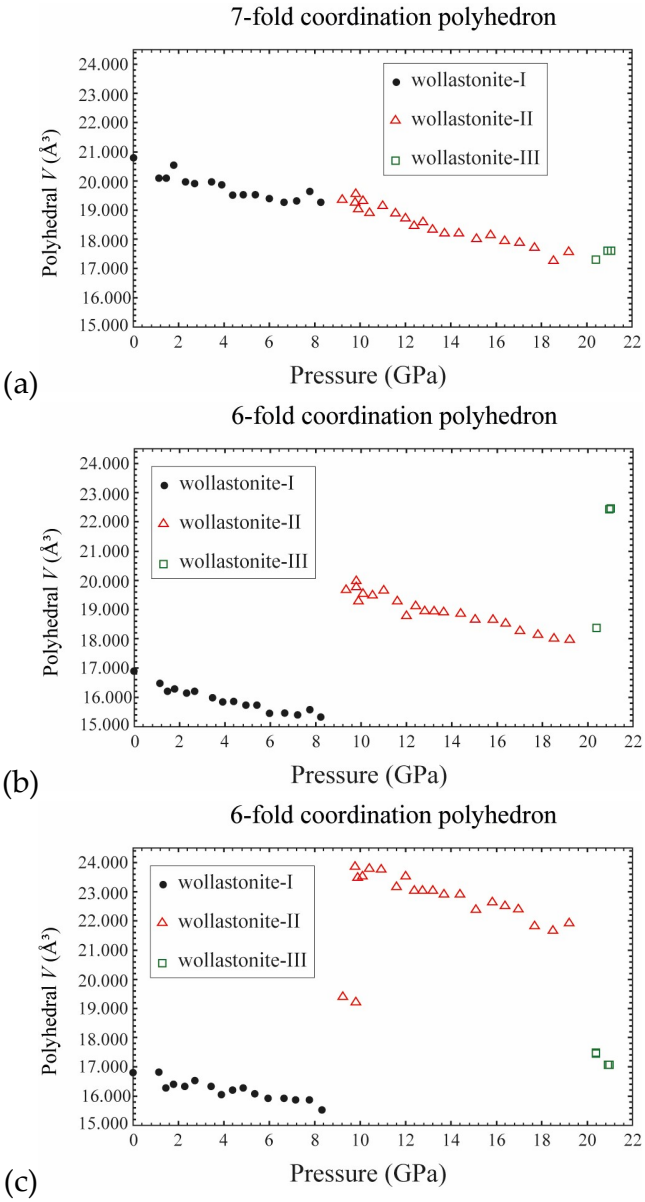

Figure S1. Volume change of the bigger wollastonite polyhedra. (**a**) 7-fold coordination polyhedron; (**b,c**) 6-fold coordinated polyhedron.

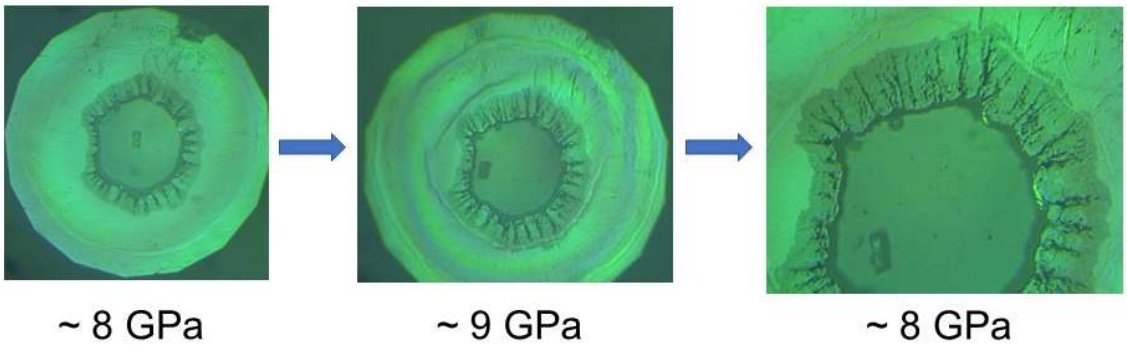

Figure S2. *In-situ* pictures of the pressure chamber loaded with a single crystal of $CaSiO_3$-walstomite, rubies as pressure standard and He as pressure transmitting medium. From the sequence of pictures, it is evident how the crystal 'jumps' from the center of the pressure chamber to the left margin. A movement is visible also in decompression.

