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The crystal structure of wagnerite

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Mineralogia. — *The crystal structure of wagnerite* (*). Nota (**) di ALESSANDRO CODA, GIUSEPPE GIUSEPPETTI e CARLA TADINI, presentata dal Socio G. CAROBBI.

RIASSUNTO. — La wagnerite $Mg_2F(PO_4)$ cristallizza nel gruppo spaziale $P2_1/c$, con 16 unità stechiometriche nella cella elementare e con costanti reticolari: $a = 9{,}644$, $b = 12{,}679$, $c = 11{,}957$, $\beta = 108^{\circ}\ 18'$.

La determinazione della struttura è stata realizzata per mezzo di fotogrammi Weissenberg dei livelli da 0 a 8 secondo l'asse b, radiazione CuK_{α}. Dai fotogrammi ottenuti si notava che i riflessi $(h\,k\,l)$ con k pari avevano una intensità media superiore a quelli con k dispari. Escludendo questi ultimi riflessi la struttura poteva riferirsi ai tre periodi reticolari: $a, b/2, c$, con una pseudocella appartenente al gruppo spaziale $I2/c$.

Basandosi su questa pseudocella ed eseguendo una sintesi di Patterson tridimensionale con i soli riflessi con k pari, si ricavarono le coordinate degli atomi di magnesio, fosforo e ossigeno. Le differenze strutturali fra le due pseudocelle costituenti la vera cella elementare furono attribuite in modo preminente agli atomi di fluoro, per le cui posizioni si avanzò una adeguata ipotesi.

Le sezioni di densità elettronica eseguite utilizzando anche i riflessi con k dispari confermarono l'ipotesi. La struttura fu successivamente raffinata con alcuni cicli di minimi quadrati sulle coordinate e sui parametri termici isotropi, raggiungendo un fattore di discordanza R di 0,064 relativo a tutti i riflessi osservati, eccetto quelli affetti da estinzione.

Nella struttura sono presenti ottaedri di coordinazione MgO_4F_2 non regolari, poliedri a coordinazione cinque MgO_4F riferibili a bipiramidi trigonali alquanto distorte ed infine gruppi tetraedrici PO_4 piuttosto regolari; essi sono collegati secondo un concatenamento tridimensionale. Ogni atomo di ossigeno partecipa alla coordinazione di due atomi di magnesio e di uno di fosforo, mentre ogni atomo di fluoro è coordinato a tre diversi atomi di magnesio. Tutte le distanze di legame rientrano nella norma.

INTRODUCTION.

Wagnerite $Mg_2F(PO_4)$ was firstly found in quartz veins traversing clay slates at Höllgraben near Warfen and at Radelgraben near Bischofshofen in Salzburg (Austria) (Fuchs, 1821) [1].

The morphological, optical, physical and chemical properties of wagnerite were studied by various Authors and reported by Dana (1951) [2]. They are summarized as follows:

monoclinic prismatic, $0.957 : 1 : 0.753$, $\beta = 108^{\circ}\ 7'$;
habit prismatic [001]; cleavages {100} and {120} imperfect;
specific gravity 3.15; luster vitreous; colour variable.

Optical data: biaxial positive, $2V = 28^{\circ}\ 24'$, $n_X = 1.568$, $n_Y = 1.572$, $n_Z = 1.582$, $Y \equiv b$, $Z \frown c = -21^{\circ}\ 30'$.

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Chemical analyses are reported from wagnerite from Werfen and Bamle and they are consistent with the stoichiometric unit $Mg_2F(PO_4)$, with some divalent Fe and Mn replacing Mg.

EXPERIMENTAL.

The X–ray diffraction data were collected by using a crystal of wagnerite from Werfen, which was ground into spherical shape ($R = 0.35$ mm).

The lattice parameters were determined by measuring, with a single crystal diffractometer, the 2θ–values of a series of high order reflections, then applying the least-squares method to the relation between the interplanar distances and the lattice parameters.

They are as follows:

$$\begin{aligned} a &= 9.644 \pm 0.007\ \text{Å} \\ b &= 12.679 \pm 0.008\ \text{Å} \\ c &= 11.957 \pm 0.008\ \text{Å} \\ \beta &= 108^\circ\ 18' \pm 9' \end{aligned}$$

that agree with those reported in literature (Strunz, 1966) [3]:

$$a = 11.92\ \text{Å} \quad , \quad b = 12.53\ \text{Å} \quad , \quad c = 9.65\ \text{Å} \quad , \quad \beta = 108^\circ\ 7'.$$

The parameters a and c were interchanged in the present work with respect to the latter data in order to achieve the conventional orientation of the International Tables.

The chemical composition assumed for the structure analysis was $Mg_2F(PO_4)$, as reported in the literature. Sixteen stoichiometric units are contained in the unit cell ($Z = 16$); the density so calculated is 3.11 g/cm^3 (observed specific gravity 3.15).

The space group is $P2_1/c$.

Equiinclinated Weissenberg photographs of the integrated reflections were taken by the multiple-film technique and CuK_α radiation, b being the rotation axis and k ranging from 0 to 8.

The evaluation of the intensities was accomplished with a Nonius microdensitometer; the independent reflections above the limits of detection were 1197 out of the 2154 ones taken into consideration.

The corrections applied to the intensities were concerned with the absorption (linear coefficient $\mu = 100\ cm^{-1}$ for CuK_α), the $\alpha_1 - \alpha_2$ spot doubling and the Lp factor.

The intensities for the different levels were approximately on the same scale because of the equal exposure times; better scale factors were obtained after the first calculation of the structure factors by applying the relation $\Sigma F_o = \Sigma F_c$ level by level, and they were improved during the least-squares refinement.

STRUCTURE ANALYSIS.

The following features were evident from a simple inspection of the Weissenberg photographs:

1) the average intensity of the general reflections with k even is much higher than that of the reflections with k odd;

2) if one assumes that the general reflections with k odd are absent, and the remaining reflections are indexed on the basis of a monoclinic pseudo-cell with $a_p = a$, $b_p = b/2$, $c_p = c$, it is possible to derive the space group I2/c according to the observed extinctions and excluding very few feeble reflections (the extinctions are as follows: $hk'l$ with $h + k' + l$ odd, $h0l$ with l odd: here $k' = k/2$).

The previous points 1) and 2) induced to think that a rough structure could be obtained by using only the general reflections with k even and by working on the pseudo-cell in the space group I2/c, $Z = 8$.

The three-dimensional Patterson synthesis calculated by using only the reflections with k even gave the positions of two non-equivalent Mg–atoms, of all the P–atoms and of four non equivalent O–atoms surrounding phosphor.

A three-dimensional electron density synthesis was successively obtained on the basis of these coordinates. The locations of the peaks were consistent with the parameters assumed for Mg, P and O, and new maxima appeared which reasonably could be attributed to F–atoms; however in the entire pseudo-cell a double number of peaks (16 on two series of non-equivalent positions) was observed for respect to what one could expect (8 on only one series of equipoints), and their average height was about half that of the O–atoms.

This observation allowed the formulation of a hypothesis on the true structure of wagnerite. One could think that in the two pseudo-cells superimposed along b, in order to form the true unit cell, all the atoms, but fluorine, occupied identical positions, whereas F–atoms lay in different places distributed among the 16 positions of the observed peaks. Eight of such positions should be occupied in the lower pseudo-cell, and the remaining in the upper one, according to the true space group. In other words the doubling of the period along b in the passage from the pseudo-cell to the true cell should be imputable mainly to the location of the F–atoms.

According to this hypothesis a model of structure was worked out in the correct space group P2$_1$/c starting from the positions of the atoms in the pseudo-cell: obviously only the F–atoms contributed to the structure factors with k odd.

The multiplicity of a general equipoint in the space group I2/c is 8, whereas it is 4 in the space group P2$_1$/c. Since the real cell contains a number of atoms double of that corresponding to the pseudo-cell, each series of equivalent positions in the latter is transformed in four series of equivalent positions in the true cell.

TABLE I.

Atomic coordinates and their standard deviations (in parentheses).

