Electronic supplementary information (ESI)

ESI Fig. 1. SEM (left) and EDX spectra (right) of $Ba_3MgTa_2O_9$ (top) and $Ba_3ZnTa_2O_9$ (bottom). Metal atom ratios are indicated.

ESI Fig. 2. Rietveld refinement of the structure of $Ba_3ZnNb_2O_9$ from powder XRD data. Observed (○), calculated (—) and difference (bottom) profiles are shown. The vertical bars indicate the positions of Bragg reflections.

ESI Table 1. Refined crystallographic data for $Ba_3ZnNb_2O_9$: space group $P\text{-}3m1$, a = 5.7866(4) Å , c = 7.1075(8) Å.

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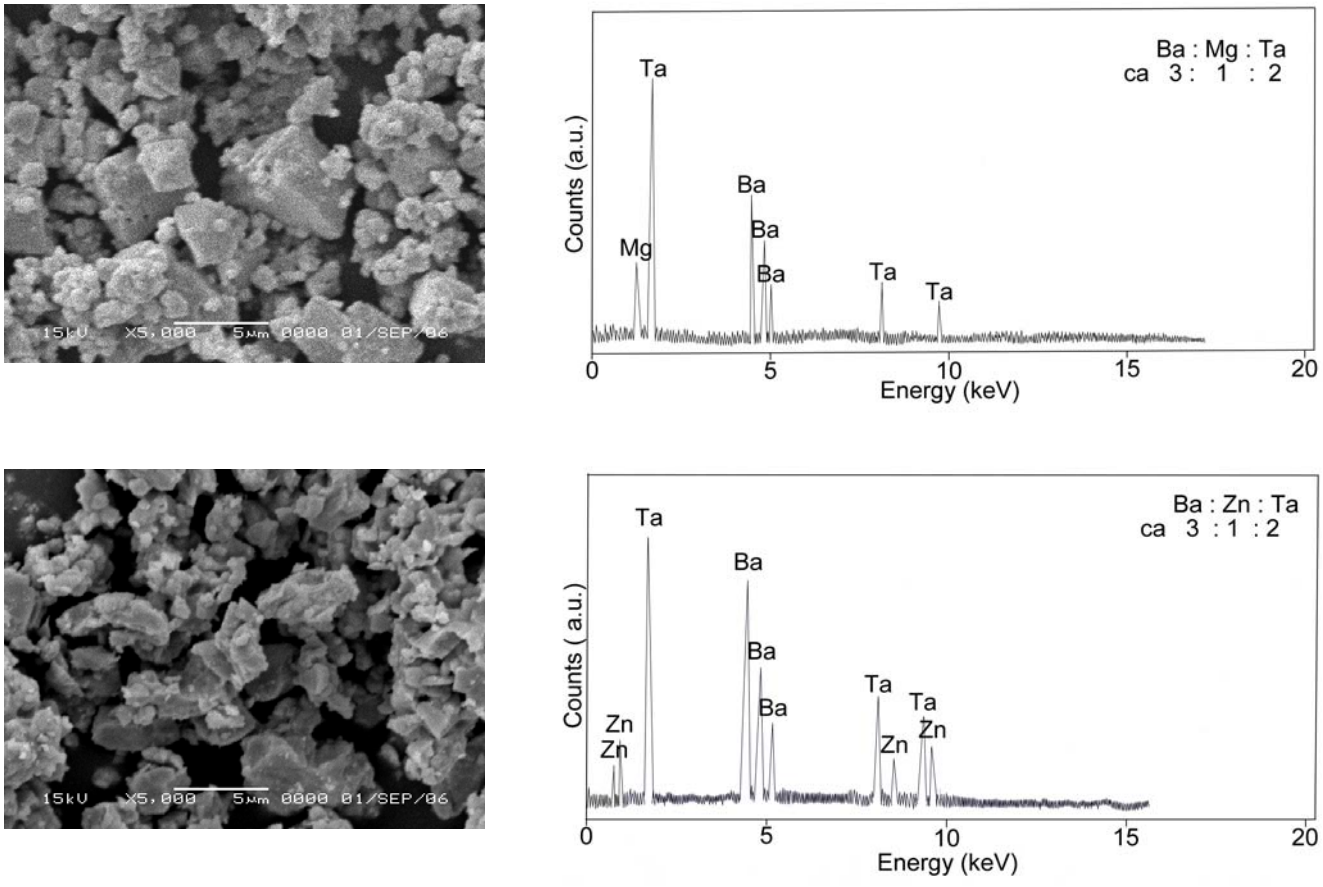
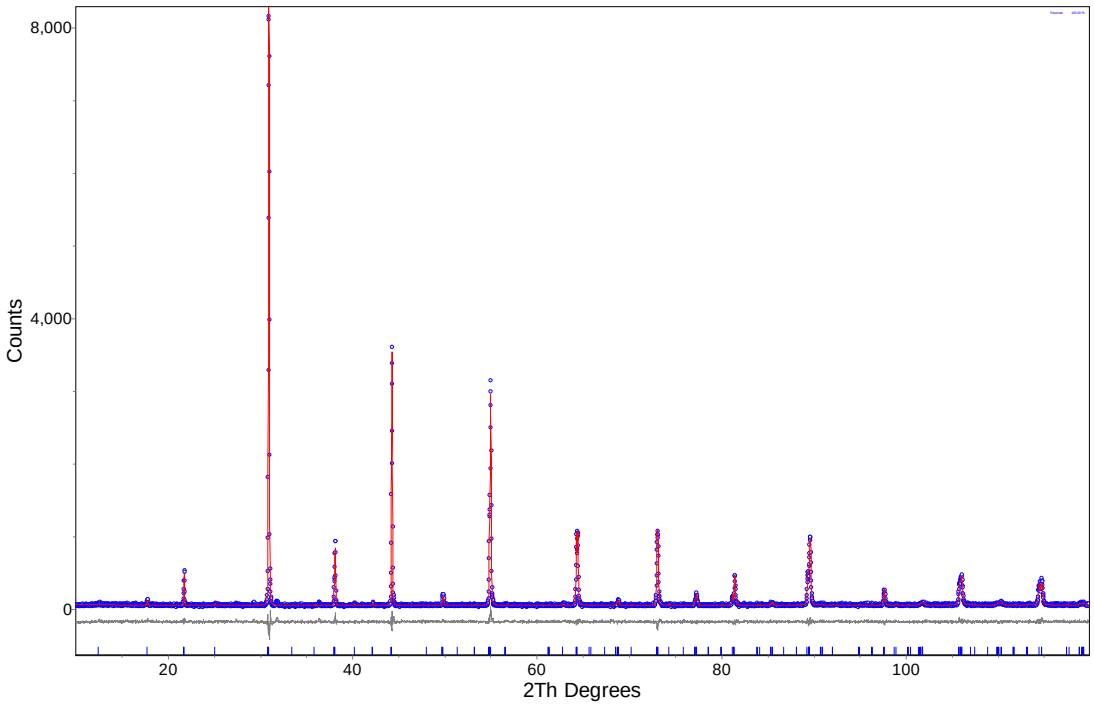


