Gold Bis-selenophenedithiolene Complexes

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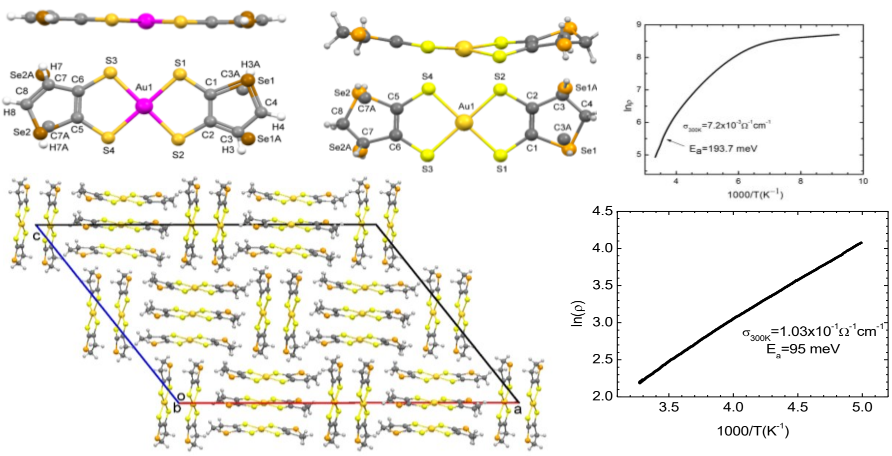
The transition metal bisdithiolene complex $[Au(\alpha\text{-tpdt})_2]^0$ is a small neutral molecule that displays a room temperature conductivity of 7 Scm^{-1} as a polycrystalline sample.[1] As the nickel complex $[Ni(tmdt)_2]$ reported by A. Kobayashi and co-workers, this molecule is also one of the first known examples of the so called Single Component Molecular Metals (SCMM).[2] The measured transport properties, characteristic of metals, are thought to rise from the intermolecular interactions in the solid state.[3] The resemblance of this materials with metals lies not only on the transport properties but also on the neutral nature of these materials. The main advantage of SCMM is the possibility of molecular engineering to develop multifunctional materials.

The purpose of this work was to develop novel gold bis-selenophenedithiolene complexes with similar structure to $[Au(\alpha\text{-tpdt})_2]^0$ but changing the peripheral sulphur atoms for selenium atoms and evaluate the impact of this structural changes in the transport properties. Two gold bisdithiolene complexes with a peripheral five member ring with selenium in the alpha position were synthesised and characterised. $[Au(\alpha\text{-spdt})_2]^0$ was obtain by oxidation with iodine of its tetrabutylammonium salt and $[Au(\alpha\text{-scpdt})_2]^0$ was obtain by electrodeposition of the respective tetrabutylammonium salt. In turn, these salts were obtain from the synthesised selenolo[2,3-*d*]-1,3-dithiole-2-thione and 5,6-dihydroselenolo[2,3-*d*]-1,3-dithiole-2-thione, respectively.[4]

Both neutral gold bis-selenophenedithiolene complexes showed a semiconducting behaviour. The transport properties of $[Au(\alpha\text{-scpdt})_2]^0$ were measure in a crystalline sample and revealed a room temperature electrical conductivity of 0.103 $S.cm^{-1}$ and an activation energy of 95 meV. On the hand the transport properties of $[Au(\alpha\text{-spdt})_2]^0$ were measure in a polycrystalline sample due to the small size of the obtained crystals. The polycrystalline sample revealed a room temperature electrical conductivity of 7.2×10^{-3} $S.cm^{-1}$ and an activation energy of 193.7 meV. The magnetic susceptibility measurements exhibited a paramagnetic behaviour, with a room temperature paramagnetic susceptibility of 1.03×10^{-4} emu/mol. In a wide range of temperatures, the values are almost temperature independent, resembling a Pauli like behaviour.



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