22nd Iranian Chemistry Conference, 23-25 August, 2023
University of Kurdistan

Construction of Organoplatinum(II) Complexes by a Tripod Phosphine Ligand: A Joint Experimental and Computational Investigation

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The chemistry of 1,1,1-tris(diphenylphosphino)methane (tppm) as a ligand is less explored [1] in comparison with bis(diphenylphosphino)methane (dppm) [2], and only a handful of studies are documented in the literature. This ligand opens up an opportunity for systematic investigation of the steric and electronic effects on chemical and physical properties, in which, by purposeful variation of the substituent groups on phosphorus, a wide array of properties can be "fine-tuned" [3]. Taking this considerable potential into account, two organoplatinum(II) complexes [PtR_2(tppm)] (R = Me, **1**, *p*-MeC_6H_4, **2**) were synthesized starting from the well-known precursor [$PtR_2(SMe_2)_2$] (R = Me, **A**, *p*-MeC_6H_4, **B**) through ligand substitution in acetone. The structures of the obtained Pt(II) complexes were characterized by NMR spectroscopy, HR ESI-MS(+), and X-ray crystallography (Figure 1). In these Pt(II) complexes, the tppm ligand is bound to the Pt center *via* monodentate-chelating mode, rendering one of the tppm's P atoms uncoordinated. In the following, computational calculations using density functional theory (DFT) and time-dependent DFT (TD-DFT) were carried out in order to gain deep insight into experimental observations.

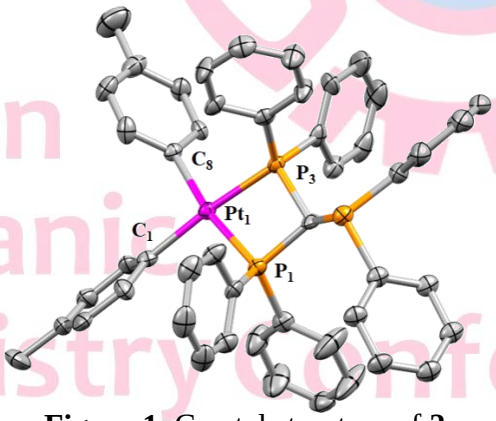


Figure 1. Crystal structure of **2**.

Keywords: Ligand substitution reaction, Organoplatinum complexes, Phosphine ligand, Theoretical calculations.

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