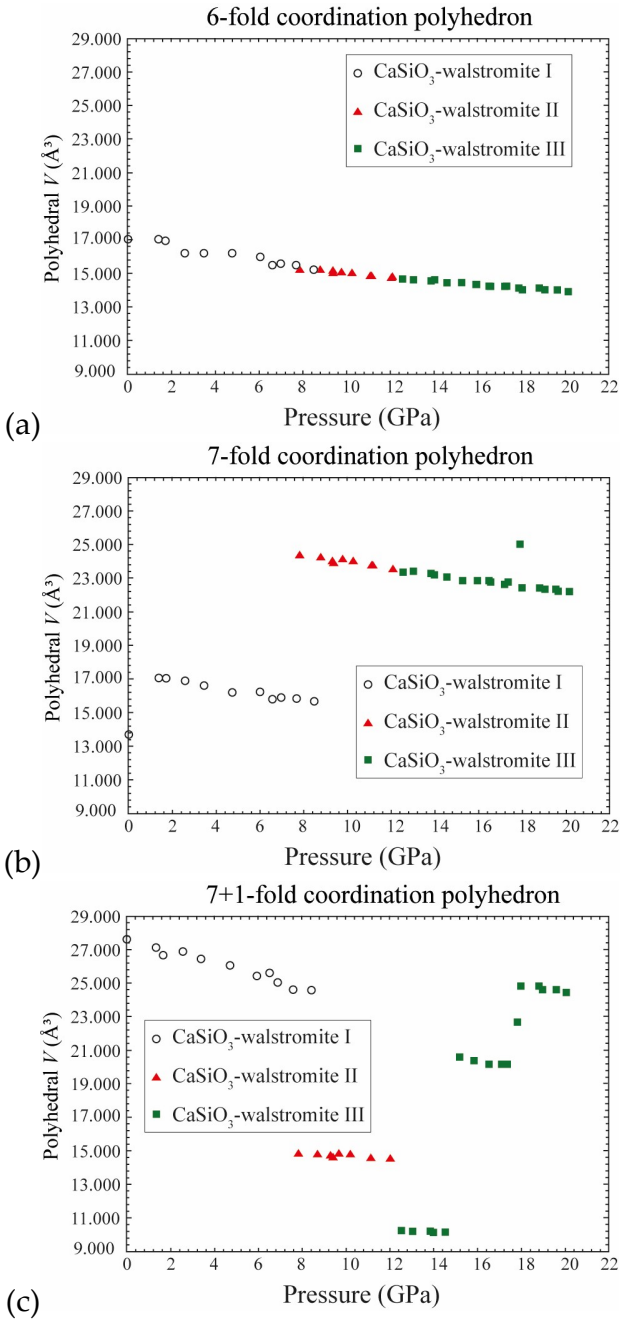

Figure S3. Volume change of the bigger $CaSiO_3$-walstromite polyhedra. (**a**) 6-fold coordinated polyhedron; (**b**) 7-fold coordination polyhedron (**c**) 7+1-fold coordination polyhedron

Table S1. Atomic coordinates, site occupancies and isotropic displacement parameters (Å^2) of the wollastonite studied in this work.

