Thermally Stable Carbazole Tagged Au(I) Mesoionic *N*-Heterocyclic Carbene Complexes with Diverse Gold–Hydrogen Bonds

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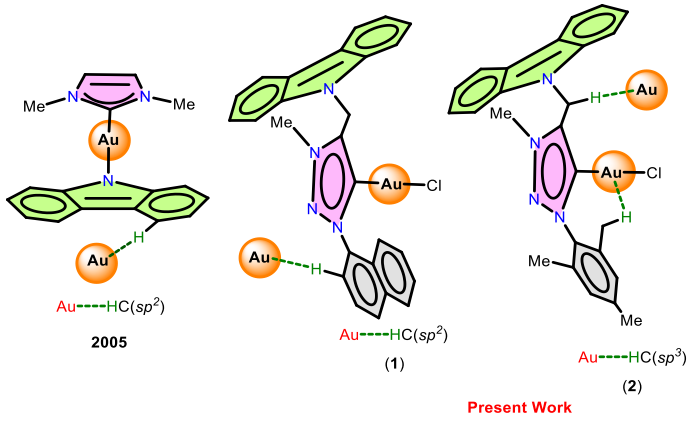
The carbazole-substituted *N*-heterocyclic carbene (NHC) gold molecules have demonstrated diverse structural features and interesting thermal properties. The role of the remotely linked carbazole group to mesoionic carbene in gold(I)-NHC complexes have been addressed in this paper. Thus, we have synthesized and characterized the neutral gold-mesoionic carbene monomers tagged with the carbazole group. The mononuclear gold(I) carbene molecules [(**L**^{1})AuCl] (**1**) and [(**L**^{2})AuCl] (**2**), where **L**^{1}**.HI** = 1-(naphth-1-yl)-3-methyl-4-(carbazolylmethyl)-1,2,3-triazolium iodide and **L**^{2}**.HI** = 1-(mesityl)-3methyl-4-(carbazolylmethyl)-1,2,3-triazolium iodide, have been synthesized and characterized. The new class of complexes depicted interesting gold-hydrogen bonding. In addition, the thermal properties of **1** and **2** were investigated. The Density Functional Theory (DFT) calculation and natural bond orbital analysis (NBO) was accomplished on a model system [(L')AuCl] (**1A**), L'=1-phenyl-4-methyl-carbazole-1,2,3-triazol-ylidene to realize the bonding situations. The calculated metrics agreed reasonably well with the experimental observations.



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