**Supporting Information**

**Synthesis of Pyridine and Oxazoline-Functionalized Vinyl Polymers by Alane-based Frustrated Lewis Pairs**

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**Materials, Reagents, and Methods**

All syntheses and manipulations of air- and moisture-sensitive materials were carried out in flamed Schlenk-type glassware on a dual-manifold Schlenk line, on a high-vacuum line, or in an inert gas-filled glovebox. NMR-scale reactions were conducted in Teflon-valve-sealed J. Young-type NMR tubes. HPLC-grade organic solvents were first sparged extensively with nitrogen during filling 20 L solvent reservoirs and then dried by passage through activated alumina (for Et₂O, THF, and CH₂Cl₂) followed by passage through Q-5 supported copper catalyst (for toluene and hexanes) stainless steel columns. Benzene-\(d_6\) and toluene-\(d_8\) were dried over sodium/potassium alloy and vacuum-distilled or filtered, whereas CD₂Cl₂ and CDCl³ were dried over activated Davison 4 Å molecular sieves. HPLC-grade DMF was degassed and dried over CaH₂ overnight, followed by vacuum distillation (CaH₂ was removed before distillation). NMR spectra were recorded on Varian Inova 300 (300 MHz, \(^1\)H; 75 MHz, \(^13\)C; 282 MHz, \(^19\)F) or a Varion 400 MHz spectrometer. Chemical shifts for \(^1\)H and \(^13\)C spectra were referenced to internal solvent resonances and are reported as parts per million relative to SiMe₄, whereas \(^19\)F NMR spectra were referenced to external CFCl₃.

Monomers 2-isopropenyl-2-oxazoline (iPOx) and 2-vinyl pyridine (2-VP) as well as other commercial reagents were purchased from Sigma-Aldrich Chemical Co. A Literature procedure¹ was modified to prepare 4-Methyl-2-isopropenyl-2-oxazoline (MiPOx). These monomers were first degassed
and dried over CaH₂ overnight, followed by vacuum distillation. The purified monomers were stored in brown bottles inside a glovebox freezer at −30 °C. N-Heterocyclic carbenes (NHCs), including 1,3-bis(2,4,6-trimethylphenyl)imidazol-2-ylidene (IMes) and 1,3-di-tert-butylimidazol-2-ylidene (I' Bu), were purchased from Strem Chemical Co. A literature procedure was used to prepare 1,3,4-triphenyl-4,5-dihydro-1H-1,2,4-triazol-5-ylidene (TPT).² Phosphines, including PMes₃, PPh₃ and P'Bu₃, as well as butylated hydroxytoluene (BHT-H, 2,6-di-tert-butyl-4-methylphenol) were purchased from Alfa Aesar Chemical Co. BHT-H was recrystallized from hexanes prior to use. P'Bu₃ was first degassed and dried over CaH₂ overnight, followed by vacuum distillation. Tris(pentafluorophenyl)borane, B(C₆F₅)₃, was obtained as a research gift from Boulder Scientific Company and further purified by recrystallization from hexanes at −30 °C. A literature procedure was used to prepare MeAl(BHT)₂.³ Al(C₆F₅)₃, as a (toluene)₀.₅ adduct, was prepared by reaction of B(C₆F₅)₃ and AlMe₃ in a 1:3 toluene/hexanes solvent mixture in quantitative yield;⁴ this is the modified synthesis based on literature procedures.⁵ Although we have experienced no incidents when handling this material, extra caution should be exercised, especially when dealing with the unsolvated form, because of its thermal and shock sensitivity.

**Isolation of Adduct (2-VP)·Al(C₆F₅)₃ (I)**

A 20 mL glass vial was charged with 2-VP (0.33 g, 3.1 mmol) and 10 mL toluene, while another vial was charged with (toluene)₀.₅:Al(C₆F₅)₃ (1.0 g, 1.7 mmol) and 5 mL toluene. The two vials were mixed via pipette at ambient temperature to give a colorless solution. The solvent was removed and the solid residue was washed by hexanes (3 × 5 mL) to give adduct I as an off-white solid in quantitative yield after drying under vacuum.

