O ₂₄)
genthelvite	<i>P4̄3n</i>	8.120		(Zn ₈ S ₂)(Be ₆ Si ₆ O ₂₄)
danalite	<i>P4̄3n</i>	8.213		(Fe ₈ S ₂)(Be ₆ Si ₆ O ₂₄)
bicchulite	<i>I4̄3m</i>	8.829		[Ca ₈ (OH) ₈](Al ₈ Si ₄ O ₂₄)
tugtupite	<i>I4̄</i>	8.640	<i>c</i> = 8.874	(Na ₈ Cl ₂)(Al ₂ Be ₂ Si ₈ O ₂₄)
tsaregorodsevitte	<i>I222</i>	8.984	<i>b</i> = 8.937 <i>c</i> = 8.927	[N(CH ₃) ₄] ₂ (Si ₁₀ Al ₂ O ₂₄)
Other sequences	Space group	<i>a</i> (Å)	<i>c</i> (Å)	Chemical formula
bystrite (ABAC...)	<i>P31c</i>	12.855	10.700	[(Na,K) ₁₄ Ca ₂](Si ₁₂ Al ₁₂ O ₄₈)(S ²⁻) ₃ · 2H ₂ O
liottite (ABABAC...)	<i>P6̄</i>	12.870	16.096	[(Na,K) ₁₆ Ca ₈](Si ₁₈ Al ₁₈ O ₇₂)(SO ₄) ₅ Cl ₄
afghanite (ABABACAC...)	<i>P31c</i>	12.801	21.412	[(Na,K) ₂₂ Ca ₁₀](Si ₂₄ Al ₂₄ O ₉₆)(SO ₄) ₆ Cl ₆
franzinite (ABCABACABC...)	<i>P321</i>	12.904	26.514	[(Na,K) ₃₀ Ca ₁₀](Si ₃₀ Al ₃₀ O ₁₂₀)(SO ₄) ₁₀ · 2H ₂ O
tounkite (unknown sequence)	<i>P6₂22</i>	12.843	32.239	[(Na,K) ₃₀ Ca ₁₈](Si ₃₆ Al ₃₆ O ₁₄₄)(SO ₄) ₁₂ Cl ₆ · 6H ₂ O
marinellite (ABCBCBACBCBC...)	<i>P6̄2c</i> or <i>P31c</i>	12.880	31.761	[(Na,K) ₄₂ Ca ₆](Si ₃₆ Al ₃₆ O ₁₄₄)(SO ₄) ₈ Cl ₂ · 6H ₂ O
giuseppettite (ABABABACBACBAC...)	<i>P6̄2c</i> or <i>P31c</i>	12.858	42.306	[(Na,K) ₅₈ Ca ₆](Si ₄₈ Al ₄₈ O ₁₉₂)(SO ₄) ₁₀ Cl ₂ · <i>n</i> H ₂ O
sacrofanite (unknown sequence)	<i>P6₃mc</i> , <i>P6̄2c</i> , or <i>P6₃/mmc</i>	12.865	74.240	[Na ₅₃ K ₂₃ Ca ₃₃](Si ₈₄ Al ₈₄ O ₃₃₆)(SO ₄) ₂₆ Cl ₆ · <i>n</i> H ₂ O

occurring among the minerals of the group. In this table, the chemical composition of channel, cages and framework is separately listed for the minerals of the cancrinite subgroup (AB... sequence), whereas the content of the cages is separated from the framework in the minerals belonging to the sodalite subgroup (ABC... sequence).

Occurrence of marinellite

The interest in feldspathoids belonging to the cancrinite-sodalite group induced us to look for crystals of giuseppettite in an ejected volcanic block from Sacrofano, Biacchella

Valley, Latium (Italy), kindly given us by the collector L. Liotti. The specimen is holocrystalline, with crystal sizes of 1 to 2 mm; it represents the product of a syntexis between a trachytic magma and the evaporitic rocks (mainly gypsum and dolomite) that made up the walls of the vent of the magmatic reservoir. Besides giuseppettite, sanidine, nepheline, häüyne, biotite, and kalsilite, we found here another mineral, which revealed to be a new member of the cancrinite-sodalite group. The new mineral was named marinellite, in memory of the late Prof. Giorgio Marinelli (1922–1993) of the Earth Science Department of the University of Pisa. The new mineral species and its name have been approved by the Commission on New Minerals and Mineral Names of the

Table 2. Electron microprobe analysis of marinellite.

Constituent	Wt.%	Range
SiO ₂	32.73(16)	32.20 – 33.11
Al ₂ O ₃	27.80(6)	27.24 – 28.23
CaO	5.14(7)	4.97 – 5.33
Na ₂ O	14.95(19)	14.15 – 15.47
K ₂ O	7.94(8)	7.85 – 7.99
SO ₃	9.84(9)	9.57 – 10.05
Cl	0.87(16)	0.84 – 0.90
H ₂ O(*)	0.93	-
Σ'	100.20	
O=Cl	0.20	
Total	100.00	
Number of atoms on the basis of 72 (Si+Al)		
Si	35.98	
Al	36.02	
Ca	6.06	
Na	31.86	
K	11.13	
S	8.12	
Cl	1.62	
H ₂ O(*)	3.41	

The reported range represents the chemical variation within the crystal, whereas the standard deviations on the weight % of the oxides (numbers in parentheses) indicate the reproducibility of the measures, as obtained for the standard minerals.

(*) The H₂O content was calculated by difference to 100 wt%.

