Coordination Study of a New Class of Imine Imidazol-2-imine Ligands to Titanium(IV) and Palladium(II)

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1 General procedures

All manipulations of air and/or moisture sensitive materials were carried out under an inert atmosphere of dinitrogen using standard Schlenk vessel techniques, or in an inert-atmosphere glove box containing dinitrogen. Dinitrogen was purified by passage through columns filled with molecular sieves (4 Å) and manganese (II) oxide suspended on vermiculite for the vacuum line. All solvents were dried by refluxing and then distilling from sodium (pentane, toluene, diethylether and THF) or CaH_2 (dichloromethane, CH_3CN and chloroform) under a positive pressure of dinitrogen and deoxygenated by bubbling dry dinitrogen through the dried solvents for twenty minutes before use. Solvents and solutions were transferred through stainless steel cannulae using a positive pressure of dinitrogen. Deuterated solvents were degassed using three freeze-pump-thaw cycles and were vacuum distilled from sodium (C_6D_6 and toluene) or CaH_2 ($CDCl_3$, CD_2Cl_2 and CD_3CN) and stored in the glove box. Filtrations of air and/or moisture-sensitive compounds were achieved by using modified stainless steel cannulae fitted with glass fiber filter discs at one end. All glassware and cannulae were dried overnight at 120 ºC for 24 h before use. NMR spectra were recorded on a Bruker DRX 600 (^1H at 600 MHz, ^{13}C at 150.9 MHz), Bruker AV 400 (^1H at 400 MHz, ^{13}C at 100 MHz) or Bruker AV 300 (^1H at 300 MHz, ^{13}C at 75.5 MHz) spectrometer and are at room temperature unless otherwise stated. The spectra were referenced internally relative to the residual protio-solvent (^1H) and solvent (^{13}C) resonances and chemical shifts were reported with respect to $\delta = 0$ for tetramethylsilane. Microanalyses were performed either by ANALEST of the Department of Chemistry, University of Toronto or by Guelph Chemical Laboratories LTD, Guelph, Ontario, Canada, N1G 5G5. Exact masses were determined by the AIMS Laboratory, Department of Chemistry, University of Toronto or microanalytical laboratory of the Department of Chemistry, McMaster University.

All reagents were purchased from Aldrich or Alfa Aesar, metal precursors from Strem ($PdCl_2$) or BDH ($TiCl_4$) and used as received unless otherwise stated. IMes·HCl,[1] IPr·HCl,[1] IMes,[2] IPr,[2] imidazol-2-imine,[3] $Pd(CH_3CN)_2Cl_2$,[4] $Pd(COD)Cl_2$[5] and $TiCl_4(THF)_2$[6] were prepared using published procedures. *N*-(2,6-Dimethylphenyl)acetimidoyl chloride was prepared by heating the starting amide and phosphorus pentachloride under vacuum in the absence of solvent[7] and the ^{1}H NMR data was compared with the literature.[8] NaO^{t}Bu was sublimed and kept in the inert-atmosphere glove box.

2 Synthesis of the ligand precursors

2.1 *N*-(1-(2,6-Dimethylphenylimino)ethyl)-1,3-bis(2,4,6-trimethylphenyl)imidazol-2-imine hydrochloride; IMesN^Imine·HCl (3a)

A solution of 1,3-bis(2,4,6-trimethylphenyl)imidazol-2-imine (6.58 g, 20.6 mmol) in toluene (50 mL) was slowly added to a solution of *N*-(2,6-dimethylphenyl)acetimidoyl chloride (3.63 g, 20.0 mmol) in toluene (20 mL) at room temperature. The reaction mixture was heated to reflux at 125 ˚C for 16 h and then cooled to room temperature. The off-white solid was filtered, washed with toluene (20 mL), diethylether (2 x 20 mL) and dried in vacuo. Yield 7.2 g (93 %). Crystals suitable for X-ray diffraction were grown by layering pentane over a saturated dichloromethane solution.

