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Crystal structure and elastic properties of parabreyite: a new high-pressure ring silicate in the $CaSiO_3$ system

Benedetta Chrappan Soldavini et al.

Correspondence to: Benedetta Chrappan Soldavini (benedetta.chrappan@unimi.it)

Supplementary materials:

Figure S1: HAADF STEM images of the two crystals from which we collected the 3D ED data merged for solving the crystal structure. The size and the location of the electron beam on the crystals is indicated by red circles. The crystal on the left shows how the crystal grain is formed by thin superimposed sheets. The relative shift between these sheets is the probable cause of the disorder. The direction of view is very close to *b**.

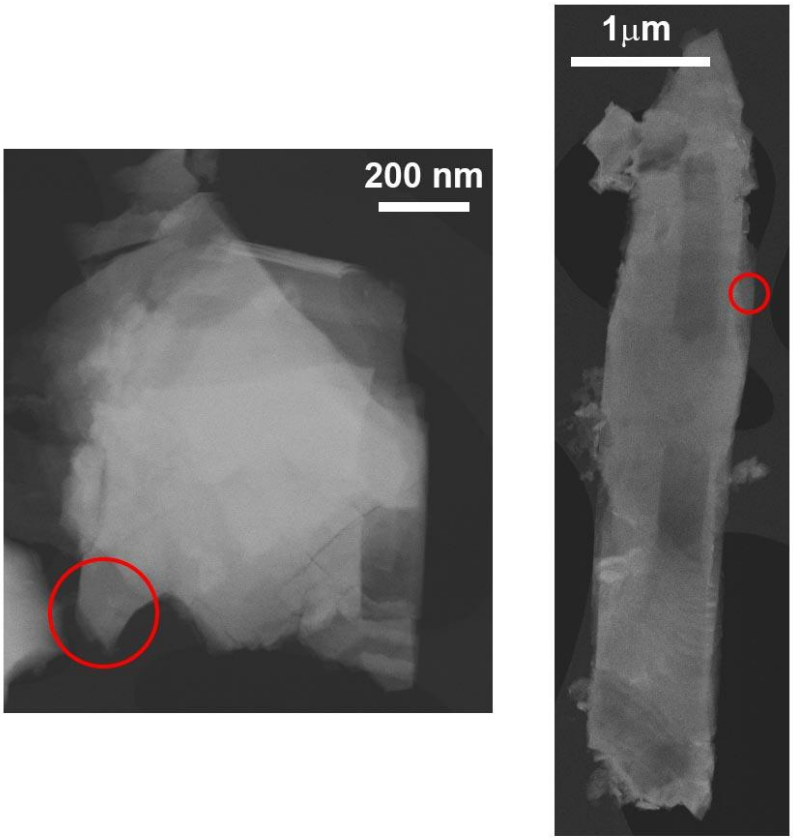


Figure S2: single crystal of parabreyite in quartz capillary for the low-to-high temperature experiment.

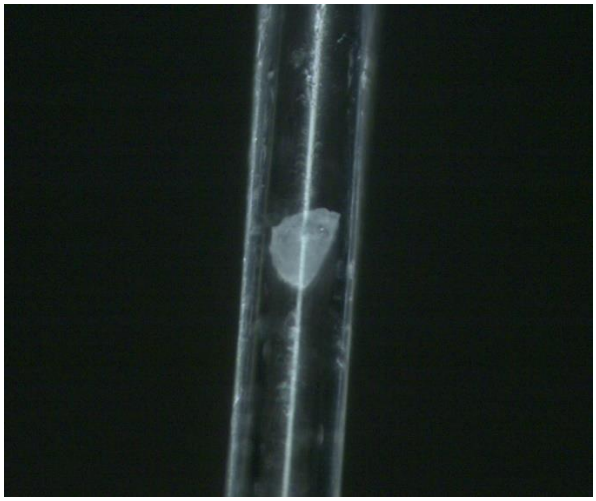
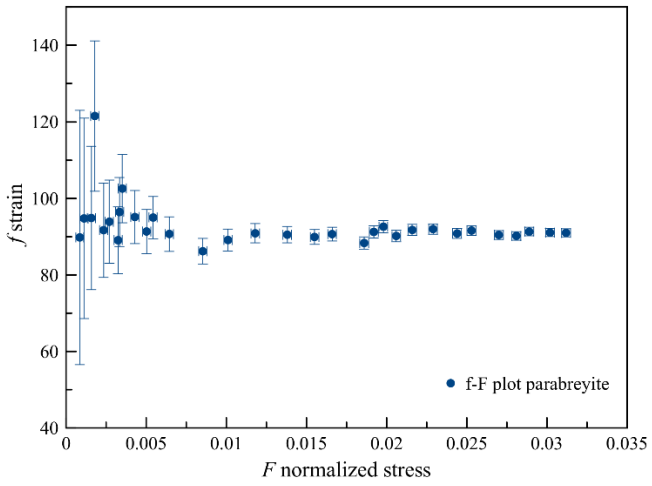


