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The crystal structure of taramellite $Ba_2(Fe,Ti,Mg)_2H_2[O_2(Si_4O_{12})]$

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With 2 figures

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Riassunto

Alcuni campioni di taramellite della California hanno reso possibile la completa determinazione della struttura cristallina di questo minerale.

I parametri della cella elementare della taramellite californiana sono: $a = 13{,}95$ Å, $b = 12{,}21$ Å, $c = 7{,}15$ Å ($\pm$ 0,1%); il gruppo spaziale *Pmmn*. E' riportata una analisi chimica comunicataci da Alfors. Una prima parte del lavoro è stata compiuta su taramellite di Candoglia (Val di Toce, Italia), che era stata oggetto di ricerche precedenti. Sono stati ripresi, con la radiazione Mo$K\alpha$, fotogrammi del cristallo oscillante lungo [010]: con i dati così ricavati sono state calcolate quattro sezioni Patterson parallele a (010) mediante le quali è stato possibile identificare le posizioni degli atomi pesanti.

Successivamente, su campioni di taramellite californiana, sono stati ripresi fotogrammi di precessione, con la radiazione Mo$K\alpha$, lungo l'asse [001] (livelli da 0 a 3) e l'asse [010] (livello 0). Con questi dati sperimentali è stata portata a termine la determinazione della struttura, cosa che si era rivelata impossibile con la taramellite di Candoglia, dato l'abito di quei cristalli. Il raffinamento, effettuato mediante diversi cicli di minimi quadrati con matrice completa su 275 riflessi di tipo *hkl*, ha dato un *R* finale, su 515 riflessi *hkl* osservati, dell' 11,9%.

Nella struttura sono presenti anelli di quattro tetraedri SiO_4, parzialmente distorti e quasi paralleli a (010). Sono pure presenti complessi ottaedrici $(Fe,Ti)O_6$ i quali, avendo due a due in comune uno spigolo, formano delle catene parallele a [010]. Il bario è circondato da almeno sei ossigeni posti a distanze che vanno da 2,73 a 3,00 Å. Gli ossigeni formano tre diversi poliedri di coordinazione irregolari intorno ai tre atomi di bario non equivalenti.

La formula che può ricavarsi da considerazioni strutturali può essere alternativamente:

$$Ba_2(Fe^{+++},Fe^{++},Ti,Mg)_2[O(Si_4O_{12})]H_2O \text{ oppure}$$

$$Ba_2(Fe^{+++},Fe^{++},Ti,Mg)_2O_2[Si_4O_{10}(OH)_2].$$

Quattro di queste unità stechiometriche sono contenute nella cella elementare.

Auszug

Die Gitterkonstanten eines kalifornischen Taramellits sind $a = 13{,}95$ Å, $b = 12{,}21$ Å, $c = 7{,}15$ Å ($\pm$ 0,1⁰/₀); $Z = 4$. Die Raumgruppe ist *Pmmn*. Aus Schwenkaufnahmen um [010] an einem Taramellit von Candoglia, Val di Toce, Italien konnten die Lagen der schweren Atome bestimmt werden. Die vollständige Strukturanalyse wurde aus 275 Reflexen des kalifornischen Minerals mittels der Präzessionsmethode und mehrfacher Verfeinerungen durchgeführt. Für 515 beobachtete Reflexe wurde zuletzt $R = 0{,}119$ gefunden.

Die Struktur ist aus SiO_4-Viererringen, die nahezu parallel (010) liegen, aufgebaut. Oktaedrische $(Fe,Ti)O_6$-Komplexe bilden, durch gemeinsame Ecken verknüpft, Ketten parallel [010]. Die Ba-Atome sind von wenigstens sechs O-Atomen in Abständen von 2,73 bis 3,00 Å umgeben. Die Koordinationspolyeder sind unregelmäßig und von verschiedener Gestalt um die drei nicht-äquivalenten Ba-Atome.

Abstract

Samples of Californian taramellite permitted the determination of the crystal structure of this mineral to be brought to completion.

The unit-cell parameters of Californian taramellite are: $a = 13.95$ Å, $b = 12.21$ Å, $c = 7.15$ Å ($\pm$ 0.1⁰/₀); space group *Pmmn*. A chemical analysis is reported. A first stage of the work was carried out on taramellite from Candoglia (Val di Toce, Italy), which was the object of preceding studies. Oscillation photographs along [010] were taken with Mo$K\alpha$ radiation: four Patterson sections, calculated with the data so obtained, permitted the identification of the positions of the heavy atoms.

[001] precession photographs (levels 0 to 3) as well as zero-level [010] precession photographs were successively taken on samples of Californian taramellite with Mo$K\alpha$ radiation. With these experimental data, the complete determination of the crystal structure, impossible with the taramellite from Candoglia because of its peculiar habit, was carried out. The refinement with several cycles of full-matrix least squares on 275 *hkl* reflections, gave a final R-factor of 0.119, on 515 observed reflections.

The structure contains rings of four tetrahedra SiO_4, partially distorted and nearly parallel to (010); octahedral complexes $(Fe,Ti)O_6$ are also present and as pairs of them share an edge, chains of octahedra are formed along [010]. Barium is surrounded by at least six oxygens lying at distances ranging from 2.73 to 3.00 Å. Three different irregular coordination polyhedra are formed around the three non-equivalent Ba atoms.

From a crystal-chemical point of view, the formula of taramellite can be written either:

$$Ba_2(Fe^{+++},Fe^{++},Ti,Mg)_2\ [O(Si_4O_{12})]\cdot H_2O \text{ or}$$

$$Ba_2(Fe^{+++},Fe^{++},Ti,Mg)_2\ O_2[Si_4O_{10}(OH)_2].$$

Four formula units are contained in the unit cell.

Introduction

In a previous paper[1], one of us reported the results of some chemical and crystallographical researches, carried out on samples of taramellite from Candoglia (Val di Toce, Italy), which was also studied by TACCONI[2]. These results can be summarized as follows:

chemical formula $Ba_4Fe_2^{+++}Fe^{++}Ti(Si_4O_{12})_2(OH)_4$,

most probable space group *Pmmn*,

lattice constants[3] $a = 13.94$ Å, $b = 12.12$ Å, $c = 7.12$ Å ($\pm 0.1\,^0/_0$), two formula units in the unit cell.

At the end of that paper[1], it was suggested that taramellite could be considered as a sorosilicate with rings of four tetrahedra SiO_4, of the same kind as those found in the mineral axinite[4]. However, as it seemed impossible to obtain good x-ray pictures from the available material, since even the smallest crystals appeared as aggregates of nearly iso-oriented individuals, the definition of the crystal structure was left unfinished.

Determination of the structure

The first stage of the structural analysis, that is the determination of the heavy-atoms positions, was carried out on samples of taramellite from Candoglia. A number of oscillation photographs along [010], with a small angle of oscillation (15°) and with Mo$K\alpha$ radiation, were taken and suitably indexed. The intensities were estimated visually and no correction was made for the absorption.

With these data, which were much better than those obtained from Weissenberg pictures on the same crystal, two Patterson projections

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[1] F. MAZZI, Riesame della taramellite. Atti della Soc. Tosc. di Sc. Nat. [A] **64** (1957) 237—245.

[2] E. TACCONI, Taramellite, nuovo silicato di ferro e bario. Rend. Acc. Lincei [5a] **17** (1908) 810—814.

