

# Coinage-metal pillarplexes hosts. Insights into host-guest interaction nature and luminescence quenching effects

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## Abstract

Host-guest chemistry is a relevant issue in materials science, which encourages further development of versatile host structures. Here the particular features of coinage-metal pillarplexes are evaluated towards formation of host-guest aggregates by the inclusion of 1,8-diaminooctane, as characterized for  $[M_8(L^{Me})_2]^{4+}$  ( $M = Ag, \text{ and, } Au$ ). The obtained results denotes the main contribution from van der Waals type interaction (50%), followed by a contribution from orbital polarization and electrostatic nature (20% and 30%), involving both orbitalary and electrostatic terms. Throughout the different coinage-metal based hosts ( $M = Cu, Ag, \text{ and } Au$ ), a similar interaction energy is found given by the large contribution of the  $\pi$ -surface from the organic ligand backbone to both van de Waals and electrostatic interactions. This suggests that a similar host structure can be obtained for the lighter copper counterpart, retaining similar how-guest features. Moreoves, the  $[Au_8(L^{Me})_2]^{4+}$  host exhibits inherent luminescent properties, involving the shortening of Au(i)-Au(i) contacts at the excited state, which is partially avoided when the guest is incorporated, accounting for the observed quenching from titration experiments. This results encourages further exploration of coinage metal hosts in the formation of inclusion complexes. © the Owner Societies 2021.