

Electronic Supplementary Information (ESI)

Highly emissive carbazole-based gold(I) complex with a long room-
temperature phosphorescence lifetime and self-reversible
mechanochromism characteristics

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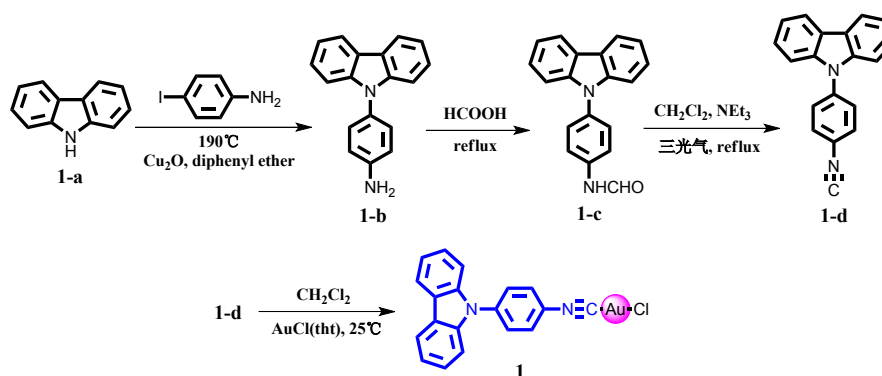
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1. Experimental Section

Materials and measurements

General: All manipulations were carried out under an argon atmosphere by using standard Schlenk techniques, unless otherwise stated. The starting material carbazole purchased from Alfa Aesar was used as received. CH_2Cl_2 was dried with CaH_2 then distilled. All other starting materials and reagents were obtained as analytical-grade from commercial suppliers and used without further purification. Compound **1-b**¹ and $\text{AuCl}(\text{tth})$ (tth = tetrahydrothiophene)² were prepared by procedures described in the corresponding literatures. ^1H NMR (400 MHz) and ^{13}C NMR (100.6 MHz) spectra were collected on American Varian Mercury Plus 400 spectrometer (400 MHz). ^1H NMR spectra are reported as followed: chemical shift in ppm (δ) relative to the chemical shift of TMS at 0.00 ppm, integration, multiplicities (s = singlet, d = doublet, t = triplet, m = multiplet), and coupling constant (Hz). ^{13}C NMR chemical shifts reported in ppm (δ) relative to the central line of triplet for CDCl_3 at 77 ppm. EI-MS was obtained using Thermo scientific DSQ II. Elemental analyses (C, H, N) were carried out with a PE CHN 2400 analyzer. Fluorescence spectra were recorded on a Fluoromax-P luminescence spectrometer (HORIBA JOBIN YVON INC.). Luminescent decay experiment was measured by Edinburgh FLS980 spectrometer. XRD studies were recorded on a Shimadzu XRD-6000 diffractometer using Ni-filtered and graphite-monochromated $\text{Cu K}\alpha$ radiation ($\lambda = 1.54 \text{ \AA}$, 40 kV, 30 mA). The solid-state surface morphology of **1** was investigated by scanning electron microscopy (SEM, Zeiss, Sigma). Absolute luminescence quantum yields were

measured by HAMAMATSU ABSOLUTE PL QUANTUM YIELD SPECTROMETER C11347. Column chromatographic separations were carried out on silica gel (200-300 mesh). TLC was performed by using commercially prepared 100-400 mesh silica gel plates (GF254) and visualization was effected at 254 nm.



Scheme S1. Synthesis of the complex **1**.

