Supporting Information for

Olefin Metathesis Catalyst: Stabilization Effect of Backbone Substitutions of N-Heterocyclic Carbene

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Materials and Methods

All reactions involving metal complexes were conducted in oven-dried glassware under a nitrogen atmosphere with anhydrous solvents, using standard Schlenk and glovebox techniques. Anhydrous solvents were obtained via elution through a solvent column drying system.\textsuperscript{1} RuCl\textsubscript{2}(PCy\textsubscript{3})\textsubscript{2}(=CHC\textsubscript{6}H\textsubscript{5}) was obtained from Materia, Inc. Silica gel used for the purification of organometallic complexes was obtained from TSI Scientific, Cambridge, MA (60 Å, pH 6.5–7.0). NMR chemical shifts are reported in ppm downfield from Me\textsubscript{4}Si, by using the residual solvent peak as internal standard for \textsuperscript{1}H and \textsuperscript{13}C, and H\textsubscript{3}PO\textsubscript{4} (δ 0.0) for \textsuperscript{31}P. Data for NMR spectra are reported as follows: chemical shift (δ ppm), multiplicity, coupling constant (Hz) and integration. IR spectra were recorded on a Perkin-Elmer Paragon 1000 Spectrophotometer. Gas chromatography data was obtained using an Agilent 6850 FID gas chromatograph equipped with a DB-Wax Polyethylene Glycol capillary column (J&W Scientific). X-ray crystallographic structures were obtained by the Beckman Institute X-ray Crystallography Laboratory of the California Institute of Technology. Crystallographic data have been deposited at the CCDC, 12 Union Road, Cambridge CB2 1EZ, U.K., and copies can be obtained on request, free of charge, by quoting the publication citation and the deposition numbers 651006 (13) and 678270 (19). The screening of the catalysts, in ring-closing metathesis (RCM), cross metathesis (CM), and ring-opening metathesis polymerization reactions (ROMP), was conducted according to literature procedures.\textsuperscript{2} The initiation kinetics studies were conducted according to literature procedures.\textsuperscript{3}

**Experimental**

4,4,5,5-Tetramethyl-1,3-diphenyl-4,5-dihydro-1H-imidazol-3-ium chloride (10)

Diamine $^4$ (2.07 g, 7.72 mmol) was dissolved in diethyl ether (20 ml) and treated with a solution of hydrogen chloride (4 M in dioxane, 7.7 ml) to precipitate the diamine hydrochloride salt. The white solid was collected by filtration and washed with copious amount of diethyl ether. The solid was placed in a flask and added triethyl orthoformate (25 ml). The resulting mixture was stirred at 130 °C for 10 min then cooled. After cooling to room temperature, the white solid was collected by filtration washing with large amount of diethyl ether and then with acetone to give the desired imidazolidinium chloride salt 10 (1.91 g, 6.07 mmol, Y = 79%).

$^1$H NMR (300 MHz, CD$_2$Cl$_2$): $\delta$ 9.37 (s, 1H), 7.69-7.66 (m, 4H), 7.54-7.52 (m, 6H), 1.46 (s, 12H).

$^{13}$C NMR (75 MHz, CD$_2$Cl$_2$): $\delta$ 156.8, 133.3, 130.4, 130.0, 128.6, 74.0, 21.5. IR: 3015 (m), 2981 (m), 1616 (s), 1585 (s), 1491 (s), 1455 (s), 1390 (m), 1292 (m), 1269 (s), 1154 (s), 1078 (w), 782 (m), 768 (m), 701 (s). HRMS Calc'd for C$_{19}$H$_{23}$N$_2$: 279.1861. Meas: 279.1852.

RuCl$_2$(4,4,5,5-Tetramethyl-1,3-diphenylimidazolin-2-ylidene)(=CH–Ph)(PCy$_3$) (12)

A mixture of 10 (288 mg, 0.915 mmol) and dry benzene (20 ml) was added KHMDS (182 mg, 0.915 mmol) under nitrogen atmosphere, and the resulting mixture was stirred at room temperature for 15 minutes, after which time, RuCl$_2$(PCy$_3$)$_2$(=CHC$_6$H$_5$) (500 mg, 0.608 mmol) was added in one portion. After stirred at room temperature for overnight, the reaction mixture was concentrated under vacuum. The dark brown residue was added dry hexane (10 ml), and the mixture was stirred at room temperature for 20 minutes. The brown precipitation was collected by filtration and washed with hexane and then with methanol to give the desired ruthenium complex 12 (275 mg, 0.335 mmol, Y = 55%). Full characterization of 12 was difficult due to its instability.

