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The crystal structure of macdonaldite

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Mineralogia. — *The crystal structure of macdonaldite* (*). Nota di ELIO CANNILLO, GIUSEPPE ROSSI e LUCIANO UNGARETTI, presentata (**) dal Socio G. CAROBBI.

RIASSUNTO. — La macdonaldite è un silicato la cui formula chimica, tratta dalla letteratura, è: $BaCa_4Si_{15}O_{35} \cdot 11\ H_2O$; quattro di queste unità stechiometriche sono contenute nella cella elementare. Il gruppo spaziale è Cmcm; le costanti reticolari, rideterminate per il presente lavoro, sono le seguenti: $a = 14{,}081$, $b = 13{,}109$, $c = 23{,}560 \pm 0{,}001$ Å.

La struttura è stata determinata attraverso l'esame della sintesi di Patterson tridimensionale e di successive sintesi di Fourier tridimensionali. Il raffinamento è stato eseguito col metodo dei minimi quadrati. Il fattore di discordanza finale per i riflessi osservati è 0.083. I poliedri di coordinazione del calcio sono ottaedri formati da atomi di ossigeno e da molecole d'acqua; questi ottaedri, mettendo in comune uno spigolo, formano catene parallele ad a. Tali catene sono collegate fra loro attraverso legami idrogeno e formano strati paralleli a (001). Tra due strati ottaedrici è posto un doppio strato tetraedrico costituito da anelli di quattro e otto tetraedri SiO_4. Gli strati tetraedrici sono del tipo apophyllite «idealizzato». L'impalcatura tetraedrica è attraversata da un doppio sistema di canali: uno parallelo a b con diametro utile di 2,1 Å, l'altro parallelo ad a con diametro utile di circa 3,4 Å. All'interno dei canali si trovano gli atomi di bario coordinati da sei ossigeni dei tetraedri e da quattro molecole d'acqua. Sono pure presenti nei canali molecole d'acqua non legate ai cationi.

Viene discussa l'analogia strutturale della macdonaldite e con le zeoliti fibrose e con i minerali rhodesite e delhayelite.

La formula chimica è modificata, sulla base dell'analisi strutturale, nel modo seguente: $BaCa_4H_2Si_{16}O_{38} \cdot (8 + x)\ H_2O$ dove x è uguale a 2,4 per il cristallo usato nella presente ricerca.

INTRODUCTION.

Macdolnaldite is one of the seven barium minerals recently found in Eastern Fresno County, California, and described by Alfors *et al.* [1]. The following data are quoted from the Authors cited above:

lattice parameters	$a = 14.06 \pm 0.01$ Å
	$b = 13.08 \pm 0.01$ Å
	$c = 23.52 \pm 0.02$ Å
space group	Cmcm
cell content	$4\ [BaCa_4Si_{15}O_{35} \cdot 11\ H_2O]$.

The mineral occurs in crystals elongated following [100].

These cleavages are present: {001} perfect, {010} good, {100} poor or a fracture.

In respect to the paper of Alfors *et al.* [1], who choose the axes setting corresponding to the convention used in Crystal Data, the reference axes have been interchanged in order to obtain an orientation consistent with the standard setting of the International Tables of X-rays Crystallography.

(*) This work was performed in the Sezione di Pavia del Centro Nazionale di Cristallografia del C.N.R., Istituto di Mineralogia dell'Università, Via Bassi 4, 27100 Pavia.

(**) Nella seduta del 19 novembre 1968.

EXPERIMENTAL.

The sample used for the crystal structure analysis was a prismatic fragment elongated following *a*. The side dimensions of the rectangular section of the sample were: 0.0200 cm (side parallel to *b*), 0.0096 cm (side parallel to *c*).

The lattice parameters were re-determinated and the values obtained are:

$$a = 14.081 \pm 0.001 \text{ Å}$$
$$b = 13.109 \pm 0.001 \text{ Å}$$
$$c = 23.560 \pm 0.001 \text{ Å}.$$

Integrated equi-inclination Weissenberg photographs of the *hkl* reflexions (*h* from 0 to 10) were taken with nickel filtered CuKα radiation, using the multiple film technique. A total of 1948 reflexions, out of the 2626 present in the CuKα limiting sphere (about 75 %) were inspected; 1428 of them were measured photometrically, 520 were too faint to be suitably measured or did not give any blackening on the films.

The intensities were corrected for the Lorentz-polarization and absorption factors and for the incipient but incomplete α_1—α_2 spot doubling. The absorption factors were obtained through an exact integration over the whole diffracting volume – considered as continuous – of the crystal; the formulas given by Cannillo and Mazzi [2] were used. The linear absorption coefficient is $\mu = 161.8 \text{ cm}^{-1}$ and the transmission factor ranges from 1 to 4 on a relative scale.

The correction for the $\alpha_1 — \alpha_2$ splitting effect was applied taking into account the integration technique which complicates the splitting effect for its diagonal direction with respect to the sides of the film.

CRYSTAL STRUCTURE ANALYSIS.

A first inspection of the Weissenberg pictures permitted to observe that the average intensity of the reflexions with $h = 2n + 1$ was noticeably lower than that of the reflexions with $h = 2n$. Furthermore, among the reflexions of the latter set, those with $h = 4n$ have the strongest intensities. The pseudo-symmetry inferred from these observations was taken into account in the course of the structure analysis.

From a three-dimensional Patterson synthesis it was possible to locate all the atoms of Ba, Ca and Si. A three-dimensional Fourier synthesis, computed giving to the Fo's the phases of the heavy atoms contributions, permitted to find the positions of the remaining atoms.

The structural model obtained in this way is self consistent only with the assumption that there are 16 Si atoms for each Ba atom in the chemical formula and no alternative structure is possible with the number of Si and O atoms of the chemical formula given by Alfors *et al.* The chemical formula will be fully discussed later.

The arrangement of the atoms in the crystal structure of macdonaldite gives a full account of the intensity differences in the sets of reflexions mentioned above. All the atoms but barium are arranged in such a way that the glide plane at $x = 1/4$ in the Cmcm space group becomes a mirror plane. Thus the contributions of these atoms to the structure factors of the reflexions with $h = 2n + 1$ are near to zero. The strong average intensity of the reflexions with $h = 4n$ is explained by the fact that many atoms are crowded on planes at $x = 0$, $x = 1/4$, $x = 1/2$ etc.

The discrepancy factor at this stage was 0.28 for all the observed reflexions.

REFINEMENT.

