Electronic Supplementary Information

$Ba_5Y_{12}Zn[O(SiO_4)]_8$: A Novel Non-Centrosymmetric Silicate with a Short Ultraviolet Cut-off Edge Featuring $[ZnSi_4O_{16}]$ and $[SiO_4]$ Units

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Table S1. The final atomic coordinates ($\times 10^4$), equivalent isotropic displacement parameters ($Å^2 \times 10^3$), and bond valence sums (BVS) for $Ba_5Y_{12}Zn[O(SiO_4)]_8$

Atom	Wyck	S.O.F	*x*	*y*	*z*	U(eq)	BVS
Ba(1)	8f	1	10000	8393(1)	10000	11(1)	2.099
Ba(2)	4d	0.5	5000	10000	7500	29(1)	2.140
Y(1)	8i	1	7916(1)	7916(1)	49(2)	8(1)	2.774
Y(2)	16j	1	6873(1)	8994(1)	4491(1)	7(1)	3.077
Zn(1)	2b	1	10000	10000	5000	14(1)	1.954
Si(1)	8i	1	8748(1)	8748(1)	4412(5)	9(1)	3.859
Si(2)	8f	1	6582(1)	10000	0	9(1)	3.968
O(1)	8i	1	9336(3)	9336(3)	3341(15)	12(2)	1.895
O(2)	16j	1	8141(3)	7044(3)	-2722(10)	9(1)	2.064
O(3)	8i	1	8703(3)	8703(3)	7422(14)	13(2)	1.705
O(4)	16j	1	7070(3)	10172(3)	2434(9)	9(1)	1.973
O(5)	16j	1	6119(3)	9305(3)	865(10)	13(1)	2.236
O(6)	16j	1	7992(3)	8936(3)	3024(10)	11(1)	2.135

U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

Table S2. Selected bond lengths (Å) and angles (deg.) for $Ba_5Y_{12}Zn[O(SiO_4)]_8$

Bond	Length	Bond	Length
Ba(1)-O(6)#1	2.674(5)	Y(2)-O(2)#1	2.210(5)
Ba(1)-O(6)#2	2.674(5)	Y(2)-O(6)	2.238(5)
Ba(1)-O(1)#3	2.804(5)	Y(2)-O(2)#17	2.276(5)
Ba(1)-O(1)#2	2.804(5)	Y(2)-O(4)#21	2.300(5)
Ba(1)-O(4)#2	2.817(5)	Y(2)-O(5)#16	2.332(5)
Ba(1)-O(4)#1	2.817(5)	Y(2)-O(5)	2.472(6)
Ba(1)-O(3)	2.852(5)	Y(2)-O(4)	2.490(5)
Ba(1)-O(3)#4	2.852(5)	Zn(1)-O(1)#22	1.970(7)
Ba(2)-O(5)#5	2.614(5)	Zn(1)-O(1)#2	1.970(7)
Ba(2)-O(5)#6	2.614(5)	Zn(1)-O(1)#23	1.970(7)
Ba(2)-O(5)#7	2.614(5)	Zn(1)-O(1)	1.970(7)
Ba(2)-O(5)#8	2.614(5)	Si(1)-O(3)	1.619(8)
Ba(2)-O(5)#11	3.053(5)	Si(1)-O(6)	1.637(6)
Ba(2)-O(5)#12	3.053(5)	Si(1)-O(6)#15	1.637(6)
Ba(2)-O(5)#13	3.053(5)	Si(1)-O(1)	1.656(8)
Ba(2)-O(5)#14	3.053(5)	Si(2)-O(4)	1.624(5)
Y(1)-O(2)	2.246(5)	Si(2)-O(4)#24	1.624(5)
Y(1)-O(2)#15	2.246(5)	Si(2)-O(5)#24	1.630(6)
Y(1)-O(2)#16	2.311(5)	Si(2)-O(5)	1.630(6)
Y(1)-O(2)#17	2.311(5)	O(3)-Si(1)-O(6)	114.8(3)
Y(1)-O(6)	2.492(6)	O(3)-Si(1)-O(6)#15	114.8(3)
Y(1)-O(6)#15	2.492(6)	O(6)-Si(1)-O(6)#15	99.5(4)
Y(1)-O(3)#18	2.514(8)	O(3)-Si(1)-O(1)	114.5(4)
O(6)-Si(1)-O(1)	105.9(3)	O(4)#24-Si(2)-O(5)#24	103.1(3)
O(6)#15-Si(1)-O(1)	105.9(3)	O(4)-Si(2)-O(5)	103.1(3)
O(4)-Si(2)-O(4)#24	111.7(4)	O(4)#24-Si(2)-O(5)	111.7(3)
O(4)-Si(2)-O(5)#24	111.7(3)	O(5)#24-Si(2)-O(5)	115.8(4)

