Supporting Information

Luminescence of an Oxonitridoberyllate: A Study of Narrow-band Cyan Emitting $Sr[Be_6ON_4]:Eu^{2+}$

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Table S1. EDS results (atom%) via Point and ID on a $Sr[Be_6ON_4]$ single crystal with platelet-like morphology (Main Figure 1)

Scan #	Sr	N	O
1	19.39	60.98	19.63
2	19.38	61.51	19.1
3	19.41	60.74	19.85
4	19.13	61.4	19.47
5	18.86	61.02	20.12
6	19.31	61.07	19.63
Average	19.25	61.12	19.63
ratio	1	3.2	1.0

Table S2. Anisotropic displacement parameters ($Å^2$) of $Sr[Be_6ON_4]$[a]

Atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Sr	0.00998(7)	0.00950(6)	0.00843(6)	0	0.00106(8)	0
Be1	0.0068(5)	0.0081(5)	0.0091(5)	-0.0005(8)	-0.0002(7)	0.0003(4)
Be2	0.0098(7)	0.0067(6)	0.0073(6)	0.0000(5)	-0.0004(6)	-0.0008(5)
Be3	0.0072(6)	0.0083(6)	0.0070(6)	-0.0001(5)	0.0004(5)	0.0008(5)
O1	0.0061(4)	0.0119(4)	0.0089(4)	0	0.0005(6)	0
N1	0.0069(4)	0.0058(3)	0.0058(4)	-0.0005(3)	0.0001(3)	-0.0003(3)
N2	0.0071(4)	0.0058(4)	0.0059(3)	-0.0003(3)	0.0009(3)	0.0003(3)

[a] e.s.d.'s in parentheses

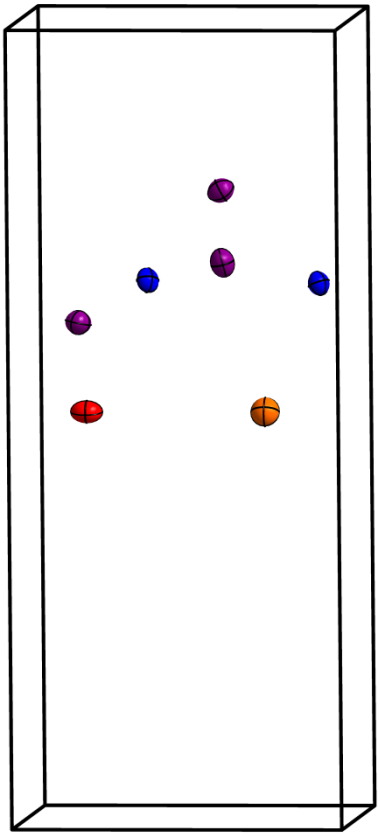

Figure S1: Presentation of the anisotropic refinement of the crystallographic positions in $Sr[Be_6ON_4]$; ellipsoids with 90% probability.

Table S3. Selected bond lengths and angles in $Sr[Be_6ON_4]$[a]

Bond name	Bond length / Å
Sr-O1 (2x)	2.6136(5)
Sr-O1 (1x)	2.6423(14)
Sr-N1 (2x)	2.7105(11)
Sr-N2 (2x)	2.9548(13)
Be1-O1 (1x)	1.5621(16)
Be1-N1 (1x)	1.783(3)
Be1-N2 (1x)	1.697(2)
Be1-N2 (1x)	1.866(2)
Be2-N1 (1x)	1.777(2)
Be2-N1 (1x)	1.913(2)
Be2-N2 (1x)	1.656(2)
Be2-N2 (1x)	1.741(2)
Be3-N1 (1x)	1.723(2)
Be3-N1 (1x)	1.761(2)
Be3-N2 (1x)	1.776(2)
Be3-N2 (1x)	1.718(2)
Angle names	**Angle / °**
O1-Sr-O1	72.70(3)
O1-Sr-N1	63.98(3)
O1-Be1-N2	114.36(12)
O1-Be1-N1	114.88(14)
N2-Be1-N1	101.37(12)
N2-Be2-N2	119.54(13)
N2-Be2-N1	122.36(12)
N2-Be2-N1	103.91(11)
N2-Be3-N1	123.15(13)
N2-Be3-N1	104.94(11)
N1-Be3-N1	107.65(11)

