

Summary**Collection Code 152489**

Struct.formula	Ca5 (Si6 O16 (O H)2) (H2 O)7	Author	Bonaccorsi, E.; Merlino, S.; Kampf, A.R.
Space Group	B 1 1 b(9)	Title of Article	The crystal structure of tobermorite 14 A (plombierite), a C - S - H phase
Unit Cell	6.735(2) 7.425(2) 27.987(5) 90. 90. 123.25(1)	Reference	Journal of the American Ceramic Society (2005) 88, p505-p512
Cell Volume	1170.43 Å ³	Formula Units per Cell	2
Temperature	room temperature	Pressure	atmospheric
PDF-numbers		R-value	0.152
Remark		Warnings & Comments	0 Warnings / 1 Comments

Details**Visualization****Chemistry****Published Crystal Structure Data****Standardized Crystal Structure Data**

Cell Parameters	6.7350 27.9870 6.7567 90.000 113.220 90.000				
Volume	1170.42	Formula Units per Cell	2	Calc. Dens.	2.23
Space Group	C 1 c 1(9)	Pearson Symbol	mS104		
Crystal System	monoclinic	Crystal Class	m	Laue Class	2/m
Wyckoff Sequence	a20				
Axis Ratios	a/b 0.2406	b/c 4.1421	c/a 1.0032		
Transformation Method	Tidy				
Transformation Info	REMARK Transformed from setting B 1 1 b.--> C c TRANS -a,c,a+b origin .85500 1/4 .25000				

Remark

EL	Lbl	OxState	WyckSymb	X	Y	Z	U	SOF
Ca	1	+2.00	4a	0.3330	0.5352	0.1750	0.0290	
Ca	2	+2.00	4a	0.3220	0.0353	0.6780	0.0290	
Si	1	+4.00	4a	0.2810	0.4252	0.1360	0.0360	
Si	2	+4.00	4a	0.0000	0.1459	0.0000	0.0460	
Si	3	+4.00	4a	0.3630	0.0749	0.2110	0.0300	
O	1	-2.00	4a	0.4050	0.3748	0.2620	0.0310	
O	2	-2.00	4a	0.5740	0.0958	0.4390	0.0420	
O	3	-2.00	4a	0.2270	0.4570	0.3040	0.0240	
O	4	-2.00	4a	0.4280	0.4565	0.0510	0.0190	
O	5	-2.00	4a	0.0080	0.2018	0.0000	0.0810	
O	6	-2.00	4a	0.3510	0.6325	0.1380	0.0620	
O	7	-2.00	4a	0.2980	0.1204	0.6950	0.0510	
O	8	-2.00	4a	0.2460	0.1248	0.1100	0.0510	
O	9	-2.00	4a	0.4680	0.0433	0.0740	0.0190	
O	10	-2.00	4a	0.1960	0.0431	0.2830	0.0520	
O	11	-2.00	4a	0.4640	0.1940	0.5190	0.1000	
O	12	-2.00	4a	0.4710	0.2530	0.0370	0.0700	0.5000
O	13	-2.00	4a	0.0600	0.2470	0.4620	0.0800	0.5000
Ca	3	+2.00	4a	0.2600	0.2481	0.2440	0.0700	0.5000
O	14	-2.00	4a	0.3410	0.2500	0.1790	0.0700	0.5000

Distances & Angles**Bibliography****Experimental Information****Warnings & Comments****Compare Published & Standardized Structure**