

An excellent cyan-emitting orthosilicate phosphor for NUV-pumped white LED application

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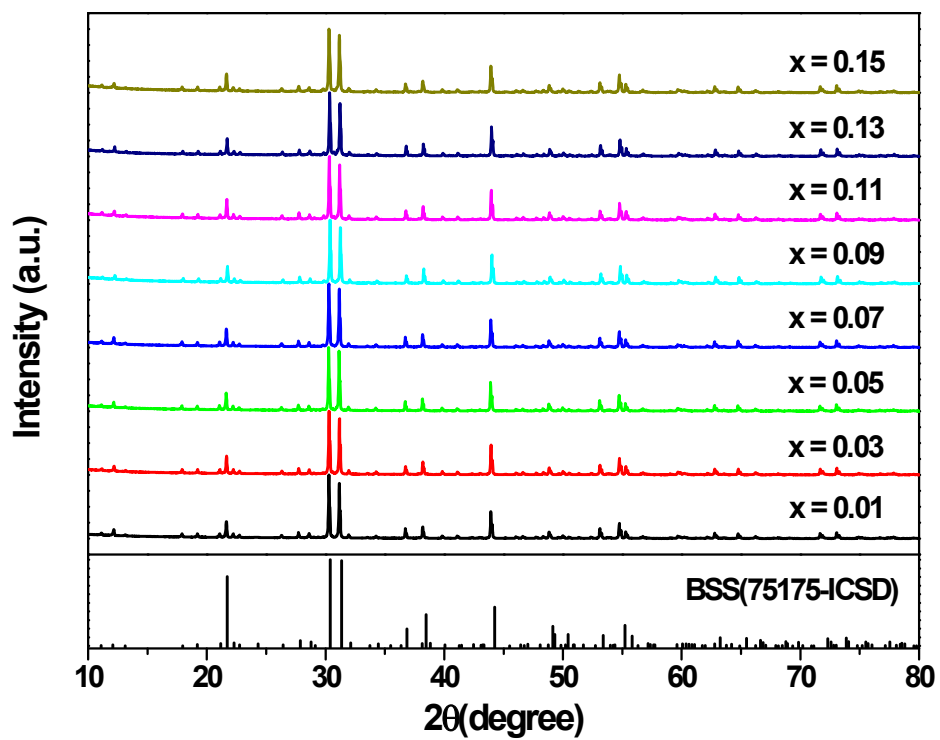


Figure S1 XRD patterns for BLS: $x\text{Ce}^{3+}$ ($x = 0.01-0.15$).