International Mineralogical Association. The specimen containing marinellite was deposited at the Museo di Storia Naturale e del Territorio, University of Pisa (catalogue no. 13216).

Appearance and physical properties

Crystals of marinellite are anhedral, transparent, colourless with vitreous lustre, white streak and Mohs' hardness of 5.5. The mineral does not fluoresce, is brittle, has conchoidal fracture, and presents poor cleavage on {001}. Twinning was not optically observed; a merohedral twinning, with (001) as twinning plane, probably occurs if the correct space group of marinellite is *P*31*c* instead of *P*62*c* (see "Structural determination and refinement").

Optically, marinellite is uniaxial positive, with $\omega = 1.495(1)$ and $\epsilon = 1.497(1)$ (in Na light). It is not pleochroic.

The density of 2.405(5) g/cm³ was obtained by sinking method in heavy liquids, to be compared with the calculated value of 2.40 g/cm³. Calculations using the Gladstone-Dale relationships and the constant reported by Mandarino (1981) indicate superior compatibility: $1 - (Kp/Kc) = -0.014$.

Chemical data

The chemical analysis of marinellite was carried out by means of a wavelength dispersive ARL/SEM-Q electron microprobe. Operating conditions were 15 kV as accelerating voltage and 20 nA as sample current; the beam diameter was

Table 3. Indexed powder pattern of marinellite (Gandolfi camera, CuK α radiation) and comparison between marinellite and tounkite powder patterns.

<i>hkl</i>	Marinellite (this work)			Tounkite (this work)		Tounkite (Ivanov <i>et al.</i> , 1992)	
	<i>d</i> _{obs}	<i>d</i> _{calc}	<i>hkl</i> ₀	<i>d</i> _{obs}	<i>hkl</i> ₀	<i>d</i> _{obs}	<i>hkl</i> ₀
						9.12	1
110	6.41	6.44	25				
105	5.51	5.52	30			5.38	1
106	4.77	4.78	5	4.86	40	4.842	40
210	4.20	4.22	42	4.15	10	4.202	1
212	4.08	4.08	6			4.125	1
213	3.92	3.919	6			3.860	1
214	3.725	3.725	100	3.722	80	3.711	100
215	3.513	3.513	80	3.537	2		
216	3.296	3.298	35	3.325	100	3.314	80
305	3.209	3.210	4	3.228	7	3.220	8
						3.191	9
217	3.089	3.088	40	3.037	60	3.035	20
						2.988	16
307	2.879	2.876	5	2.897	12	2.889	6
315	2.785	2.783	20	2.778	22	2.780	9
						2.763	4
402	2.748	2.749	6			2.747	4
0,0,12	2.645	2.644	30	2.697	65	2.687	25
				2.623	3	2.615	1
405	2.555	2.555	35	2.570	2	2.561	2
				2.532	16	2.515	3
				2.480	20	2.470	16
410	2.441	2.436	4	2.433	4	2.426	2
407	2.377	2.376	6				
				2.299	14	2.298	2
408	2.283	2.282	7			2.285	2
				2.225	5	2.212	1
				2.188	1	2.177	1
330	2.150	2.149	40	2.147	70	2.139	25
4,0,10	2.099	2.095	7	2.110	8	2.099	3
				2.070	16	2.062	4
511	2.001	2.001	2	2.015	4	2.037	2
				1.964	3	1.996	1
						1.958	2
				1.939	20	1.933	4
4,0,12	1.918	1.919	2			1.913	2
516	1.876	1.875	2	1.880	16	1.873	3
						1.854	1
$\bar{3}2$ 12	1.838	1.839	2			1.832	1
4,1,12	1.791	1.791	9	1.809	70	1.801	10
				1.778	8	1.781	1
435	1.762	1.763	3			1.770	1
						1.751	2
				1.738	12	1.731	2
				1.680	3		
				1.658	15	1.650	2
				1.629	9	1.621	2
440	1.612	1.611	4	1.612	16	1.605	4
				1.557	7	1.548	1
6,0,12	1.524	1.522	2	1.531	13	1.525	3
				1.513	16	1.506	2
710	1.479	1.479	1	1.479	7	1.472	2

30 μm . Standards used were: Amelia albite (Si), AB microcline (K, Al), An70 anorthite (Ca), stoichiometric baryte (S), blue sodalite (Na, Cl).

The following formula, recalculated on the basis of 72 (Si + Al), is derived from the chemical data reported in Table 2: $(\text{Na}_{31.86}\text{K}_{11.13}\text{Ca}_{6.06})_{\Sigma=49.05}(\text{Si}_{35.98}\text{Al}_{36.02})_{\Sigma=72}\text{O}_{144.60}(\text{SO}_4)_{8.12}\text{Cl}_{1.62}\cdot 3.41\text{H}_2\text{O}$. It may be simplified as $(\text{Na}_{31}\text{K}_{11}\text{Ca}_6)_{\Sigma=48}(\text{Si}_{36}\text{Al}_{36})_{\Sigma=72}\text{O}_{144}(\text{SO}_4)_8\text{Cl}_2\cdot 6\text{H}_2\text{O}$, where the sum of the extra-framework cations and the number of the water molecules are derived on the basis of the structural data that are reported in a next paragraph.

X-ray diffraction study

Powder X-ray diffraction study

The X-ray powder pattern (Gandolfi technique, $\text{CuK}\alpha$ radiation) of marinellite is reported in Table 3. The indexing of the reflections was performed with the help of the calculated intensities, on the basis of the structural refinement. The following hexagonal unit-cell parameters were obtained by least squares refinement: $a = 12.893(1)$ Å, $b = 31.718(5)$ Å.

