

N-Heterocyclic Carbene–Palladium Functionalized Coordination Polymer (Pd- NHC@Eu-BCI) as an Efficient Heterogeneous Catalyst in the Suzuki–Miyaura Coupling Reaction

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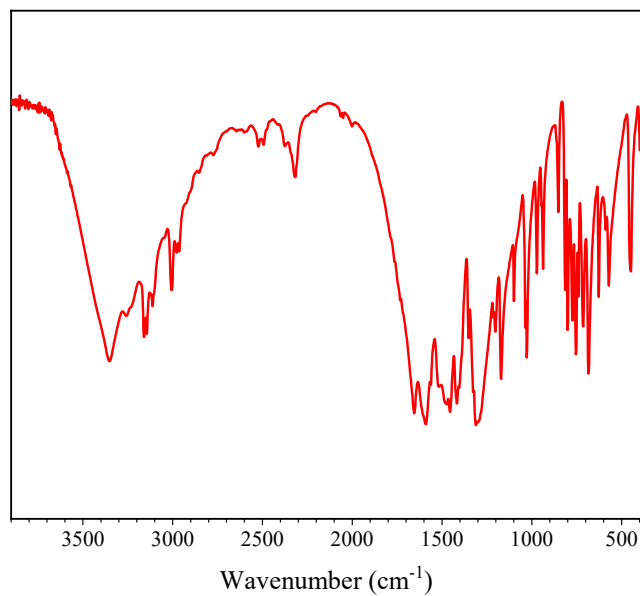


Figure S1. The IR spectrum of Eu-BCI.

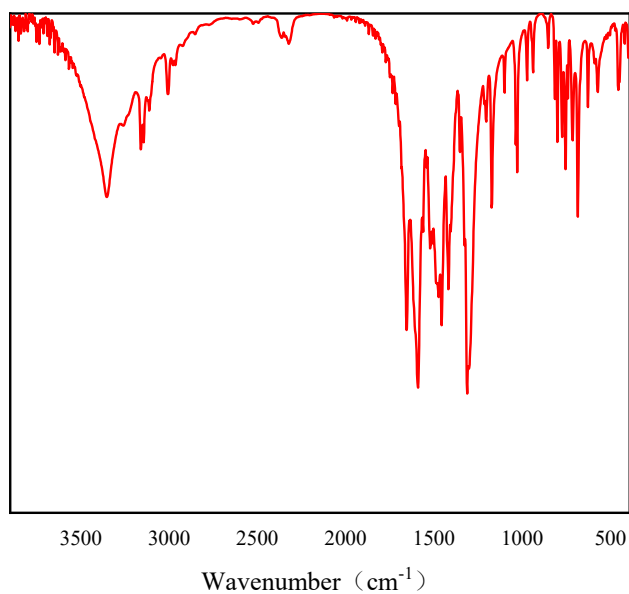


Figure S2. The IR spectrum of Pd-NHC@Eu-BCI.

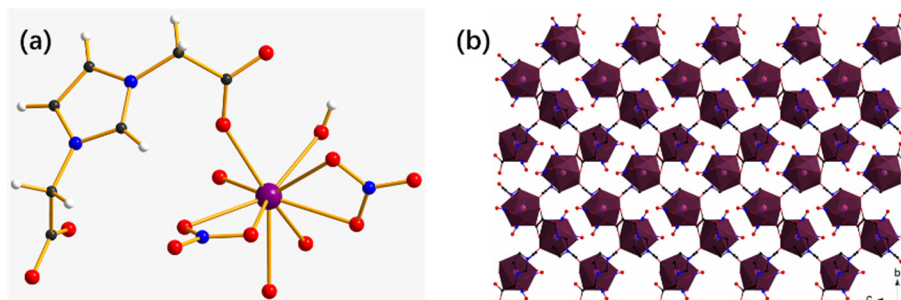


Figure S3. (a) Coordination environment of Eu(III) in Eu-BCI. (b) View of 2D layer of Eu-BCI.

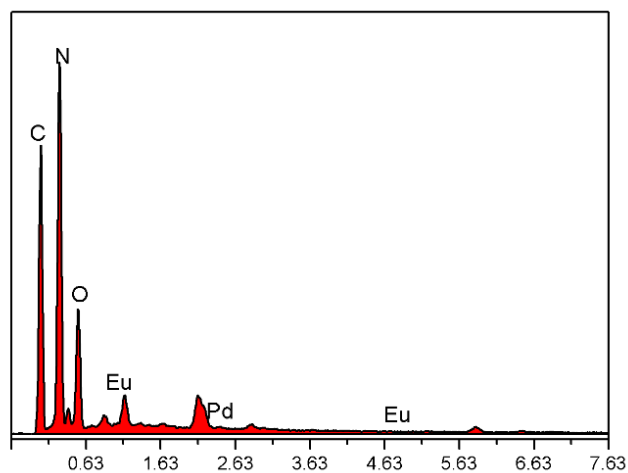


Figure S4. EDS spectrum of Pd-NHC@Eu-BCI.

