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The crystal structure of aminoffite

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Mineralogia. — *The crystal structure of aminoffite* (*). Nota (**) di ALESSANDRO CODA, GIUSEPPE ROSSI e LUCIANO UNGARETTI, presentata dal Socio G. CAROBBI.

RIASSUNTO. — L'aminoffite, silicato con formula $Ca_3(BeOH)_2Si_3O_{10}$, è tetragonale con quattro unità stechiometriche nella cella elementare; il gruppo spaziale è $P4_2/n$ e le costanti reticolari sono: $a = 9.865$, $c = 9.930$ Å. La struttura cristallina è stata studiata con i raggi X, utilizzando effetti di diffrazione registrati con la camera di Weissenberg. Le coordinate degli atomi sono state ricavate analizzando la sintesi di Patterson tridimensionale e le sintesi di Fourier tridimensionali. Le coordinate e i fattori termici anisotropi di tutti gli atomi sono stati raffinati con il metodo dei minimi quadrati (matrice completa). Il fattore di discordanza finale, per le riflessioni osservate è $R = 0.07$. L'aminoffite è un silicato a strati di tetraedri SiO_4 e BeO_4 paralleli a (001); gli strati tetraedrici sono collegati fra loro dagli atomi di Ca i cui poliedri di coordinazione, mettendo in comune degli spigoli, formano strati paralleli anch'essi a (001). Ad ogni atomo di Be è legato un ossidrile che dà luogo ad un legame idrogenico con un ossigeno legato al Si.

INTRODUCTION.

Aminoffite is a silicate identified for the first time by Hurlbut [1] at Långban (Sweden); it is associated with calcite, fluorite and barite in massive magnetite and limonite.

The data previously published [1] are:

chemical formula (analyst F. A. Gonyer): $Ca_8Be_3AlSi_8O_{28}(OH)\cdot 4\,H_2O$;
cell parameters: $a = 13.8$, $c = 9.8$ Å;
space group: $I\,4/mm$, $Z = 3$.

We are indebted to prof. C. S. Hurlbut who made this investigation possible sending us a specimen of the mineral.

EXPERIMENTAL.

An irregular fragment of roughly spherical shape (radius about cm. 0.006) was used for the structure analysis. A redetermination of the cell parameters carried out by means of Weissenberg photographs, gave the following values:

$$a = 9.865 \quad , \quad c = 9.930 \pm 0.002 \text{ Å} \quad , \quad \text{space group } P4_2/n .$$

The relationship between these values and the Hurlbut's ones (labelled a' and c') is: $a \cong a'\sqrt{2}/2$, $c \cong c'$. This chemical formula, modified by Strunz [2], was adopted: $Ca_2(Be, Al)(Si, Al)_2O_7\cdot H_2O$, $Z = 6$.

Equi-inclination Weissenberg photographs of the hkl reflexions (h from 0 to 5) were taken with CuK_α radiation, using the multiple film technique. The integrated intensities were measured photometrically. They were correct-

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

(**) Pervenuta all'Accademia il 10 ottobre 1967.

ed for the Lorentz-polarization factor, $\alpha_1 - \alpha_2$ spot doubling and absorption ($\mu = 245$ cm^{-1}, the trasmission factor varying from 7.7 to 4.4; the correction was made assuming the shape of the crystal as spherical). The observed structure factors of the different levels were put on the same scale through the relationship $|F|_{(hkl)} = |F|_{(\bar{h}\bar{k}l)}$.

Structure analysis.

It was possible to locate the atoms of Ca and Si through the examination of the three-dimensional Patterson synthesis. A successive three-dimensional Fourier synthesis allowed the attribution of the coordinates to all the oxygen

Table I.

Observed and calculated structure factors.

The sign ′ marks the reflections unobservably weak; in this case F_o derives from 0.5 I_{min}.