Structural determination and refinement

To determine the correct stacking sequence of marinellite, as well as the cationic distribution within its structural cages, an X-ray diffraction data collection was carried out. A colourless transparent crystal ($0.2 \times 0.2 \times 0.3$ mm³) was mounted on a Siemens P4 four-circle automated diffractometer, using graphite-monochromatized $\text{MoK}\alpha$ radiation. The following hexagonal unit cell was obtained through least-square refinements of 25 reflections with $20^\circ < \theta < 25^\circ$: $a = 12.880(2)$ Å, $c = 31.761(6)$ Å. Intensity data were collected in ω -scan mode up to a 2θ value of 60° , and a total of 9544

reflections were measured. Laue symmetry and systematic absences pointed to $P6_3/mmc$, $P6_3mc$ or $P\bar{6}2c$ as possible space groups. The absorption effects were empirically accounted for, on the basis of ψ -scan measurements. Information concerning the data collection and refinement are listed in Table 4.

The structure was solved in the space group $P6_3/mmc$ through direct methods (SHELX-97 package; Sheldrick, 1997). The resulting framework has an ABCBCBACBC-BC... stacking sequence of layers, where the labels A, B and C indicate the position of the six-membered rings within each layer. Following the modified Zhdanov notation (Zhdanov, 1945; Patterson & Kasper, 1959), it may be conveniently described by the symbol $11(4)11(4)11$. The same sequence is described as $(hhhcc)_2$ in the Jagodzinski-Wyckoff notation.

The occurrence of long-range ordering of Si and Al in the tetrahedral sites, in accordance with the Loewenstein rule, was recognised in all the structure refinements of the minerals of the group displaying a ratio Si/Al = 1. Such ordering probably occurs also in marinellite; anyway it cannot be realised in the space group $P6_3/mmc$. The maximal non-isomorphic subgroup of $P6_3/mmc$ that allows the alternation of Si and Al in the tetrahedral sites is $P\bar{6}2c$ but further reductions of symmetry may result due to the ordering of the extra-framework ions.

The structural refinement (by means of the SHELX-97 package; Sheldrick, 1997), assuming a perfect ordering of Si and Al within the tetrahedral sites, was performed both in the space group $P\bar{6}2c$ and $P31c$, in accordance with the indications of the observed systematic absences. In both cases, 4511 unique reflections with $R_{\text{int}} = 0.11$ were used for the refinement of 132 and 247 parameters, respectively. In the space group $P31c$ refinement, the displacement parameters of pseudo-symmetrical framework atoms were constrained to be equal, to avoid correlations among parameters and to reduce the number of variables. The former refinement converged to conventional $R = 0.189$ for 2155 reflections with $F_o > 4\sigma(F_o)$. On the other side, the structural refinement in the space group $P31c$ (assuming the occurrence of a merohedral twinning, with (001) as twin law, and refined twin fraction 0.50(1)), converged to $R = 0.098$ for the same reflections. The Hamilton test (Hamilton, 1965) indicates that the hypothesis for which the correct space group is $P\bar{6}2c$ can be strongly rejected, as it is under the 0.5% significance level.

The average T-O distances obtained in the $P31c$ refinement are 1.63(3) and 1.71(3) Å for Si-centred and Al-centred tetrahedra, respectively, whereas the same averages in the $P\bar{6}2c$ space group gave 1.65(6) and 1.68(6) Å. The numbers in parentheses refer in both the cases to the dispersion of the observed values. It is worth to note that the dispersion of the observed values is much higher in $P\bar{6}2c$ than in $P31c$. In the space group $P\bar{6}2c$, the $\langle \text{Si-O} \rangle$ and $\langle \text{Al-O} \rangle$ distances agree each other within their standard deviations, in contrast with the crystal-chemistry of this group of mineral. Such incongruity disappears if the refinement is carried out in the space group $P31c$.

The decreasing of symmetry from $P\bar{6}2c$ to $P31c$ appears as due mainly to the ordering of sulphate groups and chlo-

Table 4. Crystal and structure refinement data for marinellite.

Space group	$P31c$
Unit cell dimensions	$a = 12.880(2)$ Å $c = 31.761(6)$ Å
Volume	$4563.1(13)$ Å ³
Z	1
Wavelength	0.71073 Å
Crystal size	$0.2 \times 0.2 \times 0.3$ mm ³
θ range for data collection	1.28 to 30.00°
Index ranges	$0 \leq h \leq 17$, $-18 \leq k \leq 0$, $0 \leq l \leq 44$
Reflections collected	9544
Independent reflections	4511 [$R_{\text{int}} = 0.1220$]
Refinement method	Full-matrix least-squares on F^2
Data/restraints/parameters	4511 / 6 / 247
Twin fraction [twin plane (001)]	0.50(1)
Goodness-of-fit on F^2	1.045
Final R indices [$I > 2\sigma(I)$]	$R = 0.098^*$ $wR^2 = 0.254^{**}$
R indices (all data)	$R = 0.202^*$ $wR^2 = 0.346^{**}$

$$*R = \frac{\sum ||F_o| - |F_c||}{\sum |F_o|} \quad **wR^2 = \sqrt{\frac{\sum w(F_o^2 - F_c^2)^2}{\sum wF_o^4}}$$

Table 5. Fractional coordinates and isotropic displacement parameters U (\AA^2) for marinellite.

