Bulky and Electron-Deficient α-Iminocarboxamidato-Nickel (II) Complexes: A Study of the Steric and Electronic Effects on Ethylene Activation

Leon Skarjan, Nery Villegas-Escobar, Sebastián A. Correa, Constantin G. Daniliuc, Ricardo A. Matute, and René S. Rojas*
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Experimental

General Remarks: All manipulations were performed in an inert atmosphere using the standard glovebox and Schlenk-line techniques. All reagents were used as received from Aldrich unless otherwise specified. Ethylene was purchased from Matheson Tri-Gas (research grade, 99.99% pure). Toluene, THF, hexane, and pentane were distilled from benzophenone ketyl, and NEt₃ was dried over KOH. The NMR spectra were obtained using Bruker Avance 400 spectrometers. The chemical shifts are given in parts per million relative to TMS (δ(SiMe₄ 0 for ¹H and ¹³C) or an external standard (δ(BF₃·OEt₂) 0 for ¹¹B, δ(C₆H₅CF₃) 0 for ¹⁹F NMR, and δ(H₃PO₄) 0 for ³¹P NMR). Most NMR assignments were supported by additional 2D experiments. FT-IR spectra were acquired on a Shimadzu IRTracer-100 spectrophotometer using KBr pellets. An elemental analysis (C,H,N) was performed on an Elementar Vario EL III Analyzer.

Polymerization reactions: Polymerization reactions were performed in a 100 ml Parr reactor; The reactor was loaded in the glovebox with the desired amount of cocatalyst, either B(C₆F₅)₃ or BF₃ and 5 μmol of Ni precursor, and toluene was used as the solvent. The reactor was sealed inside the glovebox. The reactor was attached to an ethylene line, and gas was fed continuously into the reactor at a pressure of 100 or 200 psi. The pressurized reaction mixture was stirred at variable temperatures ranging from 20 to 60 °C. After 15 min, the ethylene gas was vented, and acetone was added to quench the polymerization reaction. In order to determine a possible formation of oligomers with 6-BF₃ as the catalyst, a kinetical investigation was performed by charging a Young NMR tube with a solution of 6-BF₃ (5mg) in C₆D₆. The tube was then attached to the Schlenk line and filled with ethylene, until a sufficiently high intensity of the ethylene signal was found in the ¹H NMR spectrum. ¹H NMR spectra were recorded after 5 min, 30 min and 2.5 h at room temperature.

X-ray diffraction: The data were collected and provided by Dr. Constantin G. Daniliuc; complete crystallographic details can be found in the independently recorded crystallographic information files. Data sets for compound 2 were collected with a Bruker D8 Venture PHOTON 100 diffractometer. Programs used: data collection: APEX3 V2016.1-0[¹]; cell refinement: SAINT V8.37A[²]; data reduction: SAINT V8.37A[²]; absorption correction, SADABS V2014/7[³]; structure solution SHELXT-2015[⁴]; structure refinement
For compound 3 data sets were collected with a Nonius Kappa CCD diffractometer. Programs used: data collection, COLLECT\textsuperscript{[6]}; data reduction Denzo-SMN\textsuperscript{[7]}; absorption correction, Denzo\textsuperscript{[7]}; structure solution SHELXT-2015\textsuperscript{[4]}; structure refinement SHELXL-2015\textsuperscript{[5]} and graphics, XP\textsuperscript{[8]}. \(R\)-values are given for observed reflections, and \(wR^2\) values are given for all reflections.

**Exceptions and special features:** For compound 3 four CF\(_3\) groups and for compound 2 seven CF\(_3\) groups were found disordered over two positions. Several restraints (SADI, SAME, ISOR and SIMU) were used in order to improve refinement stability. Additionally, for compound 2 a badly disordered half dichloromethane molecule was found in the asymmetrical unit and could not be satisfactorily refined. The program SQUEEZE\textsuperscript{[9]} was therefore used to mathematically remove the effect of the solvent. The quoted formula and derived parameters do not include the squeezed solvent molecule.

**Computational Details:** Molecular structures were computed using the well-tested Minnesota M06L functional for transition metal studies\textsuperscript{[10]}. The M06L functional have been found to be reliable treating Ni-complexes for olefin polymerization\textsuperscript{[11]}. Light atoms were computed using the 6-31G(d,p) Pople basis sets\textsuperscript{[12]}, while for Ni the LANL2DZ basis set with pseudo relativistic effective core potentials was employed\textsuperscript{[13]}. All structures were confirmed to be a minimum on the potential energy surface by frequency computations, getting all positive vibrational frequencies. All quantum chemistry calculations were performed using the Gaussian16 (Revision B.01) software package\textsuperscript{[14]}. Natural charges were obtained at the same level of theory, employing NBO 3.0 interfaced with Gaussian16. Molecular electrostatic potentials were obtained using the cubegen module in Gaussian16. Due to errors in thermodynamical properties by employing the harmonic oscillator approximation low low frequency modes, Gibbs free energies in solvent were computed using the quasi-rigid rotor harmonic oscillator (quasi-RRHO) approximation introduced by Grimme\textsuperscript{[15]}. Explicit Gibbs free energies were computed using:

\[
\Delta G = \Delta E + \Delta G^T_{\text{RRHO}} + \Delta \delta G^T_{\text{solv}}(X)
\]

