

## Electronic Supplementary Information (ESI) for

# **Pb[NC<sub>5</sub>H<sub>3</sub>(CO<sub>2</sub>)<sub>2</sub>]: A white light emitting single component coordination polymer revealing high quantum efficiency and thermal stability**

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## Section S1. Materials and Methods

**Materials.**  $\text{Pb}(\text{NO}_3)_2$  (99%, Daejung) and 2,6-PDC (98%, Alfa Aesar) were purchased and used without further purification.

**Synthesis of  $\text{Pb}[\text{NC}_5\text{H}_3(\text{CO}_2)_2]$ .** Single crystals of  $\text{Pb}[\text{NC}_5\text{H}_3(\text{CO}_2)_2]$  were grown through a hydrothermal reaction. 0.033 g (0.1 mmol) of  $\text{Pb}(\text{NO}_3)_2$ , 0.050 g (0.3 mmol) of 2,6-PDC, and 5 mL of deionized water were mixed. The reaction mixture was vigorously stirred for 20 min at room temperature to obtain a homogeneous solution and quickly transferred into a 23 mL Teflon-lined stainless-steel autoclave. The autoclave was subsequently sealed and heated to 180 °C for 72 h under autogenous pressure, before being cooled to room temperature at a rate of 6 °C h<sup>-1</sup>. After cooling, the crystallized product was filtered, washed with deionized water, and naturally dried overnight. Colorless rod-like crystals of  $\text{Pb}[\text{NC}_5\text{H}_3(\text{CO}_2)_2]$  were obtained in 65% yield based on  $\text{Pb}(\text{NO}_3)_2$ .

**Instrumentation.** Single crystal X-ray diffraction (SCXRD) was used to determine the structure of the synthesized  $\text{Pb}[\text{NC}_5\text{H}_3(\text{CO}_2)_2]$ . SCXRD measurements for the title compound was carried out on a Bruker BREEZE diffractometer with a 1K CCD area-detector and monochromated Mo-K $\alpha$  radiation ( $\lambda = 0.71073$  Å) at room temperature. The data reduction was performed using the Bruker SAINT program.<sup>1</sup> A colorless rod crystal of dimension,  $0.034 \times 0.038 \times 0.298$  mm<sup>3</sup> for  $\text{Pb}[\text{NC}_5\text{H}_3(\text{CO}_2)_2]$  was selected and mounted onto the end of a thin glass fiber for data collection with a narrow-frame method (an exposure time of 10 s frame<sup>-1</sup>; scan widths of 0.30° in  $\omega$ ). The obtained data were solved using the Direct method with SHELXS-97 and refined by full-matrix least-squares techniques based on  $F^2$  using SHELXL-97 within WinGX-98 crystallographic software package.<sup>2-4</sup> All atoms except for hydrogen atoms were refined with anisotropic displacement parameters and converged for  $I > 2\sigma(I)$ . Relevant crystallographic data and selected bond distances obtained from the single crystal structure refinements are tabulated in Tables S1 and S2, respectively.

**Table S1.** Crystallographic Data for  $\text{Pb}[\text{NC}_5\text{H}_3(\text{CO}_2)_2]$

formula	$\text{C}_7\text{H}_3\text{NO}_4\text{Pb}$
fw	372.29
Space group	$P2_1/n$ (No. 14)
$a$ (Å)	9.8218(2)
$b$ (Å)	5.54270(10)
$c$ (Å)	14.3601(4)
$\beta$ (°)	104.993(10)
$V$ (Å <sup>3</sup> )	755.14(3)
$Z$	4
$T$ (K)	296.0(2)
$\rho_{\text{calcd}}$ (g·cm <sup>-3</sup> )	3.274
$\lambda$ (Å)	0.71073
$R(F)^a$	0.0240
$R_w(F_o^2)^b$	0.0663

$$^a R(F) = \sum ||F_o| - |F_c|| / \sum |F_o|. \quad ^b R_w(F_o^2) = [\sum w(F_o^2 - F_c^2)^2 / \sum w(F_o^2)^2]^{1/2}.$$

**Table S2.** Selected Bond Distances (Å) for Pb[NC<sub>5</sub>H<sub>3</sub>(CO<sub>2</sub>)<sub>2</sub>]

C1–N1	1.343(6)	C7–O3	1.236(6)
C1–C2	1.388(7)	C7–O4	1.265(7)
C1–C6	1.504(7)	Pb1–N1	2.483(4)
C2–C3	1.385(8)	Pb1–O1	2.504(4)
C3–C4	1.381(9)	Pb1–O1	2.646(4)
C4–C5	1.380(8)	Pb1–O2	2.702(4)
C5–N1	1.340(6)	Pb1–O4	2.403(4)
C5–C7	1.520(8)		
C6–O1	1.272(6)		
C6–O2	1.241(6)		

Powder X-ray diffraction (PXRD) patterns were collected on a Bruker D8-Advance powder diffractometer with 40 kV and 40 mA for Cu-K $\alpha$  ( $\lambda = 1.5418 \text{ \AA}$ ) at room temperature. The well-ground polycrystalline sample of Pb[NC<sub>5</sub>H<sub>3</sub>(CO<sub>2</sub>)<sub>2</sub>] was mounted on a glass sample holder and scanned in the  $2\theta$  range 5–70° with a step time of 1 s and a step size of 0.02°. The PXRD pattern on the ground crystals revealed that the material was highly crystalline and in good agreement with the generated pattern from the single crystal data (see Fig. S1).

