Electronic supplementary information to

Red-emission over a wide range of wavelength at various temperatures from tetragonal $BaCN_2$:Eu^{2+}

Yuji Masubuchi[a]*, Sayaka Nishitani[b], Akira Hosono[b], Yuuki Kitagawa[c], Jumpei Ueda[c], Setsuhisa Tanabe[c], Hisanori Yamane[d], Mikio Higuchi[a], Shinichi Kikkawa[a]

[a]Faculty of Engineering, Hokkaido University, N13 W8, Kita-ku, Sapporo 060-8628, Japan

[b]Graduate School of Chemical Science and Engineering, Hokkaido University, N13 W8, Kita-ku, Sapporo 060-8628, Japan

[c]Graduate School of Human and Environmental Studies, Kyoto University, Yoshida-nihonmatsu-cho, Sakyo-ku, Kyoto 606-8501, Japan

[d]Institute of Multidisciplinary Research for Advanced Materials, Tohoku University, 2-1-1 Katahira, Aoba-ku, Sendai, 980-8577, Japan

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*Corresponding author: Faculty of Engineering, Hokkaido University, N13 W8, Kita-ku, Sapporo 060-8628, Japan
E-mail: yuji-mas@eng.hokudai.ac.jp

Reference:

S1) U. Berger, and W. Schnick, Synthesis, crystal structures, and vibrational spectroscopic properties of $MgCN_2$, $SrCN_2$, and $BaCN_2$. *J. Alloys Compd.,* 1994, **206**, 179-184.

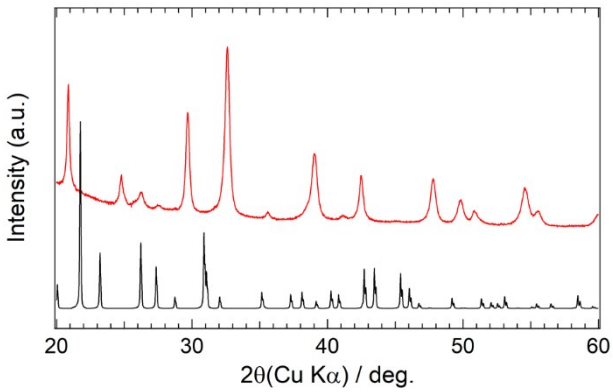

Figure S1 The powder XRD pattern of the nitrided product (red line) and the pattern calculated using the structural parameters reported by W. Schnick[S1] (black line).

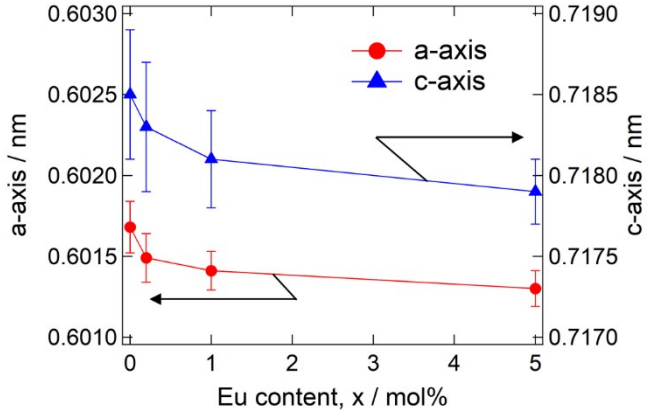

Figure S2 The Lattice parameters the tetragonal $BaCN_2$:Eu^{2+} depending on the Eu contents.

Reference:

S1) U. Berger, and W. Schnick, Synthesis, crystal structures, and vibrational spectroscopic properties of $MgCN_2$, $SrCN_2$, and $BaCN_2$. *J. Alloys Compd.,* 1994, **206**, 179-184.