[a] e.s.d.'s in parentheses

Results of MAPLE calculations [kJ/mol] for $Sr[Be_6ON_4]$; Δ = MAPLE sum of constituting binary nitrides / MAPLE sum compound.[a]

Table S4. MAPLE calculations of $Sr[Be_6ON_4]$[a]

	$Sr[Be_6ON_4]$
Sr^{2+}	1602
Be^{2+}	2834-2858
O^{2-}	2537
N^{3-}	5533- 5536
Total	43371
Δ	0.33%
Total MAPLE: SrO + 2 Be_3N_2 = 43515 kJ/mol	

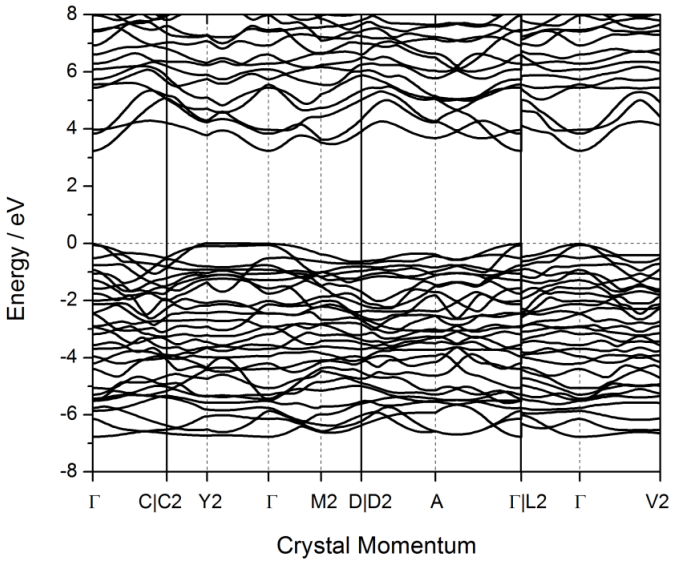

Figure S2: Band structure of $SrBe_6ON_4$ calculated using the PBEsol functional. The horizontal axis of the band structure corresponds to a path through high symmetry points in the Brillouin zone.[1]

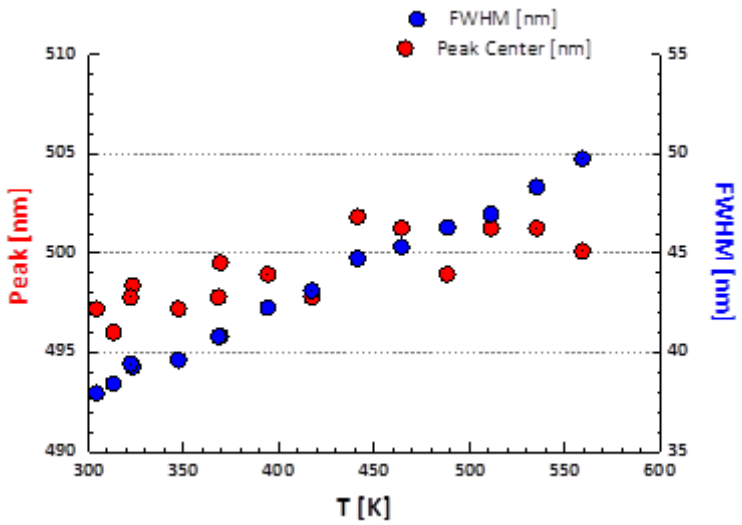

Figure S3: Temperature dependence of peak position and fwhm of $Sr[Be_6ON_4]:Eu^{2+}$ luminescence.

References

(1) Hinuma, Y.; Pizzi, G.; Kumagai, Y.; Oba, F.; Tanaka, I. Band structure diagram paths based on crystallography. *Computational Materials Science* **2017**, *128*, 140-184.