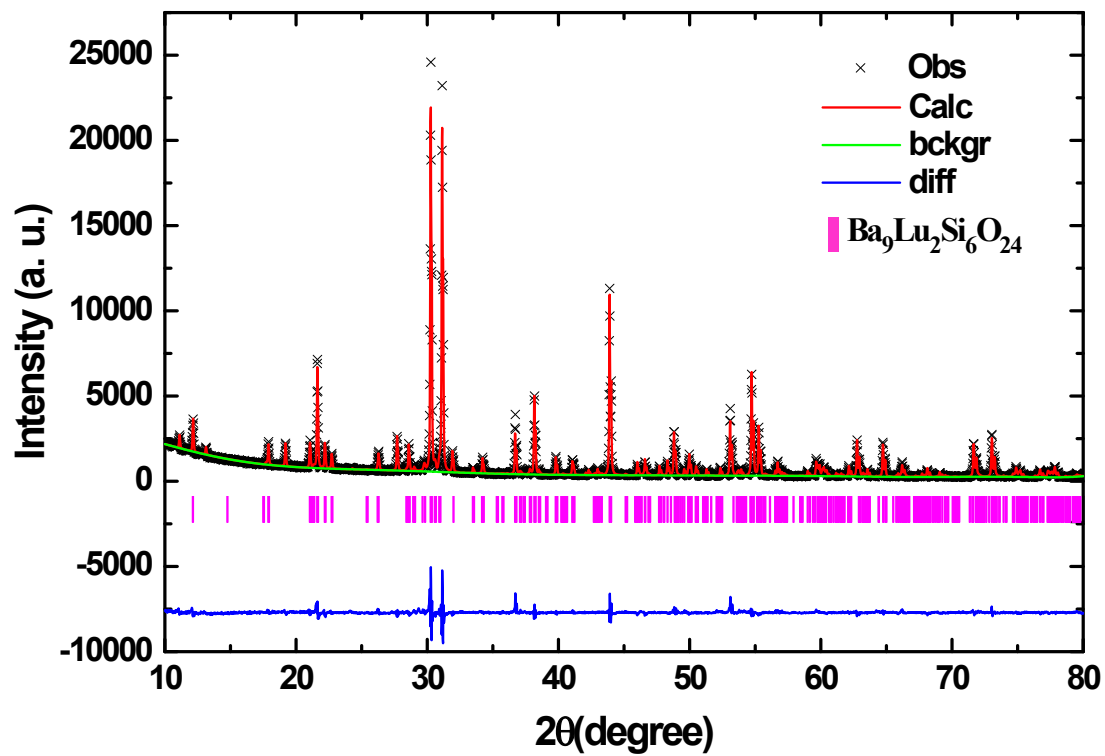


Figure S2 Rietveld refinement of BLS:5%Ce³⁺. Observed, calculated, background, difference and *hkl* of the XRD pattern are plotted in the same range. The pattern contains two phases: Ba₉Lu₂Si₆O₂₄ (magenta) and Ba₂SiO₄ (6246-ICSD, cyan).

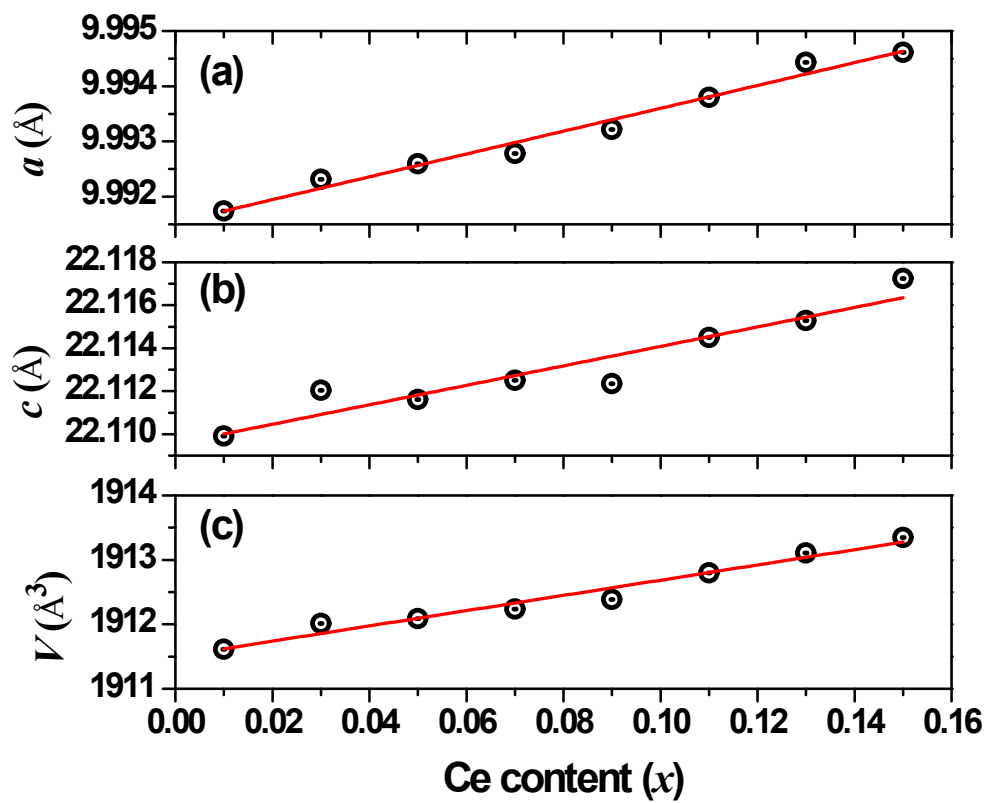


Figure S3 Refined lattice parameters a and c and unit cell volume V for BLS: $x\text{Ce}^{3+}$ ($x = 0.01-0.15$).