ESI Fig. 1



ESI Fig. 2

ESI Table 1

Refined crystallographic data for $Ba_3ZnNb_2O_9$: space group *P*-3*m*1, a = 5.78663(4) Å , c = 7.10759(8) Å.

Atom	Site	x	y	z	B(Å^2)	Occupancy
Ba1	1a	0.00000	0.00000	0.00000	0.42(4)	1
Ba2	2d	0.33333	0.66667	0.6653(5)	0.42(4)	1
Zn1	1b	0.00000	0.00000	0.50000	0.42(5)	1
Nb1	1b	0.00000	0.00000	0.50000	0.42(5)	0
Nb2	2d	0.33333	0.66667	0.1782(7)	0.42(5)	1
Zn2	2d	0.33333	0.66667	0.1782(7)	0.42(5)	0
O1	3e	0.50000	0.00000	0.00000	0.1(1)	1
O2	6i	0.177(2)	-0.177(2)	0.3251	0.1(1)	1

Reliability Factors : R_p = 8.57. R_{wp} = 11.59, R_{exp} = 10.09, χ^2 = 1.32.

Bond Lengths (Å): Ba(1) – O(1) = 2.893 (× 6), Ba(1) – O(2) = 2.911 (× 6), Ba(2) – O(2) = 2.883 (× 3), Ba(2) – O(2) = 2.896 (× 6), Ba(2) – O(1) = 2.907 (× 3), Zn(1) – O(2) = 2.164 (× 6), Nb(2) – O(1) = 2.096 (× 3), Nb(2) – O(2) = 1.885. (× 63)

Bond valence sums: Ba(1) = 2.30, Ba (2) = 2.34, Zn(1) = 1.73, Nb(2) = 5.04.