<i>site</i>	<i>x</i>	<i>y</i>	<i>z</i>	U_{iso}
Ca1	0.0	0.0	0.5256(6)	0.017(3)
Ca1b	0.0	0.0	0.507(1)	0.017(3)
Na4	0.3333	0.6667	0.159(1)	0.022(5)
Na4b	0.3333	0.6667	0.186(1)	0.022(5)
Na5	0.3333	0.6667	0.3783(9)	0.013(4)
Na5b	0.3333	0.6667	0.3553(9)	0.013(4)
Na6	0.6667	0.3333	0.102(2)	0.049(8)
Na6b	0.6667	0.3333	0.065(2)	0.049(8)
Na7	0.6667	0.3333	0.283(1)	0.030(4)
Na7b	0.6667	0.3333	0.247(1)	0.030(4)
Na8	0.6667	0.3333	0.469(1)	0.022(5)
Na8b	0.6667	0.3333	0.452(1)	0.022(5)
Na9	0.019(1)	0.511(2)	0.0161(5)	0.031(3)
Na9b	0.919(2)	0.457(3)	0.0036(6)	0.031(3)
W1	0.31(1)	0.609(5)	0.265(3)	0.09(2)
W2	0.6667	0.3333	0.357(2)	0.06(1)
W3	0.712(5)	0.34(1)	0.185(2)	0.07(2)
Si1	0.2510(7)	0.9984(9)	0.0144(3)	0.009(1)
Si2	0.9171(8)	0.5809(7)	0.0975(3)	0.009(1)
Si3	0.9164(8)	0.5839(8)	0.4302(3)	0.009(1)
Si4	0.5863(8)	0.6698(8)	0.1800(3)	0.009(1)
Si5	0.5850(7)	0.6716(8)	0.3468(3)	0.009(1)
Si6	0.5840(7)	0.9170(7)	0.7634(3)	0.008(2)
Al1	0.7480(8)	0.0022(9)	0.0132(4)	0.011(2)
Al2	0.4110(9)	0.0814(9)	0.0972(4)	0.011(1)
Al3	0.4170(9)	0.0815(9)	0.4297(4)	0.011(1)
Al4	0.5811(8)	0.9241(8)	0.1804(3)	0.008(1)
Al5	0.5798(8)	0.9230(8)	0.3455(3)	0.008(1)
Al6	0.4137(7)	0.0769(7)	0.2637(4)	0.008(2)
O1	0.333(3)	0.013(3)	0.052(1)	0.052(7)
O1b	0.327(3)	0.007(3)	0.471(1)	0.052(7)
O2	0.970(2)	0.639(2)	0.0487(5)	0.009(2)
O2b	0.995(2)	0.688(2)	0.4655(5)	0.009(2)
O3	0.217(1)	0.103(3)	0.0123(5)	0.026(2)
O3b	0.248(1)	0.120(3)	0.5250(5)	0.026(2)
O4	0.418(2)	0.212(3)	0.1062(6)	0.033(3)
O4b	0.453(2)	0.229(3)	0.4300(6)	0.033(3)
O5	0.330(2)	0.356(2)	0.1321(7)	0.013(3)
O5b	0.364(2)	0.343(2)	0.3836(6)	0.013(3)
O6	0.650(3)	0.664(3)	0.135(1)	0.036(5)
O6b	0.659(3)	0.662(3)	0.386(1)	0.036(5)
O7	0.887(2)	0.441(3)	0.0942(5)	0.033(3)
O7b	0.918(2)	0.463(3)	0.4407(5)	0.033(3)
O8	0.665(2)	0.661(2)	0.2171(8)	0.024(4)
O8b	0.647(2)	0.681(2)	0.2999(8)	0.024(4)
O9	0.360(2)	0.330(2)	0.2166(6)	0.013(3)
O9b	0.338(2)	0.354(2)	0.2994(6)	0.013(3)
O10	0.594(1)	0.795(2)	0.1873(4)	0.017(2)
O10b	0.595(1)	0.798(2)	0.3548(4)	0.017(2)
O11	0.432(2)	0.876(2)	0.1826(5)	0.019(2)
O11b	0.427(2)	0.872(2)	0.3468(5)	0.019(2)
O12	0.405(1)	0.205(2)	0.2714(4)	0.020(3)
O13	0.881(1)	0.445(2)	0.2652(6)	0.022(3)
S1	0.0	0.0	0.1163(7)	0.075(6)
OA1	0.0	0.0	0.0703(9)	0.12
OB1	0.072(6)	0.121(4)	0.131(1)	0.04(1)
S2	0.0	0.0	0.2559(4)	0.038(2)
OA2	0.0	0.0	0.3020(7)	0.12
OB2	0.038(6)	0.113(5)	0.232(2)	0.06(1)
OA2b	0.0	0.0	0.2099(7)	0.12
OB2b	0.068(5)	0.115(3)	0.277(1)	0.036(9)
S3	0.0	0.0	0.4092(4)	0.036(3)
OA3	0.0	0.0	0.450(2)	0.12
OB3	0.062(6)	0.121(3)	0.3886(9)	0.076(9)
S4	0.3333	0.6667	0.467(1)	0.11(1)
OA4	0.3333	0.6667	0.421(2)	0.12
OB4	0.40(1)	0.62(1)	0.491(3)	0.10(3)
OA4b	0.3333	0.6667	0.513(2)	0.12
OB4b	0.463(4)	0.727(8)	0.444(1)	0.04(1)
Cl5	0.372(2)	0.667(3)	0.0589(9)	0.043(7)
K1	0.2320(8)	0.1159(9)	0.1808(3)	0.050(3)
K2	0.2302(6)	0.1164(9)	0.3391(2)	0.035(2)
Na1	0.201(4)	0.401(2)	0.0856(7)	0.039(3)
Na1b	0.160(2)	0.316(1)	0.1001(4)	0.039(3)
Na2	0.6882(7)	0.844(2)	0.2608(4)	0.031(2)
Na3	0.153(2)	0.839(2)	0.4259(3)	0.020(2)

