Supporting Information

Unveiling the Mechanisms of Epoxide Polymerization with N—Al Adduct Catalysts: A Comprehensive Experimental and Theoretical Investigation.

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‡NS, AR, and GJ contributed equally.

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Experimental Details.

[1]H NMR and [13]C NMR spectra for catalysts:

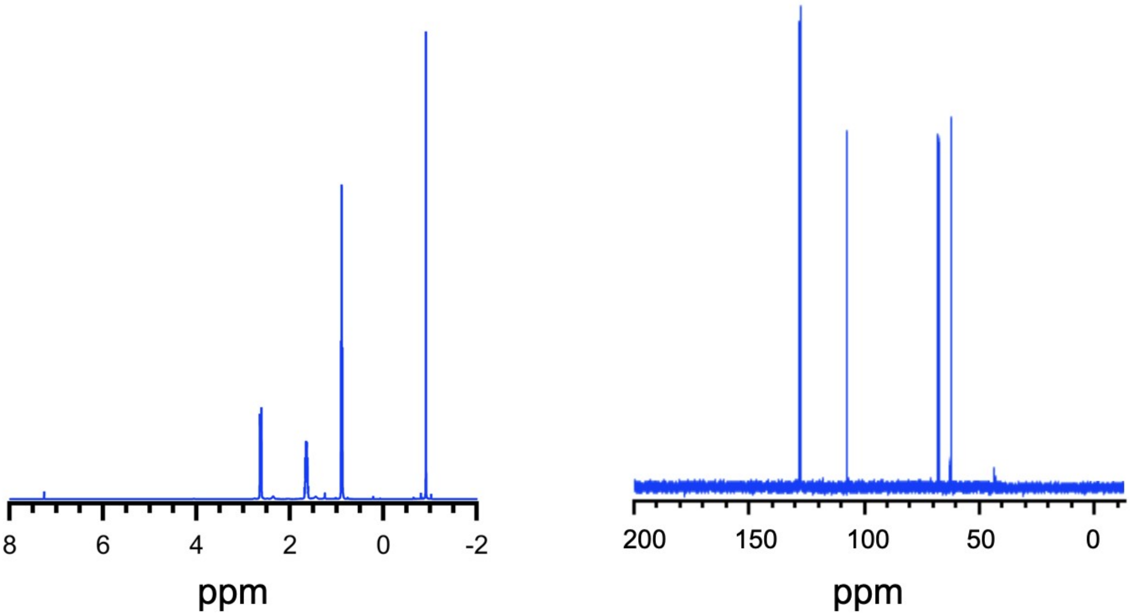


Figure S 1 Pr_3NAlMe_3: ^{1}H NMR (500 MHz, cdcl$_3$) δ 2.66 – 2.59 (m, 6H) $_3[CH_3CH_2C\underline{H_2}]NAl[CH_3]_3$, 1.70 – 1.59 (m, 6H) $_3[CH_3C\underline{H_2}CH_2]NAl[CH_3]_3$, 0.89 (t, J = 7.3 Hz, 9H) $_3[C\underline{H_3}CH_2CH_2]NAl[CH_3]_3$, -0.91 (s, 9H) $_3[CH_3CH_2CH_2]NAl[C\underline{H_3}]_3$. ^{13}C NMR (126 MHz, cdcl$_3$) δ 107.95 $_3[CH_3CH_2\underline{C}H_2]NAl[CH_3]_3$, 68.11$_3[CH_3\underline{C}H_2CH_2]NAl[CH_3]_3$, 62.87 $_3[\underline{C}H_3CH_2CH_2]NAl[CH_3]_3$, 43.62 $_3[CH_3CH_2CH_2]NAl[\underline{C}H_3]_3$.