Five cycles of least-squares calculation carried out on the observed reflexions, using the ORFLS program by Busing, Martin and Levy, with isotropic temperature factors for all the atoms, lowered the R factor to 0.11.

At this stage it was observed that two oxygen atoms, O(11) and O(17), considered as water molecules, had temperature factors exceedingly high. This fact, together with the difficulties encountered in their location, suggested the following procedure. The multipliers of all the oxygen atoms were allowed to vary in the course of a cycle of the least-squares refinement. The result was a strong diminution of the multipliers of O(11) and O(17) while the remaining oxygens showed only slight variations in both directions. Thus some doubt on the presence of those atoms arose.

In order to solve the question a structure factors calculation, without O(11) and O(17) was carried out and the relative *Fo* Fourier synthesis was examined. This one appeared very disturbed by series termination effects and gave no conclusive information. In order to eliminate such perturbations a further Fourier synthesis was computed using $Fo \cdot \exp B \frac{\sin^2 \vartheta}{\lambda^2}$ as coefficient ($B = 3.0$) instead of *Fo's*. Most of the disturbances disappeared while the maxima corresponding to O(11) and O(17) remained and their heights were those expected on the basis of the multipliers obtained from the least-squares refinement. An usual ΔF synthesis confirmed these observations. All these data were interpreted in terms of an incomplete occupation of the positions the two water molecules involved.

In the difference synthesis there was also a sure evidence that Ba and Ca had anisotropic thermal factors. The three successive least-squares cycles were computed varying the multipliers of O(11) and O(17) and using anisotropic temperature factors for Ba and Ca atoms. It has not been thought worthwhile to extend the anisotropic treatment to all the atoms because of the uncertainity on the number of water molecules and because the scale factor was not unique.

TABLE I.

Final atomic parameters and their standard deviations (in parentheses).

The letter *w* labels those oxygen atoms which are considered as belonging to water molecules. The asterisk (*) is used to distinguish the equivalent isotropic temperature factors, after Hamilton [18], of those atoms which were treated anisotropically in the refinement.

ATOMS	x/a	y/b	z/c	B
Ba	0	0.2054(1)	0.2500	0.70*(4)
Ca(1)	0	0.2522(3)	—0.0022(1)	0.55*(8)
Ca(2)	0.2500	0.2500	0	0.40*(8)
Si(1)	0.1098(3)	0.1473(2)	0.1153(1)	0.17 (4)
Si(2)	0.3895(3)	0.1406(2)	0.1170(1)	0.24 (4)
Si(3)	0.2524(3)	0.2695(2)	0.1835(1)	0.08 (4)
Si(4)	0.2522(3)	0.4642(2)	0.1025(1)	0.10 (4)
O(1)	0.1212(6)	0.2073(6)	0.0582(3)	1.14 (12)
O(2)	0.1542(6)	0.2098(6)	0.1701(3)	1.28 (12)
O(3)	0.2536(7)	0.4234(5)	0.0386(3)	1.12 (12)
O(4)	0.1568(8)	0.0352(6)	0.1149(3)	1.76 (15)
O(5)	0.2571(7)	0.3699(5)	0.1476(3)	1.21 (12)
O(6)	0.3751(6)	0.1998(6)	0.0599(3)	1.17 (12)
O(7)	0.3464(8)	0.0251(7)	0.1159(4)	2.37 (17)
O(8)	0.3419(6)	0.1974(6)	0.1714(3)	1.20 (12)
O(9)*w*	0	0.4217(15)	0.0404(8)	5.36 (43)
O(10)*w*	0	0.3830(15)	0.1825(8)	5.52 (45)
O(11)*w*	0.5000	0.3823(23)	0.1682(12)	4.63 (98)
O(12)*w*	0.5000	0.4188(17)	0.0407(9)	6.43 (51)
O(13)*w*	0.1051(12)	0.0227(10)	0.2500	2.74 (24)
O(14)	0	0.1319(7)	0.1348(4)	0.64 (16)
O(15)	0.2491(9)	0.3002(8)	0.2500	1.22 (17)
O(16)	0.5000	0.1239(8)	0.1339(4)	1.07 (18)
O(17)*w*	0.3574(26)	0.0112(26)	0.2500	6.30 (1.21)

The final R factor is 0.083 for the observed reflexions and 0.116 for all the reflexions.

The anomalous dispersion correction for barium was carried out with the method proposed by Patterson [3]; $\Delta f'$ and $\Delta f''$ are given by Cromer [4].

The secondary extinction effect appeared to be nearly negligible and no correction was applied.

TABLE II.

Analysis of the anisotropic thermal parameters.

(Root mean square thermal vibration along the ellipsoid axes (Å), magnitudes of the principal axes (Å^2) and angles (°) between the crystallographic axes and the principal axes of the vibration ellipsoid).

ATOM	r.m.s.	B	α	β	γ
Ba	0.09	0.72	0	90	90
	0.12	1.15	90	0	90
	0.05	0.22	90	90	0
Ca(1)	0.06	0.30	90	118	28
	0.12	1.16	90	28	62
	0.05	0.21	0	90	90
Ca(2)	0.05	0.23	11	90	79
	0.11	0.97	93	16	74
	0.01	0.01	100	106	19

Final atomic coordinates and thermal parameters with their standard deviations are given in Table I. The analysis of the anisotropic thermal parameters of Ba, Ca(1) and Ca(2) is reported in Table II; of course their significance is lessened by the fact that not all the atoms were treated anisotropically and that the structure factors were scaled level by level. In Table III the final observed and calculated structure factors are compared.

DISCUSSION.

The interatomic distances and bond angles are presented in Table IV as well as their standard deviations.

Calcium. Both calcium atoms in the asymmetric unit have a six-fold coordination. Ca(1) is linked to four oxygens belonging to the Si–tetrahedra and to two water molecules. Ca(2) which lies on an inversion center, is surrounded by six oxygens of the Si–tetrahedra. The coordination polyhedra of both Ca atoms could be considered as squares bipyramids rather than octahedra because there are four oxygens forming a square around Ca at distances ranging from 2.29 to 2.35 Å, and two oxygens, at opposite sides of the square, with longer Ca—O distances (from 2.42 to 2.45 Å).

TABLE III.

Structure factors of macdonaldite.

