Supporting Information

Neutral Imino-methyl Benzenesulfonate Ligated Pd(II) Complexes and Implications in Ethylene Polymerization

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1. Materials and methods:

Unless noted otherwise, all manipulations were carried out under an inert atmosphere using standard Schlenk line techniques or m-Braun glove box. Toluene was distilled from sodium/benzophenone under argon atmosphere. Dimethyl formamide and methylene chloride were distilled on calcium-hydride. Ethanol was dried on magnesium cake and was stored on molecular sieves. Ethylene (3.5 grade) was supplied by Ms. Praxair India Pvt. Ltd, Bangalore, India. Aniline, 4-methoxy aniline, 2-methoxy aniline, 2,6-diisopropyl aniline, 2-methylpropane-2-amine, adamantant-1-amine, sodium-2-formyl benzene sulfonate were supplied by sigma-aldrich or were purchased from local suppliers. [(COD)PdMeCl] was synthesized following known procedures. The polymerization was run in a Buechiglasuster cyclone 075 high pressure reactor equipped with overhead mechanical stirrer, heating/cooling jacket and pressure regulators. Solution NMR spectra were recorded on a Bruker Avance 200, 400, 500 and 700 MHz instruments. Chemical shifts are referenced to external reference TMS (\(^{1}\)H and \(^{13}\)C). Coupling constants are given as absolute values. Multiplicities are given as follows s: singlet, d: doublet, t: triplet, m: multiplet, br s: broad singlet. Mass spectra were recorded on Thermo scientific Q-Exactive mass spectrometer, the column specification is Hypersil gold C18 column 150 x 4.6 mm diameter 8 µm particle size mobile phase used is 90% methanol + 10 % water + 0.1 % formic acid. Differential scanning colorimeter (DSC) was carried out on DSC Q-10 from TA instruments at a heating and cooling rate of 10 K min\(^{-1}\). MALDI-ToF-MS was performed on AB SCIEX TOF/TOF™ 5800 and Dithranol was used as a matrix. IR spectra were recorded on Bruker VERTEX 80 spectrophotometer. The samples were prepared as Nujol mull.

**Crystallography details: Pd-Dim:** Good quality single crystal of was selected using a Leica polarizing microscope MZ75 for the single crystal X-ray diffraction study. The diffraction data measurements were carried out using a Bruker SMART APEX CCD diffractometer with graphite-monochromatized (Mo Ka = 0.71073 Å) radiation. The X-ray generator was operated at 50 kV and 30 mA. A preliminary set of cell constants and an orientation matrix were calculated from a total of 36 frames. The optimized strategy used for data collection consisted of different sets of φ and ω scans with 0.5° steps in φ/ω. The data were collected keeping the sample-to-detector distance fixed at 5.00 cm.
The X-ray data acquisition was monitored by using APEX2 program suite. All the data were corrected for Lorentz polarization and absorption effects using SAINT and SADABS programs integrated in APEX2 package. The structures were solved by direct methods and refined by full matrix least squares, based on $F^2$, using SHELX-97. Molecular diagrams were generated using Mercury programs. Geometrical calculations were performed using SHELX-97 and PLATON.

**Crystallography details: C3:** X-ray intensity data measurements of compounds SSD_C582 was carried out on a Bruker D8 VENTURE Kappa Duo PHOTON II CPAD diffractometer equipped with Incoatech multilayer mirrors optics. The intensity measurements were carried out with Mo micro-focus sealed tube diffraction source (MoKα = 0.71073 Å) at 100(2) K temperature. The X-ray generator was operated at 50 kV and 1.4 mA. A preliminary set of cell constants and an orientation matrix were calculated from three sets of 36 frames. Data were collected with $\omega$ scan width of 0.5° at different settings of $\phi$ and $2\theta$ keeping the sample-to-detector distance fixed at 5.00 cm. The X-ray data collection was monitored by APEX3 program (Bruker, 2016). All the data were corrected for Lorentzian, polarization and absorption effects using SAINT and SADABS programs (Bruker, 2016). ShelX-97 was used for structure solution and full matrix least-squares refinement on $F^2$. All the hydrogen atoms were placed in a geometrically idealized position and constrained to ride on its parent atoms. An ORTEP III view of compound was drawn with 50% probability displacement ellipsoids and H atoms are shown as small spheres of arbitrary radii.

**2. Synthesis of ligand L1-L6**

**2.1 Synthesis of sodium-2-((phenylimino)methyl)benzenesulfonate (L1):**

In a schlenk flask sodium-2-formyl benzene sulfonate (1.00 g, 4.08 mmol) was dissolved in DMF. Molecular sieves were added to this (5-6 beads) followed by aniline (0.418 g, 4.08 mmol) to immediately observe a colour change from colourless to blue. Reaction mixture was refluxed at 150 °C for 3 hours. After stirring for the desired time, reaction mixture was cooled and filtered to remove molecular sieves. Filtrate was concentrated under reduced pressure to obtain pale blue coloured residue. The crude product was washed separately with DCM (25 mL) and hexane (3 x 35 mL). The residue was dried further for 3 h under reduced pressure at room temperature to yield desired product. (1.23 g, 91%).
$^1$H NMR (500 MHz, DMSO-$d_6$) δ = 9.50 (s, 1 H), 8.15 (d, J = 6.87, 2.29 Hz, 1 H), 7.86-7.84 (m, 1 H), 7.48-7.41 (m, 4 H), 7.26-7.23 (m, 1 H), 7.18-7.17 (m, 2 H). $^{13}$C NMR (126 MHz, DMSO-$d_6$) δ = 161.2, 152.2, 148.4, 132.4, 130.3, 129.2, 129.0, 126.8, 126.5, 125.8, 120.9. ESI-MS (+Ve) C$_{13}$H$_{11}$NO$_3$NaS Calculated m/z = 284.0357 Observed m/z = 284.0350 [M+H]$^+$. IR (cm$^{-1}$) =1621 (C=N). **Elemental Analysis:** Calculated C 55.12, H 3.56, N 4.94; Found C 54.92, H 3.30, N 5.11.