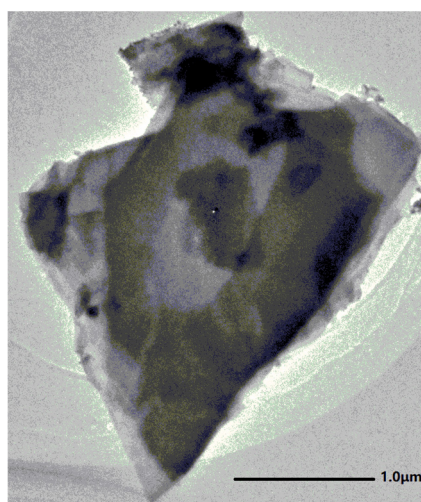


Figure S5. TEM of Pd-NHC@Eu-BCI.

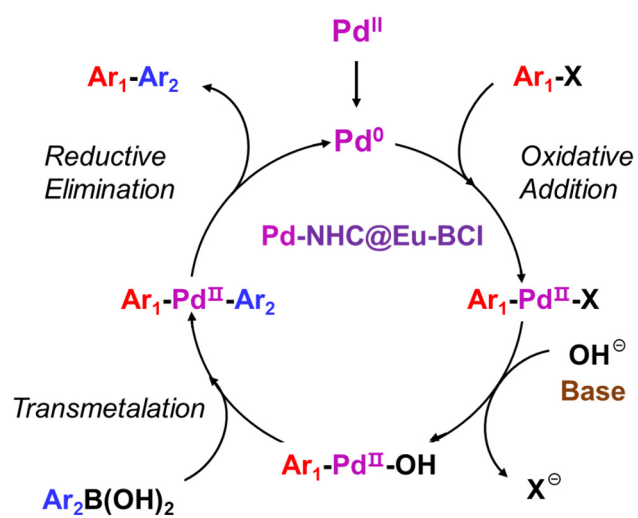


Figure S6. The proposed reaction mechanism of Suzuki-Miyaura cross-coupling catalyzed by Pd-NHC@Eu-BCI.

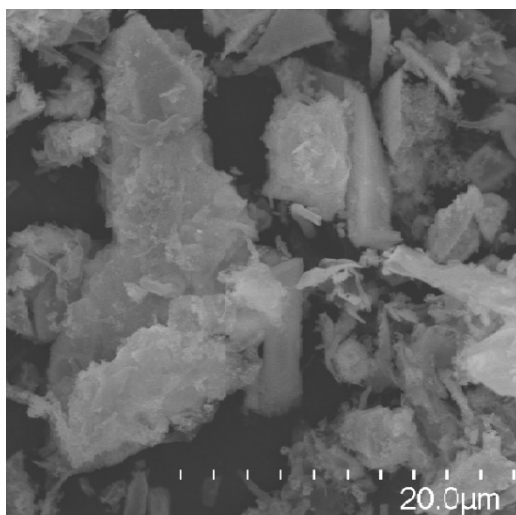


Figure S7. The SEM of Pd-NHC@Eu-BCI after five cycles.

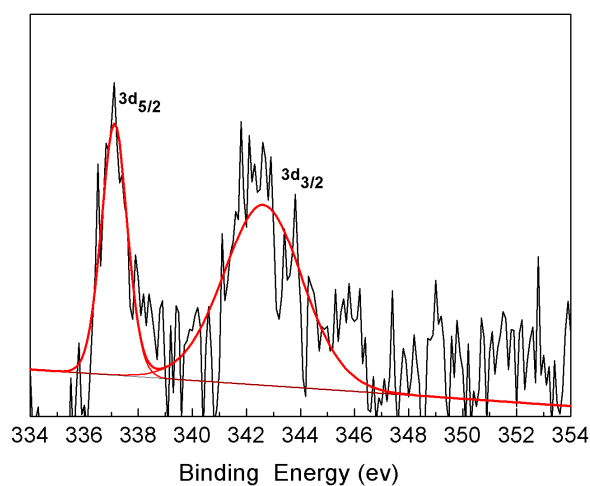
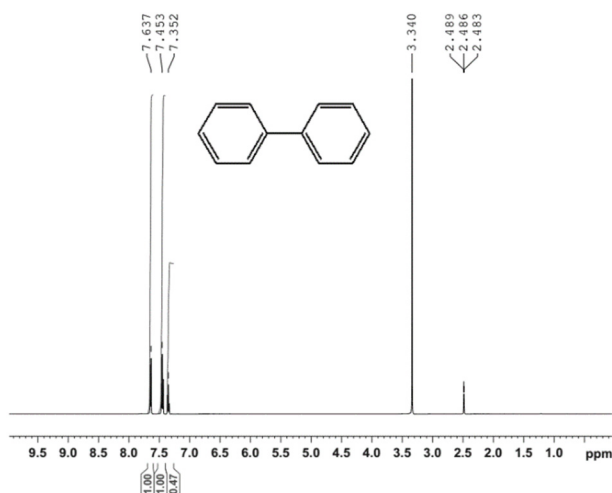