\(\Delta E\) corresponds to gas-phase energy difference, \(\Delta G^T_{\text{RRHO}}\) contains the Gibbs free and zero-point vibrational energies, while \(\Delta \delta G^T_{\text{solv}}(X)\) corresponds to the solvation energy. Quasi-RRHO were obtained using EntroPy, a python script developed by one of the authors\textsuperscript{[16]}. Solvent effects were included using the polarizable continuum model (IEF-PCM)\textsuperscript{[17]}.
The interaction energy and the physical contributions that drive the interaction of the benzyl moiety with the complex was studied using symmetry-adapted perturbation theory (SAPT).\textsuperscript{18} Computations of charge transfer effects were done by using the SAPT-CT module.\textsuperscript{19} All SAPT computations were performed at the SAPT0/def2-svp level of theory.

**Synthesis of ligands and complexes**

2-oxo-N-(2,6-bis[3,5-bis(trifluoromethyl)phenylimine]propanamide (1)

In a 50 mL flask with a magnetic stirring bar, pyruvic acid (1 eq, 2.9 mmol, 0.26 g) was diluted with 35 mL of toluene. At 0 °C, oxalyl chloride (1.0 eq, 2.9 mmol, 0.37 g) and triethylamine (1 eq, 2.9 mmol, 0.29 g) were added. The suspension was left to stir for two hours at room temperature. Then, 2,6-bis[3,5-bis(trifluoromethyl)phenyl]-aniline (1.0 eq, 2.9 mmol, 1.50 g) which was prepared as in previous reports\textsuperscript{20} and triethylamine (1.0 eq, 2.9 mmol, 0.29 g) were added. The reaction mixture was stirred overnight. The solution was filtered and the solvent was removed under vacuum. After purification by column chromatography, using silica and hexane and ethyl acetate as eluents, 570 mg of a colourless, crystalline solid were obtained (Yield: 35%).

\textsuperscript{1}H NMR (401 MHz, in CDCl\textsubscript{3}): δ 8.09 (s, 1H), 7.90 (s, 2H), 7.83 (s, 4H), 7.61 – 7.65 (m, 1H), 7.53 (d, J = 7.60 Hz, 2H), 2.25 (s, 3H)

\textsuperscript{13}C{\textsuperscript{1}H} NMR (101 MHz, in CDCl\textsubscript{3}): δ 195.7 (C\textsubscript{q}), 159.5 (C\textsubscript{q}), 140.8 (C\textsubscript{q}), 138.6 (C\textsubscript{q}), 132.1 (q, J = 33.67 Hz, C\textsubscript{q}), 131.3 (CH), 130.4 (C\textsubscript{q}), 129.4 (CH), 129.1 (d, J = 8.82 Hz, CH), 124.7 (C\textsubscript{q}), 121.9 (dt, J = 7.89 Hz, J = 3.76 Hz, CH), 23.9 (CH\textsubscript{b})

\textsuperscript{19}F NMR (376.5 MH, in CDCl\textsubscript{3}): δ -62.92 (s)
Figure S1: $^1$H NMR (400 MHz, in CDCl$_3$) of 1.

Figure S2: $^{13}$C($^1$H) NMR (101 MHz, in CDCl$_3$) of 1.
Figure S3: $^{19}$F NMR (376.5 MHz, in CDCl$_3$) of 1.

**N-(2,6-bis[3,5-bis(trifluoromethyl)phenyl]-2-(2,6-bis[3,5-bis(trifluoromethyl)phenylimine]) propanamide (2)**

In 25 mL flask with a magnetic stirring bar, 2-oxo-N-(2,6-bis[3,5-bis(trifluoromethyl)phenylimine] propanamide (1.0 eq, 539 µmol, 317 mg) and 2,6-bis[3,5-bis(trifluoromethyl)phenyl]-aniline (1.0 eq, 539 µmol, 280 mg) were dissolved in 35 mL of toluene. Then, a catalytic amount of p-toluenesulfonic acid was added. The solution was left to stir under reflux for 45 h. The solvent was removed under vacuum and the crude was washed with cold pentane. 269 mg of a slightly brown, crystalline solid was obtained (yield: 46 %).