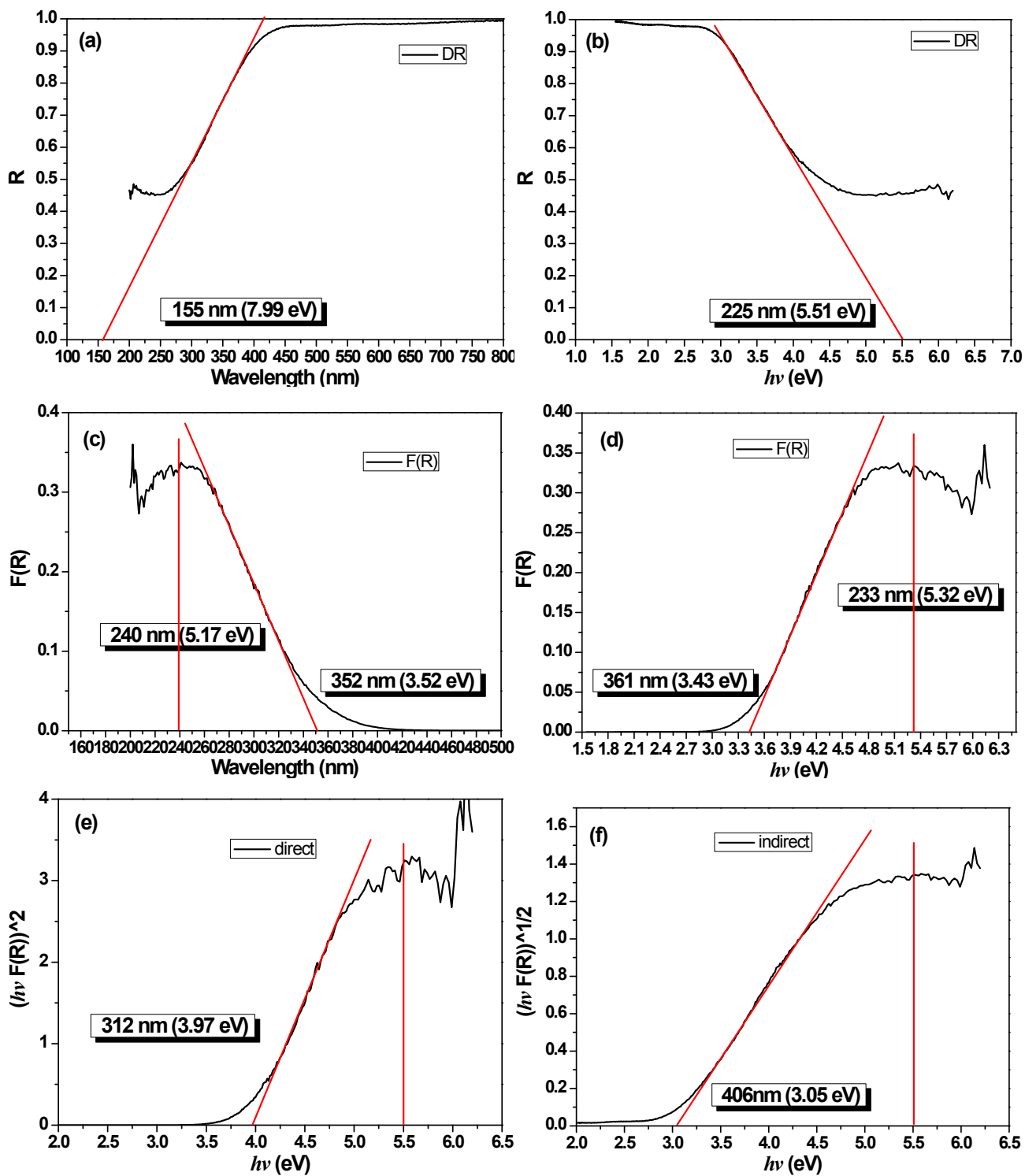


Figure S4 Optical band gap of the BLS host determined by extrapolating the DR curve (M-1) against wavelength (a) and against energy (b), the F(R) curve (M-2) against wavelength (c) and against energy (d), $(h\nu F(R))^2$ for a direct band gap (e) and $(h\nu F(R))^{1/2}$ for an indirect band gap (M-3).

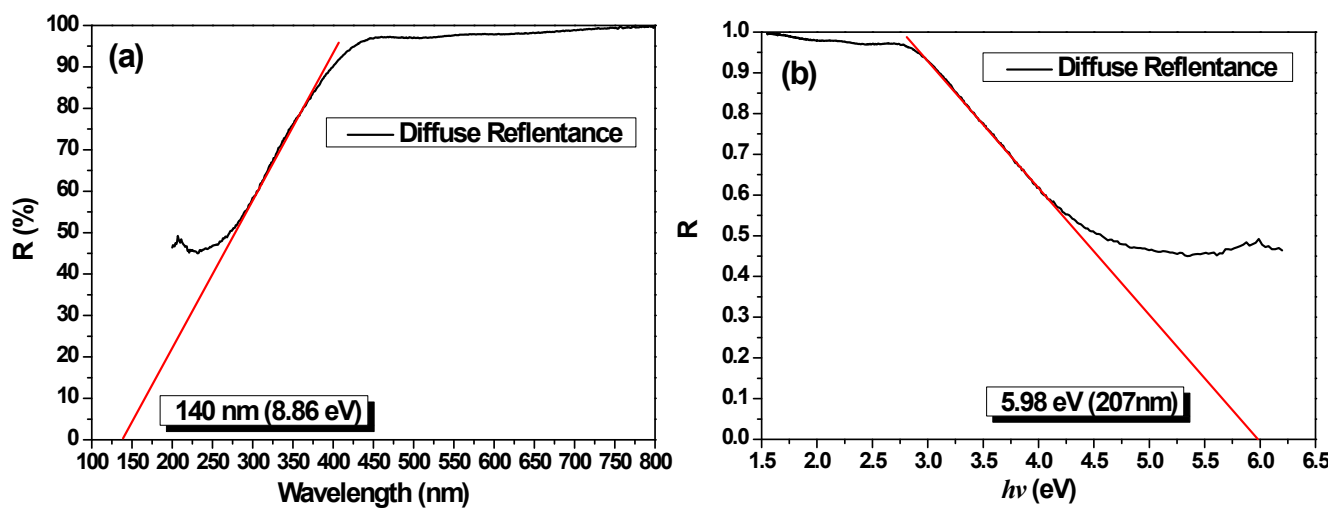


Figure S5 Optical band gap of the BYS host determined by extrapolating the R curve (M-1) against wavelength (a) and against energy (b).