Site	*x*	*y*	*z*	Site occupancies	U_{iso}
wollastonite-I					
T(1)	0.2311(5)	0.1116(2)	0.8146(4)	1	0.0082(4)
T(2)	-0.2322(5)	0.4542(2)	0.1861(4)	1	0.0078(4)
T(3)	0.5575(5)	0.2233(2)	0.3961(4)	1	0.0084(4)
Ca(1)	0.0260(4)	0.2503(2)	0.5028(3)	1	0.0093(3)
Ca(2)	0.2617(4)	-0.0772(2)	0.1981(3)	1	0.0095(3)
Ca(3)	0.2641(4)	0.4290(2)	0.2022(3)	1	0.0088(3)
O(1)	0.304(2)	0.7299(6)	0.428(1)	1	0.0100(9)
O(2)	0.404(2)	0.6300(6)	0.731(2)	1	0.012(1)
O(3)	0.330(2)	0.2269(6)	0.402(1)	1	0.0087(9)
O(4)	0.401(2)	-0.0127(6)	0.731(2)	1	0.0112(10)
O(5)	0.237(2)	0.6321(6)	0.018(2)	1	0.014(1)
O(6)	0.278(2)	0.3213(6	0.780(2)	1	0.013(1)
O(7)	0.034(2)	0.5609(6)	0.699(1)	1	0.0097(9)
O(8)	0.036(2)	0.0387(6)	0.696(1)	1	0.0106(9)
O(9)	0.238(2)	0.1264(6)	0.017(2)	1	0.012(1)
wollastonite-II					
T(1)	0.7199(9)	0.2180(4)	0.3964(4)	1	0.0073(6)
T(2)	1.1905(9)	0.2969(4)	0.0884(4)	1	0.0071(6)
T(3)	0.4721(9)	-0.0262(4)	0.3053(4)	1	0.0064(6)
T(4)	0.8184(9)	0.1378(4)	-0.0857(4)	1	0.0086(6)
T(5)	0.381(1)	0.5109(4)	0.2254(4)	1	0.0079(6)
T(6)	0.7304(9)	-0.3567(4)	0.3977(4)	1	0.0076(6)
Ca(1)	0.6327(7)	0.3263(3)	0.0961(3)	1	0.0071(5)
Ca(2)	0.3753(7)	0.1695(3)	-0.0959(3)	1	0.0070(5)
Ca(3)	1.1802(6)	-0.3332(3)	0.4174(2)	1	0.0048(4)
Ca(4)	0.9511(7)	0.5183(3)	0.2204(3)	1	0.0073(5)
Ca(5)	0.9492(6)	0.0113(3	0.2302(2)	1	0.0068(5)
Ca(6)	0.1698(6)	0.1701(3)	0.4112(2)	1	0.0058(5)
O(1)	0.834(2)	-0.355(1)	0.4894(8)	1	0.009(2)
O(2)	0.517(2)	0.130(2)	0.3657(9)	1	0.012(2)
O(3)	0.305(2)	0.351(2)	0.1730(9)	1	0.016(2)
O(4)	0.192(2)	-0.112(1)	0.5129(8)	1	0.009(2)
O(5)	0.672(2)	0.6206(9)	-0.0002(8)	1	0.004(2)
O(6)	0.535(2)	-0.232(1)	0.3768(8)	1	0.006(2)
O(7)	0.298(2)	0.714(2)	0.1654(9)	1	0.015(2)
O(8)	0.684(2)	0.128(1)	0.0060(8)	1	0.008(2)
O(9)	0.647(2)	0.426(1)	0.4080(9)	1	0.014(2)
O(10)	0.604(2)	0.017(1)	0.2086(8)	1	0.0061(2)
O(11)	1.217(2)	0.066(1)	0.1130(8)	1	0.010(2)
O(12)	0.896(2)	-0.290(1)	0.3160(8)	1	0.001(2)
O(13)	0.258(2)	0.470(2)	0.3217(8)	1	0.006(2)
O(14)	0.888(2)	0.229(1)	0.3141(8)	1	0.008(2)
O(15)	1.048(2)	0.190(2)	-0.1037(9)	1	0.016(2)

O(16)	0.960(2)	0.333(2)	0.1095(9)	1	0.014(2)
O(17)	0.239(2)	-0.037(1)	0.3109(8)	1	0.008(2)
O(18)	0.612(2)	0.527(1)	0.2043(8)	1	0.008(2)
wollastonite-III					
T(1)	0.192(2)	0.1113(4)	-0.3655(3)	1	0.0085(7)
T(2)	0.198(2)	0.1040(4)	0.1401(3)	1	0.0091(7)
T(3)	0.851(2)	0.2703(5)	0.0026(3)	1	0.0100(8)
T(4)	0.931(2)	0.1958(5)	-0.2393(3)	1	0.0109(8)

Table S1 (continued)

