Supporting Information for

A Non-Luminescent Polymorph of [(Cyclohexyl Isocyanide)$_2$Au]PF$_6$ that Becomes Luminescent Upon Grinding or Exposure to Dichloromethane Vapor

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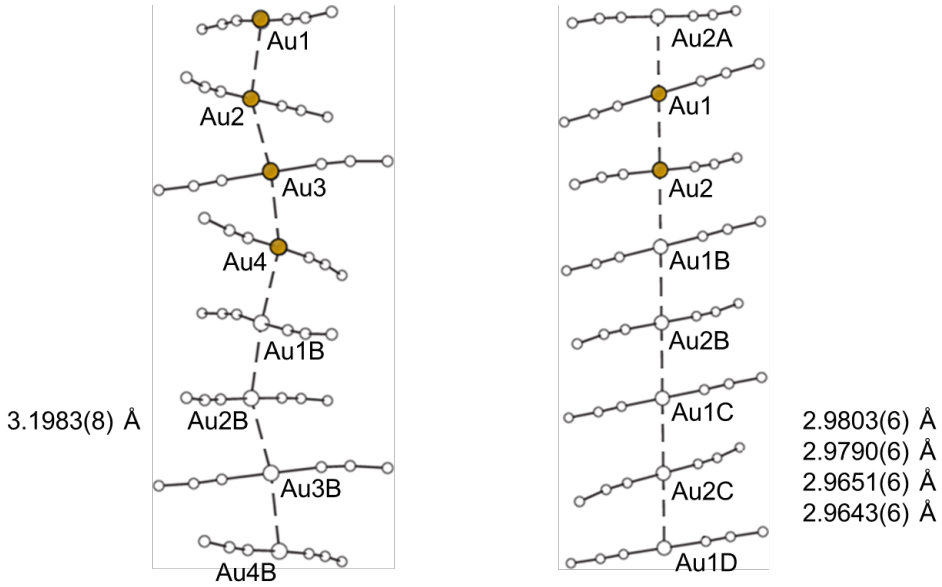

Figure SI-1. The columnar structures of green luminescent $[(C_6H_{11}NC)_2Au]PF_6$ (**1**) and blue luminescent $[(C_6H_{11}NC)_2Au]PF_6$ (**2**). For clarity, only one carbon atom of each cyclohexyl ring is shown. The aurophilic contacts are shown as solid lines and those distances are given at the bottom of the figure. From data in R. L. White-Morris, M. M. Olmstead and A. L. Balch, *J. Am. Chem. Soc.* 2003, **125**, 1033-1040.

Table 1. Crystallographic data for polymorphs of $[(C_6H_{11}NC)_2Au^I](PF_6)$

	$[(C_6H_{11}NC)_2Au^I](PF_6)$[a]	$[(C_6H_{11}NC)_2Au^I](PF_6)$[a]	$[(C_6H_{11}NC)_2Au^I](PF_6)$
color/(luminescence)/habit	Colorless (none) block	Yellow (green) plate	Colorless (blue) needle
chemical formula	$C_{14}H_{22}AuF_6N_2P$	$C_{14}H_{22}AuF_6N_2P$	$C_{14}H_{22}AuF_6N_2P$
formula weight	560.27	560.27	560.27
crystal system	monoclinic	orthorhombic	monoclinic
space group	*C*2/*c*	$P2_12_12_1$	$P2_1/c$
a (Å)	16.8465(11)	11.5235(7)	6.3644(5)
b (Å)	7.9802(5)	24.1416(15)	16.9806(15)
c (Å)	14.5677(15)	26.0516(16)	16.7224(13)
α (deg)	90	90	90
β (deg)	118.6160(10)	90	92.693(3)
γ (deg)	90	90	90
V (Å^3)	1719.2(2)	7247.4(8)	1805.2(3)
Z	4	16	4
T (K)	100(2)	91(2)	91(2)
λ (Å)	0.71073	0.71073	0.71073
ρ (g/cm^3)	2.165	2.054	2.061
μ (mm^{-1})	8.709	8.264	8.264
R_1 (obsd data)[b]	0.0128	0.055	0.019

[a]From data in R. L. White-Morris, M. M. Olmstead and A. L. Balch, *J. Am. Chem. Soc*. 2003, **125**, 1033-1040.

