

The following material did not appear in the original publication.



K L IOFO IOFC				K L IOFO IOFC				K L IOFO IOFC			
11	4	275	270	6	-12	124	132	5	-9	202	198
11	-4	32	65	6	-12	634	623	5	10	198	207
11	-5	97	100	6	-14	117	125	5	-10	198	207
11	-6	183	177	6	-14	324	305	5	-11	207	207
				6	-15	132	125	5	-12	324	321
				6	-16	323	318	5	-13	171	178
				6	-16	73	67	5	-13	171	178
				6	-17	50	45	5	-14	197	192
				6	-17	51	46	5	-14	224	227
				6	-19	100	96	5	-18	145	155
				6	0	176	172	5	-17	340	324
				6	0	147	146	5	-17	94	100
				6	0	124	119	5	-17	257	246
				6	0	200	205	5	-12	117	110
				6	0	159	153	5	-2	58	59
				6	0	31	40	5	-3	71	62
				6	0	170	167	5	-3	51	37
				6	0	235	228	5	-3	166	158
				6	0	338	332	5	-4	80	73
				6	0	103	103	5	-4	167	177
				6	0	133	119	5	-5	94	96
				6	0	92	101	5	-6	227	217
				6	0	335	334	5	-7	94	106
				6	0	101	111	5	-7	283	288
				6	0	103	102	5	-8	107	103
				6	0	114	105	5	-8	101	99
				6	0	63	61	5	-9	75	74
				6	0	53	50	5	-10	84	83
				6	0	212	209	5	-12	89	78
				6	0	187	186	5	-13	98	107
						116	121				
						70	66				
						213	208				
						224	219				
						176	168				
						90	82				
						211	210				
						162	172				
						89	91				
						93	81				
						56	67				
						216	214				
						84	76				
						238	233				
						75	65				
						71	66				
						130	140				
						174	170				
						144	150				
						61	51				
						32	23				
						288	272				
						236	232				
						247	246				
						64	61				
						239	253				
						118	128				
						113	114				
						110	114				
						113	122				
						117	122				
						300	302				
						82	84				
						145	150				
						140	151				
						197	199				
						220	210				
						166	150				
						232	257				
						306	306				
						83	79				
						93	95				
						143	137				
						33	40				
						257	272				
						40	41				
						108	116				
						353	348				
						573	573				
						46	44				
						289	276				
						376	370				
						263	249				
						107	97				
						54	54				
						134	123				
						88	82				
						422	422				
						646	635				
						60	54				
						65	50				
						67	72				
						185	188				
						69	67				
						319	327				
						180	181				
						169	178				
						103	103				
						126	137				
						56	67				
						79	86				
						67	56				
						165	159				
						85	81				
						101	108				
						270	274				
						280	274				
						155	153				
						41	27				
						246	257				

MARGARITE-2M<sub>1</sub> ATOMIC PARAMETERS IN SPACE GROUP C2/c

Atom	x	y	z	B <sub>equiv.</sub>	$\beta_{11}$	$\beta_{22}$	$\beta_{33}$	$\beta_{12}$	$\beta_{13}$	$\beta_{23}$
Ca(1)	0	0.0935(1)	1/4	0.75(3)	0.0068(5)	0.0024(2)	0.00051(3)	0	0.00025(9)	0
Al(1)	0.2517(2)	0.0837(1)	0.00012(6)	0.48(3)	0.0046(4)	0.0012(2)	0.00034(3)	0.0001(2)	0.00008(9)	0.00001(5)
T(1)	0.4644(2)	0.9263(1)	0.14367(6)	0.54(3)	0.0046(4)	0.0014(1)	0.00045(3)	-0.0001(2)	0.00018(9)	-0.00003(5)
T(2)	0.4538(2)	0.2563(1)	0.14354(6)	0.49(3)	0.0038(4)	0.0018(1)	0.00036(3)	0.0002(2)	0.00015(8)	0.00002(5)
O(1)	0.9577(6)	0.4420(3)	0.0560(2)	0.73(5)	0.005(1)	0.0026(3)	0.00064(8)	0.0012(5)	0.0003(2)	-0.0001(1)
O(2)	0.3886(6)	0.2518(3)	0.0563(2)	0.59(5)	0.0049(9)	0.0018(3)	0.00052(7)	0.0004(4)	0.0004(2)	0.0001(1)
OH(1)	0.4528(6)	0.5650(3)	0.0511(2)	0.71(5)	0.005(1)	0.0020(3)	0.00071(8)	-0.0010(5)	0.0006(2)	0.0000(1)
O(3)	0.3626(6)	0.0894(3)	0.1771(2)	0.80(5)	0.007(1)	0.0027(4)	0.00055(7)	-0.0008(5)	0.0006(2)	0.0003(1)
O(4)	0.2778(6)	0.7819(3)	0.1677(2)	0.73(5)	0.007(1)	0.0020(3)	0.00055(7)	0.0011(5)	0.0000(2)	0.0002(1)
O(5)	0.2764(6)	0.3924(3)	0.1786(2)	0.74(5)	0.006(1)	0.0021(4)	0.00055(8)	0.0003(5)	0.0002(2)	-0.0001(1)