^{1}H NMR (400 MHz, $CDCl_3$): δ 11.2 (s, 1H, N$H_{(imine)}$), 6.98 (s, 4H, *m*-C$H_{(mesityl)}$), 6.95 (br t, 1H, ^3J = 8.0 Hz, *p*-C$H_{(2,6\text{-}xylyl)}$), 6.90 (s, 2H, -NC*H*C*H*N-), 6.84 (d, 2H, ^3J = 7.7 Hz, *m*-C$H_{(2,6\text{-}xylyl)}$), 2.36 (s, 6H, *p*-C$H_{3(mesityl)}$), 2.11 (s, 3H, C$H_{3(imine)}$), 1.92 (s, 12H, *o*-C$H_{3(mesityl)}$), 1.60 (s, 6H, *o*-C$H_{3(2,6\text{-}xylyl)}$).
^{13}C{^{1}H} NMR (100.6 MHz, $CDCl_3$): δ 162.3 (s, -N$C_{(imine)}$N-), 146.8 (s, -N$C_{(imidazolin)}$N-), 140.6 (s, $C_{(mesityl)}$), 135.6 (s, *o*-$C_{(mesityl)}$), 135.1 (s, $C_{(2,6\text{-}xylyl)}$), 134.6 (s, *o*-$C_{(2,6\text{-}xylyl)}$), 129.9 (s, *p*-$C_{(mesityl)}$), 129.8 (s, *m*-C$H_{(mesityl)}$), 127.0 (s, *m*-C$H_{(2,6\text{-}xylyl)}$), 127.1 (s, *p*-C$H_{(2,6\text{-}xylyl)}$), 118.9 (s, -NCHCHN-), 21.0 (s, *p*-C$H_{3(mesityl)}$), 19.7 (s, C$H_{3(imine)}$), 17.6 (s, *o*-C$H_{3(mesityl)}$), 17.5 (s, *o*-C$H_{3(2,6\text{-}xylyl)}$)

Anal. Calcd. For $C_{31}H_{37}ClN_4 \cdot 0.15\ CH_2Cl_2$ (%): C, 72.81; H, 7.32; N, 10.90; Found (%): C, 72.81; H, 7.26; N, 10.98.

HRMS (ESI$^+$, CH_3CN): Calculated for $C_{31}H_{37}ClN_4$, *m/z* = 464.2940 $[M\text{-}Cl]^+$; Found: 464.2946 $[M\text{-}Cl]^+$

FTIR (Thin film): $\nu_{C=N}$ 1617 cm^{-1}, $\nu_{C=C}$ 1519 cm^{-1}

2.2 *N*-(1-(2,6-Dimethylphenylimino)ethyl)-1,3-bis(2,6-diisopropylphenyl)imidazol-2-imine hydrochloride, IPrN^Imine·HCl (3b)

A solution of 1,3-bis(2,6-diisopropylphenyl)imidazol-2-imine (6.33 g, 15.7 mmol) in toluene (70 mL) was slowly added to a solution of *N*-(2,6-dimethylphenyl)acetimidoyl chloride (2.71 g, 14.9 mmol) in toluene (20 mL) at room temperature. The reaction mixture was heated to reflux at 125 °C for 12 h and then cooled to room temperature. The off-white solid was filtered, washed with toluene (20 mL), diethyl ether (3 x 10 mL) and dried in vacuo. Yield 6.6 g (76 %). Crystals suitable for X-ray diffraction were grown by layering pentane over a saturated dichloromethane solution.

^{1}H NMR (400 MHz, $CDCl_3$): δ 11.35 (s, 1H, N$H_{(imine)}$), 7.56 (t, 2H, *J* = 7.8 Hz, *p*-C$H_{(2,6\text{-}diisopropylphenyl)}$), 7.30 (d, 4H, *J* = 7.8 Hz, *m*-C$H_{(2,6\text{-}diisopropylphenyl)}$), 6.95 (s, 2H, -NC*H*C*H*N-), 6.87 (t, 1H, *J* = 7.5 Hz, *p*-C$H_{(2,6\text{-}dimethylphenyl)}$), 6.73 (d, 2H, *J* = 7.4 Hz, *m*-C$H_{(2,6\text{-}dimethylphenyl)}$), 2.47 (sept, 4H, *J* = 6.8 Hz, C$H_{(2,6\text{-}diisopropylphenyl)}$), 2.25 (s, 3H, C$H_{3(Imine)}$), 1.53 (s, 6H, *o*-C$H_{3(xylyl)}$), 1.12 (d, 12H, *J* = 6.8 Hz, C$H_{3(2,6\text{-}diisopropylphenyl)}$), 1.06 (d, 12H, *J* = 6.8 Hz, C$H_{3(2,6\text{-}diisopropylphenyl)}$)