rine anions within the sodalite cages. In the space group $P\bar{6}2c$, in fact, the four sodalite cages occurring in the unit cell of marinellite are all symmetry equivalent, and the structural refinement in that space group implies a statistical distribution of sulphate groups and chlorine anions within these cages (the chemical analysis points to the occurrence of 2.12 (SO_4) and 1.62 Cl in the four sodalite cages). The ordering of these two different anions within the four cages is possible in the space group $P31c$, where the symmetry plane at $z = 1/4$ does not occur. The hexagonal Laue symmetry, on the other part, could be due to the occurrence of the twinning plane (001). The structure refinement in the space group $P31c$ supports this conclusion. In fact, the examination of the ΔF map pointed to the occurrence of several electron density maxima in two of the sodalite cages, resembling a sulphate group (S4) in two possible orientations (up and down, respectively), and of a unique large maximum in each of the other two cages, corresponding to a chlorine anion (Cl5).

Taking into account these results and the general improvement of the refinement in the space group $P31c$, as indicated by the significantly lower conventional R factor as well as by the better average tetrahedral distances and displacement parameters, we suggest that the space group of marinellite is $P31c$, and that the observed hexagonal Laue symmetry is due to the (001) twinning. Anyway, the complexity of the examined structure, the occurrence of twinning and positional disorder, and the consequent relatively high standard deviations obtained for the structural parameters require further investigations in order to obtain a definite conclusion about the correct space group.

In both the refinements it was not possible to refine temporarily the position and displacement parameters of some oxygen atoms belonging to the sulphate groups. The displacement parameters of these atoms were held fixed, and the positions of some of them were restrained to give reasonable S-O distances. The distribution of the cations is extremely complex, with splitting of the cationic sites, as commonly observed in this kind of minerals. In some cases it was possible to attribute a well definite cationic content to

Table 6. Selected bond distances (Å) involving the framework oxygen atoms in marinellite.

Si1-O1	1.55(3)	Si2-O7	1.64(4)	Si3-O7b	1.60(4)	Si4-O10	1.59(3)
Si1-O3	1.59(3)	Si2-O5	1.69(2)	Si3-O4b	1.63(4)	Si4-O8	1.59(3)
Si1-O3b	1.62(4)	Si2-O4	1.62(4)	Si3-O5b	1.66(2)	Si4-O11	1.63(3)
Si1-O1b	1.67(4)	Si2-O2	1.70(2)	Si3-O2b	1.65(2)	Si4-O6	1.66(3)
average	1.61	average	1.66	average	1.64	average	1.62
Si5-O10b	1.59(3)	Si6-O13	1.61(3)	Al1-O2	1.68(2)	Al2-O4	1.67(4)
Si5-O11b	1.62(3)	Si6-O12	1.60(3)	Al1-O2b	1.68(2)	Al2-O7	1.68(4)
Si5-O6b	1.61(3)	Si6-O9	1.65(2)	Al1-O3b	1.73(4)	Al2-O6	1.65(4)
Si5-O8b	1.66(3)	Si6-O9b	1.63(2)	Al1-O3	1.74(3)	Al2-O1	1.71(3)
average	1.62	average	1.62	average	1.71	average	1.68
Al3-O7b	1.68(4)	Al4-O11	1.70(3)	Al5-O5b	1.67(2)	Al6-O12	1.73(3)
Al3-O4b	1.72(4)	Al4-O9	1.71(2)	Al5-O9b	1.68(2)	Al6-O13	1.73(3)
Al3-O6b	1.74(3)	Al4-O5	1.71(2)	Al5-O11b	1.74(3)	Al6-O8	1.76(3)
Al3-O1b	1.69(4)	Al4-O10	1.76(3)	Al5-O10b	1.74(3)	Al6-O8b	1.77(3)
average	1.71	average	1.72	average	1.71	average	1.75
K1-O9	2.65(2)	Na1-O5	2.50(5)	Na2-O8b	2.26(3)	Na4-O11	2.46(2) x 3
K1-O2	2.70(3)	Na1-O3b	2.57(3)	Na2-O9b	2.46(3)	Na4b-O11	2.34(2) x 3
K1-O6	2.98(4)	Na1-O1	2.64(5)	Na2-O10	2.56(2)	Na4b-O10	2.91(1) x 3
		Na1-O6	2.68(5)	Na2-O8	2.62(3)		
		Na1-O2	2.87(4)	Na2-O9	2.88(3)		
K2-O12	2.90(1)	Na1b-O5	2.23(3)	Na3-O2b	2.36(3)	Na5-O11b	2.50(2) x 3
K2-O5b	2.91(2)	Na1b-O6	2.41(4)	Na3-O10b	2.48(2)		
K2-O6b	2.94(3)	Na1b-O3b	2.51(2)	Na3-O6b	2.56(4)	NaSb-O11b	2.31(2) x 3
K2-O9b	2.94(2)	Na1b-O1	2.72(4)	Na3-O1b	2.63(4)	NaSb-O10b	2.92(1) x 3
K2-O8b	2.98(3)	Na1b-O10	2.95(2)	Na3-O5b	2.80(3)		
		Na1b-O2	2.98(3)	Na3-O3	2.95(2)		
Na6-O7	2.47(2) x 3	Na8-O4b	2.68(3) x 3	Na9-O2	2.28(3)	Na9b-O2	2.54(4)
Na6-O4	2.77(2) x 3	Na8-O7b	2.94(2) x 3	Na9-O7b	2.50(2)	Na9b-O1b	2.65(5)
				Na9-O1	2.56(4)	Na9b-O7b	2.70(2)
Na6b-O7	2.63(3) x 3	NaBb-O4b	2.48(2) x 3	Na9-O1b	2.71(4)	Na9b-O1	2.79(5)
		Na8b-O7b	2.83(2) x 3	Na9-O7	2.88(2)	Na9b-O2b	2.94(4)
Na7-O13	2.46(1) x 3			Na9-O2b	2.93(3)	Na9b-O7	2.90(2)
Na7-O12	2.95(1) x 3						
Na7b-O13	2.47(2) x 3			Ca1-O3	2.46(2) x 3	Ca1b-O3	2.43(2) x 3
				Ca1-O3b	2.77(2) x 3	Ca1b-O3b	2.82(2) x 3

