

# Insight into the Stability and Electronic and Optical Properties of N-Heterocyclic Carbene Analogues of Halogen/Phosphine-Protected Au<sub>13</sub> Superatomic Clusters

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## Abstract

Atomically precise gold nanoclusters (AuNCs) belong to a relevant area offering useful templates with tunable properties toward functional nanostructures. In this work, we explored the feasible incorporation of N-heterocyclic carbenes (NHCs), as part of the protecting-ligand shell in AuNCs. Our results, which are based on the substitution of phosphine ligands in experimentally characterized AuNCs by NHCs in various eight-electron superatoms Au<sub>13</sub> and M<sub>4</sub>Au<sub>9</sub> (M = Cu, Ag), indicate similar electronic structure and stability but somewhat different optical properties. These findings support the feasible obtention of novel targets for explorative synthetic efforts featuring NHC ligands on medium-sized species based on the recurrent Au<sub>13</sub> icosahedral core. The hypothetical species appear to be interesting templates for building blocks in nanostructured materials with tuned properties, which encourage experimental exploration of ligand versatility in homo- and heterometallic superatomic clusters. © 2022 American Chemical Society. All rights reserved.