General procedure for the synthesis

Synthesis of **1-c**: A mixture of compound **1-b** (3.0 g, 11.6 mmol), formic acid (30 ml) were stirred for overnight at 110°C. After completion of present reaction, formic acid was removed from reaction system by distillation, the residual mixture was extracted with dichloromethane (3 × 30 mL), the combined organic layers were washed with brine, dried (Na₂SO₄), and concentrated in vacuo. The residues were purified by column chromatography, affording the expected pale solid product in a yield of 83%. ¹H NMR (400 MHz, CDCl₃): δ (ppm) = 8.83-8.46 (m, 1H), 8.16-8.13 (m, 2H), 7.77 (d, *J* = 8 Hz, 1H), 7.58-7.52 (m, 2H), 7.44-7.27 (m, 8H). ¹³C NMR (100 MHz, CDCl₃): δ (ppm) = 162.5, 159.1, 140.8, 140.8, 135.9, 135.8, 134.8, 134.0, 128.5, 127.8, 126.0, 126.0, 123.3, 123.3, 121.2, 120.4, 120.3, 120.1, 120.0, 109.6, 109.5. EI-MS: *m/z* = 286.16[M]⁺. Anal. Calcd. for C₁₉H₁₄N₂O: C, 79.70; H, 4.93; N, 9.78.

Found: C, 79.74; H, 4.95; N, 9.75.

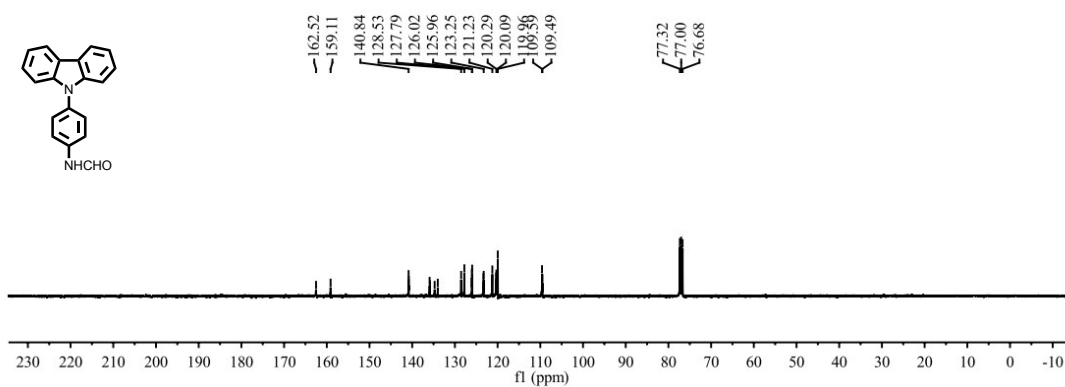
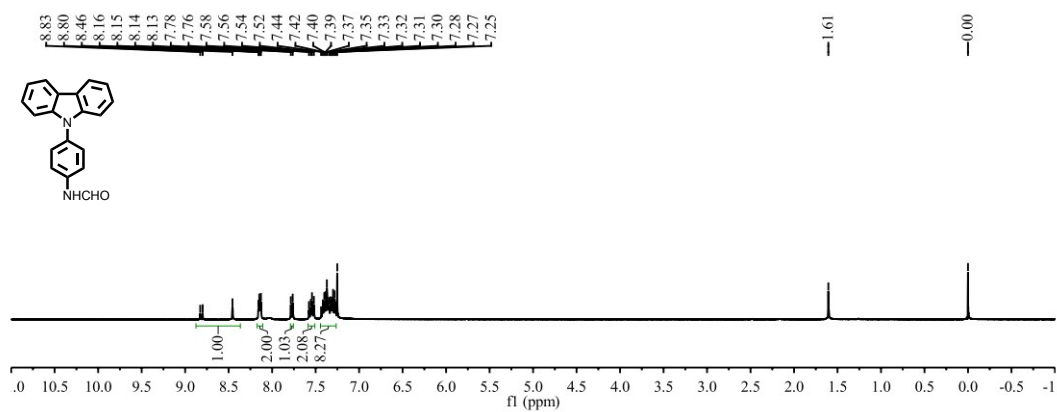
Synthesis of **1-d**: A CH₂Cl₂ suspension (15 ml) of **1-c** (1.0 g, 3.5 mmol) and triethylamine (5 ml) was cooled to 0°C. To the mixture was added dropwise a CH₂Cl₂ solution (10 ml) of triphosgene (1.16 g, 3.9 mmol). The mixture was refluxed under an argon atmosphere for 3 h, then 10% aq. Na₂CO₃ (50 ml) was added dropwise at room temperature. The mixture was extracted with dichloromethane (3 × 30 mL). The combined organic layers were washed with brine, dried (Na₂SO₄), and concentrated in vacuo. The residues were purified by column chromatography, affording the expected gray solid product in a yield of 77%. ¹H NMR (400 MHz, CDCl₃): δ (ppm) = 8.14 (d, *J* = 8 Hz, 2H), 7.63 (s, 4H), 7.45-7.30 (m, 6H). ¹³C NMR (100 MHz, CDCl₃): δ (ppm) = 165.3, 140.2, 138.7, 128.0, 127.7, 126.2, 123.7, 120.6, 120.4, 109.4. EI-MS: *m/z* = 268.14[M]⁺. Anal. Calcd. for C₁₉H₁₂N₂: C, 85.05; H, 4.51; N, 10.44. Found: C, 85.02; H, 4.55; N, 10.41.

