Structure and electronic properties of benzimidazole and cycloheptaimidazole gold N-heterocyclic carbenes

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Abstract
Two related families (one previously experimentally reported and another theoretically proposed) of gold benzimidazole (family 1) and cycloheptaimidazole (family 2) N-heterocyclic carbenes were studied due to the potential application in medicinal chemistry and the resurgence of Au based catalysis. Both families show interesting aromatic properties, which were calculated computationally using the Nucleus Independent Chemical Shift (NICS) indexes, Electron Localization Function (ELF) and the Electrostatic Potential Surface (EPS) maps. The calculation of the NICS indexes, the ELF values and EPS showed that there is a small difference between both families of studied complexes, where family 1 is slightly more aromatic that family 2. Both families showed that the carbene ring has σ aromaticity, while the six or seven membered rings showed π aromaticity. To study their spectroscopic properties, Time-Dependent Density Functional Theory (TD-DFT) calculations were performed. These calculations showed that there is almost no contribution from the metal to the observed UV–Vis transitions (all of them showed Ligand to Ligand Charge Transfer (LLCT) character), due to the high stability that the molecular orbitals (MOs) of the gold atom have in the complex.

Author keywords
Carbene; DFT; Gold; Heterocycle