minerals

Supplementary Material

Crystal Structure of Moganite and Its Anisotropic Atomic Displacement Parameters Determined by Synchrotron X-ray Diffraction and X-ray/Neutron Pair Distribution Function Analyses

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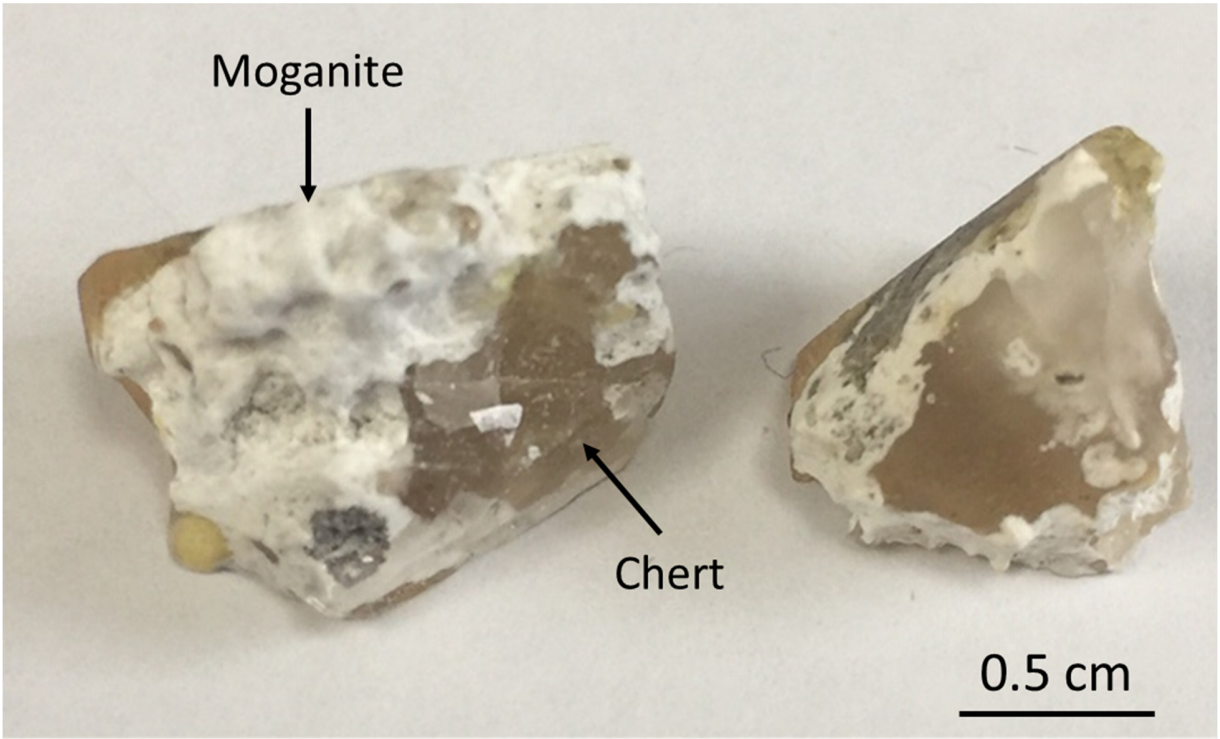

Figure S1. Moganite (white powder) coexisting with microcrystalline quartz collected from cherts found in the ignimbrite lava flows of the Mogán formation in Gran Canaria, Spain. The sample was provided by Smithsonian Institute (No. 168357).