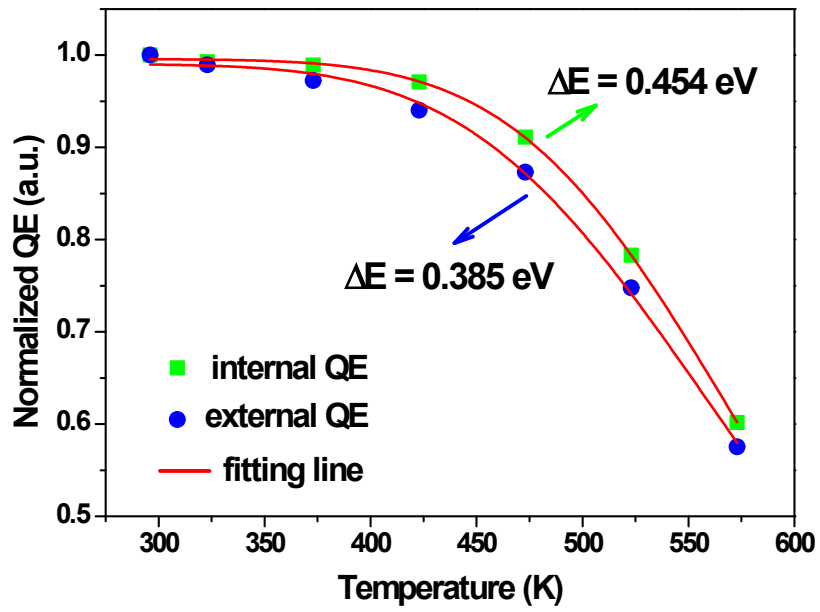


Figure S6 Temperature-dependent of normalized internal and external QEs for BLS:11%Ce³⁺ and fitting results by the Arrhenius equation.

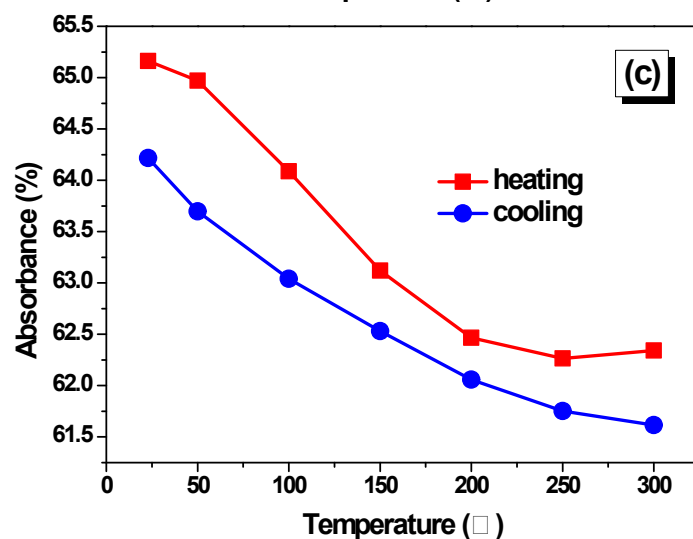
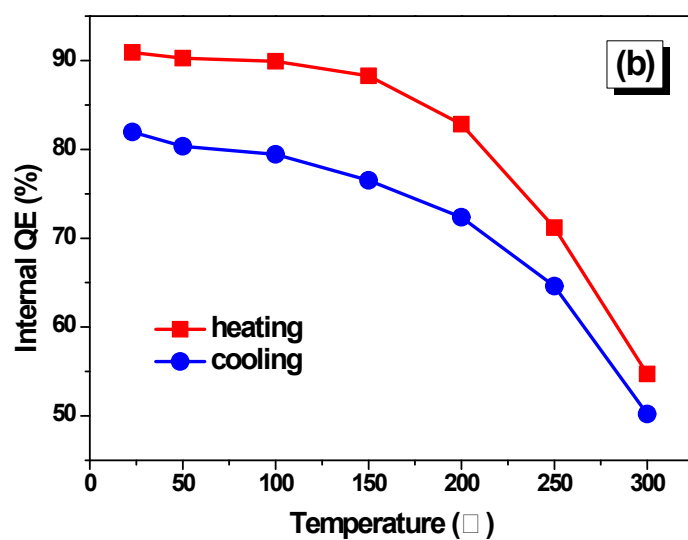
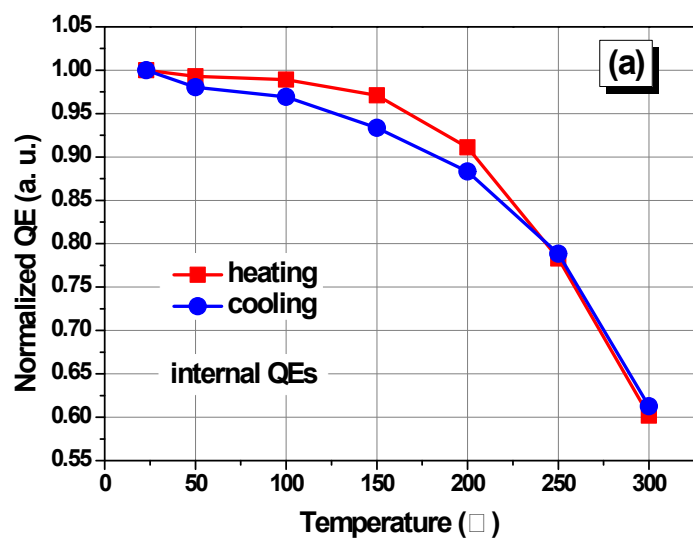


