Supplementary Information

From $Ca_3Be(SeO_3)_4$ to $SrBe(SeO_3)_2$: Two Unprecedented Alkaline Earth Metal Beryllium Selenites with Large Band Gaps and Enhanced Birefringence

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Table S1. Atomic coordinates (×10^4) and equivalent isotropic displacement parameters (Å^2×10^3) for $Ca_3Be(SeO_3)_4$ and $SrBe(SeO_3)_2$. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

$Ca_3Be(SeO_3)_4$

Atom	x	y	z	U(eq)
Se(1)	8093(1)	3989 (1)	3116(1)	12 (1)
Ca(1)	10000	2500	4516 (1)	13(1)
Ca(2)	10000	7500	3750	16(1)
O(1)	9239(5)	4423(5)	3741(2)	20 (1)
O(2)	5852(5)	4164(5)	3334(2)	19(1)
O(3)	8307(5)	6048(5)	2788 (2)	21 (1)
Be(1)	5000	2500	3750	17(2)

$SrBe(SeO_3)_2$

Atom	x	y	z	U(eq)
Sr(1)	7497(2)	2485(3)	2938(2)	11 (1)
Sr(2)	4956(2)	2542(3)	7093(2)	9(1)
Se(1)	5076(2)	2939(4)	3660(3)	13(1)
Se(2)	8301(2)	7608(4)	4398(2)	11 (1)
Se(3)	5771(2)	7662(4)	5658(2)	10(1)
Se(4)	7526(2)	2030(4)	6361 (3)	12 (1)
O(1)	4334(10)	3680(30)	2915(10)	23(4)
O(2)	5652(11)	220(30)	3319(11)	19(4)
O(3)	6000(9)	5110(30)	3434(10)	9(3)
O(4)	8358(11)	4680(30)	4021(10)	37(5)
O(5)	7242(11)	8860(30)	3998(10)	24(4)
O(6)	5468(16)	7770(30)	4714(12)	18(5)
O(7)	4716(9)	8880(20)	6097(9)	15(3)
O(8)	5742(11)	4550(30)	5898(10)	32(4)
O(9)	7895(16)	7100(30)	5349(11)	17(4)
O(10)	8086(11)	4760(30)	6731(10)	18(4)
O(11)	8437(11)	-200(30)	6626(12)	21(4)
O(12)	6752(9)	1280(30)	7110(10)	18(3)
Be(1)	6120(20)	7840(60)	3940(20)	14(7)
Be(2)	8570(20)	7030(60)	6120(20)	14(7)

Table S2. Selected bond lengths (Å) and angles (degrees) for $Ca_3Be(SeO_3)_4$ and $SrBe(SeO_3)_2$.

$Ca_3Be(SeO_3)_4$

Se(1)-O(1)	1.671(3)	Ca(2)-O(1)	2.317(3)
Se(1)-O(2)	1.715(3)	Ca(2)-O(1)#7	2.317(3)
Se(1)-O(3)	1.684(3)	Ca(2)-O(3)	2.715(4)
Ca(1)-O(1)#4	2.313(3)	Ca(2)-O(3)#2	2.715(4)
Ca(1)-O(1)	2.313(3)	Ca(2)-O(3)#7	2.715(4)
Ca(1)-O(2)#2	2.638(3)	Ca(2)-O(3)#1	2.715(4)
Ca(1)-O(2)#3	2.638(3)	O(2)-Ca(1)#1	2.638(3)
Ca(1)-O(3)#2	2.677(4)	O(2)-Be(1)	1.658(4)
Ca(1)-O(3)#3	2.677(4)	O(3)-Ca(1)#8	2.386(4)
Ca(1)-O(3)#5	2.386(4)	O(3)-Ca(1)#1	2.677(4)
Ca(1)-O(3)#6	2.386(4)	Be(1)-O(2)#9	1.658(4)