Figure S8. The Pd 3d XPS spectrum of Eu-BCI-Pd after five cycles.

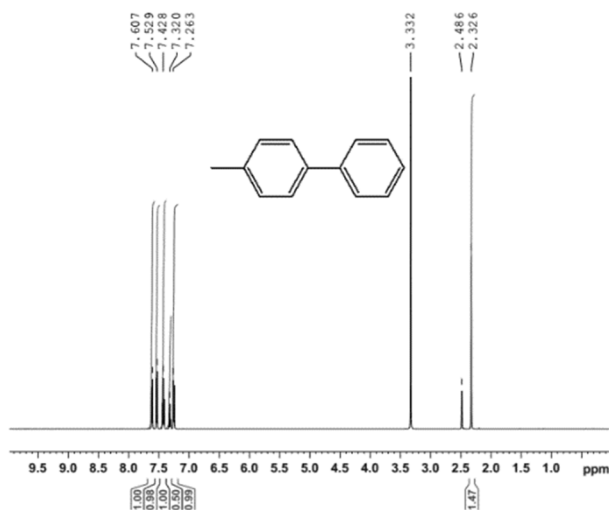
Table S1. Suzuki-Miyaura coupling of bromobenzene with phenylboronic acid catalyzed by different samples.

| Sample | Yield (%) |
|-----------------------------------|-----------|
| HBCI | 0 |
| Eu-BCI | 0 |
| Eu(NO ₃) ₃ | <5 |
| Pd(OAc) ₂ | 87 |

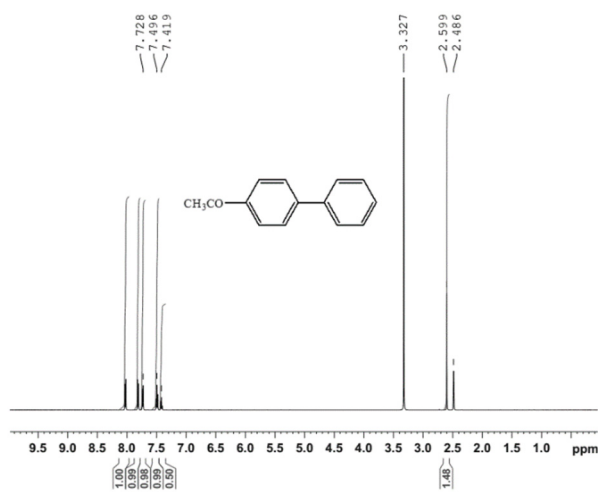
Reaction conditions: aryl halide (1.0 mmol), arylboronic acid (1.2 mmol), K₂CO₃ (2.0 mmol), EtOH (5 mL), catalyst (25 mg), temperature (80 °C), time (6 h).



Biphenyl: ^1H NMR (500 MHz, $\text{d}_6\text{-DMSO}$): $\delta = 7.35$ (t, 2H), 7.45 (t, 4H), 7.64 (d, 4H).



4-Methyl-1,1'-biphenyl: ^1H NMR (500 MHz, $\text{d}_6\text{-DMSO}$): $\delta = 2.33$ (s, 3H), 7.26 (d, 2H), 7.32 (t, 1H), 7.43 (t, 2H), 7.53 (d, 2H), 7.61 (d, 2H).



4-Acetyl-1,1'-biphenyl: ^1H NMR (500 MHz, $\text{d}_6\text{-DMSO}$): $\delta = 2.60$ (s, 3H), 7.42 (t, 2H), 7.50 (t, 2H), 7.73 (d, 2H), 7.82 (d, 2H), 8.03 (d, 2H).