Atom	x/a	y/b	z/c	B (Å^2)
Mg(1)	0.5519 (3)	0.0708 (4)	0.9131 (2)	0.71 (5)
Mg(2)	0.4661 (3)	0.0697 (4)	0.6003 (2)	0.73 (5)
Mg(3)	0.0458 (3)	0.1820 (3)	0.9195 (2)	0.47 (5)
Mg(4)	0.9648 (3)	0.1782 (4)	0.6071 (2)	0.43 (5)
Mg(5)	0.1907 (3)	0.0193 (3)	0.1900 (2)	0.35 (4)
Mg(6)	0.7896 (3)	0.0040 (3)	0.3071 (2)	0.28 (4)
Mg(7)	0.3066 (3)	0.2316 (3)	0.3134 (2)	0.54 (5)
Mg(8)	0.7069 (3)	0.2457 (3)	0.1947 (2)	0.36 (4)
P(1)	0.1165 (2)	0.0764 (3)	0.4257 (2)	0.36 (3)
P(2)	0.8787 (2)	0.0716 (3)	0.0760 (2)	0.34 (3)
P(3)	0.3836 (2)	0.1753 (3)	0.0752 (2)	0.35 (4)
P(4)	0.6200 (2)	0.1781 (3)	0.4235 (2)	0.36 (4)
O(1)	0.1766 (6)	0.1114 (6)	0.3258 (5)	0.65 (10)
O(2)	0.7981 (6)	0.0943 (6)	0.1646 (5)	0.63 (9)
O(3)	0.3160 (6)	0.1430 (7)	0.1708 (5)	0.90 (10)
O(4)	0.6921 (6)	0.1501 (7)	0.3296 (5)	0.97 (10)
O(5)	0.2436 (6)	0.0469 (6)	0.5355 (5)	0.68 (9)
O(6)	0.7674 (6)	0.0539 (6)	0.9529 (5)	0.74 (9)
O(7)	0.2635 (6)	0.2030 (6)	0.9601 (5)	0.68 (10)
O(8)	0.7387 (6)	0.2032 (6)	0.5398 (5)	0.67 (10)
O(9)	0.9858 (6)	0.0180 (7)	0.6208 (5)	0.92 (10)
O(10)	0.0227 (6)	0.0272 (7)	0.8844 (5)	0.66 (10)
O(11)	0.4843 (6)	0.2291 (7)	0.6180 (5)	0.76 (10)
O(12)	0.5190 (6)	0.2252 (7)	0.8817 (5)	0.82 (10)
O(13)	0.4731 (6)	0.0836 (8)	0.0511 (5)	0.98 (10)
O(14)	0.5190 (6)	0.0877 (8)	0.4393 (5)	1.01 (10)
O(15)	0.0265 (6)	0.1659 (7)	0.4561 (5)	0.65 (10)
O(16)	0.9831 (6)	0.1611 (8)	0.0688 (5)	0.85 (10)
F(1)	0.4171 (5)	0.0475 (5)	0.7548 (4)	1.16 (8)
F(2)	0.6706 (5)	0.0828 (5)	0.7146 (4)	1.17 (8)
F(3)	0.1724 (5)	0.1625 (5)	0.7200 (4)	1.22 (9)
F(4)	0.9139 (5)	0.2044 (5)	0.7598 (4)	1.18 (8)

In the suggested model the four series corresponding to each unique series of atoms in the pseudo-cell were still related by the symmetry of the space group $I\,2/c$; the successive refinements slightly changed this situation, showing that also the Mg, P and O–atoms give a little contribution to the reflections with k odd.

The agreement between the observed and calculated structure factors was satisfactory, thus supporting the suggested model which represented the starting point for a refinement by means of the application of six cycles of the least-squares method.

Two cycles were carried out on an Olivetti Elea 6001 computer, using a full matrix program by Sgarlata (1965) [4]. Four more cycles were carried out by using the program of Busing and Levy for the IBM 7040 computer. The reflections affected by extinction and the unobservable ones (except those with a value of F_c higher than the minimum observable) were excluded from the least-squares calculations.

During the first four cycles the positional parameters as well as the isotropic thermal factors were refined. In the fifth cycle the refining of the anisotropic thermal parameters was attempted, but several coefficients without physical significance appeared, probably showing that the number of involved parameters was too high in comparison with the available experimental data. The anisotropic refinement was no longer tried and a new cycle was carried out with isotropic thermal factors. The last changes of the parameters were, on the average, many times lower than the corresponding standard deviations: so the refinement was stopped.

The final atomic parameters and their standard deviations are listed in Table I. The observed and calculated structure factors are compared in Table II.

An overall R index, referred to the structure factors, was calculated by assigning a value of half of the minimum observed to the intensities of the 150 reflections which were visible, but below the limit of detection of the microdensitometer, furthermore a value of a quarter of the minimum observed to the intensities of the remaining 807 unobservable reflections. This overall R index dropped from 0.35 at the beginning of the refinement to 0.105 at the end.

The final R index for the observed reflections, excluding those affected by extinction, was 0.064.

DESCRIPTION OF THE STRUCTURE.

The crystal structure of wagnerite is more easily described in terms of coordination polyhedra. Three kinds of such polyhedra are present, that is: fairly regular tetrahedra PO_4, distorted octahedra MgO_4F_2 and distorted trigonal bipyramids MgO_4F, which are joined to one another by sharing either edges or vertices, in such a way as to build up a three-dimensional framework.

TABLE II.

Observed and calculated structure factors.

An asterisk marks the reflections affected by extinction. The sign ° marks the unobservable reflections and should be read as " less than ". The absent low-angle reflections were screened by the X-ray beam stop.

h	±l	$10F_o$	$10F_c$
h 0 l			
0	2	743	752
0	4	1132	-1198
0	6	*1780	-2026
0	8	*2056	-2258
0	10	718	711
0	12	658	569
0	14	117	-60
1	2	• 59	-8
1	4	• 84	13
1	-4	• 77	30
1	6	•100	17
1	-6	• 93	61
1	8	139	126
1	-8	•109	-80
1	10	•119	-42
1	-10	•119	-51
1	12	•102	-73
1	-12	•113	65
1	14	• 68	19
1	-14	123	72
2	0	460	476
2	2	*2867	4022
2	-2	524	-515
2	4	938	994
2	-4	*3804	-4946
2	6	*2687	-3120
2	-6	1893	-2042
2	8	727	729
2	-8	1944	2038
2	10	1329	-1253
2	-10	1587	1584
2	12	231	-206
2	-12	1080	976
2	-14	459	-445
3	0	• 78	33
3	2	• 87	-22
3	-2	• 78	70
3	4	•101	-61
3	-4	• 86	-47
3	6	•112	• 76
3	-6	• 97	109
3	8	•119	49
3	-8	•109	-74
3	10	•111	18
3	-10	•119	40
3	12	• 81	-23
3	-12	•113	-20
3	-14	115	131
4	0	1367	1330
4	2	2463	2708
4	-2	1529	-1614
4	4	346	270
4	-4	1435	-1452
4	6	1485	1574
4	-6	131	-86
4	8	687	-655
4	-8	1918	1906
4	10	127	-89
4	-10	555	415
4	12	592	-568
4	-12	2155	-2108
4	-14	708	-692
5	0	• 99	35
5	2	•107	16
5	-2	• 95	32
5	4	•114	-36
5	-4	•100	-40
5	6	•119	-104
5	-6	•106	-62
5	8	147	119
5	-8	•114	-24
5	10	• 90	81
5	-10	•119	-62
5	-12	•111	74
5	-14	• 87	47
6	0	707	664
6	2	730	-668
6	-2	889	-867
6	4	274	-288
6	-4	1377	-1352
6	6	781	-730
6	-6	2302	2446
6	8	206	160
6	-8	408	-355
6	10	1074	1150
6	-10	442	-331
6	-12	685	-590
6	-14	581	-561
7	0	•116	70
7	2	194	85
7	-2	•111	-40
7	4	•118	17
7	-4	•114	3
7	6	•109	-60
7	-6	•116	-38
7	8	• 86	-26
7	-8	•119	39
7	-10	•116	10
7	-12	•102	64
7	-14	• 72	-36
8	0	262	111
8	2	*2434	2718
8	-2	479	519
8	4	•109	-41
8	-4	656	-619
8	6	906	-937
8	-6	1518	-1502

