

# Computational study on the mechanism of metal-free photochemical borylation of aryl halides

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## Abstract

C-radical borylation is an significant approach for the construction of carbon-boron bond. Photochemical borylation of aryl halides successfully applied this strategy. However, precise mechanisms, such as the generation of aryl radicals and the role of base additive(TMDAM) and water, remain controversy in these reactions. In this study, photochemical borylation of aryl halides has been researched by density functional theory (DFT) calculations. Indeed, the homolytic cleavage of the C-X bond under irradiation with UV-light is a key step for generation of aryl radicals. Nevertheless, the generation of aryl radicals may also undergo the process of single electron transfer and the heterolytic carbon-halogen bond cleavage sequence, and the latter is favorable during the reaction.

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