Supporting Information

**IPr***-Oxa – A New Class of Sterically-Hindered, Wingtip-Flexible N,C-Chelating Oxazole-Donor N-Heterocyclic Carbene Ligands**

Pamela Podchorodecka, a Błażej Dziuk, b Roman Szostak, c Michal Szostak*,d and Elwira Bisz*,a

a Department of Chemistry, Opole University, 48 Oleska Street, Opole 45-052, Poland
b Department of Chemistry, University of Science and Technology, Norwida 4/6, Wrocław 50-373, Poland
c Department of Chemistry, Wrocław University, F. Joliot-Curie 14, Wrocław 50-383, Poland
d Department of Chemistry, Rutgers University, 73 Warren Street, Newark, NJ 07102, USA

[ebisz@uni.opole.pl; michal.szostak@rutgers.edu](mailto:ebisz@uni.opole.pl; michal.szostak@rutgers.edu)

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Crystallographic Analysis

Single crystals of Ag, Pd, Se and Rh complexes were collected on a Kuma KM4 diffractometer equipped with Eos CCD detector (graphite monochromatic, MoKα radiation, λ = 0.71073 Å) at room temperature. The single crystals of the complexes 5-6 were collected on a Rigaku Oxford Diffraction XtaLAB SynergyR DW diffractometer equipped with a HyPix ARC 150° Hybrid Photon Counting (HPC) detector using CuKα (λ = 1.54184 Å) at 100 K. The corrections to the Lorentz and polarization factors were applied to the reflection intensities [1]. Data were processed using the CrysAlisPro software. The structures were solved by direct methods using SHELXS and refined by full-matrix least-squares methods based F² using SHELXL [2, 3]. The hydrogen atoms were determined from the geometric concepts and refined in a riding model with isotropic temperature factors of 1.2 times the Ueq value of the parent atom. All non-hydrogen atoms were located from difference Fourier synthesis and refined by least squares method in the full-matrix anisotropic approximation. The crystallographic data for compounds and details of X-ray experiment are collected in the Supplementary information Tables. The structure drawings in ESI were prepared by using Mercury program [4]. The coordinates of atoms and other parameters for structures were deposited with the Cambridge Crystallographic Data Centre: 2180038 for [Ag(IPr*Oxa)Cl], 2180039 for [Ag(IPr*MeOOxa)Cl], 2180040 for [Pd(IPr*Oxa)Cl₂], 2180041 for [Pd(IPr*MeOOxa)Cl₂], 2180042 for [Se(IPr*Oxa)] and 2180043 for [Rh(IPr*Oxa)(CO)Cl]; 12 Union Road, Cambridge CB2 1EZ, UK (Fax, __44-(1223)336-033, E-mail deposit@ccdc.cam.ac.uk).

Figure S1. Molecular structures of [Ag(IPr*Oxa)Cl], [Ag(IPr*MeOOxa)Cl], [Pd(IPr*Oxa)Cl₂], [Pd(IPr*MeOOxa)Cl₂], [Se(IPr*Oxa)] and [Rh(IPr*Oxa)(CO)Cl] complexes. Hydrogen atoms and solvent molecules have been omitted for clarity.
IPr* – A New Class of Sterically-Hindered, Wingtip-Flexible N.C-Chelating N-Heterocyclic Carbene Ligands  Podchorodecka et al.

$\text{[Ag}(\text{IPr}^*\text{MeOx})\text{Cl}]$

$\text{[Pd}(\text{IPr}^*\text{Ox})\text{Cl}_2]$
IPr– A New Class of Sterically-Hindered, Wingtip-Flexible N,C-Chelating N-Heterocyclic Carbene Ligands

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\[ \text{[Pd(IPr-MeOOxa)Cl]}\]

\[ \text{[Se(IPr-Oxa)]} \]
[Rh(IPr\textsuperscript{Oxa})(cod)Cl]

**Table S1. Experimental details for [Ag(IPr\(^{Ox} \_Oxa\_3)\_Cl]; [Ag(IPr\(^{Me}_Oxa\_3)\_Cl]; [Pd(IPr\(^{Ox} \_Oxa\_3)\_Cl]; [Pd(IPr\(^{Me}_Oxa\_3)\_Cl]; [Se(IPr\(^{Ox} \_Oxa\_3)\_Cl]; [Rh(IPr\(^{Ox} \_Oxa\_3)\_Cl]; [Rh(IPr\(^{Me}_Oxa\_3)\_Cl];**

