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THE CRYSTAL CHEMISTRY OF SARCOLITE

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ABSTRACT

Physical, crystallographic and chemical data are given for sarcolite in contact metamorphic ejecta from Monte Somma (type locality) and from a second occurrence at Anguillara Sabazia in the Sabatini Mountains, Latium (Italy). The chemical composition can be expressed by the general formula: $(Ca,Na)_7(Na,K,Sr,Ti,Mn)_{\leq 1}(Al,Mg,Fe)_4 Si_6O_{23}[(P,Si)O_4]_{0.5}$ $[(CO_3)_a(SO_4)_bCl_c]_{0.5}(OH,F,H_2O)_{2-a-2b}$; the presence of SO_4 distinguishes the sarcolite from Anguillara Sabazia. There are two types of sarcolite at Monte Somma, one with low P and the other richer in P. Unit-cell parameters are *a* 12.378(1), *c* 15.480(8) Å for a sample from Anguillara Sabazia. For the Monte Somma samples *a* is constant at 12.350 Å, but *c* ranges from 15.453 (low-P type) to 15.477 Å (P-rich type). The Monte Somma samples have a smaller volume and a greater density. The IR spectra show clear differences in the material, owing to the vibrations of the CO_3 group, present only in the Monte Somma samples, and the SO_4 group, present only in Anguillara Sabazia samples. Sarcolite coexists with augite, hauyne and fluorite at Anguillara Sabazia, and augite, gehlenite and garnet at Monte Somma.

Keywords: sarcolite, framework silicate, physical data, chemical composition, infrared spectra, Anguillara Sabazia (Latium), Monte Somma, Italy.

SOMMAIRE

On décrit, au moyen de données physiques, cristallographiques et chimiques, la sarcolite des lithologies montrant un métamorphisme de contact, en inclusion dans les laves de Monte Somma (localité type) et d'un deuxième gisement, à Anguillara Sabazia, dans les montagnes Sabatini, au Latium (Italie). Sa composition chimique correspond à la formule générale $(Ca,Na)_7(Na,K,Sr,Ti,Mn)_{\leq 1}(Al,Mg,Fe)_4$ $Si_6O_{23}[(P,Si)O_4]_{0.5}[(CO_3)_a(SO_4)_bCl_c]_{0.5}(OH,F,H_2O)_{2-a-2b}$. La présence du SO_4 distingue la sarcolite de Anguillara Sabazia. On trouve deux types de sarcolite à Monte Somma, l'un pauvre en P, et l'autre, plus riche. Les paramères réticulaires d'un échantillon de Anguillara Sabazia sont *a* 12.378(1), *c* 15.480(8) Å. Pour les échantillons de Monte Somma, le paramètre *a* est constant à 12.350 Å, mais *c* varie de 15.453 (variété pauvre en P) à 15.477 Å (variété riche en P); ceux-ci ont un plus petit volume et une plus grande densité. Les spectres d'absorption infrarouge montrent de nettes différences parmi les échantillons, qui sont le résultat de la présence des groupes CO_3 dans les seuls échantillons de Monte Somma, et des groupes SO_4 dans l'échantillon de Anguillara Sabazia. La sarcolite coexiste avec augite, hauyne et fluorine dans ce gisement, et augite, gehlenite et grenat à Monte Somma.

(Traduit par la Rédaction)

Mots-clés: sarcolite, tectosilicate, données physiques, composition chimique, spectre d'absorption infrarouge, Anguillara Sabazia (Latium), Monte Somma, Italie.

INTRODUCTION

Sarcolite was discovered by G. Thomson in 1807 in the "erratic lavas" of Monte Somma (Breislak 1818); it was considered to be a flesh-colored variety of analcime (Haüy 1822), partly because of its very distinct pseudocubic habit. In 1824 Brooke showed that sarcolite is tetragonal and belongs to the dipyramidal class (Zambonini 1935). The remaining doubt about the validity of sarcolite as a mineral species was resolved only after the crystallographic and morphological studies by Brooke (1831), Des Cloizeaux (1844) and De Fonseca (1846), who carefully considered results of the first chemical analysis made by Scacchi (1842).

