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Non-Covalent Interactions in Molecular conductors: Gold bis-dithiolene complexes

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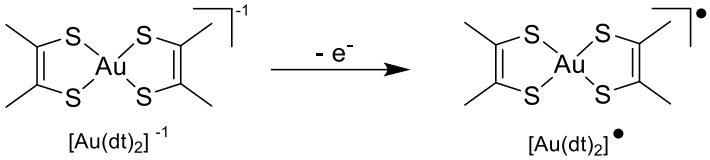
Molecular conductors, be they built out of fully organic or coordination compounds, raise a lot of interest for their applications in organic electronics and in energy storage devices.[1,2] The search for highly conducting materials, blessed with metallic or even superconducting properties is based on our ability to control intermolecular interactions between radical species in the crystalline solid state. Among such interactions, hydrogen bonds (HBs) and the so-called σ-hole interactions such as halogen bonding (XB, X = I, Br)[3] or chalcogen bonding (ChB; Ch = Se, Te)[4] can bring, thanks to their high directionality, novel solid-state architectures and associated physical properties. Neutral radical bis(dithiolene) gold complexes $[Au(dt)_2]^{\bullet}$ are known to exhibit remarkable properties, such as strong delocalization of the spin density on the two dithiolene ligands and as a consequence, these complexes are of interest for the elaboration of *single component molecular conductors.*[5] We investigated these intermolecular interactions (HB, XB, ChB) on a series of monoanionic and neutral radical gold dithiolene complexes and their influence on conducting properties.



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