Supporting Information

for

A Palladium Chelating Complex of Ionic Water-soluble Nitrogen-containing Ligand: the Efficient Precatalyst for Suzuki-Miyaura Reaction in Water

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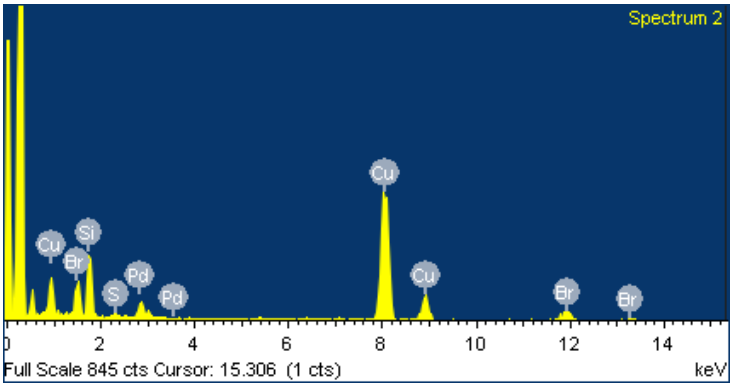

Figure S1 Energy dispersive X-ray spectrum with the use of Cu-grid of Pd NPs from the reaction catalyzed by **4.**

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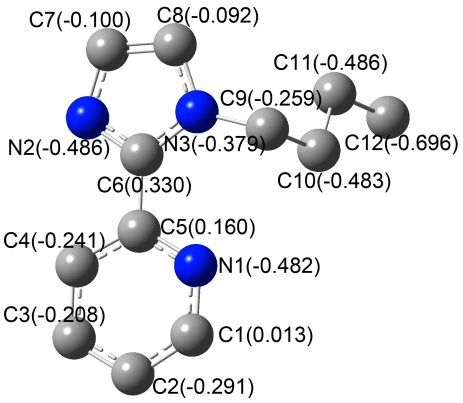
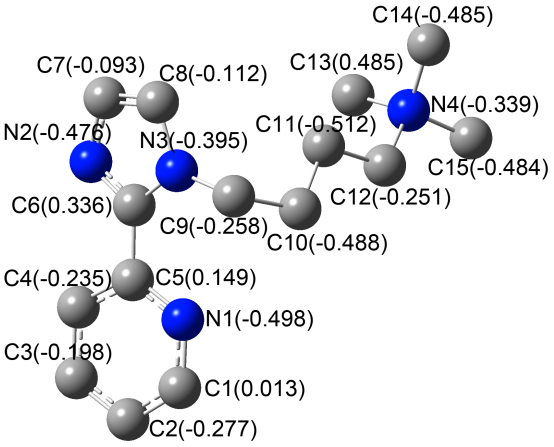
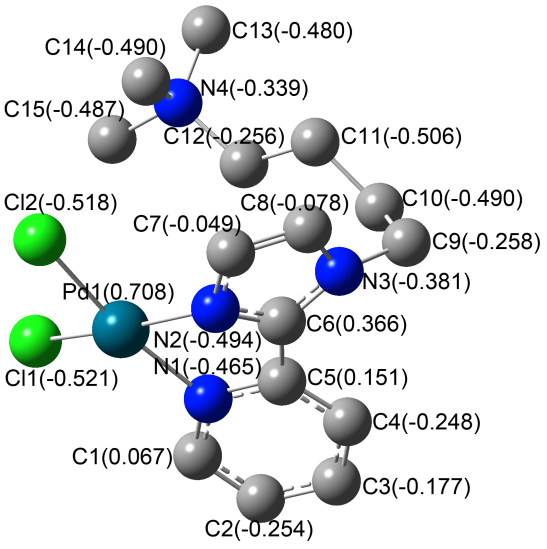


(a)

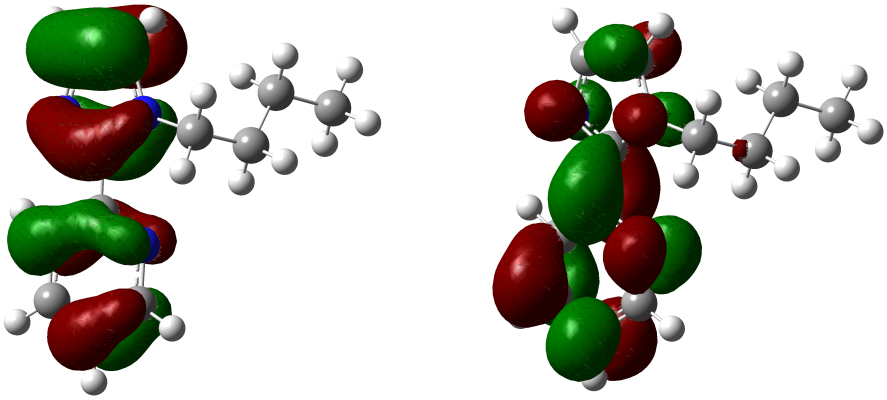


(b)



