

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

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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 %<br>wR2 = 5.08 %        |
| Final R indices (all data)           | R1 = 2.40 %<br>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.