**Figure S1:** $^1$H NMR spectrum of sodium-2-((phenylimino)methyl)benzenesulfonate (L1).
Figure S2: $^{13}$C DEPT NMR spectrum of sodium-2-((phenylimino)methyl)benzenesulfonate (L1).

Figure S3: $^{13}$C NMR of sodium (E)-2-((phenylimino)methyl)benzenesulfonate (L1).
**Figure S4**: ESI-MS of sodium-2-((phenylimino)methyl)benzenesulfonate (L1).

**Figure S5**: IR spectrum of L1 in Nujol mull.
2.2 Synthesis of sodium-2-(((4-methoxyphenyl) imino) methyl) benzenesulfonate (L2):

In a schlenk flask sodium-2-formyl benzene sulfonate (1.00 g, 4.08 mmol) was dissolved in DMF. Molecular sieves were added to this (5-6 beads) followed by 4-methoxylaniline (0.502 g, 4.08 mmol) was added to observe immediately colour change from colourless to yellow. Reaction mixture was refluxed at 150°C for 4 hours. After stirring for the desired time, reaction mixture was cooled and filtered to remove molecular sieves. Filtrate was concentrated under reduced pressure to obtain yellow coloured residue. The crude product was washed separately with DCM (25 mL) and hexane (3 x 20 mL). Product was dried further for 3 h under reduced pressure at room temperature to yield desired L2. (1.25 g, 80 %) \textbf{1H NMR} (500 MHz, DMSO-d$_6$) $\delta$ = 9.38 (s, 1H), 8.12 (br s, 1H), 7.83 (d, $J = 8.8$ Hz, 1H), 7.46 (m, 2H), 7.19 (t, $J = 7.2$ Hz, 1H), 7.05 (d, $J = 8.0$ Hz, 1H), 6.97 (t, $J = 7.4$ Hz, 1H), 6.89 (d, $J = 6.9$ Hz, 1H), 3.79 (s, 3H). \textbf{13C NMR} (126 MHz, DMSO-d$_6$) $\delta$ = 161.2 (N=CH), 152.0, 148.3, 142.2, 132.6, 130.1, 128.8, 126.7, 126.4, 120.8, 119.8, 112.0, 55.5 (-OCH$_3$). \textbf{ESI-MS} (+Ve) C$_{14}$H$_{13}$NO$_4$NaS Calculated m/z = 314.04, Observed m/z = 314.04 [M+H]$^+$, \textbf{IR} (cm$^{-1}$): 1616 (C=N). \textbf{Elemental Analysis:} Calculated C 53.67, H 3.86, N 4.47; Found C 53.51, H 3.79, N 4.94.
**Figure S6**: $^1$H NMR of sodium-2-(((4-methoxyphenyl)imino)methyl)benzenesulfonate ligand L2 (# = DMF impurities, * = H$_2$O)

**Figure S7**: $^{13}$C DEPT NMR of sodium-2-(((4-methoxyphenyl)imino)methyl) benzene sulfonate ligand L2.

**Figure S8**: $^{13}$C NMR of sodium-2-(((4-methoxyphenyl)imino)methyl) benzenesulfonate ligand L2 (# = DMF impurities).
Figure S9: ESI-MS of sodium-2-(((4-methoxyphenyl)imino)methyl) benzene sulfonate ligand L2.

Figure S10: IR of sodium-2-(((4-methoxyphenyl)imino)methyl) benzene sulfonate ligand L2.
2.3 Synthesis of sodium-2-(((2-methoxyphenyl) imino)methyl)benzenesulfonate (L3):

In a Schlenk flask sodium-2-formyl benzene sulfonate (0.208 g, 1 mmol) was dissolved in DMF. Molecular sieves were added to this (5-6 beads). To this 2-methoxyaniline (0.136 g, 1 mmol) was added. Reaction mixture was refluxed at 150° C for 6 hours. After stirring for the desired time, reaction mixture was cooled and filtered to remove molecular sieves. Filtrate was concentrated under reduced pressure. The crude product was washed separately with DCM (25 mL) and hexane (3 x 35 mL). Product was dried further for 3 h under reduced pressure at room temperature to yield desired product. (0.269 g, 86 %). ^1H NMR (400 MHz, DMSO-d6) δ = 9.41 (s, 1 H), 8.14 (br s, 1 H), 7.88 (br s, 1 H), 7.48 (br s, 2 H), 7.19 (s, 1 H), 7.05 (d, J = 7.3 Hz, 1 H), 6.97 (s, 1 H), 6.93 (s, 1 H), 3.79 (s, 3 H). ^13C NMR (101 MHz, DMSO-d6) δ = 161.2 (N=CH), 152.1, 148.1, 142.2, 132.7, 130.2, 129.1, 126.8, 126.6, 120.9, 119.9, 112.0, 55.6 (OCH3). ESI-MS (+Ve) C14H13NO4NaS Calculated m/z = 314.04, Observed m/z = 314.04 [M+H]^+.

IR (cm⁻¹) =1616 (C=N). Elemental Analysis: Calculated C 53.67, H 3.86, N 4.47; Found C 53.67, H 4.22, N 5.35.
**Figure S11:** $^1$H NMR of sodium-2-(((2-methoxyphenyl) imino) methyl) benzenesulfonate (L3) (# = dimethyl formamide solvent impurity).

**Figure S12:** $^{13}$C DEPT NMR of sodium-2-(((2-methoxyphenyl) imino) methyl) benzenesulfonate (L3).
Figure S13: $^{13}$C NMR of sodium-2-(((2-methoxyphenyl) imino) methyl) benzenesulfonate (L3) (# = DMF impurity).

