

Crystal structure and luminescence properties of the barium europium tetragermanate $\text{Ba}_2\text{Eu}_2\text{Ge}_4\text{O}_{13}$

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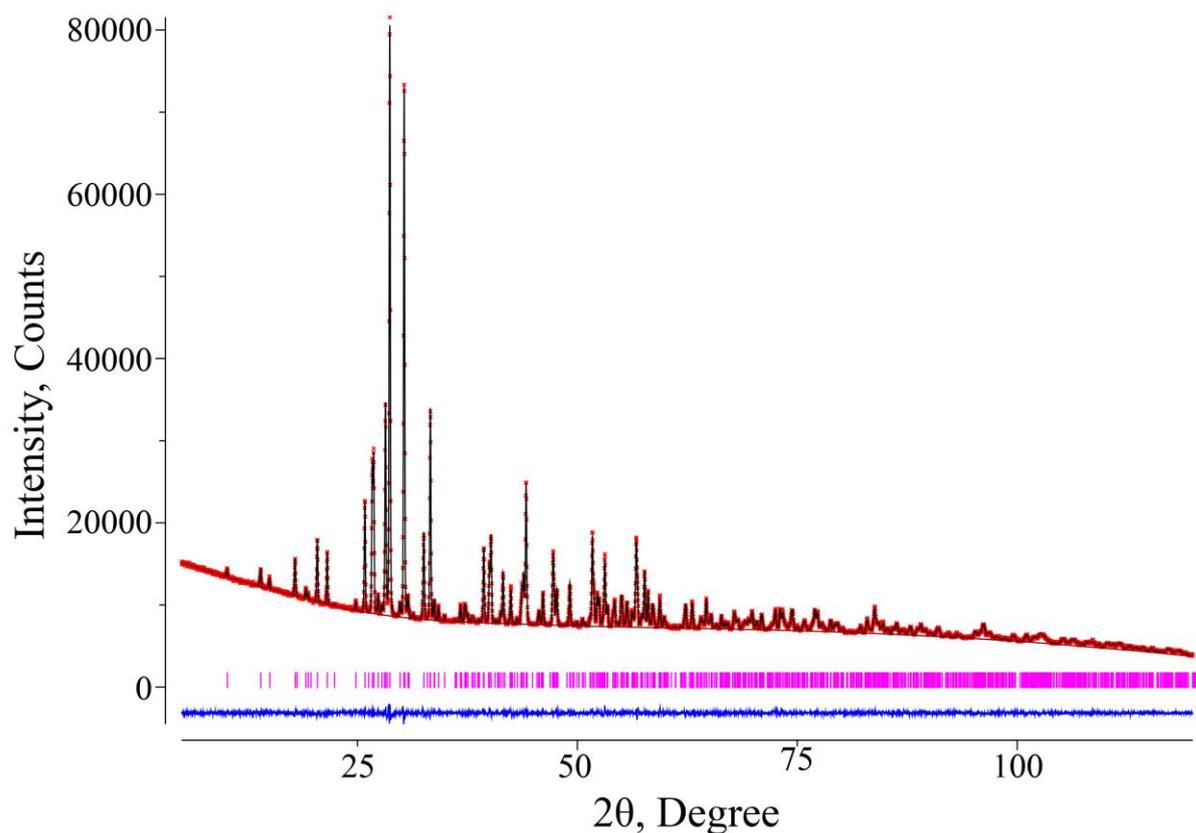


Figure S1 Experimental (crosses), calculated (solid line), and difference (bottom line) XRPD patterns for $\text{Ba}_2\text{Eu}_2\text{Ge}_4\text{O}_{13}$. Series of tick marks correspond to the Bragg reflection.

Table S1 Atom coordinates and thermal parameters (\AA^2) for $\text{Ba}_2\text{Eu}_2\text{Ge}_4\text{O}_{13}$.

Atom		x/a	y/b	z/c	Fraction	$U_{\text{iso}} \times 100$
Ba	8f	0.15677(8)	0.5035(4)	0.33266(6)	1.0	3.06(4)
Eu	8f	0.11467(9)	0.51012(34)	0.08656(5)	1.0	2.71(5)
Ge(1)	8f	0.06551(14)	0.0432(6)	0.18386(11)	1.0	2.98(8)
Ge(2)	8f	-0.12123(16)	-0.0308(6)	0.03864(12)	1.0	2.72(7)
O(1)	8f	0.0758(8)	-0.2831(18)	0.1885(6)	1.0	2.22(14)
O(2)	8f	0.1738(9)	0.2360(16)	0.1967(6)	1.0	2.22(14)
O(3)	4e	0	0.1747(25)	0.25	1.0	2.22(14)
O(4)	8f	-0.0199(8)	0.1769(16)	0.0967(6)	1.0	2.22(14)
O(5)	8f	-0.1615(8)	0.1071(16)	-0.0524(5)	1.0	2.22(14)
O(6)	8f	-0.2101(6)	-0.0539(19)	0.0964(4)	1.0	2.22(14)
O(7)	8f	-0.0667(7)	-0.3441(18)	0.0337(5)	1.0	2.22(14)

Table S2 Selected bond lengths (Å) and angles (°) for Ba₂Eu₂Ge₄O₁₃.

Bond lengths			
Ba-O(1)	2.782(10)	Eu-O(1)	2.314(10)
Ba-O(1)	3.187(10)	Eu-O(2)	2.429(10)
Ba-O(2)	2.899(10)	Eu-O(4)	2.556(10)
Ba-O(2)	2.719(11)	Eu-O(5)	2.279(8)
Ba-O(3)	2.823(8)	Eu-O(6)	2.285(8)
Ba-O(4)	3.020(10)	Eu-O(7)	2.448(10)
Ba-O(5)	2.780(10)	Eu-O(7)	2.274(9)
Ba-O(6)	3.263(10)	Average value	2.369
Ba-O(6)	2.706(10)	Expected value ^a	2.387
Ba-O(7)	3.057(9)		
Average value	2.924		
Expected value ^a	2.898		
Ge(1)-O(1)	1.761(10)	Ge(2)-O(4)	1.838(9)
Ge(1)-O(2)	1.725(10)	Ge(2)-O(5)	1.751(9)
Ge(1)-O(3)	1.787(5)	Ge(2)-O(6)	1.758(7)
Ge(1)-O(4)	1.820(9)	Ge(2)-O(7)	1.842(10)
Average value	1.773	Average value	1.797
Expected value ^a	1.760	Expected value ^a	1.760
Angles			
O(1)-Ge(1)-O(2)	122.9(6)	O(4)-Ge(2)-O(5)	105.7(4)
O(1)-Ge(1)-O(3)	114.1(6)	O(4)-Ge(2)-O(6)	101.4(4)
O(1)-Ge(1)-O(4)	117.2(5)	O(4)-Ge(2)-O(7)	110.6(4)
O(2)-Ge(1)-O(3)	101.3(5)	O(5)-Ge(2)-O(6)	120.0(4)
O(2)-Ge(1)-O(4)	100.2(5)	O(5)-Ge(2)-O(7)	111.6(4)
O(3)-Ge(1)-O(4)	97.1(4)	O(6)-Ge(2)-O(7)	106.8(5)

^aThe expected values of bond lengths are calculated as a sum of crystal radii: Ba⁺² X – 1.66 Å, Eu⁺³ VII – 1.15 Å, Ge⁺⁴ IV – 0.530 Å, O⁻² III – 1.22, O⁻² IV – 1.24 Å

[R. D. Shannon, *Acta Crystallogr.*, 1976, **A32**, 751.].