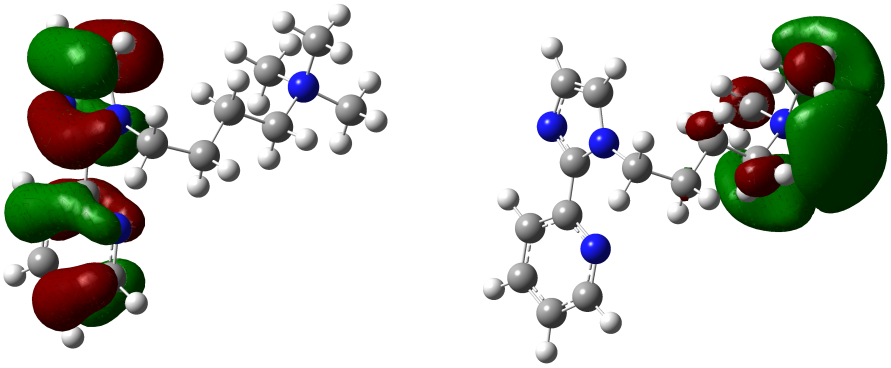
(c)

Figure S2 Charge distribution of **2a** (a); the cation in **3** (b); the cation in **4** with the national bond orbital (NBO) population analysis (B3LYP/6-31+G** for C, N, Cl, and H atoms)



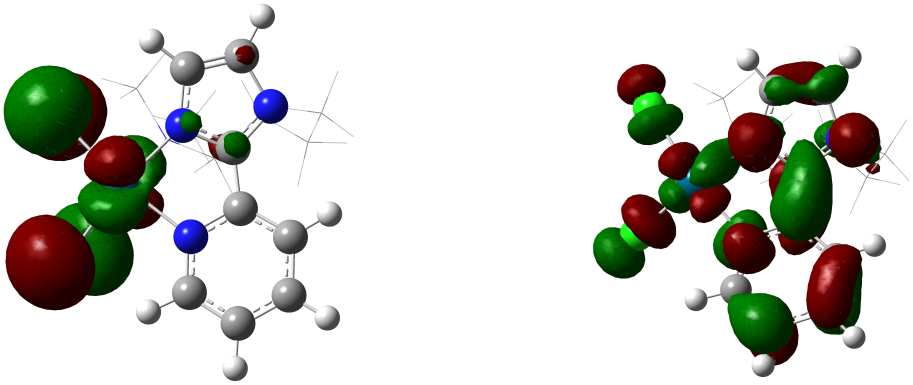
HOMO LUMO

Figure S3. HOMO (left) and LUMO (right) of **2a** (isovalue = 0.03).



HOMO LUMO

Figure S4. HOMO (left) and LUMO (right) of cation in 3 (isovalue = 0.03).



HOMO LUMO

Figure S5. HOMO (left) and LUMO (right) of cation in **4** (isovalue = 0.03).