¹H NMR (C₆D₆, 23 ºC) for I: δ 8.27 (d, J = 5.1 Hz, 1H, Py), 7.12 (dd, J = 17.1 Hz, J = 11.4 Hz, 1H, -CH=), 6.68 (t, J = 8.1 Hz, 1H, Py), 6.62 (t, J = 8.1 Hz, 1H, Py), 6.27 (t, J = 5.7 Hz, 1H,Py), 5.12 (d, J = 16.8 Hz, 1H, -C=CH₂), 4.95 (d, J = 11.1 Hz, 1H, -C=CH₂). ¹⁹F NMR (C₆D₆, 23 ºC): δ −122.44 (d, J = 17.2 Hz, 6 F, o-F), −151.45 (t, J = 19.7 Hz, 3 F, p-F), −160.8 (m, 6 F, m-F).
**Figure S1.** $^1$H NMR (C$_6$D$_6$, 23 °C) spectrum of (2-VP)·Al(C$_6$F$_5$)$_3$ (1).

**Figure S2.** $^{19}$F NMR (C$_6$D$_6$, 23 °C) spectrum of (2-VP)·Al(C$_6$F$_5$)$_3$ (1).
X-Ray Crystallographic Analysis of adduct (2-VP)·Al(C₆F₅)₃ (1)

The molecular structure of 1 has been confirmed by single-crystal X-ray diffraction analysis. Single crystals suitable for X-ray diffraction analysis, obtained by layering a solution of 2-VP (0.1 mmol) in 4 mL hexanes on an equimolar solution of (toluene)₀.₅·Al(C₆F₅)₃ in 1 mL toluene at -30 ºC, were quickly covered with a layer of Paratone-N oil (Exxon, dried and degassed at 120 ºC/10⁻⁶ Torr for 24 h) after decanting the mother liquor. A crystal was then mounted on a thin glass fiber and transferred into the cold nitrogen steam of a Bruker SMART CCD diffractometer. The structure was solved by direct methods and refined using the Bruker SHELXTL program library. The structure was refined by full-matrix least-squares on \( F^2 \) for all reflections. All non-hydrogen atoms were refined with anisotropic displacement parameters, whereas hydrogen atoms were included in the structure factor calculations at idealized positions. Selected crystallographic data for 1: \( C_{25}H_{7}AlF_{15}N \), monoclinic, space group P2(1)/c, \( a = 10.6644 (4) \) Å, \( b = 14.0645 (5) \) Å, \( c = 16.5182 (6) \) Å, \( \beta = 107.349 (2) \)°, \( V = 2364.84 (15) \) Å³, \( Z = 4 \), \( D_{\text{calc}} = 1.779 \) Mg/m³, GOF = 1.051, \( R_1 = 0.0243 \) [\( I > 2\sigma(I) \)], \( wR_2 = 0.0659 \). CCDC-972837 contains the supplementary crystallographic data for this structure. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/ data_request/cif.
**Figure S3.** X-ray crystal structure of (2-VP)·Al(C₆F₅)₃ (1). Hydrogen atoms have been omitted for clarity and ellipsoids drawn at 50% probability. Selected bond lengths [Å] and angles [°]: Al(1)-N(1) 1.9873(11), Al(1)-C(14) 1.9894(13), Al(1)-C(8) 1.9971(13), Al(1)-C(20) 2.0010(13), N(1)-Al(1)-C(14) 110.62(5), N(1)-Al(1)-C(8) 103.36(5), C(14)-Al(1)-C(8) 113.91(6), N(1)-Al(1)-C(20) 105.96(5), C(14)-Al(1)-C(20) 107.99(5), C(8)-Al(1)-C(20) 114.63(6).

**In Situ Generation of Imidazolium Pyridylaluminate l'Bu-CH₂CH=(C₅H₄N)Al(C₆F₅)₃ (2)**

A Teflon-valve-sealed J. Young-type NMR tube was charged with l'Bu (8.5 mg, 47 mmol) and 0.3 mL of C₆D₆. A 0.3 mL C₆D₆ solution of adduct 1 (29.8 mg, 47 mmol) was added to this tube via pipette at ambient temperature, and the colorless mixture was allowed to react for 10 min before analysis by NMR, which showed the clean formation of zwitterion 2 as two isomers A (major) and B (minor) in 2:1 ratio, obtained from the ¹H NMR spectrum.