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$_c$
				7	5	705	-773	-3	3	138	-150	7	0	302	-205	2	12	759	790	-6	7	' 74	-76			h 3 1		-7	2	656	633	5	5	530	-492	10	5	'102	-34
				7	6	364	-336	3	4	488	-403	-7	0	693	-717	3	1	861	-872	6	8	111	80					7	3	'130	-18	-5	5	'160	158	10	6	485	452
	h	0	1	7	7	'141	36	-3	4	813	855	7	1	304	357	-3	1	618	578	-6	8	235	243	3	0	363	-367	-7	3	206	207	5	6	'149	-129	11	1	227	233
				7	8	'128	12	3	5	238	225	-7	1	215	-261	3	2	293	-260	6	9	128	-80	3	1	' 82	-9	7	4	203	-184	-5	6	640	622	11	2	361	345
0	2	303	292	7	9	337	-372	-3	5	'100	43	7	2	743	652	-3	2	983	970	-6	9	182	178	3	2	206	-170	-7	4	267	278	5	7	'148	26	11	3	281	-292
0	4	609	668	7	10	242	-297	3	6	559	522	-7	2	1495	-1485	3	3	766	747	6	10	193	177	3	3	152	103	7	5	130	-174	-5	7	'149	214	11	4	170	62
0	6	1391	-1508	8	0	819	931	-3	6	875	-950	7	3	363	424	-3	3	487	-454	-6	10	181	192	3	4	1126	-1110	-7	5	'130	132	5	8	348	-309				
0	8	1283	1481	8	1	274	-300	3	7	'122	-48	-7	3	'116	-55	3	4	314	320	7	1	371	-418	3	5	176	163	7	6	518	-497	-5	8	487	466		h	5	1
0	10	351	-394	8	2	772	856	-3	7	284	-299	7	4	247	85	-3	4	98	-43	-7	1	244	282	3	6	954	-1008	-7	6	215	-181	5	9	366	-350				
0	12	556	551	8	3	'149	-150	3	8	229	-235	-7	4	637	647	3	5	812	-871	7	2	248	291	3	7	'130	-60	7	7	181	177	-5	9	'123	83	5	0	544	534
1	2	369	-355	8	4	237	-222	-3	8	176	196	7	5	'120	110	-3	5	667	649	-7	2	140	-129	3	8	499	-505	-7	7	'117	-6	6	0	216	-179	5	1	'132	-22
1	3	491	460	8	5	'146	- 57	3	9	'122	166	-7	5	'120	106	3	6	762	714	7	3	372	402	3	9	'124	65	7	8	298	-252	-6	0	1152	-1231	5	2	638	610
1	4	1194	-1198	8	6	'140	- 19	-3	9	'112	67	7	6	646	719	-3	6	1211	-1332	-7	3	294	-297	3	10	383	393	-7	8	340	301	6	1	216	195	5	3	'141	-47
1	5	170	-157	8	7	188	-169	3	10	511	546	-7	6	842	-855	3	7	288	298	7	4	387	436	3	11	' 85	-83	-7	9	' 84	-30	-6	1	278	278	5	4	513	-517
1	6	406	-418	8	8	'109	46	-3	10	481	-494	7	7	'111	177	-3	7	103	-141	-7	4	636	-627	4	1	169	-139	8	1	370	304	6	2	563	558	5	5	'149	-71
1	7	316	325	9	1	'148	-169	3	11	176	-190	-7	7	'111	-7	3	8	218	199	7	5	418	-446	4	1	284	-282	-8	1	612	597	-6	2	303	-184	5	6	'149	103
1	8	'126	-97	9	2	'147	-135	-3	11	' 92	-29	7	8	'101	2	-3	8	325	-323	-7	5	289	319	4	2	384	-404	8	2	173	-156	6	3	'156	121	6	1	'145	9
1	9	256	-224	9	3	'145	3	3	12	' 57	-48	7	9	' 85	-173	3	9	486	-518	7	6	547	553	4	2	293	-290	-8	2	305	310	-6	3	'156	-93	5	8	206	-199
1	10	'117	125	9	4	366	-403	-3	12	254	259	8	1	191	-140	-3	9	365	379	-7	6	647	-682	4	3	156	-98	8	3	356	-358	6	4	1114	-1152	5	9	'111	-7
1	11	'100	54	9	5	'134	-81	4	1	85	-103	-8	1	392	404	3	10	303	308	7	7	291	311	4	3	340	329	-8	3	417	-411	-6	4	527	-587	6	1	506	542
1	12	' 51	-545	9	6	391	-406	-4	1	' 82	-73	8	2	302	331	3	10	501	-508	-7	7	106	-106	4	4	284	-245	8	4	'120	63	6	5	'163	-70	-6	1	'143	45
2	0	570	-543	9	7	'107	-33	4	2	1533	-1554	-8	2	222	181	3	11	188	189	7	8	' 63	28	-4	4	486	-484	-8	4	209	193	-6	5	'163	158	6	2	145	208
2	1	717	699	9	8	214	-213	-4	2	1036	-996	8	3	' 96	-90	-3	11	117	-105	-7	8	173	-191	4	5	196	-146	8	5	255	220	6	6	'161	98	-6	2	356	-343
2	2	1087	-939	10	0	1115	-1265	4	3	' 92	-75	-8	3	487	-469	3	12	135	140	7	9	220	-212	-4	5	379	-388	-8	5	462	461	-6	6	'161	-212	6	3	'148	-176
2	3	562	515	10	1	'138	17	-4	3	209	196	8	4	549	643	4	0	233	-248	-7	9	274	300	4	6	'128	43	8	6	412	420	6	7	'153	174	-6	3	148	-26
2	4	138	120	10	2	224	269	4	4	219	101	-8	4	199	-116	4	0	269	-240	7	10	327	325	-4	6	212	209	-8	6	259	218	-6	7	'153	-64	6	4	'146	72
2	5	261	292	10	3	'131	-51	-4	4	543	-569	8	5	299	-280	4	1	437	-457	8	0	1046	-1203	4	7	188	-166	8	7	247	-262	6	8	495	-483	-6	4	455	-435
2	6	361	-361	10	4	1023	-1146	4	5	'106	-76	-8	5	318	315	-4	1	415	-405	-8	0	363	-359	-4	7	'130	165	-8	7	227	-222	-6	8	560	-535	6	5	754	707