<table>
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<th>Chemical formula</th>
<th>Crystals data</th>
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<td>(3\text{Cl} = \text{Cl}_3|\text{AgCl}_3 \cdot \text{Oxa})</td>
<td>2384.74 794.09 813.07 828.07 1192.21 802.14</td>
</tr>
<tr>
<td>(3\text{Cl} = \text{Cl}_3|\text{AgCl}_3 \cdot \text{Oxa})</td>
<td>2384.74 794.09 813.07 828.07 1192.21 802.14</td>
</tr>
<tr>
<td>(M_r)</td>
<td>10.1785 (3), 61.583 (3), 18.5412 (9)</td>
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<tr>
<td>Crystal system, space group</td>
<td>Monoclinic, (P2_1/m)</td>
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<td>Temperature (K)</td>
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<tr>
<td>No. of measured, independent and observed ([I &gt; 2σ(I)]) reflections</td>
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<tr>
<td>(R_{int})</td>
<td>0.071</td>
</tr>
<tr>
<td>((\sin \theta/\lambda)_{\text{max}}) ((\text{Å}^{-1}))</td>
<td>0.617</td>
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<tr>
<td>Refinement</td>
<td>0.079, 0.130, 0.046, 0.098, 0.041, 0.111, 0.090, 0.233, 0.030, 0.079, 0.039, 0.100, 0.079</td>
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<tr>
<td>No. of reflections</td>
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<tr>
<td>No. of parameters</td>
<td>1414</td>
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<tr>
<td>(Δρ_{\text{max}}, Δρ_{\text{min}}) ((e \text{Å}^{-3}))</td>
<td>0.46, −0.43</td>
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### Table S2. Selected geometric parameters (Å, °) for [Ag(IPr\textsuperscript{Oxa})Cl]

<table>
<thead>
<tr>
<th>Bond</th>
<th>Length (Å)</th>
<th>Angle (°)</th>
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<tbody>
<tr>
<td>Ag1A–C1A</td>
<td>2.079 (5)</td>
<td>C1A–Ag1A–C1A 175.55 (15)</td>
</tr>
<tr>
<td>Ag1A–Cl1A</td>
<td>2.3028 (16)</td>
<td>C1B–Ag1B–Cl1B 172.74 (18)</td>
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<td>Ag1B–C1B</td>
<td>2.074 (6)</td>
<td>C1C–Ag1C–C1C 178.74 (16)</td>
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<tr>
<td>Ag1B–Cl1B</td>
<td>2.288 (2)</td>
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</tr>
<tr>
<td>Ag1C–C1C</td>
<td>2.087 (5)</td>
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</tr>
<tr>
<td>Ag1C–Cl1C</td>
<td>2.3044 (18)</td>
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</table>

### Table S3. Selected geometric parameters (Å, °) for [Ag(IPr\textsuperscript{MeOOxa})Cl]

<table>
<thead>
<tr>
<th>Bond</th>
<th>Length (Å)</th>
<th>Angle (°)</th>
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</thead>
<tbody>
<tr>
<td>Ag1–C1</td>
<td>2.075 (6)</td>
<td>C1–Ag1–Cl1 173.09 (18)</td>
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<tr>
<td>Ag1–Cl1</td>
<td>2.3035 (18)</td>
<td>C1–N1–C2 111.8 (5)</td>
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<tr>
<td>N1–C1</td>
<td>1.338 (7)</td>
<td>C1–N1–C4 122.1 (5)</td>
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<tr>
<td>N1–C2</td>
<td>1.405 (8)</td>
<td>C2–N1–C4 126.0 (5)</td>
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<tr>
<td>N1–C4</td>
<td>1.447 (7)</td>
<td>C1–N2–C39–N3 144.7 (11)</td>
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<tr>
<td>N2–C1</td>
<td>1.359 (7)</td>
<td>C3–N2–C39–N3 136.3 (8)</td>
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<tr>
<td>N2–C39</td>
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<td>C1–N2–C39–O1 135.8 (7)</td>
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<td>N2–C3</td>
<td>1.411 (9)</td>
<td>C3–N2–C39–O1 143.2 (12)</td>
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### Table S4. Selected geometric parameters (Å, °) for [Pd(IPr\textsuperscript{Oxa})Cl\textsubscript{2}]

