

SUPPLEMENTARY INFORMATION

Coordination-polymer anchored single-site ‘Pd-NHC’ catalyst for Suzuki-Miyaura coupling in water

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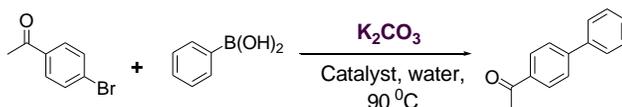
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S1.1 Hot Filtration Test

Phenyl boronic acid (146.3 mg, 1.2 mmol), 4-bromo acetophenone (200 mg, 1 mmol), potassium carbonate (414 mg, 3 mmol) and 0.1 mol % of Pd catalyst were stirred in 4 mL water at 90 °C. After 4 h, the reaction was stopped and the reaction mixture was filtered in hot condition. The filtrate was kept at 90 °C with stirring. The progress of the reaction was monitored by ¹H NMR spectroscopy.

S1.2 Hg-poisoning test



Entry	Time	Additive	Yield (%)
1	8 h	none	98
2	8 h	Hg(1 drop)	84

S1.3 Reusability Test

Phenyl boronic acid (146.3 mg, 1.2 mmol), 4-bromo acetophenone (200 mg, 1 mmol), potassium carbonate (414 mg, 3 mmol) and 0.1 mol % of Pd catalyst were stirred in 4 mL water for 8 h at 90 °C. The water layer was extracted with diethyl ether. Then, the ether extract was evaporated under vacuum and the residue was analysed by ¹H NMR spectroscopy. The catalyst was separated from the water layer by centrifugation and was washed with diethyl ether several times. It was then used for next run of catalysis without further purification.

S1.4 Characterization of the recovered Ru-CP-Pd catalyst

After hot filtration, the recovered catalyst was washed with diethyl ether. Colorless washing solution was decanted and the red solid thus obtained was dried in vacuum. The recovered catalyst was dissolved in DMF and UV-Vis Spectra was recorded and compared with the UV-Vis spectra of an unused sample of Ru-CP-Pd in DMF. In both the cases, approximately 0.1 mg of Ru-CP-Pd was dissolved in 1 mL of DMF. SEM image and EDX were also taken for recovered Ru-CP-Pd. All the analyses suggested a similar nature of both the samples.

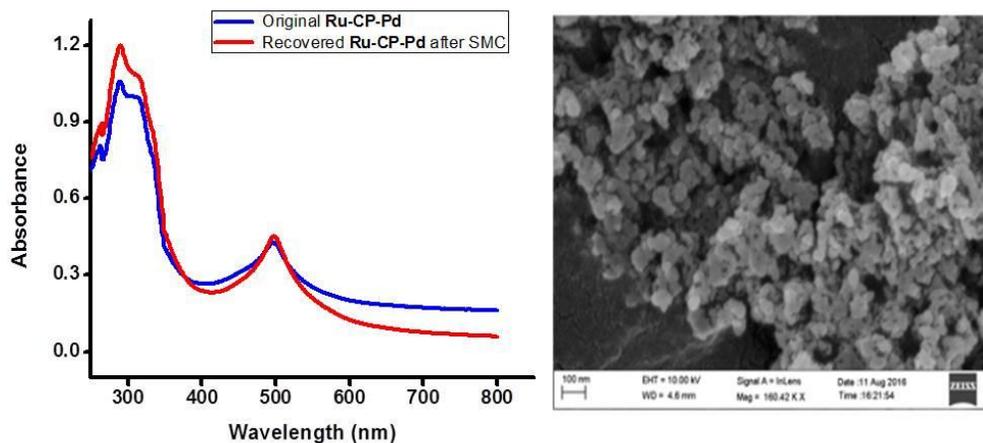


Figure S1. UV-Vis spectra of the original and recovered Ru-CP-Pd catalysts (left), and SEM image of the recovered catalyst (right).

