

Supporting Information

Cooperativity between Metal Centers in Homobimetallic Pd^{II}-NHC Complexes: Catalytic Potential Towards Hydrodefluorination

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Experimental Section

General considerations: All reactions were carried out under an inert atmosphere using standard Schlenk line and/or Glovebox techniques unless stated otherwise. All glassware was oven-dried at 130 °C overnight prior to use. The solvents used were dried, distilled, and degassed by standard methods and stored over 4 Å molecular sieves. NMR measurements were carried out on Bruker 500 MHz FT-NMR spectrometers. ESI-MS was recorded using an Agilent 6545A Q-TOF Mass spectrometer. The chemical shifts in the ¹H NMR spectra were referenced to the residual proton signals of the deuterated solvents (CDCl₃, ¹H 7.26 ppm and ¹³C{¹H} 77.2 ppm and reported relative to tetramethylsilane (TMS). The coupling constants are expressed in hertz. All other chemicals were purchased from the commercial sources and used as received without further purification.

Synthesis of [(L1)Pd^{II}Br₂Py(3-Cl)Pd^{II}Br₂Py(3-Cl)], 1. To a Schlenk tube (25 mL) equipped with a magnetic stirring bar, [L1-H₂]Br₂ (100 mg, 0.23 mmol), PdCl₂ (94.8 mg, 0.54 mmol), K₂CO₃ (96.3 mg, 0.70 mmol), and KBr (221.3 mg, 1.86 mmol) were added. A solvent mixture of acetonitrile:3-chloropyridine (10:1 mL) was then added and stirred at 70 °C for 18 h. After that, the reaction mixture was cooled and filtered through a pad of celite to obtain a clear yellow solution. Concentration followed by the addition of diethyl ether resulted in the precipitation of a compound. The precipitate was then washed with diethyl ether and dried in high vacuum to obtain a bright yellow powder that was further purified by silica gel column chromatography using dichloromethane and methanol (98:2, v:v) as eluent. Suitable single crystals for X-ray crystallographic studies were grown by slow diffusion of diethyl ether into a saturated solution of the complex in acetonitrile. Yield: 170 mg (0.17 mmol, 74%).

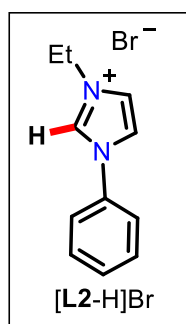
¹H NMR (500 MHz, CDCl₃) δ = 9.14 (d, *J* = 2.4 Hz, 1H), 9.04 (dd, *J* = 5.4, 1.4 Hz, 1H), 8.92 (d, *J* = 2.4 Hz, 1H), 8.76 (dd, *J* = 5.5, 1.4 Hz, 1H), 8.36 (d, *J* = 1.9 Hz, 1H), 7.80 (ddd, *J* = 8.2, 2.4, 1.3 Hz, 1H), 7.69 (ddd, *J* = 8.2, 2.4, 1.3 Hz, 1H), 7.64 (dd, *J* = 8.6, 1.9 Hz, 1H), 7.55 (d, *J* = 8.6 Hz, 1H), 7.35 (dd, *J* = 8.2, 5.4 Hz, 1H), 7.23 (dd, *J* = 8.3, 5.6 Hz, 1H), 7.18 (dd, *J* = 14.1, 2.1 Hz, 2H), 4.96 (m, 4H), 4.74 (q, *J* = 7.4 Hz, 2H), 1.79-1.69 (m, 9H) ppm.

¹³C{¹H} NMR (126 MHz, CDCl₃) δ = 163.4 (Pd^{II}-C_{NHC}), 151.9, 151.7, 150.8, 150.6, 148.1 (Pd^{II}-C_{NHC}), 138.2, 138.1, 135.1, 134.3, 134.1, 132.8, 132.7, 125.2, 125.1, 125.1, 124.3, 121.9, 121.7, 110.9, 110.4, 46.8, 44.6, 44.4, 15.6, 14.6, 14.6 ppm.

MS (ESI, positive ions): $C_{26}H_{28}N_6Pd_2Cl_2Br_4$, calculated for $[M-Br-2Py(3-Cl)+2CH_3CN]^+ m/z = 802.7828$, found: 802.7836; calculated for $[M-Br-2Py(3-Cl)+CH_3CN]^+ m/z = 761.7562$, found: 761.7642; calculated for $[M-2Br-2Py(3-Cl)-H]^+ m/z = 640.8037$, Found: 640.8052.

Anal. Calculated for **2**: C, 30.38; H, 2.75; N, 8.18. Found: C, 31.55; H, 2.0; N, 8.39.

Synthesis of $[(L2)Pd^{II}Br_2Py(3-Cl)]$, **5.** To a Schlenk tube (25 mL) equipped with a magnetic stirring bar, $[L2-H]Br$ (100 mg, 0.395 mmol), $PdCl_2$ (84 mg, 0.474 mmol), K_2CO_3 (65.4 mg, 0.474 mmol), and KBr (141 mg, 1.185 mmol) were added. A solvent mixture of acetonitrile:3-chloropyridine (10:1 mL) was then added and stirred at 70 °C for 18 h. After that the reaction mixture was cooled and filtered through a pad of celite to obtain a clear yellow solution. Concentration followed by the addition of diethyl ether resulted in precipitation of a compound. The precipitate was then washed with diethyl ether and dried in high vacuum to obtain a bright



yellow air stable powder that was further purified *via* silica gel column chromatography using dichloromethane as eluent. Yield: 172 mg (0.312 mmol, 79%).

1H NMR (500 MHz, $CDCl_3$) $\delta = 8.91$ (dd, $J = 2.3, 0.6$ Hz, 1H), 8.81 (dd, $J = 5.5, 1.4$ Hz, 1H), 8.00-7.98 (m, 2H), 7.70 (ddd, $J = 8.2, 2.4, 1.3$ Hz, 1H), 7.57 (dd, $J = 8.5, 6.9$ Hz, 2H), 7.53-7.48 (m, 1H), 7.23 (ddd, $J = 8.2, 5.5, 0.7$ Hz, 1H), 7.20 (d, $J = 2.0$ Hz, 1H), 7.12 (d, $J = 2.1$ Hz, 1H), 4.72 (q, $J = 7.4$ Hz, 2H), 1.69

(t, $J = 7.4$ Hz, 3H) ppm.

$^{13}C\{^1H\}$ NMR (126 MHz, $CDCl_3$) $\delta = 152.0, 150.9, 147.3$ ($Pd^{II}-C_{NHC}$), 139.9, 138.2, 132.8, 129.6, 129.2, 126.6, 125.2, 123.9, 121.8, 47.1, 15.9 ppm.

MS (ESI, positive ions): $C_{16}H_{16}N_3PdBr_2Cl$, calculated for $[M-Py(3-Cl)-Br+CH_3CN]^+ m/z = 399.9478$, found: 399.9490; calculated for $[M-Py(3-Cl)-Br]^+ m/z = 358.9212$, found: 358.9218; calculated for $[M-Py(3-Cl)-2Br-H+CH_3CN]^+ m/z = 318.0228$, found: 318.0230; calculated for $[M-Py(3-Cl)-2Br-H]^+ m/z = 276.9962$, found: 276.9968.