2	7	' 72	67	10	5	'113	-1	-4	5	'106	-143	8	6	'110	-84	4	2	314	323	8	1	154	-148	4	8	245	255	8	8	280	242	6	9	'115	-108	-6	5	364	312
2	8	'103	-79	10	6	160	175	4	6	523	539	-8	6	353	-338	-4	2	154	77	-8	1	151	-156	-4	8	'129	41	-8	8	163	-144	-6	9	294	269	6	6	'145	-96
2	9	' 76	-23	11	1	222	255	-4	6	407	430	8	7	203	-200	4	3	265	-231	8	2	735	827	4	9	238	-129	-8	9	490	537	6	10	261	234	-6	6	'145	-124
2	10	325	-349	11	2	'113	-19	4	7	'117	-50	-8	7	340	-363	-4	3	334	-332	-8	2	654	652	-4	9	'120	-147	9	0	224	-162	7	1	'160	-149	6	7	'135	8
2	11	149	-164	11	3	163	-178	-4	7	'117	53	8	8	' 87	-53	4	4	898	-931	8	3	' 76	9	4	10	'101	77	-9	0	463	477	-7	1	'160	-62	-6	7	'135	104
2	12	' 43	-28	11	4	' 97	44	4	8	958	1022	-8	8	138	-100	-4	4	575	-580	-8	3	' 76	-89	-4	10	340	330	9	1	410	-428	7	2	477	-464	6	8	360	-325
3	1	1077	-1061	11	5	' 83	20	-4	8	534	578	9	0	776	911	4	5	247	-254	8	4	737	-870	4	11	' 75	-103	-9	1	255	252	-7	2	671	676	-6	8	'119	18
3	2	' 64	-38	11	6	226	236	4	9	'113	-102	-9	0	' 89	26	4	5	' 69	-34	-8	4	509	-526	-4	11	' 77	78	9	2	514	528	7	3	218	193	6	9	524	526
3	3	771	739	12	0	244	-213	-4	9	'113	-70	9	1	'117	-64	4	6	383	-375	8	5	' 73	1	5	0	1275	-1295	-9	2	599	-602	-7	3	258	202	-6	9	190	183
3	4	220	187	12	1	259	-276	4	10	' 99	-95	-9	1	194	-210	-4	6	147	121	-8	5	' 73	37	-5	0	1962	2108	9	3	'123	-141	7	4	584	-616	7	0	' 87	72
3	5	959	-985	12	2	' 80	41	-4	10	240	261	9	2	198	-97	4	7	' 76	-47	8	6	653	636	5	1	486	-499	-9	3	'123	28	-7	4	298	272	-7	0	311	333
3	6	'116	-40	12	3	107	-132	4	11	' 77	-69	-9	2	444	448	-4	7	322	-346	-8	6	506	532	-5	1	441	438	9	4	'119	-26	7	5	385	-351	7	1	453	650
3	7	305	307					-4	11	' 83	17	9	3	'115	120	4	8	437	-451	8	7	' 51	-15	5	2	1040	1061	-9	4	297	274	-7	5	'160	191	-7	1	414	-417
3	8	'130	186					5	0	1121	1171	-9	3	172	-188	-4	8	247	-241	-8	7	190	191	-5	2	1165	-1228	9	5	248	-286	7	6	'153	-209	7	2	1055	1038
3	9	556	-569		h	1	1	-5	0	492	374	9	4	'112	77	4	9	' 71	-43	8	8	757	-788	5	3	294	-310	-9	5	'110	15	-7	6	'153	-21	-7	2	1177	-1147
3	10	'117	-17					5	1	183	150	-9	4	176	-189	-4	9	135	138	-8	8	435	-437	-5	3	183	176	9	6	390	425	7	7	'140	2	7	3	285	289
3	11	269	241	1	2	847	-830	-5	1	268	-259	9	5	'106	-65	4	10	257	258	9	1	' 75	-13	5	4	322	-282	-9	6	298	-309	-7	7	269	262	-7	3	235	-214
3	12	234	233	1	3	326	-279	5	2	300	-333	-9	5	231	-227	4	10	119	-109	-9	1	107	104	-5	4	480	472	10	1	257	217	7	8	322	239	7	4	641	-594
4	0	1556	1651	1	4	218	201	-5	2	167	146	9	6	217	-216	4	11	227	220	9	2	320	-381	5	5	224	-225	-10	1	538	558	-7	8	577	-537	7	4	263	249
4	1	155	-134	1	5	178	170	5	3	'101	77	-9	6	235	275	-4	11	' 82	-15	-9	2	' 76	54	-5	5	'127	131	10	2	165	161	7	9	' 94	-127	7	5	'145	115
4	2	237	-196	1	6	370	-392	-5	3	307	-315	10	1	193	123	5	1	783	-862	9	3	' 76	115	5	6	1332	1391	-10	2	177	-181	8	0	'163	48	-7	5	'145	-118
4	3	168	-158	1	7	209	-184	5	4	'106	96	-10	1	385	372	-5	1	492	465	-9	3	186	-234	-5	6	1254	-1256	10	3	190	-144	8	1	'163	-108	7	6	517	376
4	4	1356	1394	1	8	'117	64	-5	4	'115	15	10	2	198	187	5	2	180	-183	9	4	' 70	76	5	7	'130	-66	-10	3	405	-437	8	2	242	239	-7	6	914	-883
4	5	'133	-2	1	9	249	252	-5	5	'112	-12	-10	2	252	229	-5	2	261	-257	-9	4	176	-212	-5	7	'136	119	10	4	'100	75	-8	2	264	-214	7	7	218	218
4	6	577	563	1	10	428	-465	-5	5	'112	-114	10	3	234	154	5	3	965	1009	9	5	300	326	5	8	397	-351	-10	4	230	223	8	3	'160	91	-7	7	192	-53
4	7	'148	-42	1	11	222	-222	5	6	'117	-137	-10	3	490	-480	-5	3	771	-769	-9	5	320	-327	-5	8	691	684	10	5	344	372	-8	3	318	-281	7	8	330	-296
4	8	876	907	1	12	' 68	-54	-5	6	167	-159	10	4	220	-248	5	4	147	155	9	6	254	204	5	9	'111	-28	-10	5	487	529	8	4	385	276	-7	8	323	325
4	9	'142	129	2	1	165	-53	5	7	'120	26	-10	4	' 98	51	-5	4	293	-293	-9	6	291	263	-5	9	'111	20	10	6	238	-216	-8	4	922	854	8	1	540	554
