Single component molecular conductors based on closed shell Ni bis(dithiolene) and bis(diselenolene) complexes

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Metal-*bis*(dithiolene) complexes have been intensively studied as precursors of conducting materials either in multi-component or single-component molecular materials. Most of these conducting materials involve open shell species, either charged ones, as in the well-known [TTF][Ni(dmit)₂]₂,¹ or neutral radical species, such as [Au(R-thiazdt)₂].² Recently investigations carried out on the prototypal Ni(dmit)₂ have demonstrated that this closed-shell neutral Ni complex can behave as a single component molecular conductor which turns metallic under very high pressures.³ Within this frame we also demonstrated that another Ni complex, the [Ni(Et-thiazdt)₂], with an electron rich *N*-ethyl-1,3-thiazoline-2-thione-4,5-dithiolate (Et-thiazdt) ligand, could also behave as a promising single component molecular conductor.⁴ In order to explore further this family and its behavior under pressure, we considered the possibility of substituting sulfur atoms for selenium ones because such substitutions are well known to increase the band dispersion in molecular conducting systems. Thus, we decided to explore the methyl derivative [Ni(Me-thiazdt)₂], as well as the diselenolated complexes [Ni(R-thiazds)₂] (R=Me, Et), in order to unravel the effects of these structural changes on the electronic, spectral, and transport properties of the complexes. Highly conducting materials were indeed obtained from both the dithiolene and diselenolene complexes.



References

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