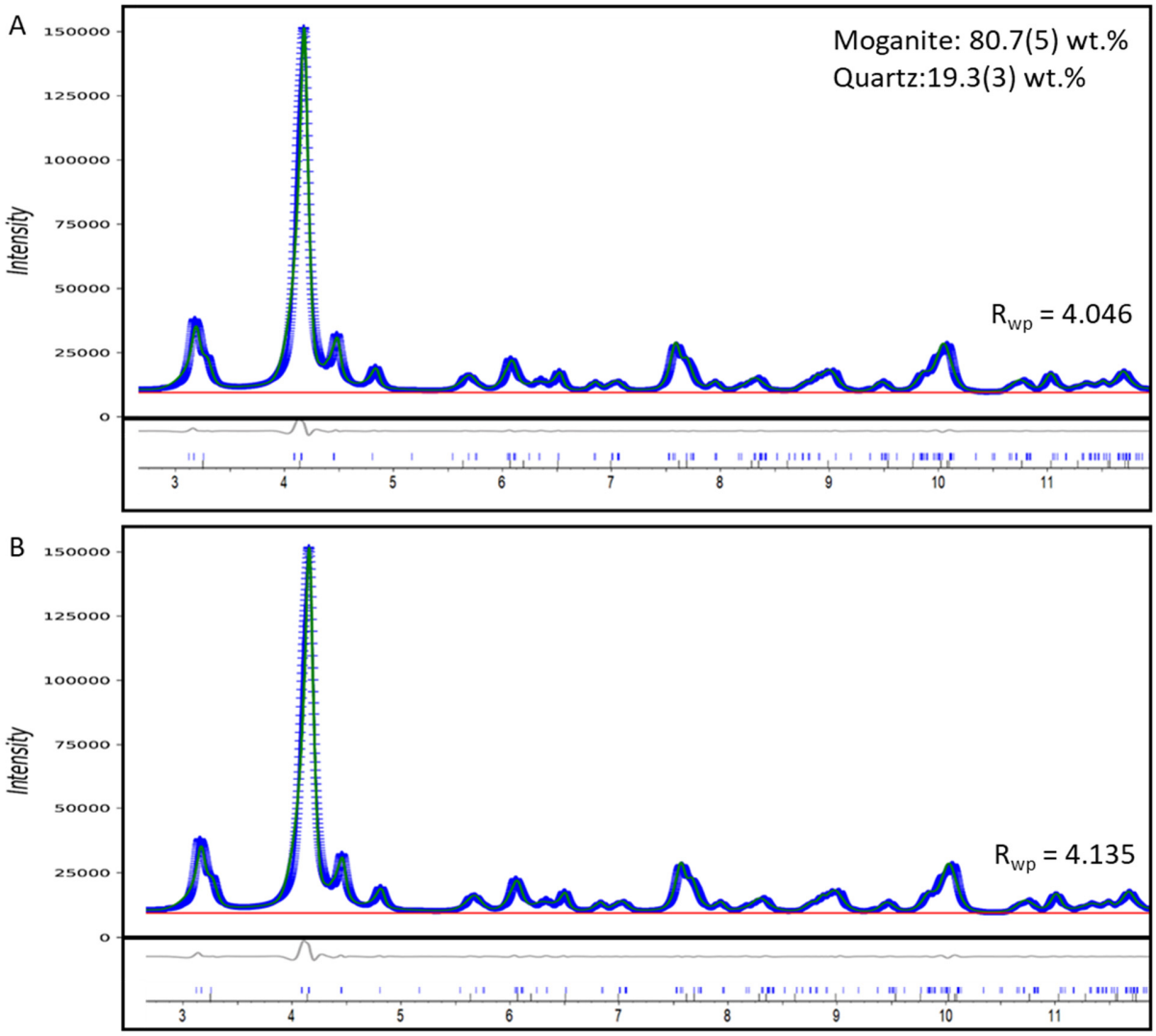

Figure S2. Synchrotron XRD pattern (APS, beamline 17-BM) of the treated sample, which is a mixture of moganite and quartz. The fitting was performed by refined structure of moganite and quartz using (A) thermal displacement parameters (U_{iso}) shown in table. 1 and (B) anisotropic atomic displacement parameters (ADPs) determined by X-ray PDF refinement (table. 3 and table S1).