Ca(2)-O(1)#1	2.317(3)	Be(1)-O(2)#10	1.658(4)
Ca(2)-O(1)#2	2.317(3)	Be(1)-O(2)#3	1.658(4)
O(1)-Se(1)-O(2)	102.83(19)	O(1)#7-Ca(2)-O(3)	118.79(11)
O(1)-Se(1)-O(3)	98.86(17)	O(1)#7-Ca(2)-O(3)#1	70.05(11)
O(3)-Se(1)-O(2)	98.54(17)	O(1)#1-Ca(2)-O(3)#7	110.85(12)
O(1)#4-Ca(1)-O(1)	81.63(19)	O(1)#2-Ca(2)-O(3)#1	118.79(12)
O(1)-Ca(1)-O(2)#2	81.50(13)	O(1)#1-Ca(2)-O(3)	70.05(11)
O(1)#4-Ca(1)-O(2)#2	72.21(12)	O(1)#1-Ca(2)-O(3)#1	60.24(11)
O(1)#4-Ca(1)-O(2)#3	81.50(13)	O(1)#2-Ca(2)-O(3)#7	70.05(11)
O(1)-Ca(1)-O(2)#3	72.21(12)	O(1)-Ca(2)-O(3)#2	70.05(11)
O(1)#4-Ca(1)-O(3)#3	70.81(12)	O(1)-Ca(2)-O(3)	60.24(11)
O(1)-Ca(1)-O(3)#3	125.33(12)	O(1)#7-Ca(2)-O(3)#2	110.85(12)
O(1)#4-Ca(1)-O(3)#5	167.11(13)	O(1)#2-Ca(2)-O(3)	110.85(12)
O(1)-Ca(1)-O(3)#5	97.50(13)	O(1)#2-Ca(2)-O(3)#2	60.24(11)
O(1)#4-Ca(1)-O(3)#2	125.33(12)	O(1)#1-Ca(2)-O(3)#2	118.79(12)
O(1)-Ca(1)-O(3)#2	70.81(12)	O(1)#7-Ca(2)-O(3)#7	60.24(11)
O(1)#4-Ca(1)-O(3)#6	97.50(13)	O(3)#1-Ca(2)-O(3)#7	129.74(9)
O(1)-Ca(1)-O(3)#6	167.11(13)	O(3)#1-Ca(2)-O(3)#2	73.82(15)
O(2)#3-Ca(1)-O(2)#2	145.15(17)	O(3)#2-Ca(2)-O(3)	129.74(9)
O(2)#3-Ca(1)-O(3)#3	57.97(11)	O(3)#1-Ca(2)-O(3)	129.74(9)
O(2)#2-Ca(1)-O(3)#3	128.99(11)	O(3)#7-Ca(2)-O(3)	73.82(15)
O(2)#3-Ca(1)-O(3)#2	128.99(11)	O(3)#2-Ca(2)-O(3)#7	129.74(9)
O(2)#2-Ca(1)-O(3)#2	57.97(11)	Se(1)-O(1)-Ca(1)	130.11(18)
O(3)#5-Ca(1)-O(2)#3	85.98(11)	Se(1)-O(1)-Ca(2)	108.19(15)
O(3)#6-Ca(1)-O(2)#3	120.49(12)	Ca(1)-O(1)-Ca(2)	121.69(15)
O(3)#5-Ca(1)-O(2)#2	120.49(12)	Se(1)-O(2)-Ca(1)#1	102.02(16)
O(3)#6-Ca(1)-O(2)#2	85.98(11)	Be(1)-O(2)-Se(1)	117.8(2)
O(3)#6-Ca(1)-O(3)#2	99.88(10)	Be(1)-O(2)-Ca(1)#1	139.38(18)
O(3)#5-Ca(1)-O(3)#3	99.88(10)	Se(1)-O(3)-Ca(1)#8	140.0(2)
O(3)#2-Ca(1)-O(3)#3	161.02(17)	Se(1)-O(3)-Ca(1)#1	101.41(16)
O(3)#6-Ca(1)-O(3)#3	65.65(14)	Se(1)-O(3)-Ca(2)	92.36(15)
O(3)#5-Ca(1)-O(3)#2	65.65(14)	Ca(1)#8-O(3)-Ca(1)#1	114.35(14)
O(3)#5-Ca(1)-O(3)#6	86.19(18)	Ca(1)#8-O(3)-Ca(2)	100.00(13)
O(1)-Ca(2)-O(1)#1	90.005(2)	Ca(1)#1-O(3)-Ca(2)	97.17(12)
O(1)#7-Ca(2)-O(1)#2	90.005(2)	O(2)#3-Be(1)-O(2)#10	111.0(3)
O(1)-Ca(2)-O(1)#7	178.95(17)	O(2)#3-Be(1)-O(2)	108.71(13)
O(1)#7-Ca(2)-O(1)#1	90.005(2)	O(2)#9-Be(1)-O(2)	111.0(3)
O(1)#2-Ca(2)-O(1)#1	178.95(17)	O(2)#9-Be(1)-O(2)#3	108.71(13)
O(1)-Ca(2)-O(1)#2	90.005(2)	O(2)#10-Be(1)-O(2)	108.71(13)
O(1)-Ca(2)-O(3)#1	110.85(12)	O(2)#9-Be(1)-O(2)#10	108.71(13)
O(1)-Ca(2)-O(3)#7	118.79(11)		

Symmetry transformations used to generate equivalent atoms:

#1 y+1/4,-x+7/4,-z+3/4 #2 -y+7/4,x-1/4,-z+3/4 #3 y+1/4,-x+3/4,-z+3/4 #4 -x+2,-y+1/2,z+0 #5 y+1/4,-x+5/4,z+1/4