Reflexions marked with an asterisk were unobservably weak; in this case Fo derives from 0.5 I_{min}.

k	l	10Fo	10Fc
0 k l			
0	4	3267	-3602
0	6*	370	373
0	8	5589	5989
0	10*	566	3
0	12	1768	1457
0	14	5634	-6101
0	16	5978	6500
0	18	3373	3470
0	20	2423	2299
0	22	1186	-1120
0	24	1603	1411
0	26*	429	819
0	28	3275	3589
2	0	4392	-5882
2	1	2988	-3444
2	3	2174	-2393
2	5	1863	1685
2	6	4129	-4709
2	7	5051	5399
2	8	1786	1331
2	9	1537	-1381
2	10	1234	1045
2	11	1171	-1074
2	12	5290	-5204
2	13	854	773
2	14	1225	-1177
2	15	3619	3601
2	16	5277	-5450
2	17	1333	-1240
2	18	941	-684
2	19	3179	-3171
2	20*	529	-675
2	21	1339	-1327
2	22	1006	-1015
2	23	2497	2673
2	24	2002	-2006
2	25	657	-478
2	26*	412	101
2	27	639	-722
2	28	1471	-1633
2	29	642	-781
4	0	3237	3158
4	1	3770	3888
4	2	287	329
4	3	3391	3391
4	4	5039	5733
4	5	2760	2750
4	6*	358	394
4	7	1378	614
4	8*	412	-275
4	9	1349	1314
4	10	2577	2296
4	11	1286	-1174
4	12	5834	5469
4	13	1486	1214
4	14*	565	-493
4	15	2749	-2455
4	16	2570	2331
4	17	1955	-1410
4	18*	552	648
4	19*	548	-4
4	20	2741	2629
4	21	1961	1883
4	22	2197	2196
4	23	1225	-1218
4	24*	457	204
4	25	952	901
4	26	1345	-1184
4	27	1230	1332
4	28	1801	2066
4	29*	270	256
6	0	554	-363
6	1	1959	-1505
6	2	2834	-2741
6	3	2500	2515
6	4	4354	-4869
6	5	2166	-2210
6	6	4291	-4411
6	7	2168	-2180
6	8	2290	2093
6	9	1683	-1489
6	10	984	-965
6	11	5490	5544
6	12	2206	-2105
6	13*	594	-193
6	14	2148	-1898
6	15*	630	-295
6	16*	611	-456
6	17	1358	-1060
6	18*	582	407
6	19	1086	846
6	20	1054	-1083
6	21	1223	-1165
6	22	3473	3584
6	23	1174	1227
6	24	698	-559
6	25	2281	-2099
6	26	843	-607
6	27	1109	1035
6	28	1059	-1207
8	0	2143	1965
8	1	1448	-908
8	2	980	1024
8	3	1592	-1401
8	4	1889	-1739
8	5	2003	2047
8	6	3209	3354
8	7*	519	284
8	8	2932	3029
8	9*	561	-472
8	10	3587	3505
8	11	3681	-3737
8	12*	617	-403
8	13	1118	987
8	14	2214	1927
8	15	2480	2001
8	16	2169	1855
8	17	824	-665
8	18	1681	1477
8	19	2081	-2122
8	20*	519	-346
8	21	1770	1647
8	22	1483	1486
8	23	992	959
8	24*	370	116
8	25	1569	1777
8	26	2327	2744
10	0	2005	-1884
10	1*	373	-287
10	2	2641	-2735
10	3	960	-839
10	4	2871	2884
10	5	1435	-1201
10	6	1457	-1501
10	7	1758	1649
10	8	3344	-3317
10	9	2738	-2608
10	10	4784	-5178
10	11*	623	-292
10	12	1872	1796
10	13	1313	1290
10	14*	644	-412
10	15	1237	1045
10	16*	599	-610
10	17*	552	-227
10	18	2787	-2864
10	19*	483	-587
10	20*	453	87
10	21*	406	-227
10	22	879	-802
10	23	2320	2516
10	24	478	407
12	0	2628	-2917
12	1*	583	-205
12	2	2205	2268
12	3	1910	1945
12	4	2442	2430
12	5	915	-785
12	6	2420	2634
12	7	2950	-3093
12	8*	602	-543
12	9*	602	671
12	10	1484	1716
12	11	1989	2094
12	12*	589	-102
12	13*	596	-614
12	14	2533	2449
12	16*	464	-188
12	17	1364	-1223
12	18	625	575
12	19	1117	1125
12	20*	317	-434
14	0	916	1220
14	1	1206	1470
14	2	1351	-1456
14	3*	566	-420
14	4*	561	-1025
14	5*	557	374
14	6	965	-1011
14	7	1459	1320
14	8*	532	4
14	9*	524	-332
14	10	2174	-2204
14	11*	503	-758
14	12	1838	-1591
14	13*	432	774
14	14	1529	-1752
14	15	1304	-1355
14	16	1012	1086
16	0	888	-752
16	1	2406	-2871
16	2*	432	818
16	3	740	-794
16	4	1534	1706
16	5	516	533
16	6	1609	1736
16	7	1236	1230
16	8*	367	244
1 k l			
1	2	722	-688
1	3	1648	2113
1	4	775	802
1	5	1717	-1914
1	6	957	-910
1	7	1942	1920
1	8	948	860
1	9	1429	-1455
1	10	815	-799
1	11	1587	1627
1	12	729	737
1	13	1342	-1457
1	14	557	-549
1	15	1667	1782
1	16*	351	208
1	17	920	-1036
1	18*	361	-337
1	19	1449	1516
1	20	705	611
1	21	1117	-1141
1	22	432	-492
1	23	1154	1212
1	24*	331	247
1	25	748	-766
1	26*	297	-346
1	27	1107	1223
1	28	416	432
1	29	677	-860
3	0	1311	-1225
3	1	1208	1260
3	2	1220	1165
3	3	857	-904
3	4	939	-964
3	5	858	913
3	6	1352	1293
3	7	1278	-1254
3	8	1380	1407
3	9	1350	1248
3	10	1226	1200
3	11	1349	-1294
3	12	1000	-908
3	13	746	640
3	14	1164	1046
3	15	1070	-1046
3	16	754	-690
3	17	523	547
3	18	893	802
3	19	863	-830
3	20	1020	-975
3	21	611	595
3	22	914	915
3	23	1042	-1047
3	24	640	-647
3	25	680	646
3	26	661	684
3	27	714	-729
3	28	731	-778
3	29	358	327
5	0	2062	2064
5	1	612	-582
5	2	1964	-2015
5	3	485	355
5	4	1537	1588
5	5	427	-363
5	6	1630	-1765
5	7*	285	306
5	8	1546	1651
5	9*	321	-385
5	10	1451	-1480
5	11	719	750
5	12	1186	1191
5	13*	403	-113
5	14	1804	-1652
5	15	644	499
5	16	1464	1481
5	17*	401	-84
5	18	1251	-1268
5	19*	388	255
5	20	1028	1024
5	21*	368	5
5	22	1172	-1185
5	23	542	530
5	24	1004	1063
5	25*	292	-225
5	26	835	-936
5	27*	239	268
5	28	615	820
7	0	1466	-1497
7	1	736	-785
7	2	1312	1425
7	3*	290	387
7	4	1052	-1135
7	5	477	-541
7	6	1184	1309
7	7	1120	1155
7	8	1037	-1065
7	9	1069	-1101
7	10	1312	1271
7	11*	396	88
7	12	1019	-968
7	13	649	-615
7	14	1457	1270
7	15	716	530
7	16	1209	-1171
7	17	644	-601
7	18	1024	970
7	19*	392	202
7	20	719	-740
7	21	707	-691
7	22	958	966
7	23	532	480
7	24	1015	-983
7	25*	258	-429
7	26	834	896
7	27*	188	-11
9	0*	338	385
9	1	839	846
9	2	814	-838
9	3	842	-871
9	4	1119	1119
9	5	908	901
9	6	590	-574
9	7	949	-942
9	8*	394	-13
9	9	1045	1088
9	10	1199	-1239
9	11	904	-600
9	13	820	864
9	14*	459	-401
9	15	807	-699
9	16*	440	308
9	17	1041	933
9	18	790	-749
9	19	563	-579
9	20	536	586
9	21	799	792
9	22	427	-380
9	23	619	-669
9	24*	392	457
9	25	767	889
11	0*	392	-342
11	1	799	-895
11	2*	393	184
11	3	1402	1539
11	4*	401	99
11	5	1290	-1437
11	6*	410	74
11	7*	418	630
11	8*	420	275
11	9	913	-1009
11	10*	427	318
11	11	1272	1321
11	12*	432	-167
11	13	1212	-1166
11	14*	436	182
11	15*	414	620
11	16*	388	68
11	17	1111	-1127
11	18*	324	18
11	19	963	1036
11	20*	268	-62
11	21	716	-892
11	22*	215	77
13	0*	403	-38
13	1	696	767
13	2*	414	367
13	3	739	-751
13	4	779	-870
13	5	771	845
13	6*	412	362
13	7*	409	-389
13	8*	406	-499
13	9	720	712
13	10*	394	400
13	11	941	-880
13	12	631	-624
13	13	872	794
13	14*	335	133
13	15*	311	-449
13	16*	278	-256
13	17	544	692
13	18	471	541
15	0*	354	311
15	1	591	-718
15	2*	351	-580
15	3*	351	109
15	4	882	1043
15	5*	240	-320
15	6*	337	-410
15	7*	335	369
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15	5*	302	-283
15	6	608	-650
15	7*	304	69
6 k l			
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0	6	589	338
0	8	1026	860
0	10	3112	-3051
0	12	1733	1700
0	14	844	737
0	16	861	865
0	18	1173	-1203
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0	22	977	-1123
0	24	2469	2733
0	26	1985	-2048
0	28	432	-477
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2	1	2387	-2557
2	2	720	668
2	3	649	613
2	4	1485	-1389
2	5	399	293
2	6	1603	1641
2	7*	353	67
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2	9	1636	-1446
2	10	1751	1547
2	11	1965	1841
2	12	2416	-2286
2	13	1286	-1193
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2	16	1490	1457
2	17	867	-592
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2	19	1955	1993
2	20	1865	-1992
2	21	390	-114
2	22	1320	1195
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2	24	1028	-1009
2	25	1034	-906
2	26	1715	2017
2	27	1624	1756
2	28	618	-716
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4	2*	277	240
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4	5	917	877
4	6	1150	-1079
4	7	2017	1941
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4	9	901	948
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4	16*	473	157
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4	19	961	-995
4	20*	427	-99
4	21*	405	-247
4	22	2443	-2558
4	23	763	-667
4	24	1567	1608
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4	26	746	925
4	27	976	-1036
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6	1	4200	-4633
6	2	730	-625
6	3	633	-214
6	4	824	748
6	5*	383	-211
6	6	1242	1220
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6	8	1553	-1522
6	9*	451	437
6	10*	473	-201
6	11	768	-768
6	12*	512	547
6	13	4173	-4124
6	14*	550	-445
6	15	4195	4164
6	16*	501	502
6	17*	479	220
6	18	868	-779
6	19	636	-467
6	20*	424	-329
6	21	1488	-1486
6	22	1199	1256
6	23	1084	1063
6	24*	315	-70
6	25	415	-221
6	26*	228	-150
8	0	1685	-1776
8	1	1697	1887
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8	5*	440	436
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8	8*	484	-140
8	9	876	866
8	10*	514	250
8	11	1621	-1456
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8	15	2340	-2184
8	16	1445	-1287
8	17	2111	2010
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8	20*	386	34
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TABLE III (*continued*).