^{13}C{^{1}H} NMR (100.6 MHz, $CDCl_3$): δ 162.1 (s, -N$C_{(imine)}$N-), 149.7 (s, -N$C_{(imidazolin)}$N-), 145.7 (s, *o*-$C_{(2,6\text{-}diisopropylphenyl)}$), 135.3 (s, *o*-$C_{(2,6\text{-}xylyl)}$), 134.7 (s, $C_{(2,6\text{-}xylyl)}$), 131.5 (s, *p*-C$H_{(2,6\text{-}diisopropylphenyl)}$), 129.9 (s, $C_{(2,6\text{-}diisopropylphenyl)}$), 127.5 (s, *m*-C$H_{(2,6\text{-}xylyl)}$), 126.9 (s, *p*-C$H_{(2,6\text{-}xylyl)}$), 124.9 (s, *m*-*p*-C$H_{(2,6\text{-}diisopropylphenyl)}$), 119.4 (s, -NCHCHN-), 28.9 (s, C$H_{(2,6\text{-}diisopropylphenyl)}$), 25.5 (s, C$H_{3(2,6\text{-}diisopropylphenyl)}$), 22.2 (s, C$H_{3(2,6\text{-}diisopropylphenyl)}$), 20.6 (s, C$H_{3(imine)}$), 17.7 (s, *o*-C$H_{3(2,6\text{-}xylyl)}$)

Anal. Calcd. For $C_{37}H_{48}ClN_4 \cdot 1.0\ CH_2Cl_2$ (%): C, 68.20; H, 7.53; N, 8.37; Found (%): C, 68.56; H, 8.04; N, 8.54.

HRMS (ESI$^+$, CH_3CN): Calculated for $C_{37}H_{48}ClN_4$, *m/z* = 548.3879 $[M\text{-}Cl]^+$; Found: 548.3870 $[M\text{-}Cl]^+$

FTIR (Thin film): $\nu_{C=N}$ 1613 cm^{-1}, $\nu_{C=C}$ 1518 cm^{-1}

3 Synthesis of the Ti(IV) and Pd(II) Complexes

3.1 *N*-(1-(2,6-Dimethylphenylimino)ethyl)-1,3-bis(2,4,6-trimethylphenyl)imidazol-2-imine teterachlorotitanium(IV); Ti(IMesN^Imine)Cl_4 (4a)

To a suspension of IMesN^Imine.HCl (**3a)** (300 mg, 0.599 mmol) in benzene (5 mL) was added sodium *tert*-butoxide (56.5 mg, 0.588 mmol) as a solid in one portion. Reaction mixture was stirred for 2 h at room temperature and then filtered through a plug of Celite. The solid was washed with benzene (1 mL) and the combined organic fractions were dried in vacuo for 1 h at room temperature. The off-white solid was redissolved in benzene (5 mL) and added dropwise to a stirred solution of $TiCl_4(THF)_2$ (192.3 mg, 0.576 mmol) in benzene (2 mL) at room temperature. The colour of the reaction mixture changed to bright red from the original yellow solution. The reaction mixture was stirred for 45 min and the precipitated brick red solid was filtered, washed with benzene (2 x 3 mL), pentane (5 mL) and dried in vacuo. Yield: 263 mg (70 %). Single crystals suitable for X-ray diffraction study were grown from a saturated CH_3Cl solution at room temperature.

^{1}H NMR (300 MHz, $CDCl_3$): δ 7.12 (s, 4H, *m*-C$H_{(mesityl)}$), 7.02 (s, 2H, -NC*H*C*H*N-), (br s, 3H, *m*-C$H_{(2,6\text{-xylyl})}$ & *p*-C$H_{(2,6\text{-xylyl})}$), 2.44 (s, 6H, *p*-C$H_{3(mesityl)}$), 2.38 (br s, 12H, *o*-C$H_{3(mesityl)}$), 2.14 (s, 6H, *o*-C$H_{3(2,6\text{-xylyl})}$), 1.69 (s, 3H, C$H_{3(imine)}$),

^{13}C{^{1}H} NMR (100.6 MHz, CD_2Cl_2): δ 175.0 (s, -NC$_{(imine)}$N-), 147.0 (s, -NC$_{(imidazolin)}$N-), 144.6 (s, $C_{(2,6\text{-xylyl})}$), 141.5 (s, *p*-$C_{(mesityl)}$), 133.8 (br s, $C_{(mesityl)}$), 133.8 (s, *o*-$C_{(2,6\text{-xylyl})}$), 131.2 (s, *o*-$C_{(mesityl)}$), 130.4 (br s, *m*-C$H_{(mesityl)}$), 129.1 (s, *m*-C$H_{(2,6\text{-xylyl})}$), 127.3 (s, *p*-C$H_{(2,6\text{-xylyl})}$), 122.2 (s, -NC*H*C*H*N-),21.4 (s, *p*-C$H_{3(mesityl)}$), 20.3 (s, *o*-C$H_{3(2,6\text{-xylyl})}$), 20.0 (s, C$H_{3(imine)}$), 19.6 (br s, *o*-C$H_{3(mesityl)}$).