[3] The values reported in the paper quoted, namely: $a = 13.95$ Å, $b = 12.01$ Å, $c = 7.07$ Å, were slightly different from those given above.

The new and more correct values of the lattice constants were obtained by means of the application of the least-squares method to the equation of the interplanar distances as functions of the unit-cell parameters, using the experimental data obtained for a number of reflections suitably indexed on an x-ray diffractogram.

In respect to the paper[1], the reference axes have been interchanged in order to obtain an orientation consistent with that given in the International Tables for X-ray Crystallography.

[4] T. ITO and Y. TAKEUCHI, The crystal structure of axinite. Acta Crystallogr. **5** (1952) 202—208.

along [001] and [010] were first calculated. As, from the first of these projections, series of maxima appeared aligned at v ranges of 1/8, four more [010] Patterson sections were calculated, respectively for $v = 0$, 1/8, 1/4 and 1/2 (Fig. 1).

All the heavy atoms present in the formula unit were situated according to the equivalent points of the space group *Pmmn*. From the examination of the Patterson sections, it appears that, whereas iron and titanium, which are apparently replaceable cations, must lie on one series of eight-fold equivalent points, barium atoms must occupy three series of equivalent points, four-fold, two-fold and two-fold respectively.

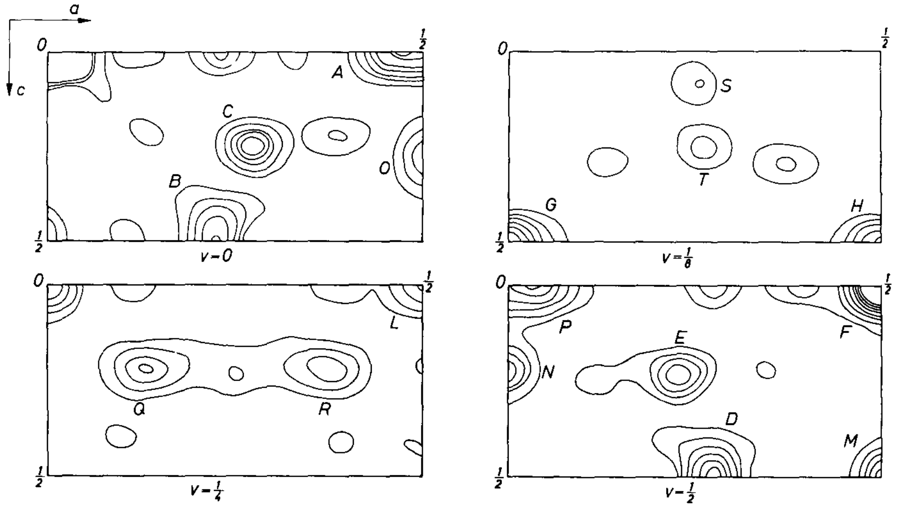

Fig. 1. Patterson sections parallel to (010)

Actually, the highest Patterson maxima, apparently due to distances between barium atoms, are on the sections at $v = 0$ and $v = 1/2$. Assuming the presence of mirror planes at $y = 1/4$ and $3/4$, there are only two possibilities of setting the barium atoms in such a way as to justify these maxima, as far as the y parameters are concerned: these are either $y = 0$ and $1/2$, or $y = 1/4$ and $3/4$. The A maximum in the section $v = 0$ shows that the distance between barium atoms at the same level is slightly less than $a/2$: this fact is not consistent with the choice of the y parameters 0 and 1/2 for the barium atoms because of the presence of symmetry centers at 000 and $\frac{1}{2}00$, as well as of (100) symmetry planes at $x = 1/4$ and $3/4$. Accordingly, a first series of four-fold positions for barium atoms can be chosen on the symmetry planes at $y = 1/4$ and $3/4$, with approximate parameters $x = 0.480$, $y = 0.250$, $z = 0$.

Taking now into consideration the B and C maxima of the section at $v = 0$, as well as the D and E maxima of the section at $v = 1/2$, one can see that their vectorial components are as follows: $(B) < a/4$, $\sim c/2$; $(C) > a/4$, $\sim c/4$; $(D) > a/4$, $\sim c/2$; $(E) < a/4$, $\sim c/4$. All these conditions are complied with if we consider such distances as occurring between a barium atom of the preceding series and one of the barium atoms lying on two sets of two-fold positions at the intersection of the (010) symmetry planes at $y = 1/4$ and $3/4$ with those (100) at $x = 1/4$ and $3/4$. The approximate parameters, which can be assigned to these further two series of barium atoms are as follows: (.250, .750, .250) and (.250, .250, .465). These parameters confirm all the considered Patterson maxima and the remaining ones: M, N, O, P, F.

The highest maxima, excluding the previously discussed ones, are at $v = 1/8$, namely $G(u = \sim 0, w = 1/2)$ and $H(u = \sim 1/2, w = 1/2)$, as well as at $v = 1/4$, that is $L(u = 1/2, w = 0)$. With the attribution of the first two maxima to vectorial distances between iron-titanium and barium and the third one to distance between equivalent iron-titanium atoms, one can assign to such atoms one series of eight-fold positions at about $x = 0$, $y = .125$, $z = \frac{1}{2}$. Also the T and S maxima at $v = 1/8$ are apparently due to Ba—(Fe,Ti) distances. Accordingly with the assumptions stated above, the parameters of all the atoms with the highest atomic numbers are now known.

Furthermore, assuming the Q and R maxima at $v = 1/4$ to be due to distances between barium and silicium, one could assign the following approximate parameters to two eight-fold sets of silicium atoms: (.375, 0, .250) and (.625, 0, .250). This assumption was subsequently found to be correct. However, the further step, that is the identification of the oxygen positions, proved to be impossible with the available data.

More recently, specimens of taramellite were found in California (Fresno County) and Canada (Yukon Territory)[5]. Thanks to the

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[5] R. M. THOMPSON and J. H. MONTGOMERY, Barium silicates from the Yukon Territory. Private communication on a paper presented at the meeting of the Mineralogical Association of Canada, April 1960; the title is recorded in Canadian Min. **6** (1960) 552.

courtesy of Professor PABST, Dr. ALFORS and Mr. MATTHEWS, it was possible to obtain samples of the Californian taramellite, on which the present study was brought to completion.

Because of the scarcity of the available material, it was impossible to carry out an accurate new chemical analysis of the Californian taramellite for the purpose of finding the actual ratios between the replaceable cations. According to ALFORS, who gave us the results of his analysis[6] the content of iron and titanium is rather different from that obtained for the samples from Candoglia. Also a noteworthy amount of magnesium is present. The structural researches, as will be seen, tend, however, to approach the preceding analysis[1].

The Californian specimen used for the complete x-ray determinations was a roughly spherical crystalline fragment of 0.2 mm in diameter. Precession photographs along [001] were taken with Mo$K\alpha$ radiation of the reflections hkl with l from 0 to 3, and similar pictures were taken for the zero level along [010].

