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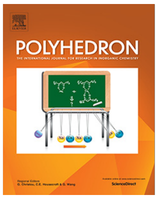

Synthesis and structural characterization of a palladium complex as an anticancer agent, and a highly efficient and reusable catalyst for the Heck coupling reaction under ultrasound irradiation: A convenient sustainable green protocol

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ABSTRACT

The complex $[Pd(paOH)_2].2Cl$ (**1**) was synthesized by the self-assembly method with palladium chloride and pyridine-2-carbaldehyde-oxime (paOH) in aqueous acetonitrile solution under ambient conditions. Complex **1** was fully characterized by FT-IR, UV–vis and NMR spectroscopic techniques, as well as elemental analysis. The single crystal X-ray structure of complex **1** indicates that the Pd(II) ion is bonded to four nitrogen atoms from two pyridine-2-carbaldehyde-oxime ligands. The molecular geometry of the Pd(II) ion in complex **1** is distorted square-planar with a trans geometry and with two free chloride ions. Using an MTT assay, the anticancer activities of the palladium complex **1** were studied with respect to human breast cancer (MCF-7) and hepatocellular carcinoma (HePG-2) cell lines. The data obtained show that complex **1** displays strong activity towards the viability and the growth of the cancer cell lines MCF-7 and HepG2. Additionally, complex **1** exhibits excellent catalytic activity for the Heck cross-coupling reaction with water as the solvent under ultrasound irradiation. Ultrasound irradiation not only enhanced the rate and the yield of the reaction, but also promoted the in *situ* generation of a well-dispersed zero-valent Pd-colloidal species as the active catalyst from complex **1**. Finally, the luminescence spectrum of complex **1** is discussed.

1. Introduction

The C—C cross-coupling reactions between aryl halide derivatives and olefins (the Heck reaction), catalyzed by a transition metal catalyst (such as palladium) under mild reaction conditions are of outstanding importance in contemporary research in organic synthesis, in which organic synthesis nowadays focuses on sustainability [1]. It is worth mentioning that the Nobel Prize in chemistry 2010 was awarded jointly to Akira Suzuki, Richard F. Heck and Ei-ichi Negishi for palladium-catalyzed C—C cross couplings in organic synthesis [2,3]. This significantly and successfully demonstrates the importance of developing C—C cross coupling reactions in current modern organic chemistry. Synthetic organic chemistry has become more important nowadays during these challenging times of "appearing new diseases." Most medicinal chemists work worldwide to introduce new organic compounds, according to a basic set of design rules, as novel organic compounds for biological screening. Therefore, there is an increasing need to develop an efficient synthetic organic methodology for important organic reactions such as "Heck C—C coupling".

In the last decade, Dawood and Kirsching introduced a catalytic activity study of a pyridine-2-carbaldehyde-oxime based Pd(II)-complex covalently anchored *via* the oxime moiety to a glass/polymer composite material for Suzuki–Miyaura cross-coupling. Although the later catalytic activity study clarified the stability and reusability of this Pd complex, which involved the microreactor technique [4], due to increasing economic and ecological pressure, investigations in modern organic synthesis are now directed to the discovery of methods that largely take into account the criterion of simplicity and sustainable chemistry [5].

On the other hand, the importance of utilizing greener solvents has permeated into all aspects of synthetic chemistry. As we know, cross-coupling reactions are preferentially carried out in highly

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