Symmetry codes: #1 y,x,z+1; #2 -y+2,x,-z+1; #3 x,y,z+1; #4 -y+2,x,-z+2; #5 x,-y+1,-z+1; #6 -x+1,y-1,-z+1; #7 -y+3/2,-x+1/2,z+1/2; #8 y-1/2,x-1/2,z+1/2; #11 y-1/2,-x+1/2,-z+1/2; #12 x,y-1,z+1; #13 -y+3/2,x-1/2,-z+1/2; #14 -x+1,-y+1,z+1; #15 y,x,z; #16 -y+3/2,x+3/2,z+1/2; #17 -x+3/2,-y+3/2,z+1/2; #18 x,y,z-1; #21 x,-y+2,-z+1; #22 -x+2,-y+2,z; #23 y,-x+2,-z+1; #24 x,-y+2,-z

Table S3. Anisotropic displacement parameters for $Ba_5Y_{12}Zn[O(SiO_4)]_8$

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Ba(1)	9(1)	11(1)	13(1)	0	2(1)	0
Ba(2)	13(1)	13(1)	61(2)	0	0	0
Y(1)	8(1)	8(1)	8(1)	-1(1)	-1(1)	1(1)
Y(2)	8(1)	7(1)	7(1)	0(1)	0(1)	0(1)
Zn(1)	9(1)	9(1)	23(1)	0	0	0
Si(1)	9(1)	9(1)	7(1)	0(1)	0(1)	0(1)
Si(2)	12(1)	8(1)	6(1)	2(1)	0	0
O(1)	10(2)	10(2)	14(4)	0(2)	0(2)	-4(3)
O(2)	10(3)	4(3)	12(3)	4(2)	-1(2)	3(2)
O(3)	16(3)	16(3)	8(4)	-1(2)	-1(2)	4(3)
O(4)	12(3)	8(3)	6(2)	-2(2)	-1(2)	1(2)
O(5)	18(3)	10(3)	12(3)	-1(2)	0(2)	-1(2)
O(6)	8(3)	12(3)	12(2)	0(2)	1(2)	-1(2)