<table>
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<tr>
<th>Bond</th>
<th>Length (Å)</th>
<th>Angle (°)</th>
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<tbody>
<tr>
<td>Pd1–C1</td>
<td>1.993 (3)</td>
<td>C1–Pd1–N3 80.31 (13)</td>
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<tr>
<td>Pd1–N3</td>
<td>2.047 (3)</td>
<td>C1–Pd1–Cl1 95.91 (10)</td>
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<tr>
<td>Pd1–Cl1</td>
<td>2.2675 (11)</td>
<td>N3–Pd1–Cl1 176.22 (9)</td>
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<td>Pd1–Cl2</td>
<td>2.3256 (12)</td>
<td>C1–Pd1–Cl2 172.42 (10)</td>
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<tr>
<td>O1–C24</td>
<td>1.327 (4)</td>
<td>N3–Pd1–Cl2 92.11 (9)</td>
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<td>O1–C26</td>
<td>1.398 (4)</td>
<td>Cl1–Pd1–Cl2 91.67 (5)</td>
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</table>

### Table S5. Selected geometric parameters (Å, °) for [Pd(IPr\textsuperscript{MeOOxa})Cl\textsubscript{2}]

<table>
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<tr>
<th>Bond</th>
<th>Length (Å)</th>
<th>Angle (°)</th>
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<tbody>
<tr>
<td>Pd1–C1</td>
<td>1.985 (10)</td>
<td>C1–Pd1–N3 79.6 (4)</td>
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<tr>
<td>Pd1–N3</td>
<td>2.067 (8)</td>
<td>C1–Pd1–Cl1 96.9 (3)</td>
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Table S6. Selected geometric parameters (Å, °) for [Se(IPr*Oxa)]

<table>
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<th>Bond</th>
<th>Distance (Å)</th>
<th>Angle (°)</th>
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<tr>
<td>Se1—C1</td>
<td>1.831 (4)</td>
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<tr>
<td>N1—C1—N2</td>
<td>104.4 (3)</td>
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<tr>
<td>N1—C1—Se1</td>
<td>127.2 (3)</td>
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<tr>
<td>N2—C1—Se1</td>
<td>128.4 (3)</td>
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<tr>
<td>C1—N2—C39—O1</td>
<td>115.4 (5)</td>
<td>−70.1 (6)</td>
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<tr>
<td>C1—N2—C39—N3</td>
<td>113.6 (5)</td>
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<tr>
<td>C3—N2—C39—N3</td>
<td>113.6 (5)</td>
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Table S7. Selected geometric parameters (Å, °) for [Rh(IPr*Oxa)(CO)Cl]

<table>
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<tr>
<th>Bond</th>
<th>Distance (Å)</th>
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<td>Rh1—C31</td>
<td>1.796 (4)</td>
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<td>Rh1—C1</td>
<td>1.976 (4)</td>
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<td>Rh1—N3</td>
<td>2.131 (3)</td>
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<td>Rh1—Cl1</td>
<td>2.3705 (11)</td>
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<td>O1—C24</td>
<td>1.336 (4)</td>
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<td>O1—C26</td>
<td>1.407 (5)</td>
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</tr>
<tr>
<td>N1—C1—Rh1</td>
<td>141.6 (3)</td>
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S8
Computational Methods

Computational Methods. All of the calculations were performed using Gaussian 09 suite of programs. All of the geometry optimizations were performed at the B3LYP level of theory in the gas phase with the 6-311++G(d,p) basis set. For geometry optimizations, we employed the X-ray structures of 1-(benzo[d]oxazol-2-yl)-3-(2,6-dibenzhydryl-4-methylphenyl)-4,5-dimethyl-1H-imidazol-3-ium and 1-(benzo[d]oxazol-2-yl)-3-(2,6-dibenzhydryl-4-methoxyphenyl)-4,5-dimethyl-1H-imidazol-3-ium or their linear metal complexes as the starting geometry and performed full optimization. The absence of imaginary frequencies was used to characterize the structures as minima on the potential energy surface. All of the optimized geometries were verified as minima (no imaginary frequencies). Energetic parameters were calculated under standard conditions (298.15 K and 1 atm). Structural representations were generated using CYLview software (Legault, C. Y. CYLview version 1.0 BETA, University of Sherbrooke). All other representations were generated using GaussView (GaussView, version 5, Dennington, R.; Keith, T.; Millam, J. Semichem Inc., Shawnee Mission, KS, 2009) or ChemCraft software (Andrienko, G. L. ChemCraft version b562a, https://www.chemcraftprog.com).

