

Thermochemically Stable Liquid-Crystalline Gold(I) Complexes Showing Enhanced Room Temperature Phosphorescence

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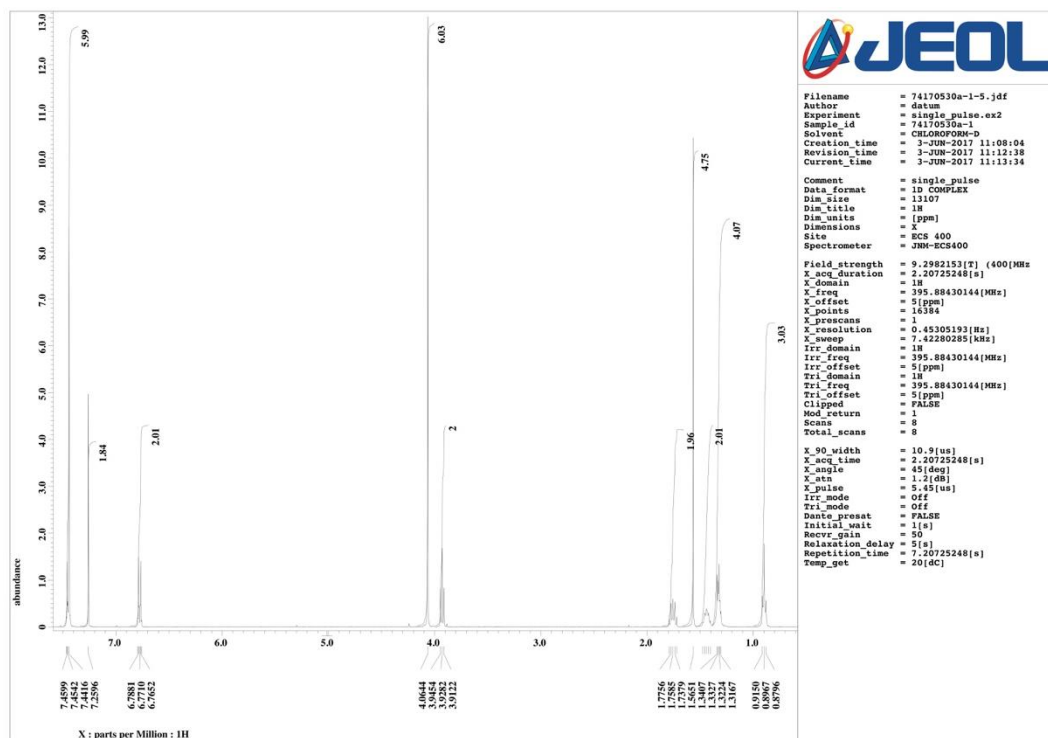


Figure S1. NMR spectrum of gold complex **3a** in CDCl₃.