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10	15	1022	911
10	16	1131	1036
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10	19	607	495
10	20	548	574
10	21*	283	-210
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12	1*	484	-373
12	2	1062	1153
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12	6*	490	-367
12	7	2468	2654
12	8*	490	-217
12	9	915	-849
12	10	1487	1505
12	11	1026	-987
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12	14*	397	559
12	15	599	540
12	16	1414	-1372
12	17	987	912
12	18	689	861
14	0*	433	134
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14	2*	431	-554
14	3*	427	-306
14	4	809	746
14	5*	422	447
14	6	833	-775
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14	12	1412	1616
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1	18*	436	-261
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1	24*	348	348
1	25	612	-680
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3	4	1028	-1186
3	5	655	764
3	6	1287	1443
3	7	882	-919
3	8	1295	-1405
3	9	704	746
3	10	1061	1032
3	11	1274	-1193
3	12	951	-962
3	13	877	826
3	14	1206	1137
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3	27	577	-724
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4	5	2092	2361
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6	7	1352	-1080
6	8	1156	985
6	9	1415	-1426
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6	12	2182	-1704
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6	17	1289	-1293
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1	4	423	466
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1	9	1094	-1049
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3	3	399	-299
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3	7	1205	-1221
3	8	774	-707
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3	11	871	-720
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8	14*	390	-282
8	15	528	-482
8	16*	334	-450
8	17	2105	2151
8	18	1175	1286
8	19	1324	-1347
8	20	758	-860
10	0*	380	85
10	1	1648	-1957
10	2	606	-654
10	3*	382	-333
10	4	1481	1555
10	5*	403	716
10	6	917	-872
10	7	769	748
10	8*	406	-234
10	9*	400	285
10	10*	400	-548
10	11*	398	-320
10	12	1574	1466
10	13	774	-926
10	14*	321	-308
10	15	1104	1153
10	16*	256	-7
10	17	611	-584
12	0*	374	51
12	1	1448	1541
12	2	579	609
12	3	1259	1011
12	4	1417	-1516
12	5	1509	-1549
12	6*	364	362
12	7*	364	317
12	8	601	-507
12	9*	350	242
12	10	1380	1364
12	11	1434	1399
12	12*	235	-5

Barium. Barium lies on a *mm* equipoint and so its coordination polyhedron is rather regular. This cation is surrounded by six oxygens lying at the corners of a slightly folded hexagon and by four water molecules. Two out of them are located above the hexagon, on a mirror plane, and two below, on another mirror plane normal to the former. The barium-oxygen system has a compact structure that is comparable with a close packed arrangement of spheres.

