

SUPPORTING INFORMATION

Mechanochemistry through extrusion: opportunities for materials design and catalysis

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Abstract: The potentialities of mechanochemistry through extrusion for nanomaterials design and organic synthesis have been herein investigated. In particular, palladium nanoparticles supported on *N*-doped carbons have been prepared via extrusion, employing chitin as carbon and nitrogen source, and ethylene glycol as a green reducing agent, in absence of solvents. The mechanochemical approach demonstrated to be effective for the reduction of Pd(II), the formation of Pd(0) nanoparticles with mean diameter within 6-10 nm, and the generation of a mesoporous network. The catalytic activity of the samples was investigated in the Suzuki-Miyaura cross-coupling reaction of iodobenzene and phenylboronic acid, also via extrusion, achieving promising results with conversion values of 81% and selectivity higher than 99%, representing a biphenyl productivity of 41 mmol g⁻¹ h⁻¹.

Keywords: Mechanochemistry, Extrusion, Catalytic nanomaterials, Suzuki-Miyaura cross-coupling reaction

List of content

- XRD data for Chitin
- Characterization of the coupling products of the Suzuki-Miyaura reaction
 - a. Biphenyl
 - b. 3-Methyl-1,1'-biphenyl

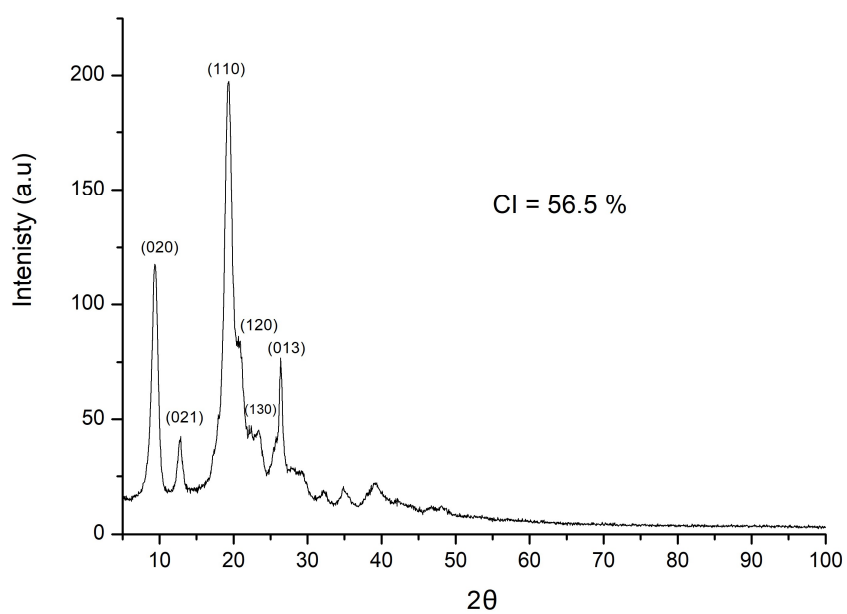


Figure S1. XRD diffractogram of a commercial sample of chitin. CI: crystallinity index