Full Reference for Gaussian 09

Table S8. HOMO and LUMO Energy Levels of IPr*-Oxa and Related NHC Ligands Calculated at the B3LYP 6-311++g(d,p) Level\textsuperscript{a,b}

<table>
<thead>
<tr>
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</tr>
</thead>
<tbody>
<tr>
<td>1\textsuperscript{a}</td>
<td>IPr*-Oxa O/carbene-syn</td>
<td>HOMO-1</td>
<td>-0.2300</td>
<td>-6.26</td>
<td>-144.33</td>
<td></td>
</tr>
<tr>
<td>2\textsuperscript{a}</td>
<td>IPr*-Oxa O/carbene-syn</td>
<td>HOMO</td>
<td>-0.2265</td>
<td>-6.16</td>
<td>-142.13</td>
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</tr>
<tr>
<td>3\textsuperscript{a}</td>
<td>IPr*-Oxa O/carbene-syn</td>
<td>LUMO</td>
<td>-0.0432</td>
<td>-1.18</td>
<td>-27.11</td>
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</tr>
<tr>
<td>4\textsuperscript{a}</td>
<td>IPr*-Oxa O/carbene-syn</td>
<td>LUMO+8</td>
<td>-0.0120</td>
<td>-0.33</td>
<td>-7.53</td>
<td>-5.93</td>
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<td>5\textsuperscript{b}</td>
<td>IPr*-Oxa N/carbene-syn</td>
<td>HOMO-1</td>
<td>-0.2296</td>
<td>-6.25</td>
<td>-144.07</td>
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<tr>
<td>6\textsuperscript{b}</td>
<td>IPr*-Oxa N/carbene-syn</td>
<td>HOMO</td>
<td>-0.2278</td>
<td>-6.20</td>
<td>-142.95</td>
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<tr>
<td>7\textsuperscript{b}</td>
<td>IPr*-Oxa N/carbene-syn</td>
<td>LUMO</td>
<td>-0.0443</td>
<td>-1.21</td>
<td>-27.80</td>
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<tr>
<td>8\textsuperscript{b}</td>
<td>IPr*-Oxa N/carbene-syn</td>
<td>LUMO+6</td>
<td>-0.0150</td>
<td>-0.41</td>
<td>-9.41</td>
<td>-5.79</td>
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<tr>
<td>9\textsuperscript{c}</td>
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<td>HOMO-1</td>
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<td>-6.22</td>
<td>-143.45</td>
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<tr>
<td>10\textsuperscript{c}</td>
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<td>HOMO</td>
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<td>-141.81</td>
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<td>11\textsuperscript{c}</td>
<td>IPr*-MeO-Oxa O/carbene-syn</td>
<td>LUMO</td>
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<td>-1.17</td>
<td>-26.98</td>
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<tr>
<td>12\textsuperscript{c}</td>
<td>IPr*-MeO-Oxa O/carbene-syn</td>
<td>LUMO+8</td>
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<td>-0.32</td>
<td>-7.41</td>
<td>-5.90</td>
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<td>HOMO-1</td>
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<td>-143.75</td>
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<tr>
<td>14\textsuperscript{d}</td>
<td>IPr*-MeO-Oxa N/carbene-syn</td>
<td>HOMO</td>
<td>-0.2266</td>
<td>-6.17</td>
<td>-142.19</td>
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<tr>
<td>15\textsuperscript{d}</td>
<td>IPr*-MeO-Oxa N/carbene-syn</td>
<td>LUMO</td>
<td>-0.0438</td>
<td>-1.19</td>
<td>-27.49</td>
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<td>16\textsuperscript{d}</td>
<td>IPr*-MeO-Oxa N/carbene-syn</td>
<td>LUMO+6</td>
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<td>-9.41</td>
<td>-5.76</td>
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<tr>
<td>17</td>
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<td>HOMO</td>
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<td>18</td>
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<td>LUMO</td>
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<td>19</td>
<td>IPr</td>
<td>HOMO</td>
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<td>-6.01</td>
<td>-139.78</td>
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<tr>
<td>20\textsuperscript{e}</td>
<td>IPr\textsuperscript{*}</td>
<td>LUMO+1</td>
<td>-0.0177</td>
<td>-0.48</td>
<td>-12.21</td>
<td>-5.53</td>
</tr>
</tbody>
</table>

