

Supporting Information

An Emitting Hofmann-type Compound: An Evidence for Interlayer Auophilic Interactions

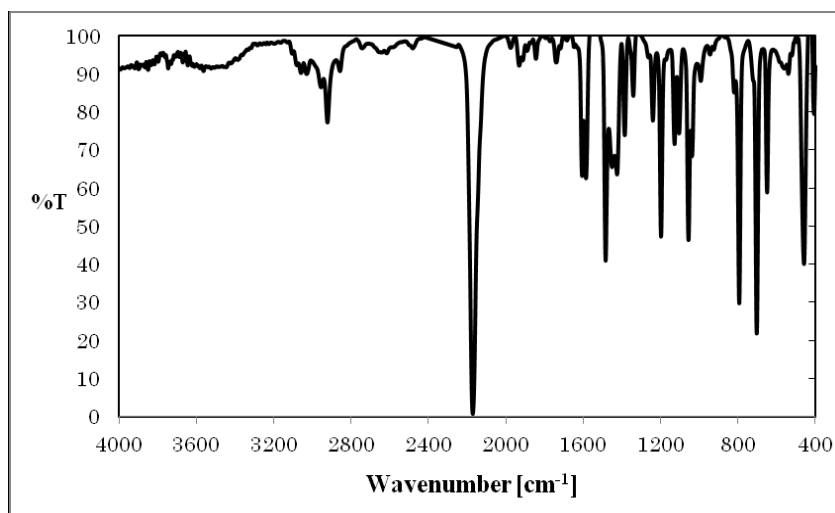
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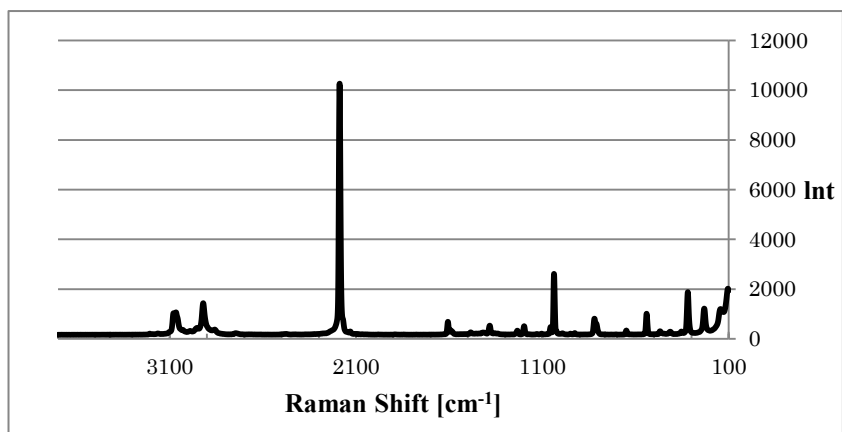
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Figure S1. Infra-red spectrum of $[\text{Cd}(\text{3-methylpyridine})_2\{\text{Au}(\text{CN})_2\}_2]_n$.



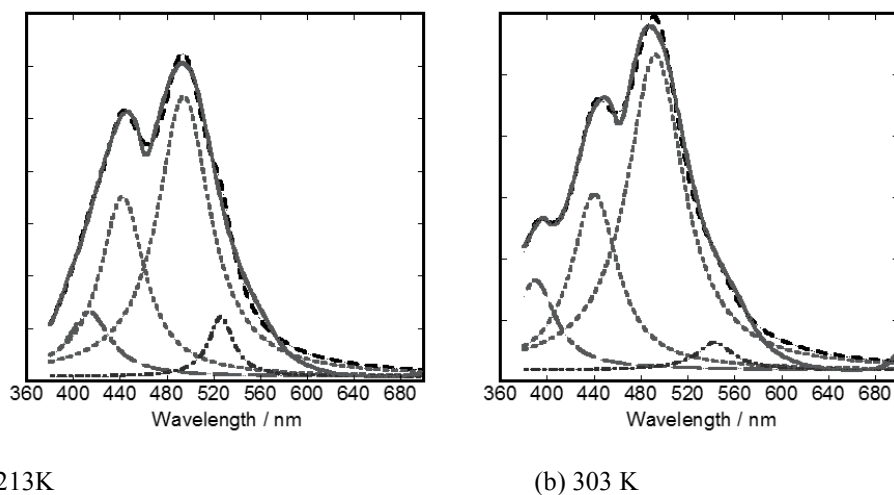
The measurement was performed on the KBr pellet at room temperature.

Figure S2. Raman spectrum of $[\text{Cd}(\text{3-methylpyridine})_2\{\text{Au}(\text{CN})_2\}_2]_n$.



