Electronic Supplementary Material (ESI) for Dalton Transactions.

Hydrogen bonding interactions in single component molecular conductors based on metal (Ni, Au) bis(dithiolene) complexes†

Hadi Hachem, Nathalie Bellec, Marc Fourmigué* and Dominique Lorcy*

Univ Rennes, CNRS, ISCR (Institut des Sciences Chimiques de Rennes) - UMR 6226, F-35000 Rennes, France. Email : marc.fourmigue@univ-rennes1.fr, dominique.lorcy@univ-rennes1.fr

Supplementary information

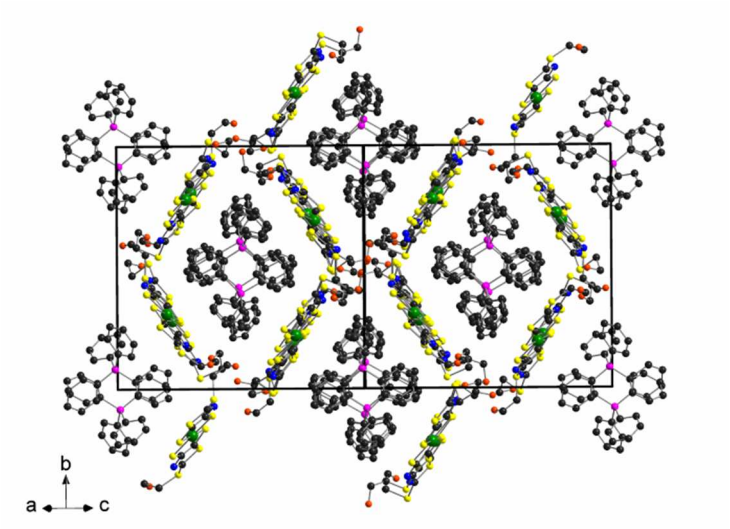

Fig. S1 Detail of the unit cell of $[Ph_4P][Au(HOEt\text{-}tzdt)_2]$

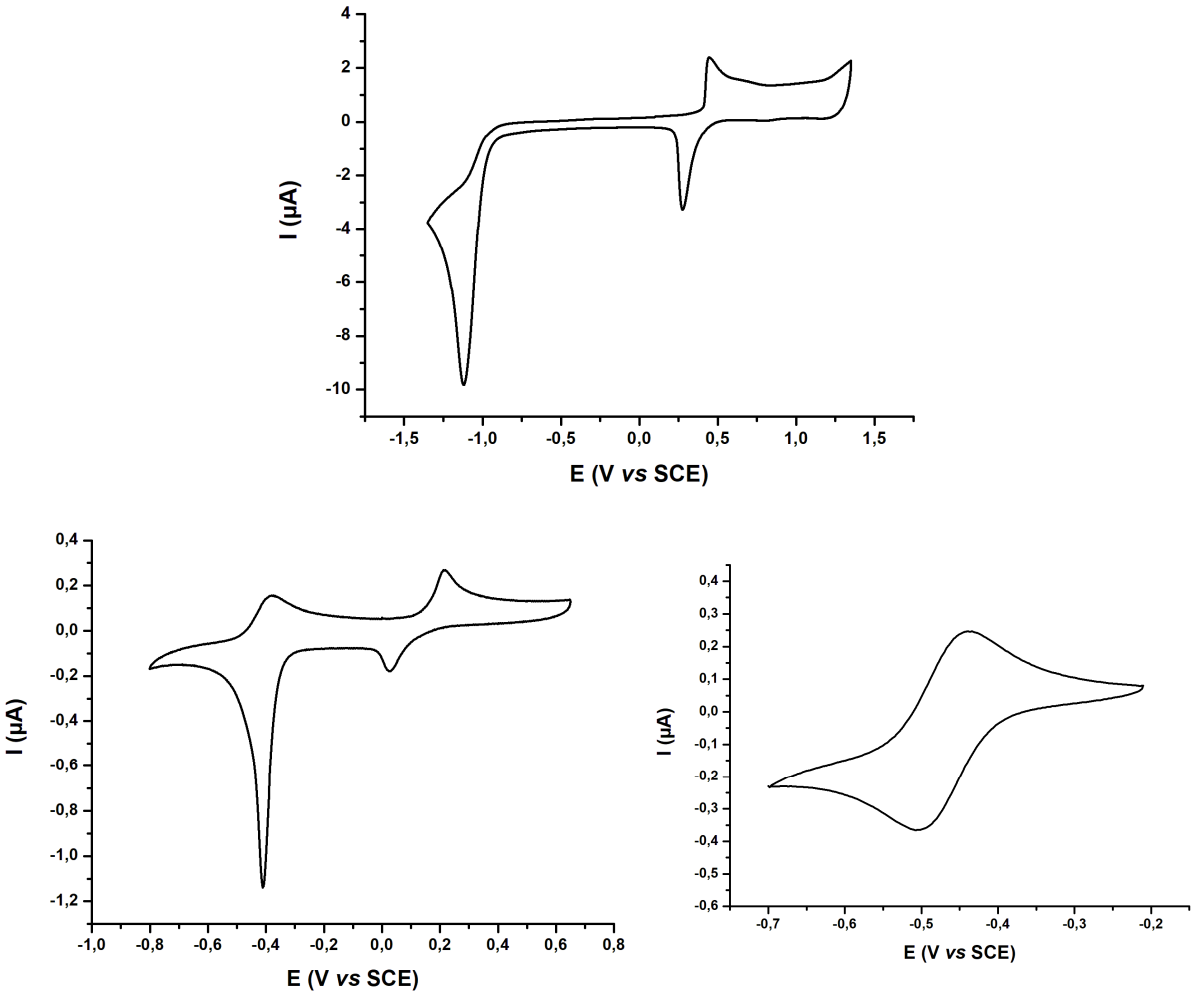

