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Synthesis and characterization of a palladium(0) complex with cyclophosphazene bearing two diphenylphosphine ligands and application in Suzuki-Miyaura cross-coupling

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TITLE: Synthesis and characterization of a palladium(0) complex with cyclophosphazene bearing two diphenylphosphine ligands and application in Suzuki-Miyaura cross-coupling

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Abstract

This paper describes the synthesis of a cyclophosphazene-based diphenylphosphine ligand and a new Pd(0) complex. Infrared spectroscopy (ATR-IR), ESI+-MS, ³¹P, ¹H and ¹³C NMR, Raman, WD-XRF, ICP-OES and TGA analysis show the coordination of two palladium atoms per unit of cyclophosphazene. A semiempirical calculation method was employed to find the lowest energy structure among the possible ones and Density Functional Theory (DFT) was used to optimize the found structure and obtain its bond angles, dihedral angles, bond lengths, atomic distances, and to calculate the vibrational spectrum (PBE/def2-TZVP(-f)). The new Pd complex showed activity in Suzuki-Miyaura cross-coupling reactions with halobenzenes and phenylboronic acid, tolerating different functional groups.

KEYWORDS: Pd(0) complexes; cyclophosphazene-based ligands; Suzuki-Miyaura cross-coupling.

1. Introduction

Palladium-catalyzed cross-coupling reactions are among the most important synthetic tools for organic chemistry, providing facile access to carbon-carbon (C-C) bond construction. In particular, the Suzuki-Miyaura C-C coupling experienced a notorious growth in both publications and patents over the past decades when compared to other classes of C-C coupling [1,2]. This approach became the most attractive due to several advantages such as mild reaction conditions and tolerance to many functional groups. The improvement of

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