Anal. Calcd. For $C_{31}H_{36}Cl_4N_4Ti$ (%): Satisfactory combustion analysis was never obtained due to the sensitive nature of the complex.

MS (ESI^+, CH_2Cl_2): Calculated for $C_{31}H_{36}Cl_4N_4Ti$, m/z = 464.29 $[M\text{-}TiCl_4]^+$; Found: 464.30 $[M\text{-}TiCl_4]^+$

3.2 *N*-(1-(2,6-Dimethylphenylimino)ethyl)-1,3-bis(2,6-diisopropylphenyl)imidazol-2-imine teterachlorotitanium(IV); Ti(IPrN^Imine)Cl_4 (4b)

To a suspension of IPrN^Imine.HCl (**3b**) (165 mg, 0.283 mmol) in benzene (5 mL) was added sodium *tert*-butoxide (26.7 mg, 0.277 mmol) as a solid in one portion. Reaction mixture was stirred for 2 h at room temperature and then filtered through a plug of Celite. The solid was washed with benzene (1 mL) and the combined organic fractions were dried in vacuo for 30 min. The off-white solid was redissolved in benzene (3 mL) and added dropwise to a stirred solution of $TiCl_4(THF)_2$ (86.9 mg, 0.260 mmol) in benzene (2 mL) at room temperature. The colour of the reaction mixture changed to bright red from the original yellow solution. The reaction mixture was stirred for 45 min and the precipitated brick red solid was filtered, washed with benzene (2 x 3 mL), pentane (10 mL) and dried in vacuo. Yield: 152 mg (76 %).

^1H NMR (400 MHz, $CDCl_3$): δ 7.55 (t, 2H, ^3J = 7.8 Hz, *p*-$CH_{(2,6\text{-diisopropylphenyl})}$), 7.39 (d, 4H, ^3J = 7.8 Hz, *m*-$CH_{(2,6\text{-diisopropylphenyl})}$), 7.30 (s, 2H, -NC*H*C*H*N-), 7.00-6.88 (m, 3H, *p*-$CH_{(2,6\text{-xylyl})}$ & *m*-$CH_{(2,6\text{-xylyl})}$), 2.95 (br s, 4H, $CH_{(2,6\text{-diisopropylphenyl})}$), 1.98 (s, 6H, *o*-$CH_{3(2,6\text{xylyl})}$), 1.64 (s, 3H, $CH_{3(\text{imine})}$), 1.46 (br d, 12 H, ^3J = 6.0 Hz, $CH_{3(2,6\text{-diisopropylphenyl})}$), 1.16 (d, 12H, ^3J = 6.7 Hz, $CH_{3(2,6\text{-diisopropylphenyl})}$)

$^{13}C\{^1H\}$ NMR (100.6 MHz, CD_2Cl_2): δ 173.9 (s, -N$C_{(\text{imine})}$N-), 148.7 (s, -N$C_{(\text{imidazolin})}$N-), 146.4 (s, *o*-$C_{(2,6\text{-diisopropylphenyl})}$), 144.5 (s, $C_{(2,6\text{-xylyl})}$), 133.9 (s, *o*-$C_{(2,6\text{-xylyl})}$), 132.1(s, *p*-$CH_{(2,6\text{-diisopropylphenyl})}$), 131.9 (s, $C_{(2,6\text{-diisopropylphenyl})}$), 129.2 (s, *m*-$CH_{(2,6\text{-xylyl})}$), 127.1(s, *p*-$CH_{(2,6\text{-xylyl})}$), 125.2 (s, *m*-$CH_{(2,6\text{-diisopropylphenyl})}$), 123.4 (s, -NCHCHN-), 29.8 (s, $CH_{(2,6\text{-diisopropylphenyl})}$), 26.6 (s, $CH_{3(2,6\text{-diisopropylphenyl})}$), 23.1 (s, $CH_{3(2,6\text{-diisopropylphenyl})}$), 20.7 (s, *o*-$CH_{3(2,6\text{-xylyl})}$), 17.9 (s, $CH_{3(\text{imine})}$).

