Identification of the Crystallographic Sites of Eu^{2+} in $Ca_9NaMg(PO_4)_7$: Structure and Luminescence Properties Study

Zhiguo Xia[*,a], Haikun Liu[a], Xia Li[b], Chengying Liu[a]

[a]*School of Materials Sciences and Technology, China University of Geosciences, Beijing 100083, China*

[b]*College of Materials Science and Engineering, Qingdao University of Science and Technology, Qingdao 266042, People's Republic of China*

Supporting Information

Table S1. *Selected interatomic bond distances[a)] of $Ca_9NaMg(PO_4)_7$:0.03Eu^{2+} phosphors.*

Ca1—O8^{i}	2.32 (2)	Ca3—O8^{iv}	2.53 (2)
Ca1—O10^{ii}	2.344 (18)	Ca3—O1	2.539 (7)
Ca1—O2^{iii}	2.440 (12)	Ca3—O10^{xiii}	2.558 (15)
Ca1—O5^{iv}	2.499 (17)	Ca3—O3^{xiv}	2.569 (13)
Ca1—O6^{i}	2.504 (17)	Na—O3^{xvi} ×3	2.353 (13)
Ca1—O7^{v}	2.51 (2)	Na—O2^{xv} ×3	2.83 (2)
Ca1—O6^{v}	2.506 (15)	Mg—O6^{xvii} ×3	2.058 (17)
Ca1—O4^{i}	2.850 (16)	Mg—O9^{xvi} ×3	2.166 (17)
Ca2—O5^{vi}	2.334 (18)	P1—O1	1.47 (2)
Ca2—O9^{vii}	2.343 (13)	P1—O2^{xv} ×3	1.555 (12)
Ca2—O2^{viii}	2.355 (12)	P2—O3	1.510 (19)
Ca2—O9^{ix}	2.478 (16)	P2—O4	1.520 (19)
Ca2—O4^{ix}	2.49 (2)	P2—O6	1.524 (9)
Ca2—O7^{vii}	2.548 (17)	P2—O5^{xviii}	1.580 (17)
Ca2—O3	2.548 (18)	P3—O7	1.504 (18)
Ca2—O8^{ix}	2.816 (16)	P3—O9	1.520 (13)
Ca3—O5^{x}	2.425 (19)	P3—O10^{xix}	1.559 (19)
Ca3—O7^{xi}	2.428 (19)	P3—O8	1.560 (15)

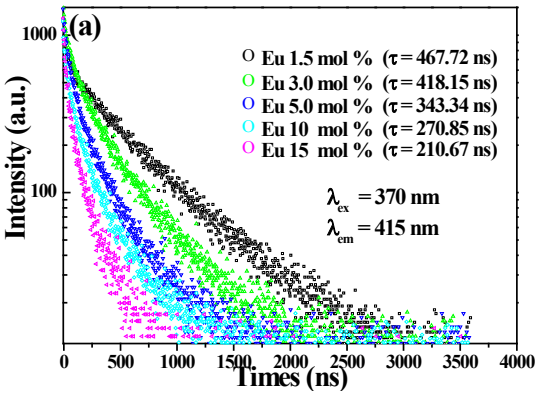
Ca3—O10^{xii}	2.439 (10)		
Ca3—O4^{vii}	2.456 (15)		

[a)]Bond distances were verified at 10^{-10} m (Å).

Symmetry codes: (i) -*x*+*y*+2/3, -*x*+4/3, *z*+1/3; (ii) *x*, *x*-*y*+1, *z*-1/2; (iii) -*y*+4/3, -*x*+2/3, *z*+1/6; (iv) -*y*+2/3, *x*-*y*+1/3, *z*+1/3; (v) -*y*+5/3, *x*-*y*+4/3, *z*+1/3; (vi) -*x*+*y*+4/3, *y*+2/3, *z*+1/6; (vii) -*x*+*y*+1/3, *y*-1/3, *z*+1/6; (viii) -*x*+*y*, -*x*+1, *z*; (ix) -*y*+4/3, -*x*+5/3, *z*+1/6; (x) *x*-2/3, *x*-*y*-1/3, *z*+1/6; (xi) *x*-1/3, *y*-2/3, *z*+1/3; (xii) -*y*+2/3, *x*-*y*+1/3, *z*-2/3; (xiii) *x*-1/3, *y*-2/3, *z*-2/3; (xiv) *x*-2/3, *x*-*y*+2/3, *z*+1/6; (xv) -*y*+1, *x*-*y*+1, *z*; (xvi) -*y*+1, *x*-*y*, *z*; (xvii) -*x*+*y*-1/3, *y*-2/3, *z*-1/6; (xviii) *x*, *y*+1, *z*; (xix) *x*, *y*, *z*-1.

Table S2. Lifetime for non-linear fitting components of $Ca_9NaMg(PO_4)_7$:*x*Eu^{2+} (*x* = 0.01 – 0.15) phosphors excited at 370 nm with the emission monitored at 415 nm, 458 nm, and 625 nm.