$^1$H NMR (400 MHz, in CDCl$_3$): δ 8.19 (s, 1H), 7.78 (s, 6H), 7.73 (s, 2H), 7.69 (s, 4H), 7.56 - 7.60 (m, 1H), 7.48 (d, $J = 7.82$ Hz, 2H), 7.44 (s, 3H), 1.20 (s, 3H)
$^{13}$C{\cite{1H}} NMR (101 MHz, in CDCl$_3$): $\delta$ 166.9 (C$_q$), 161.8 (C$_q$), 143.3 (C$_q$), 141.3 (C$_q$), 141.2 (d, J = 9.54 Hz, C$_q$), 137.2 (C$_q$), 131.9 (C$_q$), 131.7 (C$_q$), 131.96 (q, J = 33.74 Hz, C$_q$), 131.94 (q, J = 33.26 Hz, C$_q$), 129.7 (C$_q$), 129.2 (d, J = 2.9 Hz, CH), 128.9 (d, J = 2.9 Hz, CH), 128.8 (CH), 126.9 (CH), 124.6 (d, J = 5.96 Hz, C$_q$), 121.9 (d, J = 5.86 Hz, C$_q$), 121.5 (dt, J = 3.67, J = 7.34 Hz, CH), 121.2 (dt, J = 3.67, J = 7.34 Hz, CH), 119.2 (d, J = 5.86 Hz, C$_q$), 17.6 (CH$_3$)

$^{19}$F NMR (376.5 MHz, in CDCl$_3$): $\delta$ -62.99 (s), -63.05 (s)

Figure S4: $^1$H NMR (400 MHz, in CDCl$_3$) of 2.
Figure S5: $^{13}$C($^1$H) NMR (101 MHz, in CDCl$_3$) of 2.
Figure S6: $^{19}$F NMR (376.5 MHz, in CDCl$_3$) of 2.

**Elemental Analysis (%)** $\text{C}_{47}\text{H}_{22}\text{F}_{24}\text{N}_2\text{O}$ (M 1086.13 g/mol): calculated C 51.95, H 2.04, N 2.58; found C 50.96, H 2.54, N 2.62
Figure S7: Crystal structure of compound 2. (Thermals ellipsoids are shown with 15% probability.)

Table S1: Crystallographic data and structure refinement for ligand 2.

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<td>Formula weight</td>
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<td></td>
<td>α = 90°, β = 107.403(2)°, γ = 90°</td>
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<td>F(000)</td>
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</tr>
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<td>Reflections collected</td>
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<tr>
<td>Independent reflections</td>
<td>8173 [R(int) = 0.0749]</td>
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<td>Coverage of independent</td>
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reflections
Absorption correction                  multi-scan
Max. and min. transmission           0.8780 and 0.7660
Structure solution technique         direct methods
Structure solution program           SHELXL-2014/7 (Sheldrick, 2014)
Refinement method                    Full-matrix least-squares on F^2
Refinement program                   SHELXL-2014/7 (Sheldrick, 2014)
Function minimized                   \( \sum w(F_o^2 - F_c^2)^2 \)
Data / restraints / parameters       8173 / 661 / 925
Goodness-of-fit on F^2               1.082

Final R indices

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<td>0.1207</td>
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Weighting scheme

\( w = 1/[\sigma^2(F_o^2) + (0.0391P)^2 + 4.0025P] \)
\( P = (F_o^2 + 2F_c^2)/3 \)

Largest diff. peak and hole

0.327 and -0.268 e\(\text{Å}^{-3}\)

R.M.S. deviation from mean

0.052 e\(\text{Å}^{-3}\)

Table S2: Selected bond distances (Å), angles (°) and torsion angles (°) for ligand 2.

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<td>1.430(3)</td>
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<td>1.345(3)</td>
<td>N2-C41</td>
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<td>O1-C3</td>
<td>1.226(3)</td>
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<td>C1-C3</td>
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<td>C3-N2-C41</td>
<td>124.0(2)</td>
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<td>C3-N2-H2</td>
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<td>C41-N2-H2</td>
<td>116.6(18)</td>
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<td>N1-C1-C2</td>
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<td>N1-C1-C3</td>
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<td>116.1(2)</td>
<td>C1-C2-H2A</td>
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<td>H2B-C2-H2C</td>
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<td>O1-C3-N2</td>
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<td>N2-C3-C1</td>
<td>113.1(2)</td>
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<td>C16-C11-C12</td>
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<td>C16-C11-N1</td>
<td>122.0(2)</td>
</tr>
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<td>C12-C11-N1</td>
<td>117.1(2)</td>
<td>C13-C12-C11</td>
<td>119.6(2)</td>
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<td>5.1(4)</td>
<td>C11-N1-C1-C3</td>
<td>-175.0(2)</td>
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<td>C41-N2-C3-O1</td>
<td>9.8(4)</td>
<td>C41-N2-C3-C1</td>
<td>-172.4(2)</td>
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<td>N1-C1-C3-O1</td>
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<td>N1-C1-C3-N2</td>
<td>40.5(3)</td>
<td>C2-C1-C3-N2</td>
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N-(2,6-bis[3,5-bis(trifluoromethyl)phenyl]-2-(2,6-diisopropylphenylimine) propanamade (3)

In 25 mL flask with a magnetic stirring bar, 2-oxo-N-(2,6-bis[3,5-bis(trifluoromethyl)phenylimine] propanamide (1.0 eq, 461 µmol, 271 mg) and 2,6-diisopropylaniline (1.0 eq, 461 µmol, 82 mg) were dissolved in 30 mL of toluene. Then, a catalytic amount of p-toluenesulfonic acid was added. The solution was left to stir under reflux for 40 h. The solvent was removed under vacuum and the crude was washed with cold pentane. 129 mg of a yellow, crystalline solid were obtained (yield: 37 %).