Anal. Calcd. For $C_{37}H_{48}Cl_4N_4Ti$ (%): Satisfactory combustion analysis was never obtained due to the sensitive nature of the complex.

MS (ESI^+, CH_2Cl_2): Calculated for $C_{37}H_{48}Cl_4N_4Ti$, m/z = 548.39 $[M\text{-}TiCl_4]^+$; Found: 548.40 $[M\text{-}TiCl_4]^+$

3.3 *N*-(1-(2,6-Dimethylphenylimino)ethyl)-1,3-bis(2,4,6-trimethylphenyl)imidazol-2-iminedichloropalladium(II) dimer; $[Pd(IMesN^Imine)Cl_2]_2$ (5a)

To a suspension of IMesN^Imine.HCl, (**3a**) (200 mg, 0.399 mmol) in benzene (5 mL) was added sodium *tert*-butoxide (37.7 mg, 0.392 mmol) as a solid in one portion and the reaction mixture was stirred for 2 h at room temperature. The reaction mixture was then passed through a plug of Celite and the solid was washed with benzene (1 mL). The combined fractions were added dropwise to a stirred solution of $Pd(CH_3CN)_2\ Cl_2$ (101.6 mg, 0.392 mmol) in benzene (1 mL) at room temperature. The colour of the reaction mixture changed from the original yellow solution to orange brown. The reaction mixture was further stirred for 2 h and the precipitated solid was filtered, washed with benzene (2 x 3 mL). Solid was dissolved in minimum amount of dichloromethane and the solution was passed through a plug of neutral alumina. The plug was washed with dichloromethane (1 mL) and the orange brown solution was added dropwise to stirred diethyl ether (10 mL). The product was isolated as yellow brown solid, which was dried dried under high vacuum for 12 h. Yield: 190 mg (76 %).

^1H NMR (400 MHz, $CDCl_3$): δ 6.87 (s, 4H, *m*-$CH_{(mesityl)}$), 6.80 (t, 1H, ^3J = 7.2 Hz, *p*-$CH_{(2,6\text{-}xylyl)}$), 6.70 (d, 2H, ^3J = 7.4 Hz, *m*-$CH_{(2,6\text{-}xylyl)}$), 6.56 (s, 2H, -NC*H*C*H*N-), 2.39 (s, 3H, $CH_{3(imine)}$), 2.30 (s, 6H, *o*-$CH_{3(2,6\text{-}xylyl)}$), 1.82 (s, 12H, *o*-$CH_{3(mesityl)}$), 1.76 (s, 6H, *p*-$CH_{3(mesityl)}$),

$^{13}C\{^1H\}$ NMR (100.6 MHz, $CDCl_3$): δ 162.3 (s, -$NC_{(imine)}$N-), 146.4 (s, *p*-$C_{(mesityl)}$), 144.6 (s, -$NC_{(imidazolin)}$N-), 140.3 (s, *o*-$C_{(2,6\text{-}xylyl)}$), 134.9 (s, *o*-$C_{(mesityl)}$), 130.8 (s, $C_{(mesityl)}$), 130.1 (s, $C_{(2,6\text{-}xylyl)}$),

129.7 (s, *m*-*C*H$_{(mesityl)}$), 127.4 (s, *m*-*C*H$_{(2,6\text{-}xylyl)}$), 124.3 (s, *p*-*C*H$_{(2,6\text{-}xylyl)}$), 116.3 (s, -N*C*H*C*HN-), 26.3 (s, *C*H$_{3(imine)}$), 21.2 (s, *o*-*C*H$_{3(2,6\text{-}xylyl)}$), 20.2 (s, *p*-*C*H$_{3(mesityl)}$), 17.7 (s, *o*-*C*H$_{3(mesityl)}$).

Anal. Calcd. For $C_{31}H_{36}Cl_2N_4Pd$. CH_2Cl_2 (%): C, 52.87; H, 5.27; N, 7.71; Found (%): C, 51.80; H, 5.30; N, 7.79. Repeated attempts always gave lower C contents.