NMR spectra of the isolated compounds

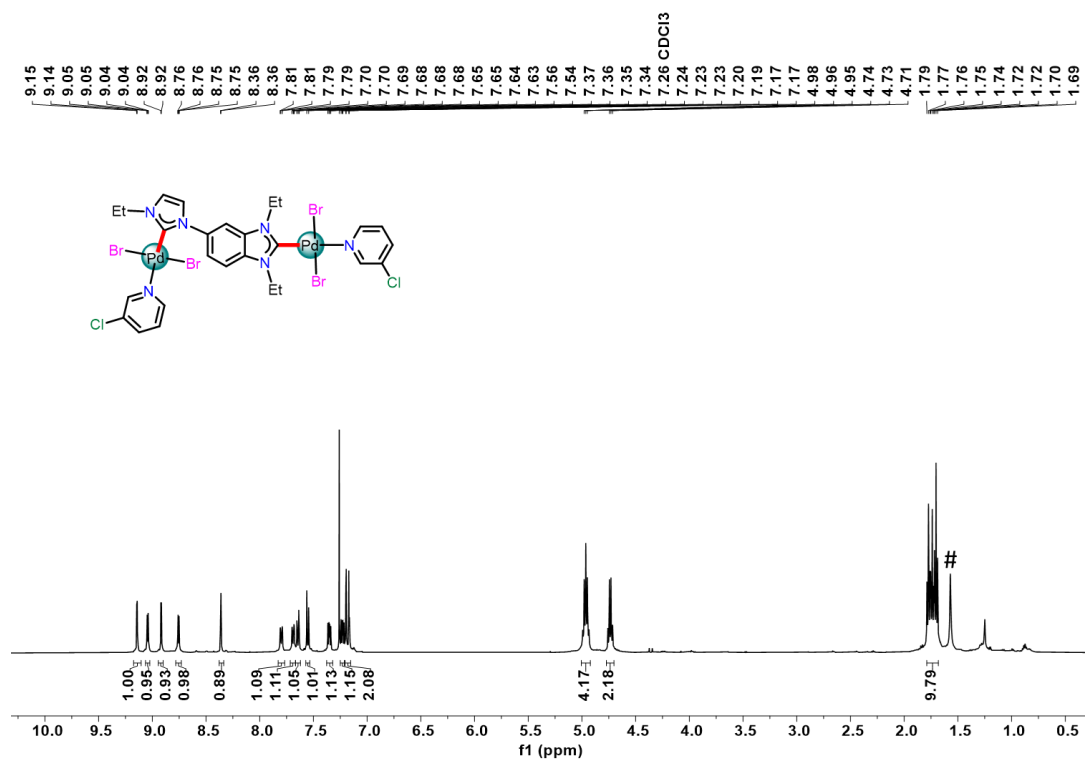


Figure S1. ¹H NMR spectrum of complex **1** in CDCl₃. # represents solvent impurity of water.

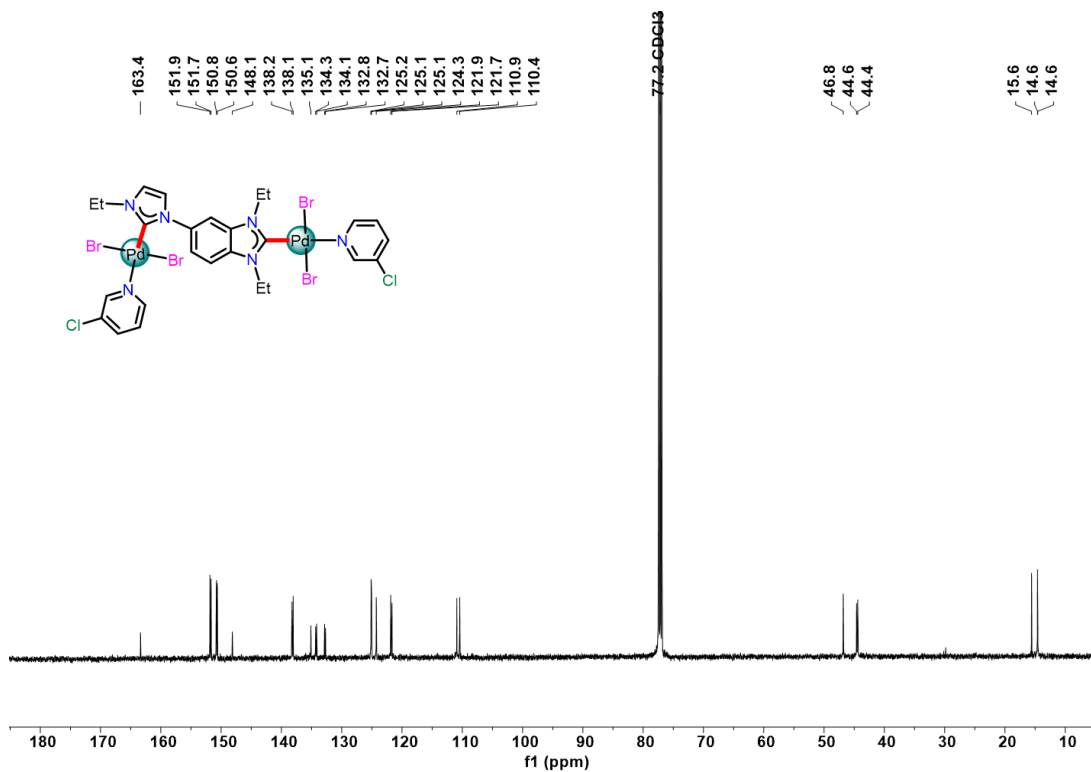


Figure S2. ¹³C NMR spectrum of complex **1** in CDCl₃.

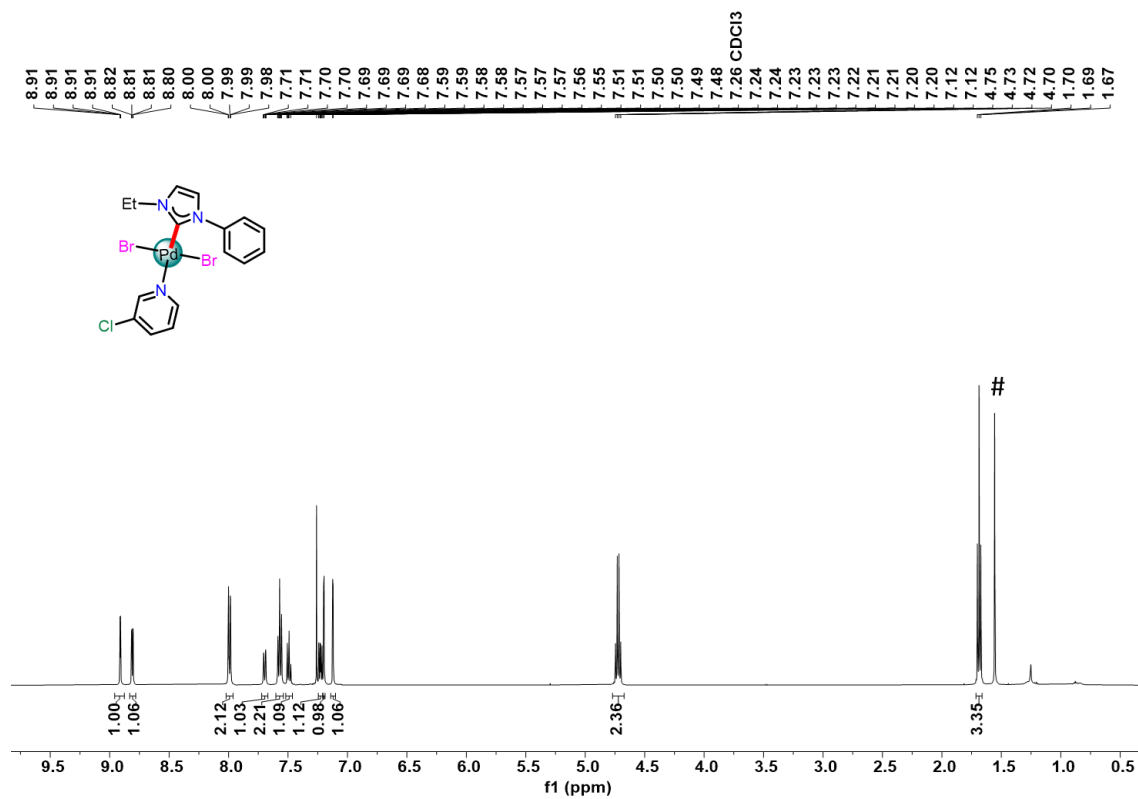


Figure S3. ¹H NMR spectrum of complex 5 in CDCl₃. # represents solvent impurity of water.