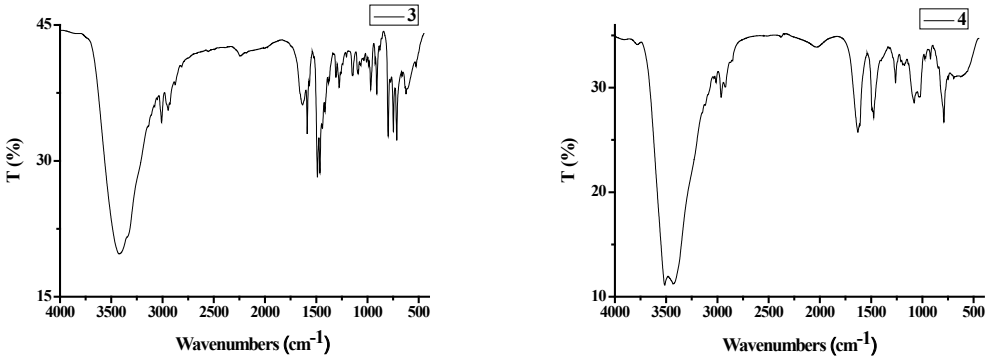


Figure S6. IR spectra of **3** and **4**

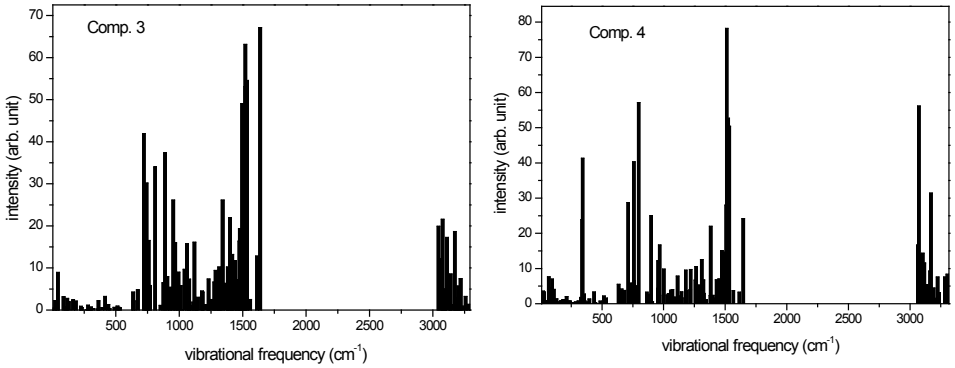


Figure S7. Calculated vibration wavenumbers (cm^{-1}) and intensities of the strongest vibrations for **3** and **4**

Table S8. Geometry coordinates of **2a**:

N	-1.34170900	-0.99973700	0.57940800
N	-0.38732900	2.34776300	-0.53010500
N	0.89278300	0.94223100	0.64710300
C	-2.39153300	-1.83127900	0.54077800
H	-2.25062900	-2.79440400	1.02766400
C	-3.60267800	-1.52154500	-0.07550100
H	-4.41861900	-2.23707900	-0.07702100
C	-3.72519200	-0.26828200	-0.68553400
H	-4.64949100	0.01923300	-1.17860900
C	-2.64921800	0.60925900	-0.65303700
H	-2.69323500	1.59222900	-1.10605600
C	-1.46315400	0.20641600	-0.00629600
C	-0.32836000	1.14100200	0.03193800
C	0.81293800	2.94404900	-0.27894600
H	1.03611600	3.94374200	-0.62456300
C	1.61857100	2.09473500	0.44678000
H	2.61997700	2.20321300	0.83516200
C	1.41825500	-0.23244600	1.36236600
H	0.61347100	-0.64310400	1.97020900
H	2.20331100	0.14255200	2.02767100
C	1.97848500	-1.32328500	0.44044400
H	2.26104600	-2.16828600	1.08427700
H	1.16909100	-1.68462400	-0.20363300
C	3.18604200	-0.90233600	-0.40613300
H	2.90842000	-0.05904700	-1.05035800
H	3.98670400	-0.53728600	0.25334200
C	3.72541600	-2.04625400	-1.27335100
H	2.95736300	-2.41293100	-1.96429000
H	4.04929400	-2.89411400	-0.65794400
H	4.58353300	-1.72209800	-1.87175200

Table S9. Geometry coordinates of the cation in **3**:

N	-2.34504100	-1.02966300	0.73803800
N	-1.86756100	2.03383600	-1.18823200
N	-0.88449000	1.54260000	0.75691200
N	3.85113700	-0.67225200	-0.47357300
C	-3.11447400	-2.12815400	0.75385700
H	-2.88994900	-2.85455100	1.53198100
C	-4.14757800	-2.36030400	-0.15278900
H	-4.73942600	-3.26739100	-0.09019200