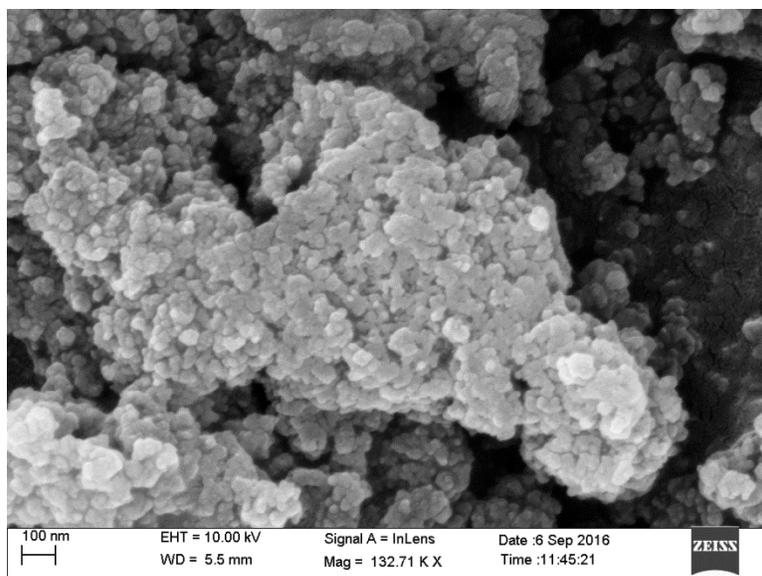
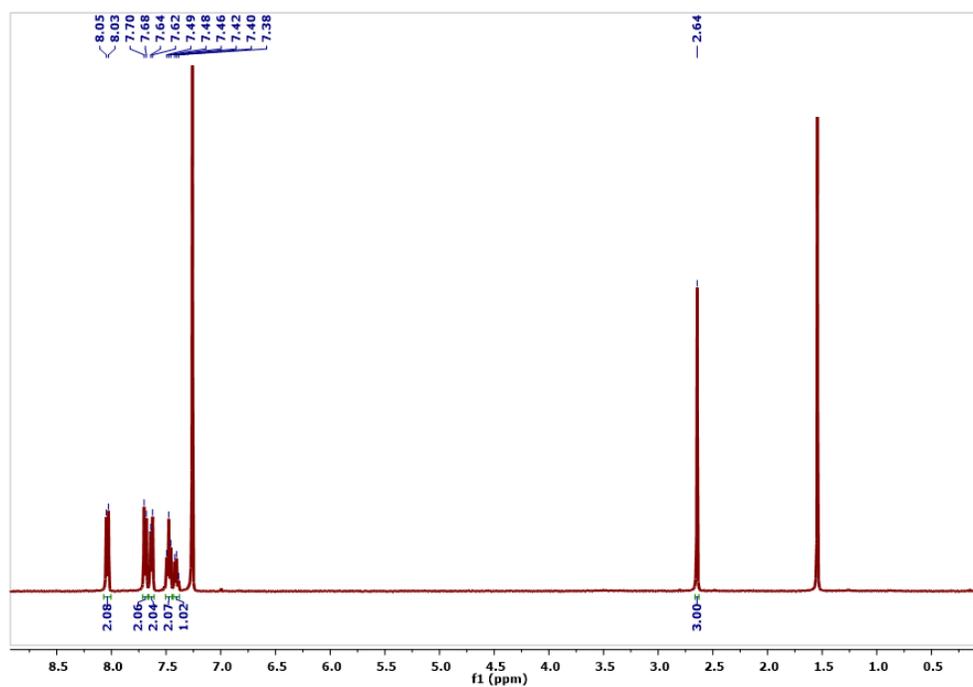
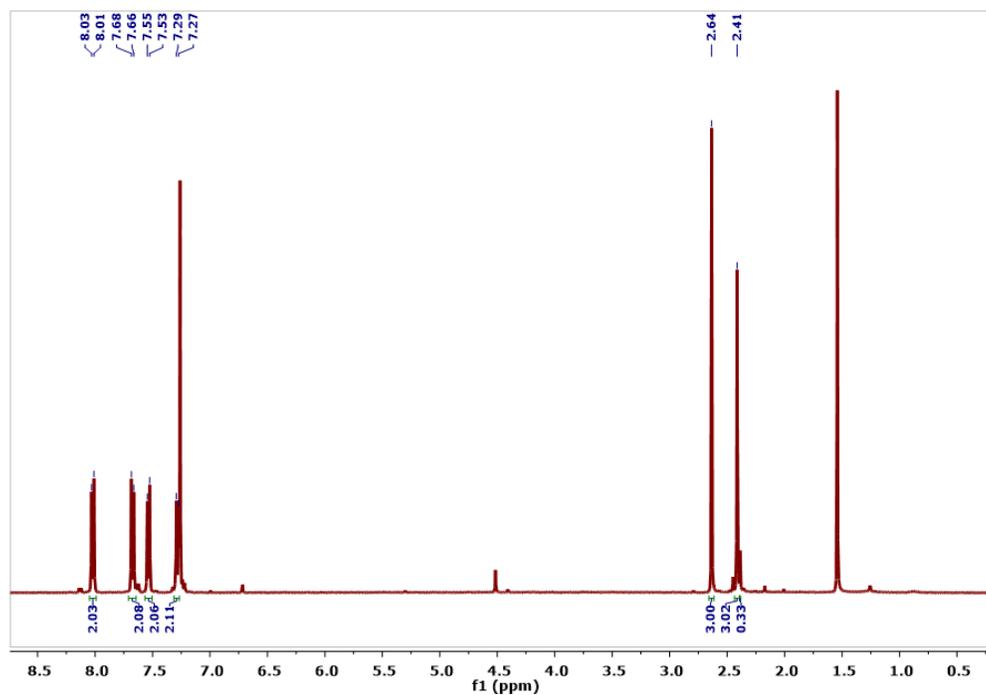