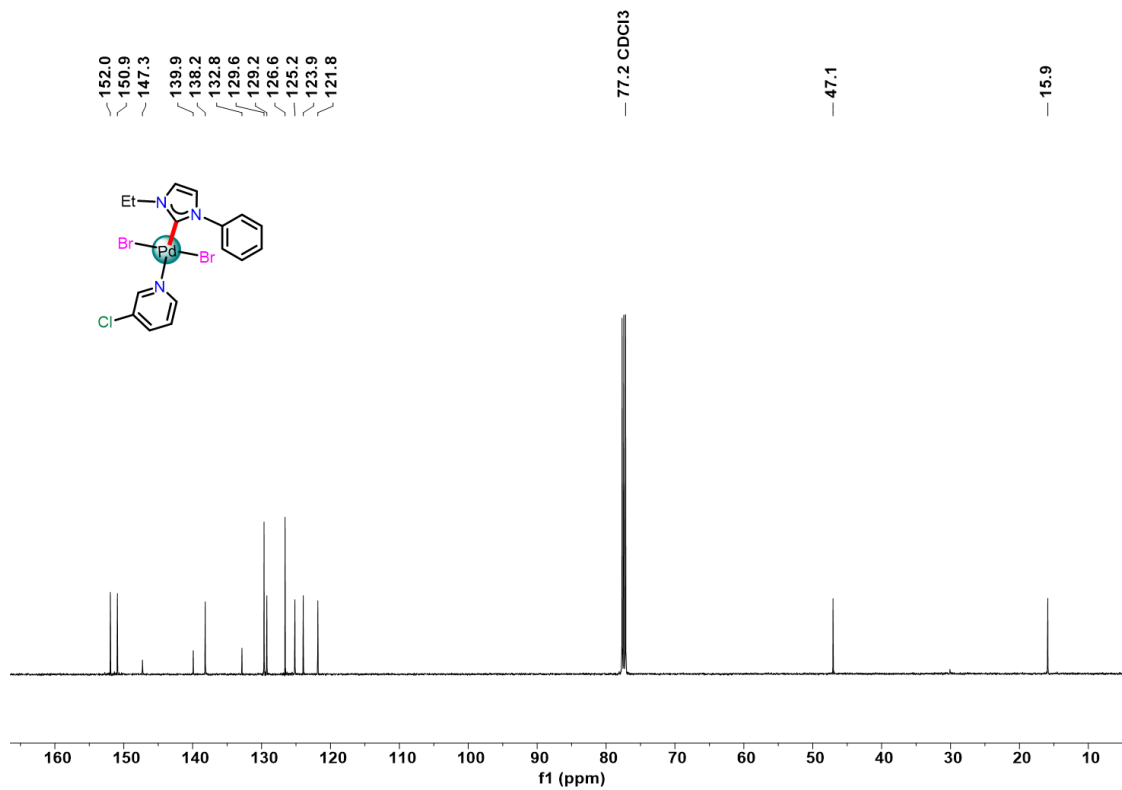


Figure S4. ¹³C NMR spectrum of complex 5 in CDCl₃.

ESI-MS (positive-ion) spectra of the synthesized metal complexes

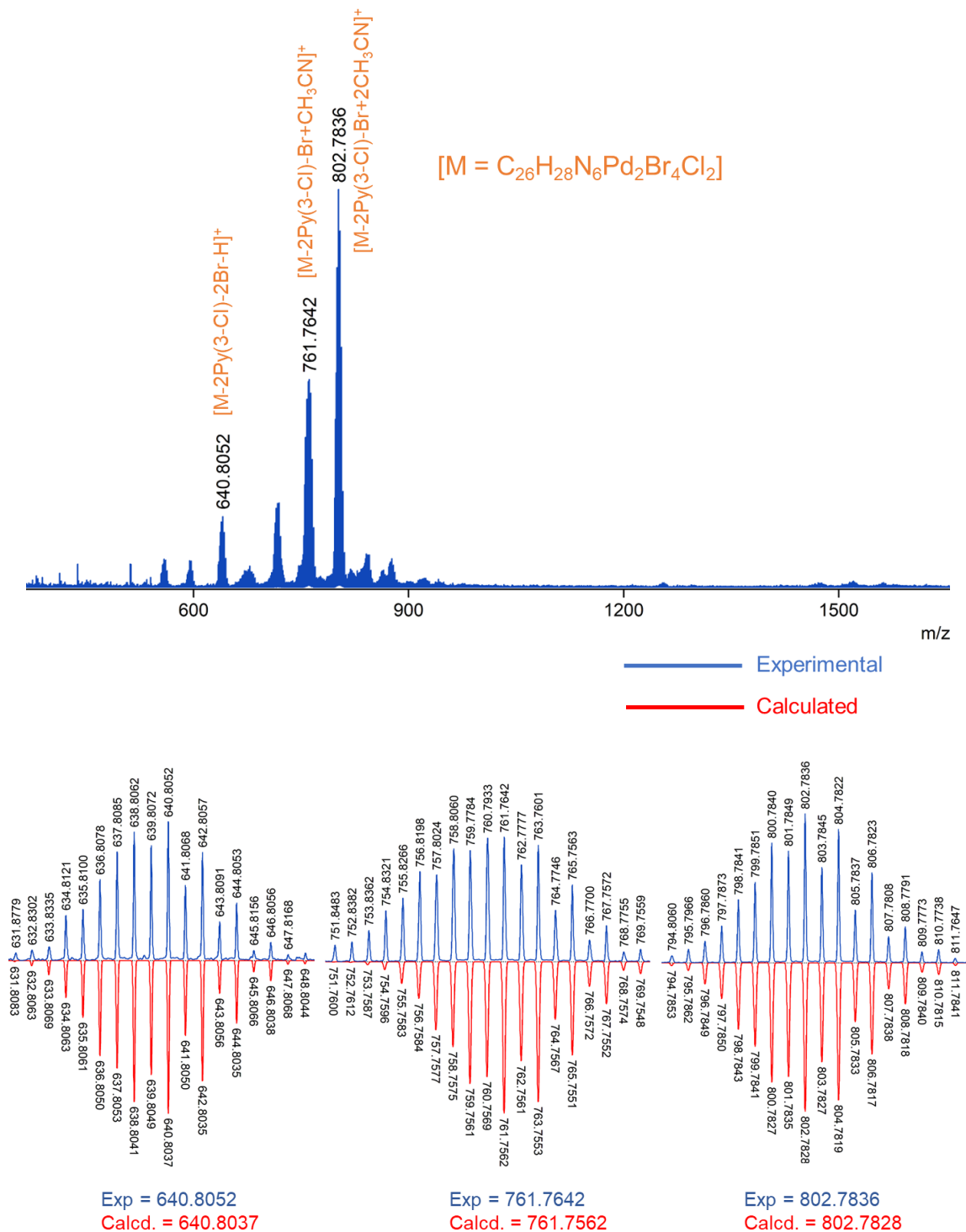


Figure S5. ESI-MS (positive ions) spectrum of the complex 1.