On these photographs the lattice parameters were again measured. The values used in the present paper are as follows:

$$a = 13.95\ \text{Å}, \quad b = 12.21\ \text{Å}, \quad c = 7.15\ \text{Å}\ (\pm\ 0.1\,^0/_0).$$

The intensities were estimated with a Nonius microdensitometer. No correction was applied for the absorption because of the small dimensions of the crystal and the radiation used. The atomic scattering factors were calculated by means of FORSYTH and WELLS' formula[7], with the constants recently published by F. H. MOORE[8]. All the cal-

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[6] These results are: SiO_2 37.9, Al_2O_3 0.4, TiO_2 11.2, Fe_2O_3 0.8, FeO 5.1, MnO 0.2, MgO 2.4, CaO 0.8, Na_2O not detected, K_2O trace, BaO 40.0, SrO trace, H_2O 1.2, total 100.0.

The values for Fe_2O_3 and FeO are the average of three wet chemical analyses made by Mr. MATTI TAVELA. The water content was determined directly on two samples by Dr. J. T. ALFORS. All other constituents, except K_2O, which was analyzed by x-ray spectrochemical methods, were determined by emission spectrochemical methods by Dr. G. W. PUTMAN. The instrumental results of the spectrographic analysis plus the wet chemical results of iron and water totaled 95.3 $^0/_0$. The analysis was calculated to total 100.0 $^0/_0$ by adding proportionate amounts to the spectrographically determinated constituents. The wet chemical values for iron and water were not adjusted in this calculation. We express our sincere thanks to Dr. ALFORS and his coworkers of the California Division of Mines and Geology for the communication of their results.

[7] J. B. FORSYTH and M. WELLS, On an analytic approximation to the atomic scattering factor. Acta Crystallogr. **12** (1959) 412–415.

[8] F. H. MOORE, Analytic constants for atomic scattering factors. Acta Crystallogr. **16** (1963) 1169–1175.

culations were carried out on the Olivetti ELEA 6001 computer of the Centro di Calcoli Numerici of the University of Pavia.

The experimental data of the Californian taramellite confirmed the coordinates previously given to the barium and iron-titanium atoms. Thus it was possible to compute some electron-density projections along [010] and [001], on which also the positions of the silicium atoms were identified more accurately. Further calculations of structure factors, as well as new electron-density projections, finally allowed the determination of the parameters of all the oxygen atoms.

Table 1. *Final coordinates*
(In fractions of cell edge)

Atom	x	y	z
Ba_1	.250	.750	.240
Ba_2	.250	.250	.462
Ba_3	.473	.250	.009
Fe,Ti	.498	.128	.525
Si_1	.366	.010	.212
Si_2	.643	.027	.211
O_1	.250	.013 —	.211
O_2	.750	.979	.275
O_3	.579	.250	.408
O_4	.578	.750	.357
O_5	.610	.963	.014
O_6	.397	.120	.332
O_7	.408	.894	.266
O_8	.651	.155	.132
O_9	.572	.003	.385

Table 2. *Standard deviations of coordinates and interatomic distances*

Atom	$\sigma(x)$	$\sigma(y)$	$\sigma(z)$
Ba	.001 Å	—	.003 Å
Fe,Ti	.003	.003 Å	.008
Si	.006	.006	.014
O	.021	.018	.034

Errors in bond lengths and angles

σ(Ba—O)	0.03 Å	σ(O—Si—O)	2°
σ(Fe,Ti—O)	0.03 Å		
σ(Si—O)	0.03 Å	σ[O—(Fe,Ti)—O]	2°

Table 3. *Interatomic distances and angles*

Si_1—O_1	1.64 Å	Ba_1—O_7	(4)*	2.83 Å
Si_1—O_6	1.65	Ba_1—O_1	(2)	2.90
Si_1—O_5	1.68	Ba_1—O_3	(2)	3.47
Si_1—O_7	1.58	Ba_1—O_8	(4)	3.21
Si_2—O_5	1.68	Ba_2—O_6	(4)	2.75
Si_2—O_2	1.67	Ba_2—O_4	(2)	2.73
Si_2—O_8	1.67	Ba_2—O_1	(2)	3.68
Si_2—O_9	1.62	Ba_2—O_2	(2)	3.37
Fe,Ti—O_6	1.98	Ba_3—O_6	(2)	3.00
Fe,Ti—O_3	2.05	Ba_3—O_5	(2)	2.85
Fe,Ti—O_4	2.02	Ba_3—O_8	(2)	2.88
Fe,Ti—O_9	2.10	Ba_3—O_4		2.71
Fe,Ti—$O_{9'}$	1.98	Ba_3—O_7	(2)	3.12
Fe,Ti—O_7	2.01	Ba_3—O_3	(2)	3.21

O_5—Si_1—O_1	101°	O_6—Fe,Ti—O_9	89°
O_1—Si_1—O_7	103°	O_6—Fe,Ti—$O_{9'}$	81°
O_1—Si_1—O_6	115°	O_6—Fe,Ti—O_7	167°
O_6—Si_1—O_7	120°	O_3—Fe,Ti—O_4	86°
O_6—Si_1—O_5	107°	O_3—Fe,Ti—O_9	94°
O_7—Si_1—O_5	110°	O_3—Fe,Ti—$O_{9'}$	173°
O_5—Si_2—O_2	108°	O_3—Fe,Ti—O_7	92°
O_2—Si_2—O_8	111°	O_4—Fe,Ti—O_9	172°
O_2—Si_2—O_9	105°	O_4—Fe,Ti—O_9	102°
O_8—Si_2—O_9	119°	O_4—Fe,Ti—O_7	97°
O_8—Si_2—O_5	100°	O_9—Fe,Ti—$O_{9'}$	79°
O_9—Si_2—O_5	113°	O_9—Fe,Ti—O_7	86°
O_6—Fe,Ti—O_3	98°	$O_{9'}$—Fe,Ti—O_7	88°
O_6—Fe,Ti—O_4	87°		

* The number in brackets indicates how many times the distance occurs. The absence of this number means that the distance occurs only once.

The agreement between calculated and observed *F*'s for the *hk*0 and *h*0*l* reflections was already good at this stage (0.18 for *R*), when the contributions of iron and titanium to the structure factors were computed in accordance with the analysis of the Italian taramellite, that is there are three Fe atoms for each Ti atom. The refinement of the structure was carried out successively with several cycles of least squares on 275 *hkl* reflections with *l* from 0 to 3, chosen with the exclusion of those apparently affected by extinction and of those whose very high or very low intensity was presumably more affected by errors in the measurements. The program for the application