The classification of sarcolite was a disputed question; at first it was considered a feldspathoid (Haüy 1822), then it was placed in the melilite group (Berman 1929) and, later, in the scapolite group (Gossner & Mussgnug 1928, Strunz 1941, 1978) because of its chemical resemblance to the marialite–meionite series. This rare species seems to have been found only at Monte Somma (Campania) and Anguillara Sabazia (Latium) (see below); in fact, the other occurrences of sarcolite mentioned in the literature [Vicentino: Vauquelin (1807, in Dana 1875), Valle dell'Allochet, Monti Monzoni: Braccio (1951)] are different minerals: the first is gmelinite, and the second, a cluster of various minerals found as a pseudomorph of quartz (Gramaccioli 1975). Giuseppetti *et al.* (1977) determined the structure of sarcolite on type material from Monte Somma.

Strüver (1885) discovered sarcolite in a single large block of contact-metamorphic ejecta that contains, in addition to sarcolite, dark green fassaitic pyroxene, garnet, wollastonite and accessory minerals, between Anguillara Sabazia and Martignano Lake, Latium. As the crystallographic and chemical data available to date have been obtained only on specimens from the type locality at Monte Somma, we decided to re-examine this species. The comparison between the specimen from Anguillara Sabazia and those from Monte Somma confirms Strüver's identification and excludes the possibility of a mislabeling or incorrect locality. In fact, some chemical differences can be documented between the specimens from the two localities.

TABLE 1. X-RAY POWDER DIFFRACTION DATA FOR SARCOLITE

ANGUILLARA SABAZIA		MONTE SOMMA					PDF 17-754	
		7501		7515				
d(Å)	I/I	d(Å)	I/I	d(Å)	I/I	h k l	d(Å)	I/I
6.186	11	6.181	14	6.193	15	2 0 0	6.19	30
5.805	6	5.770*	5	5.811*	6	1 1 2	5.78	5
5.225*	9	5.202	8	5.196	7	2 1 1	5.22	10
4.836	52	4.823	28	4.835	40	2 0 2	4.83	50
4.375	15	4.365	13	4.375	16	2 2 0	4.37	20
3.987	20	3.974	20	3.986	23	3 0 1	3.97	30
3.913	34	3.907	20	3.912	23	3 1 0	-	
-		-		-		0 0 4	3.90	30
3.774	15	3.768	9	3.777	11	2 1 3	-	
-		3.485	6	3.493	8	3 1 2	-	
3.352	78	3.343	90	3.346	91	3 2 1	3.34	80
3.281	50	3.274	46	3.278	45	2 0 4	3.28	40
3.223	40	3.215	51	3.222	55	3 0 3	3.21	50
3.005	19	2.998	51	3.003	21	1 0 5	3.00	20
2.946	86	2.941	64	2.943	66	4 1 1	2.94	60
2.900	37	2.892	23	2.898	19	2 2 4	-	
2.876*	28	-		-		4 0 2	2.89	10
2.857	82	2.853	87	2.857	80	3 2 3	2.85	70
2.764*	75	2.762	69	2.764	74	4 2 0	-	
2.752	100	2.747	100	2.750	100	3 1 4	2.75	100
2.730	20	2.724	20	2.726	17	3 3 2	-	
2.702	42	2.697	46	2.699	42	2 1 5	2.70	40
2.606	18	-		-		4 2 2	2.643	5b
2.595	26	2.589	20	2.593	23	4 1 3	-	
2.579	24	2.577	15	2.580	17	0 0 6	2.586	30
2.474	6	2.473	5	2.474	6	305,116	2.475	5
2.418	9	2.412	4	2.415	5	4 0 4	2.414	5
-		-		-		2 0 6	2.378	5
2.273	17	2.268	11	2.270	11	5 2 1	2.269	10
2.251	41	2.247	46	2.248	38	4 2 4	2.247	50
2.232	13	-		2.229	8	4 3 3	-	
-		-		-		503,226	2.228	5
2.156	21	2.150	23	2.152	19	415,316	2.153	30
-		2.102	8	2.101	13	4 4 2	-	
2.100	21	2.095	27	2.096	19	5 2 3	2.098	40
2.018	10	2.014	5	2.013	6	6 1 1	-	
1.981	4	-		-		4 0 6	-	
1.957	17	1.953	22	1.953	19	6 2 0+	1.954	30
1.935	56	1.931	35	1.933	47	0 0 8+	1.933	40
-		-		1.929*	30	3 3 6	-	
1.888	5	-		-		4 2 6	-	
1.860	13	1.857	8	1.857	11	534,327+	1.859	20
1.846	23	1.842	20	1.843	15	5 2 5+	1.843	30
1.832	6	-		1.829	6	6 3 1+	1.829	45
1.811	13	1.807	17	1.807	15	5 4 3+	1.808	30
1.780	26	1.777	18	1.778	23	4 1 7+	1.780	30
1.768	6	-		-		5 1 6	-	
1.758	6	1.753	8	1.753	8	7 0 1	-	
1.751	9	-		1.748	13	5 5 0+	1.750	20
1.735	13	1.732	13	1.733	17	3 1 8+	1.734	20
1.717	9	-		1.713	6	6 4 0+	1.713	10
-		1.697	6	-		6 1 5+	1.698	5
1.673	14	1.669	15	1.670	17	7 0 3+	1.669	40
1.669	15	-		1.667	17	4 4 6	-	
1.649	9	-		1.648	6	4 3 7+	1.647	5
-		-		-		545,536+	1.637	20
1.625	44	1.622	13	1.623	6	7 3 0	-	
1.594	17	1.591	14	1.592	23	527,554	-	

