Single and multi-component gold (bisdithiolene) complexes

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Among metal bis(dithiolene) complexes, gold complexes are particularly investigated for their ability to form single component conductors in their radical neutral form [1]. The gold bis(dithiolene) complexes involving the N-alkyl-1,3-dithiole-2-thione-4,5-dithiolate ligand (R-thiazdt) led to a variety of conducting materials. Among them, the one with R =Me, [Au(Me-thiazdt)₂], exhibits a metallic state under ambient pressure being so far the first single-component molecular metal under ambient pressure derived from such Au complexes without any TTF backbone [2]. In addition, it shows a striking stability of the metallic state finding its origin in sizable internal electron transfer from the SOMO-1 to the SOMO of the complex as well as in substantial interstack and interlayer interactions.

In order to increase the intermolecular interactions, we also studied the gold bis(diselenolene) complex analogue, as the presence of selenium atoms, thanks to stronger intermolecular interactions, generally induces a notable increase of the band dispersion in the solid state. We obtained a 1 : 2 salt which exhibits a rare charge alternation associated with the simultaneous presence of both cis and trans isomers of the gold complex in the conducting layers and shows a semiconducting behavior which turns metallic under pressure, in contrast with other 1 : 2 gold bis(dithiolene) salts [3].

Herein we show that oxidation of a gold bis(diselenolene) complex affords a mixedvalence 1 : 2 salt $[Ph_4P][Au(Me-thiazds)_2]_2$ while oxidation of the bis(dithiolene) analogue affords the corresponding neutral radical single-component conductor $[Au(Me-thiazdt)_2]$.



References

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