Synthesis of Novel Transition Metal Dithiolenes. Synthesis, Experimental and Theoretical Investigation.

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Transition-metal complexes with 1,2-dithiolene ligands have received much attention because of their capacity to give molecular metals and superconductors [1] and more recently because of their potential applications as thirdorder non-linear optical materials [2]. The importance in the chemistry of such square-planar M(dithiolene)₂ complexes is due to their ability to overlap with each other including strong electronic interactions between the units, which is a condition to obtain electronic properties, such as conductivity or even unusual magnetic behavior [3]. These M(dithiolene)₂ complexes have a similar structure to the tetrathiafulvalene (TTF) and that is the reason for further investigation in these areas [4]. Among them the metal complexes of 5, 6-dihydro-1, 4-dithiin-2, 3-dithiol (dddt) [5] are the most important due to similarities with the BEDT-TTF. BEDT-TTF [6] was permitted the synthesis of radical cation salts with a quasi two-dimensional character gave more than 750 superconductors [7] and raised their critical temperature at 14.2 K [8].

The lecture will focus in the synthesis and study of a new Transition metal 1, 2-dithiolene, similar to (dddt) (FIGURE 1). The experimental measurents will also be compared with the results from theoretical investigations by employing computational approaches, involving density functional theory and semiempirical methods [9].



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