Anguillara Sabazia	M(20)=28.67	F(30)=48.27
Monte Somma 7501	M(20)=41.63	F(30)=54.10
Monte Somma 7515	M(20)=18.50	F(30)=31.61

* not used in cell refinement as exceeding the tolerance 0.03° 2 theta; + not indexed in the PDF 17-754 card.

MATERIALS AND METHODS

Four samples from the Monte Somma – Vesuvius area and two from Anguillara Sabazia in the Sabatini volcanic complex (Latium, Italy) were investigated. All are from the collection of the Mineralogical Museum of the University of Rome. The samples from Monte Somma (7501, 7504, 7506, 7515) are from the Spada collection, listed as donated to him personally by Scacchi. The specimens from Anguillara Sabazia (17507, 17509) are part of the block found by Strüver.

The samples from both localities consist of euhedral crystals. Those from Monte Somma are flesh-colored and transparent; the crystals from Anguillara Sabazia are paler, less transparent and covered by a thin film of an unidentified product of alteration. A detailed X-ray-diffraction analysis led to the identification of the mineral association typical of the two localities: augite, haüyne and fluorite in the sample from Anguillara Sabazia, and augite, gehlenite and garnet in those from Monte Somma. Both assemblages are typical of contact-metamorphosed ejecta commonly found in both volcanic areas. The assemblage at Monte Somma suggests a temperature of formation a little higher than the assemblage at Anguillara Sabazia. This temperature, however, cannot be lower than 475°C, as haüyne is present (Van Peteghem & Burley 1962).

Indices of refraction were measured with the temperature-variation method using immersion liquids and monochromatic light (Na). The data obtained [Anguillara Sabazia: ϵ 1.612(2), ω 1.601(1); Monte Somma 7515: ϵ 1.611(4), ω 1.604(1); Monte Somma 7501: ϵ 1.613(2), ω 1.604(1)] are in agreement with those given by Ramdohr & Strunz (1978): ϵ 1.615, ω 1.604.

Density was measured using both tetrabromoethane and Clerici solution. In the former case a pychnometer was used to confirm the density of the liquid, and in the latter, the refractometer used was calibrated according to the data of Vassar (1925).

Cell parameters were calculated by means of the Hubbard *et al.* (1982) program, using as starting data the diffraction maxima measured from powder patterns obtained at ¼°2θ/min rate on a Philips PW 1050 high-angle vertical diffractometer, with Ni-filtered Cu radiation. The diffractogram, recorded at a speed of 1 cm/min, was measured twice and corrected graphically for shift against Si as an internal standard. The trial values of the cell parameters were obtained by automatic single-crystal diffractometer, while indexing proceeded automatically through at least 4 cycles of refinement.