Infrared (IR) spectrum for Pb[NC<sub>5</sub>H<sub>3</sub>(CO<sub>2</sub>)<sub>2</sub>] was performed on a Thermo Scientific Nicolet 6700 spectrometer in the spectral range 400–4000 cm<sup>-1</sup> with a resolution of 4 cm<sup>-1</sup> using KBr disk. IR data (cm<sup>-1</sup>): 3098 w, 3078 w, 1616 w, 1557 s, 1456 w, 1416 s, 1376 s, 1346 s, 1265 s, 1180 m, 1144 w, 1164 m, 1014 m, 912 s, 862 m, 812 m, 761 s, 721 s, 691 m, 661 m, 570 w, 510 m, 410 s.

UV–vis diffuse reflectance spectrum (UV–vis DRS) was recorded on a Varian Cary 500 scan UV–vis–NIR spectrophotometer over the range of 200–2500 nm at room temperature. The BaSO<sub>4</sub> plate was used as a standard (100% reflectance). The raw data were converted from reflection to absorbance by the use of the Kubelka-Munk function.<sup>5, 6</sup>

Thermogravimetric analysis (TGA) for the title compound was performed using a SCINCO TGA-N 1000 thermal analyzer. The ground sample was loaded in an alumina crucible and heated from room temperature to 900 °C at a rate of 10 °C min<sup>-1</sup> under flowing argon gas.

Elemental analysis (EA) for C, H, and N was carried out by a Carlo Erba EA1108 CHNS-O analyzer at the Organic Chemistry Research Center, Sogang University. Elemental microanalysis for Pb[NC<sub>5</sub>H<sub>3</sub>(CO<sub>2</sub>)<sub>2</sub>] obs. (calc.): C, 22.59% (22.58%); H, 0.81% (0.88%); N, 3.76% (3.70%).

Energy dispersive X-ray spectroscopy (EDX) was performed to further analyze the morphology and chemical composition, using a Horiba Energy EX-250 scanning electron microscopy (SEM) instrument attached to a Hitachi S-3400N. EDX data for Pb[NC<sub>5</sub>H<sub>3</sub>(CO<sub>2</sub>)<sub>2</sub>] exhibit approximate C:H:N:O:Pb ratios of 7:3:1:4:1. Quantitative EDX analysis data for the reported material were consistent with the refined formula from the single crystal structure refinements.

The excitation and emission spectra of Pb[NC<sub>5</sub>H<sub>3</sub>(CO<sub>2</sub>)<sub>2</sub>] were systematically recorded using a photomultiplier tube with a xenon lamp at 10, 77, and 300 K, respectively. The maximum in the excitation spectrum was used to generate the emission spectrum. Moreover, room temperature quantum yields of solid samples were measured with a Jobin Yvon fluorescence spectrometer having an additional Ulbricht sphere. The photoluminescence decay curves for Pb[NC<sub>5</sub>H<sub>3</sub>(CO<sub>2</sub>)<sub>2</sub>] were also measured at room temperature by using an in-house photoluminescence system that includes an Nd:YAG laser, a cutoff filter, and a

CCD sensor. The Commission International de l'Eclairage (CIE) in 1931 chromaticity coordinate was calculated to illuminate the fluorescent region for the title material.

### References

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Fig. S1. Calculated and experimental powder X-ray diffraction patterns of  $\text{Pb}[\text{NC}_5\text{H}_3(\text{CO}_2)_2]$