Table S4. Examples of Ba, Zn, and Y-containing silicates searched from ICSD

No	Compound	Crystal system	Space group	Cation oxides	Si-O anionic unit	n_M/n_{Si} ratio	Dimension of anionic groups	Ref.
1	α-SiO_2	Trigonal	$P3_221$		SiO_4		3D	[1]
2	$ZnSiO_3$-1	Monoclinic	$C2/c$	ZnO_4, ZnO_6	Si_2O_7	1:1	1D	[2]
3	$ZnSiO_3$-2	Orthorhombic	$Pbca$	ZnO_4	Si_2O_7	1:1	1D	[2]
4	$ZnSiO_3$-3	Monoclinic	$P2_1/c$	ZnO_4	Si_2O_7	1:1	1D	[3]
5	$ZnSiO_3$ (HP)	Monoclinic	$C2/c$	ZnO_6	Si_2O_7	1:1	1D	[3]
6	Zn_2SiO_4-1	Trigonal	$R\bar{3}H$	ZnO_4	SiO_4	2:1	0D	[4]
7	Zn_2SiO_4-2	Tetragonal	$I\bar{4}2d$	ZnO_4	SiO_4	2:1	0D	[5]
8	Zn_2SiO_4-3	Trigonal	$R\bar{3}R$	ZnO_4	SiO_4	2:1	0D	[6]
9	Zn_2SiO_4-4	Orthorhombic	$Pnma$	ZnO_4	SiO_4	2:1	0D	[7]
10	Zn_2SiO_4-5	Orthorhombic	$Pbca$	ZnO_4	SiO_4	2:1	0D	[7]
11	$Y_2(SiO_4)O$-1	Monoclinic	$C2/c$	YO_6, YO_7	SiO_4	2:1	0D	[8]
12	$Y_2(SiO_4)O$-2	Monoclinic	$I2/a$	YO_6, YO_7	SiO_4	2:1	0D	[9]
13	$Y_2(SiO_4)O$-3	Monoclinic	$P2_1/c$	YO_7, YO_8	SiO_4	2:1	0D	[10]
14	$Y_2Si_2O_7$-1	Monoclinic	$P2_1/m$	YO_6	Si_2O_7	1:1	0D	[11]
15	$Y_2Si_2O_7$-2	Monoclinic	$P2_1/a$	YO_6	Si_2O_7	1:1	0D	S11]
16	$Y_2Si_2O_7$-3	Orthorhombic	$Pnam$	YO_7	Si_2O_7	1:1	0D	[12]
17	$Y_2Si_2O_7$-4	Orthorhombic	$Pna2_1$	YO_7	Si_2O_7	1:1	0D	[13]
18	$Y_2Si_2O_7$-5	Monoclinic	$P2_1/c$	YO_6	Si_2O_7	1:1	0D	[14]
19	$Y_2Si_2O_7$-6	Triclinic	$P\bar{1}$	YO_6, YO_8	Si_2O_7, SiO_3, SiO_4	1:1	0D	[14]
20	$Y_2Si_2O_7$-7	Monoclinic	$C2/m$	YO_6	Si_2O_7	1:1	0D	[15]
21	$Y_{4.67}(SiO_4)_3O$	Hexagonal	$P6_3/m$	YO_7, YO_9	SiO_4	1.3:1	0D	[16]
22	Ba_2SiO_4	Orthorhombic	$Pmcn$	BaO_9	SiO_4	2:1	0D	[17]
23	$BaSi_4O_9$	Hexagonal	$P\bar{6}c2$	BaO_{12}	Si_7O_{22}	1:4	3D	[18]
24	Ba_3OSiO_4	Tetragonal	$I4/mcm$	BaO_{10}, BaO_8	SiO_4	3:1	0D	[19]
25	$Ba_2Si_4O_{10}$-1	Monoclinic	$C2/c$	BaO_7, BaO_8	Si_6O_{18} ring	1:2	2D	[20]
26	$Ba_2Si_4O_{10}$-2	Orthorhombic	$Pmcn$	BaO_7	Si_6O_{18}	1:2	2D	[21]
27	$BaSi_2O_5$-3	Orthorhombic	$Pcmn$	BaO_7	Si_6O_{18}	1:2	2D	[22]
28	$Ba_4Si_6O_{16}$-1	Monoclinic	$P2_1$	BaO_6, BaO_8, BaO_9	Si_6O_{18}	1:1.5	2D	[23]
29	$Ba_4Si_6O_{16}$-2	Monoclinic	$P2_1/c$	BaO_6, BaO_7	Si_6O_{18}	1:1.5	2D	[21]
30	$Ba_5Si_8O_{21}$	Monoclinic	$C2/c$	BaO_6, BaO_7	Si_6O_{18}	1:1.6	2D	[24]
31	$Ba_6Si_{10}O_{26}$	Monoclinic	$P2_1/c$	BaO_6, BaO_7	Si_6O_{18}	1:1.6	2D	[21]
32	$BaSiO_3$-1	Orthorhombic	$P2_12_12_1$	BaO_8	Si_2O_7	1:1	0D	[17]
33	$BaSiO_3$-2	Trigonal	$R\bar{3}mH$	BaO_{12}, BaO_8	Si_6O_{12}, SiO_6	1:1	2D	[25]
34	$BaSiO_3$-3	Hexagonal	$P6_3/mmc$	BaO_9	Si_7O_{18}	1:1	2D	[25]
35	$BaZnSiO_4$	Hexagonal	$P6_3$	BaO_6, BaO_9, ZnO_4	SiO_4	2:1	0D	[26]
36	$BaZn_2Si_2O_7$	Orthorhombic	$Cmc2_1$	Bao_5, ZnO_4	Si_2O_7	1.5:1	0D	[27]
37	$Ba_2ZnSi_2O_7$	Monoclinic	$C2/c$	BaO_8, ZnO_4	Si_2O_7	1.5:1	0D	[28]
38	$BaZnSi_3O_8$	Monoclinic	$P2_1/a$	BaO_8, ZnO_2	Si_6O_{18}	1:1.5	2D	[29]
39	$Ba_5Y_{12}Zn[O(SiO_4)]_8$	Tetragonal	$I\bar{4}2m$	BaO_8, YO_7, ZnO_4	SiO_4	2.3:1	0D	**This work**

Note: The determination of the crystal phase is subject to the order of time.