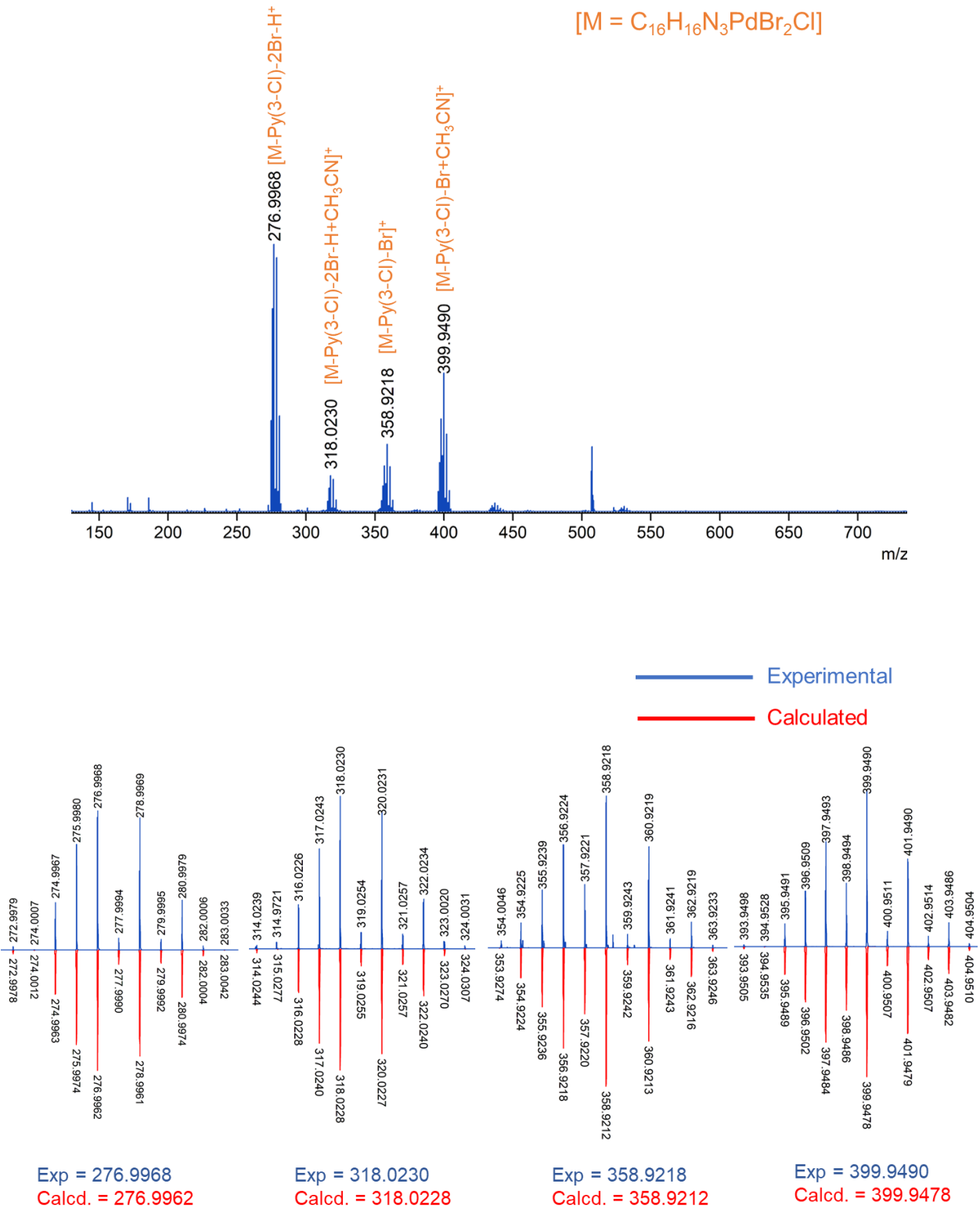
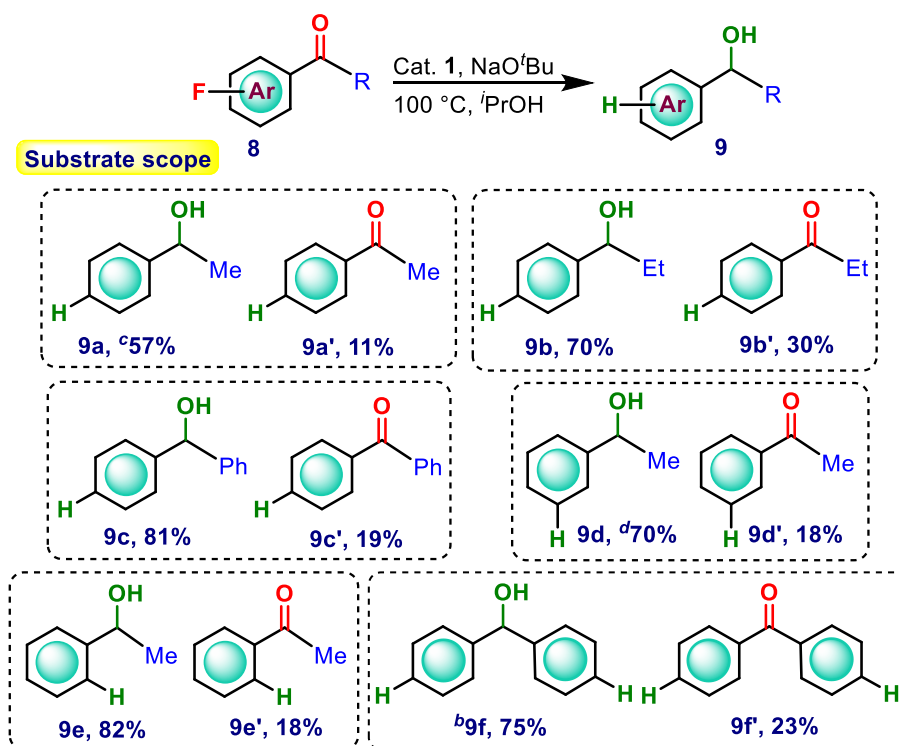


Figure S6. ESI-MS (positive ions) spectrum of the complex **5**.

General procedure for the HDF of the fluoroarenes: To an oven dried pressure tube, NaO^tBu (0.1 mmol), complex **1** (0.5 mol%) and fluoroarene (0.1 mmol) were added. Next, 2-propanol (1.5 mL) was added to it and kept in a preheated oil bath at 100 °C. After a specific reaction time, the pressure tube was taken out and cooled to room temperature. The progress of the reaction was monitored by GC-MS analysis using mesitylene as an internal standard.

General procedure for the tandem HDF and transfer hydrogenation of fluoroarenes: To an oven dried pressure tube, NaO^tBu (0.1 mmol), complex **1** (0.5 mol%) and fluoroarene (0.1 mmol) were added. Next, 2-propanol (1.5 mL) was added to it and kept in a preheated oil bath at 100 °C. After a specific reaction time, the pressure tube was taken out and cooled to room temperature. The progress of the reaction was monitored by GC-MS analysis using mesitylene as an internal standard.

Table S1. Tandem HDF and TH of fluoroarenes^a



^a**Reaction conditions:** Fluoroarene (0.1 mmol), NaO^tBu (0.1 mmol), complex **1** (0.5 mol%), *i*PrOH (1.5 mL), 24 h. ^bNaO^tBu (0.2 mmol). ^c1-(4-fluorophenyl)ethanol (**9a'**), 32%). ^d1-(3-fluorophenyl)ethanol (**9d'**), 12%). Conversions are based on GC-MS using mesitylene as internal standard.

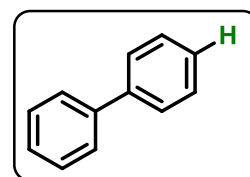
General procedure for the HDF of the trifluorotoluenes: To an oven dried pressure tube, NaO^tBu (0.3 mmol), complex **1** (1.5 mol%) and fluoroarene (0.1 mmol) were added. Next, 2-propanol (2 mL) was added to it and kept in a preheated oil bath at 100 °C. After a specific reaction time, the pressure tube was taken out and cooled to room temperature. The progress of the reaction was monitored by GC-MS analysis using mesitylene as an internal standard.

Procedure for the calculation of TON for HDF of fluorobenzene: To an oven dried pressure tube, NaO^tBu (0.2 mmol), complex **1** (0.1 mol%) and fluorobenzene (0.2 mmol) were added. Next, 2-propanol (1.5 mL) was added to it and kept in a preheated oil bath at 100 °C for 12 h. After completion of the reaction, small portion of aliquot was taken for GC-MS analysis. The data based on GC-MS analysis (using mesitylene as an internal standard) shows 41% conversion which gives TON of 410 and TOF 34.2 h⁻¹.

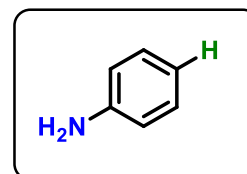
General procedure for the HDF of the fluoroarenes for the isolated products: To an oven dried pressure tube, NaO^tBu (0.3 mmol), complex **1** (0.5 mol%) and fluoroarene (0.3 mmol) were added. Next, 2-propanol (2 mL) was added to it and kept in a preheated oil bath at 100 °C. After a specific reaction time, the pressure tube was taken out and cooled to room temperature. Finally, the product was isolated by column chromatography using hexane: ethyl acetate as eluent.

