Title: Phosphinoferrocene amides and hydrazides
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Abstract: While studying functionalized phosphinoferrocene ligands, we recently turned to phosphinoferrocene carboxamides. These donors already proved to be versatile ligands for coordination chemistry and catalysis. This led us to synthesize and study the archetypal representative, 1´-(diphenylphosphino)-1-carbamoylferrocene (5), and the corresponding hydrazide 6.

This work describes the preparation of primary amide 5 and hydrazide 6 from 1´-(diphenylphosphino)-1-ferrocenecarboxylic acid (Hdpf) via the corresponding acylbenzotriazole derivative. The hydrazide was alternatively obtained from Hdpf methylester and hydrazine hydrate. Both newly synthesized compounds were characterized by spectroscopic methods (NMR, IR, and MS) and elemental analysis, and their crystal structures were determined by single-crystal X-ray crystallography. The amide was further utilized in the preparation of several palladium complexes, which were characterized in a similar manner including X-ray crystallography. One palladium complex was obtained also from the hydrazide. However, the hydrazide was used mainly as a starting material for the preparation of phosphinoferrocene heterocycles. The 1,3,4-oxadiazole derivative 7 resulting from 6 and triethyl orthoformate and 3,5-dimethyl-1,2-pyrazole 8 were prepared, structurally characterized and further used as ligands in palladium complexes.

Keywords: ferrocene, phosphines, amides, hydrazides, 1,3,4-oxadiazoles, 3,5-dimethyl-1,2-pyrazoles, coordination compounds, palladium.