The Ba—O distances range from 2.82 to 2.87 Å; these values are very near to the sum of the ionic radii of the involved atoms (2.86 Å).

Silicon. Four silicon atoms occur in the asymmetric unit of macdonaldite. One silicon shares all the oxygens with other tetrahedra; the remaining three have one oxygen unshared. The bridging Si—O bonds of the latter three silicon atoms are appreciably different from the non-bridging bonds. The mean lengths of the bridging bonds are: Si(1)—O 1.629 Å, Si(2)—O 1.626 Å, Si(4)—O 1.625 Å; the lengths of the non-bridging bonds are: Si(1)—O(1) 1.567 Å, Si(2)—O(6) 1.567 Å, Si(4)—O(3) 1.597 Å. Such differences are consistent with the *d*–*p* π-bonding hypothesis suggested by Cruickshank [5].

TABLE IV.

Interatomic distances (Å) *and angles* (°) *and their standard deviations* (*in parentheses*).

An asterisk is used to distinguish equivalent atoms. The distances preceded by the sign ′ occur twice; those preceded by ″ occur four times.

ATOMS	Bond lengths	ATOMS	Bond angles
Si(1)—O(1)	1.567 (7)	O(1)—Si(1)—O(2)	112° 33′ (28′)
—O(2)	1.651 (7)	O(1)—Si(1)—O(4)	114° 15′ (28′)
—O(4)	1.610 (8)	O(1)—Si(1)—O(14)	113° 43′ (28′)
—O(14)	1.625 (8)	O(2)—Si(1)—O(4)	107° 34′ (28′)
Si(2)—O(6)	1.567 (7)	O(2)—Si(1)—O(14)	101° 33′ (28′)
—O(7)	1.631 (9)	O(4)—Si(1)—O(14)	106° 13′ (28′)
—O(8)	1.625 (7)	O(6)—Si(2)—O(7)	113° 25′ (28′)
—O(16)	1.620 (8)	O(6)—Si(2)—O(8)	113° 22′ (28′)
Si(3)—O(2)	1.620 (9)	O(6)—Si(2)—O(16)	113° 42′ (28′)
—O(5)	1.565 (7)	O(7)—Si(2)—O(8)	106° 32′ (28′)
—O(8)	1.601 (9)	O(7)—Si(2)—O(16)	103° 37′ (28′)
—O(15)	1.617 (6)	O(8)—Si(2)—O(16)	105° 21′ (28′)
Si(4)—O (3)	1.597 (6)	O(2)—Si(3)—O(8)	110° 33′ (28′)
—O(4)*	1.621 (9)	O(2)—Si(3)—O(5)	109° 41′ (28′)
—O(5)	1.633 (7)	O(2)—Si(3)—O(15)	106° 37′ (28′)
—O(7)*	1.622 (11)	O(8)—Si(3)—O(5)	111° 26′ (28′)
Ca(1)—O(1)	′ 2.299 (8)	O(8)—Si(3)—O(15)	110° 3′ (28′)
—O(6)*	′ 2.308 (8)	O(5)—Si(3)—O(15)	108° 22′ (28′)
—O(9)w	2.437 (20)	O(5)—Si(4)—O(7)*	106° 45′ (28′)
—O(12)w	2.417 (22)	O(5)—Si(4)—O(4)*	106° 4′ (28′)
Ca(2)—O(1)	′ 2.340 (7)	O(5)—Si(4)—O(3)	111° 4′ (28′)
—O(3)	′ 2.447 (6)	O(7)*—Si(4)—O(4)*	111° 2′ (28′)
—O(6)	′ 2.350 (7)	O(7)*—Si(4)—O(3)	111° 29′ (28′)
Ba—O(2)	″ 2.874 (7)	O(4)*—Si(4)—O(3)	110° 15′ (28′)
—O(14)	′ 2.880 (9)	Si(1)—O(14)—Si(1)*	144° 4′ (56′)
—O(10)w	′ 2.820 (20)	Si(1)—O(2)—Si(3)	135° 41′ (36′)
—O(13)w	′ 2.814 (14)	Si(3)—O(15)—Si(3)*	151° (56′)
O(3)—O(3)*	2.71 (2)	Si(3)—O(5)—Si(4)	170° 24′ (36′)
O(9)w—O(9)w*	2.80 (6)	Si(3)—O(8)—Si(2)	137° 24′ (36′)
O(12)w—O(12)w*	2.87 (6)	Si(2)—O(16)—Si(2)*	147° 27′ (56′)
O(11)w—O(13)w	3.05 (3)	Si(4)—O(7)*—Si(2)*	140° 53′ (36′)
O(17)w—O(10)w*	3.06 (3)	Si(4)—O(4)*—Si(1)*	148° 28′ (36′)
O(8)—O(17)w	3.07 (3)		
O(2)—O(10)w	3.16 (2)		
O(2)—O(13)w	3.17 (1)		

The tetrahedron around Si(3) needs a more detailed discussion. Si(3) shares all its oxygens with other tetrahedra and the average Si(3)—O distance is 1.601 Å. It must be pointed out that the Si(3)—O(5) distance is the shortest of all the Si—O distances of macdonaldite. Pant and Cruickshank [6] suggest that large Si—O—Si angles " cause the bridging bonds to gain strength at the expense of peripheral bonds ". Actually the Si(4)—O(5)—Si(3) angle is 170° and this fact could explain the short Si(3)—O(5) distance. On the other hand the second bond distance, Si(4)—O(5), involved in the cited angle, is 1.633 Å. One could expect, on the basis of the cited large angle, a shorter length for the Si(4)—O(5) bridging bond, but one must take into account the different π-orders existing in the Si(4)-tetrahedron. However the average of the two Si—O(5) distance is 1.60 Å that is a value which could be expected for a Si—O—Si angle of 170°. Fig. 1 shows a plot of the Si—O—Si angles of some recently studied silicates versus the average of the two Si—O bridging bonds lengths involved. One can observe a rather regular shortening of the $\overline{\text{Si—O}}$ distances (from a value of about 1.63 Å) with the increasing of the angles (from a value of about 137°).