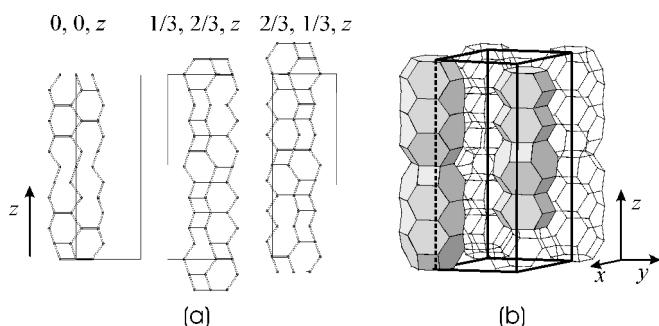


Fig. 1. (a) Schematic drawing of the framework of marinellite, as seen along $[100]$. For sake of simplicity, the columns of cages superimposed along $[0, 0, z]$, $[1/3, 2/3, z]$ and $[2/3, 1/3, z]$ are separately shown. (b) Connection of the different cages in the unit cell of marinellite. The polyhedral cages along $[0, 0, z]$ and $[1/3, 2/3, z]$ are emphasised.

each of the split sites: for example, the Na1 site is probably occupied by sodium cations, whereas the Na1b site hosts a calcium cation. In other cases, following the procedure de-

scribed in the previous works on liottite (Ballirano *et al.*, 1996), afghanite (Ballirano *et al.*, 1997) and franzinite (Ballirano *et al.*, 2000), we refined the occupancy of the split cationic sites (Ca1-Ca1b, Na9-Na9b) in terms of the scattering power of Ca; successively, we calculated the actual cationic content as percentages of Na and Ca cations, assuming the full occupancy of each set of split sites. A minor substitution of Na cation in the K2 site has been assumed, on the basis of the refined occupancy.

The final positional and displacement parameters in space group $P31c$ are reported in Table 5, whereas selected bond distances are listed in Table 6. For sake of clarity, the extra-framework cation-anion distances are reported near to the corresponding figures. The occupancies of all the extra-framework sites are reported in Table 7.

Description of the crystal structure

The marinellite framework shows an ordered distribution of Si and Al, as indicated by the average T-O distances, 1.63 and

Table 7. Population of all the extra-framework sites.

Site	Occupancy	Multi- plicity	Cell content	Na atoms	Ca atoms	K atoms	Site	Occ.	Mult.
K1	100% K	6	6 × 1 K			6	S1	100% S	2
K2	91% K	6	6 × (0.79K+0.21Na)	1.26		4.74	OA1	100% O	2
Na1	50% Na	6	6 × (0.50Ca+0.50Na)	3.00	3.00		OB1	100% O	6
Na1b	50% Ca						S2	100% S	2
Na2	100% Na	6	6 × 1 Na	6			OA2	50% O	2
Na3	100% Na	6	6 × 1 Na	6			OB2	50% O	6
Na4	50% Na	2	2 × 1 Na	2			OA2b	50% O	2
Na4b	50% Na						OB2b	50% O	6
Na5	50% Na	2	2 × 1 Na	2			S3	100% S	2
Na5b	50% Na						OA3	100% O	2
Na6	50% Na	2	2 × 1 Na	2			OB3	100% O	6
Na6b	50% Na						S4	100% S	2
Na7	50% Na	2	2 × 1 Na	2			OA4	50% O	2
Na7b	50% Na						OB4	50% O	6
Na8	50% Na	2	2 × 1 Na	2			OA4b	50% O	2
Na8b	50% Na						OB4b	50% O	6
Na9	37% Ca	6	6 × (0.31Ca+0.69Na)	4.13	1.87		Cl5	100% Cl	2
Na9b	32% Ca						W1	33% O	6
Ca1	54% Ca	2	2 × (0.58Ca+0.42Na)	0.84	1.16		W2	100% O	2
Ca1b	27% Ca						W3	33% O	6
Total				31.23	6.03	10.74			
Microprobe analysis				31.86	6.06	11.13			

1.71, respectively. The framework of marinellite is formed by two symmetry equivalent liottite cages, superimposed along $[0, 0, z]$, and by columns of base-sharing cancrinite cages and sodalite cages, along $[1/3, 2/3, z]$ and $[2/3, 1/3, z]$, as indicated in Fig. 1. Within these cages, extra-framework ions are located. The cancrinite cages host chains of H₂O molecules and sodium cations, whereas the sodalite cages host either sulphate groups or chlorine anions, surrounded by (Na, Ca) cations. Each liottite cage contains three sulphate groups, surrounded by three Na cations at the same z height, whereas three (K, Na) cations are placed in the intermediate z levels. Positional disorder involves nearly all the extra-framework cations and anions, as well as the H₂O molecules.