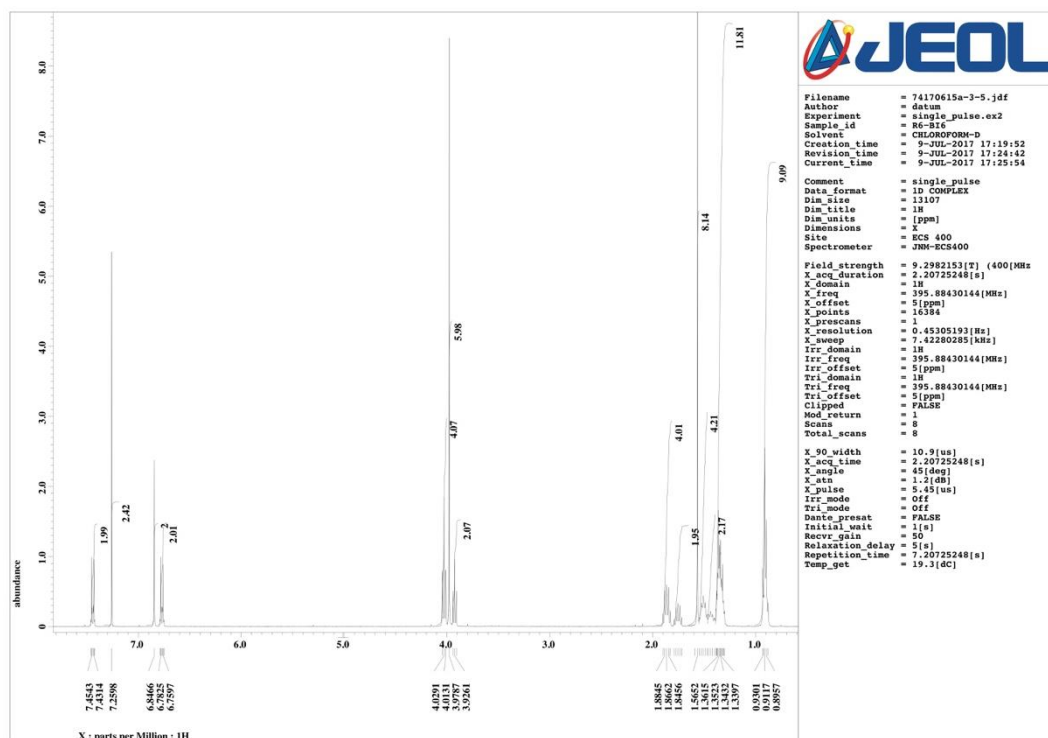
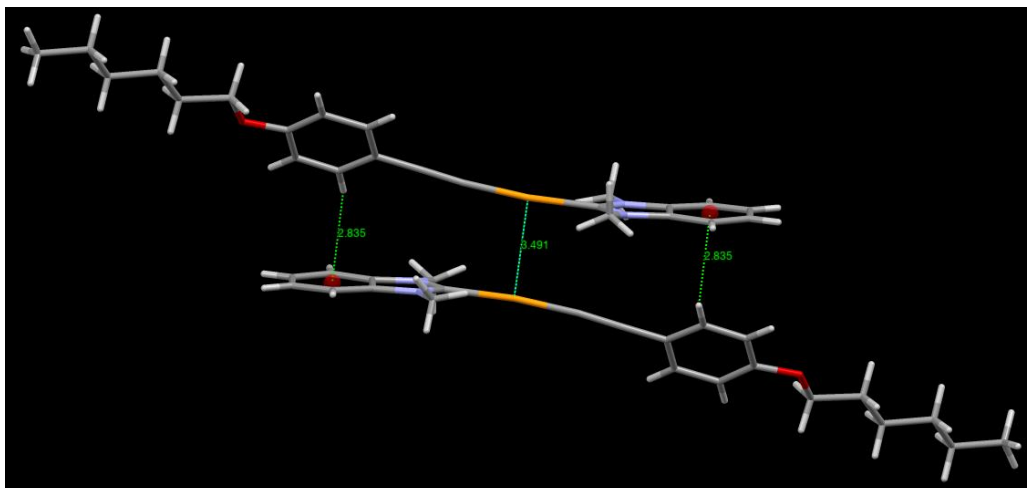


Figure S2. NMR spectrum of gold complex **3b** in CDCl₃.

Table S1. Crystallographic data for gold complexes.

Complex	1	2a	2b	3a	3b
Empirical formula	C ₂₀ H ₂₈ AuNO	C ₉ H ₁₀ AuClN ₂	C ₂₁ H ₃₄ AuClN ₂ O ₂	C ₂₃ H ₂₇ AuN ₂ O	C ₃₅ H ₅₁ AuN ₂ O ₃
Formula weight	495.40	378.61	578.93	544.43	744.74
Temperature (K)	296	298	296	296	299
Color, Habit	colorless, plate	Colorless, plate	Colorless, Needle	Colorless, needle	Colorless, needle
Crystal size (mm)	0.44 × 0.18 × 0.04	0.16 × 0.13 × 0.08	0.80 × 0.03 × 0.03	1.0 × 0.10 × 0.02	0.60 × 0.05 × 0.02
Crystal system	Triclinic	Monoclinic	Monoclinic	Monoclinic	Triclinic
$R[F^2 > 2\sigma(F^2)]$	0.045	0.0291	0.0462	0.0746	0.0423
$wR(F^2)$	0.125	0.0598	0.1488	0.2179	0.1325
Space group	<i>P</i> -1	<i>C</i> 1 2/ <i>c</i> 1	<i>P</i> 1 2 ₁ / <i>c</i> 1	<i>P</i> 1 2 ₁ / <i>n</i> 1	<i>P</i> -1
<i>Z</i>	2	8	4	8	2
<i>a</i> (Å)	7.3596(8)	20.4227 (7)	19.7051 (15)	11.6055 (6)	7.124 (2)
<i>b</i> (Å)	9.8116(2)	8.5328 (19)	6.0832 (4)	7.3649 (4)	11.986 (4)
<i>c</i> (Å)	13.9641(2)	13.7750 (5)	20.4258 (15)	50.286 (3)	21.749 (7)
α (degree)	89.373(7)	90	90	90	91.975 (10)
β (degree)	88.527(9)	123.896 (5)	100.016 (2)	90.583 (2)	99.087 (9)
γ (degree)	83.285(6)	90	90	90	105.044 (9)
<i>d</i> (g cm ⁻³)	1.721	2.524	1.595	1.683	1.402
<i>V</i> (Å ³)	1001.06 (16)	1992.52(15)	2411.1(3)	4297.9 (4)	1765.4 (9)