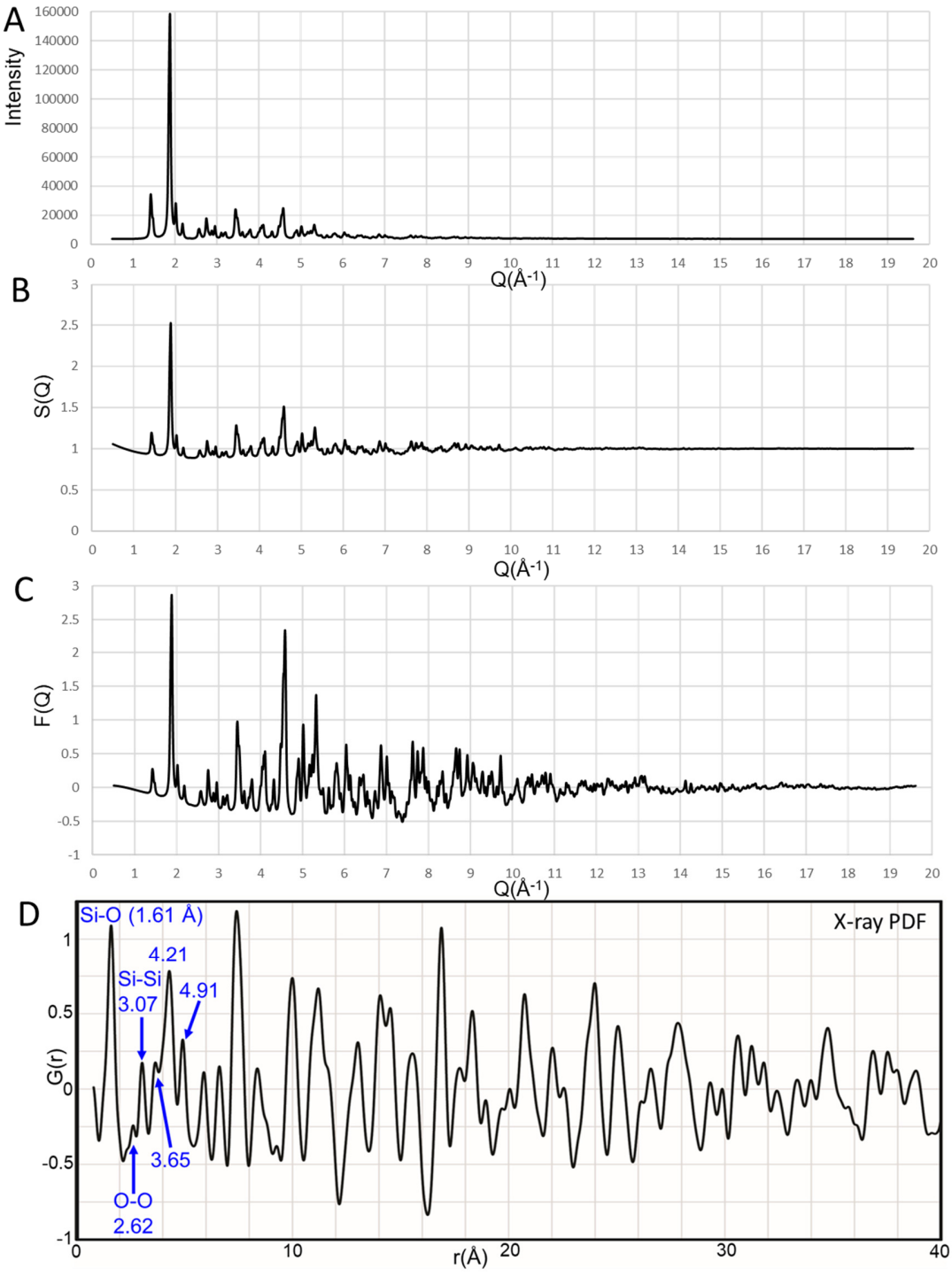

Figure S3. (**A**-**C**) Experimental results of I(Q), S(Q), and F(Q) for the studied sample obtained up to a Q_{max} of 19.6 Å^{-1}. (**D**) X-ray PDF patterns of the sample from 1 to 40 Å.