h	±l	$10F_o$	$10F_c$
8	-8	247	222
8	-10	1042	-920
8	-12	792	-736
8	-14	1189	1228
9	0	•116	15
9	2	•108	53
9	-2	158	-130
9	4	• 92	28
9	-4	•117	-64
9	6	• 69	24
9	-6	•117	-17
9	-8	•113	34
9	-10	•102	-24
9	-12	• 81	70
10	0	629	635
10	2	503	478
10	-2	1919	-2022
10	4	833	928
10	-4	1169	-1164
10	-6	611	546
10	-8	521	506
10	-10	523	604
10	-12	611	605
11	0	•116	-86
11	2	• 65	37
11	-2	• 92	-60
11	-4	• 92	57
11	-6	• 92	19
11	-8	• 81	66
11	-10	• 68	-2
12	-2	970	-1090
12	-4	138	-133
12	-6	630	696
12	-8	688	874
h 1 l			
0	2	135	-154
0	3	319	328
0	4	396	410
0	5	348	-384
0	6	147	142
0	7	•118	-74
0	8	291	292
0	9	407	-428
0	10	418	-432
0	11	135	120
0	12	194	-176
0	13	322	336
0	14	147	156
1	1	• 55	15
1	-1	• 45	17
1	2	130	-124
1	-2	• 48	22
1	3	162	-178
1	-3	• 76	-60
1	4	• 94	78
1	-4	• 87	-126
1	5	•105	-92
1	-5	122	-128
1	6	20[illegible]	188
1	-6	427	-454
1	7	237	-238
1	-7	•112	10
1	8	197	216
1	-8	•123	15
1	9	172	184
1	-9	139	-116
1	10	•132	-38
1	-10	•133	58
1	11	129	128
1	-11	163	140
1	12	202	-192
1	-12	•110	60
1	13	134	118
1	-13	• 97	-31
1	14	• 81	78
1	-14	• 85	28
2	0	• 68	-138
2	1	• 72	28
2	-1	• 66	40
2	2	• 83	-83
2	-2	• 70	-114
2	3	183	200
2	-3	162	-160
2	4	113	-100
2	-4	99	110
2	5	336	345
2	-5	399	392
2	6	498	520
2	-6	585	-590
2	7	264	-290
2	-7	502	-510
2	8	200	202
2	-8	460	464
2	9	241	-228
2	-9	286	292
2	10	198	-166
2	-10	193	-168
2	11	•132	51
2	-11	•132	-4
2	12	162	-148
2	-12	349	320
2	13	• 77	20
2	-13	358	330
2	-14	353	-348
2	-15	189	-192
3	0	• 83	-49
3	1	• 90	-89

h	±l	$10F_o$	$10F_c$
3	-1	104	-84
3	2	215	-206
3	-2	229	-258
3	3	•103	-92
3	-3	263	268
3	4	•112	17
3	-4	134	58
3	5	•120	-89
3	-5	394	-392
3	6	•125	86
3	-6	333	-328
3	7	265	-280
3	-7	297	286
3	8	368	386
3	-8	252	234
3	9	•132	4
3	-9	•129	-42
3	10	•122	-29
3	-10	126	86
3	11	•109	-19
3	-11	270	222
3	12	• 82	-4
3	-12	•127	74
3	-13	•115	65
3	-14	268	-270
3	-15	102	86
4	0	448	438
4	1	646	-630
4	-1	394	366
4	2	882	-900
4	-2	548	-536
4	3	642	604
4	-3	606	-592
4	4	364	354
4	-4	315	312
4	5	•125	-29
4	-5	175	178
4	6	•132	23
4	-6	393	-388
4	7	162	156
4	-7	420	-416
4	8	406	414
4	-8	287	264
4	9	389	-366
4	-9	•130	4
4	10	•112	89
4	-10	229	214
4	11	184	-206
4	-11	•133	89
4	12	276	-332
4	-12	•125	-79
4	-13	232	201
4	-14	140	-126
5	0	269	254
5	1	605	612
5	-1	191	-160
5	2	546	-548
5	-2	237	-256
5	3	306	-324
5	-3	200	214
5	4	•128	-29
5	-4	129	-142
5	5	203	-216
5	-5	•114	11
5	6	172	158
5	-6	116	115
5	7	•131	-16
5	-7	360	-354
5	8	•124	88
5	-8	•128	31
5	9	153	-160
5	-9	•133	5
5	10	138	172
5	-10	•134	49
5	11	136	150
5	-11	•133	-14
5	-12	198	-176
5	-13	•110	37
5	-14	• 90	-63
5	-15	94	90
6	0	142	-114
6	1	•124	-15
6	-1	302	-296
6	2	165	-144
6	-2	214	216
6	3	•131	46
6	-3	229	238
6	4	281	-292
6	-4	208	-212
6	5	138	170
6	-5	•122	38
6	6	•131	66
6	-6	193	180
6	7	261	250
6	-7	•128	89
6	8	507	506
6	-8	135	-144
6	9	283	-284
6	-9	•133	-68
6	10	126	-106
6	-10	215	216
6	-11	366	332
6	-12	268	-242
6	-13	113	-118
6	-14	127	-132
7	0	292	-300
7	1	145	-128
7	-1	389	388
7	2	•133	65

h	±l	$10F_o$	$10F_c$
7	-2	255	250
7	3	210	200
7	-3	259	-266
7	4	257	-256
7	-4	•129	-89
7	5	•127	-40
7	-5	139	-132
7	6	206	-196
7	-6	•132	97
7	7	430	-464
7	-7	•133	-1
7	8	335	362
7	-8	•134	-24
7	9	93	100
7	-9	165	146
7	-10	•130	35
7	-11	375	368
7	-12	224	-218
7	-13	171	154
7	-14	• 80	28
8	0	197	-140
8	1	255	-240
8	-1	218	-212
8	2	149	-104
8	-2	270	266
8	3	•128	-76
8	-3	153	148
8	4	393	-376
8	-4	167	-178
8	5	393	382
8	-5	333	-344
8	6	138	100
8	-6	197	138
8	7	• 82	-69
8	-7	205	182
8	8	• 68	52
8	-8	•132	54
8	-9	•130	-51
8	-10	•124	63
8	-11	203	154
8	-12	156	-120
8	-13	149	150
9	0	•127	43
9	1	152	136
9	-1	•131	-31
9	2	•121	16
9	-2	•131	-13
9	3	287	300
9	-3	•132	-1
9	4	268	-266
9	-4	•132	-61
9	5	160	-160
9	-5	250	-240
9	6	• 75	40
9	-6	•131	-61
9	-7	•127	80
9	-8	•125	70
9	-9	224	212
9	-10	•114	-13
9	-11	111	-80
9	-12	• 89	-50
9	-13	108	98
10	0	•113	62
10	1	•105	27
10	-1	198	-190
10	2	• 96	-26
10	-2	193	176
10	3	220	-246
10	-3	208	200
10	4	247	-248
10	-4	•122	-31
10	-5	261	254
10	-6	•120	-39
10	-7	•115	-50
10	-8	•113	3
10	-9	134	134
10	-10	113	-92
10	-11	• 83	18
10	-12	129	-156
11	0	111	102
11	1	131	138
11	-1	156	-174
11	2	121	-134
11	-2	•101	-82
11	-3	184	-190
11	-4	131	-132
11	-5	391	384
11	-6	255	264
11	-7	• 94	-29
11	-8	• 90	17
11	-9	376	288
11	-10	• 69	-15
12	-2	• 70	-17
12	-3	• 70	58
12	-4	• 70	31
12	-5	• 70	6
12	-6	• 68	-6
12	-7	• 65	46
12	-8	• 63	-68
h 2 l			
0	2	• 53	-25
0	3	953	-1078
0	4	• 73	-13
0	5	182	124
0	6	• 94	-29
0	7	1372	-1456
0	8	•107	-41

h	±l	$10F_o$	$10F_c$
0	9	863	858
0	10	•113	49
0	11	1275	1270
0	12	• 99	18
0	13	205	190
0	14	• 64	3
1	-1	• 48	32
1	2	621	-506
1	-2	583	664
1	3	• 68	13
1	-3	• 60	24
1	4	207	-208
1	-4	*1559	-1766
1	5	• 86	-29
1	-5	• 81	-35
1	6	514	-488
1	-6	*1778	-1796
1	7	•103	13
1	-7	• 98	-46
1	8	756	-748
1	-8	136	158
1	9	•112	51
1	-9	•110	-52
1	10	188	148
1	-10	310	306
1	11	•105	-42
1	-11	•110	4
1	12	1018	-1022
1	-12	821	790
1	13	• 70	-30
1	-13	177	154
1	-14	475	-476
2	0	• 57	-12
2	1	*1964	2378
2	-1	591	636
2	2	• 70	26
2	-2	• 56	-5
2	3	380	-276
2	-3	187	-186
2	4	• 87	42
2	-4	• 73	20
2	5	1161	-1218
2	-5	1751	1784
2	6	•103	-20
2	-6	• 91	-26
2	7	1577	-1718
2	-7	192	-164
2	8	•111	6
2	-8	•103	32
2	9	1076	-1106
2	-9	219	-190
2	10	•108	-2
2	-10	•112	-42
2	11	166	152
2	-11	•112	-67
2	12	• 85	6
2	-12	•106	66
2	13	1331	1328
2	-13	101	86
2	-14	142	-114
2	-15	226	292
3	0	*1791	-2086
3	1	• 75	-28
3	-1	• 67	4
3	2	770	776
3	-2	*1349	-1436
3	3	• 90	33
3	-3	• 73	-44
3	4	150	-88
3	-4	148	-114
3	5	•103	6
3	-5	• 85	36
3	6	1095	1144
3	-6	1120	-1104
3	7	•110	27
3	-7	• 98	-108
3	8	*1447	1544
3	-8	1903	1856
3	9	•110	37
3	-9	•109	57
3	10	637	-604
3	-10	305	-258
3	11	• 90	41
3	-11	•111	40
3	12	486	-428
3	-12	666	-618
3	-13	148	112
3	-14	403	376
4	0	• 83	-18
4	1	235	-200
4	-1	1288	-1314
4	2	• 92	-23
4	-2	• 80	-58
4	3	2323	2522
4	-3	789	-802
4	4	•103	-26
4	-4	• 86	27
4	5	678	618
4	-5	337	-320
4	6	•111	27
4	-6	• 97	-36
4	7	392	-412
4	-7	501	480
4	8	•111	-80
4	-8	•106	92
4	9	975	-912
4	-9	620	542
4	10	• 95	5
4	-10	•112	10

