

Supporting Information

**Electronic structure and photo/cathodoluminescence properties
investigation of a green emission phosphor NaBaScSi₂O₇:Eu²⁺ with
high thermal stability**

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Table S1 The effective ionic radii of Na, Ba²⁺ and Eu²⁺ ions with different coordination numbers

| | Na ⁺ (Å) | Ba ²⁺ (Å) | Eu ²⁺ (Å) |
|----------------|---------------------|----------------------|----------------------|
| 8 coordination | 1.18 | 1.42 | 1.25 |
| 9 coordination | 1.24 | 1.47 | 1.30 |

Table S2 The fitting parameters of the decay curves of NaBaScSi₂O₇:0.001Eu²⁺ excited at 300 nm and monitored at 427 and 505 nm.

| | τ_1 (s) | τ_2 (s) | A ₁ | A ₂ |
|--|--------------|--------------|----------------|----------------|
| $\lambda_{\text{ex}}=300 \text{ nm}, \lambda_{\text{em}}=427 \text{ nm}$ | 6.114E-007 | 2.170E-007 | 1041.652 | 268.818 |
| $\lambda_{\text{ex}}=300 \text{ nm}, \lambda_{\text{em}}=505 \text{ nm}$ | 8.976E-007 | 1.000E-006 | 1835.441 | -534.731 |

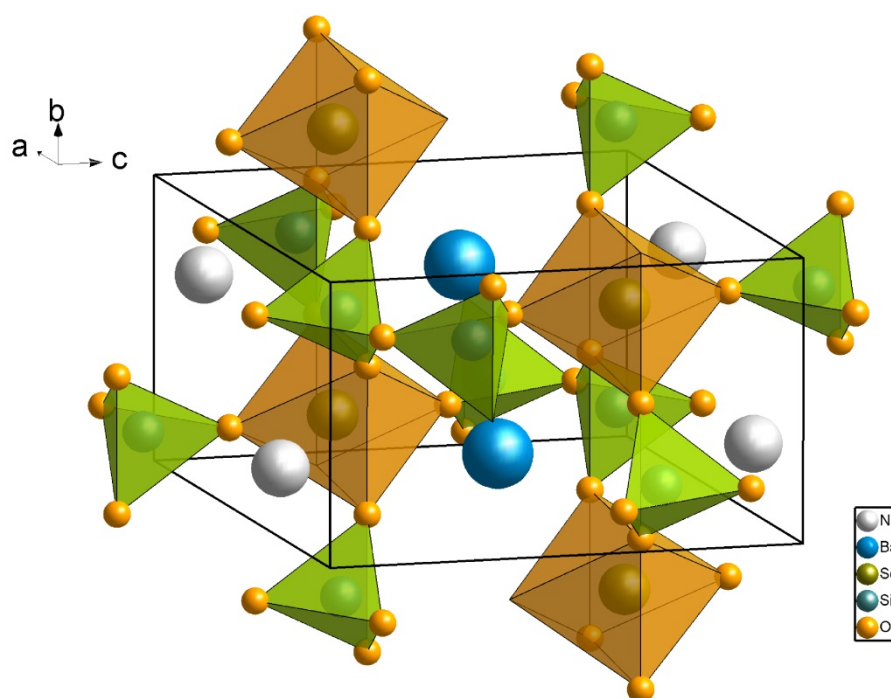


Figure S1 The crystal structure diagram of monoclinic NaBaScSi₂O₇