Electron-microprobe analyses were performed both on a Cambridge Geoscan (WDS) and a JEOL JSM-50A, using a Link energy-dispersion system. In both cases natural standards were used: orthoclase, wollastonite, rutile, olivine, celestine, silvite, apatite, jadeite, diopside and fluorite.

Infrared-absorption spectra were taken on a Perkin-Elmer 983 spectrometer using a 200 mg KBr disk containing 1 mg of sarcolite at a scanning time of 6 min. The region between 4000 and 1500 cm^{-1} was scanned at a lower speed (12 min). The KBr used had been previously heated in an oven at 200°C. The prepared disks were stored in a desiccator for 3 days before the analysis.

Thermogravimetric analyses were carried out on a Dupont Instrument. The experiments were performed in flowing air with a thermal gradient of 10°C/min in the 25–960°C temperature range, using about 10 mg of powder.

TABLE 2. PHYSICAL DATA FOR SARCOLITE

sample	a(Å)	c(Å)	V(Å^3)	Dx	Dm
ANGUILLARA SABAZIA	12.378(1)	15.480(8)	2371.8	2.89	2.91(4)
MONTE SOMMA 7501	12.350(8)	15.453(6)	2356.9	2.82	2.92(4)
MONTE SOMMA 7515	12.350(5)	15.477(8)	2360.6	2.90	2.96(2)
MONTE SOMMA GIUSEPPETTI et al.(1977)	12.343(5)	15.463(5)	2355.8	2.89	2.92

Density in g/cm^3.

X-RAY AND PHYSICAL DATA

The X-ray powder patterns of sarcolite from both Anguillara Sabazia and Monte Somma are compared with the standard pattern (PDF 17-754) in Table 1. Small differences can be observed. The Anguillara Sabazia specimen shows two fairly strong peaks at 2.876 and 2.606 Å. The Monte Somma samples show two weak peaks at about 3.48 ± 0.01 and 2.101 ± 0.001 Å, whereas the Monte Somma sample 7515 has a supplementary peak at 1.929 Å. The comparison with the PDF card, which refers to a sample from Monte Somma examined using a Debye-Scherrer camera, is satisfactory, although some weak

