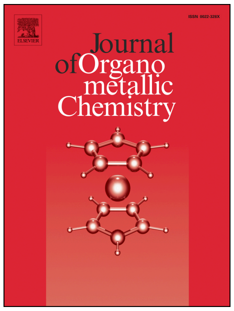

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Iridium(III)- Benzoxazolyl and Benzothiazolyl Phosphine Ligands Catalyzed Versatile Alkylation Reactions with Alcohols and the Synthesis of Quinolines and Indole

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Keywords: Iridium; Benzoxazolyl or benzothiazolyl phosphine ligands; Alkylation; Quinolines

Abstract: A series of benzoxazolyl and benzothiazolyl phosphine ligands **4a-4g** were synthesized and characterized, which prepared from commercially available 2-aminophenol / 2-aminobenzenethiol and 2-bromobenzaldehyde via cyclization and phosphination. The representative ligands **4c** and **4e** were determined by single-crystal X-ray diffraction. The corresponding iridium complexes could be generated *in situ* when $[Cp^*IrCl_2]_2$ (Cp* = pentamethylcyclopentadienyl) encountered ligands. The molecular structures of complexes **5c** and **5e** were crystallographically characterized. The dihedral angles of N(1)-C(1)-C(8)-C(9) showed an increasing twist compared with the corresponding ligand. The iridium(III) catalysts were screened, $[Cp^*IrCl_2]_2$ / **4a** proved to be the optimal catalyst, which exhibited efficient catalytic activity toward versatile alkylations including ketones, secondary alcohols and amines with primary alcohols. Additionally, the synthesis of quinolines from ketones with 2-aminobenzyl alcohol by intermolecular cyclization and indole from 2-(2-aminophenyl)ethanol by intramolecular cyclization were achieved