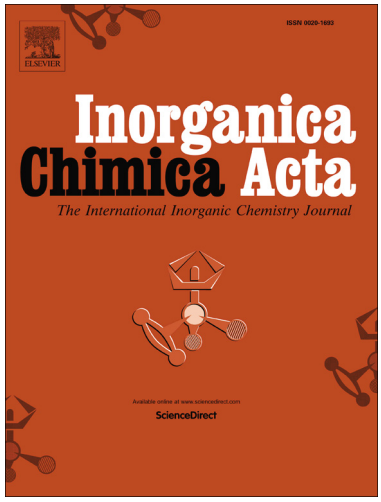

Research paper

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Palladium Complexes Bearing Pyridylthioether Ligands. Synthesis and Application as Efficient Phosphine-Free Catalysts in Suzuki-Miyaura Couplings

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Abstract

Pyridylthiother-ligated Pd(II) complexes have been synthesized and efficiently applied in Suzuki-Miyaura couplings using microwave irradiation in DMF and water. The pyridylthioether NS (NS1 and NS2) and pyridyldithiother (SNS) ligands and their corresponding palladium complexes Pd-NS1, Pd-NS2, Pd-SNS were easily synthetized and fully characterised by various analytical techniques. The molecular structures of the ligand SNS and the Pd(II) complexes Pd-NS2, Pd-SNS were unequivocally determined by single crystal X-ray diffraction analysis. From these compounds, complex Pd-SNS exhibits the ligand SNS coordinated in a *N,N*-bidentated rather than the typical SNS-pincer manner in the solid state, giving place to a seven membered palladacycle whereas in solution it behaves as a typical SNS-pincer complex. This compound was also found to be the most efficient catalyst of the series of complexes in Suzuki-Miyaura couplings with different *p*-substituted aryl bromides.

Keywords*:* Palladium complexes, sulfur based ligands, cross-coupling, Suzuki-Miyaura coupling, catalysis, Thioether ligands.
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