#6 -y+7/4,x-3/4,z+1/4 #7 -x+2,-y+3/2,z+0 #8 -y+5/4,x-1/4,z-1/4 #9 -x+1,-y+1/2,z+0 #10 -y+3/4,x-1/4,-z+3/4

$SrBe(SeO_3)_2$

Sr(1)-O(1)#2	2.575(14)	Se(4)-O(10)	1.703(16)
Sr(1)-O(2)	2.842(16)	Se(4)-O(11)	1.741(16)
Sr(1)-O(3)	2.579(14)	Se(4)-O(12)	1.692(14)
Sr(1)-O(4)	2.445(16)	O(1)-Sr(1)#6	2.575(14)
Sr(1)-O(5)#3	2.594(16)	O(1)-Sr(2)#8	2.563(16)
Sr(1)-O(10)#4	2.592(17)	O(2)-Sr(2)#11	2.637(18)
Sr(1)-O(11)#1	2.816(19)	O(2)-Be(1)#3	1.72(3)
Sr(1)-O(12)#1	2.595(14)	O(3)-Sr(2)#8	2.876(17)
Sr(2)-O(1)#5	2.563(16)	O(3)-Be(1)	1.64(3)
Sr(2)-O(2)#7	2.637(18)	O(5)-Sr(1)#9	2.594(16)
Sr(2)-O(3)#5	2.876(17)	O(5)-Be(1)	1.62(4)
Sr(2)-O(7)#3	2.531(14)	O(6)-Be(1)	1.58(4)
Sr(2)-O(8)	2.505(17)	O(7)-Sr(2)#9	2.531(14)
Sr(2)-O(10)#6	2.872(15)	O(7)-Be(2)#12	1.63(3)
Sr(2)-O(11)#6	2.598(16)	O(9)-Be(2)	1.59(4)
Sr(2)-O(12)	2.532(13)	O(10)-Sr(1)#13	2.592(17)
Se(1)-O(1)	1.659(15)	O(10)-Sr(2)#2	2.872(15)
Se(1)-O(2)	1.693(16)	O(10)-Be(2)	1.69(4)
Se(1)-O(3)	1.718(14)	O(11)-Sr(1)#10	2.816(19)
Se(2)-O(4)	1.622(14)	O(11)-Sr(2)#2	2.598(16)
Se(2)-O(5)	1.719(15)	O(11)-Be(2)#3	1.66(3)
Se(2)-O(9)	1.720(19)	O(12)-Sr(1)#10	2.595(14)
Se(3)-O(6)	1.65(2)	Be(1)-O(2)#9	1.72(3)
Se(3)-O(7)	1.733(13)	Be(2)-O(7)#14	1.63(3)
Se(3)-O(8)	1.633(15)	Be(2)-O(11)#9	1.66(3)
O(1)#2-Sr(1)-O(2)	140.5(5)	O(4)-Se(2)-O(9)	104.1(9)
O(1)#2-Sr(1)-O(3)	153.4(5)	O(5)-Se(2)-O(9)	98.8(9)
O(1)#2-Sr(1)-O(5)#3	88.7(5)	O(6)-Se(3)-O(7)	101.2(9)
O(1)#2-Sr(1)-O(10)#4	99.4(5)	O(8)-Se(3)-O(6)	105.5(8)
O(1)#2-Sr(1)-O(11)#1	121.6(5)	O(8)-Se(3)-O(7)	102.8(7)
O(1)#2-Sr(1)-O(12)#1	77.2(5)	O(10)-Se(4)-O(11)	96.7(9)
O(3)-Sr(1)-O(2)	55.6(5)	O(12)-Se(4)-O(10)	100.9(7)
O(3)-Sr(1)-O(5)#3	92.1(5)	O(12)-Se(4)-O(11)	96.1(8)
O(3)-Sr(1)-O(10)#4	106.9(4)	Sr(2)#8-O(1)-Sr(1)#6	123.2(6)
O(3)-Sr(1)-O(11)#1	71.5(4)	Se(1)-O(1)-Sr(1)#6	122.0(8)
O(3)-Sr(1)-O(12)#1	95.9(4)	Se(1)-O(1)-Sr(2)#8	110.5(7)
O(4)-Sr(1)-O(1)#2	69.4(5)	Sr(2)#11-O(2)-Sr(1)	108.5(6)
O(4)-Sr(1)-O(2)	116.2(6)	Se(1)-O(2)-Sr(1)	99.0(7)
O(4)-Sr(1)-O(3)	84.3(5)	Se(1)-O(2)-Sr(2)#11	123.8(8)
O(4)-Sr(1)-O(5)#3	82.6(6)	Se(1)-O(2)-Be(1)#3	122.6(14)
O(4)-Sr(1)-O(10)#4	168.9(5)	Be(1)#3-O(2)-Sr(1)	95.4(13)
O(4)-Sr(1)-O(11)#1	128.0(5)	Be(1)#3-O(2)-Sr(2)#11	102.8(12)
O(4)-Sr(1)-O(12)#1	82.8(5)	Sr(1)-O(3)-Sr(2)#8	108.5(6)
O(5)#3-Sr(1)-O(2)	55.7(5)	Se(1)-O(3)-Sr(1)	108.7(7)
O(5)#3-Sr(1)-O(11)#1	141.3(5)	Se(1)-O(3)-Sr(2)#8	96.3(6)
O(5)#3-Sr(1)-O(12)#1	162.5(5)	Be(1)-O(3)-Sr(1)	121.9(13)
O(10)#4-Sr(1)-O(2)	71.9(4)	Be(1)-O(3)-Sr(2)#8	95.9(13)
O(10)#4-Sr(1)-O(5)#3	97.0(5)	Be(1)-O(3)-Se(1)	120.2(14)