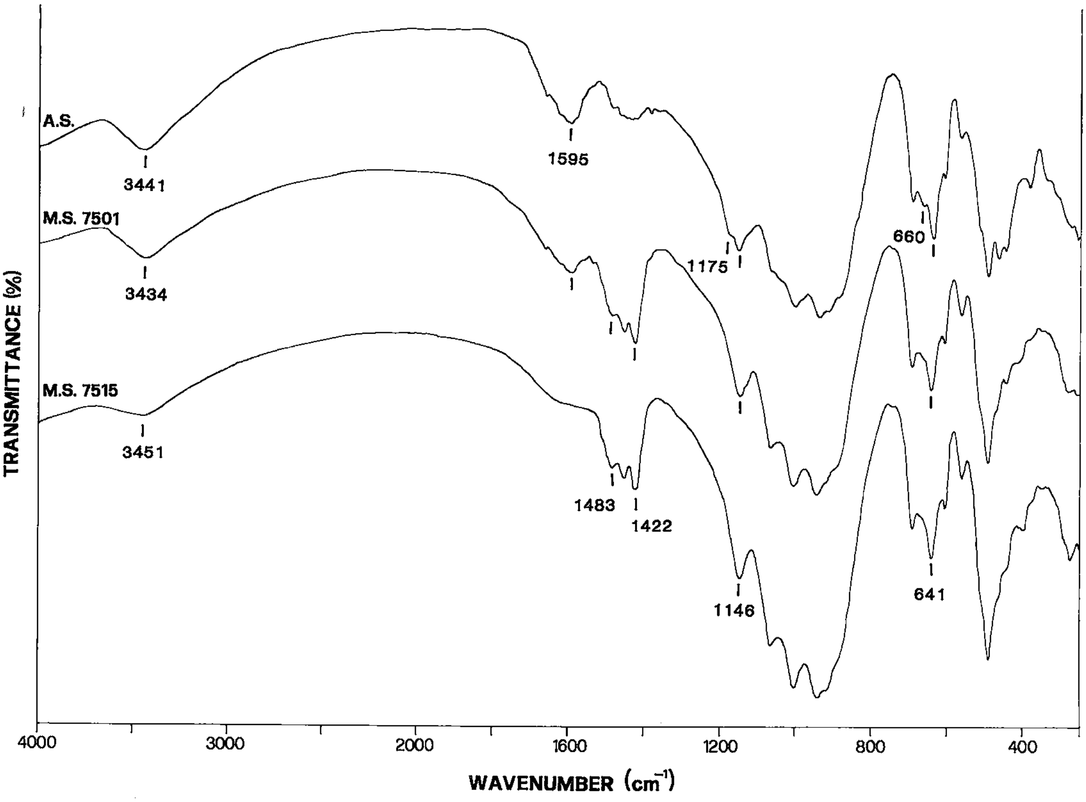

FIG. 1. Infrared absorption spectra for sarcolite (M.S.: Monte Somma, A.S.: Anguillara Sabazia).

lines had not been detected and indexing stopped at 2.098 Å. Furthermore, the peak at 3.90 Å is better indexed as (310) and the peak at 2.89 Å as (224). The published card is therefore adequate for identification, although a little inaccurate for unit-cell determination based on indexing by comparison. Cell parameters are compared in Table 2 with the values of Giuseppetti *et al.* (1977), which were obtained by single-crystal diffractometry on a sample from Monte Somma in connection with their determination of the crystal structure.

Sarcolite from Anguillara Sabazia has a larger unit-cell volume, chiefly because of a value of *a* larger than in the sample of Giuseppetti *et al.* (1977) and the other samples from Monte Somma.

The densities, calculated following the method outlined by Mandarino (1981a), in this case on the cationic ratio, are lower than the measured values, because of the lack of data on the volatile species.

INFRARED-ABSORPTION SPECTRA

The three infrared-absorption spectra reported in Figure 1 allow a direct comparison of sarcolite from the two localities. In fact, some important differences in the absorption peaks that have been identified have been confirmed by chemical analysis.

The observed variations are referred to the characteristic vibrations of SO_4^{2-}, PO_4^{3-}, CO_3^{2-}, and H_2O molecular groups. The PO_4 group, with absorption bands ν_3 at 1146 cm^{-1} and ν_4 at 641 cm^{-1} (Povarennykh 1978), is evident in the spectrum of Monte Somma material 7515. It is also present but weak in the Anguillara Sabazia spectrum.

TABLE 3. CHEMICAL COMPOSITION OF SARCOLITE

	1	2	3	4	5	6
SiO_2	35.6	36.2	34.6	34.4	36.5	36.7
Al_2O_3	18.6	19.2	18.3	18.4	17.8	19.9
TiO_2	0.14	0.09	0.1	-	-	-
FeO	0.43	0.32	0.57	0.6	0.31	-
MgO	0.38	0.29	0.33	0.3	0.26	-
CaO	34.4	34.4	33.4	32.7	32.35	32.9
SrO	0.37	0.1	0.47	0.8	-	-
MnO	0.07	0.09	0.04	0.05	0.04	-
Na_2O	2.58	3.79	3.88	4.4	4.05	5.1
K_2O	0.36	0.36	0.84	0.5	0.54	-
P_2O_5	1.60	1.44	2.96	2.9	s.a.	1.7
SO_3	3.14	0.13	0.07	-	-	-
Cl	0.01	0.01	0.02	0.04	-	0.1
CO_2	p.p.	p.	p.	p.	p.	2.0
H_2O	p.	p.	p.p.	-	-	1.6
F	1.01	1.19	1.86	2.0	-	-
total	98.69	97.61	97.51	97.09	91.85	100.0
O=F	0.43	0.50	0.78	0.84		
	98.26	97.11	96.73	96.25		

p.p. possibly present; s.a. small amount;
p. present according to IR analysis;