T(5)	1.315(2)	0.5783(4)	0.1780(2)	1	0.0074(7)
T(6)	0.947(2)	0.1912(5)	0.2619(3)	1	0.0100(8)
T(7)	0.653(2)	0.4346(5)	0.3112(3)	1	0.0093(7)
T(8)	0.854(2)	0.2790(5)	0.4947(3)	1	0.0105(8)
T(9)	0.655(2)	0.4375(4	0.1038(3)	1	0.0110(8)
T(10)	1.210(2)	0.1016(5)	0.4252(3)	1	0.0107(8)
T(11)	0.221(2)	0.1134(4	-0.0754(2)	1	0.0090(7)
T(12)	1.318(2)	0.5820(4)	0.3983(3)	1	0.0098(7)
Ca(1)	1.0808(9)	0.4026(3)	0.0928(2)	1	0.0093(6)
Ca(2)	0.6748(9)	0.0812(3)	-0.0793(2)	1	0.0093(5)
Ca(3)	0.4275(9)	0.2811(3)	0.2402(2)	1	0.0070(5)
Ca(4)	0.6596(9)	0.0817(3)	0.4146(2)	1	0.0071(5)
Ca(5)	0.6365(9)	0.0838(3)	0.1696(2)	1	0.0074(5)
Ca(6)	0.4159(9)	0.2801(3)	-0.2628(2)	1	0.0109(6)
Ca(7)	0.6422(9)	0.0963(3)	-0.3391(2)	1	0.0080(5)
Ca(8)	0.4351(9)	0.2943(3)	-0.0005(2)	1	0.0124(6)
Ca(9)	0.8768(9)	0.6001(3)	0.4157(2)	1	0.0092(5
Ca(10)	0.8758(9)	0.6159(3)	0.1538(2)	1	0.0104(6)
Ca(11)	1.0752(9)	0.4053(3)	0.3291(2)	1	0.0094(5)
Ca(12)	0.4307(9)	0.2920(3)	0.4779(2)	1	0.0107(6)
O(1)	1.135(3)	0.501(1)	0.1864(5)	1	0.006(2)
O(2)	1.339(3)	0.007(2)	0.4272(6)	1	0.014(2)
O(3)	0.832(3)	0.512(1)	0.0527(6)	1	0.009(2)
O(4)	0.343(3)	0.026(2)	-0.0820(7)	1	0.018(2)
O(5)	0.686(3)	-0.018(2)	0.3078(6	1	0.013(2)
O(6)	1.090(3)	0.287(2)	0.2422(6)	1	0.009(2)
O(7)	0.426(3)	0.403(2)	0.0958(7)	1	0.017(2)
O(8)	0.305(3)	0.006(2)	0.1976(6	1	0.014(2)
O(9)	0.938(3)	0.704(2)	0.2627(6)	1	0.011(2)
O(10)	0.349(3)	0.213(1)	-0.1087(6)	1	0.011(2)
O(11)	0.987(3)	0.130(2)	0.1797(6)	1	0.015(2)
O(12)	0.804(3)	0.318(2)	0.5881(6)	1	0.013(2)
O(13)	1.161(3)	0.494(2)	0.4333(6)	1	0.011(2)
O(14)	0.761(3)	0.537(2)	0.3009(6)	1	0.012(2)
O(15)	1.534(3)	0.593(1)	0.4360(6)	1	0.011(2)
O(16)	1.086(3)	0.285(1)	0.0022(6)	1	0.011(2)
O(17)	0.977(3)	0.135(2)	-0.3199(6)	1	0.013(2)
O(18)	0.363(3)	0.192(1)	0.3877(6)	1	0.009(2)

O(19)	0.351(3)	0.202(2)	-0.3752(6)	1	0.010(2)
O(20)	0.004(3)	0.126(2)	-0.1349(6)	1	0.016(2)
O(21)	1.125(3)	0.086(2)	0.5343(6)	1	0.012(2)
O(22)	0.708(3)	0.176(1)	0.0232(6)	1	0.008(2)
O(23)	0.358(3)	0.191(2)	0.1368(6	1	0.013(2)
O(24)	0.419(3)	0.405(1)	0.3266(6)	1	0.013(2)
O(25)	0.756(3)	0.336(2)	0.0691(7)	1	0.016(2)
O(26)	1.011(3)	0.113(2)	0.3623(6)	1	0.014(2)
O(27)	0.133(3)	0.084(2)	0.0365(6)	1	0.014(2)
O(28)	1.337(3)	0.606(1)	0.2807(6)	1	0.009(2)
O(29)	1.085(3)	0.295(2)	0.4775(6)	1	0.012(2)
O(30)	0.688(3)	0.192(1)	-0.2306(6)	1	0.005(2)
O(31)	0.760(3)	0.363(2)	0.4039(7)	1	0.021(2)
O(32)	1.220(3)	0.681(1)	0.1106(6)	1	0.010(2)
O(33)	0.285(3)	0.814(2)	0.4948(6)	1	0.012(2)
O(34)	0.288(3)	0.809(1)	0.7316(6)	1	0.007(2)

Table S1 (continued)

O(35)	0.264(3)	0.606(2)	0.7806(6)	1	0.015(2)
O(36)	0.475(3)	0.431(2)	0.8648(7)	1	0.017(2)

Table S2. Interatomic distances (Å) selected from the structural refinement of the wollastonite studied in this work.

