



Bimetallic neutral palladium (II) bis(dithiolene) complex: Unusual synthesis, structural and theoretical study

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Résumé en anglais	<p>The unusual synthesis of the dimeric dithiolene complex [PPh₃Pd(ethylene-1,2-dithiolate)]₂ (1), containing the simplest dithiolene ligand, has been achieved through the reaction between tetrathiafulvalene (TTF) and Pd(PPh₃)₄. The complex shows a folded structure in the solid state, according to single crystal X-ray analysis performed on crystals grown from two different system solvents and conditions, with a central [Pd₂S₂] ring folded about the S center dot center dot center dot S hinge by 67.9 degrees. The optimized geometry at the DFT level is in excellent agreement with the experimental structure. Moreover, TD-DFT calculations allowed the assignment of the low energy band arising at 576 nm to the HOMO - LUMO transition, between frontier orbitals having mixed metal and dithiolene character. (C) 2012 Academie des sciences. Published by Elsevier Masson SAS. All rights reserved.</p>
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