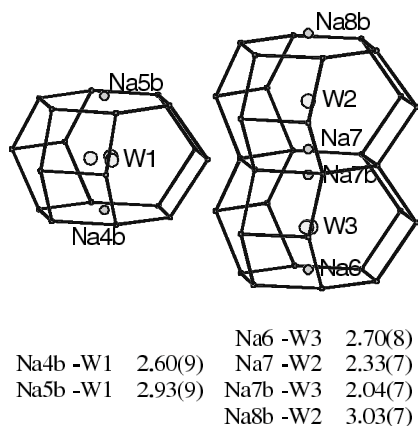


Fig. 2. Cancrinite cages in marinellite structure. The bond distances (in Å) between extra-framework atoms are indicated.

The chemical formula which results from the structural refinement is $(\text{Na}_{31}\text{K}_{11}\text{Ca}_6)_{\Sigma=48}(\text{Si}_{36}\text{Al}_{36}\text{O}_{144})(\text{SO}_4)_8\text{Cl}_2 \cdot 6\text{H}_2\text{O}$, in good agreement with the chemical analysis.

Cancrinite cages

The three symmetrically independent cancrinite cages are drawn in Fig. 2. Two of them share a common base, whereas

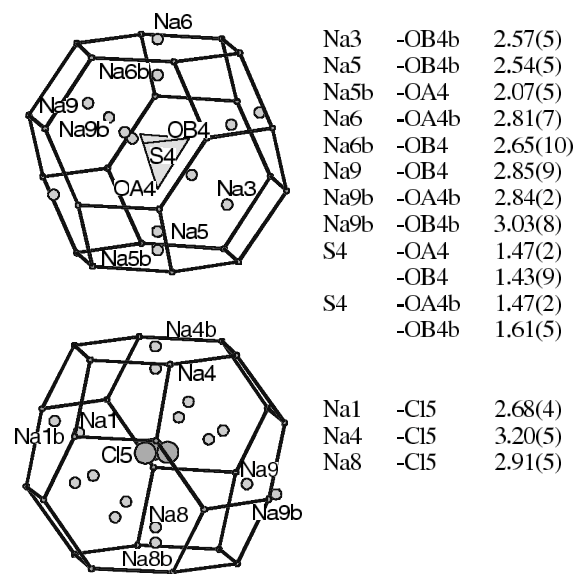


Fig. 3. Sodalite cages in marinellite structure. Only one of the two possible orientations of the S4 group is shown. The bond distances (in Å) between extra-framework atoms are indicated.

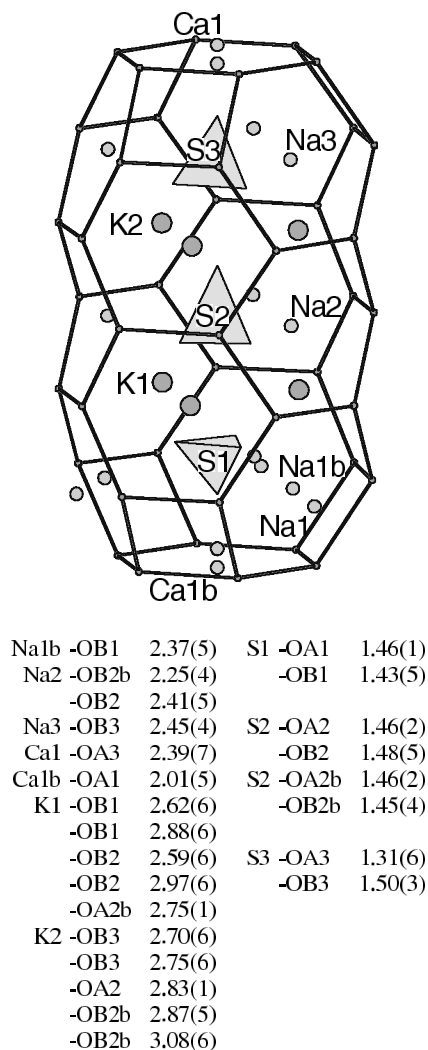


Fig. 4. Liottite cage in marinellite structure. Only one of the two possible orientations of the S2 group is shown. The bond distances (in Å) between extra-framework atoms are indicated.

the third shares both its bases with two sodalite cages. All they host H₂O molecules strongly bonded to one Na cation and weakly bonded to a second Na cation on the other side, in a similar way to what occurs in cancrinite (Jarchow, 1965), vishnevite (Hassan & Grundy, 1984), pitiglianoite (Merlino *et al.*, 1991), and franzinite (Ballirano *et al.*, 2000).

Sodalite cages

The two symmetrically independent sodalite cages are depicted in Fig. 3. The results of the structural refinement in the space group *P31c* point to an ordering of (SO₄)²⁻ groups and Cl⁻ anions within these cages, in a similar way to the ordering of (SO₄)²⁻ groups and H₂O molecules in nosean (Hassan & Buseck, 1989). The chlorine anion Cl5 is slightly displaced from the three-fold axis, towards the Na1 site; in this way, it forms two strong bonds with the sodium cations Na1 and Na8 (bond distances 2.68 Å and 2.91 Å, respectively).