O(10)#4-Sr(1)-O(11)#1	57.7(6)	Se(2)-O(4)-Sr(1)	133.7(8)
O(10)#4-Sr(1)-O(12)#1	95.5(6)	Se(2)-O(5)-Sr(1)#9	115.0(7)
O(11)#1-Sr(1)-O(2)	87.0(4)	Be(1)-O(5)-Sr(1)#9	108.2(13)
O(12)#1-Sr(1)-O(2)	140.7(5)	Be(1)-O(5)-Se(2)	134.4(14)
O(12)#1-Sr(1)-O(11)#1	56.1(4)	Be(1)-O(6)-Se(3)	131.3(19)
O(1)#5-Sr(2)-O(2)#7	95.3(6)	Se(3)-O(7)-Sr(2)#9	116.2(6)
O(1)#5-Sr(2)-O(3)#5	55.4(4)	Be(2)#12-O(7)-Sr(2)#9	108.6(13)
O(1)#5-Sr(2)-O(10)#6	139.2(5)	Be(2)#12-O(7)-Se(3)	134.6(14)
O(1)#5-Sr(2)-O(11)#6	94.3(5)	Se(3)-O(8)-Sr(2)	127.3(8)
O(2)#7-Sr(2)-O(3)#5	57.3(5)	Be(2)-O(9)-Se(2)	125.5(18)
O(2)#7-Sr(2)-O(10)#6	70.8(4)	Sr(1)#13-O(10)-Sr(2)#2	108.8(6)
O(7)#3-Sr(2)-O(1)#5	164.0(5)	Se(4)-O(10)-Sr(1)#13	126.0(7)
O(7)#3-Sr(2)-O(2)#7	95.2(5)	Se(4)-O(10)-Sr(2)#2	98.3(6)
O(7)#3-Sr(2)-O(3)#5	140.5(4)	Be(2)-O(10)-Sr(1)#13	103.7(12)
O(7)#3-Sr(2)-O(10)#6	56.2(4)	Be(2)-O(10)-Sr(2)#2	93.7(12)
O(7)#3-Sr(2)-O(11)#6	94.4(6)	Be(2)-O(10)-Se(4)	120.5(14)
O(7)#3-Sr(2)-O(12)	86.9(4)	Sr(2)#2-O(11)-Sr(1)#10	109.8(7)
O(8)-Sr(2)-O(1)#5	88.2(5)	Se(4)-O(11)-Sr(1)#10	98.7(7)
O(8)-Sr(2)-O(2)#7	170.3(5)	Se(4)-O(11)-Sr(2)#2	107.9(7)
O(8)-Sr(2)-O(3)#5	131.3(5)	Be(2)#3-O(11)-Sr(1)#10	95.9(14)
O(8)-Sr(2)-O(7)#3	79.6(5)	Be(2)#3-O(11)-Sr(2)#2	120.9(13)
O(8)-Sr(2)-O(10)#6	112.0(6)	Be(2)#3-O(11)-Se(4)	119.8(15)
O(8)-Sr(2)-O(11)#6	83.3(5)	Sr(2)-O(12)-Sr(1)#10	125.2(6)
O(8)-Sr(2)-O(12)	72.5(5)	Se(4)-O(12)-Sr(1)#10	109.0(6)
O(10)#6-Sr(2)-O(3)#5	86.2(4)	Se(4)-O(12)-Sr(2)	122.5(7)
O(11)#6-Sr(2)-O(2)#7	105.4(5)	O(3)-Be(1)-O(2)#9	104(2)
O(11)#6-Sr(2)-O(3)#5	70.2(4)	O(5)-Be(1)-O(2)#9	99.4(18)
O(11)#6-Sr(2)-O(10)#6	55.9(5)	O(5)-Be(1)-O(3)	114(2)
O(12)-Sr(2)-O(1)#5	79.6(5)	O(6)-Be(1)-O(2)#9	108.1(19)
O(12)-Sr(2)-O(2)#7	99.2(5)	O(6)-Be(1)-O(3)	110.7(19)
O(12)-Sr(2)-O(3)#5	122.3(5)	O(6)-Be(1)-O(5)	119(2)
O(12)-Sr(2)-O(10)#6	139.3(4)	O(7)#14-Be(2)-O(10)	101.0(18)
O(12)-Sr(2)-O(11)#6	155.1(6)	O(7)#14-Be(2)-O(11)#9	111(2)
O(1)-Se(1)-O(2)	102.1(8)	O(9)-Be(2)-O(7)#14	123(2)
O(1)-Se(1)-O(3)	97.7(8)	O(9)-Be(2)-O(10)	107(2)
O(2)-Se(1)-O(3)	96.2(8)	O(9)-Be(2)-O(11)#9	110.1(19)
O(4)-Se(2)-O(5)	103.1(8)	O(11)#9-Be(2)-O(10)	103(2)