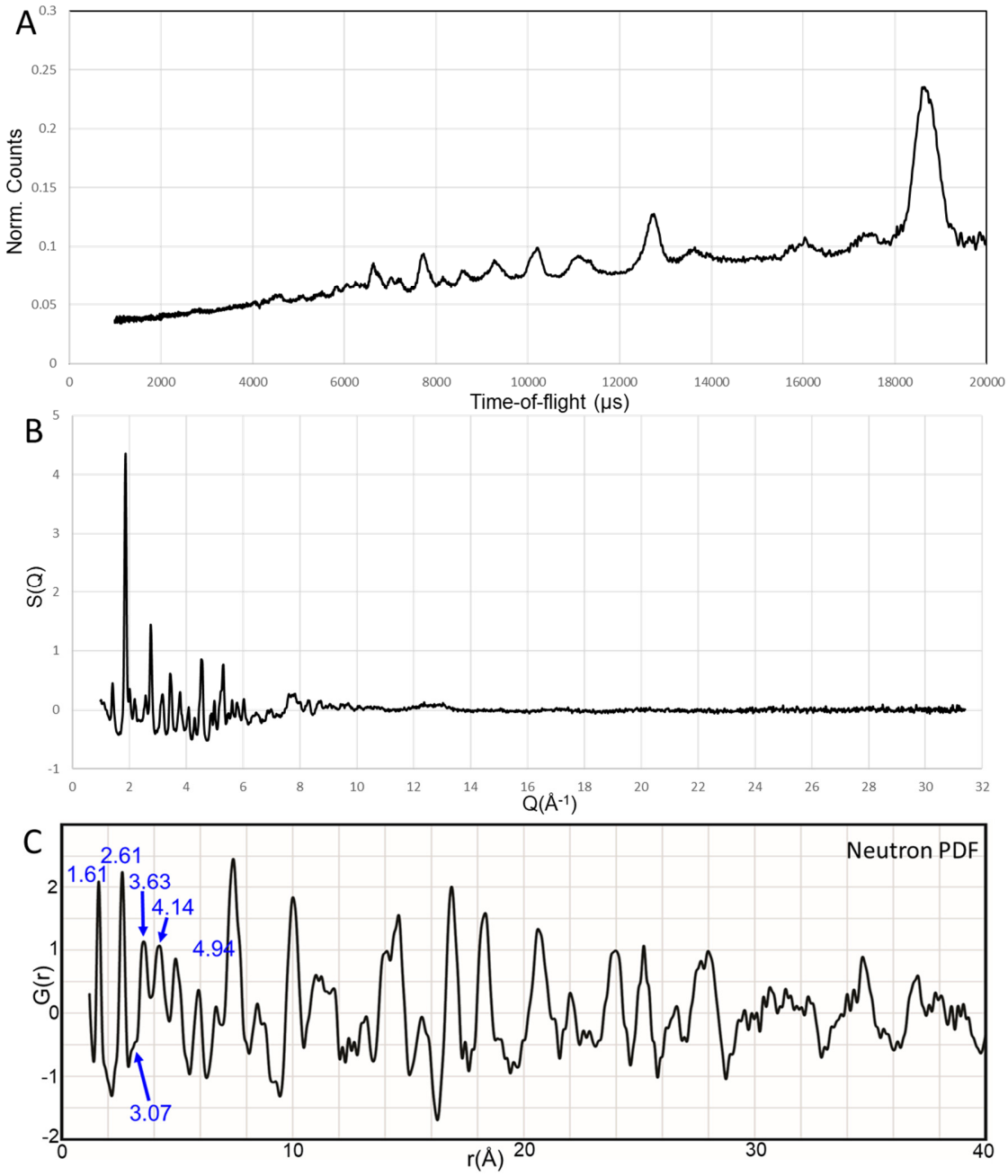

Figure S4. (A) Time-of-flight (TOF) neutron scattering profile of the sample (Beamline BL-1B, Spallation Neutron Source, Oak Ridge National Laboratory). (B) Neutron scattering structure factor S(Q) for the sample. (C) Neutron PDF pattern of the sample from 1 Å to 40 Å.