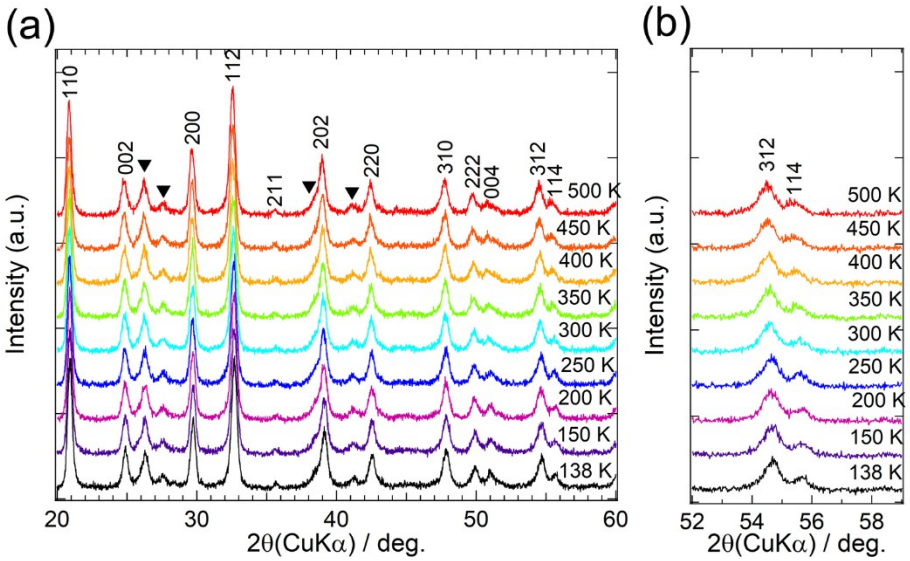

Figure S3 Temperature dependence of powder XRD patterns for $BaCN_2$:Eu. Black triangles indicate diffraction lines attributed to an impurity phase.

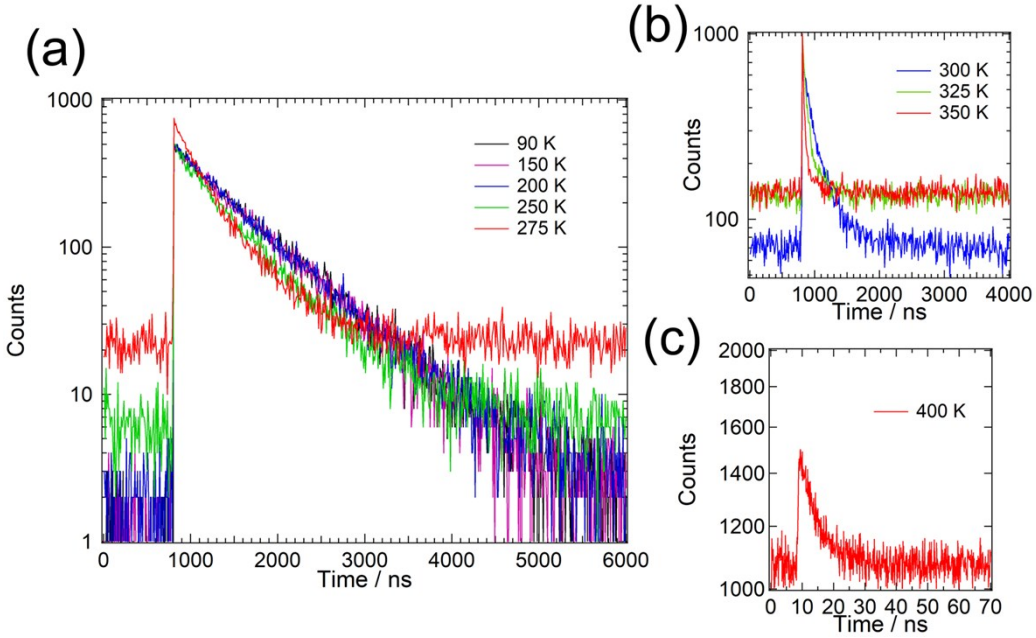

Figure S4 Luminescence decay curves monitoring 650 nm emission of $BaCN_2$:Eu at different temperatures. All decay curves were fitted using a single exponential function as mentioned in Experimental Section.