Characterization data of isolated compounds:

1,1-biphenyl (7b): Following the general procedure, the titled compound was isolated as colorless solid (42 mg, 91% yield). ¹H NMR (400 MHz, CDCl₃) δ 7.61 (d, *J* = 7.6 Hz, 4H), 7.45 (t, *J* = 7.5 Hz, 4H), 7.35 (t, *J* = 7.4 Hz, 2H) ppm. ¹³C{¹H} NMR (101 MHz, CDCl₃) δ 141.4, 128.9, 127.4, 127.3 ppm. Analytical data matches with reported data.¹



Aniline (7d): Following the general procedure, the titled compound was isolated as brown liquid (26 mg, 93% yield). ¹H NMR (500 MHz, CDCl₃) δ 7.21-7.18 (m, 2H), 6.80 (t, *J* = 7.5 Hz, 1H), 6.71 (d, *J* = 7.9 Hz, 2H), 3.66 (bs, 2H) ppm. ¹³C{¹H} NMR (126 MHz, CDCl₃) δ 146.5, 129.3, 118.6, 115.2 ppm. Analytical data matches with reported data.²



NMR spectra of the isolated products

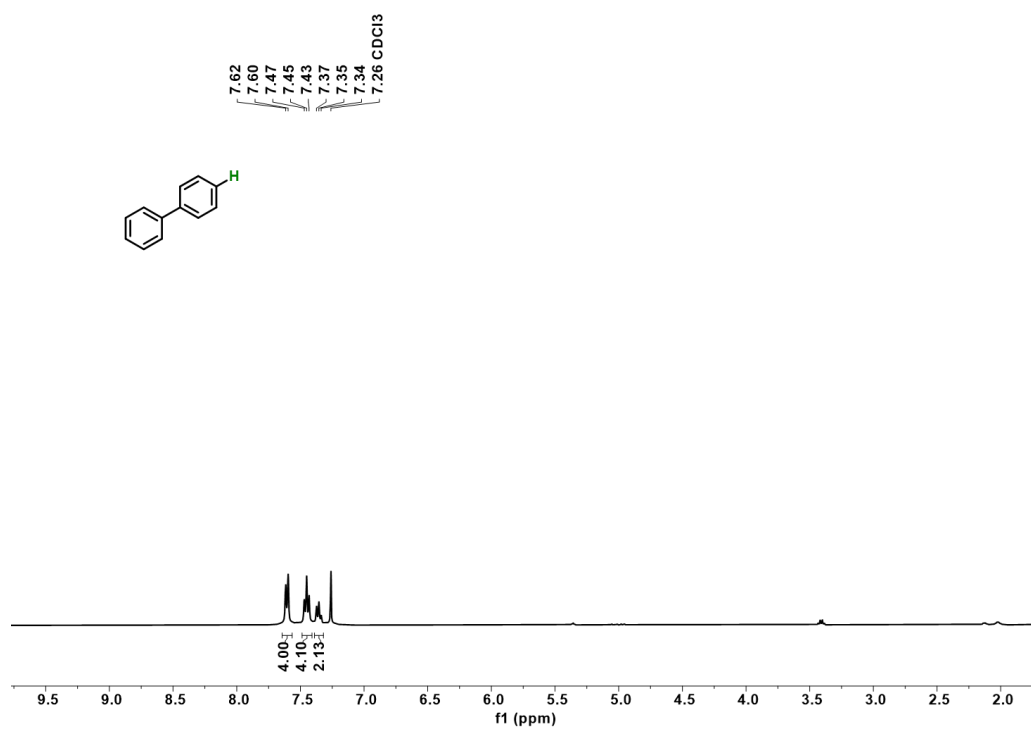


Figure S7. ¹H NMR spectrum of **7b** in CDCl₃.

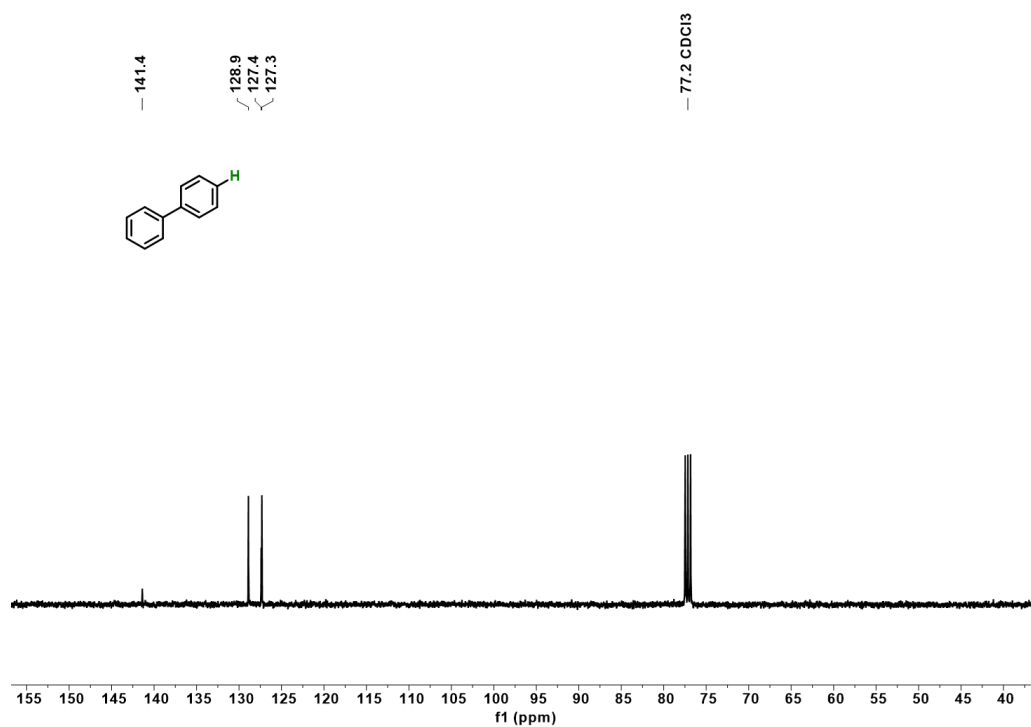


Figure S8. ¹³C{¹H} NMR spectrum of **7b** in CDCl₃.

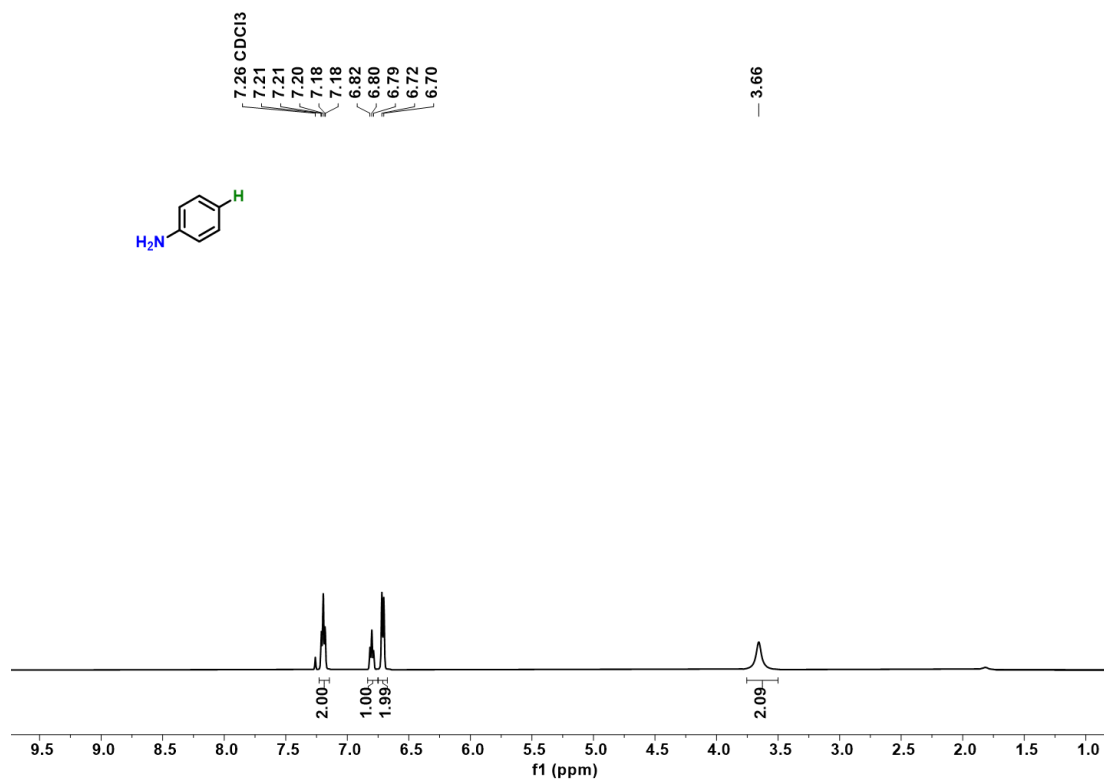


Figure S9. ^1H NMR spectrum of **7d** in CDCl_3 .