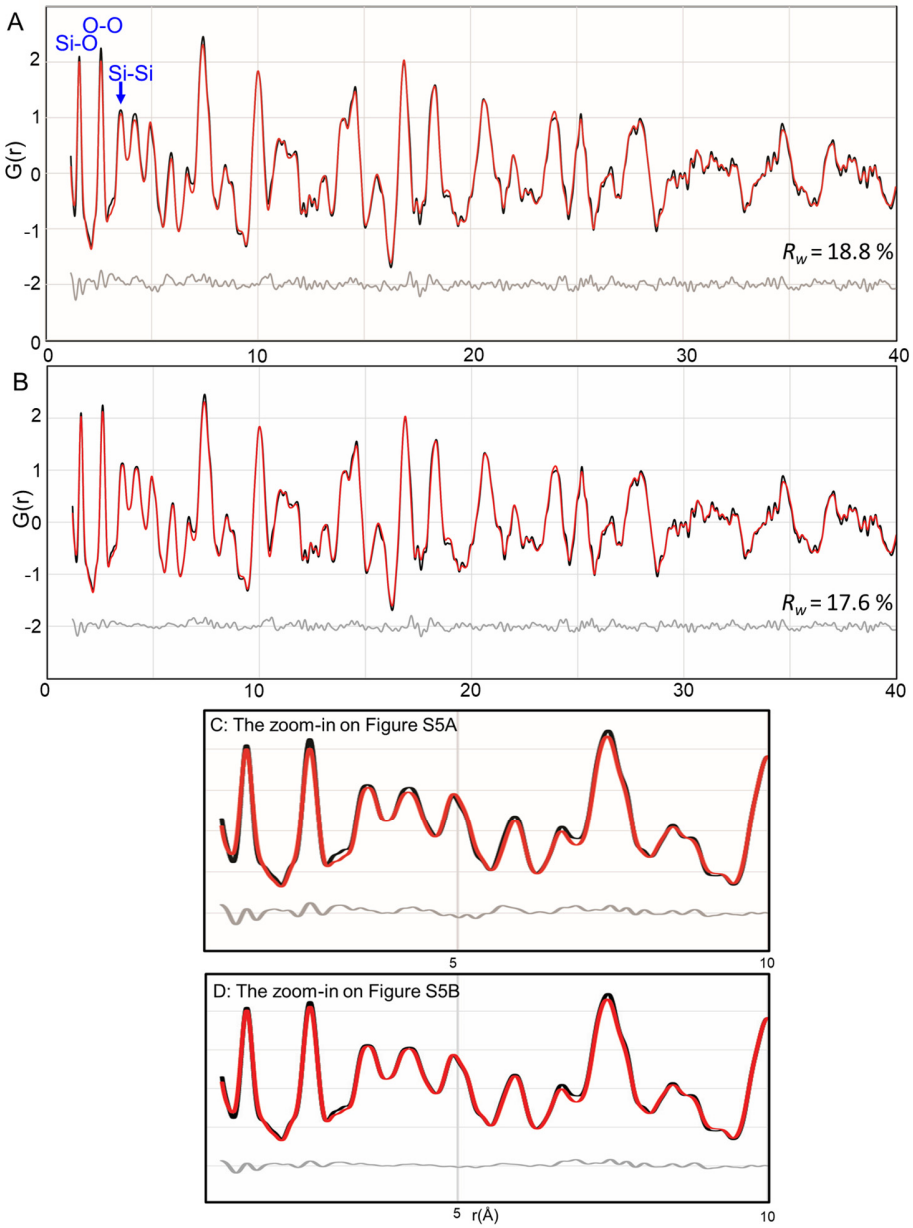

Figure S5. PDF refinement of neutron PDF patterns using two structure models of moganite with (A) full occupancy and (B) partial occupancy of O sites from 1 to 40. The zoom-in on (C) figure S5A and (D) figure S5B ranged from 1 to 10 Å. Black curve: experimental data; red curve: calculated profile; gray curve: differences between the experimental and calculated PDF patterns. Refining the occupancy of O sites in moganite improves the fitting of neutron PDF patterns, especially in short-range regimes (e.g., O-O pair at 2.61 Å), and R_w value decreases by 1.2 %.

