

Abstract

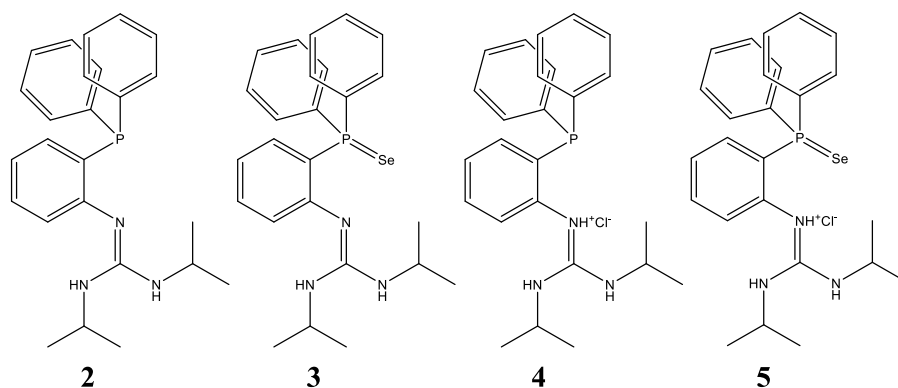
Title: Synthesis and coordination properties of phosphinoguanidine ligands

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Abstract: The aim of this work was the preparation and characterisation of a hybrid P,N-donor ligand, 2-(2-(diphenylphosphanyl)phenyl)-1,3-diisopropylguanidine (compound **2**), containing a polar guanidine moiety. Potential use of this ligand lies in the preparation of catalytically active complexes with a possible change of distribution between organic and water phase upon altering pH.



Firstly, synthesis of the starting material, (2-aminophenyl)diphenylphosphine, by copper(I)-catalysed P-C coupling reaction was optimized, up to 88% yield. Preparation of compound **2** was optimized as well. Salt **4** was prepared by protonation of **2**. In order to evaluate basicity of phosphine groups in the structure of **2** and **4** and an impact of guanidine moiety protonation, corresponding selenides **3** and **5** were prepared and the $^1J_{\text{PSe}}$ were measured. Ligand **2** was prepared by addition of (2-aminophenyl)diphenylphosphine across 1,3-diisopropylcarbodiimide. Selenide **3** was obtained from reaction of **2** with KSeCN. Salts **4** and **5** were prepared by neutralizing compounds **2** and **3** with hydrochloric acid. All novel compounds were characterized by ^1H , $^{13}\text{C}\{^1\text{H}\}$ and $^{31}\text{P}\{^1\text{H}\}$ NMR spectroscopy, IR spectroscopy and mass spectrometry. Purity of compounds was determined using elemental analysis. Structures of compounds **3**, **4** and **5** were confirmed by single crystal X-ray diffraction experiments.

Keywords: guanidine, phosphine ligands, synthesis, phosphinoselenides, guanidinium salts