4	10	547	-575	-2	1	417	-430	-5	7	'120	1	10	5	' 89	36	5	5	117	-99	9	7	374	317	5	10	403	359	-10	6	288	255	8	5	'149	3	-8	1	377	358
4	11	' 99	-40	2	2	215	199	5	8	325	267	-10	5	253	254	-5	5	' 72	-23	-9	7	428	-448	-5	10	680	-686	11	0	242	-77	-8	5	'149	-36	8	2	147	-234
5	1	1009	-1091	-2	2	309	347	-5	8	159	141	10	6	295	-322	5	6	' 75	12	9	8	253	299	5	11	167	170	11	1	' 93	53	8	6	362	356	-8	2	303	252
5	2	208	179	2	3	508	479	5	9	'106	-49	11	0	217	-187	-5	6	147	188	-9	8	193	-162	-5	11	' 72	-145	11	2	720	-764	-8	6	'137	110	8	3	599	-611
5	3	684	706	-2	3	562	562	-5	9	'106	11	11	1	215	270	5	7	966	994	10	0	194	-141	6	1	249	243	11	3	' 83	53	8	7	'121	-48	-8	3	499	-459
5	4	676	-712	2	4	419	397	5	10	530	-566	-11	1	' 92	-21	-5	7	817	-836	10	1	241	241	-6	1	190	177	11	4	' 73	-146	-8	7	255	-222	8	4	227	205
5	5	701	-722	-2	4	423	419	-5	10	324	313	11	2	479	552	5	8	176	168	-10	1	361	409	6	2	201	231						8	8	228	163	-8	4	'140	176
5	6	612	-647	2	5	181	185	5	11	' 67	-10	-11	2	511	-473	-5	8	' 74	62	10	2	352	373	-6	2	'121	-45		h	4	1	-8	8	493	505	8	5	213	220
5	7	505	517	-2	5	' 93	-16	-5	11	' 67	9	11	3	180	201	5	9	172	-149	-10	2	128	122	6	3	302	-294						9	1	'154	-25	-8	5	'131	5
5	8	463	-468	2	6	254	217	6	1	'103	95	-11	3	' 84	56	-5	9	170	-160	10	3	101	104	-6	3	256	-265	4	0	1547	1619	-9	1	'154	-12	8	6	311	249
5	9	579	-592	-2	6	584	636	-6	1	188	172	11	4	229	-206	5	10	136	-113	-10	3	175	180	6	4	'128	-141	4	1	122	9	9	2	'152	187	-8	6	428	333
5	10	138	-138	2	7	509	542	6	2	186	-183	-11	4	' 76	-154	-5	10	207	184	10	4	152	155	-6	4	'128	125	4	2	271	263	-9	2	'152	-175	8	7	617	-611
5	11	209	217	-2	7	500	561	-6	2	'106	55	11	5	' 64	-9	5	11	524	529	-10	4	187	155	6	5	249	255	4	3	292	268	9	3	'148	-166	-8	7	582	-583
6	0	1846	-1999	2	8	'103	1	6	3	220	223					-5	11	532	-573	10	5	' 55	51	-6	5	219	197	4	4	775	760	-9	3	'148	14	8	8	342	364
6	1	342	357	-2	8	305	-347	-6	3	207	-182					6	0	339	-361	-10	5	115	122	6	6	851	-886	4	5	'153	-84	9	4	200	-202	9	0	576	593
6	2	'133	35	2	9	264	285	6	4	204	-246		h	2	1	-6	0	344	313	10	6	513	592	-6	6	237	-129	4	6	'161	82	-9	4	215	179	-9	0	309	-309
6	3	'136	100	-2	9	144	123	-6	4	'113	-18					6	1	181	176	-10	6	' 57	6	6	7	215	-178	4	7	'163	147	9	5	'130	106	9	1	'137	-51
6	4	783	-788	2	10	' 92	49	6	5	182	178	2	0	191	-109	-6	1	261	239	10	7	96	100	-6	7	196	-154	4	8	547	534	-9	5	'130	29	-9	1	'137	29
6	5	'147	177	-2	10	275	309	-6	5	285	298	2	1	' 37	-3	6	2	'101	-52	11	1	314	370	6	8	'116	13	4	9	'142	-165	9	6	227	-123	9	2	'135	-224
6	6	484	522	2	11	322	335	6	6	225	-191	2	2	1554	-1630	-6	2	196	-224	-11	1	' 57	-17	-6	8	'116	-71	4	10	252	-209	-9	6	542	532	-9	2	'135	-5
6	7	'147	15	-2	11	398	417	-6	6	430	419	2	3	' 70	-42	6	3	' 70	26	11	2	169	179	6	9	'100	133	4	11	231	189	9	7	237	-259	9	3	'130	117
6	8	650	-671	-2	12	' 64	-8	6	7	193	232	2	4	1498	1544	-6	3	' 79	102	11	3	210	-233	-6	9	'100	60	5	1	450	-459	10	0	931	-969	-9	3	'130	-41
6	9	'123	43	3	0	160	70	-6	7	'117	-66	2	5	140	-125	6	4	271	292	-11	3	' 52	61	6	10	375	-406	-5	1	'107	-78	10	1	'136	-96	9	4	466	441
6	10	133	144	-3	0	596	-598	6	8	'110	124	2	6	929	-998	-6	4	290	291	11	4	140	180	-6	10	175	-144	5	2	195	-163	-10	1	'136	49	-9	4	'122	45
6	11	178	-191	3	1	357	369	-6	8	279	-311	2	7	113	102	6	5	' 79	-16	11	5	162	157	7	0	1273	-1339	-5	2	265	-262	10	2	325	223	9	5	'110	-42
7	1	441	-470	-3	1	244	-228	6	9	229	240	2	8	485	540	-6	5	286	306	12	0	'136	-159	-7	0	1433	1531	5	3	238	206	10	3	'126	-95	-9	5	'110	61
7	2	364	359	3	2	1405	1384	-6	9	166	181	2	9	' 74	-66	6	6	174	142	12	1	103	81	7	1	'127	22	-5	3	131	70	-10	3	'126	-55	9	6	94	-81
7	3	339	386	-3	2	1684	-1823	6	10	' 79	-38	2	10	99	-90	-6	6	293	-322	12	2	559	618	-7	1	'127	115	5	4	514	-494	10	4	747	-780	-9	6	299	282
7	4	267	297	3	3	167	169	6	11	186	217	2	11	' 56	82	6	7	' 71	78	12	3	92	112	7	2	961	-998	-5	4	711	718	-10	4	578	-552	10	1	336	360