Table 4. *Observed and calculated structure factors*

h	k	l	F_o	F_c
2	0	0	119.8*	177.6
4			183.3	189.7
6			95.5	- 56.0
8			378.1*	424.2
10			152.0	-125.6
12			184.0	161.8
14			54.6	- 33.8
16			99.8	74.4
18			189.0	-185.2
1	1	0	< 17.6	- 2.9
3			79.9	- 97.6
5			184.9	-178.3
7			117.9	-130.6
9			136.3	-132.8
11			145.4	-161.3
13			114.0	-102.3
15			< 48.0	- 27.1
17			< 44.6	- 20.9
0	2	0	156.5	-128.5
2			< 24.6	- 54.1
4			328.8*	-469.5
6			81.2	67.1
8			65.8	- 43.7
10			96.0	66.3
12			117.7	-108.3
14			200.5	222.5
16			< 44.6	30.0
18			95.8	97.5
1	3	0	38.7	40.4
3			74.6	88.6
5			134.4	114.7
7			155.8	172.3
9			132.7	140.0
11			75.2	68.1
13			64.8	63.5
15			70.7	82.1
0	4	0	317.7*	413.5
2			188.1	-181.0
4			144.5	121.0
6			212.3	-215.5
8			151.9	122.0
10			294.0	-343.2
12			< 46.9	- 47.1
14			157.2	-158.9
16			< 44.6	9.1
1	5	0	58.3	- 54.4
3			84.5	- 91.6
5			100.1	-106.4
7			87.0	-113.6
9			128.3	-121.6
11			115.8	-114.4
13			83.1	- 83.9
15			< 46.9	- 21.1
17			< 46.9	- 2.9
0	6	0	167.3	-172.2
2			41.2	- 39.2
4			270.8*	-326.9
6			135.7	143.1
8			55.2	- 54.2
10			65.6	37.9
12			100.9	- 82.6
14			201.9	227.3
16			< 35.6	34.8
18			104.2	106.8
1	7	0	< 44.6	42.7
3			61.2	64.9
5			66.8	62.6
7			149.9	164.7
9			150.0	164.1
11			66.0	67.7
13			53.2	51.7
15			74.3	84.1
0	8	0	392.1*	569.1
2			87.9	113.4
4			235.2	251.9
6			< 42.4	- 25.6
8			228.5	257.8
10			95.8	- 71.9
12			137.4	126.8
14			66.9	- 51.6
16			81.4	74.6
1	9	0	< 44.6	- 14.9
3			79.5	- 82.3
5			142.3	-132.3
7			63.4	- 66.9
9			82.6	- 78.0
11			134.1	-145.9
13			106.6	-100.9
0	10	0	194.7	-223.9
2			< 48.0	- 8.1
4	10	0	214.9	-238.6
6			< 46.9	15.7
8			129.1	-113.4
10			95.1	92.7
12			81.4	- 69.1
14			133.8	134.3
1	11	0	< 48.0	9.8
3			55.9	47.7
5			96.1	87.2
7			115.8	111.6
9			78.2	84.7
11			63.2	51.4
13			64.1	52.3
0	12	0	159.6	165.1
2			105.5	- 75.0
4			96.8	109.1
6			121.3	-119.9
8			59.2	30.7
10			189.3	-189.5
1	13	0	< 49.1	- 2.6
3			< 49.1	- 31.0
5			71.0	- 71.0
7			64.8	- 76.8
9			87.9	- 86.3
11			85.5	- 84.4
0	14	0	164.0	-193.4
2			< 48.0	13.9
4			104.8	-112.9
6			76.9	75.2
8			81.6	- 86.4
10			84.7	76.4
1	15	0	< 48.0	24.8
3			< 48.0	47.5
5			61.1	57.0
7			83.4	77.6
9			56.8	72.1
0	0	1	< 14.1	- 34.3
1			74.6*	118.5
2			47.8	45.9
3			88.3	95.4
4			145.4	-153.9
5			127.6	-122.8
6			112.0	122.4
7			169.4	173.4
8			49.9	- 68.7
9			63.9	- 74.7
10			102.0	- 90.9
11			< 47.8	- 13.8
12			226.8	-234.5
13			100.8	- 96.7
14			119.5	-104.0
15			114.1	105.0
16			189.4	-189.1
17			48.1	- 44.7
18			114.1	- 96.3
3	1	1	143.5*	-191.5
4			110.5	128.6
5			84.2	- 65.9
6			101.5	- 97.4
7			178.0*	-218.2
8			< 40.3	43.6
9			70.1	- 45.5
10			< 47.9	- 15.9
11			175.8	-184.9
12			59.3	69.3
13			< 51.1	- 23.0
14			< 52.1	- 38.5
15			87.5	- 84.1
2	2	1	213.9*	-271.8
3			111.6*	-142.4
4			118.1	-117.9
5			103.7	123.9
6			131.5	-165.6
7			65.0	- 55.0
8			79.4	89.8
9			84.8	94.4
10			< 45.7	- 26.8
11			87.4	- 97.3
12			91.2	94.4
13			84.2	75.2
14			< 52.1	32.1
15			< 53.1	- 38.9
16			134.4	126.8
0	3	1	78.6	- 89.9
1			30.0	- 62.1
2			85.5	100.1
3			128.3*	179.2
4			< 28.1	17.6
5			62.3	42.8
6			< 36.1	28.6
7			187.7	236.1
8	3	1	78.6	- 69.4
9			73.3	77.4
10			91.3	89.2
11			153.9	169.0
12			< 50.0	- 10.7
13			63.3	33.2
14			< 53.0	8.8
15			120.5	115.0
0	4	1	215.5*	243.6
1			53.5	- 68.5
2			267.8*	363.3
3			191.6	210.6
4			149.3	149.0
5			35.5	- 44.6
6			241.5	285.1
7			53.5	45.1
8			137.8	133.6
9			159.7	-168.2
10			144.7	144.0
11			56.6	42.5
12			73.3	- 61.9
13			< 52.1	- 28.7
14			< 53.1	12.5
15			100.3	83.6
1	5	1	< 29.4	11.9
2			93.2	- 99.2
3			191.1	-225.1
4			95.0	88.3
5			55.6	- 17.1
6			120.0	-115.7
7			147.8	-183.6
8			< 42.9	19.0
9			98.0	- 64.3
10			< 50.0	- 27.3
11			170.7	-188.7
12			< 51.1	65.8
13			71.7	- 42.7
14			81.5	- 88.1
15			98.0	- 95.2
0	6	1	65.8	- 41.7
1			116.1	114.3
2			210.2	-245.5
3			67.5	- 74.5
4			134.8	-108.7
5			105.3	98.9
6			128.2	-132.1
7			77.1	- 61.6
8			< 44.1	52.7
9			57.6	60.3
10			75.6	- 58.1
11			85.5	- 86.8
12			82.2	87.0
13			84.2	89.9
14			< 53.1	32.7
15			< 53.8	- 26.9
16			95.0	97.8
0	7	1	141.9	-149.2
1			46.6	- 58.8
2			< 36.1	43.9
3			105.8	112.8
4			< 38.9	46.5
5			< 40.3	25.6
6			< 41.6	- 8.0
7			191.3	213.2
8			86.2	- 80.5
9			86.8	68.6
10			85.5	81.6
11			117.1	116.1
12			< 52.1	- 28.6
13			< 52.6	8.3
14			< 53.1	- 48.8
15			109.6	104.8
0	8	1	53.5	- 71.8
1			119.6	-126.3
2			59.5	58.6
3			56.6	59.1
4			< 40.3	- 39.9
5			58.6	- 37.0
6			80.7	78.9
7			129.2	113.0
8			69.2	- 86.3
9			114.2	-112.2
10			73.3	- 64.5
11			< 51.0	20.8
12			168.2	-177.3
13			65.8	- 51.7
14			87.1	- 82.9
15			72.4	63.4
16			155.7	-153.7
0	9	1	50.0	39.4
1			< 40.3	50.7
2			< 41.6	- 47.8
3			130.2	-142.7
4			181.5	167.4
5	9	1	61.6	- 35.9
6			116.1	- 92.9
7			138.1	-146.3
8			< 48.9	5.7
9			< 50.0	- 29.4
10			< 51.1	12.0
11			150.5	-153.3
12			83.5	76.7
13			< 54.5	- 20.0
14			87.7	- 82.5
0	10	1	88.2	- 73.2
1			< 43.5	7.0
2			143.0	-154.8
3			121.9	-121.9
4			< 45.4	- 3.8
5			116.1	123.8
6			86.8	- 90.1
7			< 48.9	- 25.0
8			< 50.0	39.7
9			< 51.1	31.1
10			< 52.1	- 18.4
11			57.6	- 49.7
12			93.2	89.6
13			74.1	69.0
0	11	1	82.2	- 84.1
1			< 46.5	- 44.2
2			52.0	49.2
3			97.5	103.7
4			< 50.0	49.9
5			52.9	37.6
6			< 51.9	5.0
7			139.0	146.2
8			84.2	- 68.4
9			< 52.1	45.2
10			70.1	68.0
11			114.7	127.2
0	12	1	133.3	108.7
1			83.5	- 86.7
2			178.0	197.7
3			81.5	73.0
4			128.7	107.6
5			< 50.0	- 16.2
6			162.2	184.8
7			61.4	55.1
8			62.3	52.6
9			123.3	-124.0
10			73.3	70.9
0	13	1	< 50.5	- 19.8
1			< 51.1	32.8
2			< 51.1	- 47.0
3			99.1	-109.1
4			108.5	88.7
5			< 52.1	- 27.4
6			102.0	-100.6
7			114.2	-124.5
8			< 53.1	- 8.7
9			< 53.8	- 35.2
10			< 54.1	6.2
11			113.1	-122.9
0	14	1	89.4	- 70.0
1			< 52.1	22.6
2			151.6	-143.1
3			81.5	- 56.1
4			55.6	- 37.7
5			112.2	99.7
6			82.2	- 92.4
0	0	2	88.3*	113.3
1			< 16.5	44.7
2			296.0*	396.8
3			42.6	50.5
4			310.5	355.2
5			126.8	-106.4
6			180.8	199.4
7			< 35.5	- 37.8
8			52.4	21.8
9			49.2	45.4
10			162.5	161.9
11			< 51.9	- 7.2
12			< 54.8	26.1
13			< 57.3	21.0
14			86.0	- 60.6
15			< 62.8	- 11.9
16			< 64.0	- 34.1
17			< 64.0	- 45.0
18			< 64.8	57.0
19			< 64.8	- 41.2
5	1	2	228.6*	-274.5
6			137.5	-122.8
7			< 36.0	1.5
8			< 41.0	13.2
9			266.4	-273.0
10			< 48.9	- 19.4
11			< 51.9	- 7.3