Characterization data

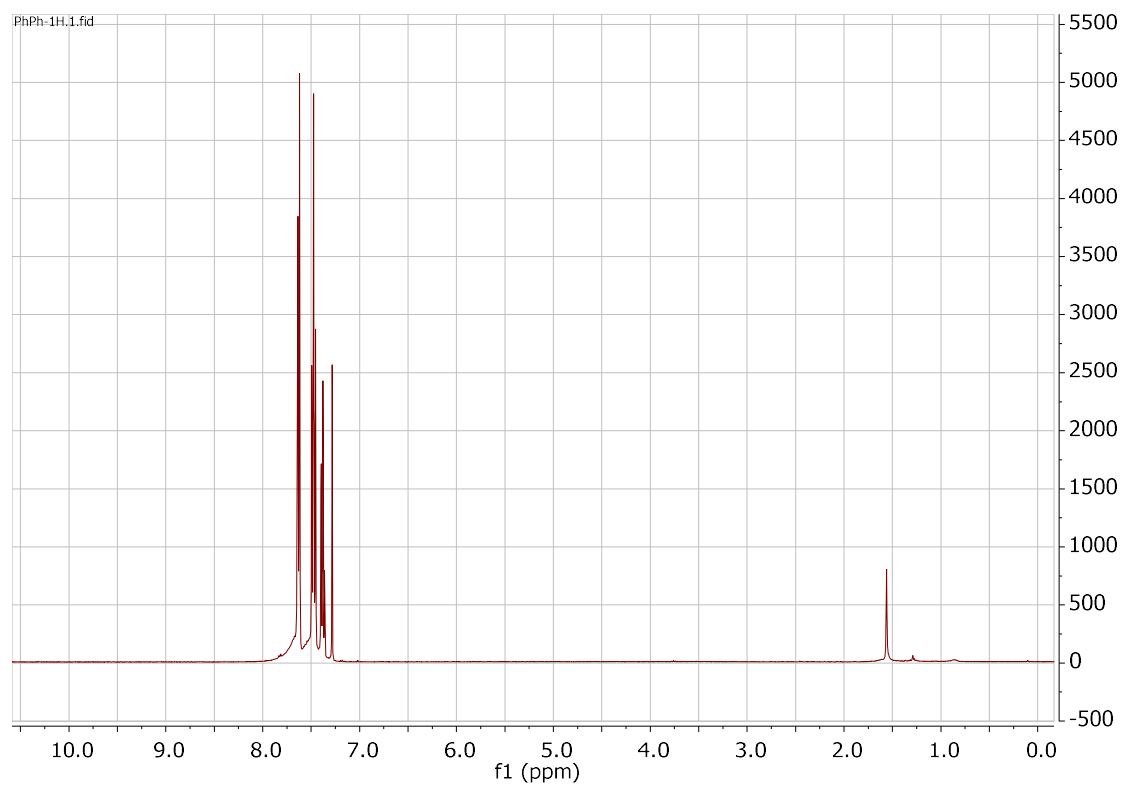


Figure S2. ^1H NMR of biphenyl. ^1H NMR (400 MHz, 298 K, $\text{DMSO}-d_6$) δ 9.62 (s, 1H), 8.10 (d, 1H), 7.54 (t, 1H), 6.78 (d, 1H).