Figure S3: Eulerian finite strain (f_e) vs. normalized stress (F_e) plot for the different high-pressure runs.



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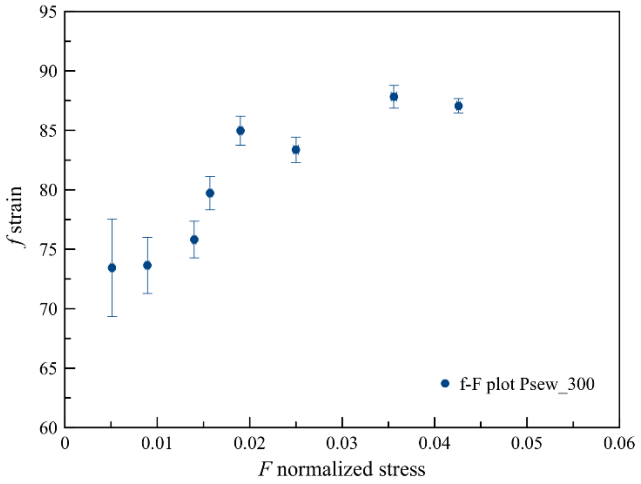

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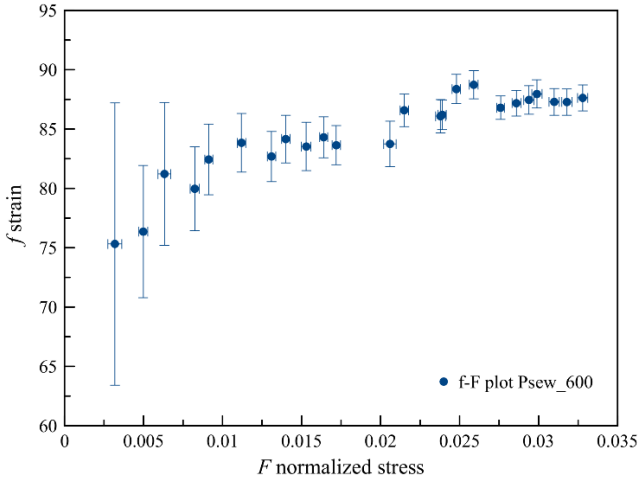

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Table S1: Details of 3D ED data collection and kinematical refinement.

Experimental details (Crystal Data)	
Crystal system, space group	Triclinic, *P-1*
Temperature (K)	293
a, b, c (Å)	8.2(1), 9.3(1), 10.5(1)
α,β,γ (°)	74(1),90(1),77(1)
Radiation type	Electron, λ= 0.0335 Å
3D ED data collection	PEDT
Precession semiangle	1°
Tilt range of the two merged data sets (°)	101; 105
Data resolution (Å)	0.7
	Kinematical Refinement
No. of: measured, independent and observed reflections	5217, 2864, 2013
R_{int} (all)	12.2%
Coverage up to 0.7Å	63%
Parameters	121
R_{obs}, wR_{obs} (%), S	37.8, 68.04, 4.79
R_{all}, wR_{all} (%)	42.0, 72.8