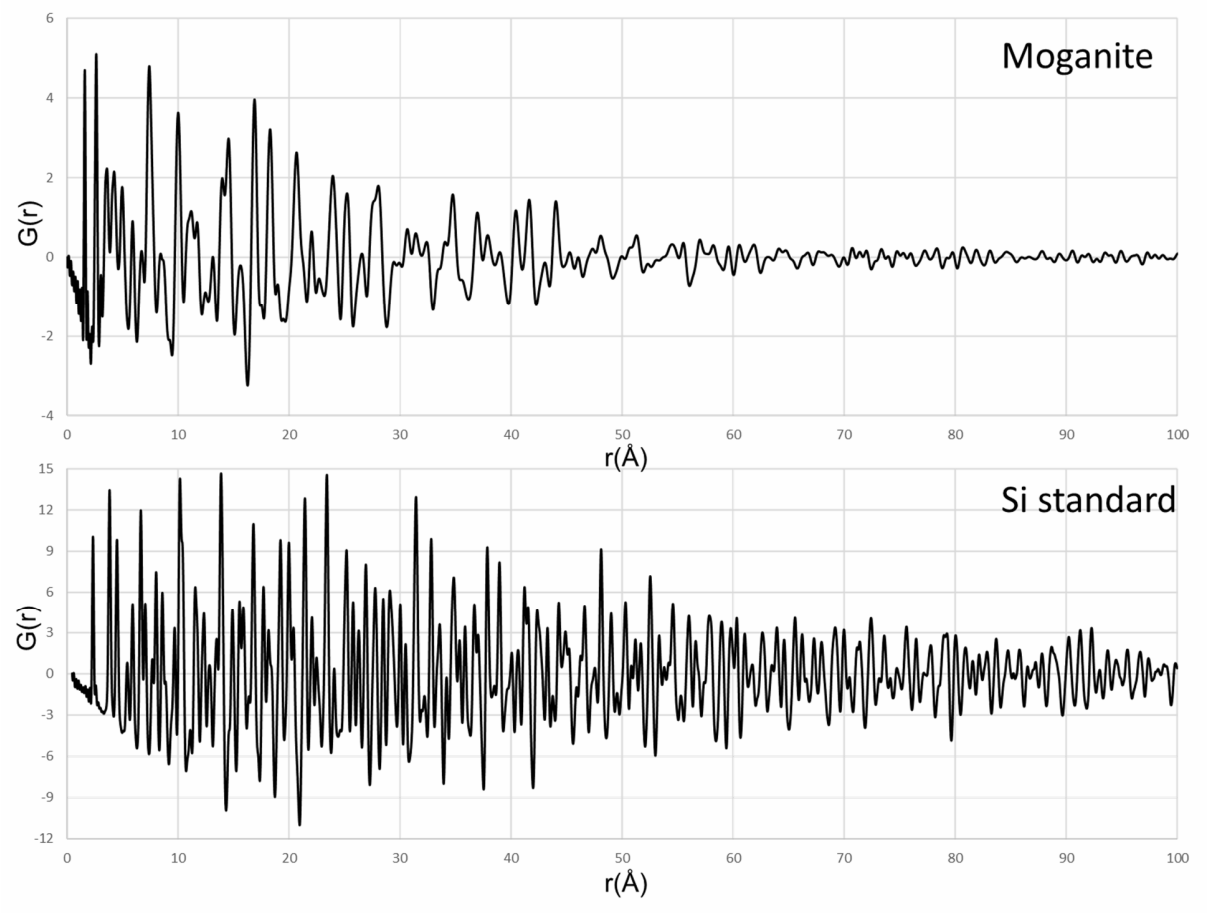

Figure S6. Neutron PDF patterns of moganite and Si standard from 0.5 to 100 Å. The particle size of moganite estimate ~ 6 nm by the experimental PDF pattern.