Table 4. *(Continued)*

h	k	l	F_o	F_c
12	1	2	< 54.8	17.0
13			209.6	-191.6
14			< 59.5	- 59.9
15			< 61.4	25.6
16			< 62.8	26.8
17			110.8	- 95.5
18			< 64.5	- 14.3
19			101.8	80.8
5	2	2	< 24.5	- 24.1
6			87.9*	-124.7
7			< 37.0	43.1
8			126.4	-113.1
9			< 45.6	- 29.8
10			130.4	109.3
11			< 52.1	41.3
12			< 55.1	74.1
13			< 57.5	4.0
14			< 59.6	1.8
15			< 61.4	38.2
16			< 62.8	62.1
17			< 64.0	- 28.6
18			171.3	146.6
19			< 64.4	1.1
4	3	2	67.9	- 55.0
5			229.1*	280.6
6			< 34.6	- 2.4
7			< 39.0	18.1
8			75.7	- 65.9
9			244.6	258.3
10			< 50.0	46.7
11			< 52.7	0.4
12			< 55.5	- 51.3
13			195.7	167.3
14			< 60.0	- 18.0
15			65.6	65.8
16			< 63.0	- 44.9
17			105.6	88.6
18			< 64.5	21.1
19			89.1	- 66.2
2	4	2	102.8	120.5
3			120.3	-143.4
4			< 28.6	6.2
5			< 32.7	- 16.3
6			104.1	- 97.0
7			< 41.0	10.0
8			138.6	-158.7
9			< 47.8	34.6
10			< 50.9	16.1
11			< 53.6	- 0.7
12			70.8	- 93.2
13			< 58.5	7.6
14			194.1	-191.3
15			< 62.0	- 28.2
16			162.3	-175.6
17			< 64.2	- 8.5
18			93.8	- 57.5
0	5	2	37.6	51.6
1			188.4	-211.9
2			37.5	- 41.0
3			42.4	41.5
4			68.6	71.1
5			175.9	-203.0
6			< 39.9	- 13.8
7			< 43.0	22.6
8			< 46.4	40.2
9			230.8	-255.8
10			< 51.9	- 16.4
11			< 54.4	- 4.3
12			55.1	68.0
13			177.9	-157.1
14			< 60.6	- 8.7
15			< 62.1	38.9
16			< 63.1	38.5
17			< 64.2	- 67.6
18			< 64.5	8.8
0	6	2	200.6	-212.9
1			< 32.7	- 21.4
2			75.0	- 88.6
3			< 35.2	33.0
4			60.1	- 52.8
5			< 39.9	- 42.2
6			76.4	-102.9
7			51.1	58.0
8			94.0	79.6
9			< 50.5	- 6.5
10			97.2	94.2
11			< 55.5	14.9
12			90.2	90.6
13			< 59.6	- 1.6
14			< 61.2	28.2
15			< 62.5	44.6
16			< 63.4	54.9
17			< 64.3	54.9
18			120.3	117.6
0	7	2	80.2	- 67.7
1			135.9	127.1
2			85.5	88.8
3			98.7	- 89.5
4			< 40.4	45.7
5			232.8	270.0
6			< 44.9	35.2
7			< 47.0	6.6
8			< 49.5	- 51.5
9			197.0	198.1
10			85.5	70.3
11			< 56.5	7.0
12			< 58.5	- 10.5
13			194.4	176.7
14			< 61.2	8.2
15			< 62.6	- 39.6
16			< 63.3	- 12.1
17			117.3	96.7
18			< 63.7	37.0
0	8	2	106.0	121.2
1			< 40.4	- 8.0
2			195.7	241.0
3			< 41.8	- 60.0
4			224.2	246.0
5			< 45.4	- 14.4
6			133.7	160.6
7			< 49.0	- 31.3
8			< 51.1	29.1
9			< 53.3	6.8
10			86.0	76.5
11			< 57.4	4.1
12			< 59.2	29.2
13			< 60.9	28.9
14			< 62.1	- 12.5
15			< 62.9	- 31.6
16			< 63.6	- 36.1
17			< 64.0	- 34.7
18			< 62.9	7.5
0	9	2	< 43.0	- 38.2
1			155.2	-158.8
2			55.8	- 55.7
3			< 44.6	45.8
4			< 46.3	38.7
5			149.0	-166.0
6			98.2	-100.4
7			< 51.1	- 10.0
8			< 53.1	- 15.2
9			228.2	-228.7
10			< 56.7	- 1.0
11			< 58.7	0.6
12			< 60.0	26.5
13			157.1	-139.2
14			< 62.4	- 66.0
15			< 63.6	12.6
16			< 63.6	17.9
17			80.2	- 74.0
0	10	2	186.5	-199.8
1			44.8	- 49.2
2			122.8	-129.6
3			< 47.5	17.5
4			68.7	- 46.9
5			< 50.1	21.9
6			< 51.4	- 51.2
7			< 53.1	23.4
8			76.3	- 67.5
9			< 56.6	- 43.4
10			< 58.1	- 7.1
11			< 59.6	40.6
12			< 61.1	44.7
13			< 62.1	21.1
14			< 62.7	47.4
15			< 63.6	11.8
16			< 63.5	51.0
17			< 62.6	- 23.7
18			87.4	68.5
0	11	2	< 49.4	- 36.7
1			116.1	101.6
2			< 49.6	36.7
3			50.1	- 72.2
4			< 51.4	- 23.8
5			165.7	184.1
6			< 54.0	6.3
7			< 55.3	- 2.2
8			< 56.8	- 53.4
9			170.7	175.7
10			< 59.6	32.9
11			< 60.8	11.5
12			< 62.0	- 19.8
13			129.9	124.0
14			< 63.1	- 14.2
15			< 63.1	- 59.3
16			< 62.8	- 45.0
17			88.5	76.4
