Supporting Information

$Ba_{33}Zn_{22}Al_8O_{67}$ with a framework of $([O(Zn/Al)_4]/Ba)(Zn/AlO_4)_4$ motifs

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Table S1. Atomic displacement parameters (Å^2) for $Ba_{33}Zn_{22}Al_8O_{67}$

Table S2. Ba–O and Zn/Al–O interatomic distances (Å) for $Ba_{33}Zn_{22}Al_8O_{67}$

Table S3. Isotropic chemical shift δ, quadrupolar coupling constant C_Q, and asymmetry parameter η.

Figure S1. Result of Rietveld analysis for the synthesized powder sample of $Ba_{33}Zn_{22}Al_8O_{67}$

Table S1. Atomic displacement parameters (Å^2) for $Ba_{33}Zn_{22}Al_8O_{67}$

Label	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Ba1	0.0226(2)	0.0159(2)	0.0158(2)	0	0	−0.00125(8)
Ba2	0.0138(1)	0.0119(1)	0.0118(2)	0	0	−0.0019(2)
Ba3a	0.0176(2)	0.0176(2)	0.0176(2)	−0.0002(2)	−0.0002(2)	−0.0002(2)
Ba3b	0.0318(3)	0.0318(3)	0.0318(3)	−0.0094(3)	−0.0094(3)	−0.0094(3)
Ba4/O1	0.0294(4)	0.0294(4)	0.0294(4)	0	0	0
Zn1	0.0089(2)	0.0089(2)	0.0089(2)	0.0001(2)	0.0001(2)	0.0001(2)
Zn/Al2	0.0120(2)	0.0120(2)	0.0120(2)	0.0003(2)	0.0003(2)	0.0003(2)
Zn/Al3	0.0118(2)	0.0118(2)	0.0118(2)	−0.0013(2)	−0.0013(2)	−0.0013(2)
Zn/Al4	0.0108(2)	0.0108(2)	0.0108(2)	0.0005(2)	0.0005(2)	0.0005(2)
Zn/Al5	0.0115(2)	0.0115(2)	0.0115(2)	0	0	0
O2	0.018(2)	0.028(2)	0.019(2)	−0.002(2)	−0.005(2)	−0.002(2)
O3	0.017(2)	0.019(2)	0.023(2)	−0.005(2)	−0.002(2)	−0.003(2)
O4	0.03(2)	0.008(6)	0.03(2)	0.010(5)	−0.01(2)	−0.004(5)
O5	0.0165(8)	0.0165(8)	0.0165(8)	−0.0014(9)	−0.0014(9)	−0.0014(9)
O6	0.017(2)	0.017(2)	0.017(2)	0	0	0

Table S2. Ba–O and Zn/Al–O interatomic distances (Å) for $Ba_{33}Zn_{22}Al_8O_{67}$

Ba1–O3	2.883 (3) × 4	Zn/Al1–O3	1.988 (3) × 3
Ba1–O2	2.923 (3) × 4	Zn/Al1–O1	1.933 (2)
Average	2.903	Average	1.974
Ba2–O3	2.669 (3) × 2	Zn/Al2–O2	1.953 (3) × 3
Ba2–O2	2.722 (3) × 2	Zn/Al2–O6	2.0124 (7)
Ba2–O5	2.7378 (2) × 2	Average	1.968
Ba2–O4	3.85(6) × 2		
Ba2–O4	3.92(6) × 2	Zn/Al3–O4*	1.82 (1) × 3
Ba2–O4	4.23(6) × 2	Zn/Al3–O2	1.880 (3) × 3
Average	3.032	Average	1.865
Ba3a–O3	2.619 (3) × 3	Zn/Al4–O3	1.905 (3) × 3
Ba3a–O4*	2.55 (5) × 3	Zn/Al4–O5	1.918 (4)
Ba3a–O4*	2.84 (7) × 3	Average	1.908
Ba3a–O4*	2.91 (2) × 3		
Average	2.693	Zn/Al5–O5	1.943 (4) × 4
		Average	1.943

Ba3b–O3	2.978 (3) × 3
Ba3b–O4*	2.25 (4) × 3
Ba3b–O4*	2.52 (7) × 3
Bab–O4*	2.58 (2) × 3
Average	2.714
Ba4–O3	3.197 (3) × 12
Average	3.197

* split site

Table S3. Isotropic chemical shift δ, quadrupolar coupling constant C_Q, and asymmetry parameter η.

	Peak I	Peak II	Peak III	Peak IV
δ_{iso} [ppm]	80.9	81.8	83.7	88.3
C_Q (= e^2qQ/h) [MHz]	1.47	2.63	1.9	2.66
η	1.0	0.05	0.527	0.099

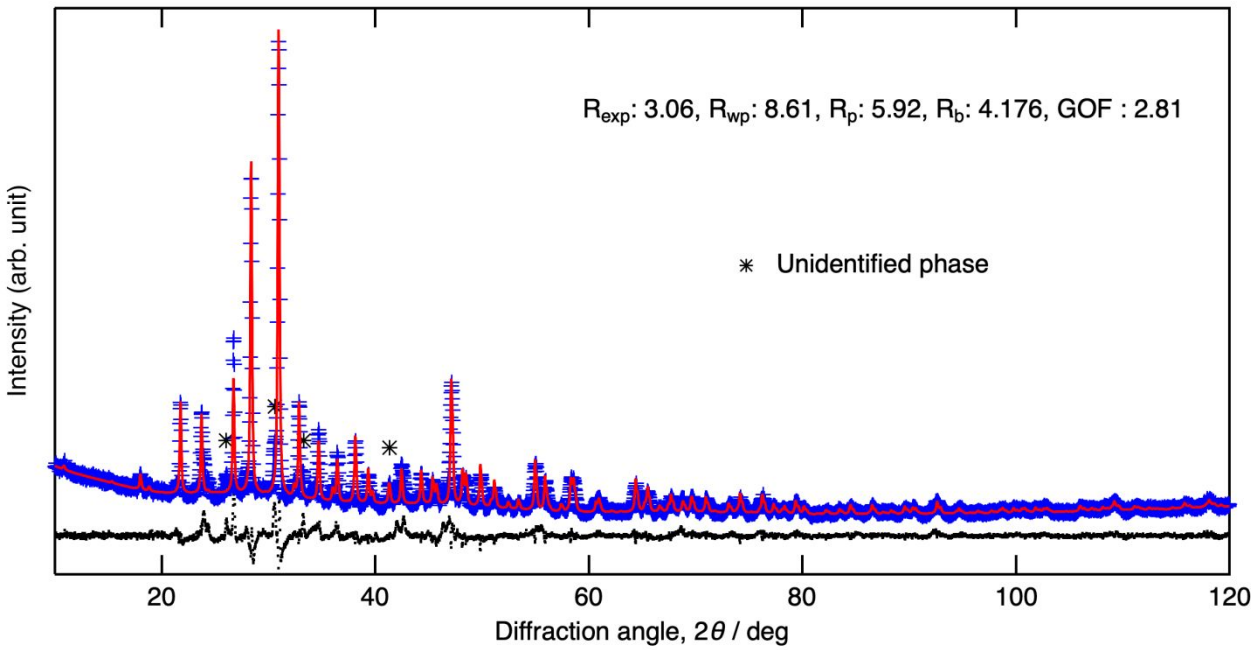

Figure S1. Result of Rietveld analysis for the synthesized powder sample of $Ba_{33}Zn_{22}Al_8O_{67}$