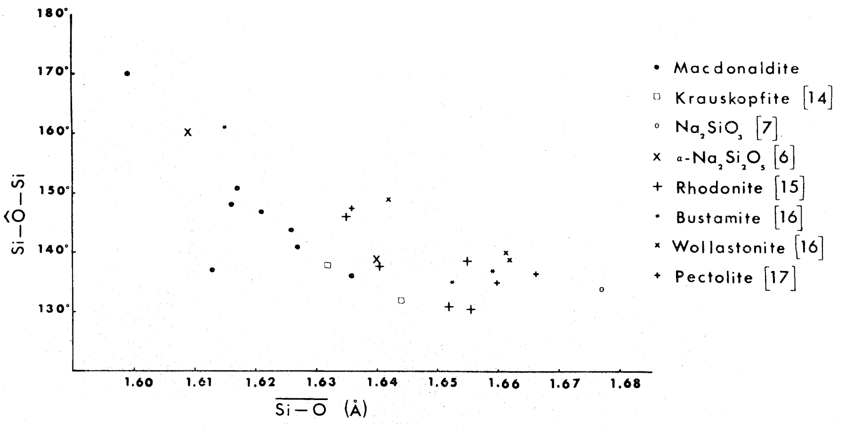

Fig. 1. – Plot of the average of the two Si—O distances involved in one Si—O—Si angle versus the Si—O—Si angle for some recently studied silicates.

The O—Si—O angles range from 101° to 114°. By plotting the mean lengths of any pair of bonds forming an angle at Si, against the O···O distances, the results of this work fit the corresponding curve given by McDonald and Cruickshank [7].

Balance of electrostatic valences. The balance of electrostatic valences computed in the usual way, assigning a bond strength of 1.00 to tetrahedral Si—O bonds, 1/3 to Ca—O bonds and 1/5 to Ba—O links, give some unacceptable results: O(2) and O(14) are " overbonded " (2.20) while O(1), O(6) and O(3) are " underbonded " (1.66, 1.66 and 1.33 respectively). The valences get balanced if one accept the suggestion of Zachariasen [9] that " the observed bond lengths uniquely determine the bond strengths ". In this way O(1) and O(6), which form with silicon non-bridging bonds of 1.57 Å, would have a bond strength greater than 1.00; O(2) and O(14) which form with silicon bridging bonds of 1.62–1.63 Å, would have a bond strength less than 1.00. As Pant [8] observes "...the two theories *(d–p* π–bonding theory and the method of balancing of valences) for the Si—O bonds are not exclusive. π–bonding in Si—O bonds may be part of the mechanism whereby valency balance is achieved".

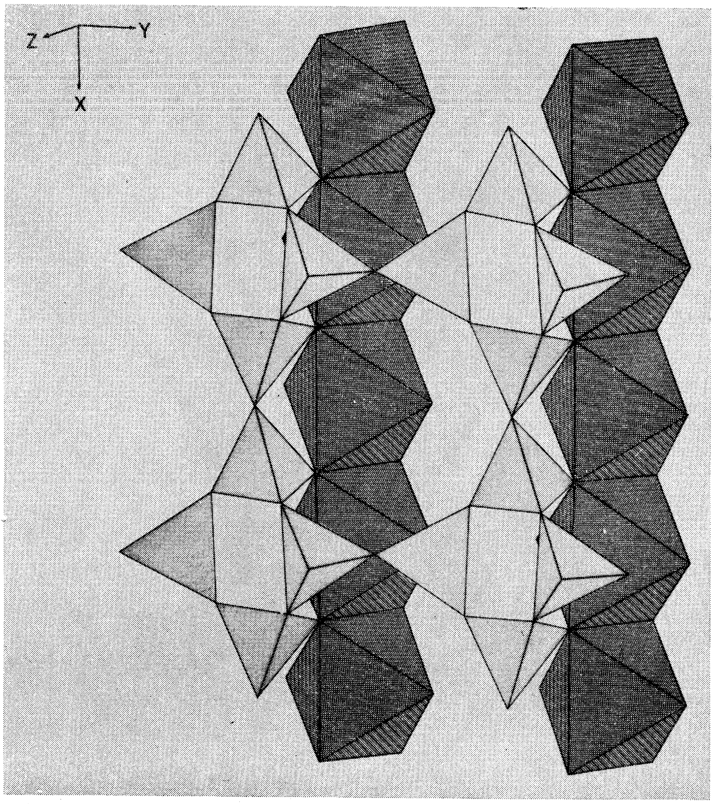

Fig. 2. – Perspective view of the chains of Ca–octahedra and of a layer of tetrahedra. The rings of four and eight tetrahedra are shown; the layer is doubled by a mirror plane parallel to *xy*.

For the case of O(3) it is necessary to spend some more words. In fact, for this atom the valences balance is not achieved even with the application of the cited method; O(3) is linked to Si(4) with a non-bridging bond of 1.597 Å and to Ca(2); in such a way the positive charge reaching this oxygen is about 1.4 that is far from 2.0. On the other hand, if this atom is considered to be a hydroxyl group, it would be "overbonded" (1.4 + 1.0). Furthermore, the chemical formula would have an excess of positive charges. The O(3)—O(3′) distance of 2.70 Å is the shortest distance between oxygens not belonging to the same coordination polyhedron and surely represents a hydrogen bond, but it seems too long (Zachariasen [9]) for the hypothesis of a hydrogen atom occurring midway between O(3) and O(3′). Thus the possibility of a statistical distribution of one hydrogen between the two equivalent O(3) seems to be the more convenient one. This assumption permits to get balanced the valences of O(3) and the sum of positive and negative charges in the chemical formula.

Description of the structure. The crystal structure of macdonaldite is characterized by the presence of double layers of Si—tetrahedra connected by layers of Ca—octahedra (1).