$^1$H NMR (500 MHz, C$_6$D$_6$): $\delta$ 19.61 (d, $J$ = 3.8 Hz, 1H), 8.11 (d, $J$ = 6.7 Hz, 2H), 7.36-6.67 (m, 13H), 2.25-2.18 (m, 3H), 1.68-1.54 (m, 15H), 1.34-1.25 (m, 6H), 1.17-1.06 (m, 9H), 0.87 (s, 6H), 0.85 (s, 6H).

$^{13}$C NMR (125 MHz, C$_6$D$_6$): $\delta$ 300.8, 217.2, 216.6, 151.8, 139.3, 137.9, 133.9,

131.1, 129.5, 129.4, 129.2, 129.1, 128.7, 128.5, 128.3, 128.0, 127.8, 127.7, 70.8, 70.7, 70.5, 33.4, 29.6, 28.5, 28.4, 27.1, 22.5, 22.0. $^{31}$P NMR (121 MHz, C$_6$D$_6$): $\delta$ 22.35.

RuCl$_2$(4,4,5,5-Tetramethyl-1,3-diphenylimidazolin-2-ylidene)(=CH–$^{1}$PrPh) (13)

A mixture of 12 (200 mg, 0.240 mmol), $\alpha$-isopropoxy-$\beta$-methylstyrene (14) (64 mg, 0.365 mmol), and $p$-toluenesulfonic acid (51 mg, 0.268 mmol) in benzene was stirred at 40 °C for 1 hour. After cooled to room temperature, the mixture was evaporated under vacuum and the residue was washed with methanol. The green solid thus obtained was recrystallized from benzene/n-pentane to give 13 as a dark green, crystalline solid (65 mg, 0.109 mmol, Y = 45%). X-ray quality crystal was obtained by a slow diffusion of pentane into a benzene solution.

$^1$H NMR (500 MHz, C$_6$D$_6$): $\delta$ 16.62 (s, 1H), 8.27 (d, $J$ = 7.5 Hz, 2H), 7.56 (d, $J$ = 7.1 Hz, 2H), 7.42 (t, $J$ = 7.7 Hz, 2H), 7.26 (t, $J$ = 7.3 Hz, 1H), 7.17-7.03 (m, 4H), 6.96 (dd, $J$ = 7.5, 1.6 Hz, 1H), 6.66 (t, $J$ = 7.3 Hz, 1H), 6.38 (d, $J$ = 8.3 Hz, 1H), 4.49 (sept, $J$ = 6.2 Hz, 1H), 1.38 (d, $J$ = 6.2 Hz, 6H); 0.97 (s, 6H), 0.91 (s, 6H). $^{13}$C NMR (125 MHz, CD$_2$Cl$_2$): $\delta$ 296.1 (d, $J_{C-H}$ = 22 Hz), 208.0, 152.8, 144.0, 140.5, 138.7, 132.5, 131.4, 130.4, 129.7, 129.2, 129.2, 128.9, 128.5, 128.5(4), 128.5(3), 128.4(8), 122.6, 121.8, 113.2, 75.0, 71.5, 70.3, 22.3, 22.2, 21.8, 21.7. IR: 3062 (w), 2979 (m), 2935 (w), 1589 (m), 1494 (s), 1453 (m), 1396 (s), 1370 (s), 1289 (m), 1267 (s), 1152 (s), 1114 (m), 954 (m), 938 (m), 844 (w), 808 (w), 770 (m), 748 (m), 714 (s) cm$^{-1}$. HRMS Calc'd for C$_{29}$H$_{34}$Cl$_2$N$_2$ORu: 598.1092. Meas: 598.1070.

N-Mesityl-2-methyl-2-(phenylamino)propanamide (15)