0	12	2	< 52.1	10.9
1			< 52.3	- 21.0
2	12	2	< 52.8	37.6
3			59.3	- 72.7
4			< 54.1	19.4
5			< 55.1	1.5
6			< 56.3	- 8.3
7			< 57.4	3.8
8			< 58.8	- 70.3
9			< 59.6	16.2
10			< 60.8	- 60.0
11			< 62.0	- 12.3
12			75.7	- 69.1
13			< 63.1	16.5
14			99.7	- 86.7
15			< 62.8	- 20.4
16			124.8	-121.9
17			< 60.2	- 12.4
0	13	2	< 55.1	- 1.8
1			110.3	-111.2
2			< 55.4	- 14.8
3			< 56.0	36.9
4			59.3	70.4
5			150.4	-141.7
6			< 58.5	- 58.5
7			< 59.3	2.5
8			< 60.4	12.8
9			142.8	-148.0
10			< 62.1	8.4
11			< 62.6	12.1
12			< 63.3	49.6
13			119.6	-124.4
14			< 62.9	- 18.9
15			< 60.5	16.1
0	14	2	68.7	- 61.2
1			< 57.8	- 33.9
2			< 58.0	- 69.1
3			< 58.5	- 0.5
4			59.3	- 46.6
5			< 59.5	8.5
6			< 60.4	30.8
7			< 62.5	32.7
8			< 61.9	- 9.7
9			< 62.6	- 20.4
10			< 62.8	14.4
11			< 63.5	15.9
12			68.5	68.2
13			< 62.9	9.0
14			69.3	66.4
15			< 60.4	14.5
0	15	2	61.7	- 46.9
1			109.8	96.6
2			< 60.7	46.3
3			< 61.0	- 26.7
4			< 61.3	31.1
5			122.4	127.2
6			< 62.1	17.3
7			< 62.6	- 11.2
8			< 62.9	- 39.7
9			137.1	145.3
10			< 63.7	39.7
11			< 63.4	15.2
12			< 62.6	- 5.1
13			107.2	101.7
0	16	2	107.5	125.6
1			< 62.4	- 22.1
2			100.8	114.5
3			< 62.7	- 46.8
4			118.2	99.1
5			< 63.1	22.8
6			112.9	97.5
7			< 63.6	- 23.1
8			< 63.8	46.3
0	0	3	< 17.5	- 30.1
1			120.7	99.5
2			183.1	199.7
3			88.3	84.5
4			< 20.9	- 42.3
5			80.0	31.0
6			132.2	- 95.2
7			110.0	- 87.7
8			176.4	-192.8
9			< 56.6	- 38.3
10			72.7	- 74.0
11			< 61.2	- 36.9
12			127.5	-133.3
13			< 62.9	8.2
14			176.8	-159.2
15			< 64.6	- 11.3
16			186.8	-177.5
7	1	3	127.0	-147.9
8			69.0	- 74.1
9			102.3	- 90.7
10			116.0	124.3
11			118.5	-127.1
12			85.6	- 75.9
13	1	3	< 58.1	- 47.4
14			126.2	112.2
15			< 58.7	- 74.2
16			< 59.3	- 25.2
17			< 62.0	19.8
18			109.9	93.6
19			< 64.6	2.9
6	2	3	191.3	-184.6
7			< 25.6	21.8
8			< 33.1	- 4.3
9			< 39.1	- 7.2
10			65.2	24.7
11			81.6	61.9
12			121.9	128.0
13			< 56.5	- 14.8
14			< 59.2	- 28.7
15			< 61.1	- 4.2
16			100.9	107.0
17			64.6	5.1
6	3	3	62.9	- 37.3
7			196.7	197.8
8			135.7	154.5
9			69.2	70.0
10			90.1	- 98.5
11			135.2	127.9
12			92.1	77.1
13			< 56.4	47.4
14			< 59.3	- 43.0
15			71.1	81.6
16			75.4	79.3
17			< 66.4	14.5
5	4	3	60.2	33.9
6			166.2	200.7
7			69.2	- 56.2
8			< 40.5	- 23.8
9			< 44.5	- 16.5
10			110.4	131.5
11			< 53.0	- 36.8
12			< 55.8	3.2
13			< 58.4	- 27.2
14			< 60.7	17.9
15			< 62.5	- 42.0
16			< 64.3	- 65.5
17			< 66.0	43.4
3	5	3	112.9	-124.0
4			204.5	-249.1
5			94.5	- 77.6
6			109.4	113.3
7			133.2	-141.2
8			105.8	-101.5
9			110.0	- 93.2
10			< 50.9	36.3
11			146.9	-131.5
12			112.5	-120.1
13			81.9	- 50.7
14			99.9	97.8
15			68.5	- 71.8
16			76.9	- 83.3
0	6	3	177.0	-176.8
1			< 26.5	- 1.0
2			154.2	-190.7
3			64.0	39.1
4			< 33.5	23.5
5			< 36.2	- 30.0
6			157.3	-163.5
7			89.9	43.4
8			< 45.5	- 24.6
9			< 48.5	34.8
10			< 51.2	- 2.1
11			< 54.1	33.4
12			116.2	98.3
13			< 58.9	- 35.3
14			< 60.9	- 18.9
15			< 62.9	9.2
16			100.5	104.6
17			< 66.0	11.4
0	7	3	154.6	179.3
1			74.1	- 51.3
2			85.7	- 97.8
3			85.0	102.2
4			< 37.7	12.2
5			106.5	87.4
6			93.8	-102.6
7			127.9	142.1
8			91.8	99.4
9			< 50.2	35.9
10			103.6	-112.3
11			129.5	129.9
12			< 58.2	35.9
13			< 59.1	43.5
14			< 62.0	- 59.1
15			< 63.9	48.8
16			< 65.0	22.4