¹H NMR (C₆D₆, 23 ºC) for 2A: δ 7.40 (d, J = 6.0 Hz, 1H, Py), 6.74 (s, br, 1H, Py), 6.55 (t, J = 7.1 Hz, 2H, NCCH=), 5.81 (d, J = 8.4 Hz, 1H, Py), 5.38 (s, br, 1H, =CH), 3.22 (s, br, 2H, CH₂), 0.73 (s, br, 18H, tBu). 2B: δ 7.40 (d, J = 6.0 Hz, 1H, Py), 6.74 (s, br, 1H, Py), 6.55 (t, J = 7.1 Hz, 2H, NCCH=), 5.81 (d, J = 8.4 Hz, 1H, Py), 5.38 (s, br, 1H, =CH), 3.31 (s, br, 2H, CH₂), 1.45 (s, br, 18H, tBu). ¹⁹F NMR (C₆D₆, 23 ºC): δ −121.8 (d, J = 18.3 Hz, 6 F, o-F), −156.5 (t, J_E,F = 19.7 Hz, 3 F, p-F), −162.8 (m, 6 F, m-F).
Figure S4. $^1$H NMR (C$_6$D$_6$, 23 °C) spectrum of the in situ-generated (crude) tBu-CH$_2$CH=(C$_3$H$_2$N)Al(C$_6$F$_5$)$_3$ (2) as a mixture of two isomers.
**Figure S5.** $^{19}$F NMR (C$_6$D$_6$, 23 °C) spectrum of the in situ-generated (crude) $^{t}$Bu-CH$_2$CH=(C$_5$H$_4$N)Al(C$_6$F$_5$)$_3$ (2) as a mixture of two isomers. The peaks for some excess of the (2-VP)-alane adduct 1 (−122.4, −151.5, −160.8) were also present.

**X-Ray Crystallographic Analysis of $^{t}$Bu-CH$_2$CH=(C$_5$H$_4$N)Al(C$_6$F$_5$)$_3$·CH$_2$Cl$_2$ (2)**

The molecular structure of 2 has been confirmed by single crystal X-ray diffraction analysis. A 20 mL glass vial was charged with (2-VP)·Al(C$_6$F$_5$)$_3$ (0.16 mmol) and 4 mL CH$_2$Cl$_2$, while another vial was charged with $^{t}$Bu (0.16 mmol) and 10 mL hexanes. The two vials were cooled to −30°C and the solution of $^{t}$Bu was layered on the (2-VP)·Al(C$_6$F$_5$)$_3$ solution via pipette at low temperature. The vial was stored in the freezer for one week and crystals of 2 were formed. The crystals were quickly covered with a layer of Paratone-N oil (Exxon, dried and degassed at 120 °C/10$^{-6}$ Torr for 24 h) after decanting the mother liquor. A crystal was then mounted on a thin glass fiber and transferred into the cold nitrogen steam of a Bruker SMART CCD diffractometer. The structure was solved by direct methods and refined using the Bruker SHELXTL program library. The structure was refined by full-matrix least-squares on $F^2$ for all reflections. All non-hydrogen atoms were refined with anisotropic displacement parameters, whereas hydrogen atoms were included in the structure factor calculations at idealized positions. There was a disordered CH$_2$Cl$_2$ solvent molecule found in the crystal lattice. Selected crystallographic data for 2·CH$_2$Cl$_2$: C$_{37}$H$_{29}$AlCl$_2$F$_{15}$N$_3$, monoclinic, space group P2(1)/c, $a = 11.6507$ (7) Å, $b = 16.8033$ (10) Å, $c = 19.1096$ (12) Å, $\beta = 94.747$ (3)°, $V = 3728.3$ (4) Å$^3$, $Z = 4$, $D_{calc} = 1.601$ Mg/m$^3$, GOF = 1.060, $R1 = 0.0512$ [$I > 2\sigma(I)$], $wR2 = 0.1482$. CCDC-972835 contains the supplementary crystallographic data for this structure. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif.
Figure S6. X-ray crystal structure of $2 \cdot \text{CH}_2\text{Cl}_2$. Hydrogen atoms and CH$_2$Cl$_2$ molecule have been omitted for clarity and ellipsoids drawn at 50% probability. Selected bond lengths [Å] and angles [°]: Al(1)-N(3) 1.906(2), Al(1)-C(31) 2.011(3), Al(1)-C(19) 2.010(3), Al(1)-C(25) 2.027(3), C(6)-C(5) 1.359(4), C(5)-C(4) 1.521(4), C(4)-C(1) 1.500(4), N(3)-Al(1)-C(31) 114.85(11), N(3)-Al(1)-C(19) 105.02(11), C(31)-Al(1)-C(19) 113.21(11), N(3)-Al(1)-C(25) 109.59(11), C(31)-Al(1)-C(25) 100.09(11), C(19)-Al(1)-C(25) 114.36(11).