(1) Anguillara Sabazia, EMPA WDS-analysis
(2) Monte Somma 7501, EMPA EDS-analysis
(3) Monte Somma 7515, EMPA WDS-analysis
(4) Monte Somma, EMPA (Livingstone 1984; an.n.10)
(5) Monte Somma, EMPA (Giuseppetti et al.1977;an.n.8)
(6) theoretical as given by Giuseppetti et al. (1977) on the basis of the structural refinement

The ν_3 and ν_4 vibrations due to the SO_4 group (1175 and 660 cm^{-1}) (Schwarcz & Speelman 1965) are present only in the spectrum of the Anguillara Sabazia sarcolite. However, the most important difference concerns the presence in the Monte Somma samples of abundant CO_3 made conspicuous by the asymmetrical ν_3 vibrations at 1422 and 1483 cm^{-1} (Schwarcz & Speelman 1965). Vibrations at these frequencies are almost entirely absent in the other spectrum.

The approximate amount of CO_2 present in the Monte Somma samples is about 3% if the plot given by Schwarcz & Speelman (1965, Fig. 5) for scapolite can be extrapolated to sarcolite. To a first approximation, this amount is the difference between the totals in the chemical analyses. Some water is present, as indicated by the stretching vibration in the region 3451–3434 cm^{-1}, and bending, at 1640–1592 cm^{-1}. In Monte Somma sample 7515, water seems to be present in trace amounts, whereas in the Anguillara Sabazia sample, the vibrations at 3441 and 1595 cm^{-1} are particularly evident.

THERMOGRAVIMETRIC ANALYSIS

TGA curves show an accumulated loss in weight to 960°C of 2.50% in Anguillara Sabazia sample and of 2.90% in Monte Somma sample 7515. In particular, the Anguillara Sabazia sarcolite is characterized by a continuous and gradual loss, whereas the Monte Somma sample has two clear steps (at about 300 and 700°C), probably due to the presence of CO_2 (Graziani & Lucchesi 1982, Fig. 2) and to the higher content of P_2O_5 and F.

CHEMICAL COMPOSITION

The compositions of the samples from Anguillara Sabazia (5 points on two crystals) and Monte Somma (3 points on 7515 and 4 on 7501) are shown in Table 3, where they are compared with some recent data from the literature on Monte Somma specimens (Giuseppetti *et al.* 1977, Livingstone 1984), all obtained by microprobe.

Some differences in the concentration of S, P, Na and F between the Monte Somma and Anguillara Sabazia samples can be pointed out. In particular, the Anguillara Sabazia sample is depleted in Na with respect to the Monte Somma samples, whereas it is strongly enriched in SO_3. The P content is variable: the Anguillara Sabazia sample compares well with most of the Monte Somma samples, but 7515 has a P_2O_5 content that is almost double that of all the others and is similar to the sample analyzed by P. Hill, quoted by Livingstone (1984). Even the F content is higher in Monte Somma 7515 sample with respect to the Anguillara Sabazia sample. Moreover, it is important to consider the difference between the totals obtained: this can be related to the different amounts of the other volatiles (such as H_2O and CO_2) that cannot be detected by electron-microprobe analysis, but could be documented by IR spectroscopy.

DISCUSSION

The crystal structure of sarcolite from Monte Somma, as resolved by Giuseppetti *et al.* (1977), consists of layers of tetrahedra roughly parallel to (001), connected by Si_2O_7 groups. The framework of tetrahedra has large cavities around the mirror planes, that are partly occupied by anionic groups. Isolated $(Si,P)O_4$ and CO_3 groups occupy the largest cavities. Other smaller cavities are incompletely filled by hydroxyl groups or water molecules.

Which element is to be used to calculate the structural formula is a disputed question. Giuseppetti *et al.* (1977) suggested a basis of 6 Ca atoms, as only this element shows consistency in all the analyses carried out on sarcolite. Livingstone (1984) suggested 27 (O + F) atoms, as he found a fluorine content (not considered by the former authors during their structural studies) "that raises some serious doubts concerning the validity of certain aspects of the sarcolite structure".

