

PALLADIUM(II) COMPLEXES BASED ON N,S-DONOR LIGANDS: SYNTHESIS AND MOLECULAR STRUCTURES

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Phenyl(chloro)dithioformate is treated with pyrazole derivatives and phenyl(Pz-1-carbodithioate) ligands (Pz = pyrazole (**1**), 3-methylpyrazole (**2**), and 3,5-dimethylpyrazole (**3**)) are obtained. These ligands are treated with PdCl₂ in acetonitrile and complexes of the general formula Pd(L)Cl₂ form in an essentially quantitative yield. The ligands are found to be N,S-bidentate linkers, and 5-membered palladacycles are obtained. Precursors **1-3** are oily materials and characterized by ¹H and ¹³C NMR spectroscopy. Due to a partial solubility of Pd complexes, the complete set of NMR data cannot be collected. The structural elucidation is also accompanied by elemental and mass spectrometric analyses. Solid-state structures of complexes **5** and **6** are determined by X-ray diffraction. The data obtained for complexes **5** and **6** are also calculated by DFT using the *TURBOMOLE* program package. Experimental and calculated data sets are found to be in close agreement with each other.

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