Synthesis of **1**: A mixture of AuCl(tht) (0.25 g, 0.78 mmol) and **1-d** (0.2 g, 0.75 mmol) was stirred in CH₂Cl₂ (20 ml) over night under an argon atmosphere at room temperature. After completion of present reaction, the solvent was evaporated. A small amount of CH₂Cl₂ was added, and then a lot of n-hexane was added. Collecting the white solid product by suction filtration. Yield = 81%. ¹H NMR (400 MHz, CDCl₃): δ (ppm) = 8.15 (d, *J* = 8 Hz, 2H), 7.80 (s, 4H), 7.47-7.42 (m, 4H), 7.37-7.33 (m, 2H). Anal. Calcd. for C₁₉H₁₂AuClN₂: C, 45.57; H, 2.42; N, 5.59. Found: C, 45.62; H, 2.48; N, 5.55.

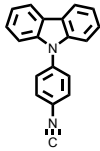
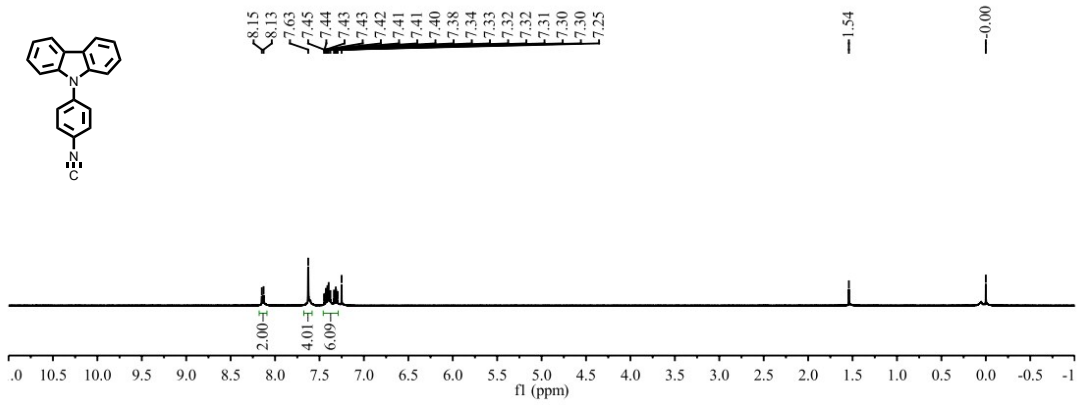
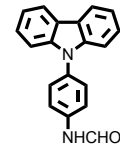
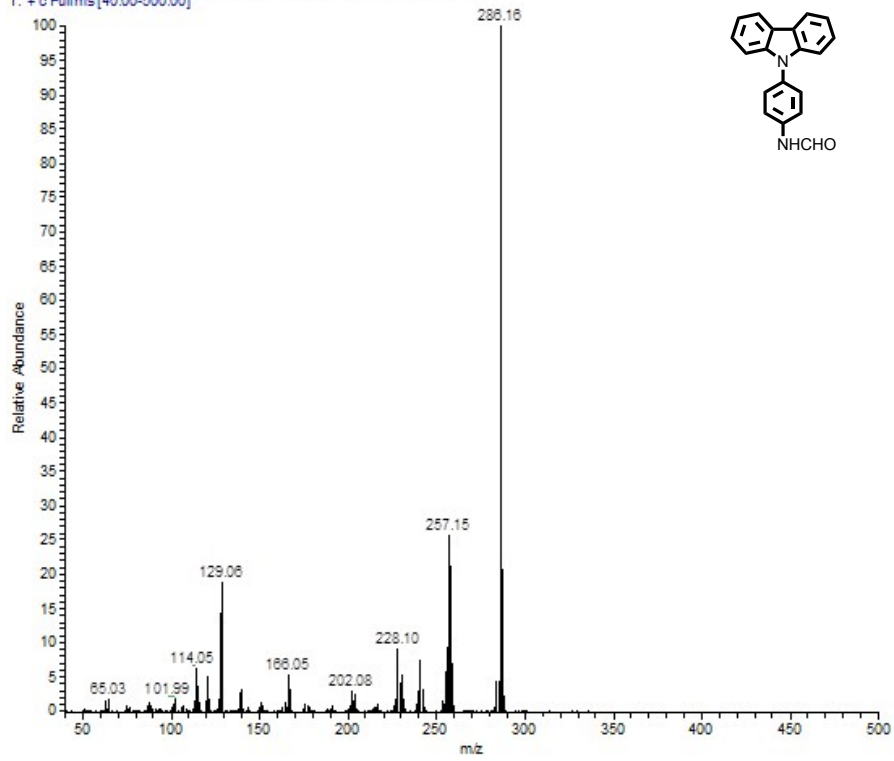
2. References