Giuseppetti *et al.* (1977) intentionally omitted elements present only in small amounts such as K, Fe, Mg and Mn, and considered that they occupy the site identified as *Me*. They also did not consider the possible replacement of Ca by Na. Even though some details were left uncertain, the sarcolite structure appears to be correct. Therefore, neither basis of calculation of the formula is completely satisfactory. As in many formulae, Al appears to be deficient; considering the theoretical value of 4, we suggest a calculation on the basis of 4(Al + Fe + Mg), *i.e.*, we assume that the small amount of Fe and Mg, always present, occupies the tetrahedral site instead of the *Me* site. Recent structural refinements carried out by F. Mazzi (pers. comm.) on Anguillara Sabazia and Monte Somma 7515 samples seem to support the substitution of Al by heavier atoms.

A comparison between the formula of Anguillara Sabazia samples and that of Monte Somma shows that Ca is always more than 6. Therefore, we propose that some Ca replaces Na with respect to the theoretical occupancy. The *Me* site, supposed to be filled by Na, appears to have a variable occupancy, ranging from 0.47 in Anguillara Sabazia up to 1.00 in Monte Somma composition 5 (Table 4). The tetrahedral site, assumed to be occupied by an equal amount of Si and P (Anguillara Sabazia and Monte Somma 7501 reveal such an occupancy), can be mainly occupied by P in Monte Somma 7515 and in composition 4 (Table 4).

TABLE 4. CHEMICAL FORMULAE OF SARCOLITE BASED ON 4 (Al+Fe+Mg)

	1	2	3	4	5	6
Ca	6.45	6.32	6.34	6.19	6.41	6.00
Na	0.55	0.68	0.66	0.81	0.59	1.0
Na	0.32	0.58	0.67	0.70	0.86	0.7
K	0.08	0.08	0.19	0.11	0.13	-
Sr	0.04	0.01	0.05	0.08	-	-
Ti	0.02	0.01	0.02	-	-	-
Mn	0.01	0.01	0.01	0.01	0.01	-
Al	3.84	3.88	3.83	3.83	3.88	4.00
Fe	0.06	0.05	0.08	0.09	0.05	-
Mg	0.10	0.07	0.09	0.08	0.07	-
Si	6.00	6.00	6.00	6.00	6.00	6.00
Si	0.23	0.20	0.12	0.08	0.75	0.25
P	0.24	0.21	0.44	0.43	-	0.25
S	0.41	0.02	0.01	-	-	-
Cl	0.003	0.001	0.01	0.01	-	0.04
C	(0.09)	(0.48)	(0.48)	(0.49)	-	0.46
H	(0.53)	(0.84)	(0.46)	(0.39)	-	1.8
F	0.56	0.64	1.04	1.12	-	

numbers as in Table 3.

As already noted by Livingstone (1984) the Si/Al ratio shows marked variability. However, the (Si + P)/Al ratio seems to be nearly constant, confirming that Si and P occupy the same structural position.

The site 0.5, 0.5, 0, supposed to be mainly filled by CO_3 groups and minor chlorine, is almost completely occupied by SO_4 tetrahedra in the Anguillara Sabazia sarcolite, as appears from the infrared absorption spectra (Fig. 1), where the respective bands seem to vary inversely with the proportion of CO_3 groups.

No significant variation in the calculated formula can be attributed to the presence of F in the site already indicated as occupied by OH and H_2O (Giuseppetti *et al.* 1977). In sarcolite, as in many other minerals, OH can be replaced in all proportions by F. In fact, in the Anguillara Sabazia and Monte Somma 7501 samples, this site is approximately one-half filled by F, whereas in Monte Somma 7515 and no. 4 it is a little more than two-thirds filled by F. The total number of oxygen atoms in the unit formula is 28 if the largest cavities are fully occupied by oxidized anions (SiO_4, PO_4, CO_3 SO_4), and they drop to 27 if the site of the CO_3 and SO_4 is vacant, as supposed by Livingstone (1984).