Fig. S2 CVs of $[Ph_4P][Au(HOEt\text{-}tzdt)_2]$ (top) and $[Ph_4P][Ni(HOEt\text{-}tzdt)_2]$ (bottom left) and scan of the first oxidation process of $[Ph_4P][Ni(HOEt\text{-}tzdt)_2]$ (bottom right) in CH_2Cl_2 with 0.1M NBu_4PF_6, at 100 $mV.s^{-1}$

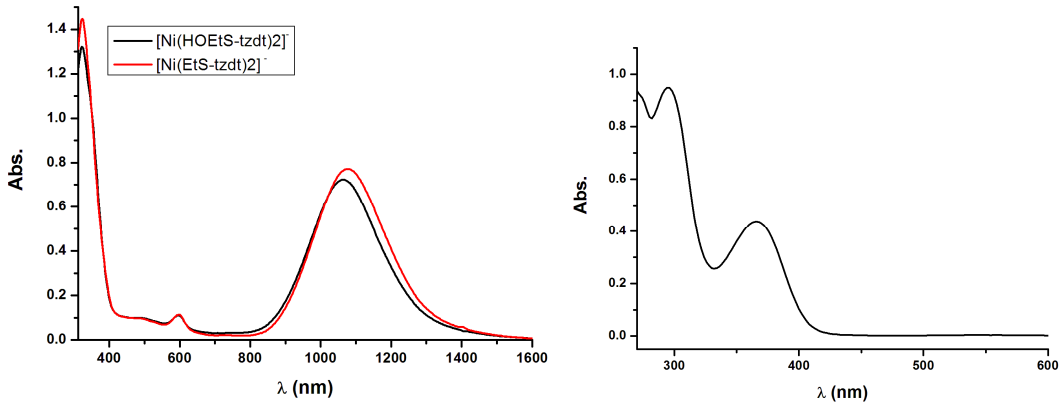

Fig S3 UV-vis-NIR spectra of $[Ni(RS\text{-}tzdt)_2]^{-1}$ (R = EtOH, Et) (left), and UV-vis Spectrum of $[Au(HOEtS\text{-}tzdt)_2]^{-1}$ (right).

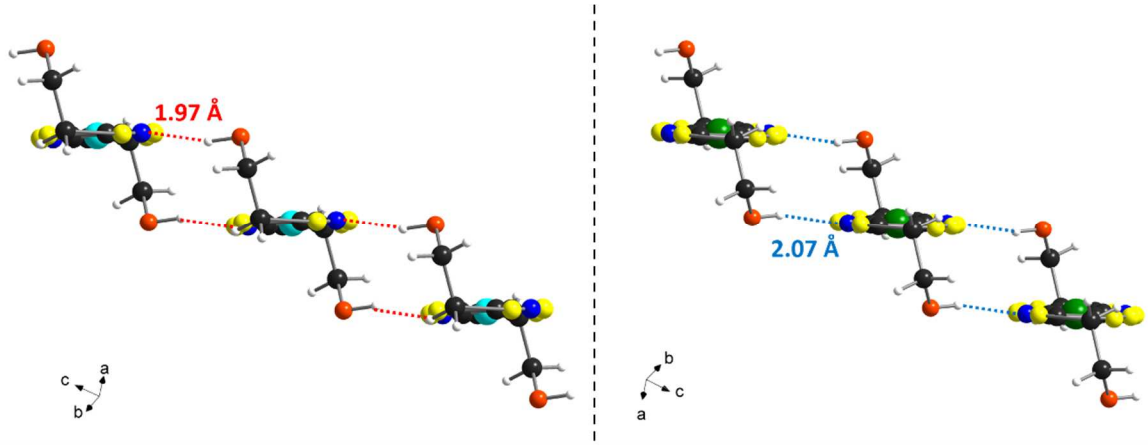

Fig S4 Hydrogen-bonded chains of $[Ni(HOEtS\text{-}tzdt)_2]^0$ (left), and $[Au(HOEtS\text{-}tzdt)_2]^{0\bullet}$ (right) running along *c*.