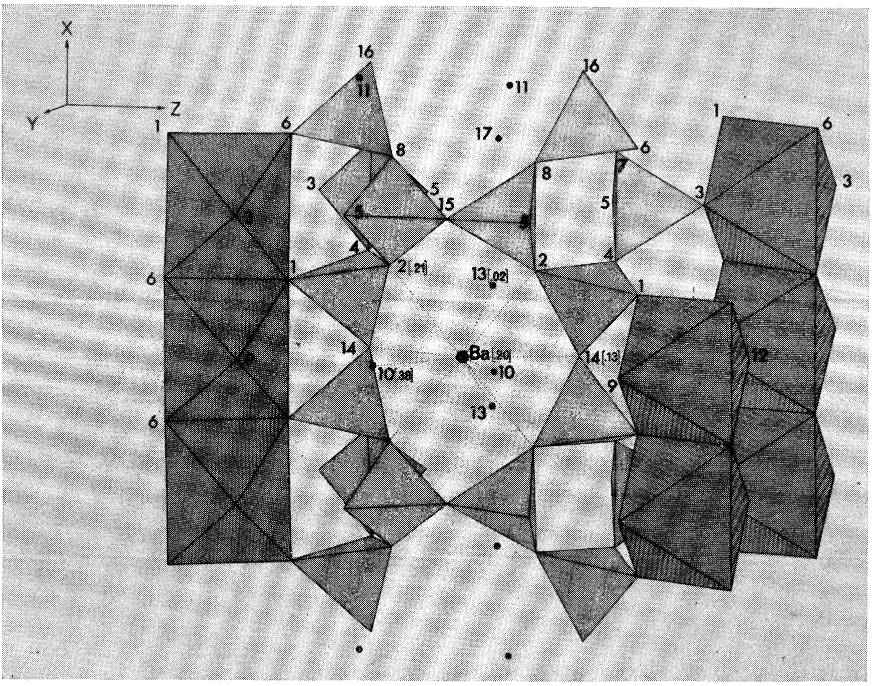

Fig. 3. – Perspective view of the structure following *b*. The ring of tetrahedra normal to *b* is shown. The small black circles represent water molecules occurring in the channels and those linked to barium. The number in square parentheses are the *y* coordinates. The chains of octahedra occur at $z = 0$ and $1/2$.

The Ca—octahedra, sharing two opposite edges, form chains parallel to *a*. The chains are linked to one another with hydrogen bonds and give rise to sheets parallel to (001) and occurring at $z = 0$ and $z = 1/2$.

The tetrahedral framework is located between two of such octahedral sheets. The basic unit of the silicate framework is a ring of four tetrahedra. The rings are linked together to form a corrugated layer of tetrahedra parallel to (001) (See fig. 2). The presence of the mirror plane at $z = 1/4$

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(1) The coordination polyhedra of calcium have been described as square bipyramids, but in the course of this description they will be designated more simply as octahedra.

makes the layer doubled. Each single layer is very similar to the " idealized " apophyllite layer which is derived from the condensation of wollastonite chains through the xonotlite ribbon. The doubling of the layers produces two sets of channels built up by eight-membered rings of tetrahedra: one set is parallel to *a* with a free diameter of 3.4 Å and the other is parallel to *b* with a free diameter of 2.1 Å (figs. 3 and 4). The barium atoms and the water molecules not linked to calcium occur in these channels.

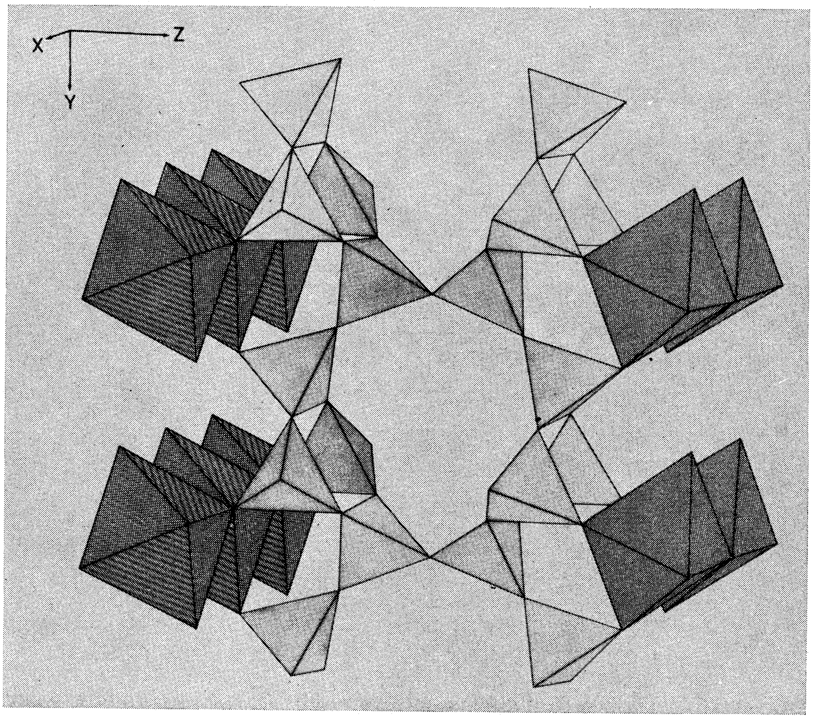

Fig. 4. – Perspective view of the structure showing the ring of tetrahedra that forms channels parallel to *a*.

The fact that the thermogravimetric curve of macdonaldite resembles those of mesolite and scolecite [1] and the presence of such channels, suggested the possibility of some relationship between fibrous zeolites and macdonaldite. In effect some structural arguments give strength to this hypothesis. Fig. 5 (left) shows the structural feature characteristic of natrolite [10] and of all the fibrous zeolites: it is a ring of four tetrahedra (two Si and two Al) with alternate vertices pointing upwards and downwards; a fifth Si–tetrahedon links the upper vertices and, repeated 6.6 Å below, the lower ones to form a sort of string parallel to *c*. The vertices labelled 1 to 4 connect together neighbouring strings thus forming a three-dimensional tetrahedral framework. The openings among neighbouring chains give place to a double system of channels (with free diameter of 2.08 and 2.6 Å) formed by eight-membered rings of tetrahedra. Fig. 5 (right) shows the four Si–tetrahedra and one of the two Ca–octahedra contained in the asymmetric unit of macdonaldite. This group could be derived from that showed in the left part of the figure by substituting in this one the tetrahedron labelled 4 with an octahedron. The figs. 3 and 4 permit to see how this structural feature of macdonaldite (four tetrahedra and one octahedron) is repeated in the structure and the role played by the octahedra of the second Ca atom.

The water molecules. Water is present in the coordination polyhedra of barium and calcium and, as " free " or zeolitic water, in the channels of the tetrahedral framework. Ca(1) is linked to two water molecules, O(9) and O(12) lying on a mirror plane. Each of these water molecules form a hydrogen bond which together with that occurring between O(3) and O(3′) contributes to hold together the chains of Ca–octahedra.

