Supporting Information

Ipso-Nitration of Arylboronic Acids with Chlorotrimethylsilane - Nitrate Salts

G. K. Surya Prakash*, Chiradeep Panja, Thomas Mathew, Vijayalakshmi Surampudi, Nicos A. Petasis, and George A. Olah*

Loker Hydrocarbon Research Institute and Department of Chemistry, University of Southern California, Los Angeles, California 90089-1661, USA

General:

Unless otherwise mentioned, all other chemicals were purchased from commercial sources. Commercially available analytical grade DCM was used as the solvent. Chlorotrimethylsilane was distilled and stored in freezer prior to use. All the nitro products are known and are well characterized by comparing their spectral data with those of the authentic samples.

^1H , ^{13}C and ^{19}F NMR spectra were recorded on superconducting NMR spectrometers at 200 or 300 MHz. ^1H NMR chemical shifts were determined relative to internal $(\text{CH}_3)_4\text{Si}$ (TMS) at δ 0.0 or to the signal of a residual protonated solvent: CDCl_3 . ^{13}C NMR chemical shifts were determined relative to internal TMS at δ 0.0 or to the ^{13}C signal of solvent: CDCl_3 at δ 77.0. ^{19}F NMR chemical shifts were determined relative to internal CFCl_3 at δ 0.0. Mass spectra were recorded on a GC-MS spectrometer with a mass selective detector at 70 eV.

Typical procedure for the *ipso*-nitration of arylboronic acids using TMSCl/nitrate salts:

In a Teflon bottle, to arylboronic acid (1 mmol) in dichloromethane (10 mL), nitrate salt (2.2 mmol) and TMSCl (2.2 mmol) were added and closed. The heterogeneous mixture was stirred vigorously at room temperature till the reaction went to completion as monitored by TLC. After completion of the reaction, the mixture was filtered and washed with water (2x 10 mL) and brine solution (10 mL) and then dried over anhydrous Na_2SO_4 . Solvent was removed under reduced pressure to get the nitroarenes, in almost NMR pure grade. The products were well characterized by comparing their spectral data with those of the authentic samples.