Table 4. *(Continued)*

h	k	l	F_o	F_c
0	8	3	< 38.1	- 19.8
1			64.9	62.5
2			110.8	123.9
3			< 40.0	30.1
4			< 41.9	- 29.6
5			< 43.6	9.7
6			< 45.5	- 7.9
7			81.7	- 57.9
8			137.6	-143.2
9			< 52.1	- 2.6
10			< 54.5	5.9
11			< 56.6	- 40.3
12			114.8	-106.6
13			< 60.9	- 10.7
14			102.4	- 86.6
15			< 64.1	- 2.3
16			154.0	-160.8
0	9	3	< 41.3	- 42.8
1			52.0	- 36.4
2			95.6	112.5
3			118.8	-116.7
4			147.1	-146.2
5			< 46.1	- 29.3
6			151.9	145.7
7			81.7	-101.1
8			< 52.1	- 25.9
9			94.9	- 81.2
10			85.2	83.6
11			100.3	- 90.8
12			84.0	- 74.0
13			< 61.9	- 42.3
14			117.6	127.5
15			< 64.3	- 65.6
16			< 65.1	- 33.6
0	10	3	85.0	- 57.6
1			< 45.2	13.1
2			115.3	-138.7
3			64.8	54.6
4			< 47.7	- 5.3
5			< 50.7	- 14.3
6			85.9	- 82.6
7			< 52.6	11.0
8			< 54.5	13.7
9			< 56.2	14.2
10			< 58.0	- 19.0
11			< 59.6	28.3
12			110.1	106.8
13			< 62.6	- 20.2
14			< 63.9	30.3
15	10	3	< 65.1	18.4
0	11	3	144.1	167.4
1			< 48.5	- 26.7
2			< 49.4	- 55.9
3			72.3	80.4
4			< 51.3	46.9
5			< 52.4	50.0
6			< 53.3	- 0.1
7			118.9	134.1
8			111.7	123.7
9			< 57.8	54.1
10			86.0	- 97.2
11			104.3	93.5
12			< 62.5	38.2
0	12	3	105.2	79.5
1			< 51.0	57.2
2			186.8	202.3
3			< 52.1	10.7
4			134.7	115.8
5			< 54.1	- 19.1
6			124.7	143.0
7			< 56.6	- 36.8
8			< 58.1	- 11.3
9			< 59.7	22.2
10			< 61.2	60.9
11			< 62.5	- 53.7
12			< 63.5	- 7.3
0	13	3	88.7	- 91.1
1			< 54.1	1.3
2			< 54.5	30.5
3			< 54.8	- 58.9
4			136.6	-152.3
5			< 56.6	- 45.1
6			98.0	84.1
7			87.1	-106.8
8			< 61.1	- 60.5
9			< 62.0	- 67.7
10			< 62.9	16.1
11			104.9	- 71.5
12			104.1	-106.0
0	14	3	100.1	- 82.6
1			< 56.7	16.7
2			114.9	-133.9
3			< 57.9	23.8
4			< 58.5	- 18.0
5			80.3	- 36.9
6			< 59.2	- 71.0
7	14	3	< 60.1	30.9
8			< 61.1	- 7.1
9			< 61.7	49.0
10			< 62.5	- 52.8
11			< 65.0	5.6
0	15	3	87.1	94.5
1			< 61.5	- 6.7
2			< 61.5	- 56.4
3			< 61.9	85.7
4			< 62.5	18.2
5			< 62.5	33.6
6			< 63.2	- 50.2
7			< 63.8	68.2
8			< 64.2	66.3
9			< 64.7	32.4
10			< 65.6	- 70.9
11			104.4	100.9
0	0	4	348.5*	419.5
1			57.5	67.7
2			81.0	71.9
3			142.6	-154.4
4			263.1	271.5
5			66.2	67.6
6			46.9	55.3
7			113.4	-115.4
8			273.2	292.1
9			62.8	64.1
10			68.5	- 52.7
11			58.0	- 70.6
12			97.3	52.1
13			< 42.5	19.7
14			119.1	- 95.1
15			116.1	-101.4
16			< 43.2	46.0
0	0	5	194.6	193.6
1			133.4	-149.3
2			52.7	53.8
3			63.7	81.9
4			81.4	- 78.8
5			117.1	-142.5
6			< 42.5	15.4
7			78.6	73.7
8			43.4	17.2
9			103.0	-118.3
10			169.1	-129.5
11			100.0	97.2
12			136.8	-129.7
13			60.3	- 84.4
14	0	5	42.1	- 27.9
15			55.9	45.5
16			71.1	- 73.0
0	0	6	166.7	116.9
1			< 43.4	24.4
2			190.0	208.8
3			< 43.7	- 3.0
4			82.6	70.9
5			< 43.9	19.2
6			150.2	150.5
7			73.1	- 61.6
8			76.6	34.9
9			79.3	- 58.9
10			60.5	84.5
11			78.4	- 73.0
12			63.2	- 52.7
13			< 42.7	4.4
0	0	7	< 44.8	- 30.8
1			< 45.6	- 26.2
2			85.6	85.3
3			< 44.8	- 24.7
4			76.8	86.2
5			< 44.8	- 44.0
6			< 44.8	- 6.1
7			< 45.0	- 23.8
8			77.3	- 80.7
9			< 44.1	- 29.1
10			48.3	31.8
11			< 42.2	- 1.0
12			48.2	- 37.2
0	0	8	130.6	140.3
1			81.0	86.6
2			90.2	89.6
3			57.7	- 74.9
4			160.5	112.9
5			< 43.9	41.6
6			< 43.2	9.1
7			102.0	-133.6
8			< 41.6	27.4
9			< 39.8	28.9
10			< 36.8	1.7
0	0	9	115.6	168.3
1			< 40.8	- 59.7
2			< 40.4	- 5.3
3			58.9	54.7
4			< 39.1	16.7
5			68.8	- 96.3

* Low values due to extinction

of the least-squares method, (with full matrix and isotropical temperature factor for each atom) for the ELEA 6001 computer, was kindly given us by Professor SGARLATA. During the course of the refinement, different curves of the atomic scattering factors for the replaceable cations (iron—titanium—magnesium) were successively assumed on the basis of the available analyses. The best agreement between F_0's and F_c's was obtained with the assumption of an equal content of iron and titanium as replaceable cations, a composition which is closer to that of Italian taramellite than to that previously given for the Californian specimen. Actually, the agreement became worse and the temperature factor of these atoms assumed negative values when we took into account the measured amount of titanium and the presence of magnesium found by ALFORS. With the best agreement we got an $R = 0.10$ for the 275 observed reflections used in the refinement. At this final stage, the R factor, computed on 515 observed *hkl* reflections (excluding some few reflections apparently affected by extinction) was 0.119.

An average temperature factor was assigned to each atomic species; the obtained values are as follows:

$$B_{\mathrm{Ba}} = 0.61\,,\quad B_{\mathrm{Fe,Ti}} = 0.63,\quad B_{\mathrm{Si}} = 0.10,\quad B_{\mathrm{O}} = 0.49\ \text{Å}^2.$$

The final parameters are given in Table 1. The errors in the parameters, according to the method of CRUICKSHANK[9] are shown in Table 2. In Table 3 bond distances and angles are summarized, and the comparison between observed and calculated structure factors is given in Table 4.

Discussion of the structure

The present study has completely confirmed the hypothesis put forward in the preceding paper[1] that taramellite is a sorosilicate. In the structure are present rings of four tetrahedra SiO_4, partially distorted and nearly parallel to (010). The average lengths of the Si—O bonds for the two non-equivalent tetrahedra of the asymmetrical unit are respectively 1.64 and 1.66 Å.

Octahedra are formed by iron-titanium and oxygen atoms; the distance between these cations and the surrounding oxygen atoms ranges from 1.98 to 2.10 Å. As each such coordination polyhedron shares two edges with its two opposite neighbours, chains of octahedra are formed along [010] (Fig. 2*a* and *b*). These chains may be the cause of the fibrous habit of taramellite from Candoglia.