h	±l	$10F_o$	$10F_c$
4	11	566	-578
4	-11	131	-90
4	12	• 55	63
4	-12	•106	12
4	-13	265	-262
4	-14	• 79	5
5	0	1100	1108
5	1	• 98	30
5	-1	• 91	-36
5	2	2304	-2476
5	-2	435	-398
5	3	•105	-22
5	-3	• 91	-39
5	4	992	-920
5	-4	1505	1490
5	5	•111	38
5	-5	• 98	-12
5	6	491	456
5	-6	2277	2212
5	7	•111	-2
5	-7	•110	1
5	8	369	324
5	-8	375	-302
5	9	• 95	36
5	-9	•111	27
5	10	682	736
5	-10	•112	-58
5	11	• 64	25
5	-11	200	136
5	-12	799	-732
5	-13	• 93	44
5	-14	749	-666
6	0	•104	-34
6	1	1198	-1214
6	-1	772	-734
6	2	•108	15
6	-2	•101	-5
6	3	•110	-18
6	-3	257	226
6	4	•112	32
6	-4	•103	49
6	5	1126	1112
6	-5	1843	1862
6	6	•109	-10
6	-6	•105	25
6	7	426	386
6	-7	1857	1890
6	8	• 93	-20
6	-8	•111	-40
6	9	448	-446
6	-9	237	-202
6	10	• 62	-1
6	-10	•112	9
6	-11	1323	-1250
6	-12	137	-98
6	-13	491	-406
6	-14	• 73	-46
7	0	200	-160
7	1	•114	-54
7	-1	•109	-47
7	2	389	-382
7	-2	1397	1380
7	3	•113	38
7	-3	•108	40
7	4	736	-778
7	-4	139	-54
7	5	•106	-12
7	-5	•109	-8
7	6	1075	-1110
7	-6	748	-740
7	7	• 90	-17
7	-7	•112	71
7	8	1204	1188
7	-8	•112	-8
7	9	• 60	57
7	-9	•112	8
7	-10	1599	-1490
7	-11	•105	50
7	-12	594	584
7	-13	• 81	-12
7	-14	542	516
8	0	•112	-20
8	1	861	-820
8	-1	281	-274
8	2	•111	-52
8	-2	•112	36
8	3	804	-790
8	-3	1074	1084
8	4	•104	20
8	-4	•112	-17
8	5	207	-220
8	-5	1897	1976
8	6	• 85	19
8	-6	•112	93
8	7	653	678
8	-7	711	-696
8	8	• 50	-34
8	-8	•111	-29
8	-9	1223	-1170
8	-10	•104	20
8	-11	1140	-1072
8	-12	• 88	-12
8	-13	492	-414
9	0	1386	1414
9	1	•105	-20
9	-1	•110	-23
9	2	635	626
9	-2	•110	7
9	3	• 95	-10

h	±l	$10F_o$	$10F_c$
9	-3	•111	23
9	4	821	-866
9	-4	442	420
9	5	• 74	43
9	-5	•108	40
9	6	466	-474
9	-6	863	-790
9	-7	•108	33
9	-8	327	-286
9	-9	• 99	32
9	-10	770	744
9	-11	• 84	21
9	-12	216	-236
9	-13	• 59	-44
10	0	• 96	-40
10	1	• 89	38
10	-1	1140	1172
10	2	• 84	2
10	-2	•102	61
10	3	130	-108
10	-3	1373	1410
10	4	• 64	-13
10	-4	•102	22
10	-5	231	-156
10	-6	101	-21
10	-7	693	-630
10	-8	• 96	-46
10	-9	1380	-1382
10	-10	• 80	-60
10	-11	321	-272
11	0	97	80
11	1	• 66	-23
11	-1	• 80	-38
11	2	132	124
11	-2	283	-282
11	-3	• 85	51
11	-4	1366	-1440
11	-5	• 85	58
11	-6	534	546
11	-7	• 80	-2
11	-8	• 75	36
11	-9	• 70	-48
11	-10	467	504
12	-2	• 57	26
12	-3	136	-154
12	-4	• 58	52
12	-5	553	-624
12	-6	• 57	-21
12	-7	580	-630
h 3 l			
0	2	247	-266
0	3	312	-336
0	4	373	394
0	5	267	264
0	6	114	-128
0	7	•114	93
0	8	•121	-27
0	9	198	190
0	10	138	-120
0	11	•122	-43
0	12	•110	-85
0	13	292	-298
0	14	133	-130
1	1	177	190
1	2	225	232
1	-2	100	60
1	3	203	-194
1	-3	• 64	-72
1	4	328	-338
1	-4	93	-72
1	5	•100	43
1	-5	146	134
1	6	133	-130
1	-6	136	135
1	7	320	318
1	-7	274	254
1	8	•122	-27
1	-8	210	-216
1	9	336	324
1	-9	167	148
1	10	154	134
1	-10	252	-264
1	11	•116	-9
1	-11	176	-156
1	12	262	270
1	-12	162	-146
1	13	255	-274
1	-13	579	-550
1	-14	273	260
2	0	334	-338
2	1	272	-276
2	-1	161	152
2	2	401	428
2	-2	131	134
2	3	320	332
2	-3	• 77	-4
2	4	220	-232
2	-4	• 85	88
2	5	111	-110
2	-5	161	150
2	6	•116	-10
2	-6	•102	-95
2	7	226	212
2	-7	441	446
2	8	194	200
2	-8	153	148
2	9	305	312

h	±l	$10F_o$	$10F_c$
2	-9	•124	47
2	10	206	-196
2	-10	•127	-33
2	11	•112	0
2	-11	198	-192
2	12	• 96	-29
2	-12	•117	45
2	13	221	-258
2	-13	460	-454
2	-14	162	-154
3	0	349	-366
3	1	188	220
3	-1	408	-422
3	2	276	284
3	-2	402	436
3	3	182	-166
3	-3	398	404
3	4	•107	-85
3	-4	255	-270
3	5	•114	-39
3	-5	307	-330
3	6	121	-146
3	-6	498	506
3	7	•125	13
3	-7	774	806
3	8	276	-280
3	-8	392	-378
3	9	496	486
3	-9	260	-236
3	10	397	392
3	-10	•126	122
3	11	• 98	12
3	-11	•125	-20
3	12	128	132
3	-12	260	-234
3	-13	459	-444
3	-14	263	246
4	0	214	214
4	1	141	154
4	-1	404	-414
4	2	267	-302
4	-2	344	-366
4	3	•104	-69
4	-3	393	386
4	4	•116	57
4	-4	295	316
4	5	173	-166
4	-5	•102	-77
4	6	272	262
4	-6	•109	-51
4	7	190	182
4	-7	286	272
4	8	156	-152
4	-8	193	190
4	9	177	180
4	-9	•124	-98
4	10	•104	52
4	-10	•126	100
4	11	114	120
4	-11	513	-476
4	-12	•118	-13
4	-13	163	-166
4	-14	• 85	-69
5	0	240	-260
5	1	392	412
5	-1	350	-334
5	2	313	332
5	-2	185	176
5	3	302	-278
5	-3	287	272
5	4	•122	-100
5	-4	298	-284
5	5	•125	23
5	-5	•110	37
5	6	•126	-21
5	-6	•114	64
5	7	•123	-98
5	-7	168	136
5	8	320	-312
5	-8	196	-174
5	9	368	354
5	-9	•125	10
5	10	• 84	20
5	-10	269	-276
5	11	197	246
5	-11	684	-648
5	-12	187	192
5	-13	177	-148
5	-14	• 90	64
6	0	121	128
6	1	197	204
6	-1	218	200
6	2	261	-282
6	-2	309	302
6	3	290	-264
6	-3	237	-228
6	4	•125	97
6	-4	•116	-86
6	5	120	152
6	-5	606	582
6	6	•123	-107
6	-6	272	268
6	7	177	-168
6	-7	250	-238
6	8	203	176
6	-8	247	-250
6	9	185	180
6	-9	140	-136
6	10	• 63	24