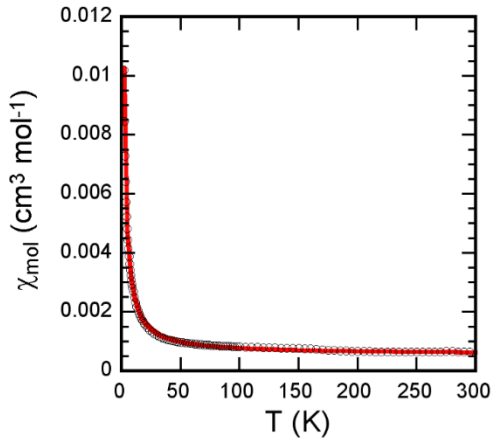

Fig S5. Temperature dependence of the magnetic susceptibility of [Au(HOEt-tzdt)$_2$].

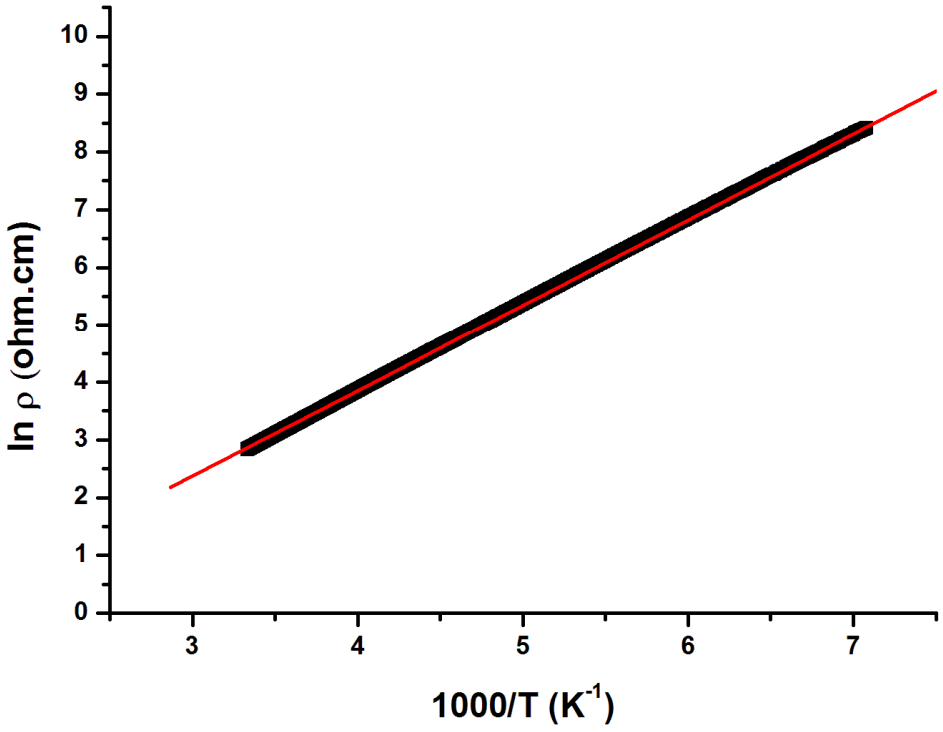

Fig S6. Resistivity data of [Au(HOEt-tzdt)$_2$] The red line is the fit to the data giving the activation energie E_a.

Band structure calculation

The exponents, contraction coefficients, and atomic parameters are detailed below

STO **Ni**4s. 4p. 3d.
-9.170000 1.825000 1.00000
-5.150000 1.125000 1.00000
-13.490000 5.750000 0.568300 2.000000 0.629200

STO **Pt** 6s. 6p. 5d.
-9.077000 2.554000 1.00000
-5.475000 2.554000 1.00000
-12.590000 6.013000 0.633400 2.696000 0.551300

STO **Au** 6s. 6p. 5d.
-10.920000 2.602000 1.00000
-5.550000 2.584000 1.00000
-15.076000 6.163000 0.685100 2.794000 0.569600

STO **S** 3s. 3p.
-20.000000 2.662000 0.556400 1.688000 0.487300
-13.300000 2.338000 0.521200 1.333000 0.544300

STO **Se** 4s. 4p.
-20.500000 3.138700 0.616250 1.889960 0.512890
-13.200000 2.715040 0.550890 1.511400 0.572150

STO **C** 2s. 2p.
-21.400000 1.625000 1.00000
-11.400000 1.625000 1.00000

STO **H** 1s.
-13.600000 1.300000 1.00000

STO **N** 2s. 2p.
-26.000000 1.950000 1.00000
-13.400000 1.950000 1.00000