wollastonite-I	
T(1)-O(4)	1.609(9)
-O(6)	1.660(7)
-O(8)	1.613(9)
-O(9)	1.580(10)
<*T*(1)-O>	1.615
T(2)-O(2)	1.619(11)
-O(5)	1.597(9)
-O(6)	1.642(5)
-O(7)	1.619(10)
<*T*(2)-O>	1.619
T(3)-O(1)	1.598(9)
-O(2)	1.675(9)
-O(3)	1.614(10)
-O(4)	1.678(6)
<*T*(3)-O>	1.641
Ca(1)-O(1)	2.446(10)
-O(3)	2.358(10)
-O(6)	2.653(9)
-O(7)	2.439(6)
-O(7)	2.359(8)
-O(8)	2.415(8)
-O(8)	2.342(6)
<*Ca*(1)-O>	2.430
Ca(2)-O(1)	2.552(8)
-O(3)	2.450(6)
-O(4)	2.456(10)
-O(5)	2.269(6)
-O(8)	2.338(10)
-O(9)	2.298(8)
<*Ca*(2)-O>	2.394
Ca(3)-O(1)	2.495(6)
-O(2)	2.423(11)
-O(3)	2.426(8)
-O(5)	2.311(8)
-O(7)	2.316(10)
-O(9)	2.357(6)
<*Ca*(3)-O>	2.388
wollastonite-II	
T(1)-O(2)	1.635(15)
-O(4)	1.535(13)
-O(9)	1.631(10)
-O(14)	1.609(14)
<*T*(1)-O>	1.603
T(2)-O(3)	1.635(16)
-O(5)	1.559(13)
-O(11)	1.642(8)
-O(16)	1.593(15)
<*T*(2)-O>	1.607

Table S2 (continued)

T(3)-O(2)	1.644(14)
-O(6)	1.678(10)
-O(10)	1.615(14)
-O(17)	1.559(15)
<*T*(3)-O>	1.624
T(4)-O(7)	1.630(13)
-O(8)	1.585(14)
-O(11)	1.643(11)
-O(15)	1.576(15)
<*T*(4)-O>	1.608
T(5)-O(3)	1.644(14)
-O(7)	1.643(10)
-O(13)	1.580(14)
-O(18)	1.562(15)
<*T*(5)-O>	1.607
T(6)-O(1)	1.570(15)
-O(6)	1.593(13)
-O(9)	1.643(10)
-O(12)	1.588(14)
<*T*(6)-O>	1.599
Ca(1)-O(3)	2.447(14)
-O(5)	2.530(14)
-O(5)	2.275(8)
-O(8)	2.207(12)
-O(10)	2.459(9)
-O(16)	2.212(15)
-O(18)	2.423(12)
<*Ca*(1)-O>	2.365
Ca(2)-O(5)	2.341(12)
-O(7)	2.431(14)
-O(8)	2.605(14)
-O(8)	2.275(8)
-O(10)	2.398(13)
-O(15)	2.203(15)
-O(18)	2.394(9)
<*Ca*(2)-O>	2.378
Ca(3)-O(1)	2.354(8)
-O(1)	2.491(14)
-O(4)	2.396(12)
-O(6)	2.487(14)
-O(12)	2.467(14)
-O(13)	2.294(12)
-O(17)	2.366(9)
<*Ca*(3)-O>	2.408
Ca(4)-O(3)	2.797(14)
-O(7)	2.707(13)
-O(12)	2.236(12)
-O(13)	2.589(14)
-O(14)	2.252(9)
-O(15)	2.396(10)
-O(16)	2.367(14)
-O(18)	2.294(15)
<*Ca*(4)-O>	2.455
Ca(5)-O(10)	2.349(15)

Table S2 (continued)	
-O(11)	2.401(13)
-O(12)	2.271(8)
-O(14)	2.263(11)
-O(15)	2.649(14)
-O(16)	2.583(9)
-O(17)	2.319(14)
< *Ca*(5)-O>	2.405
Ca(6)-O(1)	2.225(12)
-O(2)	2.424(14)
-O(4)	2.243(9)
-O(4)	2.609(14)
-O(13)	2.318(8)
-O(14)	2.415(14)
-O(17)	2.390(12)
< *Ca*(6)-O>	2.375
wollastonite-III	
T(1)-O(5)	1.603(17)
-O(17)	1.63(2)
-O(19)	1.619(19)
-O(21)	1.619(13)
<*T*(1)-O>	1.618
T(2)-O(8)	1.598(17)
-O(11)	1.58(3)
-O(23)	1.592(19)
-O(27)	1.634(13)
<*T*(2)-O>	1.602
T(3)-O(16)	1.56(3)
-O(22)	1.581(18)
-O(25)	1.615(18)
-O(32)	1.664(11)
<*T*(3)-O>	1.604
T(4)-O(9)	1.599(18)
-O(17)	1.632(16)
-O(20)	1.651(12)
-O(30)	1.60(3)
<*T*(4)-O>	1.620
T(5)-O(1)	1.575(19)
-O(28)	1.616(12)
-O(32)	1.665(15)
-O(36)	1.53(2)
<*T*(5)-O>	1.597
T(6)-O(6)	1.598(19)
-O(11)	1.652(16)
-O(26)	1.642(12)
-O(34)	1.55(3)
<*T*(6)-O>	1.610
T(7)-O(14)	1.570(18)
-O(24)	1.58(3)
-O(31)	1.627(15)
-O(35)	1.660(15)
<*T*(7)-O>	1.610
T(8)-O(12)	1.605(14)
-O(29)	1.54(3)
-O(31)	1.653(14)