Figure S7 Temperature dependence of normalized internal QEs (a), internal QEs (b) and absorbance (c) for BLS:11%Ce³⁺.

Table S1 Rietveld refinement and Crystal data for Ba₉Lu_{2-x}Ce_xSi₆O₂₄ ($x = 0.01-0.15$).

x	a	c	V	R_{WP}	R_P	χ^2
$x = 0.01$	9.991742	22.109903	1911.613	7.87%	5.89%	5.104
$x = 0.03$	9.992314	22.112038	1912.016	10.4%	7.55%	8.682
$x = 0.05$	9.992594	22.111609	1912.086	7.74%	6.07%	4.416
$x = 0.07$	9.992785	22.112505	1912.236	9.05%	6.68%	6.658
$x = 0.09$	9.993217	22.112343	1912.388	9.23%	7.25%	6.268
$x = 0.11$	9.993797	22.114502	1912.797	10.9%	8.58%	8.946
$x = 0.13$	9.994432	22.115292	1913.108	10.8%	8.71%	9.958
$x = 0.15$	9.994613	22.117237	1913.346	11.4%	8.90%	8.961

Table S2 Atomic Parameters, x , y , z , occupancy, Uiso and Wyckoff position for Ba₉Lu₂Si₆O₂₄:5%Ce³⁺.

atom	x	y	z	Occupancy	Uiso*100	Wyckoff position
Ba1	0.00000(0)	0.00000(0)	0.00000(0)	1.0000	0.82(3)	3a
Ba2	0.33330(0)	0.66670(0)	0.00420(1)	1.0000	0.57(7)	6c
Ba3	0.03203(0)	0.67011(8)	0.10848(5)	1.0000	0.77(1)	18f
Lu	0.00000(0)	0.00000(0)	0.16383(5)	1.0000	2.53(1)	6c
Si	0.33854(5)	0.01357(8)	0.07356(3)	1.0000	2.86(4)	18f
O1	0.35161(6)	0.05826(1)	0.00330(7)	1.0000	6.72(6)	18f
O2	0.49420(1)	0.14148(0)	0.10621(8)	1.0000	2.04(4)	18f
O3	-0.03290(3)	0.16891(2)	0.10333(8)	1.0000	0.40(0)	18f
O4	0.16581(9)	0.47469(8)	0.09243(3)	1.0000	0.69(2)	18f

Table S3 Selected Bond Distances for Ba₉Lu₂Si₆O₂₄:5%Ce³⁺.

Bond	Distance (Å)	Bond	Distance (Å)
Ba1-O1 (6×)	3.298(4)	Ba3-O1	2.548(7)
Ba1-O3 (6×)	2.861(1)	Ba3-O2	2.981(6)
Ba2-O1 (3×)	2.893(4)	Ba3-O2	3.065(7)
Ba2-O2 (3×)	3.115(3)	Ba3-O2	3.086(8)
Ba2-O4 (3×)	2.776(6)	Ba3-O3	2.929(7)
Lu-O2	2.163(0)	Ba3-O3	3.038(3)
Lu-O3	2.225(7)	Ba3-O3	3.176(6)
Si-O1	1.589(1)	Ba3-O4	2.703(2)
Si-O2	1.671(3)	Ba3-O4	2.718(5)
Si-O3	1.653(6)	Ba3-O4	3.113(1)
Si-O4	1.629(1)		