Symmetry transformations used to generate equivalent atoms:

#1 -x+3/2,y+1/2,z-1/2 #2 x+1/2,-y+1/2,z #3 x,y-1,z #4 -x+3/2,y-1/2,z-1/2 #5 -x+1,-y+1,z+1/2 #6 x-1/2,-y+1/2,z #7 -x+1,-y,z+1/2 #8 -x+1,-y+1,z-1/2 #9 x,y+1,z #10 -x+3/2,y-1/2,z+1/2 #11 -x+1,-y,z-1/2 #12 x-1/2,-y+3/2,z #13 -x+3/2,y+1/2,z+1/2 #14 x+1/2,-y+3/2,z

Table S3. Anisotropic displacement parameters ($Å^2×10^3$) for $Ca_3Be(SeO_3)_4$ and $SrBe(SeO_3)_2$.

The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U_{11} + ... + 2hka^* b^* U_{12}]$

$Ca_3Be(SeO_3)_4$

	U11	U22	U33	U23	U13	U12
Se(1)	12(1)	11(1)	14(1)	-1(1)	0(1)	1(1)
Ca(1)	17(1)	13(1)	8(1)	0	0	2(1)
Ca(2)	12(1)	12(1)	25(1)	0	0	0
O(1)	26(2)	13(2)	22(2)	7(1)	-10(1)	-3(1)
O(2)	11(2)	17(2)	28(2)	3(1)	1(1)	0(1)
O(3)	29(2)	18(2)	18(2)	7(1)	6(1)	4(1)
Be(1)	15(4)	15(4)	22(6)	0	0	0

$SrBe(SeO_3)_2$

	U11	U22	U33	U23	U13	U12
Sr(1)	13(2)	11(2)	9(2)	0(1)	0(1)	0(1)
Sr(2)	4(1)	13(2)	8(2)	-1(1)	2(1)	0(1)
Se(1)	9(1)	20(1)	10(1)	3(2)	2(1)	1(1)
Se(2)	9(1)	21(2)	5(2)	0(1)	0(1)	0(1)
Se(3)	6(1)	13(2)	10(2)	0(1)	2(1)	0(1)
Se(4)	7(1)	21(1)	6(1)	-2(2)	-1(1)	1(1)
O(1)	18(8)	34(9)	16(8)	2(7)	-6(6)	-1(6)
O(2)	32(10)	6(7)	20(9)	-5(6)	10(7)	-3(7)
O(3)	14(4)	5(4)	9(5)	-4(3)	2(4)	2(3)
O(4)	30(11)	32(9)	48(11)	-29(8)	-15(8)	22(7)
O(5)	20(8)	30(9)	20(9)	-2(7)	3(7)	0(7)
O(6)	13(6)	25(7)	16(7)	2(5)	-1(5)	-6(5)
O(7)	6(7)	16(7)	22(9)	-14(6)	6(6)	-6(6)
O(8)	45(11)	24(8)	28(10)	10(7)	19(8)	6(7)
O(9)	12(6)	26(6)	14(7)	3(5)	-2(5)	1(5)
O(10)	27(9)	18(8)	7(8)	-3(6)	1(7)	1(7)
O(11)	26(6)	10(6)	27(7)	0(5)	-8(5)	-4(5)
O(12)	18(6)	16(5)	20(6)	9(5)	1(5)	-3(4)
Be(1)	11(9)	16(9)	13(9)	-2(6)	0(6)	0(6)
Be(2)	13(9)	14(8)	14(9)	-5(6)	-1(6)	1(6)

Table S4. Direction and magnitude of the dipole moment of $[SeO_3]^{2-}$ groups in $Ca_3Be(SeO_3)_4$ and $SrBe(SeO_3)_2$.

