

Cyclic trinuclear copper(i), silver(i), and gold(i) complexes: A theoretical insight

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The metal-ligand, M-L, bonding situation in cyclic trinuclear complexes, CTCs, of copper(i), silver(i), and gold(i) was investigated in terms of the energy decomposition analysis (EDA-NOCV) and natural bond orbitals (NBOs). The anisotropy of the induced current density (ACID) and magnetic response were employed to evaluate the effect of electronic conjugation and metal-metal interactions in CTCs. The EDA-NOCV results show that the M-L bonding is stronger in gold(i) than in copper(i) or silver(i) complexes. Au⁺-L bonds present an elevated covalent character when compared with Cu⁺-L and Ag⁺-L bonds. The NBO analysis confirms the elevated covalent character observed for Au⁺-L bonds, indicating that the ligand-metal donation, L → M, and the metal-ligand back-donation, M → L, are more stabilizing in gold(i) than in copper(i) or silver(i) complexes. Both ACID and the magnetic response calculations reveal that there are cyclic conjugations in the ligands and a strong diatropic ring current indicating the presence of aromaticity. However, there is no through-bond M-L conjugation between the ligands and the metallic centers, as indicated by the absence of a continuous anisotropy boundary surface involving M-L bonds. This journal is © The Royal Society of Chemistry 2015.