$^1$H NMR (400 MHz, in CDCl$_3$): $\delta$ 8.81 (s, 1H), 7.97 (s, 4H), 7.93 (s, 2H), 7.62 (t, J = 7.34, 1H), 7.53 (d, J = 7.58 Hz, 2H), 7.04 (s, 3H), 1.97 (spt, J = 6.78 Hz, 2H), 1.78 (s, 3H), 0.95 (d, J = 6.85 Hz, 6H), 0.74 (d, J = 6.85 Hz, 6H)

$^{13}$C{1H} NMR (101 MHz, in CDCl$_3$): $\delta$ 163.8 (C$_q$), 162.9 (C$_q$), 143.6 (C$_q$), 141.6 (C$_q$), 139.9 (C$_q$), 135.3 (C$_q$), 131.91 (C$_q$), 131.89 (q, J = 33.26 Hz, C$_q$), 131.2 (CH), 129.3 (d, J = 3.67 Hz, C$_q$), 129.0 (CH), 125.1 (CH), 123.3 (CH), 122.1 (C$_q$), 121.7 (dt, J = 3.76 Hz, J = 7.89 Hz, CH), 28.4 (CH), 22.8 (CH$_3$), 22.4 (CH$_3$), 15.4 (CH$_3$)

$^{19}$F NMR (376.5 MHz, in CDCl$_3$): $\delta$ -62.85 (s)
Figure S8: $^1\text{H}$ NMR (400 MHz, in CDCl$_3$) of 3.

Figure S9: $^{13}\text{C}\{^1\text{H}\}$ NMR (101 MHz, in CDCl$_3$) of 3.
Figure S10: $^{19}$F NMR (376.5 MHz, in CDCl$_3$) of 3.

Elemental Analysis (%) $C_{37}H_{30}F_{12}N_2O$ (M 746.63 g/mol): calculated C 59.52, H 4.05, N 3.75; found C 59.26, H 4.20, N 3.68
Figure S11: Crystal structure of compound 3. (Thermals ellipsoids are shown with 15% probability.)

Table S3: Crystallographic data and structure refinement for ligand 3.

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<td>Wavelength</td>
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<td>Crystal size</td>
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<td>Crystal habit</td>
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<td>Crystal system</td>
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<td>Space group</td>
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<td>Unit cell dimensions</td>
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Absorption correction: multi-scan
Max. and min. transmission: 0.9890 and 0.9830
Structure solution technique: direct methods
Structure solution program: SHELXL-2014/7 (Sheldrick, 2014)
Refinement method: Full-matrix least-squares on F^2
Refinement program: SHELXL-2014/7 (Sheldrick, 2014)
Function minimized: Σ w(Fo^2 - Fc^2)^2
Data / restraints / parameters: 5961 / 300 / 590
Goodness-of-fit on F2: 1.105
Final R indices: 5281 data; I>2σ(I)
R1 = 0.0485, wR2 = 0.1082
all data
R1 = 0.0589, wR2 = 0.1171
Weighting scheme:
w=1/[σ^2(Fo^2)+(0.0434P)^2+2.2126P]
where
P=(Fo^2+2Fc^2)/3
Absolute structure parameter: 0.2(4)
Largest diff. peak and hole: 0.195 and -0.243 eÅ^-3
R.M.S. deviation from mean: 0.048 eÅ^-3

Table S4: Selected bond distances (Å), angles (°) and torsion angles (°) for ligand 3.

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<td>1.484(6)</td>
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<td>C2-H2B</td>
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<table>
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<tr>
<td>N1-C1-C3-N2</td>
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</tr>
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</table>
The following reactions were carried out in the glove box.

**Potassium N- (2,6-bis[3,5-bis(trifluoromethyl)phenyl]) -2- (2,6-bis[3,5-bis(trifluoromethyl)phenylimine]) propanamidate (4)**

In a large vial with a magnetic stirring bar, N- (2,6-bis[3,5-bis(trifluoromethyl)phenyl]) -2- (2,6-bis[3,5-bis(trifluoromethyl)phenylimine]) propanamide (1.0 eq, 107 µmol, 116 mg) and potassium hydride (9.3 eq, 990 µmol, 40 mg) were suspended in THF. The reaction mixture was stirred for two hours. The solution was filtered through Celite® and the solvent was removed under vacuum. 115 mg of a slightly brown solid were obtained (Yield: 96%).

**¹H NMR** (400 MHz, in THF-d₈): δ 8.20 (s, 4H), 8.01 (s, 4H), 7.64 (s, 2H), 7.59 (s, 2H), 7.45 (d, J = 7.58 Hz, 2H), 7.29-7.25 (m, 3H), 7.01 (t, J = 7.58 Hz, 1H), 1.45 (s, 3H)
Potassium N-(2,6-bis[3,5-bis(trifluoromethyl)phenyl]) -2-(2,6-diisopropylphenylimine) propanamidate (5)

In a large vial with a magnetic stirring bar, N-(2,6-bis[3,5-bis(trifluoromethyl)phenyl]) -2-(2,6-diisopropylphenylimine) propanamide (1.0 eq, 173 µmol, 129 mg) and potassium hydride (3.2 eq, 556 µmol, 22 mg) were suspended in THF. The reaction mixture was stirred for two hours. The solution was filtered through Celite® and the solvent was removed under vacuum. The crude was washed with hexane. 72 mg of a slightly yellow solid were obtained (Yield: 53%).