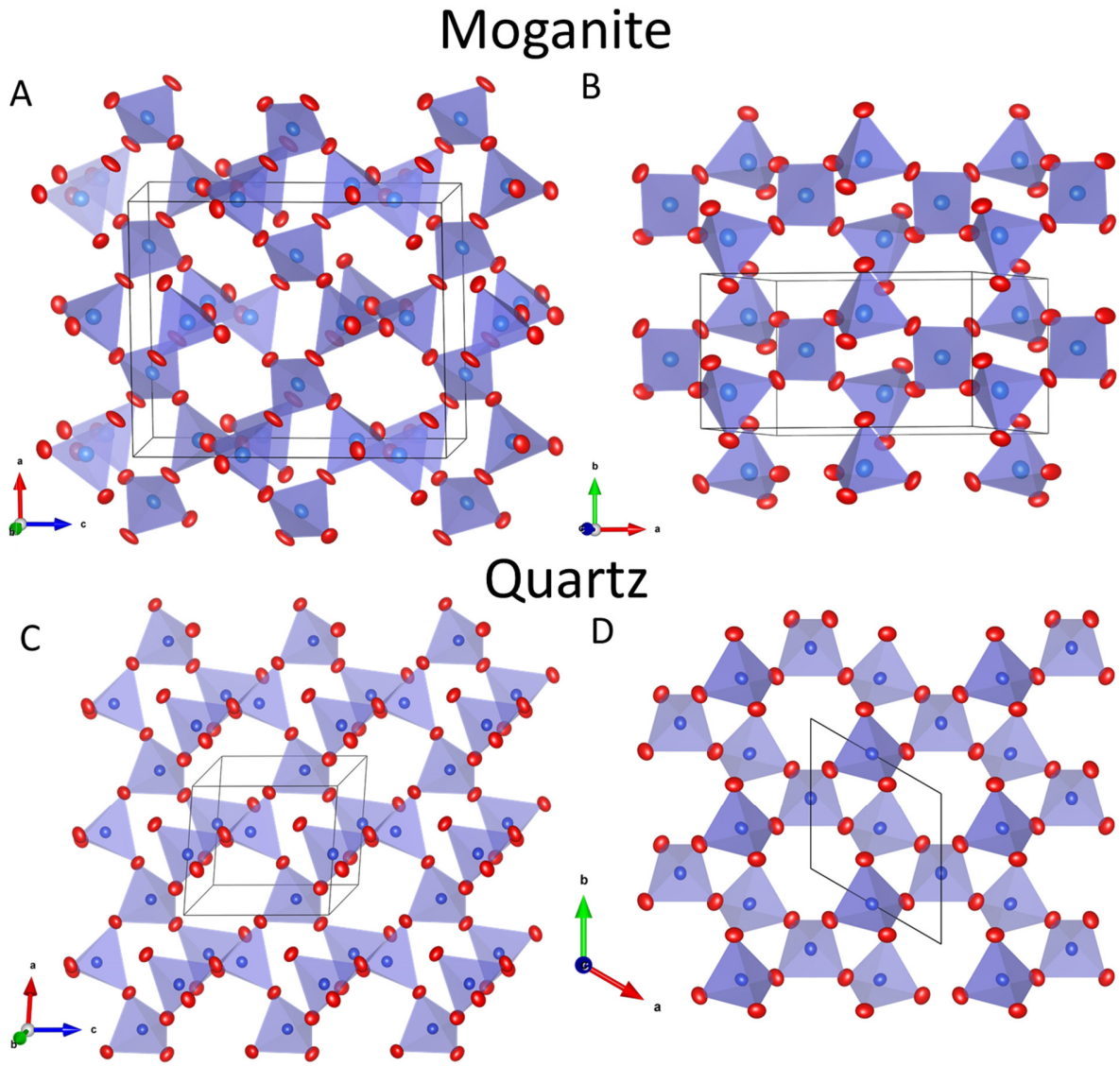

Figure S7. Crystal structures of moganite (**A**,**B**) and quartz (**C**,**D**) from X-ray PDF refinement. The models include the displacement ellipsoids drawn with a probability of 80% (blue atoms are silicon, and red atoms are oxygen).

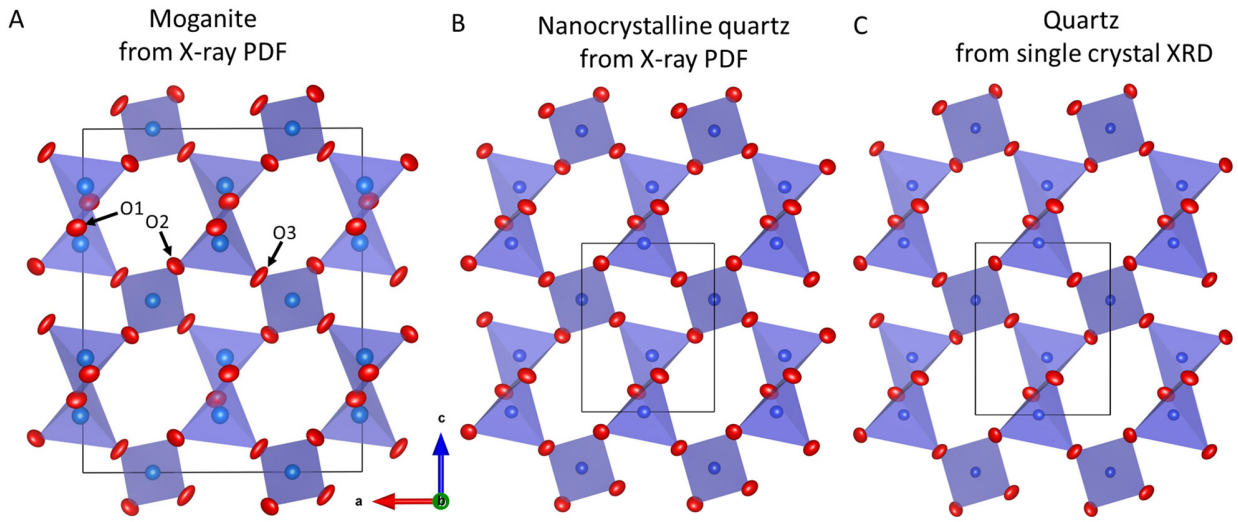

Figure S8. Crystal structures of moganite (this study), nano-crystalline quartz (this study), and bulk quartz (Kihara, 1990) projected along *b*-axes.

Table S1. Unit-cell parameters, atomic coordinates, and anisotropic atomic displacement parameters of nano-crystalline quartz from X-ray and neutron PDF refinement compared with previously reported quartz structures.

