Supplementary Materials

Table S1. Unit cell parameters, bond distances, bond angles and tetrahedral volume of tetragonal cristobalite ($P4_12_12$) from Rietveld refinement, compared to the (1) Downs & Palmer, (1994) and (2) Pluth et al. (1985).

	(This study)	**(1)**	**(2)**
a (Å)	4.9727(6)	4.9717(4)	4.9709(1)
c	6.9257(5)	6.9223(3)	6.9278(2)
Si-O X 2	1.600(3)	1.6026(1)	1.599(2)
Si-O_1 X 2	1.607(3)	1.6034(1)	1.606(2)
Average	1.603(3)	1.6030(1)	1.603(2)
O-O	2.607(5)	2.6098(2)	2.606(2)
O-O_1 X 2	2.598(2)	2.5969(2)	2.596(2)
O-O_{11} X 2	2.627(3)	2.6261(1)	2.625(2)
O-O_{111}	2.651(6)	2.6494(1)	2.651(2)
Average	2.618(4)	2.6175(2)	2.616(2)
Si-O1-Si (°)	146.6(2)	146.50(1)	146.7(1)
TeT Volume ($Å^3$)	2.114(4)	2.1126(2)	2.111(2)

Table S2. Atomic coordinates and anisotropic thermal displacement parameters of tetragonal cristobalite ($P4_12_12$) calculated by Rietveld method and PDF refinement.

Atom	**x**	**y**	**z**	$\mathbf{U_{11}}$	$\mathbf{U_{22}}$	$\mathbf{U_{33}}$	$\mathbf{U_{12}}$	$\mathbf{U_{13}}$	$\mathbf{U_{23}}$
Si	0.3007(3)	0.3007(3)	0	0.0089(2)	0.0086(2)	0.0088(2)	-0.001(1)	0.002(1)	-0.002(1)
O	0.2390(5)	0.1041(2)	0.1787(4)	0.0289(6)	0.0094(3)	0.0178(4)	-0.002(1)	0.006(2)	0.001(1)
Lattice parameters: a = 4.9727(6) Å and c = 6.9257(5) Å									