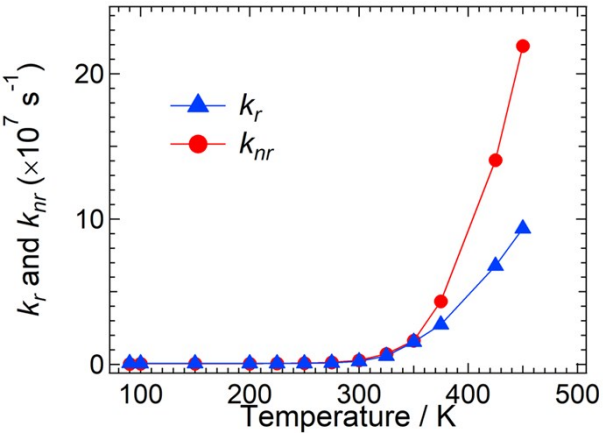

Figure S5 Radiative rate constant (k_r) and nonradiative rate constant (k_{nr}) at different temperatures calculated using both the lifetime (τ) and the estimated quantum efficiency (QE). The QE values at different temperatures were estimated from the integrated emission intensity ratio shown in Fig. 5b and the QE value at room temperature (42%).

The QE and τ are expressed as

$$QE = \frac{k_r}{k_r + k_{nr}} \qquad (S1)$$

and

$$\tau = \frac{1}{k_r + k_{nr}} \qquad (S2)$$

From equations S1 and S2, we calculated k_r and k_{nr} values at each temperature.

Table S1 Crystal data and refinement result for $BaCN_2$ at 90 K

Chemical formula	$BaCN_2$
Formula weight, M_r (g mol^{-1})	177.37
Crystal form, color	Plate, Translucent colorless
Crystal size, mm^3	0.075×0.062×0.014
Radiation wavelength, λ (nm)	0.071073
Temperature, T (K)	90
Crystal system	Tetragonal
Space group	*I*4/*mcm* (No. 140)
Unit-cell dimensions, a (nm)	0.60028(2)
c (nm)	0.71519(3)
Unit-cell volume, V (nm^3)	0.25771(2)
Z	4
Calculated density, D_{cal} (Mg m^{-3})	4.572
Absorption coefficient, μ (mm-1)	15.057
Absorption correction	MULTI-SCAN (TWINABS)[S2]
Limiting Indices	$-5 \le h \le 5$
	$-7 \le k \le 7$
	$-9 \le l \le 9$
Number of reflections	228
Weight parameters, *a, b*	0.0066, 7.6297
Goodness-of-fit on F^2, S	1.195
$R1,\omega R2(I > 2\sigma(I))$	0.0257, 0.0493
$R1,\omega R2$(all data)	0.0332, 0.0517

$R1 = \Sigma||F_O|-|F_C||/\Sigma|F_O|$. $\omega R2 = [\Sigma\omega(F_O^2 - F_C^2)^2/\Sigma(\omega F_O^2)^2]^{1/2}$, $\omega = 1/[\sigma^2(F_O^2)+(aP)^2 + bP]$, where F_O is the observed structure factor, F_C is the calculated structure factor, σ is the standard derivation of F_C^2, and $P=(F_O^2+2F_C^2)/3$. $S=[\Sigma\omega(F_O^2-F_C^2)^2/(n-p)]^{1/2}$, where n is the number of reflections and p is the total number of parameters refined.

Reference:

S2) TWINABS (version 2012/1). Bruker AXS Inc., Madison, Wisconsin (USA) 2012.

Table 2 Atomic coordinates for $BaCN_2$ at 90 K.

Atom	Site	Occ.	*x*	*y*	*z*	U_{iso}
Ba	4*a*	1	0	0	0.25	0.0060(3)
C	4*d*	1	0.5	0	0	0.006(3)
N	8*h*	1	0.3548(14)	0.1452(14)	0	0.006(2)

U_{iso} / $\times 10^{-2}$ nm^2 (= Å^2)