

Facile synthesis of N- (4-bromophenyl)-1- (3-bromothiophen-2-yl)methanimine derivatives via Suzuki cross-coupling reaction: their characterization and DFT studies

ABSTRACT

A variety of imine derivatives have been synthesized via Suzuki cross coupling of N-(4-bromophenyl)-1-(3-bromothiophen-2-yl)methanimine with various arylboronic acids in moderate to good yields (58–72%). A wide range of electron donating and withdrawing functional groups were well tolerated in reaction conditions. To explore the structural properties, Density functional theory (DFT) investigations on all synthesized molecules (3a–3i) were performed. Conceptual DFT reactivity descriptors and molecular electrostatic potential analyses were performed by using B3LYP/6-31G(d,p) method to explore the reactivity and reacting sites of all derivatives (3a–3i).

Keyword: Imines; Thiophene; Suzuki coupling; Density functional theory; Computational; Reactivity

