Effect of the bis-cyclometallisation ligand and temperature on luminescence of gold(III) complexes

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A novel class of luminescent cyclometallated gold(III) alkynyl complexes has been demonstrated to possess electroluminescence (EL) properties and has been employed in the roles of electrophosphorescent emitters or dopants of organic light-emitting diodes (OLEDs) with high brightness and efficiency\textsuperscript{[1-3].}

This work focuses on the effect of the bis-cyclometallisation ligand in order to investigate how ligand affects the luminescence properties of the resulting gold (III) complexes\textsuperscript{[4]}. Our complexes include a diphenyl-pyridine metallacycle with a terminal R1 group and an alkynyl ligand bearing a radical R2, namely [Au(HC^N(R1)^CH)(C≡CR2)]. Absorption and emission properties of our compounds were performed by density functional theory (DFT) and TD-DFT calculations, using the hybrid functional PBE0 associated with a double zeta basis of atomic orbitals, in addition with the polarization functions LANL2DZ, as implemented in the Gaussian 09 package.

Obtained results show that the nature of the ligands influences greatly the geometry and the molecular orbital borders. In addition, the phosphorescence wavelength of these complexes was estimated. It appears to be dependent on both the surrounding environment and the nature of the R1 and R2 end groups. Temperature effects have been considered to improve the simulated spectrum, when is taken into account, the simulated and observed spectra fit much better.

References

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