[b]$R_1 = (\Sigma||F_o| - |F_c||)/\Sigma|F_o|$

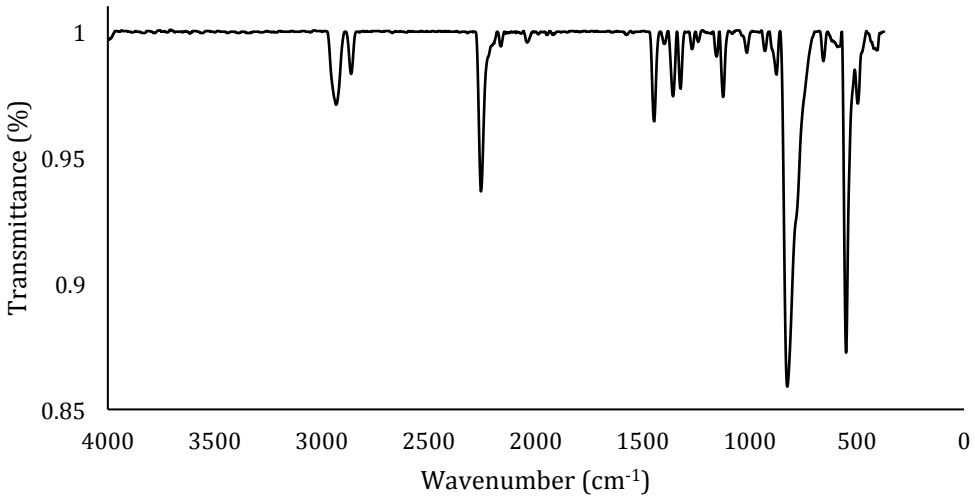

Figure SI-2. Infrared spectrum of the colorless, non-luminescent polymorph of $[(C_6H_{11}NC)_2Au]PF_6$ with the isonitrile stretching band at 2257 cm^{-1} and P-F vibrations at 828 and 556 cm^{-1}.

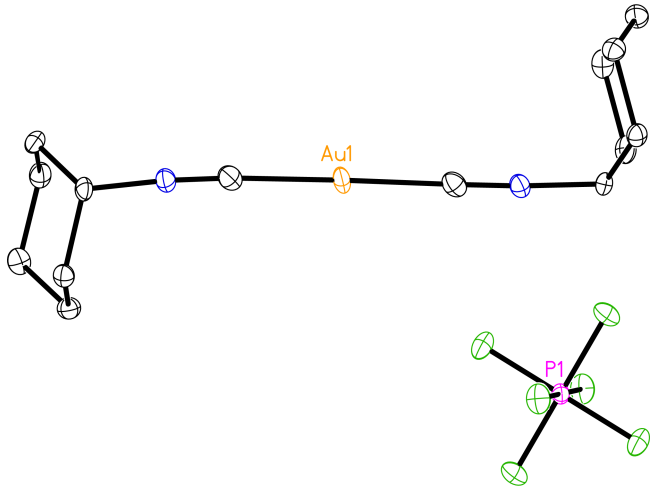

Figure SI-3. The molecular structure of the colorless, non-luminescent polymorph of $[(C_6H_{11}NC)_2Au]PF_6$. Hydrogen atoms are omitted for clarity. Thermal ellipsoids are drawn at 50%. Atom colors are: Au, orange; C, black; N, blue; P, purple; F, green. Selected bond distances (Å): Au1-C1, 1.975(2); N1-C1, 1.140(3); N1-C2, 1.455(3); P1-F1, 1.6065(12); P1-F2, 1.6060(13); P1-F3, 1.6032(11). Selected bond angles (deg); C1-Au1-C1', 177.90(11); N1-C1-Au1, 176.71(19); C1-N1-C2, 176.0(2); N1-C2-C7, 109.44(16); N1-C2-C3, 108.20(16).