	Species	D_x	D_y	D_z	Magnitude
	$[SeO_3]^{2-}$	-2.348	8.341	5.000	10.004
	$[SeO_3]^{2-}$	-8.342	-2.349	-5.000	10.006
	$[SeO_3]^{2-}$	2.346	-8.341	5.004	10.006
	$[SeO_3]^{2-}$	8.342	2.347	-5.002	10.005
	Absolute value addition	**21.377**	**21.378**	**20.005**	**/**
	$[SeO_3]^{2-}$	-7.399	-5.270	0.707	9.111
	$[SeO_3]^{2-}$	3.506	-0.286	9.531	10.160
	$[SeO_3]^{2-}$	4.081	0.323	-9.989	10.796
	$[SeO_3]^{2-}$	-7.486	-4.458	-2.305	9.012
Layer 1	$[SeO_3]^{2-}$	-7.399	5.270	0.707	9.111
	$[SeO_3]^{2-}$	3.506	0.286	9.531	10.160
	$[SeO_3]^{2-}$	4.081	-0.323	-9.989	10.796
	$[SeO_3]^{2-}$	-7.486	4.458	-2.305	9.012
	Absolute value addition	**44.942**	**20.676**	**45.064**	**/**
	$[SeO_3]^{2-}$	7.399	5.270	0.707	9.111
	$[SeO_3]^{2-}$	-3.506	0.286	9.531	10.160
	$[SeO_3]^{2-}$	-4.081	-0.323	-9.989	10.796
	$[SeO_3]^{2-}$	7.486	4.458	-2.305	9.012
Layer 2	$[SeO_3]^{2-}$	7.399	-5.270	0.707	9.111
	$[SeO_3]^{2-}$	-3.506	-0.286	9.531	10.160
	$[SeO_3]^{2-}$	-4.081	0.323	-9.989	10.796
	$[SeO_3]^{2-}$	7.486	-4.458	-2.305	9.012
	Absolute value addition	**44.942**	**20.676**	**45.064**	**/**

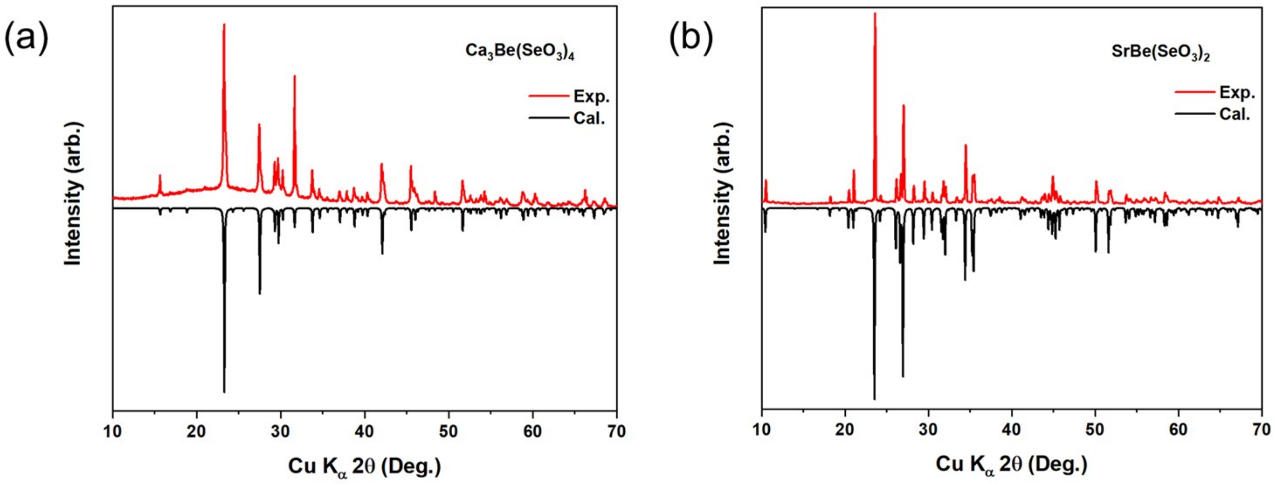

Figure S1. Powder X-ray diffraction for (a) $Ca_3Be(SeO_3)_4$ and (b) $SrBe(SeO_3)_2$.