$^{13}$C NMR data:
- C$_{14}$H$_{13}$O$_4$N$_2$NaS = 314.0457 ppm
- m/z values and relative abundances:
  - 314.043 R=61502
  - 317.3047 R=60307
  - 321.3148 R=55202
  - 315.0489 R=45700
  - 324.9789 R=45100
  - 319.2842 R=43900
  - 312.3257 R=44800
  - 310.3101 R=54900
  - 308.9127 R=60502
- RT: 1.00  AV: 1  NL: 5.90E5
- T: FTMS + p ESI Full ms [100.0000-1500.0000]
2.4 Synthesis of sodium-2-(((2,6-diisopropylphenyl)imino)methyl) benzenesulfonate (L4):

In a schlenk flask sodium-2-formyl benzenesulfonate (0.416 g, 2 mmol) was dissolved in DMF. Molecular sieves were added to this (5-6 beads). To this 2,6-diisopropylaniline (0.354 g, 2 mmol) was added. Reaction mixture was refluxed at 150°C for 6 hours. After stirring for the desired time, reaction mixture was cooled and filtered to remove molecular sieves. Filtrate was concentrated under reduced pressure. The crude product was washed separately with DCM (25 mL) and hexane (3 x 35 mL). Product was dried further for 3 h under reduced pressure at room temperature to yield desired L4. (0.522 g, 71%)

$^1$H NMR (400 MHz, DMSO-$d_6$) δ = 9.08 (s, 1 H, N=CH), 8.21-8.20 (m, 1 H), 7.84 (m, 1 H), 7.51 (d, $J = 3.7$ Hz, 2 H), 7.12-7.10 (m, 3 H), 3.58 (s, 2 H), 1.07 (d, $J = 6.7$ Hz, 12 H). $^{13}$C NMR (126 MHz, DMSO-$d_6$) δ = 162.7 (s, N=CH), 149.6, 148.5, 136.9, 132.1, 130.2, 128.8,
126.8, 126.1, 123.6, 122.6, 27.3, 23.2. **ESI-MS** (+Ve) C\textsubscript{19}H\textsubscript{23}NO\textsubscript{3}NaS Calculated m/z = 368.12

Observed m/z = 368.12 [M+H]\textsuperscript{+}. **IR** (cm\textsuperscript{-1}) = 1632 (C=N). **Elemental Analysis:** Calculated C 62.11, H 6.04, N 3.81; Found C 62.09, H 5.64, N 3.75.

**Figure S16:** \textsuperscript{1}H NMR of sodium-2-(((2,6-diisopropylphenyl)imino)methyl) benzenesulfonate (L4) (# = solvent Impurity).
Figure S17: $^{13}$C DEPT NMR of sodium-2-(((2,6-diisopropylphenyl)imino)methyl) benzenesulfonate (L4).

Figure S18: $^{13}$C NMR of sodium-2-(((2,6-diisopropylphenyl) imino)methyl) benzenesulfonate (L4).
Figure S19: ESI-MS of sodium-2-(((2,6-diisopropylphenyl)imino)methyl) benzenesulfonate (L4).

Figure S20: IR of sodium-2-(((2,6-diisopropylphenyl)imino)methyl) benzenesulfonate (L4).
2.5 Synthesis of sodium-2-(((tert-butylimino)methyl)benzenesulfonate (L5):

In a schlenk flask sodium-2-formyl benzene sulfonate (0.416 g, 2 mmol) was dissolved in DMF. Molecular sieves were added to this (5-6 beads). To this 2-methylpropan-2-amine (0.146 g, 2 mmol) was added. Reaction mixture was stirred for 12 hours. After stirring for the desired time, reaction mixture was filtered to remove molecular sieves. Filtrate was concentrated under reduced pressure. The crude product was washed with hexane (3 x 5 mL). Product was dried further for 3 h under reduced pressure at room temperature to yield desired product (0.339 g, 64 %). $^1$H NMR (500 MHz, DMSO-$d_6$) $\delta = 9.24$ (s, 1 H), 7.98 (s, 1 H), 7.81 (s, 1 H), 7.37 (s, 2 H), 1.23 (s, 9 H). $^{13}$C NMR (126 MHz, DMSO-$d_6$) $\delta = 155.6$ (-N=C), 147.2, 133.5, 129.0, 128.8, 126.7, 126.1, 57.1, 29.8 (CH$_3$). ESI-MS (+Ve) C$_{11}$H$_{15}$NO$_3$NaS Calculated m/z = 264.06 Observed m/z = 264.06 [M+H]$^+$. IR (cm$^{-1}$) = 1635 (C=N). **Elemental Analysis:** Calculated C 50.18, H 5.36, N 5.32; Found C 50.10, H 5.10, N 5.78.
Figure S21: $^1$H NMR of sodium-2-((tert-butylimino)methyl)benzenesulfonate (L5) (# = DMF Impurity, *water impurity).

Figure S22: $^{13}$C DEPT NMR of sodium-2-((tert-butylimino)methyl)benzenesulfonate (L5).
**Figure S23.** $^{13}$C NMR of sodium-2-((tert-butylimino)methyl)benzenesulfonate (L5).

**Figure S24.** ESI-MS of sodium-2-((tert-butylimino)methyl)benzenesulfonate (L5).
2.6. Synthesis of Sodium-2-(((3s,5s,7s)-adamantan-1-yl)imino)methyl)benzenesulfonate (L6):

Sodium-2-formyl benzene sulfonate (0.208 g, 1 mmol) was taken into schlenk flask having magnetic stir bar. (3s, 5s, 7s) - adamantan-1-amine (0.151 g, 1 mmol) was added to the above flask followed by addition of 5 mL of ethanol. The reaction mixture was refluxed for 5 h under constant stirring at 78 °C. After this time the reaction mixture was allowed to cool to room temperature. At room temperature, ethanol was evaporated under reduced pressure. The crude product was washed with hexane and dried further for 3 h under reduced pressure at room temperature. The yield of product obtained was 78 % (0.265 g).

\(^1\)H NMR (400 MHz, DMSO-\textit{d}_6) \(\delta = 9.21\) (s, 1 H), 7.98-7.96 (m, 1 H), 7.78-7.76 (m, 1 H), 7.35-7.33 (m, 2 H), 2.12 (br s, 3 H), 1.72-1.66 (m, 12 H). \(^1\)C NMR (101 MHz, DMSO-\textit{d}_6) \(\delta = 155.7, 147.8, 133.9, 129.3, 129.0, 127.0, 126.2, 57.6, 43.4, 36.6, 29.3\). IR (cm\(^{-1}\)) = 1634
Elemental Analysis: Calculated C 59.81, H 5.91, N 4.10; Found C 60.10, H 5.85, N 4.22.