$^1$H NMR (400 MHz, in THF-d$_8$): δ 8.30 (s, 4H), 7.98 (s, 2H), 7.30 (d, J = 7.58 Hz, 2H), 7.04-6.99 (m, 3H), 6.90 (t, J = 7.58 Hz, 1H), 2.39 (quin, J = 7.09 Hz, 2H), 0.95 (d, J = 7.09 Hz, 12H)
Figure S13: $^1$H NMR (400 MHz, in THF-$d_8$) of 5.

[N- (2,6-bis[3,5-bis(trifluoromethyl)phenyl]) -2- (2,6-bis[3,5-bis(trifluoromethyl)phenylimine]) propanamidato-$K^2$–$Ν,O$] ($η^1$–benzyl)
(trimethylphosphine) nickel (II) (6)

In a large vial with a magnetic stirring bar, Potassium N- (2,6-bis[3,5-bis(trifluoromethyl)phenyl]) -2- (2,6-bis[3,5-bis(trifluoromethyl)phenylimine]) propanamidate (1.0 eq, 102.2 µmol, 115 mg) was dissolved in toluene. The precursor Ni($h^1$-benzyl)Cl(PMe$_3$) (1.0 eq, 102.2 µmol, 35 mg) was added and the reaction was left to stir for two hours. The solvent was removed under vacuum and the crude was recrystallized in a mixture of toluene and hexane. 88 mg of a red, crystalline solid were obtained (Yield: 66%).
$^1$H NMR (400 MHz, in C$_6$D$_6$): δ 8.49 (s, 4H), 8.03 (s, 4H), 7.82 (s, 2H), 7.78 (s, 2H), 6.92-6.88 (m, 2H), 6.79-6.87 (m, 5H), 6.65-6.71 (m, 4H), 1.32 (d, J = 4.89 Hz, 2H), 1.16 (s, 3H), 0.51 (d, J = 10.80 Hz, 9H)

$^{13}$C{H} NMR (101 MHz, in C$_6$D$_6$): δ 180.9 (C$_q$), 162.7 (C$_q$), 148.4 (C$_q$), 146.4 (C$_q$), 143.5 (C$_q$), 141.9 (C$_q$), 140.5 (C$_q$), 132.6 (C$_q$), 132.0 (q, J = 33.01 Hz, C$_q$), 131.9 (C$_q$), 131.2 (q, J = 32.77 Hz, C$_q$), 131.0 (C$_q$), 130.5 (d, J = 2.93 Hz, CH), 129.7 (d, J = 2.93 Hz, CH), 129.3 (CH), 128.9 (CH), 125.8 (C$_q$), 124.5 (CH), 123.1 (C$_q$), 121.7-121.9 (m, C$_q$), 120.4-120.7 (m, C$_q$), 18.6 (CH$_3$), 12.4 (d, J = 29.34 Hz, C$_q$), 9.1 (d, J = 30.81 Hz, CH$_2$)

$^{19}$F NMR (376.5 MHz, in C$_6$D$_6$): δ -62.20, -62.60 (s)

$^{31}$P NMR (161.98 MHz, in C$_6$D$_6$): δ -8.62 (s)

Figure S14: $^1$H NMR (400 MHz, in C$_6$D$_6$) of 6.
Figure S15: $^{13}$C($^1$H) NMR (101 MHz, in C$_6$D$_6$) of 6.
Figure S16: $^{13}$C DEPT 135 (101 MHz, in C$_6$D$_6$, green), compared to $^{13}$C{${}^1$H} NMR (101 MHz, in C$_6$D$_6$, red) of 6. The highlighted signal on the top left corner of the inlet shows the benzyl group’s CH$_2$ signal assignment.
Figure S17: $^1$H-$^{13}$C HSQC NMR (400 MHz, in C$_6$D$_6$) of 6. The highlighted signal on the top left corner of the inlet shows the benzyl group’s CH$_2$ signal correlation.
Figure S18: $^1$H-$^1$H NOESY NMR (400 MHz, in $\text{C}_6\text{D}_6$) of 6.
Figure S19: $^{19}$F NMR (376.5 MHz, in C$_6$D$_6$) of 6.

Figure S20: $^{31}$P NMR (161.98 MHz, in C$_6$D$_6$) of 6.

