

[Au(α -spdt) $_2$] 0 : a Gold Bisdithiolene Complex with a Selenophene Ligand

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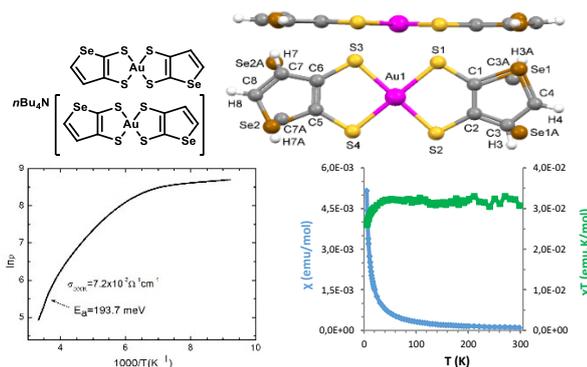
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[Au(α -tpdt) $_2$] 0 , which is a transition metal bisdithiolene complex (the inorganic analogues of tetrathiafulvalenes (TTF)), is one of the first known examples of the so called Single Component Molecular Metals (SCMM). This small neutral molecule displays a room temperature conductivity of 7 S cm⁻¹ as a polycrystalline sample. The observed transport properties, typical of a metal, are believed to arise from the intermolecular interactions in the solid state.^[1] Apart from the transport properties, SCMM also share with typical elemental metals the fact of being a neutral specie. One of the main features of the transition metal bisdithiolene complexes is the possibility of molecular engineering to develop multifunctional materials.

The aim of this work was to design and develop a new SCMM by replacing the thiophene for a selenophene ring in the structure of [Au(α -tpdt) $_2$] 0 . We present [Au(α -spdt) $_2$] 0 , a new neutral gold bisdithiolene complex with a semiconductor behaviour. This complex was obtained by oxidation of its precursor, the salt *n*Bu₄N[Au(α -spdt) $_2$], which, in turn, was obtained from selenolo[2,3-*d*]-1,3-dithiole-2-thione.^[2,3]

The transport properties of [Au(α -spdt) $_2$] 0 reveal a semiconducting behaviour, with a room temperature electrical conductivity of 7.2x10⁻³ S.cm⁻¹ and an activation energy of 193.7 meV. The magnetic susceptibility measurements indicate a paramagnetic behaviour of [Au(α -spdt) $_2$] 0 with a room temperature paramagnetic susceptibility of 1.03x10⁻⁴ emu/mol. The values are almost temperature independent, in a wide range of temperatures, resembling a Pauli like behaviour.

[Au(α -spdt) $_2$] 0 , and its precursor, *n*Bu₄N[Au(α -spdt) $_2$], are just the first members of a new family of transition metal bisdithiolene and bisdiselenolene complexes with selenophene ligands, that we intend to study.



[1] D. Belo, H. Alves, E.B. Lopes, M.T. Duarte, V. Gama, R.T. Henriques, M. Almeida, A. Pérez Benítez, C. Rovira, C., J. Veciana, *Chem. Eur. J.*, **2001**, 7, 511.

[2] M. Andrade, R. Silva, I. Santos, E. Lopes, S. Rabaça, L. Pereira, J. Coutinho, J. Telo, C. Rovira, M. Almeida and D. Belo, *Inorg. Chem. Front.*, **2017**, 4, 270.

[3] T. Jigami, K. Takimiya and T. Otsubo, *J. Org. Chem.*, **1998**, 63, 8865.