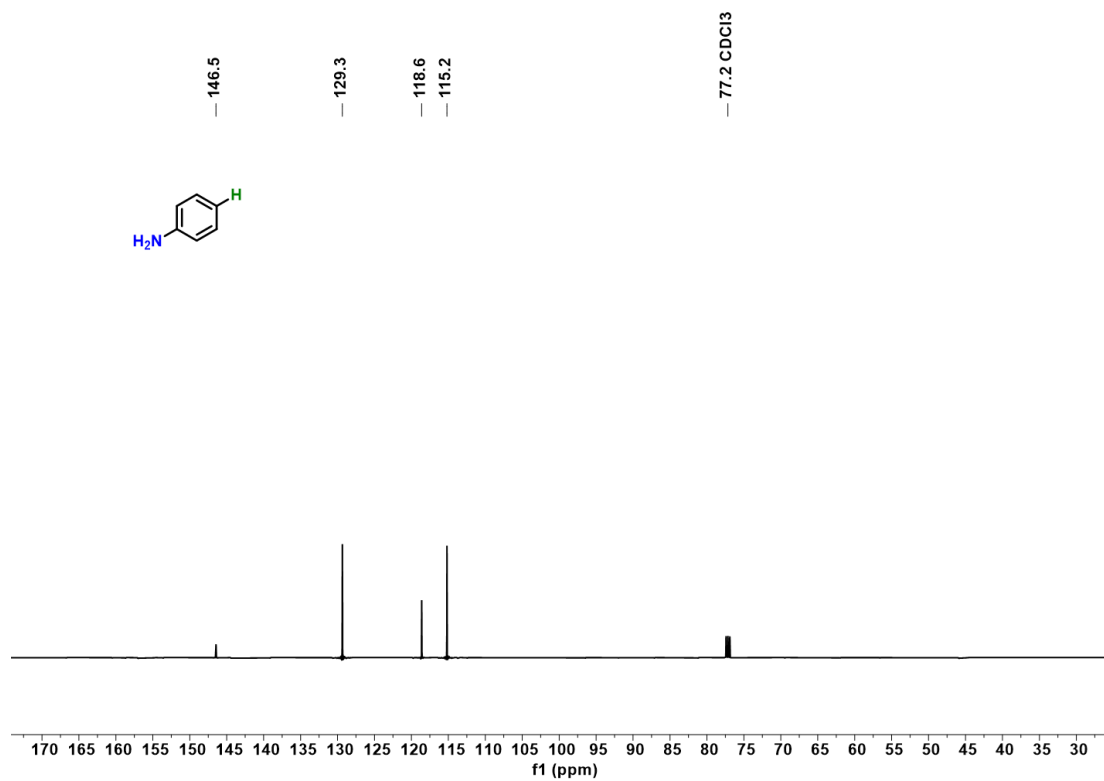


Figure S10. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **7b** in CDCl_3 .

Table S2: Optimization conditions for the HDF of fluorobenzene.^a

Entry	Base	Base (equiv.)	Cat. (mol%)	Temp. (°C)	Conv. (%)
1	NaO ^t Bu	2	1	100	100
2	NaO ^t Bu	1.5	0.5	100	100
3	NaO^tBu	1	0.5	100	96
4	NaO ^t Bu	1	0.5	80	74
5	KO ^t Bu	1	0.5	100	81
6	K ₂ CO ₃	1	0.5	100	1
7	Cs ₂ CO ₃	1	0.5	100	9
8	NaOAc	1	0.5	100	0
9	NaTMAH	1	0.5	100	0

Reaction conditions: Fluorobenzene (0.1 mmol), catalyst **1** (x mol%), base (x equiv.) in 2-propanol (1.5 mL), 12 h. Conversions were determined by GC-MS using mesitylene as internal standard. NaTMAH = sodium trimethylacetate hydrate.

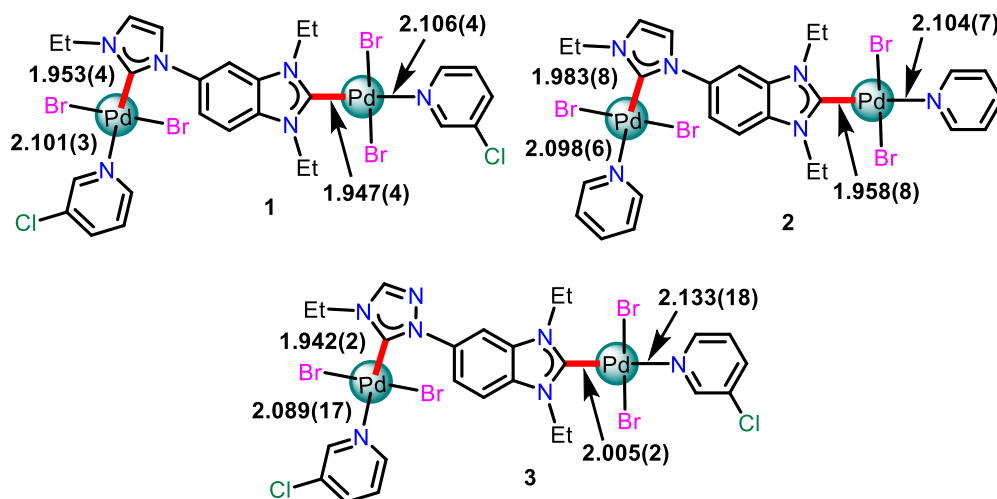


Figure S11: Selected bond lengths (Å) of Pd-C and Pd-N in the complexes **1-3**.

Calculation of cooperativity index (α):

Cooperativity index was calculated using equations I and II. Here, A_o and A_p are the % conversion using the bimetallic complex **1** (entry 1, Table 1, 96% conversion) and the combination of mono-metallic fragments **4** (13% conversion) and **5** (5% conversion) (entries 4-5, Table 1), respectively. The cooperativity index (α) for the present system was calculated to be 8.67.

$$\bar{A} = \frac{A_p}{n} \quad (\text{I})$$

$$\alpha = \frac{A_o - A_p}{\bar{A}} \quad (\text{II})$$

Figure S12: Calculation of cooperativity index (α).

Single crystal X-ray Crystallography:

Single crystal X-ray diffraction data were collected on a Bruker AXS Kappa APEX3 diffractometer equipped with PHOTON-II detector using MoK α radiation ($\lambda = 0.71073 \text{ \AA}$). Crystals were selected using a polarizing optical microscope and then mounted in a crystal-mounting loop using Paraton oil. The mounted crystal was then placed on a goniometer head and the crystal is centered with the help of a video microscope. The automatic cell determination routine, with 24/36 frames (10 sec exposure time per frame) at two/three different orientations of the detector, respectively was employed to collect reflections for unit cell determination. The collected reflections were indexed using inbuilt APEX software^{3a} to obtain the unit cell parameters. Further, intensity data for structure determination were collected through an optimized strategy, which gave an average 4-fold redundancy for the reflections. The program Bruker-S SAINT^{3b} was used for integrating the frames and multi-scan absorption correction was applied using the program SADABS.^{3c} The structure was solved by SHELXT^{3d} and refined by full-matrix least squares techniques on F^2 using SHELXL^{3e-f} computer program incorporated in WinGX^{3g} system. The non-hydrogen atoms were refined anisotropically. All hydrogen atoms were fixed at chemically meaningful positions and riding model refinement was applied. The graphical representations were performed using the program Mercury.^{3h}

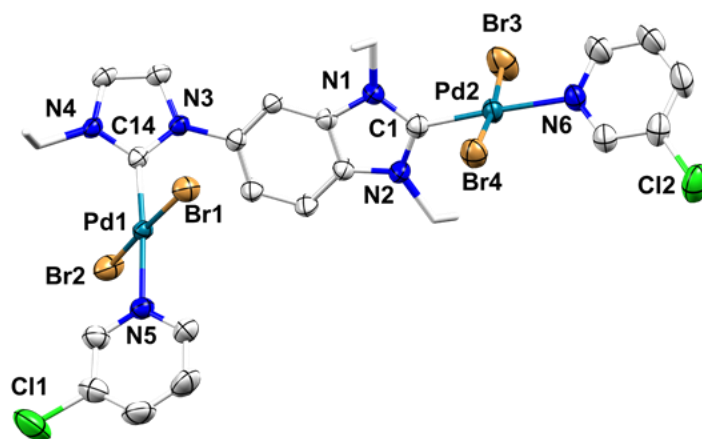


Figure S13: Ellipsoid representation (at 40% probability level) of the molecular structure of complex **1**. Hydrogen atoms are removed and *N*-ethyl groups are shown in capped stick for clarity.