**Elemental Analysis (%)** C$_{58}$H$_{40}$F$_{24}$N$_2$OPNi (M 1326.58 g/mol): calculated C 52.51, H 3.04, N 2.11; found C 51.96, H 3.24, N 2.22
[N-(2,6-bis[3,5-bis(trifluoromethyl)phenyl]) -2- (2,6 -diisopropylphenylimine) propanamidato-K^2–N,O] (η^1–benzyl) (trimethylphosphine) nickel (II) (7)

In a large vial with a magnetic stirring bar, Potassium N-(2,6-bis[3,5-bis(trifluoromethyl)phenyl]) -2- (2,6 -diisopropylphenylimine) propanamide (1.0 eq, 92 µmol, 72 mg) was dissolved in toluene. The precursor Ni(h^1-benzyl)Cl(PMe_3) (1.0 eq, 92 µmol, 31 mg) was added and the reaction was left to stir for two hours. The solvent was removed under vacuum and the crude was recrystallized in a mixture of toluene and hexane. 65 mg of a red, crystalline solid were obtained (Yield: 73%).

^1H NMR (400 MHz, in C_6D_6): δ 8.07 (s, 4H), 7.85 (s, 2H), 7.34-7.36 (m, 2H), 6.89-7.02 (m, 9H), 3.09 (spt, J = 6.77 Hz, 2H), 1.64 (s, 3H), 1.25 (d, J = 6.85 Hz, 2H), 0.98 (d, J = 6.85 Hz, 3H), 0.39 (d, J = 10.27 Hz, 9H)

^13C{1H} NMR (101 MHz, in C_6D_6): δ 179.3 (C_q), 165.6 (C_q), 150.2 (C_q), 148.2 (C_q), 144.5 (C_q), 141.0 (C_q), 140.0 (C_q), 132.1 (C_q), 131.5 (q, J = 32.77 Hz, C_q), 130.5 (CH), 130.3 (d, J = 2.94 Hz, CH), 130.1 (CH), 128.3 (CH), 128.0 (CH), 126.0 (C_q), 124.4 (CH), 124.2 (C_q), 123.4 (CH), 120.78 (qui, J = 7.70 Hz, J = 3.48 Hz, CH), 28.9 (CH), 24.32 (CH_3), 24.15 (CH_3), 12.24 (CH_3), 12.14 (d, J = 27.88 Hz, CH_2), 10.03 (d, J = 28.61 Hz, CH_3)

^19F NMR (376.5 MHz, in C_6D_6): δ -62.32 (s)

^31P NMR (161.98 MHz, in C_6D_6): δ -9.56 (s)
Figure S21: $^1$H NMR (400 MHz, in C$_6$D$_6$) of 7.
Figure S22: $^{13}$C{1H} NMR (101 MHz, in C$_6$D$_6$) of 7.
Figure S23: $^{13}$C DEPT 135 (101 MHz, in C$_6$D$_6$, green), compared to $^{13}$C$^{[1]}$H NMR (101 MHz, in C$_6$D$_6$, red) of 7.
Figure S24: $^1$H-$^{13}$C HSQC NMR (400 MHz, in C$_6$D$_6$) of 7.

Figure S25: $^1$H-$^1$H NOESY NMR (400 MHz, in C$_6$D$_6$) of 7.
Figure S26: $^{19}$F NMR (376.5 MHz, in C$_6$D$_6$) of 7.

Figure S27: $^{31}$P NMR (161.98 MHz, in C$_6$D$_6$) of 7.

Elemental Analysis (%) C$_{47}$H$_{45}$F$_{12}$N$_2$OPNi (M 971.52 g/mol): calculated C 58.11, H 4.67, N 2.88; found C 58.96, H 4.54, N 3.22
BF$_3$ adduct of Benzyl((1Z,2E)-1,2-bis((3,3''',5,5'''-tetrakis(trifluoromethyl)-[1,1':3',1''-terphenyl]-2'-yl)imino)propoxy)phosphinenickel

In a large vial with a magnetic stirring bar, Benzyl((1Z,2E)-1,2-bis((3,3''',5,5'''-tetrakis(trifluoromethyl)-[1,1':3',1''-terphenyl]-2'-yl)imino)propoxy)phosphinenickel (1.0 eq, 27.5 µmol, 36 mg) was dissolved in C$_6$D$_6$. Boron trifluoride diethyl etherate (5.1 eq, 140.2 µmol, 19.9 mg) was added and the reaction mixture was heated to 50 °C for 18h. The solvent was evaporated and 9 mg of a yellow solid were obtained (Yield: 25%).

Figure S28: $^1$H NMR (400 MHz, in C$_6$D$_6$) of 6-BF$_3$ (BF$_3$ adduct of 6, red), compared to the spectrum of 6 (400 MHz, in C$_6$D$_6$, green). It is evident that a significant shift of all aromatic signals occurs. Notably, the methyl group signal of the phosphine ligand can no longer be found, suggesting the successful formation of the η$_3$ complex.
Figure S29: $^{13}$C($^1$H) NMR (101 MHz, in C$_6$D$_6$) of 6-BF$_3$.

Figure S30: $^{11}$B NMR (160 MHz, in C$_6$D$_6$) of 6-BF$_3$. 
Figure S31: $^1$H NMR (400 MHz, in C$_6$D$_6$) of polymerization attempt with 6-BF$_3$, 2.5 h at room temperature after charging of ethylene (5.25 ppm), compared to the spectrum of 6-BF$_3$ (400 MHz, in C$_6$D$_6$, green). No signals that may be attributed to oligomers can be observed. Furthermore, the signals in the aromatic region, including the benzyl group, remain unchanged.
Quantum Chemistry Computations

Free Gibbs reaction enthalpies

Table S5: Computed Free Gibbs reaction enthalpies of the adduct formation.