Figure S26: $^1$H NMR of sodium-2-(((3s,5s,7s)-adamantan-1-yl)imino)methyl)benzenesulfonate (L6).
Figure S27: $^{13}$C DEPT NMR of sodium-2-(((3s,5s,7s)-adamantan-1-y1)imino) methyl)benzenesulfonate (L6).

Figure S28: $^{13}$C NMR of sodium-2-(((3s,5s,7s)-adamantan-1-y1)imino) methyl)benzenesulfonate (L6).
**Figure S29:** IR spectrum of sodium-2-(((3s,5s,7s)-adamantan-1-yl)imino)methyl)benzenesulfonate (L6).

### 3. Synthesis of palladium complexes:

#### 3.1 Complexation of L3 with palladium, first attempt:

In a schlenk flask, sodium-2-(((4-methoxyphenyl)imino)methyl)benzenesulfonate L3 (0.100 g, 0.319 mmol) and [(COD)PdMeCl] (0.084 g, 0.319 mmol) was dissolved in dry DMSO at room temperature and stirred for four hours. Volatiles were evaporated under reduced pressure to yield brown coloured residue (0.165 g).

**$^1$H NMR** (400 MHz, DMSO-$d_6$, 298 K) $\delta$ = 9.49 (s, 1H), 8.12 (s, 1H), 7.82 (s, 1H), 7.44 (s, 2H), 7.18 (s, 2H), 7.00 (m, 2H), 3.77 (m, 3H), 0.95 (s, 3H).
3.2 Synthesis of [(DMSO)PdCH₂Cl]₂ dimer (Pd-Dim):

50 mg of [(COD)PdMeCl] (0.188 mmol) was dissolved in dry DMSO at room temperature. Reaction was stirred for 4 hours at room temperature. Solvent was evaporated under reduced pressure to obtain yellow coloured powder in quantitative yield (96.59 %). \(^1\)H NMR (500 MHz, CDCl₃, 298 K) \(\delta = 2.53\) (s, 12H), 0.95 (s, 6H). The above dimer (0.300 gm) was dissolved in 10 mL of DCM and flask was kept for slow evaporation. After 2 days, suitable crystals for X-ray analysis were obtained.
Figure S31: $^1$H NMR spectrum of [(DMSO)PdMeCl]$_2$ at 200 MHz in CDCl$_3$.

Figure S32: Molecular structure of [(DMSO)PdMeCl]$_2$ (Pd-Dim).
Table S1. Comparison of important bond distance [Å] and bond angles [°] (Pd-Dim).

| Bonds[Å]/Angles [°] | Pd-Dim | Reference 4     |
|---------------------|--------|-----------------|
| Pd1-Cl1a            | 2.47 Å | 2.44 Å          |
| Pd1-Cl1             | 2.36 Å | 2.39 Å          |
| Cl1-Pd1-Cl1a        | 86.30° | 85.38°         |

3.3 Synthesis of [Lu$_2$PdMeCl] complex:

In a schlenk flask [(COD)PdMeCl] (0.458 g, 1.72 mmol) was dissolved in dry dichloromethane (DCM) and lutidine (0.268 g, 2.5 mmol) was added to it at room temperature. Reaction was stirred for 3 hours and 30 minutes at room temperature. Solvent was evaporated under reduced pressure and washed with hexane (3 × 10 mL) to obtain off yellow coloured powder. This was dissolved in DCM and filtered through celite bed to obtain off yellow coloured Pd complex in 97 % yield. $^1$H NMR (200 MHz, CDCl$_3$, 298 K) δ = 7.51 (t, $J = 7.69$ Hz, 2H), 7.11 (d, $J = 7.62$ Hz, 4H), 3.36 (s, 12H), 0.196 (s, 3H).

![Figure S33: $^1$H NMR of [Lu$_2$PdMeCl] at 200 MHz in CDCl$_3$.](image-url)
3.4 Preparation of 2-((4-methoxyphenyl) imino) methyl) benzenesulfonato ligated Palladium (II) complex (C1):

\[\text{[(COD)PdMeCl]}\ 0.100\ g,\ 0.38\ mmol\] was taken in Schlenk flask having magnetic stir bar which was followed by addition of AgBF\(_4\) (0.0737 g, 0.38 mmol) and 10 mL dry DCM. The reaction mixture was stirred for 2 hours at RT. Sodium-2-((4-methoxyphenyl)imino)methyl) benzenesulfonate (0.1189 g, 0.38 mmol) and 5 mL of dry DCM was added to the above Schlenk flask. After 15 min, 44 μL of lutidine (0.38 mmol) was added to the reaction mixture followed by the constant stirring for 30 Min. Reaction mixture was filtered by using cannula filtration. The filtrate was evaporated and dried for 3 hours under reduced pressure at room temperature. The yield of obtained product complex C1 was 56% (0.150 g). \(^1\)H NMR (400 MHz, CDCl\(_3\)) \(\delta = 8.91\) (br s, 1H), 8.25 (d, \(J = 5.06\) Hz, 1H), 7.67 (d, \(J = 8.76\) Hz, 2H), 7.59 (m, 2H), 7.45 (t, \(J = 7.68\) Hz, 1H), 6.98-6.94 (m, 5H), 3.85 (s, 3H), 2.68 (br s, 6H), 0.06 (s, 3H). \(^{13}\)C NMR (101 MHz, CDCl\(_3\)) \(\delta = 169.7\) (-N=CH), 159.7, 159.6, 144.4, 138.1, 133.5, 130.7, 130.3, 130.1, 128.8, 128.5, 127.3, 123.8, 122.7, 122.5, 114.4, 55.7 (OCH\(_3\)), 28.1, 27.5, -8.1 (Pd-CH\(_3\)). ESI-MS (+Ve) C\(_{22}\)H\(_{25}\)N\(_2\)O\(_4\)NaS Calculated \(m/z = 519.05\), Observed \(m/z = 519.05\) [M+H]\(^+\). IR (cm\(^{-1}\)): 1614 (C=N). **Elemental Analysis:**

Calculated C 50.92, H 4.66, N 5.40; Found C 50.70, H 4.88, N 5.74.
Figure S34: $^1$H NMR of 2-(((4-methoxyphenyl) imino) methyl) benzenesulfonato palladium (II) complex (C1) in CDCl$_3$.

