

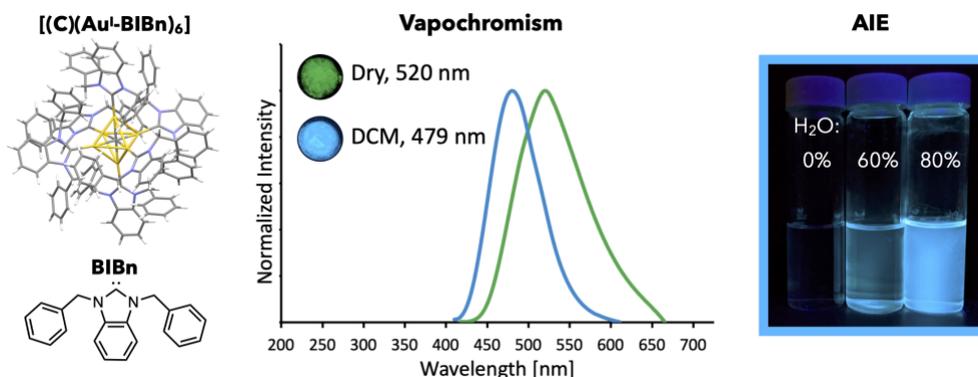
## Vapochromism and Aggregation-Induced Luminescence in An *N*-Heterocyclic Carbene-Protected Carbon-Centered Hexagold(I) Cluster

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Element-centered gold(I) clusters represent a unique class of molecules with stable hypervalent main-group elements. Since Schmidbaur et al. reported a carbon-centered phosphine-supported hexagold(I) cluster in 1988,<sup>1</sup> the diversity and development of this group of materials has attracted much attention. Our group has pioneered the construction of carbon-centered hexagold(I) clusters supported by *N*-heterocyclic carbene (NHC) ligands, and has shown that their stability, luminescent properties, and versatility are improved compared to the phosphine analogues. In this study, we synthesized a new carbon-centered hexagold(I) cluster supported by 1,3-dibenzylbenzimidazolylidene (BIBn), [(C)(Au<sup>I</sup>-BIBn)<sub>6</sub>](BF<sub>4</sub>)<sub>2</sub>, and found that it exhibits unique photophysical properties such as vapochromism and aggregation-induced emission (AIE).

First, this complex was synthesized according to the reported procedures,<sup>2,3</sup> and its structure was characterized by NMR spectroscopy and single crystal XRD analysis. Under photoirradiation at 365 nm, it showed turquoise emission after vacuum drying or contact with low polar solvents such as Et<sub>2</sub>O, *n*-hexane, and toluene, and blue emission was observed upon contact with CH<sub>2</sub>Cl<sub>2</sub>, CHCl<sub>3</sub>, and acetone. It is noteworthy that in the case of anion exchange from BF<sub>4</sub><sup>-</sup> to large BPh<sub>4</sub><sup>-</sup>, the solid emits blue light regardless of the dryness or wetness of the solvent used. Moreover, aggregation-induced luminescence was observed in a water-methanol solution with an emission maximum at 482 nm. We expect that this work will lead to a better understanding of the relationship between the luminescence properties of NHC-supported gold(I) clusters and the ligand structures.



1) H. Schmidbaur et al. *Angew. Chem., Int. Ed.* **1988**, 27, 11, 1544; 2) M. Shionoya et al. *Organometallics*, **2018**, 37, 2007; 3) M. Shionoya et al. *J. Organomet. Chem.*, **2020**, 917, 121271.