

# Supplementary Materials: *N*-Heterocyclic Carbene Coinage Metal Complexes Containing Naphthalimide Chromophore: Design, Structure, and Photophysical Properties

Pierre-Henri Lanoë, Btissam Najjari, Florine Hallez, Geoffrey Gontard and Hani Amouri

Table S1: Crystallographic data for complex **1c**.

Empirical formula	C <sub>20</sub> H <sub>19</sub> N <sub>3</sub> O <sub>2</sub> ClAu
Formula weight	565.80
Temperature	200(1) K
Wavelength	0.71073 Å
Crystal system	Triclinic
Space group	P -1
Unit cell dimensions	a = 9.3874(2) Å
	b = 9.8339(2) Å
	c = 12.0913(2) Å
	α = 69.669(1)°
	β = 70.888(1)°
	γ = 76.465(1)°
Volume	979.82(3) Å <sup>3</sup>
Z	2
Crystal size	0.25 x 0.15 x 0.05 mm <sup>3</sup>
Density (calculated)	1.918 g.cm <sup>-3</sup>
F(000)	544
Absorption coefficient	7.663 mm <sup>-1</sup>
Absorption correction	Semi-empirical from equivalents
Min. and max. transmission	0.36 and 0.84
θ range for data collection	2.23° to 30.57°
Index ranges	-13 ≤ h ≤ 13
	-14 ≤ k ≤ 14
	-17 ≤ l ≤ 17
Reflections collected	29802
R(int)	1.87 %

Completeness	99.6 %
Refinement method	Full-matrix least-squares on $F^2$
Data / parameters / restraints	5978 / 246 / 0
Goodness-of-fit on $F^2$	1.089
Final R indices [ $I > 2\sigma(I)$ ]	R1 = 2.09 % wR2 = 5.08 %
Final R indices (all data)	R1 = 2.40 % wR2 = 5.20 %
Largest difference peak	2.07 e. $\text{\AA}^{-3}$
Largest difference hole	-0.59 e. $\text{\AA}^{-3}$

Figure S1. Absorption spectrum of the azolium salt  $L^1-H^+ I^-$  in  $CH_3CN$  versus  $CH_2Cl_2$  solution at same concentration and at room temperature.