atoms and showed some features indicating incongruencies in the chemical formula. In fact, as one can see from the chemical formula given by Strunz, six (Be, Al) atoms are present in the unit cell; these atoms in the space, group $P4_2/n$, can be located only in special positions with fourfold and twofold multiplicity. But the presence of atoms in those positions gave rise to (Be, Al)—Ca and (Be, Al)—Si distances too short to be possible. Furthermore the Fourier syntesis showed no maximum in those positions, but only one (in a position with eight-fold multiplicity) at the center of a tetrahedron built-up by oxygen atoms: it has been assumed that this maximum was due to the presence of an atom of Be. With this assumption the number of atoms of Be per unit cell was eight and not six, but the structural model obtained in this way was self-consistent and was submitted to the least-squares refinement. Four cycles of isotropic three-dimensional least squares (full matrix) dropped the R. factor from 0.26 to 0.08 for the observed amplitudes. The secondary extinction effect was negligible, so no extinction correction was applied. The anisotropic refinement (two cycles) lowered the R factor to 0.071. The observed and calculated structure factors are compared in Table I. Positional and thermal parameters are listed in Table II.

TABLE II.

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

M is the equipoint multiplicity and W is the Wyckoff notation. Final anisotropic thermal parameters and their standard deviations (in parentheses); the thermal factor is in the form: $\exp[-10^{-4}(h^2b_{11}^2 + k^2b_{22}^2 + l^2b_{33}^2 + 2hkb_{12} + 2hlb_{13} + 2klb_{23})]$; $\bar{u}$: r.m.s. thermal vibrations along the ellipsoid axes (Å); $\hat{A}$, $\hat{B}$, $\hat{C}$, angles (°) among the crystallographic axes and the principal axes of the vibration ellipsoid; B_H: equivalent isotropic temperature factors after Hamilton [8].