In Situ Generation of Imidazolium pyridylaluminate IMes-CH$_2$CH=($C_5H_4N$)Al(C$_6F_5$)$_3$ (3)

A Teflon-valve-sealed J. Young-type NMR tube was charged with IMes (14.7 mg, 48 mmol) and 0.3 mL of C$_7$D$_8$. A 0.3 mL C$_7$D$_8$ solution of adduct 1 (30.5 mg, 47 mmol) was added to this tube via pipette at ambient temperature, and the colorless mixture was allowed to react for 10 min before analysis by NMR, which showed the formation of zwitterion 3 as two isomers A (major) and B (minor) in 2:1 ratio, obtained from the $^{19}$F NMR spectrum.

$^1$H NMR (C$_7$D$_8$, 23 ºC): $\delta$ 7.64 (s, 1H, Py), 6.82-6.57 (m, 3H, Py), 6.33 (s, br, 4H, Ph), 5.93 (s, br, 1H, CH=), 5.66 (s, br, 2H, NCH=), 3.64 (t, $J = 15.0$ Hz), 2.97 (d, $J = 16.8$ Hz), 2.65 (d, $J = 13.5$ Hz) (2H,}
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\[ \text{[2.21(s), 2.04(s), 1.94(s), 1.82(s), (18H, Me)]}. \] \[ \text{\(^{19}\)F NMR (C}_7\text{D}_8, 23 \degree\text{C}) \text{ for 3A}: \delta -120.8 \text{ (d, } J = 18.0 \text{ Hz, 6 F, o-F), } -157.0 \text{ (t, } J = 19.6 \text{ 3 F, p-F), } -163.2 \text{ (m, 6 F, m-F).} \] 

\[ \text{3B}: \delta -117.6 \text{ (d, } J = 15.8 \text{ Hz, 6 F, o-F), } -155.6 \text{ (t, } J = 19.5 \text{ 3 F, p-F), } -162.8 \text{ (m, 6 F, m-F).} \]

**Figure S7.** \(^1\)H NMR (C\(_7\)D\(_8\), 23 °C) spectrum of the in situ-generated (crude) IMes-CH\(_2\)CH=(C\(_5\)H\(_4\)N)Al(C\(_6\)F\(_5\))\(_3\) (3) as a mixture of two isomers.

**Figure S8.** \(^{19}\)F NMR (C\(_7\)D\(_8\), 23 °C) spectrum of the in situ-generated (crude) IMes-CH\(_2\)CH=(C\(_5\)H\(_4\)N)Al(C\(_6\)F\(_5\))\(_3\) (3) as a mixture of two isomers.