h	±l	$10F_o$	$10F_c$
6	-10	208	-178
6	-11	340	-316
6	-12	•109	-114
6	-13	167	-146
6	-14	• 78	-55
7	0	162	156
7	1	•125	-78
7	-1	355	342
7	2	138	142
7	-2	386	-400
7	3	•126	2
7	-3	465	-482
7	4	•126	33
7	-4	535	546
7	5	142	-132
7	-5	627	624
7	6	•112	-21
7	-6	286	-272
7	7	183	-186
7	-7	137	-102
7	8	232	-220
7	-8	•126	81
7	-9	206	-164
7	-10	142	-108
7	-11	245	-208
7	-12	•106	79
7	-13	150	-128
7	-14	104	124
8	0	173	-180
8	1	225	-226
8	-1	•126	99
8	2	329	310
8	-2	239	250
8	3	418	424
8	-3	•125	-1
8	4	336	-326
8	-4	198	178
8	5	267	-248
8	-5	225	-222
8	6	• 96	-49
8	-6	356	-350
8	7	• 75	-102
8	-7	162	134
8	-8	•124	52
8	-9	321	-300
8	-10	•114	-23
8	-11	141	-112
8	-12	114	120
8	-13	120	122
9	0	•120	-31
9	1	•117	-24
9	-1	•123	-18
9	2	214	-218
9	-2	•123	-105
9	3	460	466
9	-3	169	160
9	4	558	560
9	-4	205	-192
9	5	394	-380
9	-5	178	-156
9	6	173	-176
9	-6	•123	-54
9	-7	•119	-70
9	-8	•118	-13
9	-9	225	-208
9	-10	•104	-8
9	-11	443	-410
9	-12	244	234
9	-13	171	212
10	0	457	466
10	1	284	276
10	-1	326	-336
10	2	145	-136
10	-2	•112	-89
10	3	• 75	-34
10	-3	119	104
10	4	• 65	68
10	-4	195	-186
10	-5	•112	108
10	-6	•112	-84
10	-7	•107	-105
10	-8	225	-200
10	-9	98	-3
10	-10	107	114
10	-11	180	-186
11	0	154	-160
11	1	156	168
11	-1	• 85	-61
11	2	• 60	60
11	-2	163	-154
11	-3	235	-236
11	-4	198	190
11	-5	218	194
11	-6	• 94	96
11	-7	163	-156
11	-8	119	122
11	-9	• 72	-15
11	-10	• 62	-37
12	-2	• 60	56
12	-3	153	-182
12	-4	177	-190
12	-5	142	156
12	-6	• 60	55
h 4 l			
0	2	966	-944
0	3	• 65	8
0	4	139	139

h	±l	$10F_o$	$10F_c$
0	5	• 84	-14
0	6	680	658
0	7	•101	-56
0	8	249	230
0	9	•111	-108
0	10	655	670
0	11	•107	31
0	12	776	-780
0	13	191	150
1	1	471	390
1	2	• 63	18
1	-2	• 51	-31
1	3	• 71	53
1	-3	1409	1576
1	4	• 78	29
1	-4	• 71	-23
1	5	*1657	-1870
1	-5	443	-356
1	6	• 99	17
1	-6	• 93	-18
1	7	435	444
1	-7	1505	-1554
1	8	•109	-7
1	-8	•106	-55
1	9	550	526
1	-9	1997	-2172
1	10	•109	22
1	-10	•111	-4
1	11	878	856
1	-11	425	-366
1	12	• 88	-15
1	-12	•100	16
1	13	121	-32
1	-13	1026	1058
1	-14	• 63	-21
2	0	638	-602
2	1	• 65	-13
2	-1	• 50	-12
2	2	*1385	-1578
2	-2	936	920
2	3	• 80	-10
2	-3	• 68	52
2	4	325	-306
2	-4	1188	-1194
2	5	• 97	15
2	-5	• 82	4
2	6	705	-716
2	-6	710	678
2	7	•109	-26
2	-7	• 98	105
2	8	1106	1128
2	-8	1316	1312
2	9	•110	-80
2	-9	•109	-90
2	10	488	454
2	-10	1280	-1258
2	11	• 96	-26
2	-11	•109	-74
2	12	• 80	-55
2	-12	467	442
2	13	• 63	92
2	-13	198	-164
2	-14	• 73	-6
3	0	• 71	16
3	1	*1643	2006
3	-1	767	-718
3	2	• 83	-16
3	-2	• 71	20
3	3	271	-212
3	-3	772	-780
3	4	• 96	31
3	-4	• 80	35
3	5	950	-952
3	-5	2228	-1992
3	6	•108	-52
3	-6	• 94	30
3	7	487	-486
3	-7	1888	-1928
3	8	•110	-23
3	-8	•104	9
3	9	336	-328
3	-9	704	664
3	10	•100	-75
3	-10	•111	-14
3	11	572	532
3	-11	1852	1796
3	12	• 65	36
3	-12	•103	2
3	-13	1339	1310
3	-14	• 75	11
4	0	1088	1084
4	1	• 90	-58
4	-1	• 82	18
4	2	860	864
4	-2	1183	-1154
4	3	• 98	-6
4	-3	• 84	83
4	4	1626	-1712
4	-4	1279	1234
4	5	•108	50
4	-5	• 92	-5
4	6	352	366
4	-6	446	-388
4	7	•110	20
4	-7	•102	44
4	8	•108	97
4	-8	637	-578
4	9	•100	-48
4	-9	•109	-39

Continued: TABLE II.

