Synthesis and characterization of N-heterocyclic carbene-M···OEt_2complexes (M = Cu, Ag, Au). Analysis of solvated auxiliary-ligand free $[(NHC)M]^+$species

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Abstract
We report the synthesis, characterization and computational analysis of coinage metal-ether complexes supported by N-heterocyclic carbenes (NHC), SIPr and Et2CAAC. The related water adducts are also included. The [(NHC)M]+(M = Cu, Ag, Au) species show the noteworthy ability to bind Et2O and H2O. This interaction towards Et2O and H2O is partly ascribed to a σ-hole bonding with an almost linear disposition, taking advantage of the enhanced σ-hole potential evaluated for such [(NHC)M]+ species. This enhanced ability is larger than those found for non-covalent interactions involving main group species.

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