Crystallographic Data

Compound	1
CCDC No.	2301305
Empirical formula	C ₅₆ H ₆₆ Br ₈ Cl ₄ N ₁₂ OPd ₄
Formula weight	2129.88
Temperature (K)	297(2)
Crystal system	Monoclinic
Space group	C2/c
a (Å)	29.200(2)
b (Å)	8.5804(6)
c (Å)	28.6903(18)
α (°)	90
β (°)	96.068(3)
γ (°)	90
V (Å ³)	7178.0(8)
Z	4
D calc (Mg/m ³)	1.971
F (000)	4104
μ (mm ⁻¹)	5.634
θ Range (°)	3.270 to 27.116
Crystal size (mm ³)	0.117 x 0.101 x 0.092
No. of total reflns collected	146462
No. of unique reflns [I > 2 σ (I)]	7890
Data/restraints/parameters	7890 / 1 / 384
Goodness-of-fit on F ²	1.078
Final R indices [I > 2 σ (I)]	R1 = 0.0342, wR2 = 0.0914
R indices (all data)	R1 = 0.0426, wR2 = 0.0972

Electrochemical analysis of the metal complexes:

The electrochemical measurements, differential pulse voltammetry (DPV) of the synthesized complexes **1**, **2**, and **3** were carried out at ambient temperature using Orignalys OGF01A potentiostat instrument. The measurements of all the complexes (0.01 mM) were performed at a sweep rate of 100 mV/sec in CH₂Cl₂ using Bu₄NPF₆ (0.1 M) as supporting electrolyte with three electrode configurations e.g. counter electrode: Pt foil; working electrode: Glassy carbon (6 mm diameter); reference electrode: saturated Calomel electrode (Hg/HgCl₂). All the measurements were calibrated externally using Ferrocene ($E_{1/2}$, Fc/Fc⁺ = 1.20 volts vs. Hg/Hg²⁺).

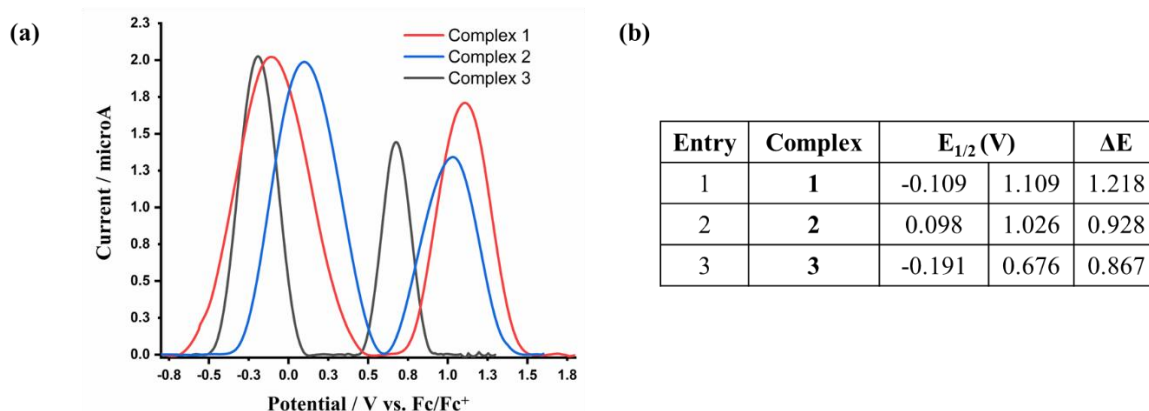
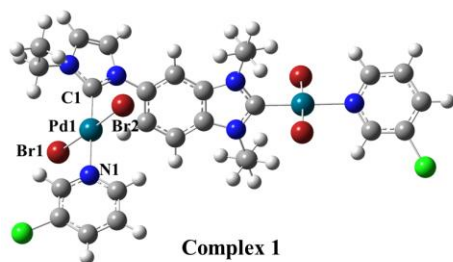


Figure S14: (a) Differential Pulse Voltammetry (DPV) plot of the complexes **1-3**. (b) Electrochemical data obtained from DPV (referenced to Fc/Fc⁺).

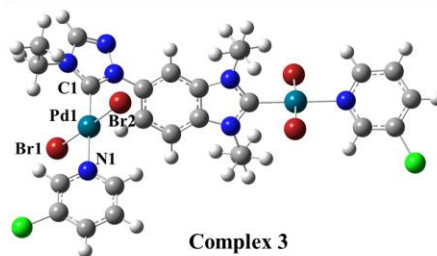
Computational data

All the calculations were performed using the Gaussian 16, Revision B.01 program.⁴ All structures were optimized with B3LYP⁵ functional. Metals (Pd) were treated with SDD (Stuttgart-Dresden)⁶ basis set with an effective core potential, while the other atoms were treated using 6-31G**,⁷ a double- ζ Pople type basis set. Further, the solvent (toluene) effect was incorporated by using CPCM solvent model, scrf=(cpcm, solvent = toluene). Dispersion effects were incorporated by using the D3 version of Grimme's dispersion with Becke-Johnson damping with the keyword "Empiricaldispersion=GD3BJ".⁸ ESP charges were calculated using the keywords "pop=mk" and "pop=saveesp".



Complex 1

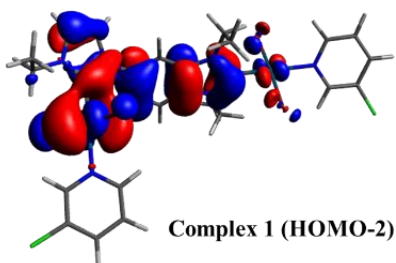
	ESP charges
Pd1	0.098753
Cl1	-0.066226
Br1	-0.452704
Br2	-0.456237
N1	-0.200522
Overall	-1.076936



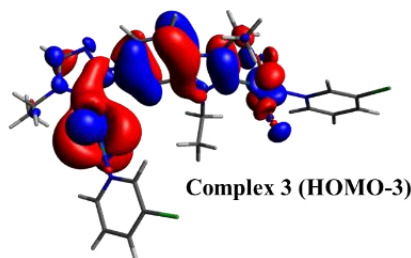
Complex 3

	ESP charges
Pd1	0.065670
Cl1	0.005674
Br1	-0.451508
Br2	-0.442623
N1	-0.132842
Overall	-0.955629

Figure S15: ESP charge distribution of the complexes **1** and **3**. DFT calculations were performed at the B3LYP/SDD (for metals) or 6-31G** (for non-metals) level of theory.



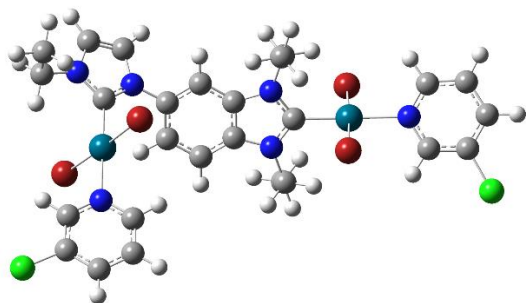
Complex 1 (HOMO-2)



Complex 3 (HOMO-3)

Figure S16: Orbital distribution of the complexes **1** (HOMO-2) and **3** (HOMO-3). DFT calculations were performed at the B3LYP/SDD (for metals) or 6-31G** (for non-metals) level of theory.