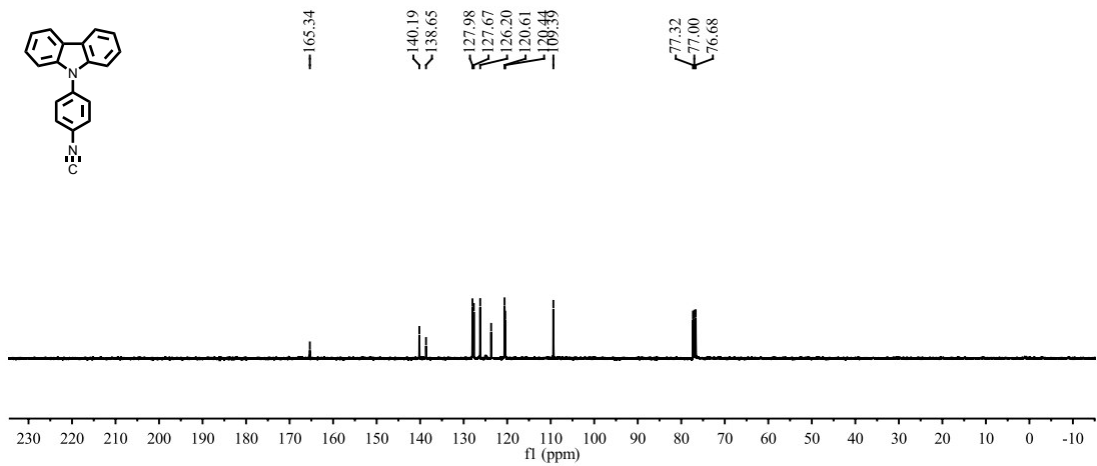
- 1 C.-G. Zhen, Z.-K. Chen, Q.-D. Liu, Y.-F. Dai, R. Y. C. Shin, S.-Y. Chang and J. Kieffer, *Adv. Mater.*, 2009, **21**, 2425-2429.
- 2 R. Uson, A. Laguna, M. Laguna, D. A. Briggs, H. H. Murray and J. P. Fackler, *Inorg. Synth.*, 1989, **26**, 85-91.