Table S2: Parabreyite compressibility

Step	***P (GPa)***	***a* (Å)**	***b* (Å)**	***c* (Å)**	***α* (°)**	***β* (°)**	***γ* (°)**	***V* (Å³)**
0	0.0001	8.1713(2)	9.3318(2)	10.4382(2)	73.902(2)	89.8888(19)	77.489(2)	745.14(3)
1	0.23(5)	8.161(2)	9.369(5)	10.419(3)	73.80(4)	90.13(2)	77.31(4)	744.6(4)
2	0.32(5)	8.157(2)	9.367(5)	10.415(3)	73.83(4)	90.14(2)	77.33(4)	744.0(4)
3	0.45(5)	8.152(2)	9.367(5)	10.408(2)	73.84(4)	90.17(2)	77.30(4)	743.0(4)
4	0.65(5)	8.149(2)	9.355(5)	10.400(2)	73.84(4)	90.13(2)	77.35(4)	741.3(4)
5	0.77(5)	8.146(2)	9.355(5)	10.393(2)	73.84(4)	90.14(2)	77.35(4)	740.5(4)
6	0.98(5)	8.142(2)	9.353(5)	10.382(3)	73.83(4)	90.14(2)	77.33(4)	739.1(4)
7	1.25(5)	8.136(2)	9.343(5)	10.368(2)	73.84(4)	90.13(2)	77.36(4)	737.0(4)
8	1.41(5)	8.131(3)	9.330(5)	10.362(3)	73.87(4)	90.13(2)	77.42(5)	735.4(4)
9	1.59(5)	8.131(2)	9.329(5)	10.356(2)	73.84(4)	90.09(2)	77.35(4)	734.5(4)
10	1.81(5)	8.123(2)	9.321(5)	10.341(2)	73.83(4)	90.10(2)	77.43(4)	732.3(4)
11	2.30(5)	8.102(2)	9.308(4)	10.312(2)	73.90(3)	90.21(2)	77.51(3)	727.8(4)
12	2.83(5)	8.096(2)	9.295(5)	10.288(2)	73.89(4)	90.16(2)	77.49(4)	724.5(4)
13	3.40(5)	8.085(2)	9.273(5)	10.266(2)	73.95(4)	90.12(2)	77.61(4)	720.9(4)
14	4.00(5)	8.072(2)	9.259(5)	10.238(2)	73.92(4)	90.12(2)	77.64(4)	716.7(4)
15	4.51(5)	8.056(2)	9.248(5)	10.213(2)	73.97(4)	90.18(2)	77.74(4)	713.1(4)
16	4.90(5)	8.055(3)	9.225(5)	10.204(2)	73.99(4)	90.11(2)	77.80(4)	710.8(4)
17	5.40(5)	8.036(3)	9.213(5)	10.177(2)	74.00(4)	90.20(2)	77.89(4)	706.7(4)

18	5.77(5)	8.038(3)	9.201(5)	10.165(2)	74.01(4)	90.12(2)	77.98(4)	705.5(4)
19	6.17(5)	8.028(3)	9.185(5)	10.151(2)	74.01(4)	90.11(2)	78.06(4)	702.6(4)
20	6.61(5)	8.025(3)	9.174(5)	10.134(2)	74.03(3)	90.09(2)	78.14(4)	700.6(4)
21	7.05(5)	8.019(3)	9.153(5)	10.122(2)	74.04(4)	90.04(2)	78.26(4)	698.1(4)
22	7.49(5)	8.010(3)	9.135(5)	10.104(2)	74.03(4)	90.05(2)	78.38(4)	695.0(4)
23	7.85(5)	8.003(3)	9.129(5)	10.090(2)	74.05(4)	90.04(2)	78.47(4)	693.3(4)
24	8.35(5)	7.991(3)	9.117(5)	10.067(2)	74.05(4)	90.08(2)	78.53(4)	689.9(4)
25	8.72(5)	7.985(3)	9.105(5)	10.054(2)	74.04(4)	90.08(2)	78.61(4)	687.7(4)
26	9.12(5)	7.977(3)	9.102(5)	10.039(2)	74.07(4)	90.09(2)	78.67(4)	686.1(4)
27	9.54(5)	7.971(3)	9.087(5)	10.024(2)	74.07(4)	90.07(2)	78.78(4)	683.7(4)
28	9.89(5)	7.967(3)	9.077(5)	10.013(2)	74.06(4)	90.06(2)	78.80(4)	681.8(4)
29	6.07(5)	8.032(2)	9.206(5)	10.153(2)	73.99(4)	90.17(2)	77.92(4)	704.2(4)
30	0.66(5)	8.156(2)	9.357(5)	10.405(2)	73.84(4)	90.08(2)	77.35(4)	742.5(4)