X-ray PDF refinement: a = 4.9156(4) Å and c = 5.4052(4) Å (Space group $P3_221$)										
Atom	***Occ.***	***x***	***y***	***z***	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Si1	1	0.4690(5)	0	0	0.0104(5)	0.0086(3)	0.0093(4)	0.0042(5)	-0.0002(1)	0.0002(1)
O1	1	0.4134(6)	0.2671(4)	0.1192(3)	0.0201(6)	0.0154(4)	0.0144(4)	0.0101(5)	-0.0033(3)	-0.0040(6)
Neutron PDF refinement: a = 4.9151(5) Å and c = 5.4044(4) Å										
Atom	*Occ.*	*x*	*y*	*z*	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Si1	1	0.4693(5)	0	0	0.0095(5)	0.0075(2)	0.0082(4)	0.0030(4)	-0.0002(1)	0.0002(1)
O1	1	0.4132(5)	0.2668(5)	0.1196(3)	0.0188(5)	0.0125(3)	0.0118(3)	0.0075(3)	-0.0031(3)	-0.0038(6)
Quartz by Rietveld refinement with high-resolution powder XRD (Antao et al. 2008): a = 4.91344 Å and c = 5.40512 Å										
Atom	*Occ.*	*x*	*y*	*z*	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Si1	1	0.4700	0	0	0.00733	0.00590	0.00535	0.00294	0.00027	0.00055
O1	1	0.4146	0.2678	0.1197	0.01200	0.01050	0.01180	0.00650	-0.00290	-0.00400
Quartz by single-crystal XRD (Kihara, 1990): a = 4.9137 Å and c = 5.4047 Å										
Atom	*Occ.*	*x*	*y*	*z*	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Si1	1	0.4697	0	0	0.00734	0.00560	0.00666	0.0028	-0.00017	-0.00035
O1	1	0.4133	0.2672	0.1188	0.01642	0.01193	0.01258	0.00936	-0.00303	-0.00478

Table S2. Unit-cell parameters, atomic coordinates, and anisotropic atomic displacement parameters of two structure models of moganite (full occupancy and partial occupancy of O sites) determined by neutron PDF refinement.

Neutron PDF refinement: a = 8.7357(13) Å, b = 4.8675(15) Å, c = 10.719(3) Å, and β = 90.20(3)° (R_w = 18.8 %)										
Atom	***Occ.***	***x***	***y***	***z***	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Si1	1	0.25	0.9733(4)	0	0.0095(5)	0.0098(5)	0.0104(5)	0	-0.004(1)	0
Si2	1	0.0089(5)	0.2511(7)	0.1664(4)	0.0115(4)	0.0127(4)	0.0108(3)	0.0005(1)	-0.0003(1)	-0.0005(1)
O1	1	0.9774(5)	0.0648(7)	0.2873(4)	0.0207(5)	0.0101(3)	0.0122(3)	-0.0024(3)	-0.0012(2)	0.0037(6)
O2	1	0.1678(4)	0.1713(4)	0.1003(4)	0.0155(4)	0.0216(6)	0.0124(4)	0.0033(4)	0.0015(2)	-0.0011(2)
O3	1	0.8699(8)	0.2304(7)	0.0674(7)	0.0202(5)	0.0128(4)	0.0225(6)	-0.0016(2)	-0.0073(6)	-0.0014(1)
Neutron PDF refinement: a = 8.7357(13) Å, b = 4.8675(15) Å, c = 10.719(3) Å, and β = 90.20(3)° (R_w = 17.6 %)										
Atom	*Occ.*	*x*	*y*	*z*	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Si1	1	0.25	0.9733(4)	0	0.0098(5)	0.0098(4)	0.0109(5)	0	-0.004(1)	0
Si2	1	0.0089(5)	0.2512(6)	0.1664(4)	0.0112(3)	0.0125(4)	0.0104(3)	0.0006(1)	-0.003(1)	-0.005(2)
O1	1.06(1)	0.9776(5)	0.0649(6)	0.2873(4)	0.0205(5)	0.0102(3)	0.0120(5)	-0.0023(2)	-0.0015(3)	0.0038(5)
O2	1.06(1)	0.1681(5)	0.1712(5)	0.1005(4)	0.0161(6)	0.0212(5)	0.0129(4)	0.0035(4)	0.0019(2)	-0.0014(3)
O3	1.06(1)	0.8699(8)	0.2303(6)	0.0674(6)	0.0198(5)	0.0131(4)	0.0226(7)	-0.0021(3)	-0.0081(5)	-0.0014(2)

References

1. Antao, S. M., Hassan, I., Wang, J., Lee, P. L., & Toby, B. H. (2008). State-of-the-art high-resolution powder X-ray diffraction (HRPXRD) illustrated with Rietveld structure refinement of quartz, sodalite, tremolite, and meionite. The Canadian Mineralogist, 46(6), 1501-1509.
2. Kihara, K. (1990) An X-ray study of the temperature dependence of the quartz structure. European Journal of Mineralogy, 63-78.