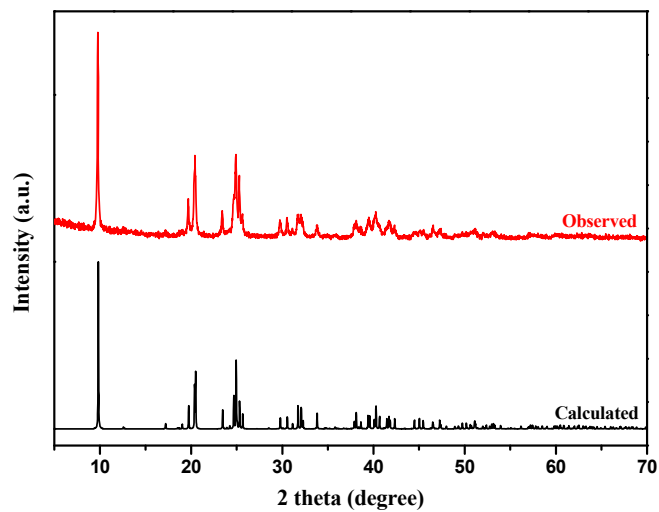


Fig. S2. Infrared spectrum of  $\text{Pb}[\text{NC}_5\text{H}_3(\text{CO}_2)_2]$

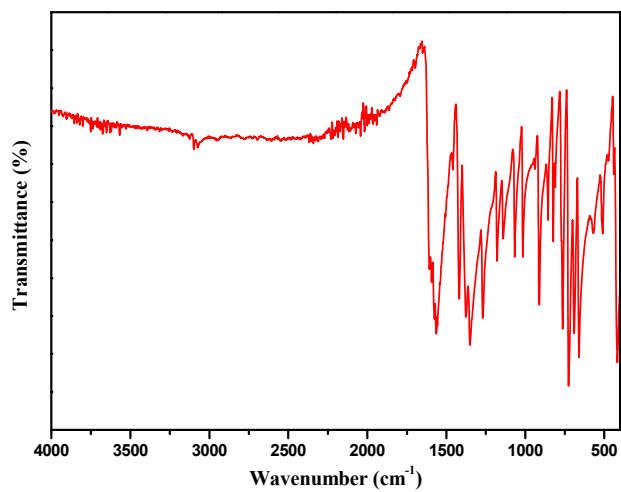


Fig. S3. Energy dispersive X-ray spectral data for  $\text{Pb}[\text{NC}_5\text{H}_3(\text{CO}_2)_2]$

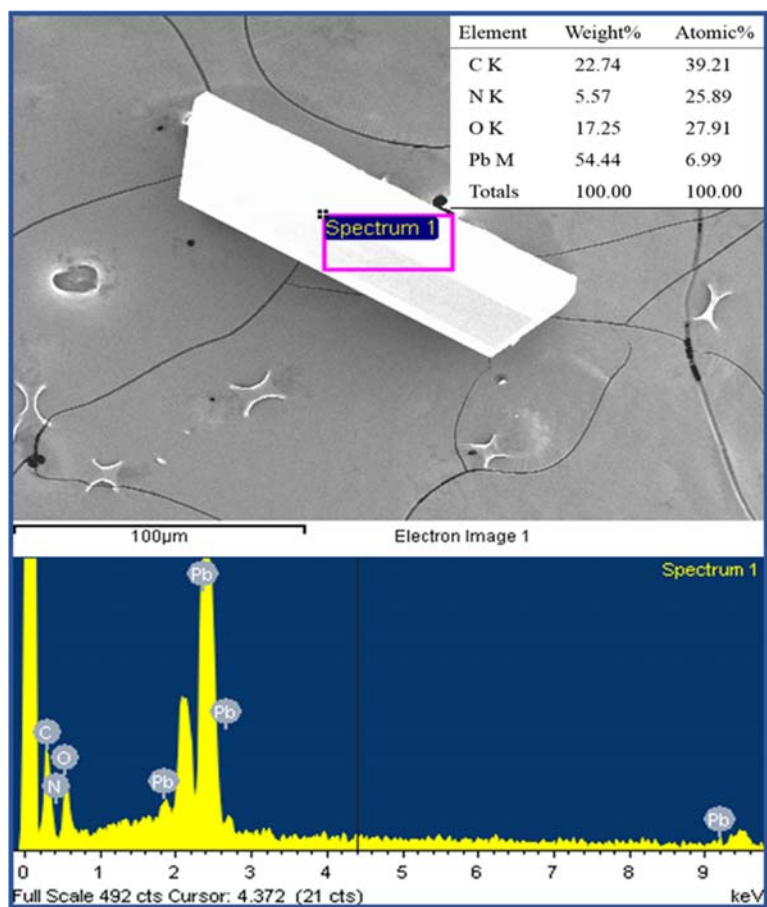


Fig. S4. UV-vis diffuse reflectance spectrum of  $\text{Pb}[\text{NC}_5\text{H}_3(\text{CO}_2)_2]$

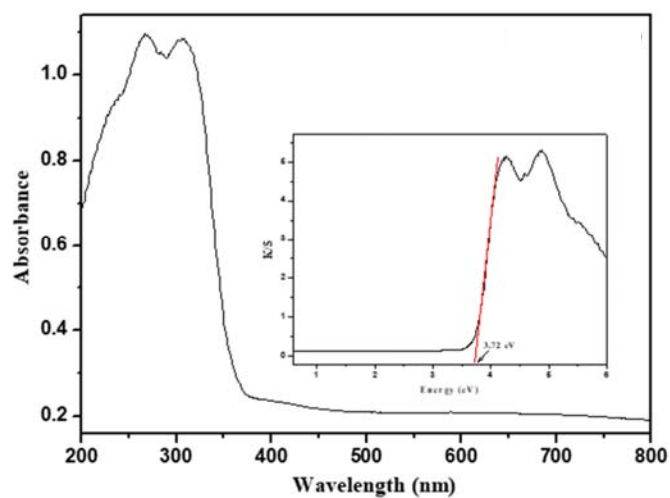


Fig. S5. Emission spectra of  $\text{Pb}[\text{NC}_5\text{H}_3(\text{CO}_2)_2]$  at various temperatures.

