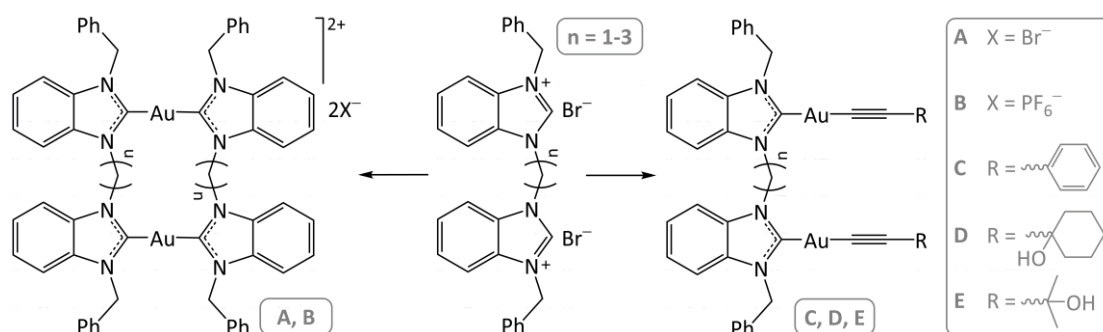


# Homo- and heteroleptic gold complexes based on bidentate N-Heterocyclic carbene ligands: some features of the photophysical properties

Elena Grachova<sup>1</sup>, Alexander Penney<sup>1</sup>, Vladimir Sizov<sup>1</sup> and Sergey Tunik<sup>1</sup>

<sup>1</sup> St. Petersburg State University, Russian Federation

We prepared a series of structurally similar homo- and heteroleptic dinuclear Au(I) complexes supported by non-rigid bidentate NHC ligands and systematically investigated their photophysical properties in different media, while paying special attention to the effect of the diNHC linker length, counterions and the nature of alkynyl ligands on the photophysics.



In particular, it has been found that:

- In methanolic solution, the emission profiles of complexes **A** and **B** demonstrate remarkable changes upon the addition of excess Br<sup>-</sup>. [1]
- **A** and **B** are emissive in the solid state, and the nature of counterion has a pronounced effect on the photophysical characteristics, such as emission wavelength and quantum yield.
- **A** exhibit reversible luminescent mechano- and vapochromism toward methanol triggered by an amorphous-to-crystalline phase transition.
- **C** show noticeable luminescent solvatochromism on changing the solvent from CH<sub>2</sub>Cl<sub>2</sub> to MeCN.
- **D** and **E** are non-emissive in CH<sub>2</sub>Cl<sub>2</sub>, but demonstrate dual luminescence in MeCN solution.
- Solid state emission of **C**, **D** and **E** depends dramatically on the nature of alkynyl ligands, and luminescence maximum of **C** is considerably redshifted relative to those of **D** and **E**.

As evidenced by a detailed computational study, aurphilicity plays a determining role in the photophysical properties of these compounds in solution, where the formation of exciplexes between the complex and counterions (**A** and **B**) or solvent molecules (**A**–**E**) was demonstrated to significantly decrease the Au–Au distance in the triplet excited state.

In the solid, the space conformation of the complex molecule, intramolecular interactions, and packing effects become more important to control the photophysics of the investigated dinuclear Au(I)-NHC complexes.

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