3a



3b

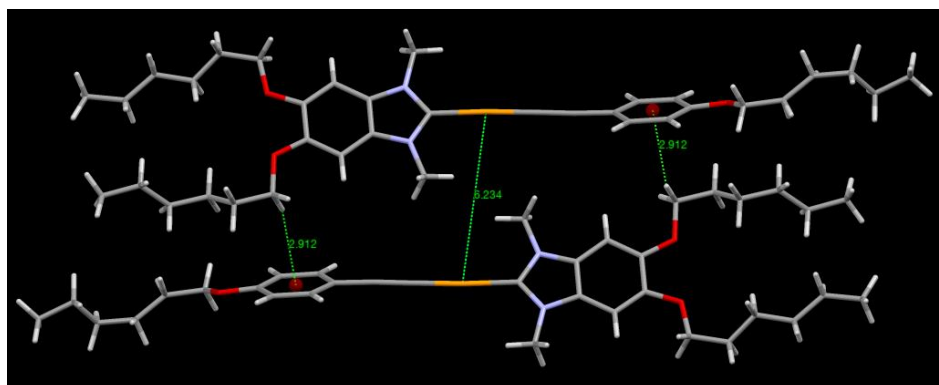


Figure S3. Packing structures of gold complexes **3a** and **3b**. Color legend: Grey, carbon; red, oxygen; blue, nitrogen; orange, gold. Red ball indicates a center of the phenyl ring.