Figure S35: $^{13}$C DEPT NMR of C1 in CDCl$_3$. 
Figure S36: $^{13}$C NMR of 2-(((4-methoxyphenyl) imino) methyl) benzenesulfonato palladium (II) complex (C1) in CDCl$_3$.

Figure S37: ESI-MS of 2-(((4-methoxyphenyl) imino) methyl) benzenesulfonato palladium (II) complex (C1).
Figure S38: IR of 2-(((4-methoxyphenyl) imino) methyl) benzenesulfonato palladium (II) complex (C1).

3.5 Preparation of 2-(((2,6-diisopropylphenyl)imino)methyl) benzenesulfonato ligated palladium (II) complex (C2):

Sodium-2-(((2,6-diisopropylphenyl)imino)methyl)benzenesulfonate (0.177 g, 0.477 mmol) was taken in Schlenk flask having magnetic stir bar. [([Lu]_2PdMeCl] (0.209 g, 0.572 mmol) was added to the above the Schlenk flask followed by addition of 10 mL of dry DCM. The reaction mixture was stirred for 5 h at RT followed by precipitation by addition of 30 mL of hexane. Precipitate was filtered out by using cannula filtration. The filtrate is evaporated and dried for 3 h under reduced pressure at room temperature. The yield of obtained product complex C2 was 84 % (0.243 g).$^1$H NMR (400 MHz, CDCl$_3$) $\delta$ = 8.78 (s, 1H), 8.31 (d, $J$ = 7.33 Hz, 1H), 7.66 (m, 1H), 7.49-7.42 (m, 2H), 7.35-7.29 (m, 3H), 7.13 (d, $J$ = 7.75 Hz, 1H), 7.01 (d, $J$ = 7.75 Hz, 2H), 3.73 (quint, $J$ = 13.1 Hz, 6.58 Hz, 2H), 2.76 (s, 6H),
1.47 (d, J = 6.65 Hz, 6H), 1.37 (d, J = 6.65 Hz, 6H), 0.09 (s, Pd-CH₃, 3H). ¹³C NMR (101 MHz, CDCl₃) δ = 174.9 (-N=CH), 160.5, 160.3, 159.8, 146.3, 144.3, 141.7, 138.1, 138.0, 137.5, 133.6, 130.3, 130.1, 128.2, 128.0, 126.9, 124.5, 122.5, 28.2, 27.1, 26.6, 24.2, -7.2 (Pd-CH₃). ESI-MS (+Ve) C₂₇H₃₅N₂O₃NaS Calculated m/z = 573.13, Observed m/z = 573.15 [M+H]⁺. IR (cm⁻¹): 1628 (C=N). Elemental Analysis: Calculated C 56.59, H 5.98, N 4.89; Found C 56.19, H 6.30, N 5.11.

**Figure S39:** ¹H NMR of 2-(((2,6-diisoproplyphenyl)imino)methyl) benzenesulfonato palladium (II) complex (C2).
**Figure S40:** $^{13}$C DEPT NMR of 2-(((2,6-diisopropylphenyl)imino)methyl) benzenesulfonato palladium (II) complex (C2).

**Figure S41:** $^{13}$C NMR of Sodium-2-(((2,6-diisopropylphenyl)imino)methyl) benzenesulfonato palladium (II) complex (C2).
Figure S42: ESI-MS of \(2-((2,6\text{-diisopropylphenyl})\text{imino})\text{methyl})\) benzenesulfonato palladium (II) complex (C2).

Figure S43: IR of \(2-((2,6\text{-diisopropylphenyl})\text{imino})\text{methyl})\) benzenesulfonato palladium (II) complex (C2).
3.6 Preparation of 2-((tert-butylimino)methyl)benzenesulfonato complex (C3):

(0.100 g, 0.477 mmol) [Pd(COD)MeCl] (0.100 g, 0.38 mmol) was taken in schlenk flask having magnetic stir bar followed by addition of AgBF\(_4\) (0.0737 g, 0.38 mmol) and 10 mL dry DCM. The reaction mixture was stirred for 2 h at RT. sodium 2-((tert-butylimino)methyl)benzenesulfonate (0.100 g, 0.38 mmol) and 10 mL of dry DCM was added to the above Schlenk flask. After 15 min, 44 μL of lutidine (0.38 mmol) was added to the reaction mixture followed by the constant stirring for 2 h. Reaction mixture was filtered by passing through celite bed. The filtrate is evaporated and residue obtained was reprecipitated using DCM and hexane mixture. Residue obtained after cannula filtration was dried for 3 h under vacuum at room temperature. The yield of obtained product complex C1 was 55% (0.0.098 g). Suitable crystals for single crystal XRD were grown by layering hexane on the DCM solution of the complex C3 at -25 °C.

\( ^{1}H\) NMR (400 MHz, CDCl\(_3\)) \( \delta = 8.84\) (s, 1H, \( HC=\text{N} \)), 8.27 (d, \( J = 7.19\) Hz, 1H), 7.62-7.54 (m, 2H), 7.47 (t, \( J = 7.65\) Hz, 1H), 7.37 (d, \( J = 7.01\) Hz, 1H), 7.04 (d, \( J = 6.54\) Hz, 1H), 6.93 (d, \( J = 6.56\) Hz, 1H), 3.27 (s, 3H, Lutidine CH\(_3\)), 2.14 (s, 3H, Lutidine CH\(_3\)), 1.73 (s, 9H, tert. CH\(_3\)) 0.17 (s, 3H, Pd-CH\(_3\)). \( ^{13}C\) NMR (101 MHz, CDCl\(_3\)) \( \delta = 167.2\) (-N=CH), 160.2, 159.8, 145.5, 137.9, 135.0, 130.2, 129.3, 128.4, 126.4, 122.7, 122.4, 65.1 [C(CH\(_3\))], 30.9 (tert. CH\(_3\)), 27.4 (Lutidine CH\(_3\)), 25.8 (Lutidine CH\(_3\)), -12.6 (Pd-CH\(_3\)). IR (cm\(^{-1}\)) : 1605 (C=N). ESI-MS (+Ve) C\(_{19}\)H\(_{27}\)N\(_3\)O\(_3\)PdS [M+H]\(^{+}\) Calculated m/z = 469.0777; Observed m/z = 469.0786. **Elemental Analysis:** Calculated C 48.67, H 5.59, N 5.97; Found C 48.73, H 5.55, N 6.12.
Figure S44: $^1$H NMR for C3 in CDCl$_3$ (400 MHz).
Figure S45: $^{13}$C NMR of C3 in CDCl$_3$ (100 MHz).
Figure S46: DEPT NMR of C3 in CDCl$_3$ (100 MHz).