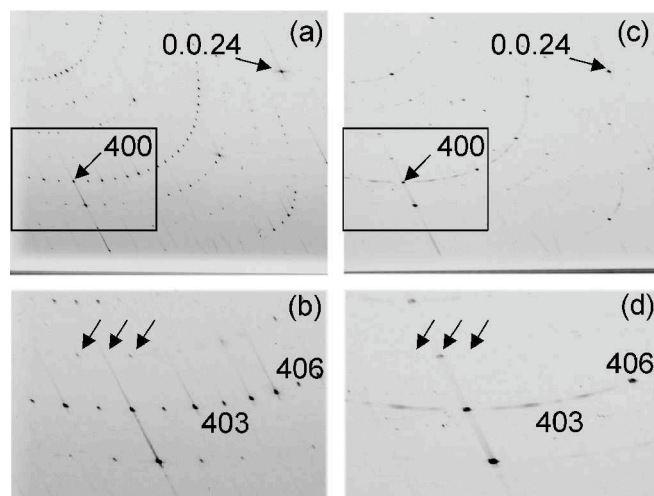


Fig. 5. Parts of (*h0l*) Weissberg photographs for marinellite (a, b) and tounkite (c, d). In (a) and (c) the positions of the (400) and (0.0.24) reflections were marked for reference. In the enlarged views, (b) and (d), some noticeable differences in the intensity and shape of the reflections are outlined.

Liottite cage

The liottite cage (Fig. 4) contains three sulphate groups; one of them (S2) may statistically assume two different orientations. Three Na cations are located around each sulphate group. The Na cations around the S1 group are distributed into two split sites, Na1 and Na1b. Such splitting may be due to the occurrence of the chlorine anion Cl5 into the neighbour sodalite cage, which may itself occupy three symmetrically equivalent positions. As regards the cationic sites located between the sulphate groups, they host mainly K cations and a minor fraction of Na cations (Table 7). The atomic distribution inside the liottite cage closely resembles that occurring in liottite structure (Ballirano *et al.*, 1996).

Discussion

The minerals of the cancrinite-sodalite group display a more or less complex sequence of layers. As reported in Table 1, many minerals have an ABAB... stacking sequence (cancrinite subgroup), and many others display the well known sequence ABC... (sodalite subgroup). Several other phases exist, which show more complex sequences of layers and, consequently, parameters *c* that are multiples of the basic *c* parameter of cancrinite. From a theoretical point of view, the number of possible ways of stacking layers greatly increases with the number *N* of the layers themselves (Patterson & Kasper, 1959). However, up to now, phases having equal *c* parameters (and therefore equal number *N* of layers) but different stacking sequences were not found for *N* > 3, in the cancrinite-sodalite group. On the contrary, the mineral we studied has the same number of layers of tounkite (Ivanov *et al.*, 1992), as indicated by their similar *c* parameters, but a definitely different crystal structure. We guessed that by comparing the intensity of the (*hkl*) reflections of the two

minerals, as the crystal structure of tounkite is yet unknown. This evaluation has been performed both on the powder patterns (Table 3), and on (*0kl*) Weissenberg photographs (Fig. 5), as well as on the whole set of intensity data, collected by us for both the minerals.

In Table 3 the Gandolfi pattern of marinellite is compared with both the Gandolfi pattern we collected from a crystal of tounkite (kindly given us by Dr. Saposhnikov, who formerly described the mineral; Ivanov *et al.*, 1992) and the published powder pattern of tounkite (Ivanov *et al.*, 1992), respectively. In order to evaluate the intensities of both the Gandolfi patterns, and to compare them, the films were scanned and the data were transformed in a file containing *I* vs. 2θ , by means of the program X-ray (Nguyen & Jeanloz, 1993). Finally, the positions and the areas of the peaks were found through a fitting program. The differences between the first (marinellite) and the second (tounkite) couple of columns of Table 7 are remarkable.

The different intensities of the reflections are well detectable also in the (*0kl*) Weissenberg photographs, partially reported in Fig. 5. Anyway, a definitive check was carried out by collecting the X-ray diffraction intensities from a single crystal of tounkite, through a conventional automated 4-circle diffractometer as well as in the X-ray Diffraction Beamline at the Elettra synchrotron facility. The latter collection was performed on a very small crystal, to avoid the possible occurrence of twinning or mixed phases. Any trial to refine the positional parameters of the marinellite-like framework using the collected tounkite intensity data failed, as the conventional reliability index *R* never decreased below 45%.

All these data indicated that the stacking sequences of layers in marinellite and tounkite are different. It is worth to note that the proposed space group of tounkite, $P6_22$ (Ivanov *et al.*, 1992), not only is incompatible with the stacking sequence that we determined for marinellite, but also with all the other 41 possible ordered sequences of 12 layers, having hexagonal or trigonal symmetry (Patterson & Kasper, 1959).

Conclusions

Although the structural investigation on marinellite is still in progress, the reported preliminary results clearly indicate that the framework of marinellite is topologically different from those of all the other members of the cancrinite-sodalite group, giving rise to a different arrangement of structural cages. The framework of marinellite is composed by columns of liottite cages along $[0, 0, z]$ and columns of sodalite and cancrinite cages along $[1/3, 2/3, z]$ and $[2/3, 1/3, z]$. The distribution of the anions and cations within these cages is in agreement with the crystal chemistry of the cancrinite-sodalite group of minerals.

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