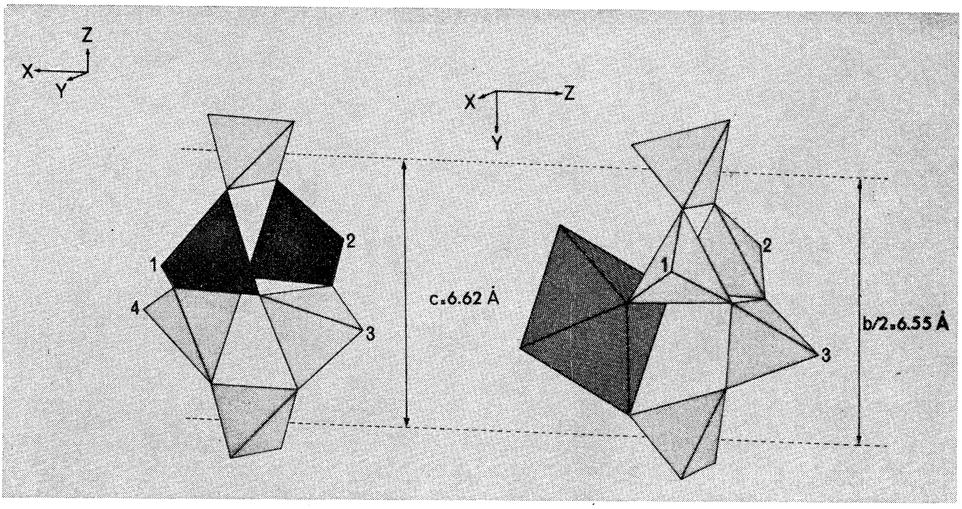

Fig. 5. – Left: the structural feature characteristic of fibrous zeolites; dark tetrahedra are AlO_4 groups. Right: the structural feature of macdonaldite built up by four Si–tetrahedra and by one Ca–octahedra; the Ca atom involved is that labelled Ca(1).

The water molecules occurring in the channels and not linked to the cations are labelled O(11) and O(17). They occupy two positions, on mirror planes, related by a pseudo-mirror plane to those of O(10) and O(13). The occupancy is 64 % for O(11) and 56 % for O(17); the unit cell contains 9.6 of such water molecules. They are linked very weakly to the water molecules belonging to the coordination polyhedron of barium and to some oxygens of the Si–tetrahedra.

It must be pointed out that there is room in the channels for other atoms (cations or water) and the number of free water molecules could vary without disturbing the structure.

Chemical formula. On the basis of all the considerations made in the preceding discussions and of the fact that the number of H_2O linked to calcium and barium could not be varied without important changes in the structure, the chemical formula of macdonaldite can be written as follows:

$$4\,[BaCa_4H_2Si_{16}O_{38}\cdot(8+x)H_2O]$$

where x is the number of free water molecules; in the case of the present work $x = 2.4$.

This formula is somewhat different from that given by Alfors *et al.* [1]. However the chemical analysis calculated from it does not diverge from the experimental analyses more than that calculated from the formula published by the mentioned Authors (Table V).

TABLE V.

Oxides in wt. %	1	2	3	4	5
SiO_2	61.1	62.1	61.00	61.00	62.23
Al_2O_3	0.06				
TiO_2	0.01	0.03			
FeO	<0.01	0.1	0.96		
MgO	<0.05	0.10			
CaO	14.8	14.95	15.3	15.19	14.53
BaO	10.2	9.0	9.3	10.38	9.93
H_2O	13.7	13.7	13.7	13.42	13.30
Total . . .	100.0	100.0	100.3	100.00	100.00

Analyses 1, 2 and 3 are published by ALFORS *et al.* [1].

1, 2: analyses made by G. W. Putman by *d–c* arc emission spectrograph methods;

3: wet chemical analysis made by M. Tavela;

4: chemical analysis calculated from the chemical formula given by ALFORS *et al.* [1], $4\,[BaCa_4Si_{15}O_{35}\cdot 11\,H_2O]$;

5: chemical analysis calculated from the chemical formula given in this work, $4\,[BaCa_4H_2Si_{16}O_{38}\cdot 10.4\,H_2O]$.

CONCLUSION.

The description of the crystal structure made previously in terms of double layers of tetrahedra appears to be more suitable than that emerging from the comparison with the fibrous zeolites for a convenient introduction of macdonaldite in the Zoltai classification of silicates [11]. The crystal structure of this silicate, characterized by double layers of the apophyllite type, fills a gap in the series of structure families having as common feature the wollastonite chain. Table VI shows the two series of structure families that can be derived respectively from the pyroxene chain and from the wollastonite chain: in the second series, the place corresponding to the " double sheets " subtype, the same as the hexagonal celsian family, was empty.

TABLE VI.

	PYROXENE CHAIN		WOLLASTONITE CHAIN	
	Structure family	Repeat unit or loop of tetrahedra	Structure family	Repeat unit or loop of tetrahedra
Single chain	Pyroxenes	2	Wollastonite	3
Double chain	Amphiboles	6	Xonotlite	8
Single sheet	Micas	6	Apophyllite	4–8
Double sheet.	Hexagonal celsian	4–6	Macdonaldite	4–8

TABLE VII.

MINERAL	CELL DIMENSIONS	CHEMICAL FORMULA
Macdonaldite . . .	$a = 14.08$ $b = 13.11$ $c = 23.56$ Å	$4[BaCa_4H_2Si_{16}O_{38} \cdot 10.4\ H_2O]$
Rhodesite	$c = 14.10$ $b = 13.08$ $a = 23.8$ Å	$4[K_2Na_2Ca_4Si_{16}O_{38} \cdot 12\ H_2O]$
Delhayelite	$b = 7.04$ $a = 13.05$ $c = 24.65$ Å	

Probably macdonaldite is not the sole member of this structure family. Two minerals have crystallographic, physical and chemical properties similar to those of macdonaldite. They are rhodesite [12] and delhayelite [13] which can be compared also with fibrous zeolites. In Table VII are reported the crystallographic and chemical properties of these two silicates and of macdonaldite. The chemical formula of delhayelite is not so immediately comparable with that of macdonaldite as is that of rhodesite. The number of cations in this one is greater than that of macdonaldite, but it must be observed that the number of Ca, Si and O, the atoms which build up the foundamental part of the structure, is the same and that in the structure of macdonaldite there is room for other cations or water molecules. However only the structural analysis could confirm or discard the hypothesis.

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