2-bromo-2-methylpropanoyl bromide (4.50 g, 19.57 mmol) was added to a mixture of 2,4,6-trimethylaniline (2.41g, 17.78 mmol), triethylamine (3.60 g, 35.56 mmol), and CH$_2$Cl$_2$ (20 ml) at 0 °C under Ar atmosphere. The cooling bath was removed after the addition was completed, and the reaction mixture was stirred at room temperature for 1.5 hour, after which time the mixture was diluted with CH$_2$Cl$_2$ (20 ml) and added aqueous solution of NH$_4$Cl. After the aqueous phase was separated, the organic layer was washed with brine and dried over anhydrous MgSO$_4$. Filtration and concentration of the
filtrate gave 2-bromo-N-mesityl-2-methylpropanamide as a pale yellow solid (5.05g, 17.78 mmol, 100%). A solution of this amide (284 mg, 1.00 mmol) in dry THF (5 ml) was added to a mixture of sodium hydride (60% in mineral oil, 80 mg, 2.00 mmol), aniline (112 mg, 1.20 mmol) and THF (5 ml), and the resulting mixture was stirred for overnight at room temperature. The mixture was then added an aqueous solution of NH$_4$Cl (15 ml), extracted with ethyl acetate (20 ml × 2), and the combined organic layer was washed with brine then dried over anhydrous Na$_2$SO$_4$. After filtration, the filtrate was concentrated under vacuum, and the residue was purified by column chromatography on silica (eluent: Hexane/Ethyl acetate = 5/1 ~ 4/1) to give 15 as a white solid (255 mg, 0.86 mmol, Y = 86%).

$^1$H NMR (300 MHz, CDCl$_3$): $\delta$ 8.35 (s, 1H), 7.25-7.17 (m, 2H), 6.84-6.71 (m, 5H), 3.98 (s, 1H), 2.23 (s, 3H), 2.11 (s, 6H), 1.63 (s, 6H). $^{13}$C NMR (75 MHz, CDCl$_3$): $\delta$ 173.8, 144.5, 136.4, 134.8, 131.0, 129.0, 119.2, 116.2, 58.4, 26.2, 20.8, 18.6. IR: 3341 (m), 3310 (s), 2987 (w), 1666 (s), 1607 (m), 1488 (s), 1376 (m), 1318 (m), 1264 (m), 1210 (m), 1162 (m), 850 (m), 749 (s), 696 (m) cm$^{-1}$. HRMS Calc'd for C$_{19}$H$_{24}$N$_2$O: 297.1967. Meas: 297.1956.

1-Mesityl-4,4-dimethyl-3-phenyl-4,5-dihydro-1H-imidazol-3-ium chloride (16)

A solution of 15 (100 mg, 0.337 mmol) in dry dimethoxyethane (2 ml) was added lithium aluminum hydride (80 mg, 2.1 mmol), and the mixture was refluxed for 1 day. After cooling to room temperature, the reaction was quenched by adding H$_2$O (0.08 ml), 15% aqueous NaOH (0.08 ml), and H$_2$O (0.24 ml) successively. The white precipitation was filtered off and the filtrate was purified by column chromatography on silica (eluent: Hexane/Ethyl acetate = 10/1) to give N$_1$-mesityl-2-methyl-N$_2$-phenylpropane-1,2-diamine as a pale yellow solid (54 mg, 0.192 mmol, Y = 57%). The diamine (1.45 g, 5.14 mmol) was converted to the corresponding dihydrochloride salt (1.83 g, 5.14 mmol, 100%) by treating with HCl solution (4 M in dioxane). A mixture of this salt (500 mg, 1.4 mmol) and triethyl orthoformate (4.7 ml) was stirred at 130 ºC for 5 min then cooled. After cooling to room temperature, the white precipitation was collected by filtration washing with large amount of diethyl ether and then with acetone to give the desired imidazolidinium chloride salt 16 (367 mg, 1.12 mmol, Y = 80%).

$^1$H NMR (300 MHz, CDCl$_3$): $\delta$ 9.76 (s, 1H), 7.65-7.62 (m, 2H), 7.49-7.47 (m, 3H), 6.92 (s, 2H), 4.13 (s, 2H), 2.39 (s, 6H), 2.27 (s, 3H), 1.69 (s, 6H). $^{13}$C NMR (75 MHz, CDCl$_3$): $\delta$ 158.4, 140.2,
134.9, 132.3, 130.2, 129.9, 129.8, 127.4, 68.6, 63.7, 26.7, 20.9, 18.1. IR: 3401 (m), 2975 (w), 1624 (s), 1592 (m), 1301 (w), 1263 (m), 1219 (m), 856 (w), 776 (w) cm\(^{-1}\). HRMS Calc’d for C\(_{20}\)H\(_{25}\)N\(_2\): 293.2018. Meas: 293.2021.

**RuCl\(_2\)(1-Mesityl-4,4-dimethyl-3-phenylimidazolin-2-ylidene)(=CH–Ph)(PCy\(_3\)) (18) and RuCl\(_2\)(1-Mesityl-4,4-dimethyl-3-phenylimidazolin-2-ylidene)(=CH–p-\text{PrPh}) (19)**

The phosphine complex 18 and the phosphine-free complex 19 was prepared from 16 according to the procedure described for the synthesis of 13. X-ray quality crystal of 19 was obtained by a slow diffusion of pentane into a CH\(_2\)Cl\(_2\) solution.