Lifetime	*x* = 0.01	*x* = 0.03	*x* = 0.05	*x* = 0.10	*x* = 0.15
τ at 415 nm (ns)	467.72	418.15	343.34	270.85	210.67
τ at 458 nm (ns)	483.21	457.23	386.18	285.56	242.30
τ at 625 nm (ns)	995.70	866.68	759.10	616.78	521.59



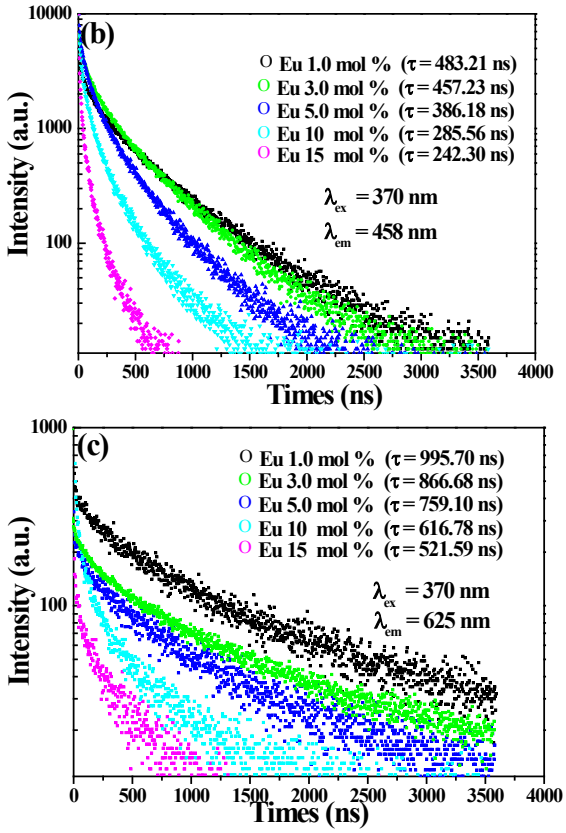


Figure S1. Decay curves of Eu^{2+} emission in $Ca_9NaMg(PO_4)_7$: xEu^{2+} phosphors under excitation at 370 nm with different monitoring wavelengths are shown in (a) λ_{em}= 415 nm, (b) λ_{em}= 458 nm, and (c) λ_{em}= 625 nm, respectively.

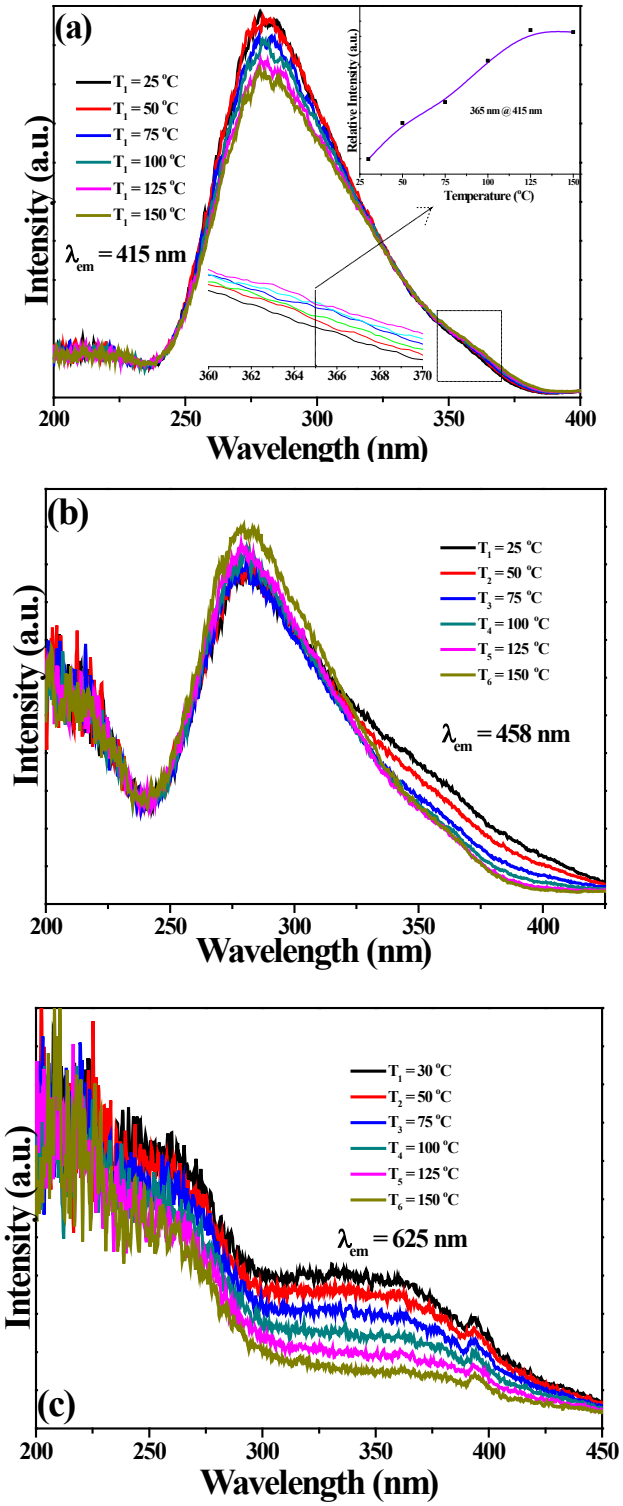


Figure S2. The PLE spectra of $Ca_{8.97}NaMg(PO_4)_7$:0.03Eu^{2+} phosphor with different excitation wavelengths under different temperatures in the range of 30–150 °C are shown in (a) λ_{em}= 415 nm, (b) λ_{em}= 458 nm, and (c) λ_{em}= 625 nm, respectively.