Barium, as said above, lies on three series of equivalent positions and forms with the oxygen atoms three different kinds of coordination polyhedra. Ba_1 is surrounded by four O atoms lying nearly at the corners of a square, and by two more O atoms at a greater distance, but practically in the same plane as the preceding ones, so that the six oxygen atoms form a slightly irregular hexagon. Also Ba_2 is coordinated with six oxygen atoms, which are arranged at the corners of a sort of distorted trigonal prism. The coordination polyhedron of Ba_3 is rather irregular: it may be considered as a trigonal prism with a non-basal "centered" face, or as an octahedron with a "centered" face. As one can see in Table 3, other oxygen atoms lie around barium atoms at distances larger than 3.12 Å, and they should not take part in the coordination of such cations.

The chemical formula of taramellite shows the presence of OH^- ions; however, in the last stage of the work some striking arguments

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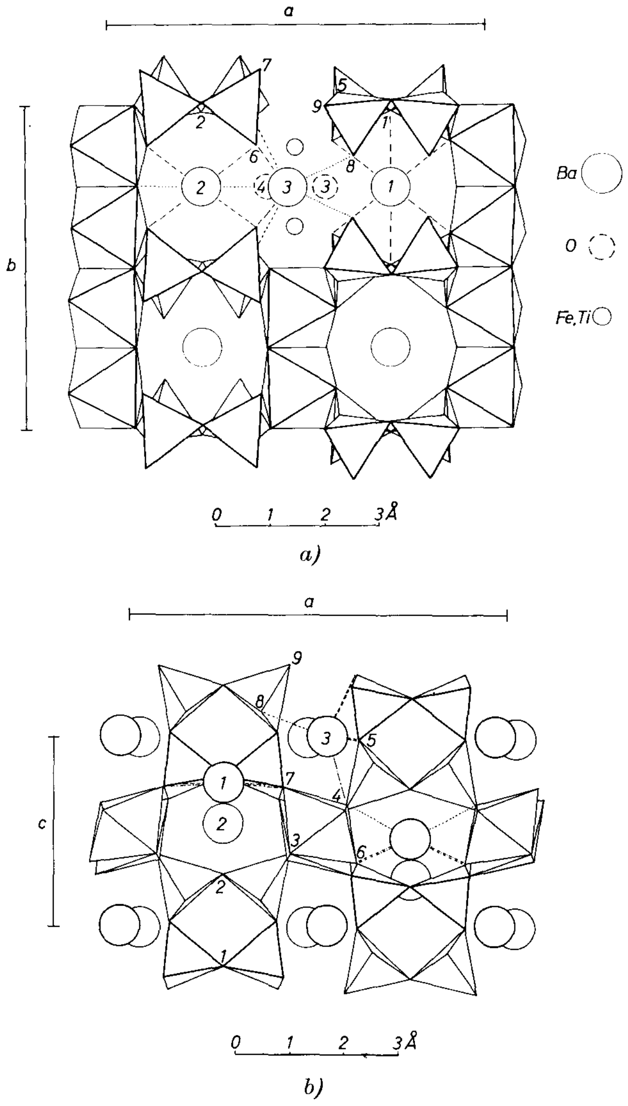
[9] D. W. CRUICKSHANK, The accuracy of electron density maps in x-ray analysis with special reference to dibenzyl. Acta Crystallogr. 2 (1949) 65—82.

suggested that the hydrogen atoms could be distributed in a more satisfactory different way. The first of these arguments is that the distance (2.49 Å) between 0_3, which lies on a symmetry plane, and the two 0_8 atoms situated out of the same plane, is too small to be



a)

b)

Fig. 2. *a)* Projection of the structure of taramellite along [001]. In the upper part of the figure the octahedra have been omitted to show the coordination of Ba_3. *b)* Projection of the structure of taramellite along [010]

Table 5. *Electrostatic valency table*

Anion	Balancing cations	$\frac{\text{Charges of cation}}{\text{Coordination number}}$	Total charges surrounding anion
O_1	Ba_1	1/3	2.333
	Si_1	1	
	Si_1	1	
O_2	Si_2	1	2.000
	Si_2	1	
O_3 (as OH)	H	1	2.000
	Fe,Ti	1/2	
	Fe,Ti	1/2	
O_3 (as H_2O)	H*	1/2	2.000
	H*	1/2	
	Fe,Ti	1/2	
	Fe,Ti	1/2	
O_4 (as OH)	H	1	2.619
	Fe,Ti	1/2	
	Fe,Ti	1/2	
	Ba_2	1/3	
	Ba_3	2/7	
O_4 (as O)	Fe,Ti	1/2	1.619
	Fe,Ti	1/2	
	Ba_2	1/3	
	Ba_3	2/7	
O_5	Si_1	1	2.286
	Si_2	1	
	Ba_3	2/7	
O_6	Si_1	1	2.119
	Ba_2	1/3	
	Ba_3	2/7	
	Fe,Ti	1/2	
O_7	Si_4	1	1.833
	Ba_1	1/3	
	Fe,Ti	1/2	
O_8	Si_2	1	1.286
	Ba_3	2/7	
O_8 **	Si_2	1	1.786
	Ba_3	2/7	
	H	1/2	
O_9	Si_2	1	2.000
	Fe,Ti	1/2	
	Fe,Ti	1/2	

* Assuming that the hydrogens of H_2O form hydrogen bonds with O_8 and that the positive charge of hydrogen is roughly equally divided between the oxygen of H_2O and O_8.

** Assuming that O_8 is linked to O_3 (H_2O) by a hydrogen bond.

the distance between oxygens not coordinated around the same cation: so, in order to justify such a distance, we may suppose the existence of hydrogen bonds between O_3 and the two O_8 atoms. This assumption gains in probability if we suppose that O_3 is a water molecule with its hydrogens out of the mirror plane on opposite sides so as to form two hydrogen bonds with the O_8 atoms. If on the contrary O_3 is considered to be an hydroxyl, it should be linked by two hydrogen bonds with only one hydrogen, which is rather improbable. Another argument is that if O_3 and O_4 are thought to be OH^- ions, the balance of the electrostatic charges of O_4 and O_8 is unsatisfactory, while, as can be seen in Table 5, PAULING's rule is better fulfilled if we assume that O_3 is H_2O and O_4 a free oxygen. Furthermore these assumptions are consistent with the following structural feature: O_4 is strictly linked not only to (Fe,Ti), but also to Ba, whereas O_3 is linked only to (Fe,Ti) and not to Ba (Ba_1—O_3 = 3.47 Å, Ba_3—O_3 = 3.21 Å). These facts can be explained if we assume that O_4 is a free oxygen and O_3 is a molecule of water with its more positive side directed toward Ba and its more negative side (taking also into account that the hydrogens are partially neutralized by the hydrogen bonds) directed toward iron-titanium.

On the basis of the considerations stated above, the chemical formula of taramellite could be $Ba_2(Fe^{+++},Ti,Fe^{++},Mg)_2[O(Si_4O_{12})]\cdot H_2O$ Four of these formula units are present in the unit cell.

An alternative formula was suggested by Professor A. PREISINGER during the meeting of the Società Mineralogica Italiana (Pisa, September 1964), that is;

$$Ba_2(Fe^{+++},Fe^{++},Ti,Mg)_2O_2[Si_4O_{10}(OH)_2].$$

This possibility does not change the above written considerations: the only difference is that the hydrogen atoms could be more tightly bound to two oxygens (O_8) of the Si-O rings, rather than to the oxygen (O_3) of the supposed water molecule.

The alternative cannot be solved with our available data.