Figure S47: ESI-MS of C3.
**Figure S48:** IR spectrum of L5 ligated palladium (II) complex (C3).

**Figure S49:** Molecular structure of C3 (50% probability thermal ellipsoids).
### Table S2. Crystal data table for C3.

|                  | SSD_C_582               |
|------------------|-------------------------|
| **Formula**      | C₁₉H₂₆N₂O₃PdS          |
| **Mᵣ**          | 468.88                  |
| **Crystal Size, mm** | 0.33×0.16×0.10        |
| **Temp. (K)**    | 100(2)                  |
| **Crystal Syst.**| Tetragonal              |
| **Space Group**  | I4₁/a                   |
| **a/Å**          | 16.9821(5)              |
| **b/Å**          | 16.9821(5)              |
| **c/Å**          | 27.6108(19)             |
| **α[^°]**        | 90                      |
| **β[^°]**        | 90                      |
| **γ[^°]**        | 90                      |
| **V/Å³**         | 7962.7(7)               |
| **Z**            | 16                      |
| **Dₐ₁₉c/g cm⁻³** | 1.564                   |
| **μ/mm⁻¹**       | 0.099                   |
| **F(000)**       | 3840                    |
| **Ab. Correct.** | multi-scan              |
| **Tₘᵢ₉ν/Tₘₐₓ**   | 0.722/0.902             |
| **2θₘₐₓ**        | 61                      |
| **Total reflections** | 245568                  |
| **Unique reflections** | 6082                   |
| **Observed reflections** | 5595                   |
| **h, k, l (min, max)** | (-24, 24), (-24, 24), (-39, 30) |
| $R_{int}$ | 0.0696 |
| $R_{sig}$ | 0.0173 |
| No. of parameters | 241 |
| No. of restraints | 0 |
| $R1 \ [I > 2\sigma(I)]$ | 0.0217 |
| $wR2[I > 2\sigma(I)]$ | 0.0520 |
| $R1 \ [all \ data]$ | 0.0251 |
| $wR2 \ [all \ data]$ | 0.0541 |
| goodness-of-fit | 1.059 |
| $\Delta \rho_{max}, \Delta \rho_{min}(\text{eÅ}^{-3})$ | +0.573, -0.498 |
| CCDC No. | 1911214 |

**Table S3.** Bond lengths [Å] and angles [°] for mo_ssd_c_582_0ma_a (C3).

| Bond | Length/Angle |
|------|--------------|
| Pd(1)-C(19) | 2.0111(14) |
| Pd(1)-N(1) | 2.0546(11) |
| Pd(1)-N(2) | 2.0643(12) |
| Pd(1)-O(1) | 2.1963(10) |
| S(1)-O(2) | 1.4437(14) |
| S(1)-O(3) | 1.4440(15) |
| S(1)-O(1) | 1.4821(11) |
| S(1)-C(4) | 1.7886(15) |
| N(1)-C(7) | 1.2714(17) |
| N(1)-C(8) | 1.5130(18) |
| N(2)-C(18) | 1.350(2) |
| N(2)-C(14) | 1.3521(19) |
| C(1)-C(2) | 1.386(2) |
| C(1)-C(6) | 1.388(2) |
| C(1)-H(1) | 0.9500 |
| C(2)-C(3) | 1.386(2) |
| C(2)-H(2) | 0.9500 |
| C(3)-C(4) | 1.392(2) |
| C(3)-H(3) | 0.9500 |
| C(4)-C(5) | 1.3978(19) |
| C(5)-C(6) | 1.3996(18) |
| C(5)-C(7) | 1.4805(19) |
| C(6)-H(6) | 0.9500 |
| C(7)-H(7) | 0.9500 |
| C(8)-C(11) | 1.515(2) |
| C(8)-C(9) | 1.529(2) |
| C(8)-C(10) | 1.532(3) |
| C(9)-H(9A) | 0.9800 |
| C(9)-H(9B) | 0.9800 |
| C(9)-H(9C) | 0.9800 |
C(10)-H(10A) 0.9800
C(10)-H(10B) 0.9800
C(10)-H(10C) 0.9800
C(11)-H(11A) 0.9800
C(11)-H(11B) 0.9800
C(11)-H(11C) 0.9800
C(12)-H(12A) 0.9800
C(12)-H(12B) 0.9800
C(12)-H(12C) 0.9800
C(13)-C(14) 1.499(3)
C(12)-H(12A) 0.9800
C(12)-H(12B) 0.9800
C(12)-H(12C) 0.9800
C(13)-C(15) 1.499(2)
C(13)-H(13A) 0.9800
C(13)-H(13B) 0.9800
C(13)-H(13C) 0.9800
C(14)-C(15) 1.499(2)
C(15)-C(16) 1.397(2)
C(15)-H(15) 0.9500
C(16)-C(17) 1.397(2)
C(16)-H(16) 0.9500
C(17)-C(18) 1.397(2)
C(17)-H(17) 0.9500
C(19)-H(19A) 0.9800
C(19)-H(19B) 0.9800
C(19)-H(19C) 0.9800
C(19)-Pd(1)-N(1) 91.41(5)
C(19)-Pd(1)-N(2) 89.03(5)
N(1)-Pd(1)-N(2) 179.12(5)
C(19)-Pd(1)-O(1) 175.93(6)
N(1)-Pd(1)-O(1) 90.59(4)
N(2)-Pd(1)-O(1) 89.02(4)
O(2)-S(1)-O(3) 115.28(10)
O(2)-S(1)-O(1) 110.59(8)
O(3)-S(1)-O(1) 112.65(8)
O(2)-S(1)-C(4) 105.18(8)
O(3)-S(1)-C(4) 106.32(7)
O(1)-S(1)-C(4) 106.04(6)
S(1)-O(1)-Pd(1) 120.33(6)
C(7)-N(1)-C(8) 117.81(12)
C(7)-N(1)-Pd(1) 119.52(10)
C(8)-N(1)-Pd(1) 122.58(9)
C(18)-N(2)-C(14) 119.42(13)
C(18)-N(2)-Pd(1) 121.00(10)
C(14)-N(2)-Pd(1) 119.52(10)
C(2)-C(1)-C(6) 119.85(14)
C(2)-C(1)-H(1) 120.1
C(1)-C(6)-H(1) 120.1
C(3)-C(2)-C(1) 120.04(15)
C(3)-C(2)-H(2) 120.0
C(1)-C(2)-H(2) 120.0
C(2)-C(3)-C(4) 120.54(14)
C(2)-C(3)-H(3) 119.7
C(4)-C(3)-H(3) 119.7
C(3)-C(4)-C(5) 119.82(13)
C(3)-C(4)-S(1) 118.66(11)
C(5)-C(4)-S(1) 121.37(11)
C(4)-C(5)-C(6) 119.06(13)
C(4)-C(5)-C(7) 122.04(12)
C(6)-C(5)-C(7) 118.70(12)
C(1)-C(6)-C(5) 120.68(13)
C(1)-C(6)-H(6) 119.7