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22 **Table S3**: Pseudowollastonite compressibility

300µm DAC								
Step	***P (GPa)***	***a* (Å)**	***b* (Å)**	***c* (Å)**	***α* (°)**	***β* (°)**	***γ* (°)**	***V* (Å^3)**
0	0.0001	11.8166(8)	6.8456(3)	10.5177(7)	90	111.287(7)	90	792.75(8)
1	1.15(5)	11.734(3)	6.803(3)	10.494(2)	90	111.23(3)	90	780.8(4)
2	2.06(5)	11.678(3)	6.772(2)	10.469(2)	90	111.17(2)	90	772.0(4)
3	3.41(5)	11.613(3)	6.729(3)	10.435(2)	90	111.11(3)	90	760.6(4)
4	4.06(5)	11.585(3)	6.710(2)	10.438(2)	90	111.12(3)	90	756.8(4)
5	5.32(5)	11.537(2)	6.686(3)	10.414(2)	90	111.06(2)	90	749.6(4)
6	7.05(5)	11.459(3)	6.637(4)	10.382(2)	90	111.04(3)	90	736.9(5)
7	11.13(5)	11.313(3)	6.540(4)	10.343(3)	90	110.86(3)	90	715.1(6)
8	13.64(5)	11.222(3)	6.493(3)	10.295(2)	90	110.79(3)	90	701.3(4)
600µm DAC								
Step	***P (GPa)***	***a* (Å)**	***b* (Å)**	***c* (Å)**	***α* (°)**	***β* (°)**	***γ* (°)**	***V* (Å^3)**
0	0.0001	11.813(4)	6.8461(8)	10.5161(15)	90	111.26(3)	90	792.5(3)
1	0.73(5)	11.74(2)	6.8263(12)	10.517(5)	90	111.34(12)	90	785(1)
2	1.17(5)	11.752(8)	6.8009(8)	10.485(3)	90	111.29(5)	90	780.8(6)
3	1.59(5)	11.696(14)	6.7992(8)	10.493(3)	90	111.25(8)	90	777.7(9)
4	2.06(5)	11.702(8)	6.7736(7)	10.469(3)	90	111.27(6)	90	773.3(6)
5	2.36(5)	11.694(7)	6.7632(8)	10.469(3)	90	111.32(5)	90	771.3(5)
6	2.99(5)	11.668(7)	6.7427(7)	10.458(3)	90	111.31(0)	90	766.5(5)
7	3.46(5)	11.641(7)	6.7291(6)	10.445(3)	90	111.28(0)	90	762.4(5)
8	3.78(5)	11.620(7)	6.7239(7)	10.440(3)	90	111.21(0)	90	760.4(5)
9	4.13(5)	11.609(8)	6.7108(7)	10.432(3)	90	111.24(50)	90	757.5(6)
10	4.49(5)	11.575(7)	6.7078(7)	10.424(3)	90	111.09(50)	90	755.1(5)
11	4.71(5)	11.572(8)	6.6973(7)	10.424(3)	90	111.18(50)	90	753.2(5)
12	5.73(5)	11.486(12)	6.6807(7)	10.419(4)	90	111.09(80)	90	745.9(8)
13	6.22(5)	11.521(6)	6.6553(7)	10.407(3)	90	111.21(5)	90	743.9(5)
14	6.89(5)	11.484(8)	6.6427(8)	10.385(3)	90	111.09(6)	90	739.2(6)
15	6.93(5)	11.486(8)	6.6404(6)	10.386(3)	90	111.10(6)	90	739.0(5)

