

Terminal AuN and AuO Units in Organometallic Frames

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Early transition metals (TM) readily form compounds containing terminal nitride and oxo ligands. The multiple bonds formed with these electron-poor metals, e.g. $M\equiv N$ and $M\equiv O$, are not possible with electron-rich late-TMs owing to population of π^* MOs.^[1] This feature greatly destabilizes the MX unit ($X = N, O$). Thus, in gold chemistry, for instance, just a handful of terminal oxo derivatives have been detected in the gas phase or in inert matrices: $(AuO)^{q+}$ ($q = -1, 0, 1, 2$), $OAuF_n$ ($n = 1, 2$), $(OAuO)^{q-}$ ($q = 0, 1$), and $[OAu(OBO)]^-$.^[2-5] They all contain hard ligands and exhibit low coordination numbers (<4).

We found that the trifluoromethyl group, CF_3 , which is an organic hard ligand, is able to stabilize not only the terminal AuO unit in the gas phase, but also the terminal AuN unit (Figure 1). The structural and electronic properties of these unusual organogold derivatives are examined by calculation. These compounds boldly defy the conventional rules to assign oxidation states.

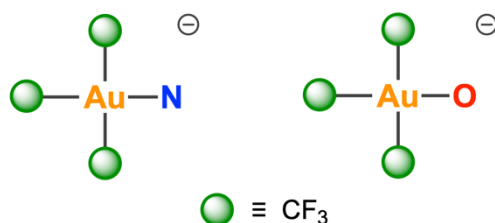


Figure 1: Organogold compounds with AuN and AuO terminal units.

References

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