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<th>$\Delta \Delta G^0$ of step 1 (kcal mol(^{-1}))</th>
<th>$\Delta \Delta G^0$ of step 2 (kcal mol(^{-1}))</th>
<th>$\Delta G^0$ of complete adduct formation (kcal mol(^{-1}))</th>
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<td>B(C(_6)F(_5))(_3): -8.0</td>
<td>B(C(_6)F(_5))(_3): 1.3</td>
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<td></td>
<td></td>
<td>BF(_3): -17.5</td>
<td>BF(_3): -11.0</td>
</tr>
<tr>
<td>7</td>
<td>5.9</td>
<td>B(C(_6)F(_5))(_3): -16.9</td>
<td>B(C(_6)F(_5))(_3): -8.3</td>
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<tr>
<td></td>
<td></td>
<td>BF(_3): -21.4</td>
<td>BF(_3): -15.6</td>
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</table>

The change in coordination, the phosphine removal, and the change from N,O to N,N coordination was found to be an endothermic process (Table S5). In particular, the results suggest a reduction of the Gibbs free energy from 9.2 kcal mol\(^{-1}\) to 5.9 kcal mol\(^{-1}\), when exchanging the bulky 3,5-bis(trifluoromethyl)phenyl substituent for the less sterically demanding iPr substituent in the ligand. The endothermic free energies imply that the activation energies for the transformation are higher for 6 than for 7. First, the larger energy barrier in the N,O to N,N coordination mode takes place through a C–C bond torsion, which is sterically hindered primarily by the CF\(_3\) substituents in L1 that fight against this torsion, effectively increasing the activation energy of the process. Conversely, when 3,5-bis(trifluoromethyl)phenyl is substituted by iPr in 7, the steric repulsion decreases considerably, effectively lowering the energy associated with the conformational change around the C–C bond.
London dispersion interactions

It was found that 6 and 7 are more stable than the inversion products due to stabilizing London dispersion interactions. In Figure S32, the NCI indexes computed for 6 and 6-inv are shown as representatives. The key dispersion interactions that were observed to stabilize both 6 and 7 correspond to the one triggered by the benzyl moiety with both the methyl groups of the phosphine ligand as well as the 3,5-bis(trifluoromethyl)phenyl moiety.

Figure S32: Noncovalent interaction (NCI) for 6, 7, 6-inv, and 7-inv in color code.
in the ligand. On the other hand, the reduced thermodynamic stability of the inversion products (6-inv and 7-inv) may be explained by the lack of the phosphine ligand and its long-range stabilization effect. Interestingly, the new η1-benzyl substituent facilitates dispersion interactions with the phenyl moiety in L1 (or L2). At the same time, the removal of the phosphine ligand allows intensifying the CH···CH, CH···CF, and CF···CF interactions within the R1 and R2 moieties in 6-inv and 7-inv.

**Bond distances**

![Molecular structures of 6-BF3, 6-B(C6F5)3, 7-BF3, and 7-B(C6F5)3 with bond distances and angles.]

*Figure S33: Optimized DFT molecular structures for the formation of the adducts of 6 and 7 with BF3 and B(C6F5)3.*
The B–O bond distances (Figure S33) were found to be 1.675 Å and 1.576 Å in 6-BF$_3$ and 6-B(C$_6$F$_5$)$_3$, respectively. Interestingly, the less congested BF$_3$ generates a thermodynamically more stable adduct through a longer B–O bond distance. Longer B–O bond distances were obtained for 7-BF$_3$ (1.609 Å) compared to 7-B(C$_6$F$_5$)$_3$ (1.585 Å), with 7-BF$_3$ as the more stable product.

Steric plots

Figure S34: Steric plots for 6-inv, 7-inv and b-inv in color code. Steric plots computed using SambVCA 2.1 web application.

To explore the coordination of the boron Lewis acids to the oxygen atoms, we computed steric plots and free volume percentage ($\%V_{\text{free}}$) using the oxygen atom as the origin of coordinates for 6-inv and 7-inv, as depicted in Figure S34, compared with b-inv. The $\%V_{\text{free}}$ in b-inv is 57.1, considerably larger than the values obtained for 6-inv and 7-inv. However, 7-inv has a larger free space compared to 6-inv for coordination of the Lewis acids, as expected due to the bulkier nature of the ligand. In 6-inv, this result arises due to two highly polarizing -F atoms (within -CF$_3$) close to the oxygen atom, which interacts with the boron acid. Conversely, as a consequence of the change of the 3,5-bis(trifluoromethyl)phenyl moiety for the less bulky iPr ligand, both -CF$_3$ groups are further apart from each other, increasing the free volume for a potentially easier Lewis acid
coordination. Considering the steric plots computed using a spheric radius of 6Å, a more favorable interaction can be anticipated with the smaller BF$_3$ acid, which has a radius of ~2.6 Å in contrast to ~10 Å of B(C$_6$F$_5$)$_3$. Moreover, although the adducts with B(C$_6$F$_5$)$_3$ could be optimized to be a minimum on the potential energy surface, the low free space hinders a dynamical interaction with the catalysts, being even further constrained at higher temperatures.