Atom	M	W	x/a	y/b	z/c	b_{11}	b_{22}	b_{33}	b_{12}	b_{13}	b_{23}	$\bar{u}$	$\hat{A}$	$\hat{B}$	$\hat{C}$	B_H
Ca(1)	8	g	0.0644 (2)	0.0622 (2)	0.2421 (2)	10 (2)	25 (2)	24 (2)	4 (2)	9 (2)	0 (2)	0.110 0.120 0.050	91° 28' 63° 19' 26° 43'	23° 25' 68° 35' 99° 2'	113° 22' 35° 21' 114° 55'	0.77
Ca(2)	4	e	0.2500 (0)	0.7500 (0)	0.2596 (3)	8 (3)	12 (3)	17 (2)	0 (3)	0 (0)	0 (0)	0.080 0.089 0.066	82° 59' 90° 7° 2'	7° 1' 90° 97° 1'	90° 0° 90°	0.48
Si(1)	8	g	0.0373 (3)	0.7384 (3)	0.0297 (3)	9 (3)	13 (3)	16 (3)	0 (2)	0 (0)	0 (0)	0.081 0.090 0.063	112° 33' 96° 47' 23° 7'	30° 5' 71° 37' 67° 4'	108° 49' 19° 2' 92° 47'	0.50
Si(2)	4	f	0.2500 (0)	0.2500 (0)	0.0106 (4)	5 (4)	11 (4)	22 (3)	4 (5)	0 (0)	0 (0)	0.080 0.104 0.038	63° 26' 90° 26° 34'	26° 34' 90° 116° 34'	90° 0° 90°	0.50
Be	8	g	0.0348 (16)	0.7343 (16)	0.5299 (16)	39 (16)	42 (17)	26 (12)	-18 (18)	9 (13)	-9 (14)	0.106 0.176 0.102	60° 34' 130° 2' 125° 56'	44° 59' 46° 31' 99° 19'	59° 28' 109° 37' 37° 31'	1.39
O(1)	8	g	0.3942 (7)	0.6239 (7)	0.0920 (7)	36 (8)	18 (7)	31 (7)	-7 (6)	9 (7)	5 (6)	0.121 0.146 0.077	115° 16' 35° 35' 66° 41'	56° 23' 96° 23' 34° 22'	44° 20' 55° 9' 113° 44'	1.11
O(2)	8	g	0.1247 (7)	0.6106 (7)	0.0881 (7)	19 (7)	24 (7)	29 (7)	3 (7)	12 (6)	14 (6)	0.095 0.150 0.063	134° 12' 66° 43' 126° 44'	45° 15' 57° 38' 117° 50'	97° 47' 41° 42' 49° 21'	0.94
O(3)	8	g	0.2674 (7)	0.3869 (7)	0.1000 (7)	8 (7)	19 (7)	39 (8)	-4 (7)	-7 (6)	2 (6)	0.098 0.142 0.052	103° 56' 101° 50' 18° 26'	16° 34' 84° 2' 74° 35'	98° 48' 13° 17' 80° 7'	0.86
O(4)	8	g	0.6181 (7)	0.7726 (7)	0.0897 (7)	30 (8)	16 (7)	32 (7)	2 (7)	4 (6)	-3 (6)	0.117 0.132 0.086	37° 36' 54° 22' 100° 21'	75° 23' 92° 35' 14° 51'	123° 43' 35° 45' 79° 28'	1.02
O(5)	8	g	0.7127 (8)	0.4643 (8)	0.1380 (7)	34 (8)	45 (9)	40 (8)	15 (8)	-6 (7)	-8 (7)	0.132 0.172 0.107	75° 2' 59° 10' 35° 1'	68° 53' 42° 39' 125° 1'	26° 17' 116° 17' 90° 17'	1.55
O(6)	8	g	0.9664 (7)	0.2651 (7)	0.1352 (6)	34 (8)	19 (7)	24 (6)	5 (8)	7 (6)	3 (6)	0.112 0.133 0.083	120° 22' 31° 35' 97° 52'	67° 25' 68° 39' 31° 55'	39° 23' 67° 52' 120° 43'	1.00
H	8	g	0.3840	0.6500	0.1370	B = 2.50										

As the refinement confirmed the hypothesis made above, the following chemical formula can be adopted for aminoffite: $Ca_3(BeOH)_2Si_3O_{10}$; four of these formula units are contained in the unit cell. The presence of the OH group linked to Be was inferred on the basis of the electrostatic valences Pauling's rule which is well fulfilled for all the atoms. However only a new chemical analysis could give a definitive picture of the details of the chemical formula. Unfortunately the available amount of crystals was too small to permit a new analysis.