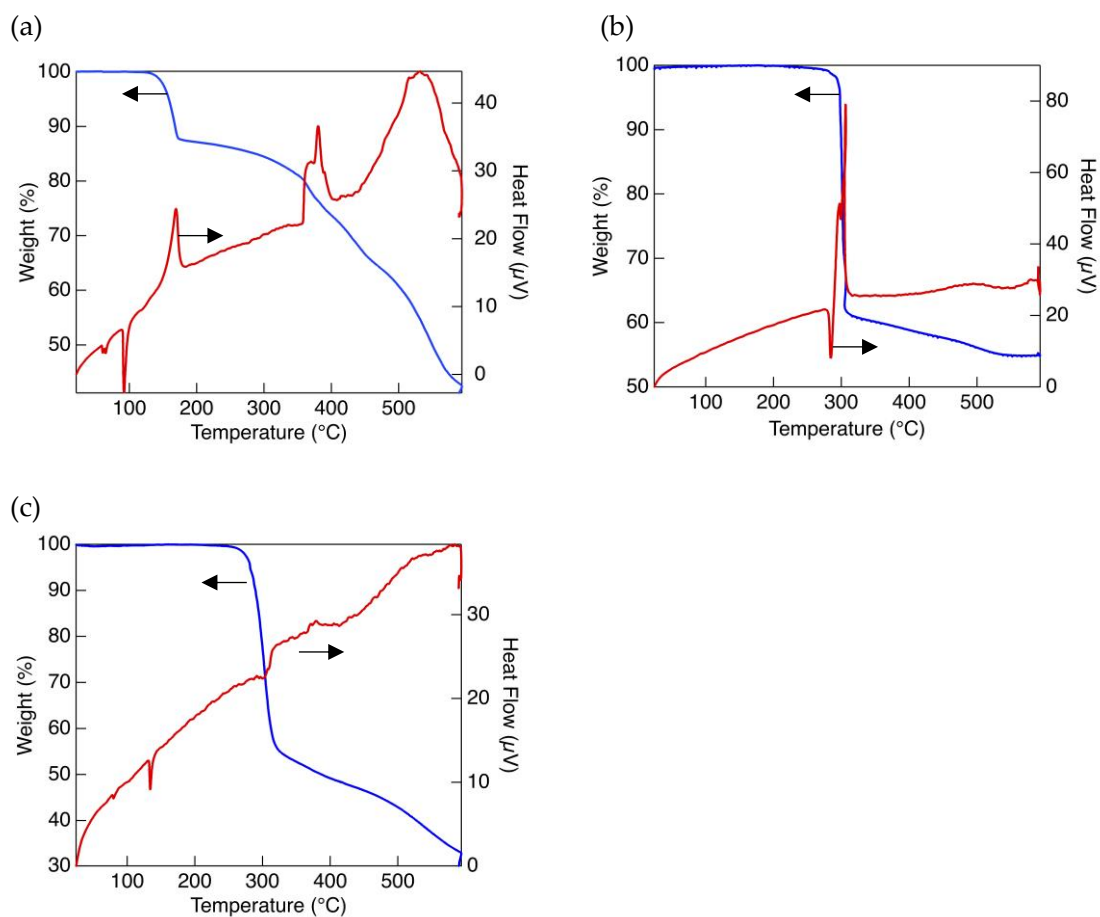


Figure S4. TG/DTA thermograms of complexes **1** and **2** in air (heating rate = $5.0\text{ }^{\circ}\text{C min}^{-1}$): (a), **1**; (b), **2a**; (c), **2b**.

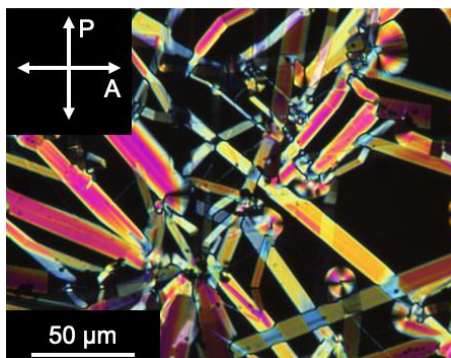


Figure S5. A POM image of the complex **3b** observed at $200\text{ }^{\circ}\text{C}$ using a higher magnification. White arrows represent the directions of the polarizer and the analyzer of POM. Uniform batonnet texture and focal conic texture showing dark region and/or lines parallel to the polarizer or the analyzer.

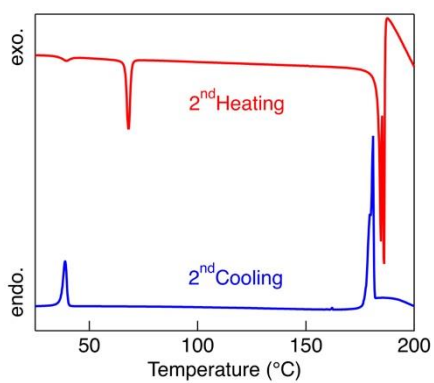


Figure S6. DSC thermograms of complexes **3a**. Scanning rate: 5.0 °C min⁻¹.

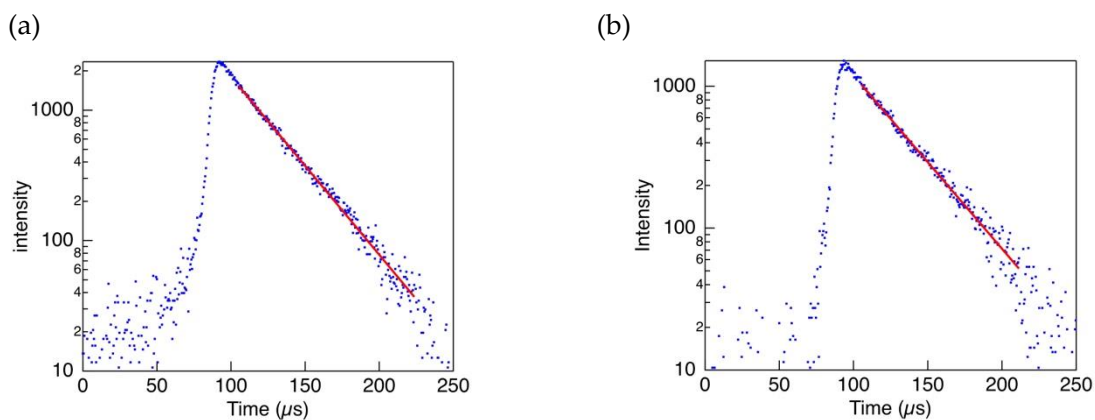


Figure S7. Photoluminescence decay profiles of complexes in crystal: (a), **3a**; (b), **3b**. Wavelength range of luminescence was 400–600 nm. The measurement was carried out using a laser pulse at 355 nm (4 ns, FWHM; 10 Hz).