

Mixed-valence gold bis(diselenolene) complex turning metallic under pressure

Yann Le Gal,^a HengBo Cui,^{b,c} Pere Alemany,^d Enric Canadell,^{e*} Reizo Kato,^b Thierry Roisnel,^a Vincent Dorcet,^a Marc Fourmigué^a and Dominique Lorc^{a*}

a Univ Rennes, CNRS, ISCR (*Institut des Sciences Chimiques de Rennes*) - UMR 6226, F-35000 Rennes, France

b Condensed Molecular Materials Laboratory, RIKEN, Wako-shi, Saitama 351-0198, Japan

c New permanent address : Department of Physics, Sungkyunkwan University, Suwon 16419, Republic of Korea.

d Departament de Ciència de Materials i Química Física and Institut de Química Teòrica i Computacional (IQTCUB), Universitat de Barcelona, Martí i Franquès 1, 08028 Barcelona, Spain;

e Institut de Ciència de Materials de Barcelona, ICMAB-CSIC, Campus de la UAB, 08193 Bellaterra, Spain.

Supplementary Information

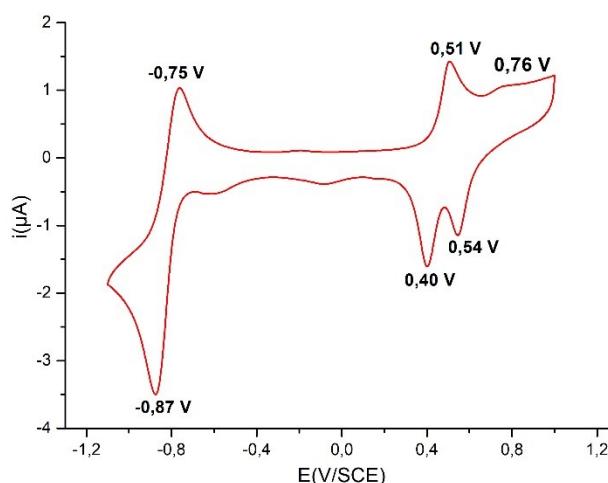


Figure S1. Cyclic voltammogram of $[\text{Ph}_4\text{P}][\text{Au}(\text{Me-thiazds})_2]$ recorded in $\text{CH}_2\text{Cl}_2\text{-Bu}_4\text{NPF}_6$ 0.1 M at a platinum electrode, scan rate 100 mVs⁻¹.

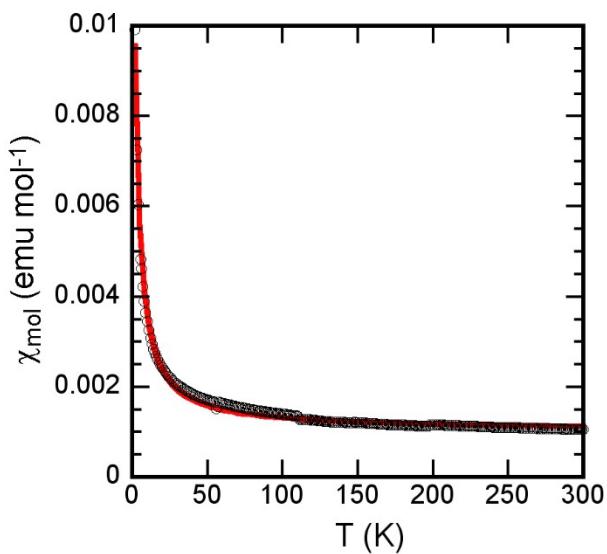


Figure S2. Temperature dependence of the magnetic susceptibility of $[\text{PPh}_4][\text{Au}(\text{Me}-\text{thiazds})_2]_2$. The red curve is a fit to the Curie-Weiss law (see text).

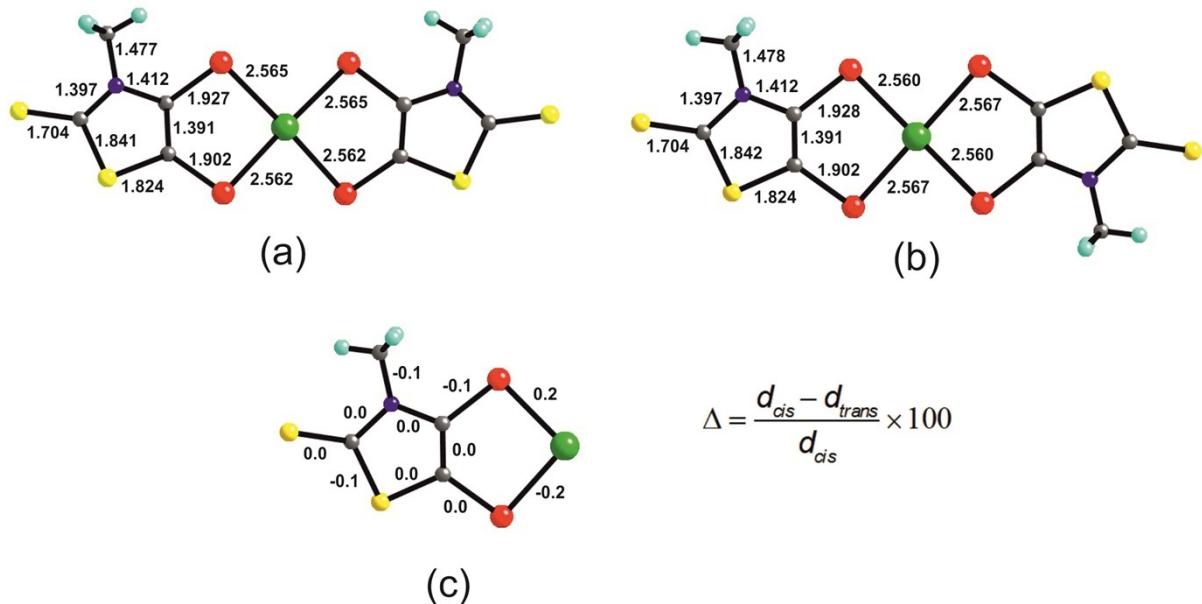


Figure S3. DFT optimized geometries for the isolated *cis* (a) and *trans* (b) isomers of the gold complex and bond distance differences between the *cis* and *trans* structures in % with respect to the *cis* geometry (c).