Table S2 (continued)

-O(33)	1.554(19)
<*T*(8)-O>	1.589
T(9)-O(3)	1.601(18)
-O(7)	1.58(3)
-O(25)	1.779(18)
-O(35)	1.705(12)
<*T*(9)-O>	1.667
T(10)-O(2)	1.592(19)
-O(18)	1.589(18)
-O(21)	1.619(12)
-O(26)	1.577(19)
<*T*(10)-O>	1.594
T(11)-O(4)	1.51(2)
-O(10)	1.593(17)
-O(20)	1.652(19)
-O(27)	1.651(11)
<*T*(11)-O>	1.602
T(12)-O(12)	1.691(19)
-O(13)	1.581(18)
-O(15)	1.54(3)
-O(28)	1.636(10)
<*T*(12)-O>	1.612
Ca(1)-O(1)	2.187(14)
-O(3)	2.198(10)
-O(3)	2.250(18)
-O(6)	2.344(11)
-O(7)	2.27(3)
-O(16)	2.356(15)
-O(25)	2.38(2)
<*Ca*(1)-O>	2.283
Ca(2)-O(4)	2.423(11)
-O(4)	2.31(3)
-O(8)	2.338(14)
-O(20)	2.32(2)
-O(22)	2.227(14)
-O(27)	2.614(18)
-O(30)	2.336(10)
<*Ca*(2)-O>	2.3666
Ca(3)-O(6)	2.22(3)
-O(7)	2.339(12)
-O(18)	2.207(10)
-O(23)	2.224(15)
-O(24)	2.382(15)
-O(34)	2.264(19)
-O(35)	2.521(19)
<*Ca*(3)-O>	2.308
Ca(4)-O(2)	2.298(10)
-O(2)	2.32(2)
-O(5)	2.332(15)
-O(18)	2.490(19)
-O(21)	2.732(18)
-O(26)	2.42(2)
-O(33)	2.225(15)
-O(34)	2.289(10)

Table S2 (continued)	
<*Ca*(4)-O>	2.389
Ca(5)-O(4)	2.229(17)
-O(5)	2.163(11)
-O(8)	2.41(2)
-O(11)	2.39(3)
-O(22)	2.216(10)
-O(23)	2.373(19)
-O(34)	2.363(15)
<*Ca*(5)-O>	2.306
Ca(6)-O(9)	2.34(3)
-O(10)	2.211(10)
-O(14)	2.790(17)
-O(15)	2.687(10)
-O(19)	2.202(14)
-O(28)	2.235(18)
-O(30)	2.181(19)
<*Ca*(6)-O>	2.378
Ca(7)-O(2)	2.162(15)
-O(5)	2.39(2)
-O(8)	2.208(11)
-O(17)	2.29(3)
-O(19)	2.431(19)
-O(30)	2.322(14)
-O(33)	2.317(10)
<*Ca*(7)-O>	2.303
Ca(8)-O(7)	2.313(16)
-O(10)	2.213(14)
-O(16)	2.29(3)
-O(22)	2.446(19)
-O(23)	2.186(11)
-O(25)	2.454(19)
-O(32)	2.725(18)
-O(36)	2.375(12)
<*Ca*(8)-O>	2.376
Ca(9)-O(9)	2.342(10)
-O(12)	2.37(2)
-O(13)	2.40(2)
-O(13)	2.245(10)
-O(14)	2.189(15)
-O(15)	2.27(3)
-O(29)	2.397(15)
<*Ca*(9)-O>	2.315
Ca(10)-O(1)	2.342(19)
-O(3)	2.319(14)
-O(9)	2.262(15)
-O(10)	2.795(17)
-O(14)	2.244(11)
-O(16)	2.332(10)
-O(32)	2.44(2)
-O(36)	2.42(3)
<*Ca*(10)-O>	2.395
Ca(11)-O(1)	2.181(9)
-O(6)	2.324(16)
-O(13)	2.239(15)

