

Insights into metal-ligand and metal-metal interaction in coinage metal triangles.
Insights of d10-d10, d10-d8 and d8-d8 contacts from $[\text{Au}_3\text{In}(\text{CH}_3\text{N}=\text{COCH}_3)_3]$
($n = 2, 4, 6$) via relativistic DFT calculations

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The successive addition of one, two and three equivalents of iodide to $[\text{Au}_3(\text{CH}_3\text{N}=\text{COCH}_3)_3]$, gives rise to the $[\text{Au}_3\text{In}(\text{CH}_3\text{N}=\text{COCH}_3)_3]$ ($n = 2, 4, 6$) oxidized systems. Such structures have been studied by using scalar relativistic DFT calculations and TD-DFT. Our results demonstrate a stronger ligand-to-metal charge donation, which increases in covalency. The long metal-metal contacts observed through the series result from the similarly population of bonding, non-bonding and slightly anti-bonding combinations of the 6s-Au atomic shells in the $[\text{Au}_3]^{n+}$ core, leading to distances in the range of the sum of their van der Waals radii for all the systems. © 2016 Elsevier B.V. All rights reserved.