h	±l	$10F_o$	$10F_c$	h	±l	$10F_o$	$10F_c$	h	±l	$10F_o$	$10F_c$	h	±l	$10F_o$	$10F_c$	h	±l	$10F_o$	$10F_c$	h	±l	$10F_o$	$10F_c$	h	±l	$10F_o$	$10F_c$	h	±l	$10F_o$	$10F_c$	h	±l	$10F_o$	$10F_c$	h	±l	$10F_o$	$10F_c$
4	10	132	-102	9	-5	167	-94	3	-3	215	-210	7	7	•80	66	1	-11	•90	52	6	-1	839	-814	0	7	•102	74	5	2	379	-386	11	-2	134	176	4	-8	928	-838
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4	-12	1038	-996	9	-8	•110	22	3	-5	201	194	7	-9	191	-152	1	-13	•64	70	6	-3	423	386	0	11	155	144	5	4	286	298	11	-6	58	-58	4	-10	•107	26
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8	-1	•111	92	2	-2	495	-466	6	-4	179	162	0	6	•88	34	4	-12	•83	20	10	1	•66	44	3	-11	234	208	8	-12	187	-208	3	-6	•102	8	8	-6	235	-248
8	2	569	544	2	3	•83	82	6	5	181	190	0	7	461	-418	4	-13	147	98	10	-1	434	440	3	-12	161	-148	9	0	198	204	3	7	•112	-10	8	-7	•101	-22
8	-2	381	-330	2	-3	403	-406	6	-5	•107	56	0	8	•97	70	5	0	*2150	2460	10	2	•59	26	3	-13	106	94	9	1	315	-306	3	-7	1084	1034	8	-8	1145	1086
8	3	•104	0	2	4	•91	54	6	6	•107	46	0	9	848	868	5	1	•91	-70	10	-2	•80	-2	4	0	259	260	9	-1	•94	76	3	8	•106	-44	8	-9	•93	66
8	-3	•111	18	2	-4	463	494	6	-6	•108	60	0	10	•96	30	5	-1	•86	30	10	-3	502	504	4	1	239	262	9	2	200	-196	3	-8	•110	58	8	-10	317	288
8	4	592	-614	2	5	•99	-46	6	7	•98	-46	0	11	190	188	5	2	1817	1978	10	-4	•80	-72	4	-1	381	-398	9	-2	164	-166	3	9	•97	-110	8	-11	•69	-46
8	-4	405	354	2	-5	218	218	6	-7	•112	-94	0	12	•78	-28	5	-2	1632	-1604	10	-5	533	520	4	2	292	-284	9	3	•70	-34	3	-9	331	-244	9	0	•91	-10
8	5	•92	-28	2	6	•106	-114	6	8	•88	32	0	13	330	296	5	3	•108	-24	10	-6	•80	-6	4	-2	462	-482	9	-3	•95	104	3	10	•83	-58	9	1	133	124
8	-5	•111	-36	2	-6	211	-186	6	-8	•115	-66	1	0	*1395	1708	5	-3	•88	-78	10	-7	98	-62	4	3	204	-200	9	4	187	-210	3	-10	•107	-12	9	-1	•94	84
8	6	286	292	2	7	•111	-36	6	9	225	-248	1	1	•49	-36	5	4	810	812	10	-8	•70	38	4	-3	432	422	9	-4	171	130	3	11	529	736	9	2	•82	-14
8	-6	•110	-92	2	-7	453	-450	6	-9	294	244	1	2	*1330	-1562	5	-4	1794	-1806	10	-9	965	-968	4	4	•103	-86	9	-5	160	146	3	-11	•830	-758	9	-2	•99	90
8	7	•64	-48	2	8	•114	-28	6	-10	406	-374	1	-2	*1335	1558	5	5	•99	24	10	-10	•55	-18	4	-4	143	128	9	-6	•93	-92	3	-12	•87	-4	9	3	340	358
8	-7	•110	-79	2	-8	319	310	6	-11	186	172	1	3	•69	26	5	-5	•91	56	11	0	63	48	4	5	279	-294	9	-7	•87	-54	3	-13	508	-514	9	-3	638	-624
8	-8	977	910	2	9	338	-334	6	-12	•96	8	1	-3	•61	-76	5	6	692	-670	11	-1	•54	28	4	-5	150	-122	9	-8	•86	-76	4	0	679	636	9	-4	•96	14
8	-9	•107	27	2	-9	•112	12	6	-13	70	-110	1	4	792	760	5	-6	1365	-1344	11	-2	407	448	4	6	230	210	9	-9	•79	-62	4	1	•99	36	9	-5	683	644
8	-10	433	-396	2	10	291	-260	6	-14	86	-76	1	-4	1568	-1644	5	7	•91	-32	11	-3	•59	-18	4	-6	227	-212	9	-10	•67	30	4	-1	•92	-4	9	-6	•95	2
8	-11	•92	-48	2	-10	156	-148	7	0	•113	-30	1	5	•86	-6	5	-7	•96	-16	11	-4	252	264	4	7	•103	-6	9	-11	•60	-48	4	2	745	-814	9	-7	•90	-54
8	-12	419	-396	2	11	•103	108	7	1	•115	-116	1	-5	•77	-36	5	8	1529	-1640	11	-5	•59	36	4	-7	•103	60	10	0	159	142	4	-2	318	260	9	-8	•84	-48
8	-13	•67	41	2	-11	225	198	7	-1	•112	-104	1	6	1318	-1372	5	-8	406	-328	11	-6	519	522	4	8	254	230	10	1	255	298	4	3	•106	-10	9	-9	678	-588
9	0	•105	-30	2	12	224	228	7	2	•114	66	1	-6	278	286	5	9	•73	40	11	-7	•55	2	4	-8	177	176	10	-1	•75	-38	4	-3	•95	90	9	-10	•70	0
9	1	688	698	2	-12	•101	6	7	-2	200	-190	1	7	•95	52	5	-9	•99	44	11	-8	282	-406	4	9	185	160	10	2	74	-98	4	4	1196	-1332	10	0	586	638
9	-1	539	488	2	-13	255	232	7	3	227	-222	1	-7	•91	12	5	10	113	116					4	-9	158	124	10	-2	•77	44	4	-4	1112	1102	10	-1	•74	-38
9	2	•100	-82	2	-14	•70	-60	7	-3	•110	106	1	8	875	876	5	-10	1447	1340			h 7 1		4	10	143	-138	10	-3	•77	-28	4	5	•111	-66	10	-2	584	606
9	-2	•108	7	3	0	185	-176	7	4	435	434	1	-8	138	-114	5	-11	•90	86					4	-10	198	172	10	-4	•80	80	4	-5	•102	56	10	-3	•80	-2
9	3	253	-256	3	1	293	-320	7	-4	287	278	1	9	•98	-32	5	-12	192	140	0	2	146	-122	4	-11	117	100	10	-5	•80	-86	4	6	181	-168	10	-4	356	334
9	-3	282	232	3	-1	90	60	7	5	389	398	1	-9	•99	8	5	-13	•69	-2	0	3	•68	-32	4	-12	142	138	10	-6	121	102	4	-6	982	-898	10	-5	•80	32
9	4	•84	43	3	2	587	668	7	-5	•112	-64	1	10	1399	1464	5	-14	215	190	0	4	134	120	5	0	198	-202	10	-7	336	-336	4	7	•106	-22	10	-6	460	450
9	-4	•108	-11	3	-2	•73	84	7	6	150	-118	1	-10	569	-506	6	0	•95	74	0	5	•88	-50	5	1	275	-254	10	-8	274	-266	4	-7	•109	2	10	-7	•72	-46
9	5	424	-456	3	3	500	538	7	-6	•114	50	1	11	•84	-24	6	1	977	-1000	0	6	161	158	5	-1	287	-270	10	-9	224	230	4	8	239	-244	10	-8	797	-906

Each O–atom is shared by one tetrahedron and two Mg–polyhedra, whereas each F–atom is the common corner of three Mg–polyehdra. In this way the tetrahedra have each of their vertices common to those of two Mg–polyhedra.

Fig. 1 is a schematic picture of the connections among the eight non-equivalent Mg–atoms by means of the O– and F–atoms. All the oxygens are also coordinated by the P–atoms not inserted in the figure.

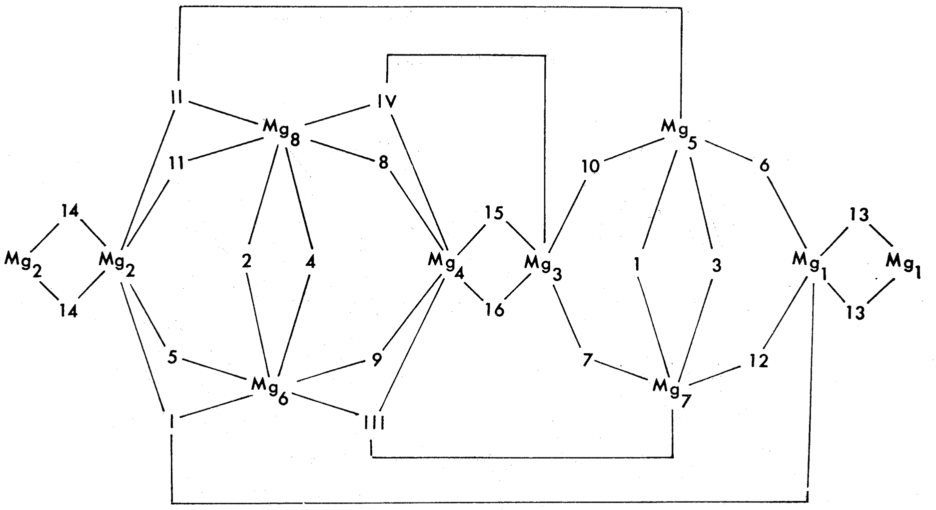

Fig. 1. – Schematic picture of the connections among the Mg–atoms. The Arabic numerals denote the O–atoms, whereas the Roman numerals refer to the F–atoms; this convention holds the following figures.

The following considerations, based on this figure, can be made:

1) Each of the octahedra Mg(2), Mg(4), Mg(6), Mg(8) shares three edges with as many octahedra, except Mg(4) which shares one edge with the trigonal bipyramid Mg(3). Two of the shared edges are formed between oxygen and fluorine and the third between two oxygen atoms.

2) Each of the trigonal bipyramids Mg(1), Mg(5), Mg(7) shares one edge with a similar polyhedron (only the trigonal bipyramid Mg(5) does not show this feature and shares one edge with an octahedron, Mg(4)). Each trigonal bipyramid shares also two vertices, occupied by O–atoms, with two more trigonal bipyramids, and a vertex, formed by an F–atom, with two octahedra.