C	-4.39444900	-1.39234300	-1.13113000
H	-5.19112700	-1.52899800	-1.85616700
C	-3.61283000	-0.24305300	-1.15917400
H	-3.77164100	0.54206400	-1.88852500
C	-2.59331100	-0.09584800	-0.20044800
C	-1.77863300	1.13063900	-0.21664700
C	-1.02754300	3.05432100	-0.84651800
H	-0.92331100	3.93593400	-1.46332600
C	-0.40892100	2.77520100	0.35058600
H	0.27830100	3.34383000	0.95971300
C	-0.42201100	0.86318300	1.97081200
H	-1.27938700	0.42325300	2.47985300
H	0.00599300	1.63601500	2.61662300
C	0.60559200	-0.24553500	1.69038700
H	0.93919100	-0.64469600	2.65683200
H	0.08131200	-1.05262500	1.16883700
C	1.81420300	0.23083600	0.86269600
H	1.43931400	0.72505700	-0.03893000
H	2.38338500	0.97338900	1.43361600
C	2.69440800	-0.96051100	0.49808000
H	2.10149800	-1.74143900	0.01424400
H	3.16264600	-1.39119000	1.38758600
C	4.63386500	-1.94949000	-0.65712800
H	3.96961800	-2.71811100	-1.05345900
H	5.03297100	-2.26360100	0.30781800
H	5.45118700	-1.76784200	-1.35596700
C	4.77016400	0.38640600	0.08006000
H	5.62285200	0.49384000	-0.59122400
H	5.11174700	0.07627300	1.06838100
H	4.23415800	1.33133500	0.14795700
C	3.32785700	-0.22992000	-1.81875200
H	4.17324900	-0.10823300	-2.49679900
H	2.80151100	0.71662500	-1.71270600
H	2.64956400	-0.99316400	-2.20151800

Table S10. Geometry coordinates of the cation in **4**:

Pd	0.53412200	-1.46818300	0.54005100
Cl	0.20435100	-2.97533000	-1.19977300
Cl	-1.20968700	-2.35676500	1.79598500
N	1.99324200	-0.37832100	-0.49781300
N	0.72211600	0.21462100	1.77272200
N	0.65175000	2.40830400	1.45875700
N	-3.06351300	0.43899500	-1.22324600
C	2.80276200	-0.83738700	-1.46145800

H	2.66668200	-1.87915500	-1.73219000
C	3.74474000	-0.01239600	-2.07988900
H	4.39132500	-0.42061900	-2.84862900
C	3.83870000	1.32067500	-1.68253500
H	4.57136400	1.98163900	-2.13471100
C	2.99131700	1.79877100	-0.67955000
H	3.07251600	2.82230600	-0.33283600
C	2.07036100	0.92311700	-0.10169900
C	1.16714500	1.22278600	1.01318100
C	-0.04989700	0.75029600	2.76757900
H	-0.51830000	0.12849400	3.51530900
C	-0.10355000	2.10996100	2.58521800
H	-0.60166400	2.88563500	3.14735400
C	0.41823400	3.61390500	0.64105100
H	1.36916400	4.08441800	0.38095500
H	-0.12207700	4.31704400	1.27902200
C	-0.38417300	3.29278800	-0.64012400
H	-0.56805900	4.24295600	-1.15216400
H	0.26078700	2.71535300	-1.31140200
C	-1.73022700	2.53686700	-0.41621000
H	-1.84810100	2.29057600	0.64255400
H	-2.55994400	3.19698500	-0.68483600
C	-1.76344700	1.24617500	-1.24938100
H	-0.99209000	0.54946600	-0.90965200
H	-1.58225300	1.46597000	-2.30569200
C	-2.82695800	-0.83216700	-2.01603100
H	-2.01888400	-1.40646600	-1.55638500
H	-2.56212300	-0.56027500	-3.03886800
H	-3.74804500	-1.41593900	-2.01212200
C	-4.18672300	1.20947900	-1.86277100
H	-5.07138100	0.57261600	-1.89362800
H	-3.89719900	1.48694200	-2.87751900
H	-4.40282100	2.10131800	-1.27568500
C	-3.45203500	0.05291200	0.18566300
H	-4.34990500	-0.56396800	0.13027500
H	-3.66496100	0.95415600	0.75946300
H	-2.64561100	-0.52730200	0.64222600

S11 Characterization data for coupling products:

4-Nitrobiphenyl

^{1}H NMR: δ 8.33 (d, *J* =8.8 Hz, 2H), 7.77 (d, *J* =8.8 Hz, 2H), 7.65 (t, *J* =7.5 Hz, 2H), 7.53-7.47 (m, 3H); ^{13}C NMR: δ 147.65, 147.14, 138.81, 129.15, 128.90, 127.80, 127.38, 124.10

Biphenyl-4-carbonitrile

^{1}H NMR: δ 7.77-7.70 (m, 4H), 7.63-7.60 (m, 2H), 7.53-7.45 (m, 3H); ^{13}C NMR: δ 145.70, 139.21, 132.59, 129.10, 128.65, 127.74, 127.23, 118.90, 110.97.