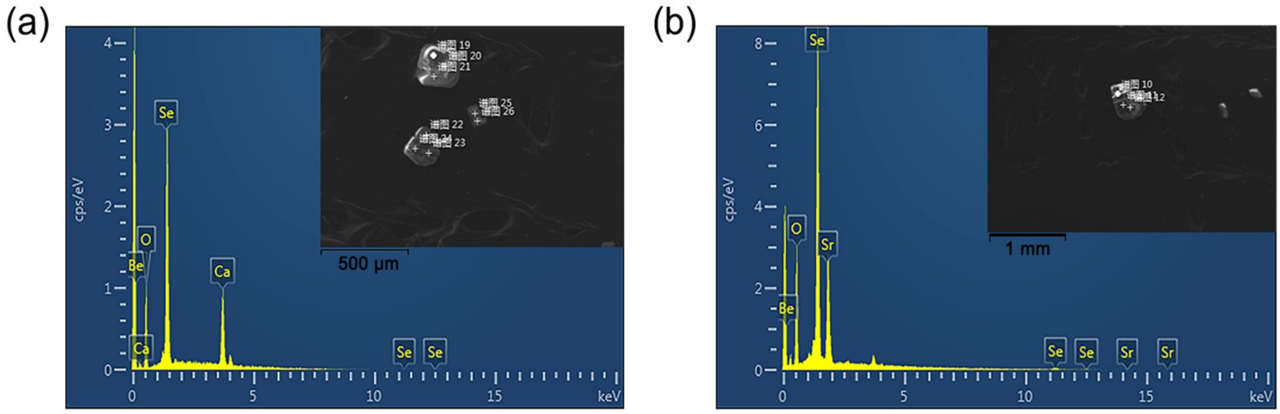

Figure S2. Energy dispersive X-ray spectroscope (EDS) analysis for $Ca_3Be(SeO_3)_4$ (a) and $SrBe(SeO_3)_2$ (b).

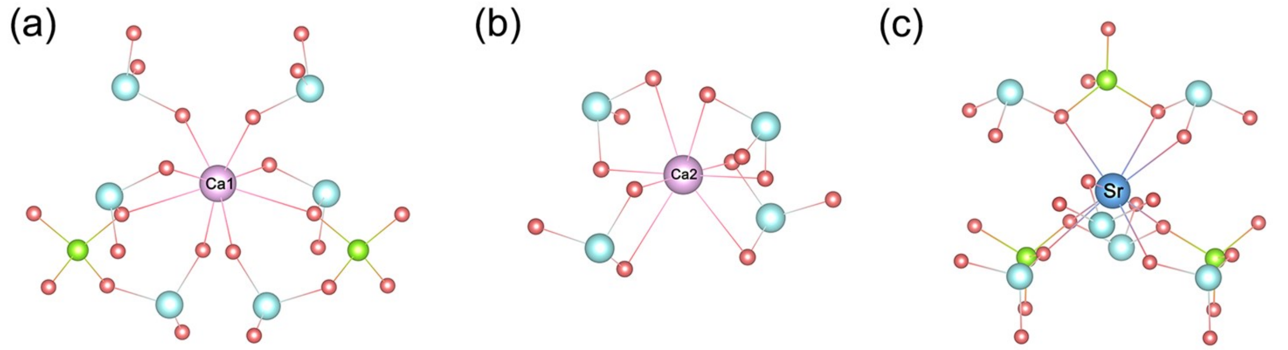

Figure S3. Atomic coordination forms of Ca-O (a,b) and Sr-O (c).

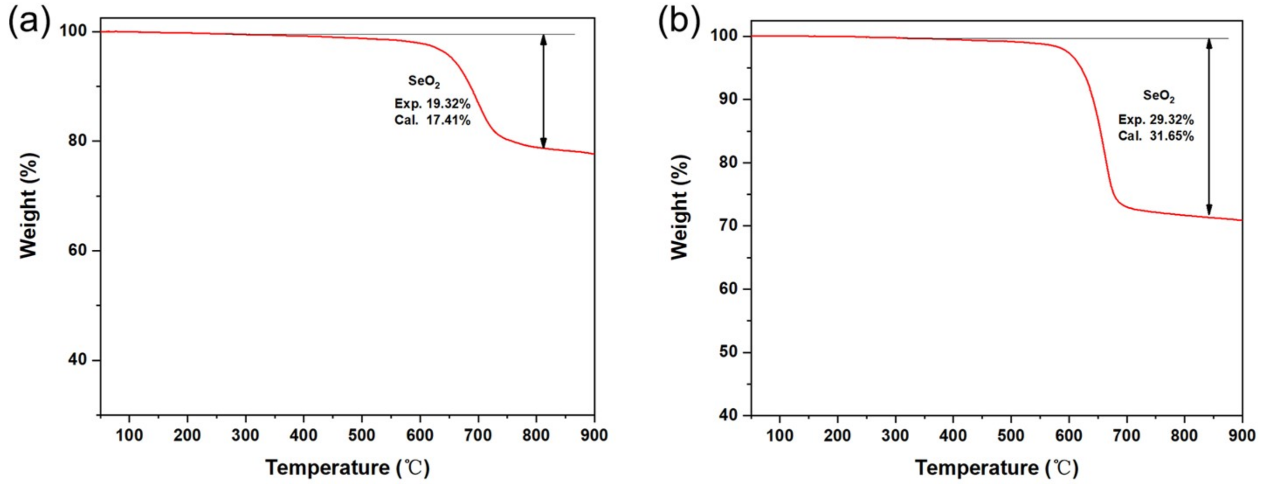

Figure S4. Thermogravimetric (TG) analysis for $Ca_3Be(SeO_3)_4$ (a) and $SrBe(SeO_3)_2$ (b).