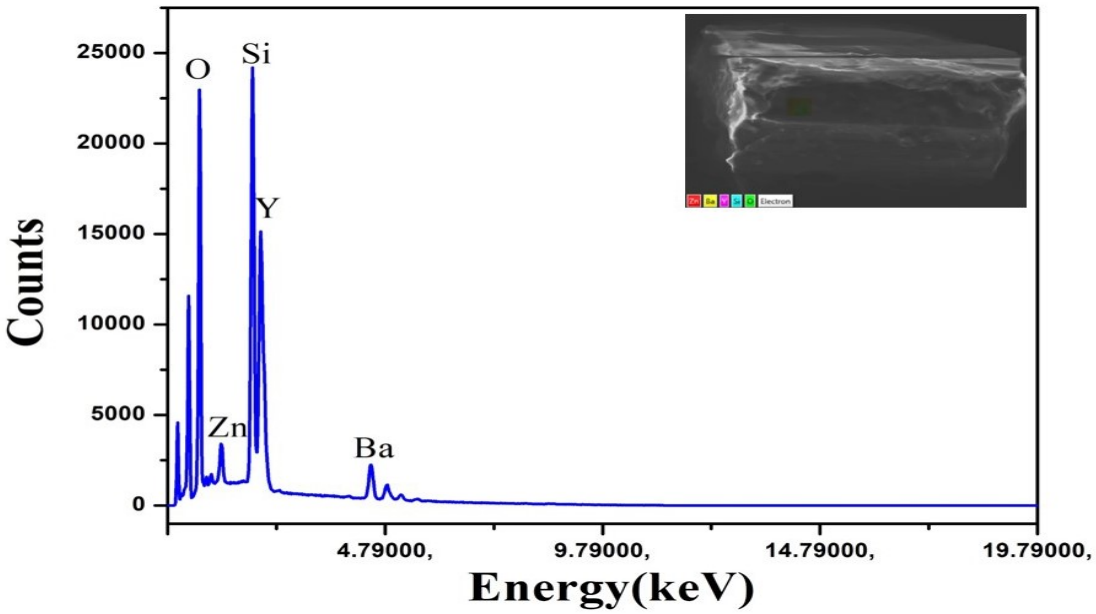

Figure S1 Energy dispersive X-ray spectroscopic (EDS) spectrum of $Ba_5Y_{12}Zn[O(SiO_4)]_8$