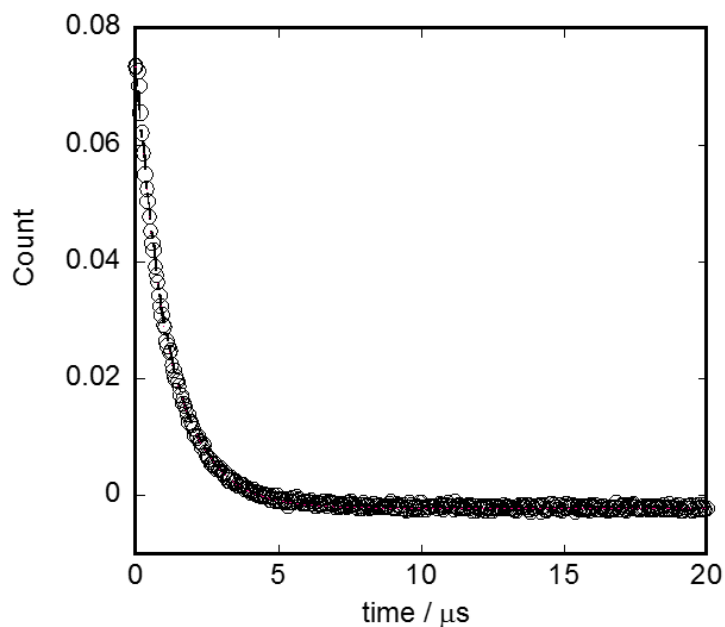
The measurement was performed on the powder sample at room temperature with a NRS-5100 Laser-Raman spectrophotometer (JASCO, Japan). The excitation wavelength was 532 nm.

Figure S3. The decomposition of the observed emission spectra from $[\text{Cd}(\text{3-methylpyridine})_2\{\text{Au}(\text{CN})_2\}_2]_n$ at 303 K and 213 K into four composite bands.



The observed emission spectra at 303 K (right) and 213 K (left) were decomposed into four composite bands. The initial peak position of each band was taken from the peaks or a shoulder in the emission spectrum experimentally observed at 303 K. The best values of the peak position and intensity was chosen independently so that the summed spectra (dotted curves) reproduced well the observed ones at both temperatures. According to the simulated spectra, the relative area of each band was obtained as 0.13 (P_1), 0.26 (P_2), 0.52 (P_3) and 0.09 (P_4) at 303 K and 0.11 (P_1), 0.29 (P_2), 0.52 (P_3) and 0.08 (P_4) at 213 K, respectively. The calculation was done using Origin (OriginPro7.5J).

Figure S4. The decay curve of the emission from $[\text{Cd}(\text{3-methylpyridine})_2\{\text{Au}(\text{CN})_2\}_2]_n$.



The decay of the emission was monitored at 490 nm, when the compound was irradiated by a laser pulse at 360 nm with the width less than 50 ns. The decay curve was expressed in terms of a single exponential with a relaxation time of 1.26 μs. The sample was maintained at 243 K.

Table S1. Crystal Data for [Cd(3-methylpyridine)₂{Au(CN)₂}]₂·n

Crystal data	[Cd(3-methylpyridine) ₂ {Au(CN) ₂ }] ₂ ·n
Empirical formula	C ₁₆ H ₁₄ Au ₂ Cd ₁ N ₆
Formula weight	796.67
Temperature	298(2) K
Crystal system	Monoclinic
Space group	P2 ₁ /c
a / Å	9.1208(5)
b / Å	15.7138(9)
c / Å	14.9519(8)
β / °	102.7620(10)
V / Å ³	2090.0(2)
Z	4
Density (calculated) / Mg m ⁻³	2.532
Absorption coefficient / mm ⁻¹	15.022
F(000)	1432
Crystal size / mm ³	0.38 x 0.30 x 0.25
Reflections collected	15427
Independent reflections	6104 [R(int) = 0.0338]
Goodness-of-fit on F ²	0.979
Final R indices [I > 2σ(I)]	R1 = 0.0351, wR2 = 0.0705
R indices (all data)	R1 = 0.0641, wR2 = 0.0795
Largest diff. peak and hole / e.Å ⁻³	0.745 and -2.598

The crystal structure of [Cd(3-methylpyridine)₂{Au(CN)₂}]₂·n was determined using a BRUKER APEXII SMART CCD area-detector diffractometer with monochromated Mo Kα radiation (λ = 0.71073 Å) at 298 K. The diffraction data was treated using SMART and SAINT, and absorption correction was performed using SADABS.¹⁾ The structure was solved by using direct methods with SHELXTL.²⁾ All non-hydrogen atoms were refined anisotropically, and the hydrogen atoms were generated geometrically.

- 1) G. M. Sheldrick, SADABS, *Program for Empirical Absorption Correction for Area Detector Data*, University of Göttingen, Göttingen, Germany, **1996**.
- 2) G. M. Sheldrick, SHELXS-97, *Program for the Solution of Crystal Structures*, University of Göttingen, Göttingen, Germany, **1997**.