Figure S2. SEM image of original unused Ru-CP-Pd.

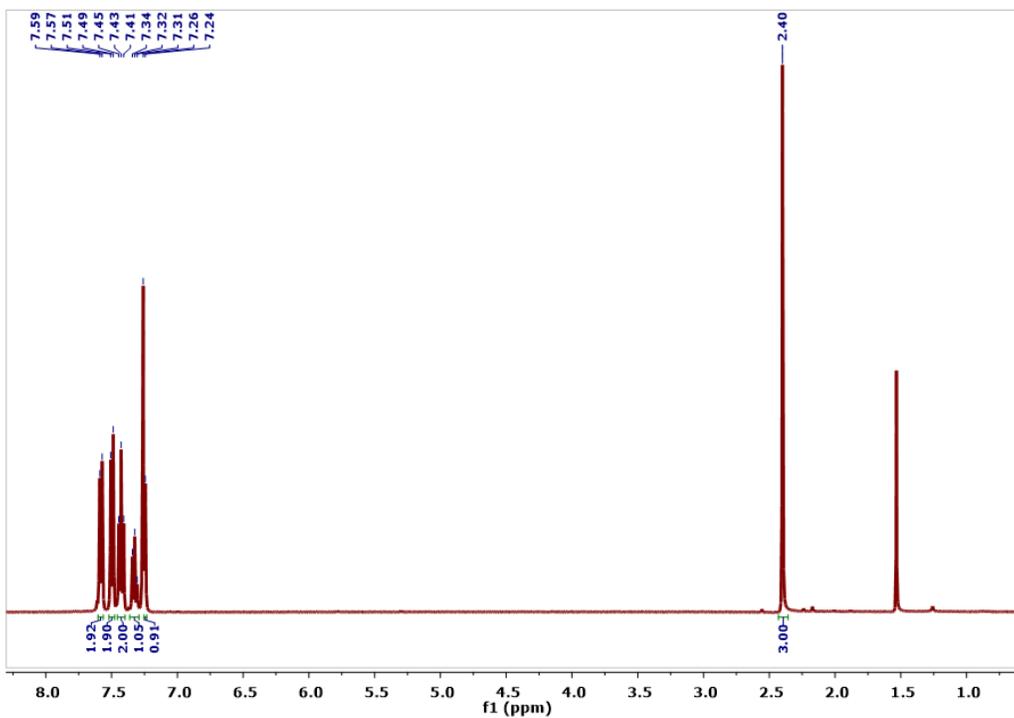
S1.5 ^1H NMR spectra of the coupling products