\(\text{\^{1}H NMR (500 MHz, CD}_2\text{Cl}_2): \delta 19.14 (s, 1H), 8.77 (br s, 1H), 7.89-7.87 (m, 2H), 7.51 (t, } J = 7.6 \text{ Hz, 2H), 7.44 (tt, } J = 7.4, 1.2 \text{ Hz, 1H), 7.39 (t, } J = 7.4 \text{ Hz, 1H), 7.10 (t, } J = 7.6 \text{ Hz, 2H), 6.71 (br s, 2H), 5.84 (br s, 1H), 3.66 (br s, 2H), 2.65-1.99 (m, 5H), 1.91 (s, 3H), 1.94-1.87 (m, 3H), 1.53-1.47 (m, 9H), 1.36 (s, 6H), 1.39-1.23 (m, 6H), 0.98-0.89 (m, 16H). \text{\^{13}C NMR (125 MHz, CD}_2\text{Cl}_2): \delta 296.8, 218.1, 217.5, 151.8, 138.3, 137.7, 136.9, 136.1, 135.0, 129.7, 129.4, 129.1, 128.9, 128.6, 128.2, 65.9, 65.2, 32.7, 32.5, 29.2, 28.3, 28.2, 27.7, 26.7, 21.2, 18.8. IR (CD\(_2\)Cl\(_2\)): 2931 (s), 2852 (m), 1987 (w), 1487 (m), 1447 (m), 1400 (m), 1301 (m), 1175 (m), 778 (w) cm\(^{-1}\). HRMS Calc’d for C\(_{45}\)H\(_{63}\)Cl\(_2\)N\(_2\)PRu: 834.3150. Meas: 834.3165.**

\(\text{\^{1}H NMR (500 MHz, C}_6\text{D}_6): \delta 16.49 (s, 0.5H), 16.48 (s, 0.5H), 7.99-7.96 (m, 2H), 7.57-7.49 (m, 4H), 7.10 (d, } J = 0.6 \text{ Hz, 2H), 6.91 (d, } J = 4.4 \text{ Hz, 2H), 6.86 (d, } J = 8.1 \text{ Hz, 1H), 4.90 (sept, } J = 6.2 \text{ Hz, 1H), 3.91 (s, 2H), 2.46 (s, 3H), 2.33 (s, 6H), 1.47 (s, 6H), 1.22 (d, } J = 6.2 \text{ Hz, 6H). \text{\^{13}C NMR (125 MHz, CD}_2\text{Cl}_2): } \delta 297.6 (d, } J_{\text{C-H}} = 18 \text{ Hz), 209.9, 152.6, 145.1, 139.4, 138.9, 138.1, 136.5, 135.6, 130.1, 1230.0, 129.4, 128.9(0), 128.8(6), 122.9, 122.5, 113.4, 75.4, 66.0, 65.5, 27.8, 21.8, 21.5, 18.5. IR: 2967 (m), 1589 (m), 1572 (m), 1489 (m), 1472 (m), 1450 (m), 1380 (s), 1317 (m), 1286 (s), 1207 (m), 1179 (m), 1154 (m), 1113 (s), 1031 (w), 931 (m), 877 (w), 805 (w), 770 (w), 754 (m), 699 (m) cm\(^{-1}\). HRMS Calc’d for C\(_{34}\)H\(_{44}\)Cl\(_2\)N\(_2\)ORu: 612.1249. Meas: 612.1229.**
**RhCl(CO)₂(4,4,5,5-Tetramethyl-1,3-diphenylimidazolin-2-ylidene) (32a)**

The imidazolidinium salt 16 (33 mg, 0.10 mmol), KHMDS (20 mg, 0.10 mmol), and toluene (2 ml) was stirred at room temperature under N₂ for 15 min, and added to a suspension of [RhCl(COD)]₂ (20 mg, 0.04 mmol) in toluene (1 ml). The resulting mixture was stirred at room temperature for 1.5 hour, and then the solvent was removed under vacuum. The residue was purified by column chromatography on TSI silica (eluent: 2% EtOH in CH₂Cl₂) to give [(NHC)RhCl(COD)] 31a as a yellow powder. A solution of 31a in CH₂Cl₂ (3 ml) was bubbled with CO for 1 hour. The mixture was then concentrated under vacuum and the residue was washed with dry hexane (2 ml × 3). The resulting solid was dried under vacuum to give 32 (26 mg, 0.055 mmol, Y = 76% two steps).