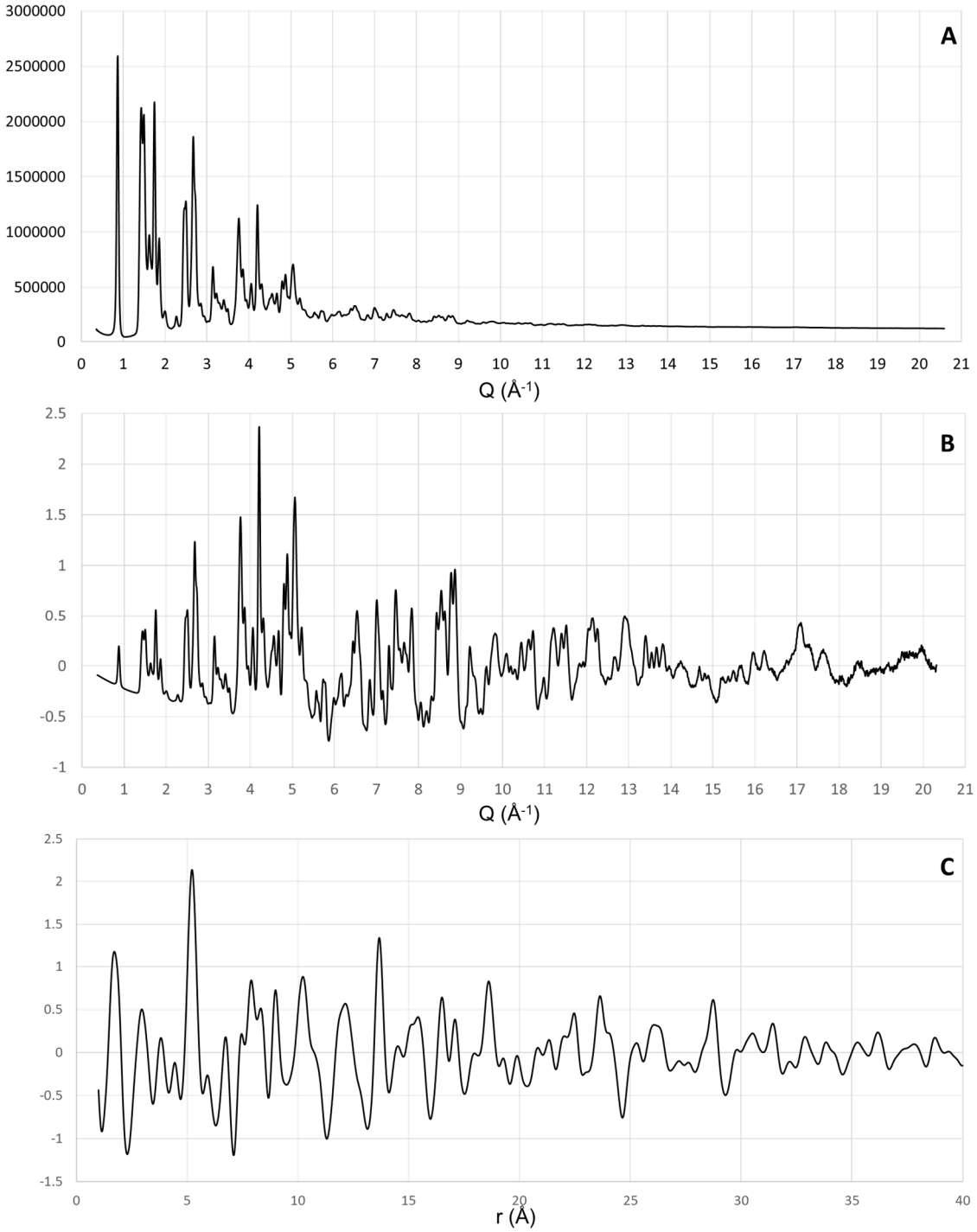

Figure S1. X-ray PDF analysis of (A) I(Q), (B) F(Q), and (C) G(r) for a kaolinite sample from Murfreesboro, Arkansas, USA.

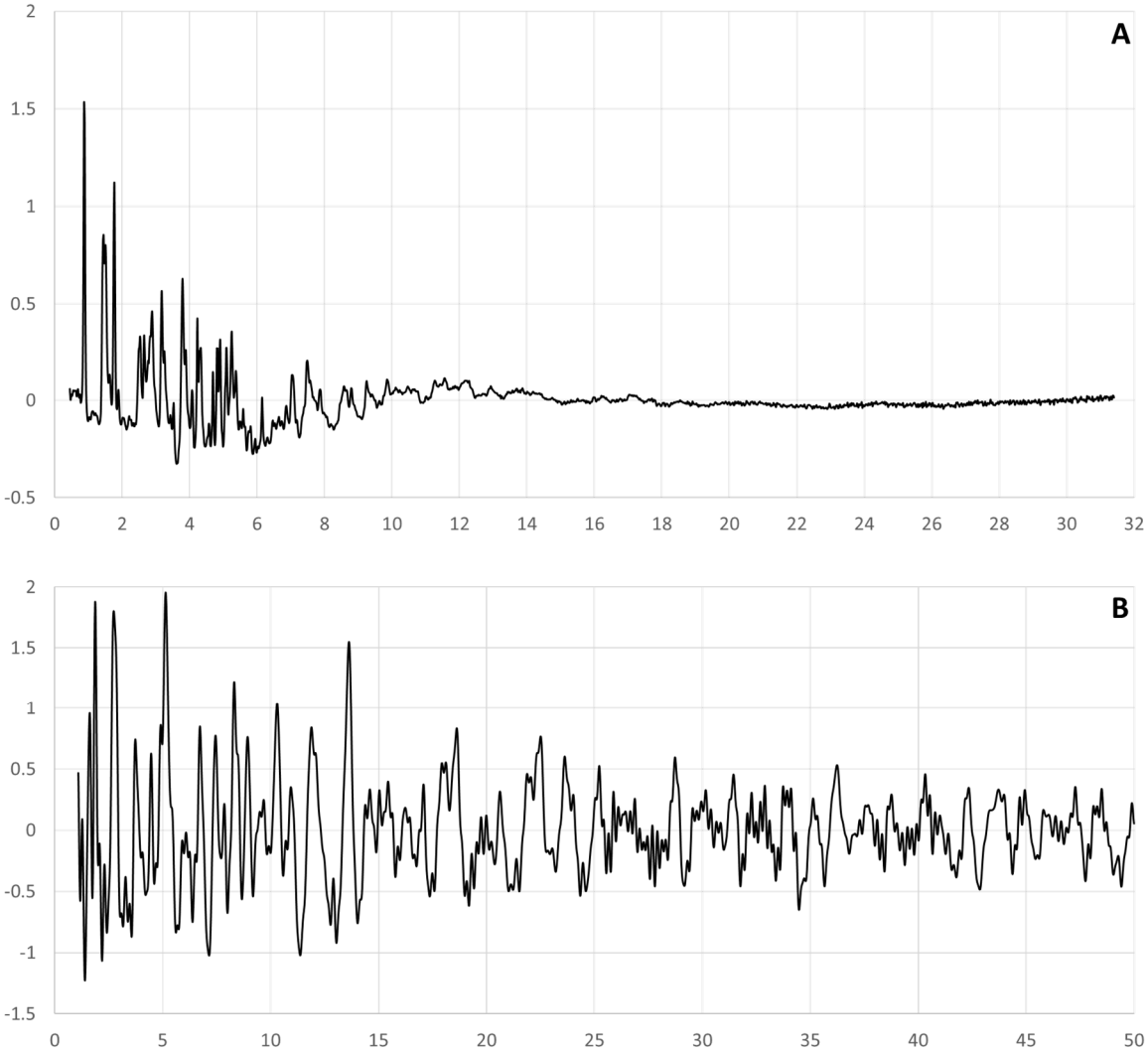

Figure S2. Neutron PDF analysis of (**A**) S(Q) and (**B**) G(r) for a kaolinite sample from Murfreesboro, Arkansas, USA.

References

Bish, D.L.; Von Dreele, R.B. Rietveld refinement of non-hydrogen atomic positions in kaolinite. *Clays Clay Miner* **1989**, *37*, 289-296.

Downs, R.T.; Palmer, D.C. The pressure behavior of α cristobalite. *American Mineralogist* **1994**, *79*, 9-14.