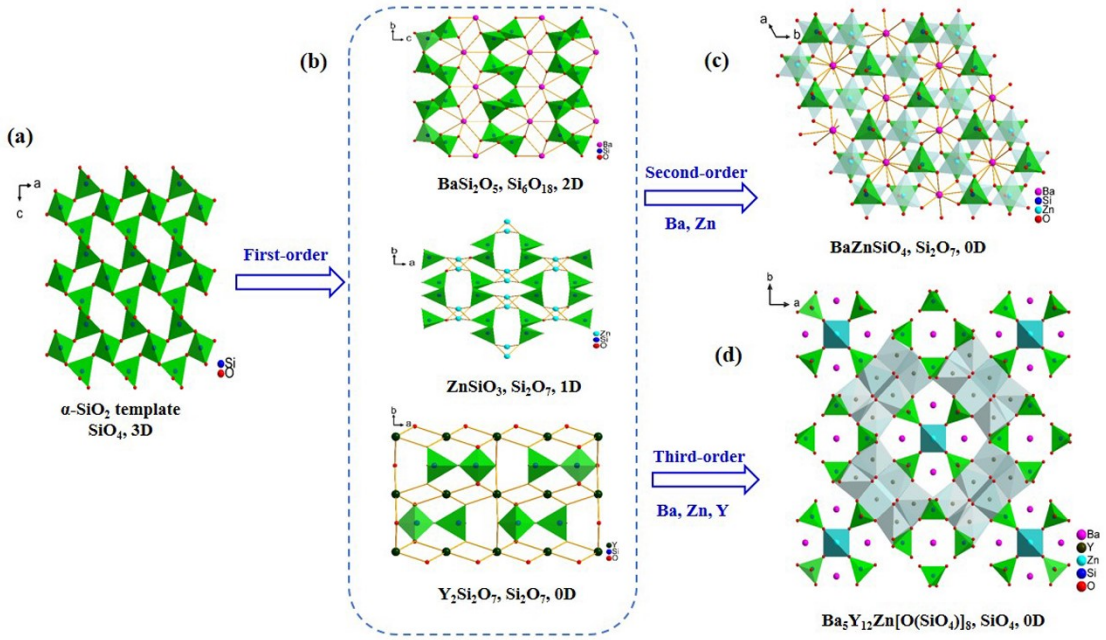

Figure S2 The structural evolution of anionic groups from (a) 3D network of α-SiO_2 down the *b*-axis to (b) 2D layers, 1D chains, 0D infinite groups of $BaSi_2O_5$, $ZnSiO_3$, $Y_2Si_2O_7$ crystals to (c, d) 0D isolated SiO_4 units of $BaZnSiO_4$ and $Ba_5Y_{12}Zn[O(SiO_4)]_8$ crystals down the *c*-axis.

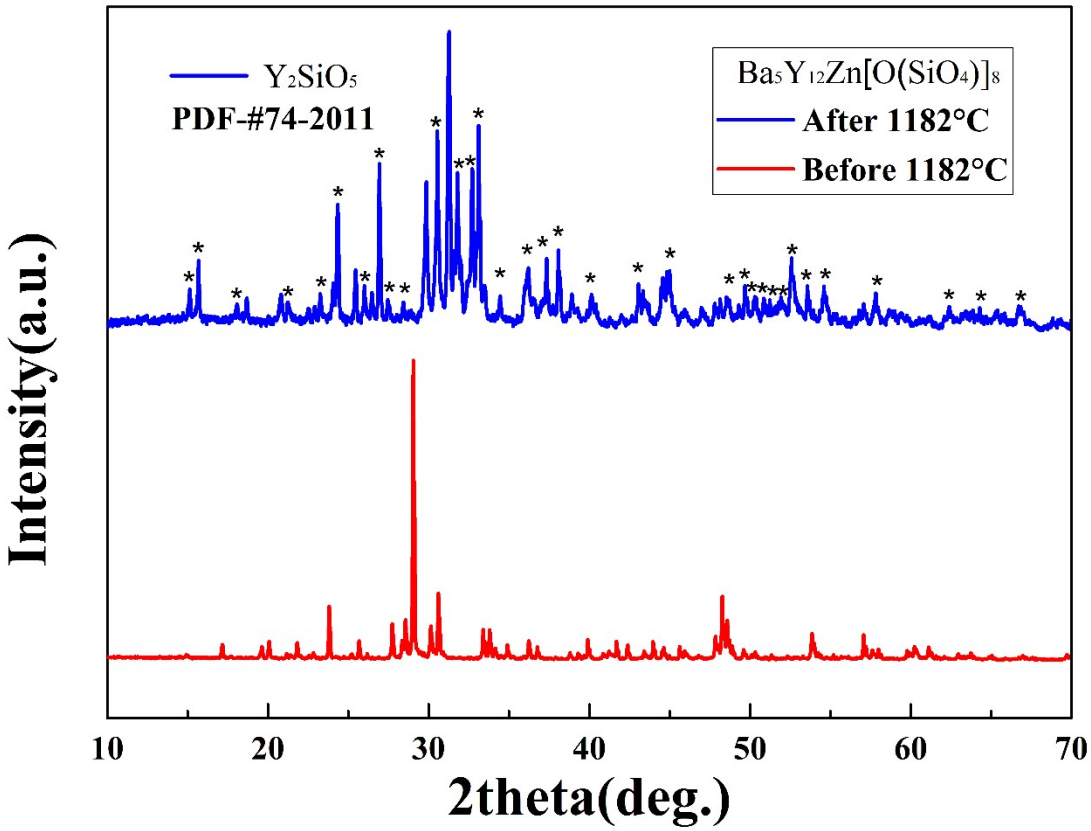

Figure S3 Experimental powder X-ray diffraction pattern of $Ba_5Y_{12}Zn[O(SiO_4)]_8$

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