HRMS (ESI$^+$, CH_3CN): Calculated for $C_{62}H_{72}Cl_4N_8Pd_2$, *m/z* = 1245.3009 $[M\text{-}Cl]^+$; Found: 1245.2864 $[M\text{-}Cl]^+$

FTIR (Thin film): $\nu_{C=N}$ 1595 cm^{-1}, $\nu_{C=C}$ 1519 cm^{-1}

3.4 *N*-(1-(2,6-Dimethylphenylimino)ethyl)-1,3-bis(2,6-diisopropylphenyl)imidazol-2-imine dichloropalladium(II) dimer; [Pd(IPrN^Imine)Cl$_2$]$_2$ (5b)

To a suspension of IPrN^Imine**.**HCl (**3b**) (215 mg, 0.368 mmol) in benzene (4 mL) was added sodium *tert*-butoxide (36.1 mg, 0.376 mmol) as solid in one portion and the reaction mixture was stirred for 2 h at room temperature. The reaction mixture was then passed through a plug of Celite and the solid was washed with benzene (1 mL). The combined organic fractions were added dropwise to a stirred solution of $Pd(CH_3CN)_2Cl_2$ (93.4 mg, 0.357 mmol) in benzene (2 mL) at room temperature. The colour of the reaction mixture changed from the original yellow solution to orange brown and the reaction mixture was stirred for 2 h. The precipitated solid was filtered, washed with benzene (2 x 3 mL), pentane (3 mL) and dried in vacuo. Yield: 198 mg (76 %). Single crystals suitable for X-ray diffraction study were grown by layering pentane onto a saturated CH_2Cl_2 solution.

^{1}H NMR (400 MHz, $CDCl_3$,): δ 7.45 (t, 2H, ^3J = 7.7 Hz, *p*-C*H*$_{(2,6\text{-}diisopropylphenyl)}$), 7.23 (d, 4H, ^3J = 7.8 Hz, *m*-C*H*$_{(2,6\text{-}diisopropylphenyl)}$), 6.76 (m, 2H, -NC*H*C*H*N- & 1H, *p*-C*H*$_{(2,6\text{-}xylyl)}$), 6.62 (d, 2H, ^3J = 7.4 Hz, *m*-C*H*$_{(2,6\text{-}xylyl)}$), 2.59 (s, 3H, C*H*$_{3(imine)}$) 2.48 (m, 4H, C*H*$_{(2,6\text{-}diisopropylphenyl)}$), 1.47 (s, 6H, *o*-C*H*$_{3(2,6xylyl)}$), 1.03 (d, 12 H, ^3J = 6.5 Hz, C*H*$_{3(2,6\text{-}diisopropylphenyl)}$), 1.01 (d, 12H, ^3J = 6.5 Hz, C*H*$_{3(2,6\text{-}diisopropylphenyl)}$)

$^{13}C\{^1H\}$ NMR (100.6 MHz, $CDCl_3$): δ 162.7 (s, -N$C_{(imine)}$N-), 150.1 (s, -N$C_{(imidazolin)}$N-), 146.7 (s, *o*-$C_{(2,6\text{-diisopropylphenyl})}$), 146.4 (s, $C_{(2,6\text{-xylyl})}$), 135.5 (s, *o*-$C_{(2,6\text{-xylyl})}$), 131.6 (s, $C_{(2,6\text{-diisopropylphenyl})}$), 131.3 (s, *p*-$CH_{(2,6\text{-diisopropylphenyl})}$), 128.2 (s, *m*-$CH_{(2,6\text{-xylyl})}$), 125.1 (s, *m*-*p*-$CH_{(2,6\text{-diisopropylphenyl})}$), 124.8 (s, *p*-$CH_{(2,6\text{-xylyl})}$), 119.0 (s, -NCHCHN-), 29.3 (s, $CH_{(2,6\text{-diisopropylphenyl})}$), 27.9 (s, $CH_{3(imine)}$), 25.8 (s, $CH_{3(2,6\text{-diisopropylphenyl})}$), 22.7 (s, $CH_{3(2,6\text{-diisopropylphenyl})}$), 20.5 (s, *o*-$CH_{3(2,6\text{-xylyl})}$)

Anal. Calcd. For $C_{37}H_{48}Cl_2N_4Pd$ (%): C, 61.20; H, 6.66; N, 7.72; Found (%): C, 60.92; H, 6.51; N, 7.84.

HRMS (ESI$^+$, CH_3CN): Calculated for $C_{37}H_{48}Cl_2N_4Pd$, *m/z* = 653.2829 $[M\text{-}Cl_2]^+$; Found: 653.2779 $[M\text{-}Cl_2]^+$

FTIR (Thin film): $\nu_{C=N}$ 1599 cm^{-1}, $\nu_{C=C}$ 1518 cm^{-1}

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