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A comparative study of Pd/Pt-cyclopropa[60]fullerenes compounds with ambidentate phosphorous ylide ligands; Synthesis and DFT calculations

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Functionalization of fullerenes C_{60} and investigation of their new properties, in particular biological and reactivity studies of these compounds have attracted the attention of academic researchers in the past decades [1]. Although there are many reports of metallofullerenes [2], few studies have focused on the Pd/Pt-cyclopropa[60]fullerene complexes bearing phosphorus ligands [3]. Among them, the simple mono- and diphosphines are the most widely used ligands coordinated to C_{60} and neutral Pd(0)/Pt(0) core which form metallacyclopropa[60]fullerene complexes [4]. Versatile functionalized diphosphines, especially α-keto stabilized phosphorus ylides can coordinate to transition metal ions through the terminal PPh_2 group and/or formally negatively charged carbanion [5]. In this work, reaction of C_{60} with [Pd/Pt$(dba)_2$] (dba= dibenzylideneacetone) and phosphorus ylides [$Ph_2P(CH_2)_nPPh_2C(H)C(O)C_6H_4$-*m*-OMe] (n=1, (**L^1**); n=2, (**L^2**)) gave the new Pd/Pt-[60]fullerene complexes These complexes have been fully characterized by spectroscopic methods (^{1}H, ^{13}C and ^{31}P) and other conventional techniques such as IR, elemental analysis and mass spectrometry. Theoretical studies confirmed the P,C-chelation and P-coordination behaviors of ligands **L^1 and L^2**, respectively.

Keywords: Synthesis, Pd/Pt-[60]fullerene complexes, Phosphorus ylide, DFT studies, Multinuclear NMR

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