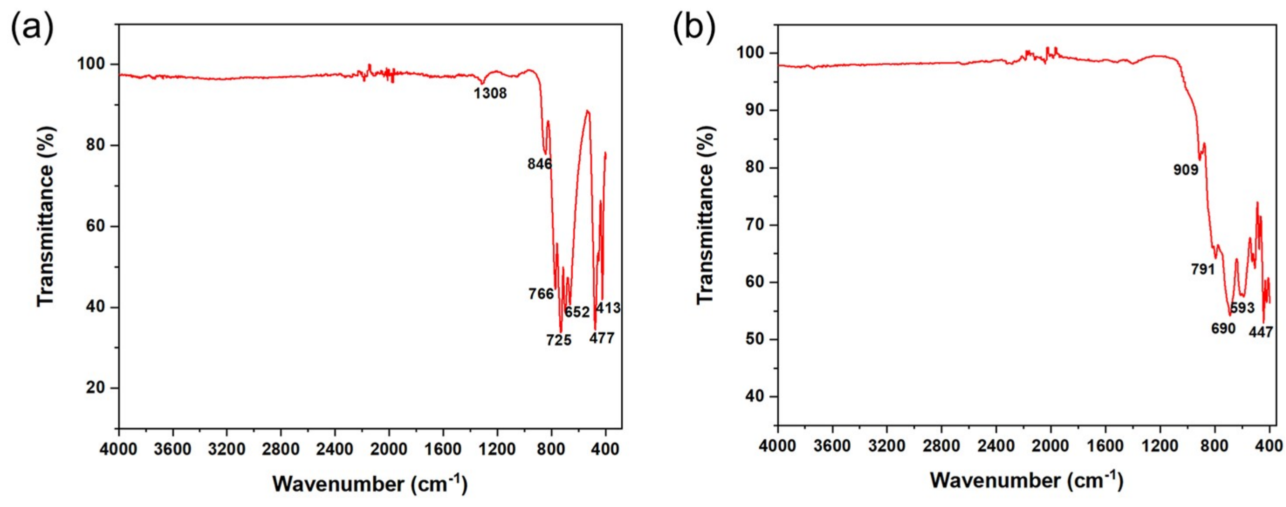

Figure S5. IR spectra for $Ca_3Be(SeO_3)_4$ (a) and $SrBe(SeO_3)_2$ (b).

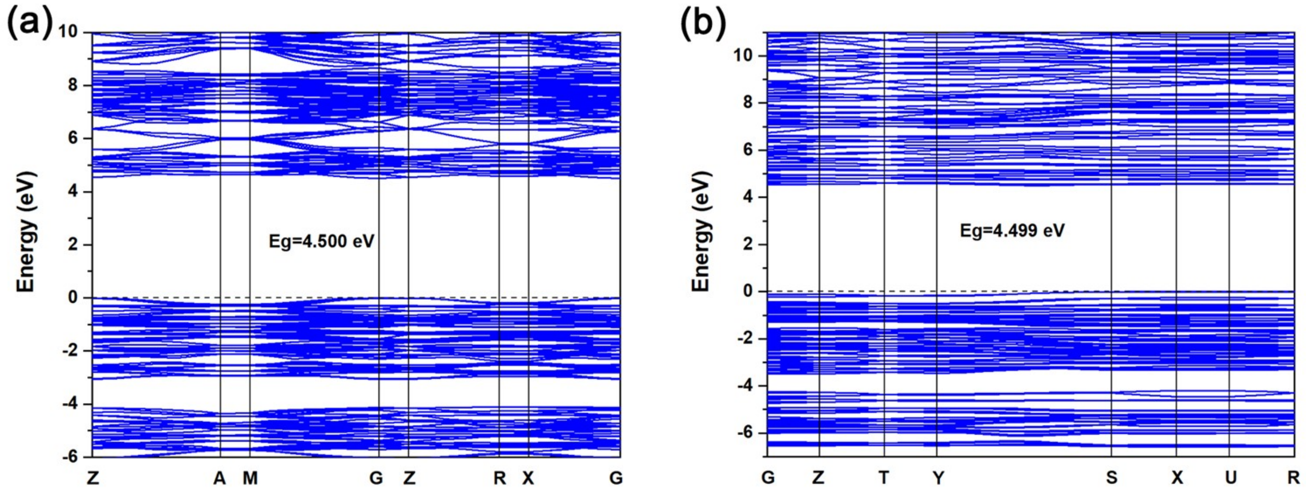

Figure S6. Calculated band structure for $Ca_3Be(SeO_3)_4$ (a) and $SrBe(SeO_3)_2$ (b).