3. Copies of NMR spectra and Mass spectra

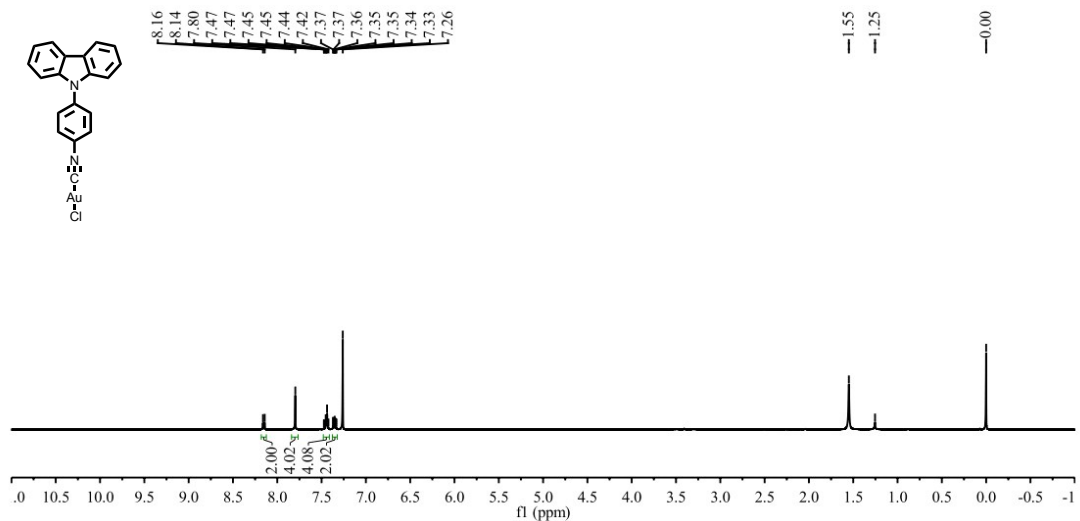
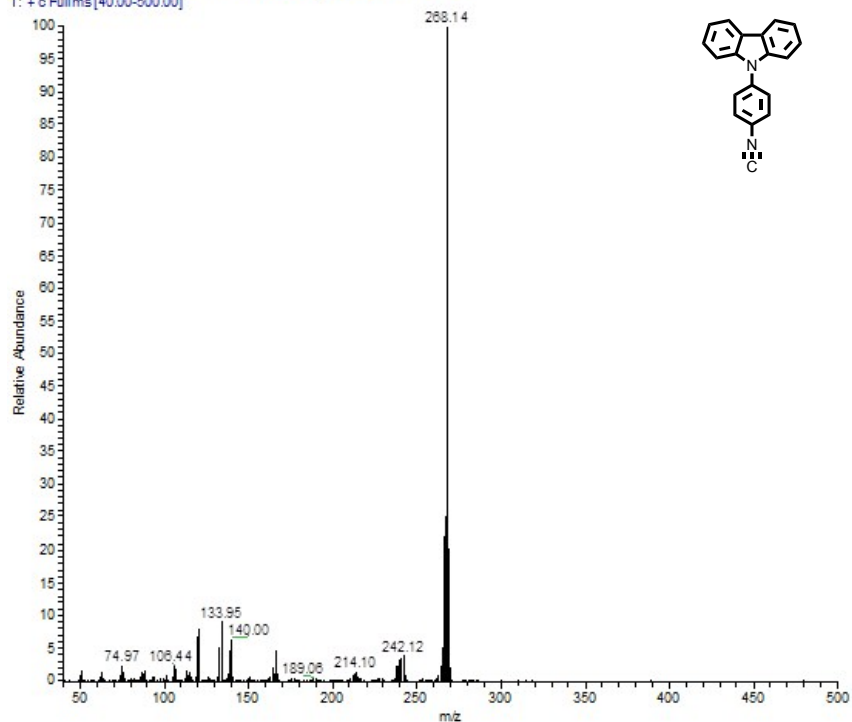


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4. The picture with test result of luminescent decay experiment