MARGARITE-2M<sub>1</sub> BOND LENGTHS AND ANGLES IN SPACE GROUP Cc

Bond lengths (Å)				Bond angles (°)			
Tetrahedron T(1)							
to	0(1)	1.722(7)	0(1)--0(3)	2.839(8)	0(1)--0(3)	109.7(4)	
	0(3)	1.749(7)		0(4)	2.907(8)	0(4)	113.9(3)
	0(4)	1.746(7)		0(5)	2.840(8)	0(5)	108.8(3)
	0(5)	<u>1.771(7)</u>	0(3)--0(4)	2.866(8)	0(3)--0(4)	110.2(4)	
	Mean	1.747		0(5)	2.818(9)	0(5)	106.3(3)
	(= 0.853 Al)		0(4)--0(5)	<u>2.837(8)</u>	0(4)--0(5)	<u>107.5(3)</u>	
			Mean	2.851	Mean	109.4	
Tetrahedron T(11)							
to	0(11)	1.628(8)	0(11)--0(33)	2.653(9)	0(11)--0(33)	109.5(4)	
	0(33)	1.622(7)		0(44)	2.677(8)	0(44)	110.6(4)
	0(44)	1.627(7)		0(55)	2.664(9)	0(55)	110.6(4)
	0(55)	<u>1.613(7)</u>	0(33)--0(44)	2.658(8)	0(33)--0(44)	109.8(4)	
	Mean	1.623		0(55)	2.642(8)	0(55)	109.6(4)
	(= 0.092 Al)		0(44)--0(55)	<u>2.600(9)</u>	0(44)--0(55)	<u>106.7(4)</u>	
			Mean	2.649	Mean	109.5	
Tetrahedron T(2)							
to	0(2)	1.636(7)	0(2)--0(3)	2.685(9)	0(2)--0(3)	110.7(3)	
	0(3)	1.629(7)		0(4)	2.694(8)	0(4)	111.3(3)
	0(4)	1.627(6)		0(5)	2.698(8)	0(5)	110.9(3)
	0(5)	<u>1.640(7)</u>	0(3)--0(4)	2.619(8)	0(3)--0(4)	107.0(3)	
	Mean	1.633		0(5)	2.634(9)	0(5)	107.4(4)
	(= 0.153 Al)		0(4)--0(5)	<u>2.666(9)</u>	0(4)--0(5)	<u>109.4(3)</u>	
			Mean	2.666	Mean	109.5	
Tetrahedron T(22)							
to	0(22)	1.713(7)	0(22)--0(33)	2.792(9)	0(22)--0(33)	107.7(3)	
	0(33)	1.744(7)		0(44)	2.886(8)	0(44)	113.0(4)
	0(44)	1.747(7)		0(55)	2.827(9)	0(55)	110.0(3)
	0(55)	<u>1.738(7)</u>	0(33)--0(44)	2.833(8)	0(33)--0(44)	108.5(3)	
	Mean	1.736		0(55)	2.792(9)	0(55)	106.6(4)
	(= 0.785 Al)		0(44)--0(55)	<u>2.869(9)</u>	0(44)--0(55)	<u>110.8(4)</u>	
			Mean	2.833	Mean	109.4	
Interlayer cation Ca(1)							
to	0(3)	2.421(8)			3.396(7)		
	0(4)	2.486(7)			3.530(7)		
	0(5)	2.426(7)			3.374(7)		
	0(33)	2.426(7)			3.428(7)		
	0(44)	2.491(7)			3.533(7)		
	0(55)	<u>2.476(7)</u>			<u>3.328(7)</u>		
	Mean	2.454		Mean	3.432		
	Inner			Outer			

Octahedron M(2)				T(1) to T(2)		
to	0(1)	1.860(7)	0(1)--0(2)	2.770(8)	around 0(3)	119.3(5)
	0(2)	1.948(7)	0(22)	2.830(8)	0(4)	125.4(4)
	OH(1)	1.910(7)	OH(1)	2.724(9)	0(5)	<u>117.8(4)</u>
	0(11)	1.930(7)	0(2)--OH(1)	2.802(9)	Mean	120.8
	0(22)	1.872(7)	OH(11)	2.838(9)		
	Oh(11)	<u>1.900(8)</u>	0(11)-OH(1)	2.813(9)		
Mean	1.903		0(22)	2.775(9)		
			OH(11)	2.753(9)	T(11) to T(22)	
			0(22)-OH(11)	<u>2.736(9)</u>	around 0(33)	119.9(4)
			Mean	2.782	0(44)	126.6(4)
			unshared		0(55)	<u>120.4(4)</u>
					Mean	122.3
			0(1)--0(11)	2.462(6)		
			0(2)--0(22)	2.458(5)		
			OH(1)-OH(11)	<u>2.363(5)</u>		
			Mean	2.428		
			shared			
Octahedron M(3)						
to	0(1)	1.885(7)	0(1)--0(2)	2.761(9)		
	0(2)	1.975(6)	OH(1)	2.837(9)		
	OH(1)	1.897(7)	OH(11)	2.785(9)		
	0(11)	1.990(7)	0(2)--0(11)	3.001(8)		
	0(22)	1.857(7)	OH(1)	2.793(8)		
	OH(11)	<u>1.883(8)</u>	0(11)-0(22)	2.754(9)		
Mean	1.915		OH(11)	2.795(9)		
			0(22)-OH(1)	2.753(8)		
			OH(11)	<u>2.769(10)</u>		
			Mean	2.805		
			unshared			

End of supplemental material.