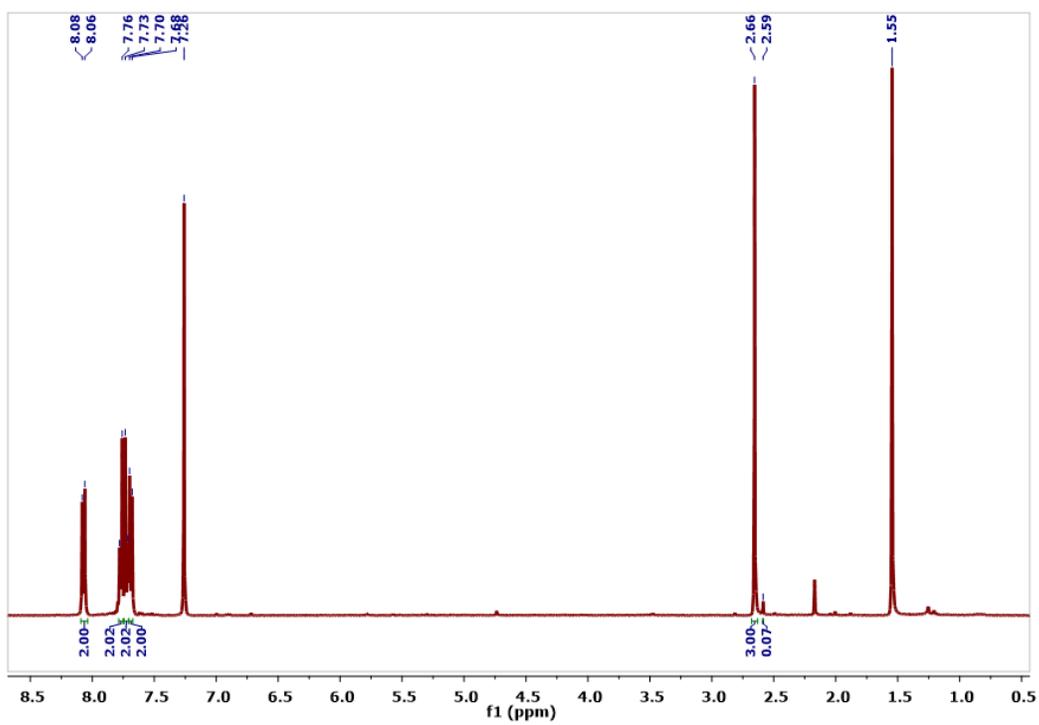
^1H NMR spectrum of 1-([1, 1'-biphenyl]-4-yl)ethan-1-one (400 MHz, CDCl_3).



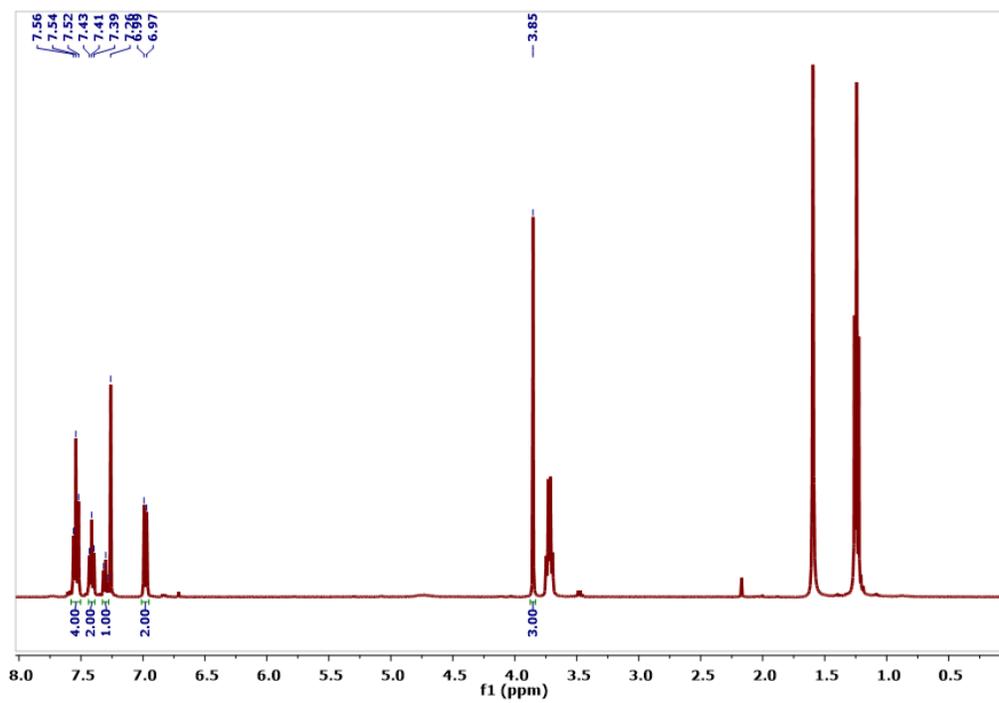
^1H NMR spectrum of 1-(4'-methyl-[1, 1'-biphenyl]-4-yl)ethan-1-one (400 MHz, CDCl_3).



¹H NMR spectrum of 4-methyl-1, 1'-biphenyl (400 MHz, CDCl₃).



¹H NMR spectrum of 4'-acetyl-[1, 1'-biphenyl]-4-carbonitrile (400 MHz, CDCl₃).



¹H NMR spectrum of 4-methoxy-1, 1'-biphenyl (400 MHz, CDCl₃).