Title: Synthesis and characterization of bidentate P,N-donor ferrocene ligand

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The main goal of this thesis was the preparation and characterization of ferrocene ligand 4-[1'-(diphenylphosphino)ferrocen-1-yl]morpholine (compound 3). Compared to structurally similar compounds, compound 3 offers greater geometrical flexibility which might have a positive effect in some applications, for example in catalysis by transition metal complexes.

Two new compounds were synthesized along the synthetic route of phosphinoamine 3, the protected amine 1 and morpholine derivate 2. Selenide 4 was prepared in order to determine the basicity of compound 3 via the direct scalar interaction of ⁷⁷Se with ³¹P. The synthesis comprised phosphinylation of 1,1'-dibromoferrocene, protection of the obtained 1-bromo-1'-(diphenylphosphino)ferrocene with sulfur, azidation and immediate reduction to protected amine 1. Morpholine derivate 2 was subsequently synthesized by cyclization reaction with bis(2-chloroethyl)ether. Phosphinoamine 3 was obtained by deprotection of compound 2 with Raney nickel. Finally, selenide 4 was obtained by the reaction of 3 with KSeCN. All newly prepared compounds were analyzed by NMR and transmission IR spectroscopy and by ESI mass spectrometry. The purity of compounds was verified by elementary analysis. Compounds 1, 2 and 3 were further analyzed by X-ray diffraction which provided detailed structures of the compounds.

Keywords: phosphine ligands, ferrocene, hybrid ligands, structure elucidation.