3) The Mg(1) trigonal bipyramid as well as the Mg(2) octahedron share an edge with the centrosymmetric equivalent polyhedra.

Because of the fairly large dimensions of the unit cell edges, a drawing of the entire structure with the connections among the atoms in the various directions proved to be unattainable with sufficient clearness. So it was preferred to represent the polyhedra contained into limited slabs of the unit cell, projected on a plane normal either to the *b*–axis (figg. 2 and 3) or to the *c*–axis (figg. 4 and 5). With this representation the three-dimensional picture of the structure is partially lost, but the sharing of the polyhedra in two-dimensions appears very clear.

In fig. 2 the sheet of polyhedra around $y = 0$ in a range comprised between $\pm 0.2\,b$ is shown. They appear symmetrical with respect to the symmetry centers lying at $y = 0$. The evident feature of the structure in this range is given by the running along *c* of chains formed by pairs of similar polyhedra, connected by edges (alternatively Mg(1) trigonal bipyramids and Mg(2) octahedra), which share a vertex. Each chain is joined on both sides to two other chains having the same *c*–direction, formed by the following sequence: a Mg(5) trigonal bipyramid, a P(1) tetrahedron, a Mg(6) octahedron and a P(2) tetrahedron. The three chains are connected together by either the O(5)F(1) edge or the O(6) and F(2) vertices shared among different kinds of polyhedra. The connections between the polyhedra of the adjacent cells are given by the O(9) and O(10) vertices.

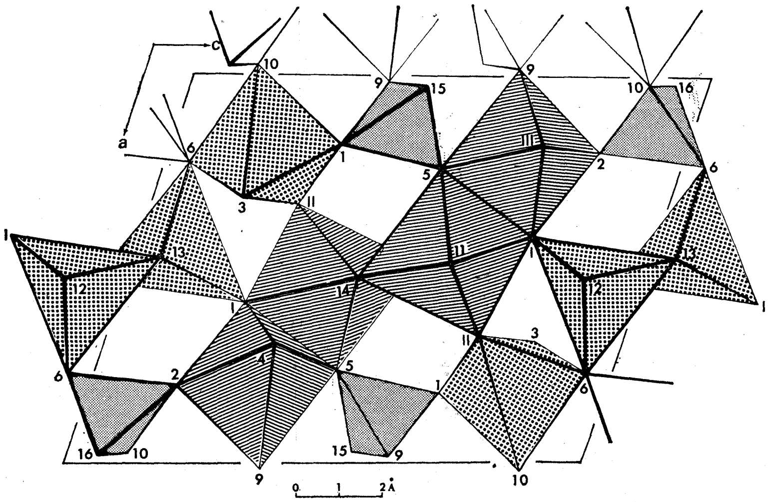

Fig. 2. – Projection on a plane normal to *b* of a cell slab in the range $\pm 0.2\,b$ around $y = 0$.

Fig. 3 shows the sheet of polyhedra around $y = 1/4$ in a range of $\pm 0.2\,b$. They are symmetrical with respect to a 010 slide plane *c* lying at $y = 1/4$. The distribution of polyhedra is similar to that of fig. 2. This fact is a consequence of the pseudosymmetry of the lattice, which, as shown above, can be described with a body-centered pseudo-cell having a period $b/2$. So, if a translation of 1/4 of period along [212] is given to the plane of polyhedra of fig. 2, the plane of polyhedra of fig. 3 is obtained. However some of the Mg–polyhedra change their coordination, in such a way that those of the central chain are alternatively Mg(4) octahedra and Mg(3) trigonal bipyramids, whereas the two chains from both sides of the preceding chain are not anymore equivalent: the former showing only Mg(8) octahedra, the latter only Mg(7) bipyramids. The connections among different chains in this slab are due

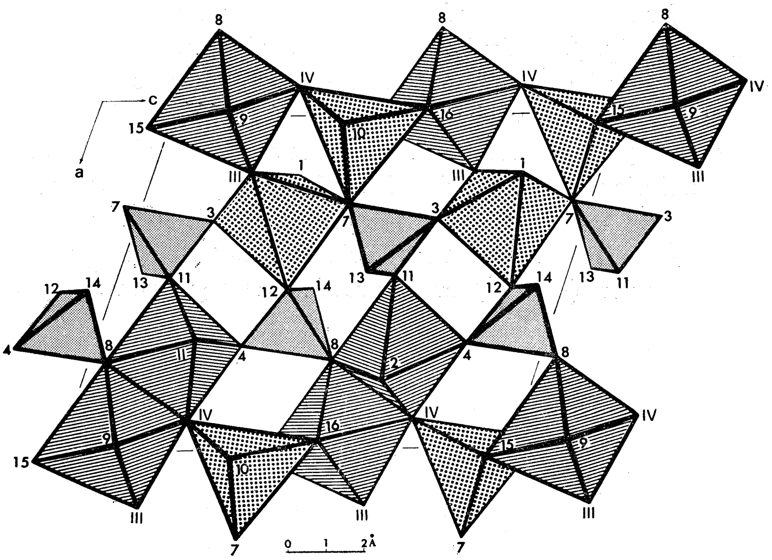

Fig. 3. – Projection on a plane normal to *b* of a cell slab in the range $\pm$ 0.2 *b* around $y = 1/4$.

to vertices shared by various polyhedra, with the exception of the junction due to the O(4) O(8) edge between the Mg(4) and Mg(8) octahedra.

The polyhedra connections in the *b*–direction are more evident in fig. 4 ($z = 0$, cell slab $\pm$ 0.2 *c*) and fig. 5 ($z = 1/4$, cell slab $\pm$ 0.2 *c*). In both figures

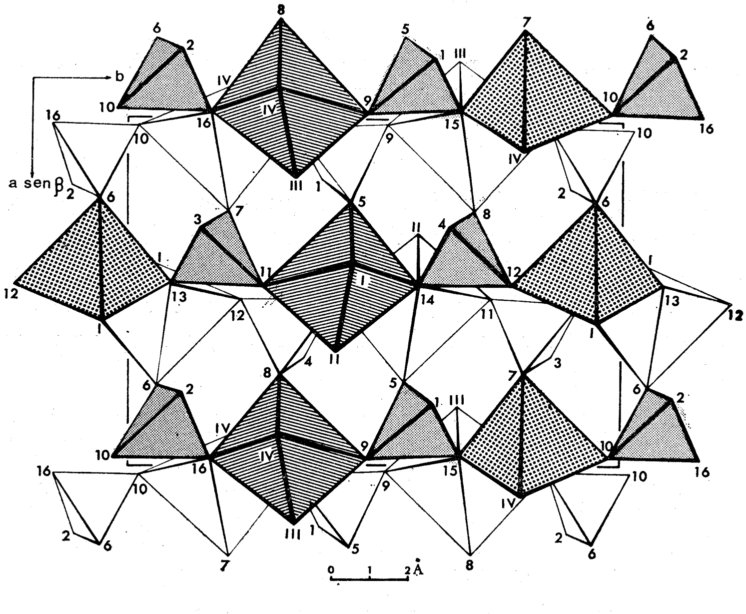

Fig. 4. – Projection on a plane normal to *c* of a cell slab in the range $\pm$ 0.2 *c* around $z = 0$.

the polyhedra form chains along *b*, which resemble those of fig. 2; particularly the two chains of fig. 5, equivalent by a screw-diad, are similar in their connections to the central chain along *c* of the fig. 2, whereas those of fig. 4 are analogous to the remaining chains along *c* of fig. 2.

Figg. 4 and 5 show clearly the pseudosymmetry of the lattice, which allows its description on the basis of a cell with parameters *a*, *b*/2 and *c*. All the atoms, but fluorine, repeat themselves at distances nearly equal to *b*/2. It is just the disposition of the fluorine atoms that is responsible for the different coordination (either 5 or 6) around the Mg atoms.

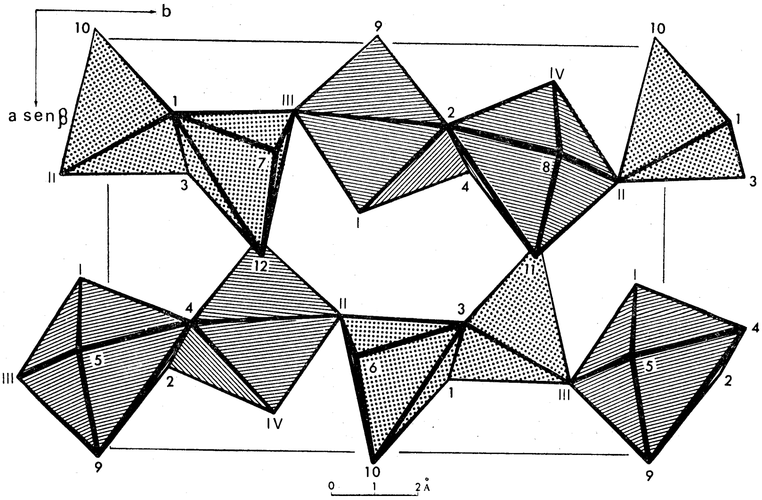

Fig. 5. – Projection on a plane normal to *c* of a cell slab in the range $\pm\ 0.2\,c$ around $z = 1/4$.