\textsuperscript{a} HOMO-1 due to required orbital symmetry. HOMO corresponds to π-donor orbital. LUMO+8 due to required orbital symmetry.
\textsuperscript{b} HOMO-1 corresponds to π-donor orbital. LUMO+6 due to required orbital symmetry.
**1a 2,6-Dibenzhydryl-4-methylaniline**

![Chemical Structure](image)

**NMR Spectra**

- **1H NMR (500 MHz, CDCl₃)**
  - δ 7.39, 7.26, 7.23, 7.19, 7.10, 7.06, 5.45, 3.27, 2.01

- **13C NMR (125 MHz, CDCl₃)**
  - δ 142.90, 139.78, 132.63, 129.38, 129.18, 128.60, 52.51, 21.17
1b 4-Methoxy-2,6-bis(diphenylmethyl)aniline
2a 1-(2,6-Dibenzhydryl-4-methylphenyl)-4,5-dimethyl-1H-imidazole
\[ 2b \text{ } 1-(2,6-\text{Dibenzhydryl}-4\text{-methoxyphenyl})-4,5\text{-dimethyl-1H-imidazole} \]
3a 1-(Benzo[d]oxazol-2-yl)-3-(2,6-dibenzhydryl-4-methylphenyl)-4,5-dimethyl-1H-imidazol-3-ium chloride
3b 1-(Benzo[d]oxazol-2-yl)-3-(2,6-dibenzhydryl-4-methoxyphenyl)-4,5-dimethyl-1H-imidazol-3-ium chloride
4a 1-(Benzo[d]oxazol-2-yl)-3-(2,6-dibenzhydryl-4-methylphenyl)-4,5-dimethylimidazol-2-ylidene)silver(I) chloride
4b 1-(Benzo[d]oxazo[2-yl]-3-(2,6-dibenzhydryl-4-methoxyphenyl)-4,5-dimethylimidazol-2-ylidene)silver(I) chloride
5a Dichloro(1-(benzo[d]oxazol-2-yl)-3-(2,6-dibenzhydryl-4-methylphenyl)-4,5-dimethylimidazol-2-ylidene)palladium(II)
5b Dichloro(1-((benzo[\text{d}]oxazol-2-yl)-3-((2,6-dibenzhydryl-4-methoxyphenyl)-4,5-dimethylimidazol-2-ylidene)palladium(II)
6a (1-(Benzo[d]oxazol-2-yl)-3-(2,6-dibenzhydryl-4-methylphenyl)-4,5-dimethylimidazol-2-ylidene)selenone
6a (1-(Benzo[d]oxazol-2-yl)-3-(2,6-dibenzhydryl-4-methylphenyl)-4,5-dimethylimidazol-2-ylidene)selenone, $^{77}$Se NMR
7a Chlorocarbonyl[1-(benzo[d]oxazol-2-yl)-3-(2,6-dibenzhydryl-4-methylphenyl)-4,5-dimethylimidazol-2-ylidene]rhodium(I)
Ag(I)–NHC-catalyzed three component coupling: 1-(1-Cyclohexyl-3-phenylprop-2-ynyl)piperidine
Pd–NHC-catalyzed Heck coupling reaction: (E)-1-(4-Styrylphenyl)ethenone
Pd–NHC-catalyzed Heck coupling reaction: (E)-1-Methoxy-4-styrylbenzene
IPr*Oxa O/carbene syn

Energy: -1977.013688 au

Sum of electronic and thermal Energies: -1976.275129 au

Geometry:

N  -0.11889600  -0.00668800  0.51515500
N  -2.22539500  0.00681600  0.79229200
C  -1.26534200  0.01987500  -0.20601600
C  -0.32686800  -0.03644200  1.91461800
C  -1.66986700  -0.03160100  2.10026400
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Sum of electronic and thermal Energies: -1976.271677 au

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Sum of electronic and thermal Energies: -2051.498512 au

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$\text{IPr}^\text{S39}$ – A New Class of Sterically-Hindered, Wingtip-Flexible N,C-Chelating N-Heterocyclic Carbene Ligands

Podchorodecka et al.
**IPr**\(^{\text{MeOxa}}\) N/carbene syn

Energy: -2052.239341 au

Sum of electronic and thermal Energies: -2051.495089 au

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