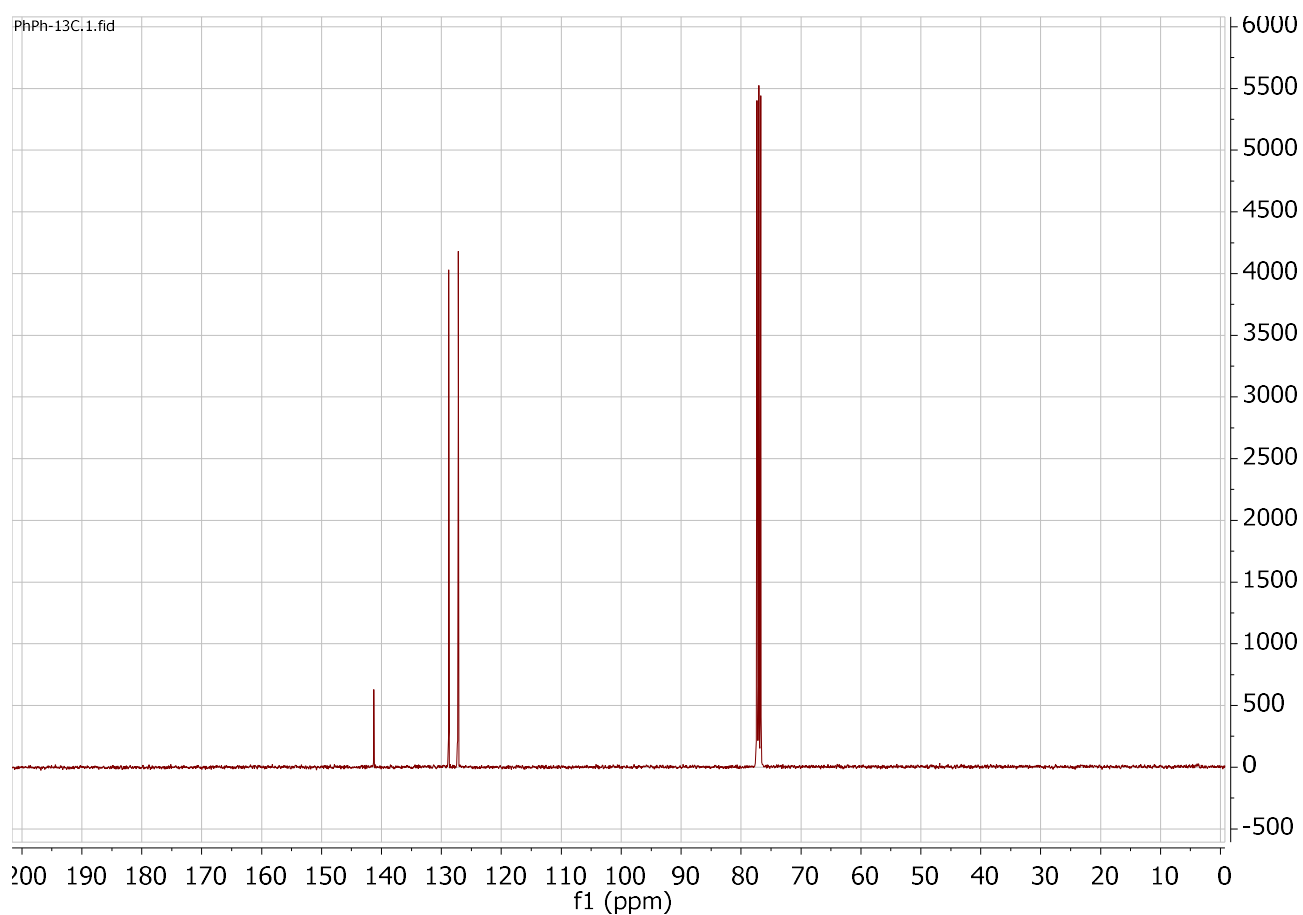


Figure S3. ^{13}C NMR of biphenyl. ^{13}C NMR (101 MHz, 298 K, $\text{DMSO-}d_6$) δ 178.39, 152.50, 149.17, 122.96, 112.89.

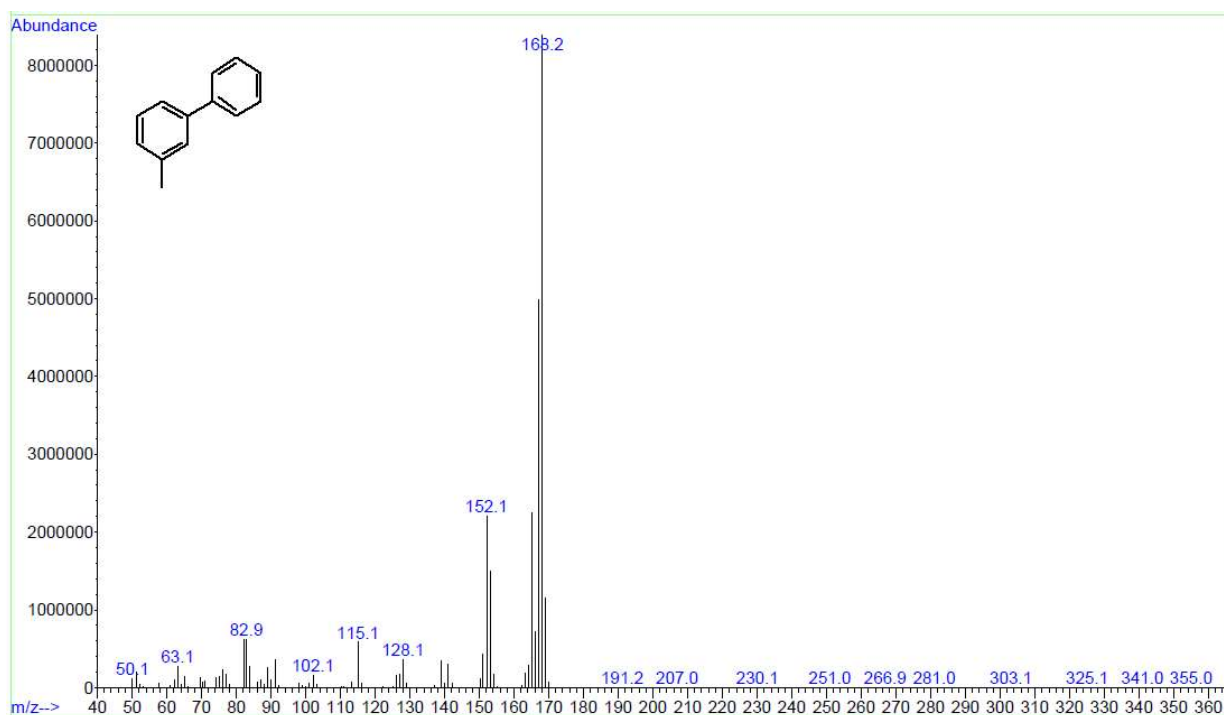


Figure S4. MS spectra (EI, 70 eV) of 3-Methyl-1,1'-biphenyl.