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## ACCEPTED MANUSCRIPT

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<sub>2</sub>]<sub>2</sub> (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<sub>2</sub>]<sub>2</sub> / 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

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