Finally, we suggest the following general formula for sarcolite: $(Ca,Na)_7(Na,K,Sr,Ti,Mn\ldots)_{\leq 1}(Al,Fe,Mg)_4Si_6O_{23}[(PO_4)(SiO_4)]_{0.5}[(CO_3)_a(SO_4)_bCl_c]_{0.5}(OH,F,H_2O)_{2-a-2b}$. The site occupied by F, OH and H_2O is in mutual relationship with the site of CO_3 or SO_4. Where the latter is empty, the occupancy of the former is 2. Every CO_3 group causes an equivalent vacancy in the site of OH, F and H_2O, and every SO_4 a double vacancy in the same site because of its greater dimension (C–O_3: 1.28–1.35, S–O_4: 1.47–1.50 Å, Povarennykh 1972).

The formula takes into account the variations observed in sarcolite from the two localities known so far; it is used to calculate the C and H ions reported between brackets in Table 4 by considering the site fully occupied. According to the infrared absorption spectra, some water is present in variable amount in all the specimens; in Monte Somma 7515 it appears in trace amounts, and it is present in higher amounts in the other samples. Values obtained using the proposed formula are effectively different, ranging from 0.39% H_2O in Monte Somma 7515 up to 0.46% in the Anguillara Sabazia sample.

Also, the estimated amount of CO_2 in Monte Somma 7515 is in good agreement with the calculated value (2%). Adding these values to our analyses, the total becomes closer to the theoretical composition. Moreover, the discrepancy between calculated and measured densities (Table 2) becomes smaller if the calculated CO_2 and H_2O are included in the formula weight (D_x Anguillara Sabazia: 2.92; D_x Monte Somma 7515:2.97).

The compatibility index (Mandarino 1981b) is -0.015 for sarcolite from Anguillara Sabazia, -0.007 for Monte Somma 7501 and 0.003 for Monte Somma 7515 sample. It was calculated using $D_{meas.}$, as D_x does not take into account the presence of CO_2 and H_2O.

We tentatively explain the observed larger unit-cell volume in the Anguillara Sabazia sample as due to the replacement of triangular CO_3 groups, which occurs along the *c* axis, by the tetrahedral SO_4 groups.

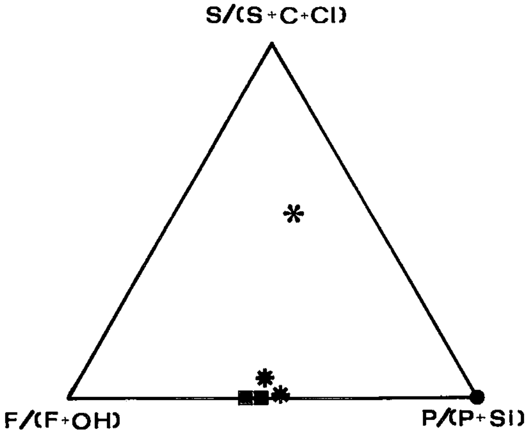

FIG. 2. Composition of sarcolite expressed in terms of S/(S+C+Cl), P/(P+Si), F/(F+OH). Symbols: asterisk: Anguillara Sabazia, "compound" asterisk: Monte Somma (this work), square: Monte Somma (Livingstone 1984), circle: theoretical composition.

In conclusion, there are two kinds of sarcolite from the type locality Monte Somma: one with lower and one with higher P content. The crystal structure was solved by Giuseppetti *et al.* (1977) on a low-P crystal, similar to our sample 7501 and to the theoretical composition. On the contrary, Livingstone (1984) analyzed a specimen with a high content of phosphorous, similar to our specimen 7515.

Sarcolite from Anguillara Sabazia is very close to the theoretical composition, but reveals one peculiarity: the presence of SO_3 instead of CO_2. No specimens of Monte Somma in the old or recent literature reveal such a feature. This can be illustrated in a plot of the proportion of S/(S+C+Cl), P/(P+Si) and F/(F+OH) (molar basis) in a triangular diagram (Fig. 2), where the apices represent three different structural sites. The sample from Anguillara Sabazia falls far from the points for the Monte Somma samples.

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