1-(Biphenyl-4-yl)ethanone

^{1}H NMR: δ 8.06 (d, *J* =8.0 Hz, 2H), 7.71 (d, *J* = 8.3Hz, 2H), 7.65 (d, *J* = 7.3 Hz, 2H), 7.50 (t, *J* = 7.2 Hz, 2H), 7.43 (t, *J* = 7.4 Hz, 1H), 2.67 (s, 3H); ^{13}C NMR: δ 197.71, 145.81, 139.91, 135.91, 128.94, 128.90, 128.22, 127.27, 127.23, 26.62.

4-Methoxy-4'-nitrobiphenyl

^{1}H NMR: δ 8.29 (d, *J* =8.3 Hz, 2H), 7.71 (d, *J* = 8.4Hz, 2H), 7.60 (d, *J* = 8.2 Hz, 2H), 7.04 (d, *J* = 8.4 Hz, 2H), 3.90 (s, 3H); ^{13}C NMR: δ 160.48, 147.22, 146.60, 131.11, 128.56, 127.07, 124.13, 114.63, 55.42.

3-Methyl-4'-nitrobiphenyl

^{1}H NMR: δ 8.31 (d, *J* =8.8 Hz, 2H), 7.75 (d, *J* = 8.8Hz, 2H), 7.46-7.39 (m, 3H), 7.29 (s,1H), 2.47 (s, 3H); ^{13}C NMR: δ 147.82, 147.07, 138.88, 138.79, 129.65, 129.05, 128.11, 127.78, 124.50, 124.04, 21.49.

4-Fluoro-4'-nitrobiphenyl

^{1}H NMR: δ 8.32 (d, *J* =8.8 Hz, 2H), 7.72 (d, *J* = 8.8Hz, 2H), 7.64-7.61 (m, 2H), 7.21 (t, *J* = 8.6Hz, 2H); ^{13}C NMR: δ 164.62, 162.14, 147.12, 146.57, 134.95, 129.18, 129.10, 127.65, 124.17, 116.30, 116.09; ^{19}F NMR: δ: -112.75.

1-(4'-Methoxybiphenyl-4-yl)ethanone

^{1}H NMR: δ 8.03 (d, *J* =8.3Hz, 2H), 7.67 (d, *J* = 8.3Hz, 2H), 7.60(d, *J* = 8.6Hz, 2H), 7.03 (d, *J* = 8.6Hz, 2H), 3.89 (s, 3H), 2.65 (s, 3H); ^{13}C NMR: δ 197.65, 159.95, 145.38, 135.33, 132.28, 128.93, 128.35, 126.61, 114.43, 55.37, 26.56.

1-(4'-Fluorobiphenyl-4-yl)ethanone

^{1}H NMR: δ 8.05 (d, *J* = 8.4Hz, 2H), 7.67-7.60 (m, 4H), 7.18 (t, *J* = 8.6Hz, 2H), 2.66 (s, 3H); ^{13}C NMR: δ 197.60, 164.4, 161.90, 144.75, 136.01, 135.90, 128.96, 128.89, 127.07, 116.02, 115.80, 26.61; ^{19}F NMR: δ: -114.06.

1-(3'-Methylbiphenyl-4-yl)ethanone

^{1}H NMR: δ 8.05 (d, *J* =8.4 Hz, 2H), 7.70 (d, *J* =8.4 Hz, 2H), 7.45 (d, *J* =8.1Hz, 2H), 7.38 (t, *J* =7.5Hz, 1H), 7.24(d, *J* =7.4Hz, 1H), 2.66 (s, 3H), 2.46 (s, 3H); ^{13}C NMR: δ 197.73, 145.96, 139.89, 138.60, 135.83, 128.97, 128.85, 128.03, 127.22, 124.39, 26.62, 21.50.

1-(4'-Methylbiphenyl-4-yl)ethanone

^{1}H NMR: δ 8.04 (d, *J* =8.4 Hz, 2H), 7.70 (d, *J* =8.5 Hz, 2H), 7.56 (d, *J* =8.2 Hz, 2H), 7.31 (d, *J* =7.9Hz, 2H), 2.66 (s, 3H), 2.44 (s, 3H); ^{13}C NMR: δ 197.69, 145.74, 138.23, 136.99, 135.66, 129.68, 128.89, 127.10, 126.95, 26.60, 21.14.