S41
Symmetry transformations used to generate equivalent atoms:

Table S4. Torsion angles [°] for mo_ssd_c_582_0ma_a (C3).

| Torsion angle [°] | Equivalent Transformation |
|------------------|---------------------------|
| O(2)-S(1)-O(1)-Pd(1) | 147.13(9) |
| O(3)-S(1)-O(1)-Pd(1) | -82.29(9) |
| C(4)-S(1)-O(1)-Pd(1) | 33.61(9) |
| C(6)-C(1)-C(2)-C(3) | -0.4(3) |
| C(1)-C(2)-C(3)-C(4) | 0.0(3) |
| C(2)-C(3)-C(4)-C(5) | -0.3(2) |
| C(2)-C(3)-C(4)-S(1) | 175.27(14) |
| O(2)-S(1)-C(4)-C(3) | -8.87(15) |
| O(3)-S(1)-C(4)-C(3) | -131.55(14) |
| O(1)-S(1)-C(4)-C(3) | 108.33(13) |
| O(2)-S(1)-C(4)-C(5) | 166.65(13) |
| O(3)-S(1)-C(4)-C(5) | 43.97(14) |
| O(1)-S(1)-C(4)-C(5) | -76.15(13) |
| C(3)-C(4)-C(5)-C(6) | 1.1(2) |
| S(1)-C(4)-C(5)-C(6) | -174.37(11) |
| C(3)-C(4)-C(5)-C(7) | 175.83(14) |
| S(1)-C(4)-C(5)-C(7) | 0.37(19) |
| C(2)-C(1)-C(6)-C(5) | 1.2(2) |
| C(4)-C(5)-C(6)-C(1) | -1.5(2) |
| C(7)-C(5)-C(6)-C(1) | -176.45(13) |
| C(8)-N(1)-C(7)-C(5) | -175.40(13) |
| Pd(1)-N(1)-C(7)-C(5) | 1.30(18) |
| C(4)-C(5)-C(7)-N(1) | 62.32(19) |
| C(6)-C(5)-C(7)-N(1) | -122.92(15) |
| C(7)-N(1)-C(8)-C(11) | 150.80(15) |
| Pd(1)-N(1)-C(8)-C(11) | -25.79(18) |
| C(7)-N(1)-C(8)-C(9) | 30.9(2) |
| Pd(1)-N(1)-C(8)-C(9) | -145.65(12) |
| C(7)-N(1)-C(8)-C(10) | -89.07(17) |
| Pd(1)-N(1)-C(8)-C(10) | 94.34(14) |
| C(18)-N(2)-C(14)-C(15) | -1.4(2) |
| Pd(1)-N(2)-C(14)-C(15) | 175.95(11) |
| C(18)-N(2)-C(14)-C(13) | 178.29(15) |
| Pd(1)-N(2)-C(14)-C(13) | -4.40(19) |
| N(2)-C(14)-C(15)-C(16) | 1.2(2) |
| C(13)-C(14)-C(15)-C(16) | -178.44(16) |
| C(14)-C(15)-C(16)-C(17) | 0.4(2) |
| C(15)-C(16)-C(17)-C(18) | -1.7(2) |
| C(14)-N(2)-C(18)-C(17) | 0.0(2) |
| Pd(1)-N(2)-C(18)-C(17) | -177.29(12) |
| C(14)-N(2)-C(18)-C(12) | 178.95(16) |
| Pd(1)-N(2)-C(18)-C(12) | 1.7(2) |
| C(16)-C(17)-C(18)-N(2) | 1.6(2) |
| C(16)-C(17)-C(18)-C(12) | -177.35(18) |

Symmetry transformations used to generate equivalent atoms:
4. Ethylene polymerization with C1-C3:
The ethylene polymerization was carried out in a 250 mL stainless steel high pressure reactor (Buechi) equipped with mechanical stirrer and heating/cooling jacket. Prior to the experiment, the reactor was heated in vacuum to 90°C for 60 minutes, cooled to room temperature and was filled with argon. Reactor was flushed with ethylene (3 times) and was charged with 100 ml of toluene under positive ethylene stream. Next, the reactor was pressurized and saturated with ethylene for 30 minutes at desired reaction temperature before it was cooled to room temperature. A catalyst solution (25 mg, 48 μmol in 5 ml DCM) was introduced into the reactor at room temperature. The reactor was then pressurized to desired ethylene pressure with stirring and appropriate temperature was reached within 1-5 minutes. After polymerization the excess ethylene was slowly vented off and the reactor was allowed to cool down to room temperature. The precipitated solid was separated and resultant solution was evaporated in vacuum to obtain waxy mass, which was further dried under reduced pressure at 50 °C for 8 hours or until constant weight obtained. Important polymerization experiments using C1-C3 are summarized in table 2.