**Natural Charges**

![Natural charges diagram](image)

Figure S35: Natural charges for (a) Adduct formation of Ni(II) species with B(C$_6$F$_5$)$_3$ and BF$_3$ acids. (b) Two arbitrarily chosen steps of adduct formation. The first step is associated with the loss of the phosphine ligand, a change of the coordination mode from $N,O$ to $N,N$ and the benzyl ligand’s hapticity switching from $\eta^1$ to $\eta^3$.  

L1 : 3,5-bis(trifluoromethyl)phenyl
Interestingly, for complexes 6 and 7, the natural charge \( Q \) of Ni (Figure S35) is equal for both compounds, suggesting that the acryl rests R\(^1\) of the \( \alpha \)-iminocarboxamidato ligand do not affect the electronic properties of the metal center within the N,O coordination mode. To examine if the fluorine atoms indeed play an innocent role in the complex, all fluorine atoms were exchanged by hydrogen atoms. Surprisingly, \( Q_{Ni} \) for hydrogenated versions of 6 and 7 was found to be 0.364 |e| and 0.327 |e|, respectively. Even though a depletion of electron density due to the introduction of F atoms at the ligand is expected, the calculations suggest that the hydrogen-substituted ligand produces a stronger withdrawing effect in the N,O coordination mode when compared to the complex with CF\(_3\) groups.

It is worth noting that the desired removal of electron density from the metal is achieved when changing from the N,O to the N,N coordination mode. As expected, the more positive metal center is obtained with 6 (\( Q_{Ni} \) is 0.535 |e| in 6 versus 0.527 |e| in 7) due to the more electron-withdrawing nature of ligand L1. Importantly, these values are clearly suggesting a more positively charged Ni centers when compared to the reference system b (\( Q_{Ni} \)= 0.494 |e|), indicating that the desired removal of electron density can be achieved through introduction of remote substituents.

Surprisingly, \( Q_{Ni} \) is 0.553 |e| for 6-BF\(_3\) and 0.541 for 6-B(C\(_6\)F\(_5\))\(_3\), which is in contrast to the expected increase in electrophilicity due to the electron removing effect of a Lewis acid.

Global DFT Descriptors

Chemical potential (\( \mu \)) was computed using the energy of the highest occupied molecular orbital (HOMO) and lowest occupied molecular orbital (LUMO) orbitals as \( \mu = (\epsilon_{HOMO} + \epsilon_{LUMO})/2 \). On the other hand, the donor-acceptor hardness (\( \Delta \eta_{DA} \)) quantifies the affinity between the donor (ethylene) and the acceptor (nickel complexes) species to interact. In general, small values of \( \Delta \eta_{DA} \) indicate high reactivity between the donor and acceptor. The \( \Delta \eta_{DA} \) index was computed as \( \Delta \eta_{DA} = (\epsilon_{LUMO(acceptor)} - \epsilon_{HOMO(donor)})/2 \). As it can be concluded from the values in Table S6, the Lewis acid adducts become more reactive towards ethylene in comparison with the naked complexes. However, when the BCF acid is used, higher complex-ethylene interactions are expected to take place. However, it is worth mentioning that according to the values of chemical potential 6-BF\(_3\) should show a stronger interaction with ethylene compared to the experimentally active b catalyst. Similarly, when the donor-acceptor energies are taken into account, it is
clear that the proposed systems and their Lewis adducts should perform better than the b catalyst by showing lower $\Delta \eta_{DA}$ values. This is a clear example in which DFT descriptors fail to give a consistent interpretation and prediction of reactivity due to the steric hindrance caused by ligands, preventing the reaction with ethylene, although the electronic requirements are met.

Table S6: Chemical potential and donor-acceptor energies for systems under discussion. All values are reported in kcal mol$^{-1}$.

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Table S7: Symmetry-adapted perturbation theory energetics for systems under discussion in main text.

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## XYZ coordinates for optimized DFT structures

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H  -0.935278  -1.205201  1.183134
C  -1.441354  -3.252423  0.971411
C  -1.511488  -3.989717  1.355972
H  -1.701959  -0.945725  3.561285
H  -2.171158  -2.651127  3.566514
H  -0.481926  -2.204377  3.329754
H  -2.154915  -3.987917  1.355972
H  -0.430373  -3.593952  1.224919
H  -1.532108  -3.225446  -0.117776
C  -4.805807  -0.267574  -2.090424
H  -3.898130  0.241435  -2.449395
C  -5.991526  0.649232  -2.355485
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b-inv
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H  1.565221  1.089108  -3.613284
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C    0.947906  -1.379835   0.982615
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H    2.604019  -2.525503  1.727333
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C    5.183503   0.078237   1.152788
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H  -1.256373  -0.747731  -4.664614  
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References:

[8]XP–Interactive molecular graphics (version 5.1), Madison, Wisconsin, USA.