16	7.42(5)	11.464(7)	6.6335(7)	10.385(3)	90	111.06(0)	90	737.0(5)
17	7.82(5)	11.464(8)	6.6197(6)	10.378(3)	90	111.12(5)	90	734.7(5)
18	8.21(5)	11.423(6)	6.6133(6)	10.368(2)	90	111.00(5)	90	731.2(4)
19	8.59(5)	11.413(7)	6.6041(8)	10.365(3)	90	111.04(4)	90	729.1(5)
20	8.90(5)	11.409(8)	6.5930(8)	10.364(4)	90	111.09(5)	90	727.4(6)
21	9.12(5)	11.395(8)	6.5934(8)	10.357(3)	90	111.02(6)	90	726.4(6)
22	9.44(5)	11.367(9)	6.5897(8)	10.351(3)	90	110.94(6)	90	724.1(6)
23	9.73(5)	11.374(8)	6.5762(7)	10.344(3)	90	110.98(6)	90	722.4(6)
24	10.1(5)	11.352(8)	6.5694(8)	10.345(4)	90	110.96(6)	90	720.5(6)

Table S4: Parabreyite thermal expansion

Step	***T (K)***	***a* (Å)**	***b* (Å)**	***c* (Å)**	***α* (°)**	***β* (°)**	***γ* (°)**	***V* (Å^3)**
1	100	8.1860(2)	9.3471(3)	10.4621(3)	73.865(2)	89.870(2)	77.560(3)	749.52(4)
2	120	8.1871(2)	9.3487(3)	10.4625(3)	73.863(2)	89.874(2)	77.554(3)	749.74(4)
3	140	8.1882(2)	9.3496(3)	10.4632(3)	73.860(2)	89.877(2)	77.556(3)	749.96(4)
4	160	8.1893(2)	9.3504(3)	10.4643(3)	73.865(2)	89.879(2)	77.557(3)	750.21(4)
5	180	8.1908(2)	9.3523(3)	10.4651(3)	73.862(2)	89.881(2)	77.553(3)	750.53(4)
6	200	8.1919(2)	9.3529(3)	10.4664(3)	73.866(2)	89.882(2)	77.552(3)	750.80(4)
7	220	8.1935(2)	9.3543(3)	10.4681(3)	73.862(2)	89.882(2)	77.551(3)	751.16(4)
8	240	8.1949(2)	9.3558(3)	10.4691(3)	73.861(2)	89.884(2)	77.552(3)	751.47(4)
9	260	8.1965(2)	9.3569(3)	10.4707(3)	73.864(2)	89.886(2)	77.549(3)	751.82(4)
10	280	8.1981(2)	9.3591(3)	10.4718(3)	73.860(2)	89.887(2)	77.546(3)	752.20(4)
11	300	8.1998(2)	9.3608(3)	10.4728(3)	73.863(2)	89.892(2)	77.545(3)	752.57(4)
12	302	8.2009(3)	9.3608(3)	10.4744(3)	73.866(3)	89.893(3)	77.503(3)	752.66(4)
13	322	8.2022(3)	9.3625(3)	10.4755(3)	73.865(3)	89.893(3)	77.505(3)	753.00(4)
14	373	8.2072(3)	9.3668(3)	10.4801(3)	73.865(3)	89.895(3)	77.501(3)	754.12(4)
15	423	8.2118(3)	9.3717(3)	10.4844(3)	73.869(3)	89.904(3)	77.505(3)	755.27(4)
16	473	8.2171(3)	9.3774(3)	10.4887(3)	73.862(3)	89.910(3)	77.506(3)	756.49(4)
17	522	8.2223(3)	9.3821(3)	10.4938(3)	73.866(3)	89.916(3)	77.507(3)	757.73(4)
18	573	8.2274(3)	9.3879(4)	10.4987(3)	73.860(3)	89.924(3)	77.506(3)	759.00(5)
19	623	8.2326(3)	9.3934(4)	10.5033(4)	73.868(3)	89.930(3)	77.498(3)	760.26(5)
20	673	8.2381(3)	9.3987(4)	10.5084(4)	73.868(3)	89.940(3)	77.503(3)	761.57(5)
21	724	8.2434(4)	9.4043(4)	10.5141(4)	73.860(3)	89.947(3)	77.497(4)	762.87(5)
22	766	8.2468(4)	9.4107(4)	10.5187(4)	73.870(3)	89.942(3)	77.504(4)	764.10(5)