Cartesian coordinates of all the optimized geometries:

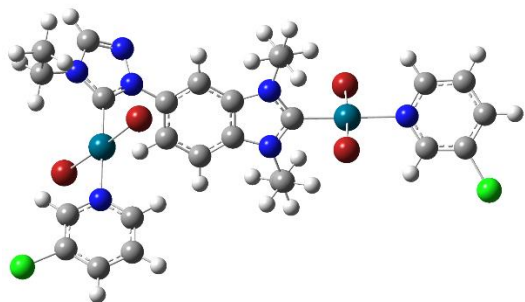


Complex 1

6	2.549160000	-0.708068000	0.363189000
6	0.504500000	-1.619099000	0.132636000
6	-0.633104000	-2.291937000	-0.300102000
1	-0.659788000	-2.867741000	-1.216412000
6	-1.771420000	-2.141259000	0.487770000
6	-1.784611000	-1.367898000	1.661647000
1	-2.704381000	-1.292942000	2.228938000
6	-0.640855000	-0.692466000	2.081542000
1	-0.647997000	-0.092891000	2.983665000
6	0.501295000	-0.827377000	1.294205000
6	2.252480000	0.556422000	2.501160000
1	1.460630000	1.275632000	2.726665000
1	3.112497000	1.111858000	2.123909000
6	2.625190000	-0.275357000	3.725100000
1	2.967178000	0.384330000	4.527373000
1	1.766803000	-0.845220000	4.092019000
1	3.427863000	-0.973552000	3.473459000
6	2.198680000	-2.108825000	-1.684122000
1	1.800189000	-3.126145000	-1.721126000
1	3.287319000	-2.176684000	-1.660715000
6	1.719785000	-1.271307000	-2.867284000
1	2.026766000	-1.746916000	-3.802883000
1	0.629821000	-1.177541000	-2.870804000

1	2.155595000	-0.270046000	-2.818050000
6	-4.440027000	-4.247885000	-0.657616000
1	-4.994048000	-5.120878000	-0.961607000
6	-4.123038000	-2.060400000	-0.222513000
6	-6.375524000	-2.668217000	-1.100827000
1	-6.759921000	-1.889124000	-0.440517000
1	-6.976196000	-3.567888000	-0.952055000
6	-6.394519000	-2.219110000	-2.558699000
1	-7.421797000	-1.996303000	-2.860871000
1	-5.786650000	-1.319549000	-2.687106000
1	-6.002977000	-3.002517000	-3.214158000
6	-5.783346000	2.552611000	0.105144000
1	-6.629548000	1.878932000	0.064340000
6	-5.947211000	3.930397000	0.214625000
6	-4.833684000	4.763626000	0.292368000
1	-4.950742000	5.836987000	0.384617000
6	-3.573063000	4.172309000	0.248470000
1	-2.675216000	4.775872000	0.307485000
6	-3.471930000	2.791160000	0.123758000
1	-2.514313000	2.289257000	0.069343000
6	6.920467000	1.495002000	-0.011497000
1	6.213472000	2.186092000	0.428710000
6	8.245656000	1.851381000	-0.243220000

6	9.119972000	0.946217000	-0.840018000
1	10.152002000	1.216539000	-1.030346000
6	8.623740000	-0.309846000	-1.181140000
1	9.261937000	-1.049720000	-1.649322000
6	7.294015000	-0.614114000	-0.911456000
1	6.871256000	-1.583866000	-1.140233000
7	1.785964000	-1.522186000	-0.405179000
7	1.781448000	-0.283478000	1.395364000
7	-2.986092000	-2.752878000	0.050318000
7	-5.015096000	-2.981051000	-0.642233000
7	-4.559903000	2.003070000	0.057588000
7	6.462620000	0.276662000	-0.340885000
17	-7.562589000	4.593428000	0.259467000
17	8.789972000	3.445717000	0.218130000
35	-2.987940000	0.134126000	-2.164357000
35	-5.687749000	-0.435058000	1.976138000
35	5.086657000	-2.290621000	1.253527000
35	3.626879000	1.801824000	-1.151071000
46	-4.346507000	-0.103982000	-0.092858000
46	4.428600000	-0.230694000	0.031151000
6	-3.162441000	-4.108801000	-0.222119000
1	-2.379820000	-4.829740000	-0.054066000



Complex 3

6	2.664570000	-0.623218000	0.349580000
6	0.619539000	-1.532686000	0.112408000
6	-0.505420000	-2.236845000	-0.302411000
1	-0.499439000	-2.917321000	-1.143788000
6	-1.674031000	-1.994890000	0.415281000
6	-1.731571000	-1.112088000	1.507301000
1	-2.668560000	-0.984505000	2.035469000
6	-0.599871000	-0.404102000	1.904620000
1	-0.638834000	0.279211000	2.744081000
6	0.573048000	-0.624213000	1.185211000
6	2.281412000	0.860512000	2.329286000
1	1.474322000	1.585585000	2.461867000
1	3.146199000	1.392615000	1.930347000
6	2.621926000	0.150670000	3.636500000
1	2.933511000	0.886051000	4.383444000
1	1.756381000	-0.391083000	4.028366000

1	3.437116000	-0.560017000	3.476878000
6	2.401699000	-2.241717000	-1.543870000
1	1.967459000	-3.243899000	-1.499483000
1	3.482643000	-2.341617000	-1.436470000
6	2.037102000	-1.525037000	-2.841052000
1	2.398568000	-2.104613000	-3.694974000
1	0.953722000	-1.409970000	-2.938114000
1	2.497220000	-0.533735000	-2.864438000
6	-4.108207000	-4.216020000	-0.665435000
1	-4.500200000	-5.178154000	-0.958091000
6	-4.056619000	-2.046781000	-0.240416000
6	-6.264718000	-2.928584000	-1.054585000
1	-6.734908000	-2.262841000	-0.329089000
1	-6.716899000	-3.917283000	-0.957196000
6	-6.393178000	-2.390483000	-2.475586000
1	-7.451684000	-2.297830000	-2.733473000
1	-5.924485000	-1.406433000	-2.557437000
1	-5.918705000	-3.065290000	-3.193626000
6	-6.141551000	2.380683000	0.103660000
1	-6.924632000	1.637489000	0.026690000
6	-6.425826000	3.737794000	0.223098000
6	-5.389940000	4.661234000	0.344162000

1	-5.601177000	5.719488000	0.443115000
6	-4.082438000	4.180522000	0.334355000
1	-3.241879000	4.857676000	0.427719000
6	-3.859136000	2.814985000	0.198740000
1	-2.861225000	2.396374000	0.171187000
6	7.076260000	1.495353000	-0.052497000
1	6.362228000	2.230955000	0.294259000
6	8.413178000	1.816516000	-0.267348000
6	9.297357000	0.851427000	-0.743564000
1	10.338905000	1.093407000	-0.919613000
6	8.798202000	-0.426584000	-0.983963000
1	9.443609000	-1.213008000	-1.356634000
6	7.455792000	-0.692108000	-0.737176000
1	7.029292000	-1.675026000	-0.890086000
7	1.927743000	-1.506980000	-0.366131000
7	1.853884000	-0.084897000	1.292461000
7	-2.871971000	-2.641884000	-0.007424000
7	-4.857070000	-3.064563000	-0.647291000
7	-4.874283000	1.939265000	0.088813000
7	6.615316000	0.255652000	-0.283667000
17	-8.091918000	4.260113000	0.224724000
17	8.959774000	3.442644000	0.061391000

35	-3.169576000	0.258515000	-2.167551000
35	-5.772360000	-0.612563000	1.975212000
35	5.141561000	-2.156125000	1.467009000
35	3.834034000	1.747590000	-1.312083000
46	-4.473085000	-0.127351000	-0.088137000
46	4.562334000	-0.196005000	0.054997000
7	-2.882345000	-3.994360000	-0.276579000

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