Tunable Emission Color of Polymorphic Gold(I) Isocyanide Complexes

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Organic materials with aggregation-induced emission (AIE) are demonstrated to be promising as optoelectronic devices. Generally, single molecule organic luminescent material only exhibits one emission color according to Kasha's rule, which cause a limitation for multifunctional material. Since the luminescence properties is strongly dependent on the aggregated structure, it is desirable to control the aggregated structure to obtain the desired luminescence properties. Polymorphic material which possesses more than one crystalline phase, can be utilized to obtain multi-color emission from one chromophore. Another method to tune the emission color is by applying external stimuli (e.g., mechanical force, heat, pressure) which also related to the change in aggregated structure. Such mechano-responsive materials can endow various applicability in sensors, probes, and memory devices.¹ Gold complex is a promising material to induce both efficient luminescence in aggregated states and stimuli-responsive luminescence behavior owing to the unique Au–Au (aurophilic) system. Indeed, numerous studies have reported various gold complexes with luminescence color sensitivity toward external stimuli.²

In this study, we designed and synthesized gold complexes having biphenyl or cyclohexylphenyl and isocyanide ligands (Figure 1a). This type of complexes having ligand with less steric hindrance around Au atoms is favorable to manifest aurophilic interaction. Photophysical behaviors of the gold complexes in various states were discussed based on not only their primary structures but also aggregated structure. Both complexes are AIE-active where strong room-temperature phosphorescence (RTP) was observed in the crystal. Interestingly, **CP** exhibited intriguing stimuli-responsive luminescence by having both polymorphism and mechanochromic luminescence properties. High-contrast luminescence color tuning was observed in **CP** by simply controlling the recrystallization conditions (Figure 1b). Such polymorphism-dependent emission color is likely to attribute to the change in the aggregated structure between crystal polymorphs as well as the ground crystal.



Figure 1. (a) Molecular structures of **BP** and **CP** gold(I) complexes. (b) Excitation and emission spectra of **CP** crystal polymorphs (**CP-B** and **CP-G**). Solid line, emission spectra ($\lambda_{ex} = 320$ nm); dashed line, excitation spectra. (c) Photographs of **CP-B** and **CP-G** bulk crystal under UV irradiation ($\lambda_{ex} = 365$ nm).

- 1) Hajime Ito et al., Angew. Chem. Int. Ed., 2013, 52, 12828.
- 2) Kaori Fujisawa et al., Sci Rep., 2015, 5, 7934