**General Polymerization Procedures**

Polymerizations were performed either in 25 mL flame-dried Schlenk flasks interfaced to the dual-manifold Schlenk line for runs using external temperature bath, or in 30 mL glass reactors inside the glovebox for ambient temperature (ca. 25 °C) runs. In a typical polymerization procedure, a predetermined amount of a LA, such as (toluene)\(_{0.5}\)·Al(C\(_6\)F\(_5\))\(_3\), or iPOx·Al(C\(_6\)F\(_5\))\(_3\), or 2-VP·Al(C\(_6\)F\(_5\))\(_3\), or
B(C₆F₅) was first dissolved in the monomer (0.5 mL for iPOx or 0.51 mL for 2-VP, 200 equiv relative to the LB) and 3.1 mL of solvent (CH₂Cl₂ or toluene) inside a glovebox. Benzene (0.369 g, 4.73 mmol) was added an internal standard to each reactor if needed. The polymerization was started by rapid addition of a solution of a LB (1 equiv of a phosphine or an NHC) in 1.0 mL of solvent (CH₂Cl₂ or toluene) via a gastight syringe to the above mixture containing the LA and monomer under vigorous stirring. The amount of the monomer was fixed for all polymerization. After the measured time interval, a 0.2 mL aliquot was taken from the reaction mixture via syringe and quickly quenched into a 4-mL vial containing 0.6 mL of undried “wet” CDCl₃ stabilized by 250 ppm of BHT-H; the quenched aliquots were later analyzed by ¹H NMR to obtain the percent monomer conversion data. After the polymerization was stirred for the stated reaction time and then the polymer was immediately precipitated into 200 mL of hexane, stirred for 1 h, filtered, washed with hexane, and dried in a vacuum oven at 50 °C overnight to a constant weight.

**Polymer Characterizations**

Polymer number-average molecular weights (Mₙ) and molecular weight distributions (D = Mₘ/Mₙ) were measured by gel permeation chromatography (GPC) analyses carried out at 40 °C and a flow rate of 1.0 mL/min, with DMF as the eluent, on a Waters University 1500 GPC instrument equipped with one PLgel 5 µm guard and three PLgel 5 µm mixed-C columns (Polymer Laboratories; linear range of molecular weight = 200–2,000,000). The instrument was calibrated with 10 PMMA standards, and chromatograms were processed with Waters Empower software (version 2002).
Figure S9. A representative GPC trace of the polymer produced by the FLP system (run 16, Table 1).

Table S1. Crystal data and structure refinement for (2-VP)·Al(C₆F₅)₃ (1).

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S11
Completeness to theta = 25.03 100.0 %

Absorption correction Semi-empirical from equivalents

Max. and min. transmission 0.9632 and 0.8994

Refinement method Full-matrix least-squares on F^2

Data / restraints / parameters 4172 / 0 / 407

Goodness-of-fit on F^2 1.051

Final R indices [I>2sigma(I)] R1 = 0.0243, wR2 = 0.0646

R indices (all data) R1 = 0.0259, wR2 = 0.0659

Largest diff. peak and hole 0.293 and -0.209 e.A^-3

Table S2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for (2-VP)·Al(C₆F₅)₃ (1). U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

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**Table S3.** Bond lengths [Å] and angles [deg] for (2-VP·Al(C$_6$F$_5$)$_3$ (1).
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Table S4. Crystal data and structure refinement for 2·CH₂Cl₂.

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Crystal system, space group  
Monoclinic, P2(1)/c

Unit cell dimensions  
a = 11.6507(7) Å  alpha = 90 deg.
b = 16.8033(10) Å  beta = 94.747(3) deg.
c = 19.1096(12) Å  gamma = 90 deg.

Volume  
3728.3(4) Å³

Z, Calculated density  
4, 1.601 Mg/m³

Absorption coefficient  
0.307 mm⁻¹

F(000)  
1816

Crystal size  
0.51 x 0.40 x 0.33 mm

Theta range for data collection  
2.13 to 25.03 deg.

Limiting indices  
-13<=h<=13, -19<=k<=20, -22<=l<=22

Reflections collected / unique  
56102 / 6589 [R(int) = 0.0303]

Completeness to theta = 25.03  
100.0 %

Absorption correction  
Semi-empirical from equivalents

Max. and min. transmission  
0.9045 and 0.8595

Refinement method  
Full-matrix least-squares on F²

Data / restraints / parameters  
6589 / 0 / 524

Goodness-of-fit on F²  
1.060

Final R indices [I>2sigma(I)]  
R1 = 0.0512, wR2 = 0.1427

R indices (all data)  
R1 = 0.0581, wR2 = 0.1482

Largest diff. peak and hole  
1.454 and -0.950 e Å⁻³

S16
Table S5. Atomic coordinates ( x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for 2 CH₂Cl₂. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

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Table S6. Bond lengths [Å] and angles [deg] for $2\cdot$CH$_2$Cl$_2$.

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