The coordination number five for magnesium is rather unusual, but a lower coordination number for this atom is known (e.g. four in melilite). Tarbuttite (Cocco, Fanfani, Zanazzi, 1966) [5], a mineral with chemical formula $Zn(OH)PO_4$, similar to wagnerite but with a different structure, contains Zn atoms with coordination number five, analogous to that found for magnesium in wagnerite.

The bond distances (Table III) range into the limits reported in literature. The distance Mg—F in each trigonal bipyramid (on the average: 1.953 Å) is somewhat shorter than the two corresponding ones in each octahedron (on the average: 2.076 Å); the interaction between the strongly electronegative F–atoms of the same octahedron can account for this feature.

The bond angles (Table III) are practically regular in the P–tetrahedra, but show noteworthy deviations in the octahedra and in the trigonal bipyramids, thus justifying their definition as distorted polyhedra.

TABLE III.

Bond distances and angles and their standard deviations (in parentheses).

Mg(1)	F(1)	O(6)	O(13)	O(13)*	O(12)					
	1.953 (5) Å	1.992 (6) Å	2.028 (7) Å	2.034 (10) Å	1.999 (10) Å					
O(12)	87° 1' (17')	104° 1' (21')	89° 48' (21')	163° 35' (19')						
O(13)*	88° 22' (18')	91° 43' (20')	78° 50' (21')							
O(13)	119° 41' (15')	116° 19' (16')								
O(6)	127° 50' (19')									
									81° 40' (14')	F(1)
								94° 31' (19')	79° 17' (16')	O(11)
							166° 47' (20')	97° 12' (19')	96° 22' (17')	O(14)*
						81° 3' (20')	87° 11' (20')	178° 12' (24')	98° 6' (15')	O(14)
					100° 56' (16')	85° 16' (20')	102° 57' (20')	79° 15' (15')	160° 54' (19')	O(5)
				2.060 (6) Å	2.152 (7) Å	2.066 (10) Å	2.033 (10) Å	2.064 (6) Å	2.022 (6) Å	
				O(5)	O(14)	O(14)*	O(11)	F(1)	F(2)	Mg(2)

Mg(3)	F(4)	O(16)	O(7)	O(10)	O(15)					
	1.954 (5) Å	2.073 (7) Å	2.018 (6) Å	2.004 (10) Å	1.999 (10) Å					
O(15)	89° 49' (17')	82° 5' (21')	88° 56' (20')	168° 4' (19')						
O(10)	86° 41' (16')	90° 40' (22')	102° 37' (21')							
O(7)	121° 38' (19')	111° 51' (16')								
O(16)	125° 41' (16')									
									85° 30' (14')	F(3)
								78° 21' (16')	97° 43' (19')	O(9)
							164° 56' (20')	96° 6' (16')	95° 31' (19')	O(16)
						85° 19' (19')	104° 14' (20')	162° 24' (19')	78° 54' (14')	O(8)
					103° 0' (16')	79° 28' (20')	86° 57' (21')	94° 29' (15')	174° 24' (23')	O(15)
				2.076 (7) Å	2.097 (6) Å	2.107 (10) Å	2.042 (10) Å	2.042 (4) Å	2.061 (6) Å	
				O(15)	O(8)	O(16)	O(9)	F(3)	F(4)	Mg(4)

Mg(5)	F(2)	O(10)	O(3)	O(6)	O(1)					
	1.951 (6) Å	2.055 (6) Å	2.036 (9) Å	2.092 (8) Å	2.038 (8) Å					
O(1)	96° 51' (17')	101° 35' (18')	80° 44' (20')	169° 19' (23')						
O(6)	84° 51' (17')	86° 44' (17')	88° 37' (20')							
O(3)	104° 45' (16')	136° 8' (20')								
O(10)	118° 10' (22')									
									79° 52' (16')	F(1)
								79° 30' (16')	85° 11' (19')	O(5)
							163° 25' (25')	99° 38' (15')	111° 5' (19')	O(2)
						96° 18' (18')	91° 6' (16')	153° 15' (25')	74° 23' (18')	O(9)
					120° 26' (20')	75° 56' (20')	87° 31' (20')	84° 25' (16')	163° 39' (17')	O(4)
				2.132 (9) Å	2.083 (6) Å	2.075 (8) Å	2.107 (7) Å	2.005 (8) Å	2.184 (8) Å	
				O(4)	O(9)	O(2)	O(5)	F(1)	F(3)	Mg(6)

Mg(7)	F(3)	O(12)	O(1)	O(7)	O(3)					
	1.953 (6) Å	2.027 (6) Å	2.008 (9) Å	2.096 (8) Å	2.067 (8) Å					
O(3)	95° 26' (17')	100° 17' (18')	80° 43' (20')	167° 33' (22')						
O(7)	86° 22' (18')	89° 49' (17')	86° 54' (20')							
O(1)	104° 17' (16')	132° 37' (22')								
O(12)	116° 39' (22')									
									79° 42' (16')	F(2)
								82° 6' (19')	80° 46' (15')	O(8)
							161° 49' (25')	116° 2' (19')	100° 48' (15')	O(4)
						75° 5' (20')	86° 59' (20')	163° 32' (18')	86° 27' (16')	O(2)
					118° 23' (20')	96° 54' (18')	88° 50' (16')	73° 50' (18')	152° 44' (25')	O(11)
				2.077 (6) Å	2.187 (9) Å	2.058 (8) Å	2.073 (7) Å	2.227 (8) Å	2.003 (5) Å	
				O(11)	O(2)	O(4)	O(8)	F(2)	F(4)	Mg(8)

P(1)	O(1)	O(5)	O(9)	O(15)				
	1.547 (7) Å	1.534 (5) Å	1.539 (8) Å	1.539 (8) Å				
O(15)	110° 14' (28')	109° 37' (23')	108° 16' (23')					
O(9)	107° 17' (24')	111° 37' (27')						
O(5)	109° 46' (20')							
							109° 41' (20')	O(6)
						110° 28' (26')	109° 42' (25')	O(10)
					105° 16' (23')	109° 1' (24')	112° 39' (28')	O(16)
				1.537 (8) Å	1.553 (8) Å	1.541 (5) Å	1.525 (7) Å	
				O(16)	O(10)	O(6)	O(2)	P(2)

P(3)	O(3)	O(7)	O(11)	O(13)				
	1.538 (7) Å	1.535 (5) Å	1.536 (8) Å	1.528 (8) Å				
O(13)	109° 30' (31')	108° 28' (23')	109° 7' (23')					
O(11)	109° 28' (24')	109° 45' (27')						
O(7)	110° 31' (20')							
							109° 19' (20')	O(8)
						110° 6' (27')	109° 17' (24')	O(12)
					105° 35' (23')	111° 11' (23')	111° 18' (28')	O(14)
				1.553 (8) Å	1.547 (8) Å	1.531 (5) Å	1.536 (7) Å	
				O(14)	O(12)	O(8)	O(4)	P(4)

The electrostatic equilibrium of the structure is fairly well attained, as shown in Table IV. The greatest difference between the charge of an anion and the sum of the electrostatic valences around it is nearly 4 % for seven O–atoms and lower for the remaining anions.

TABLE IV.

Electrostatic balance.

Coordinated anions	Coordinating cations	Sum of the charges around each anion
O(1), O(3), O(6), O(7), O(10), O(12), O(13)	Mg^{V} Mg^{V} P	$2/5 + 2/5 + 5/4 = 2.050$
O(2), O(4), O(5), O(8), O(9), O(11), O(14)	Mg^{VI} Mg^{VI} P	$1/3 + 1/3 + 5/4 = 1.917$
O(15), O(16)	Mg^{V} Mg^{VI} P	$2/5 + 1/3 + 5/4 = 1.983$
F(1), F(2), F(3), F(4)	Mg^{V} Mg^{VI} Mg^{VI}	$2/5 + 1/3 + 1/3 = 1.067$

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