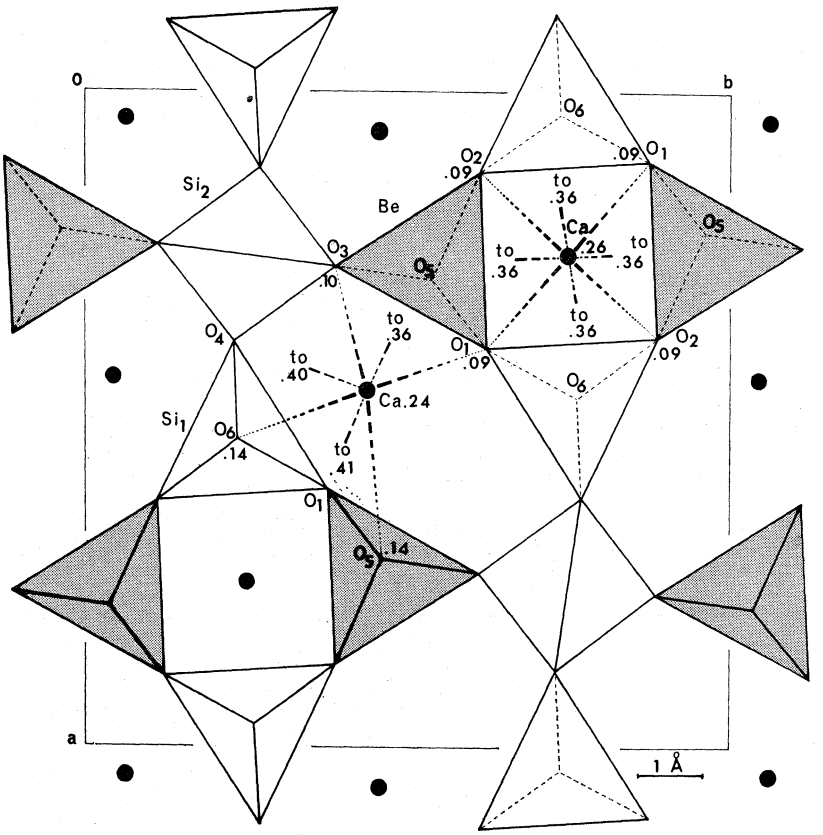

Fig. 1 *a*. – Schematic view of the crystal structure of aminoffite and key to the identification of the atoms and their coordination. One half of the content of the unit cell is projected on (001). The layer of tetrahedra is around $z \cong 0$; the black circles are Ca atoms at $z \cong 1/4$.

Description of the structure.

The two non-equivalent Si atoms have a tetrahedral coordination. Each Si_1 and Si_2 tetrahedron shares respectively three and four oxygens with other tetrahedra. The Si—O bond lengths are in good agreement with those found in other silicates (see Table III). The Be tetrahedron is built up by three oxy-

gens shared with the Si tetrahedra and one OH group labelled O_5. The O_5—O_6 distance of 2.87 Å could be referred to a hydrogen bond between OH and the unshared oxygen O_6. The tetrahedra form six-membered and four-membered rings which, connected with one another, give rise to layers parallel to (001) (fig. 1). These layers are held together by the Ca atoms occurring halfway between them (fig. 2). Ca_2 is linked to four oxygens belonging to a tetraedral layer and four belonging to the other; these eight oxygens form a square antiprism whose bases have sides of different length (2.64 and 2.84 Å respectively). The Ca_2—O distances range from 2.375 to 2.517 Å.

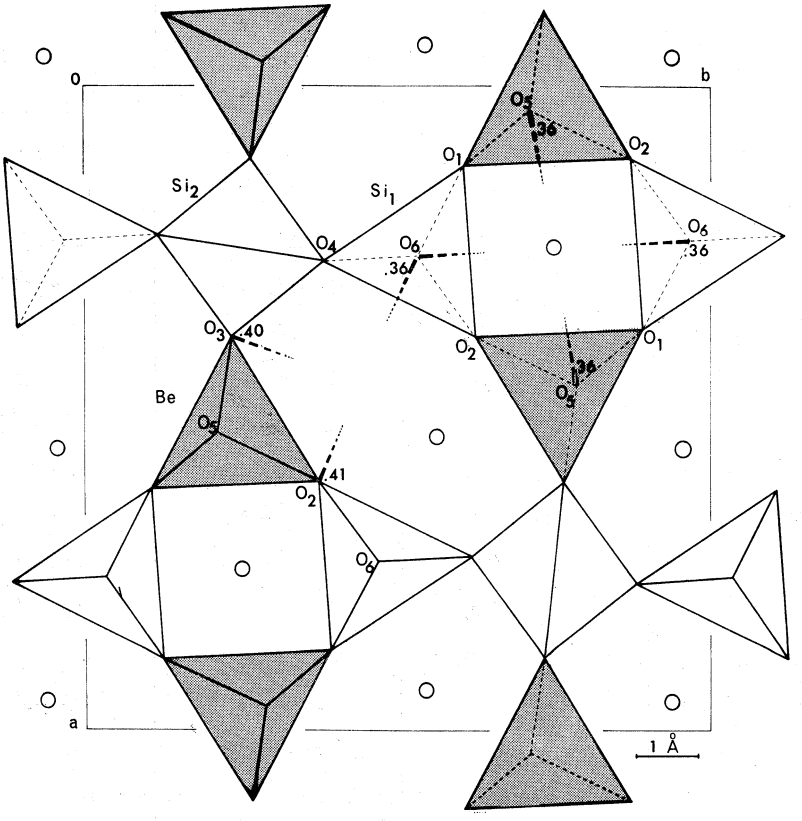

Fig. 1*b*. – The layer of tetrahedra around $z \cong 1/2$ (one half of the content of the cenit cell) is projected on (001). Open circles represent Ca atoms at $z \cong 3/4$.

The seven oxygens bonded to Ca_1 form a coordination polyhedron that could be described as a square antiprism lacking a corner. The Ca_1—O distances range from 2.359 to 2.752 Å. The coordination polyhedra of Ca atoms give rise, by sharing some edges, to layers parallel to (001). The presence of these layers and of those made up by the tetrahedra account for the (001) cleavage.