¹H NMR (500 MHz, CD₂Cl₂): δ 7.49-7.36 (m, 10H), 1.28 (s, 6H), 1.27 (s, 6H). ¹³C NMR (125 MHz, CD₂Cl₂): δ 202.8 (J_C–Rh = 40 Hz), 187.0 (J_C–Rh = 54 Hz), 183.6 (J_C–Rh = 76 Hz), 138.3, 131.7, 129.3, 129.1, 128.9, 72.1, 22.0, 21.9. IR (CD₂Cl₂): 2078, 1996 cm⁻¹. HRMS Calc’d for C₂₁H₂₂ClN₂O₂Rh: 472.0425. Meas: 472.0402.

**RhCl(CO)₂(1-Mesityl-4,4-dimethyl-3-phenylimidazolin-2-ylidene) (32b)**

The imidazolidinium 16 (33 mg, 0.10 mmol) was treated as described above to give 32b (32 mg, 0.066 mmol, Y = 94% two steps).

¹H NMR (500 MHz, CD₂Cl₂): δ 7.49-7.47 (m, 4H), 7.36 (s, 1H), 6.98 (br s, 2H), 3.77 (br s, 2H), 2.42 (br s, 6H), 2.33 (s, 3H), 1.46 (s, 6H). ¹³C NMR (125 MHz, CD₂Cl₂): δ 204.4 (J_C–Rh = 40 Hz), 186.5 (J_C–Rh = 54 Hz), 183.8 (J_C–Rh = 75 Hz), 139.2, 137.8, 135.5, 131.7, 129.9, 129.2, 129.1, 128.9, 67.3, 65.4, 27.6, 21.4. IR (CD₂Cl₂): 2079, 1996 cm⁻¹. HRMS Calc’d for C₂₂H₂₄N₂O₂Rh: 451.0893. Meas: 451.0889.
Standard Activity Test: RCM Reactions

All tests were performed according to the experimental procedure described by Ritter et al.$^1$

At 30 °C, CD$_2$Cl$_2$ (0.1 M)

At 60 °C, C$_6$D$_6$ (0.1 M)
At 30 °C, CD₂Cl₂ (0.1 M)

At 60 °C, C₆D₆ (0.1 M)
At 30 °C, CD₂Cl₂ (0.1 M)

At 60 °C, C₆D₆ (0.1 M)
CM Reactions

\[
\text{Ph} = 26 \quad + \quad \text{AcO} = 27 \quad \xrightarrow{\text{catalyst (2.5 mol\%)}} \quad \text{Ph} = 28 \quad (E/Z)
\]

![Graph showing conversion over time for CM Reactions](image)

ROMP of Cyclooctadiene

\[
\text{29} \quad \xrightarrow{\text{catalyst (0.1 mol\%)}} \quad \text{30}
\]

![Graph showing conversion over time for ROMP of Cyclooctadiene](image)
**Initiation Studies**

The initiation kinetics studies of compound 13 were conducted according to literature procedures.²

![Reaction Scheme](image)

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<td>11.9 (± 1.7)</td>
<td>15.2 (± 0.8)</td>
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<td>( \Delta S^\ddagger ) (e.u.)</td>
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<td>-19 (± 3)</td>
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<td>( \Delta G^\ddagger ) (kcal/mol)</td>
<td>21.0 (± 0.1)</td>
<td>20.7 (± 0.01)</td>
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<td>( k_{init} )</td>
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**Eyring Plot**

![Eyring Plot](image)

The equation for the Eyring plot is:

\[
y = 11898x - 29.936 \\
R^2 = 0.9848
\]
NMR Spectra

$^1$H-NMR of 12
$^{13}\text{C}$-NMR of 12
$^{31}$P-NMR of 12
$^1$H-NMR of 13
$^{13}$C-NMR of 13
$^{1}$H-NMR of 18
$^{31}\text{P}-\text{NMR of 18}$
$^{1}$H-NMR of 19
$^{13}$C-NMR of 19
$^1$H-NMR of 32a
$^{13}$C-NMR of 32a
$\text{H-NMR of 32b}$
$^{13}$C-NMR of 32b
X-Ray Structural Analysis

Minimum Overlap View of 13

Selected Bond Lengths [Å] and Angles [°] for 13

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Minimum Overlap View of 19

Selected Bond Lengths [Å] and Angles [°] for 19

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