Table S5. Insertion polymerization of ethylene catalyzed by neutral Pd(II) complex C1.

| Entry | Press. (bars) | Temp. (°C) | Time (h) | Yield (g) a | TOF (mol of PE/mol of Pd/h) | Tm (°C) a |
|-------|---------------|------------|----------|------------|----------------------------|------------|
| 1     | 10            | 40         | 1        | ND         | ND                        | ND         |
| 2     | 15            | 80         | 2        | 0.027b     | 20                        | ND         |
| 3     | 5             | 95         | 2        | 0.020      | 15                        | ND         |
| 4     | 15            | 95         | 2        | 0.075c     | 56                        | 125        |
| 5     | 25            | 95         | 2        | 0.106c     | 79                        | ND         |

Conditions: C1: 0.025 g (48μmol in 5 mL dichloromethane), Solvent: Toluene (100 mL), a-determined after evaporating volatiles from the reaction content and subtracting the weight of catalyst from total solid obtained. b: 2 mg of precipitated polyethylene was observed, c: 5 mg of precipitated polyethylene was observed.
Figure S50: $^1$H NMR spectrum of a low molecular weight polyethylene fraction produced in run 4, table S5 (in CDCl$_3$).

Figure S51: MALDI-ToF-MS spectrum of a polyethylene produced in run 4, table S5.
Table S6. Permutations and combinations with ethylene insertion in a Pd-Me (or Pd-H) bond of C1. As evident, repeat unit mass of 28 Da or multiples of this number could be observed. Underlined molar masses could be observed in the MALDI-ToF-MS spectrum. ET: Ethylene (-CH\(_2\)-CH\(_2\)-) repeat unit.

| Sr.No | (ET)\(n\) | C1 (g/mol) + nET (Pd-Me) Calculated | C1 (g/mol) + nET (Pd-H) Calculated |
|-------|-------------|-------------------------------------|-------------------------------------|
| 1     | 0           | 518.93                              | 504.90                              |
| 2     | 1           | 546.98                              | 532.92                              |
| 3     | 2           | 575.04                              | 561.01                              |
| 4     | 3           | 603.09                              | 589.06                              |
| 5     | 4           | 631.14                              | 617.11                              |
| 6     | 5           | 559.19                              | 645.17                              |
| 7     | 6           | 687.25                              | 673.22                              |
| 8     | 7           | 715.30                              | 701.28                              |
| 9     | 8           | 743.36                              | 729.33                              |
| 10    | 9           | 771.41                              | 757.38                              |
| 11    | 10          | 799.46                              | 785.44                              |
| 12    | 11          | 827.52                              | 813.49                              |
| 13    | 12          | 855.57                              | 841.55                              |
| 14    | 13          | 883.63                              | 869.60                              |
| 15    | 14          | 911.68                              | 897.65                              |
| 16    | 15          | 939.73                              | 925.71                              |
| 17    | 16          | 979.79                              | 953.76                              |
| 18    | 17          | 995.84                              | 981.82                              |
| 19    | 18          | 1023.90                             | 1009.87                             |
| 20    | 19          | 1051.95                             | 1037.92                             |
| 21    | 20          | 1080.00                             | 1065.98                             |
| 22    | 21          | 1108.06                             | 1094.03                             |
| 23    | 22          | 1136.11                             | 1122.09                             |
| 24    | 23          | 1164.17                             | 1148.75                             |
| 25    | 24          | 1192.22                             | 1178.79                             |
| 26    | 25          | 1220.27                             | 1206.25                             |
| 27    | 26          | 1248.33                             | 1234.30                             |
| 28    | 27          | 1276.38                             | 1262.36                             |
| 29    | 28          | 1304.44                             | 1290.41                             |
| 30    | 29          | 1332.49                             | 1318.46                             |
| 31    | 30          | 1360.54                             | 1346.52                             |
| 32    | 31          | 1388.60                             | 1374.57                             |
| 33    | 32          | 1418.65                             | 1402.63                             |
| 34    | 33          | 1444.71                             | 1430.68                             |
| 35    | 34          | 1472.76                             | 1458.73                             |
| 36    | 35          | 1500.81                             | 1486.79                             |
| 37    | 36          | 1528.87                             | 1514.84                             |
| 38    | 37          | 1556.92                             | 1542.90                             |
| 39 | 38  | 1584.98 | **1570.95** |
|----|-----|---------|-------------|
| 40 | 39  | 1613.03 | 1599.00     |
| 41 | 40  | 1641.08 | 1627.06     |
| 42 | 41  | 1669.14 | 1655.11     |
| 43 | 42  | 1697.19 | 1683.17     |
| 44 | 43  | **1725.25** | 1711.22   |
| 45 | 44  | 1753.30 | 1739.27     |
| 46 | 45  | 1781.35 | 1767.33     |
| 47 | 46  | 1809.41 | 1795.38     |
| 48 | 47  | 1837.46 | 1823.44     |
| 49 | 48  | 1865.52 | 1851.49     |
| 50 | 49  | 1893.57 | 1879.54     |
| 51 | 50  | **1921.62** | 1906.70   |
| 52 | 51  | 1949.68 | 1935.65     |
| 53 | 52  | **1977.73** | 1963.71   |
| 54 | 53  | 2005.79 | 1991.76     |
| 55 | 54  | 2033.84 | 2019.81     |

**Figure S52:** DSC heating (2nd) curve of polyethylene (Table S5, run 4).

### 5. References:

1. Sheldrick, G. M. *Acta Crystallogr., Sect. A: Found. Crystallogr.* **2008**, *64*, 112-122.
2. Macrae, C. F.; Bruno, I. J.; Chisholm, J. A.; Edgington, P. R.; McCabe, P.; Pidcock, E.; RodriguezMonge, L.; Taylor, R.; van de Streek, J.; Wood, P. A. J. Appl. Crystallogr. 2008, 41, 466-470.
3. Spek A. L. Acta Crystallogr., Sect. D: Biol. Crystallogr. 2009, 65, 148-155.
4. Bruker (2016). APEX2, SAINT and SADABS. Bruker AXS Inc., Madison, Wisconsin, USA.
5. Farrugia, L. J. J. Appl. Cryst. 1997, 30, 565-565.