TABLE III.

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

The asterisk is used to distinguish equivalent atoms. The distances preceded by the sign '' occur twice.

Atoms	Bond lengths	Atoms	Bond angles
Si_1—O_2	1.632 (7)	O_1—Si_1—O_2	106° 44′ (23′)
Si_1—O_6	1.638 (7)	O_1—Si_1—O_4	107° 33′ (23′)
Si_1—O_1	1.638 (7)	O_1—Si_1—O_6	113° 50′ (23′)
Si_1—O_4	1.648 (7)	O_2—Si_1—O_4	108° 11′ (23′)
		O_2—Si_1—O_6	110° 29′ (23′)
		O_4—Si_1—O_6	109° 50′ (23′)
Si_2—O_3	'' 1.625 (7)	O_3—Si_2—O_4	110° 58′ (25′)
Si_2—O_4	'' 1.653 (7)	O_3—Si_2—O_3^*	113° 43′ (25′)
		O_3—Si_2—O_4^*	107° 28′ (25′)
		O_4—Si_2—O_4^*	105° 59′ (25′)
Be—O_3	1.614 (17)	O_1—Be—O_2	105° 28′ (1°)
Be—O_1	1.661 (17)	O_1—Be—O_3	108° 7′ (1°)
Be—O_5	1.680 (17)	O_1—Be—O_5	105° 36′ (1°)
Be—O_2	1.683 (17)	O_2—Be—O_3	105° 14′ (1°)
		O_2—Be—O_5	116° 13′ (1°)
		O_3—Be—O_5	115° 34′ (1°)
Ca_1—O_2	2.359 (7)	Atoms	Bond lengths
Ca_1—O_3	2.385 (7)		
Ca_1—O_6	2.393 (7)	Ca_2—O_5	'' 2.375 (7)
Ca_1—O_6^*	2.429 (7)	Ca_2—O_6	'' 2.381 (7)
Ca_1—O_1	2.441 (7)	Ca_2—O_1	'' 2.514 (7)
Ca_1—O_3^*	2.647 (7)	Ca_2—O_2	'' 2.517 (7)
Ca_1—O_5	2.752 (7)		

The crystal structure of aminoffite is similar to those of melilites (3,4), meliphanite [5] and leucophanite [6]. The general feature common to all these silicates is the presence of layers of tetrahedra parallel to (001) connected by Ca or Ca and Na atoms. Consequently the *c* sides of the unit cells of the minerals written above and of aminoffite have nearly the same dimensions.

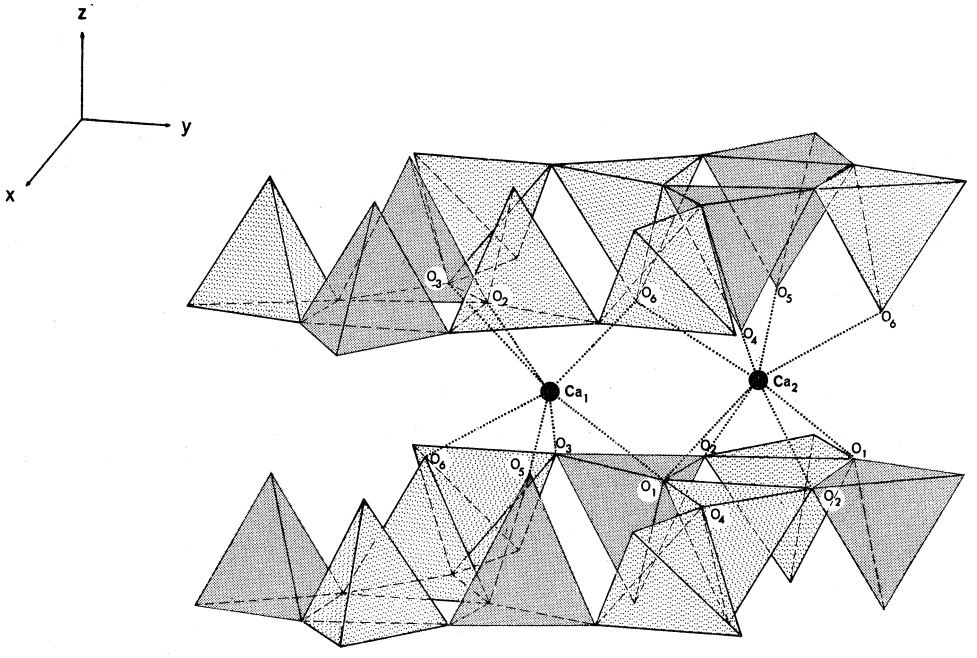

Fig. 2. – Perspective view of the layers of tetrahedra showing the coordination of Ca atoms. Dotted tetrahedra: Si; dashed tetrahedra: Be.

The tetrahedral sheets of melilites, meliphanite and leucophanite are built up by rings of five tetrahedra while those of aminoffite consist of rings of four and six tetrahedra. Owing to these differences, aminoffite cannot be classified in the same " structure family " [7] as melilites, but in a particular " structure family " of single sheet silicates with tetrahedral loops of four and six members.

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