Table S2 (continued)	
-O(14)	2.769(19)
-O(24)	2.26(3)
-O(29)	2.304(10)
-O(31)	2.328(19)
-O(35)	2.753(18)
<*Ca*(11)-O>	2.395
Ca(12)-O(15)	2.282(15)
-O(18)	2.182(15)
-O(19)	2.222(11)
-O(24)	2.347(10)
-O(29)	2.27(3)
-O(31)	2.486(19)
-O(33)	2.39(2)
<*Ca*(12)-O>	2.311

Table S3. Atomic coordinates, site occupancies and isotropic displacement parameters (Å^2) of the $CaSiO_3$-walstromite studied in this work.

Site	*x*	*y*	*z*	Site occupancies	U_{iso}
$CaSiO_3$-walstromite-I					
T(1)	0.6076(3)	0.3377(4)	0.2930(9)	1	0.0066(5)
T(2)	0.2705(3)	0.7729(4)	-0.0137(9)	1	0.0082(5)
T(3)	-0.0424(3)	0.9775(5)	0.3015(9)	1	0.0087(5)
Ca(1)	0.0752(2)	0.4203(3)	0.3355(7)	1	0.0087(4)
Ca(2)	0.5852(3)	0.2296(4)	0.6498(7)	1	0.0126(4)
Ca(3)	0.2369(3)	0.2557(3)	0.0009(7)	1	0.0106(4)
O(1)	0.1289(9)	0.599(2)	0.062(2)	1	0.009(2)
O(2)	0.614(1)	0.160(2)	0.899(2)	1	0.014(2)
O(3)	0.1396(9)	0.112(2)	0.260(2)	1	0.010(2)
O(4)	0.0411(9)	0.728(2)	0.407(2)	1	0.011(2)
O(5)	0.4511(9)	0.690(2)	-0.132(2)	1	0.011(2)
O(6)	-0.2660(9)	0.527(2)	0.258(2)	1	0.013(2)
O(7)	-0.1356(9)	0.994(2)	0.141(2)	1	0.012(2)
O(8)	0.4163(9)	0.380(2)	0.406(2)	1	0.012(2)
O(9)	-0.2456(9)	1.094(2)	0.390(2)	1	0.011(2)
$CaSiO_3$-walstromite-II					
T(1)	0.2325(2)	0	0.5270(2)	1	0.0048(4)
T(2)	0.1318(2)	0.3170(2)	0.1835(2)	1	0.0051(3)
Ca(1)	0.3326(2)	0	0.1754(2)	1	0.0066(4)
Ca(2)	0.5	-0.2389(2)	0.5	1	0.0064(4)
Ca(3)	0.0538(2)	0	-0.1530(2)	1	0.0080(4)
O(1)	0.3589(6)	0	0.4525(6)	1	0.010(2)
O(2)	0.1512(4)	0.1641(6)	0.0753(5)	1	0.0095(8)
O(3)	0.3566(6)	0	-0.0926(6)	1	0.007(1)
O(4)	-0.0875(6)	0	-0.4047(6)	1	0.008(1)
O(5)	0.2375(4)	0.1628(5)	0.6538(4)	1	0.0061(7)
O(6)	0.4941(4)	-0.1981(5)	0.2369(5)	1	0.0079(8)
$CaSiO_3$-walstromite-III					
T(1)	0.5278(2)	0.0013(3)	0.2323(2)	1	0.0057(3)
T(2)	0.1848(2)	-0.3110(2)	0.1304(2)	1	0.0060(4)
T(3)	0.1776(2)	-0.8202(2)	0.6334(2)		0.0071(4)
Ca(1)	0.17724(12)	0.0015(2)	0.3321(2)	1	0.0081(2)
Ca(2)	0.49632(16)	0.2393(2)	0.5006(2)	1	0.0074(2)
Ca(3)	-0.1542(2)	0.0034(2)	0.0606(2)	1	0.0088(2)
O(1)	0.4551(4)	0.0023(6)	0.3596(4)	1	0.0089(7)
O(2)	0.0817(5)	-0.1488(6)	0.1414(5)	1	0.0105(9)
O(3)	0.0628(5)	-0.6772(6)	0.6618(5)	1	0.0098(9)
O(4)	-0.0903(4)	0.0072(7)	0.3571(4)	1	0.0095(7)
O(5)	-0.4049(4)	-0.0013(6)	-0.0858(4)	1	0.0095(7)
O(6)	0.6569(5)	-0.1599(6)	0.2351(5)	1	0.0076(9)
O(7)	0.3468(5)	0.6671(6)	0.2640(5)	1	0.0092(9)
O(8)	0.2302(5)	0.2015(5)	0.4952(5)	1	0.0096(9)
O(9)	0.2419(5)	-0.3033(5)	0.9932(4)	1	0.0091(9)

Table S4. Interatomic distances (Å) selected from the structural refinement of the $CaSiO_3$-walstromite studied in this work.

$CaSiO_3$-walstromite-I	
T(1)-O(5)	1.66(3)
-O(6)	1.605(9)
-O(8)	1.592(14)
-O(9)	1.682(8)
<*T*(1)-O>	1.636
T(2)-O(1)	1.592(8)
-O(2)	1.610(18)
-O(5)	1.665(15)
-O(7)	1.709(11)
<*T*(2)-O>	1.644
T(3)-O(3)	1.612(8)
-O(4)	1.610(9)
-O(7)	1.64(2)
-O(9)	1.675(13)
<*T*(3)-O>	1.633
Ca(1)-O(1)	2.430(18)
-O(3)	2.332(14)
-O(4)	2.369(17)
-O(4)	2.330(14)
-O(6)	2.323(9)
-O(8)	2.355(10)
<*Ca*(1)-O>	2.357
Ca(2)-O(2)	2.22(2)
-O(3)	2.507(7)
-O(4)	2.542(7)
-O(6)	2.608(11)
-O(8)	2.480(9)
-O(8)	2.416(17)
<*Ca*(2)-O>	2.462
Ca(3)-O(1)	2.446(8)
-O(1)	2.480(13)
-O(2)	2.591(10)
-O(2)	2.585(8)
-O(3)	2.340(17)
-O(5)	2.672(14)
-O(6)	2.353(16)
-O(7)	2.689(17)
<*Ca*(3)-O>	2.520
$CaSiO_3$-walstromite-II	
T(1)-O(1)	1.587(7)
-O(4)	1.577(6)
-O(5)(x2)	1.685(5)
<*T*(1)-O>	1.633
T(2)-O(2)	1.575(5)
-O(3)	1.669(4)
-O(5)	1.672(4)
-O(6)	1.596(5)
<*T*(2)-O>	1.628

Table S4 (continued)

Ca(1)-O(1)	2.333(6)
-O(2)(x2)	2.244(5)
-O(3)	2.386(6)
-O(6)(x2)	2.241(5)
<*Ca*(1)-O>	2.282
Ca(2)-O(1)(x2)	2.352(4)
-O(4)(x2)	2.481(4)
-O(5)(x2)	2.563(4)
-O(6) (x2)	2.276(5)
<*Ca*(2)-O>	2.418
Ca(3)-O(2)(x2)	2.352(5)
-O(2)(x2)	2.696(5)
-O(3)	3.001(7)
-O(4)	2.269(5)
-O(6)(x2)	2.514(5)
<*Ca*(3)-O>	2.549
$CaSiO_3$-walstromite-III	
T(1)-O(1)	1.563(5)
-O(5)	1.577(4)
-O(6)	1.672(6)
-O(7)	1.678(6)
<*T*(1)-O>	1.623
T(2)-O(2)	1.567(5)
-O(4)	1.660(6)
-O(7)	1.672(5)
-O(9)	1.582(5)
<*T*(2)-O>	1.620
T(3)-O(3)	1.563(6)
-O(4)	1.660(6)
-O(6)	1.677(5)
-O(8)	1.580(6)
<*T*(3)-O>	1.620
Ca(1)-O(1)	2.309(4)
-O(2)	2.227(5)
-O(3)	2.224(5)
-O(4)	2.355(4)
-O(8)	2.236(5)
-O(9)	2.216(5)
<*Ca*(1)-O>	2.261
Ca(2)-O(1)	2.314(5)
-O(1)	2.338(5)
-O(5)	2.465(5)
-O(5)	2.417(5)
-O(6)	2.529(5)
-O(7)	2.519(5)
-O(8)	2.271(5)
-O(9)	2.238(5)
<*Ca*(2)-O>	2.386
Ca(3)-O(2)	2.547(6)
-O(2)	2.299(5)
-O(3)	2.925(6)
-O(3)	2.313(5)

Table S4 (continued)

-O(4)	2.902(5)
-O(5)	2.262(4)
-O(6)	2.965(6)
-O(7)	2.995(6)
-O(8)	2.484(5)
-O(9)	2.276(5)
<*Ca*(3)-O>	2.618