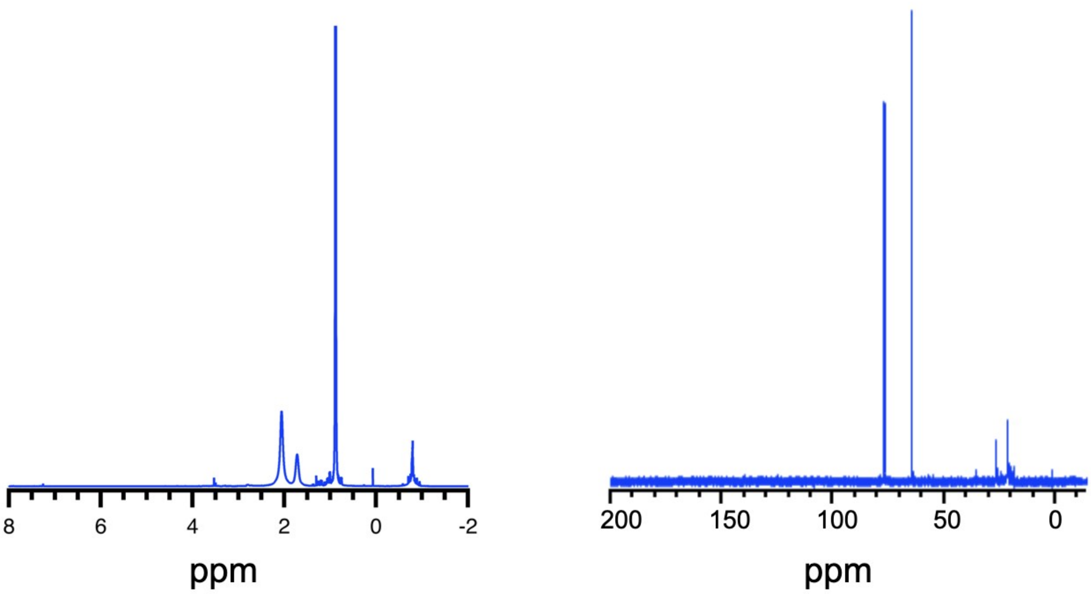


Figure S 2 ^{1}H NMR and ^{13}C NMR for iBu_3NAlEt_3: ^{1}H NMR (500 MHz, cd$_2$cl$_2$) δ 2.25 (b, 6H) $_3[(CH_3)_2CHC\underline{H_2}]NAl[CH_2CH_3]_3$, 1.86-1.83 (b, 3H) $_3[(CH_3)_2C\underline{H}CH_2]NAl[CH_2CH_3]_3$, 1.09 (t, J = 8.0 Hz, 9H) $_3[(CH_3)_2CHCH_2]NAl[CH_2C\underline{H_3}]_3$, 0.94 (d, J = 6.6 Hz, 18H) $_3[(C\underline{H_3})_2CHCH_2]NAl[CH_2CH_3]_3$, 0.26

(q, J = 8.0 Hz, 6H) $_3[(CH_3)_2CHCH_2]NAl[C\underline{H_2}CH_3]_3$. ^{13}C NMR (126 MHz, cd_2cl_2) δ 64.38 $_3[(CH_3)_2CH\underline{C}H_2]NAl[CH_2CH_3]_3$, 25.77 $_3[(CH_3)_2\underline{C}HCH_2]NAl[CH_2CH_3]_3$, 19.21 $_3[(CH_3)_2\underline{C}HCH_2]NAl[CH_2CH_3]_3$, 13.51 $_3[(\underline{C}H_3)_2CHCH_2]NAl[CH_2CH_3]_3$, 8.64 $_3[(CH_3)_2CHCH_2]NAl[CH_2\underline{C}H_3]_3$, 0.52 $_3[(CH_3)_2CHCH_2]NAl[\underline{C}H_2CH_3]_3$.

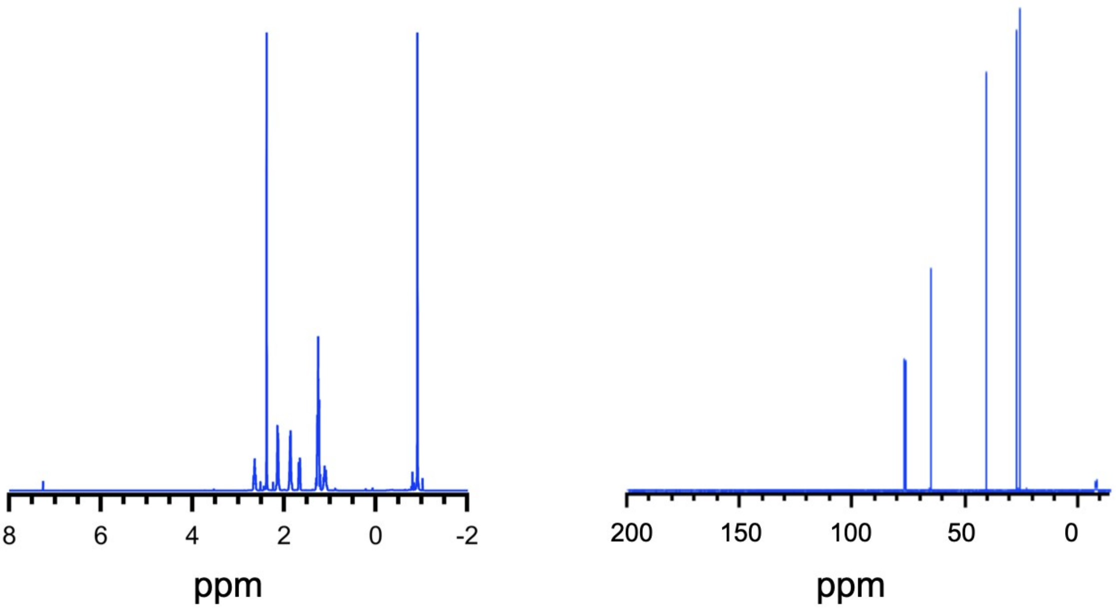


Figure S 3 ^{1}H NMR and ^{13}C NMR for $CyMe_2NAlMe_3$: ^{1}H NMR (500 MHz, $cdcl_3$) δ 2.70–2.58 (m, 1H) $_3[(CH_3)_2\underline{Cy}]NAl[CH_3]_3$, 2.38 (s, 6H), $_3[(C\underline{H_3})_2Cy]NAl[CH_3]_3$, 2.19-2.07 (m, 2H), 1.92-1.80 (m, 2H), 1.69-1.62 (m, 2H), and 1.35-1.04 (m, 6H) $_3[(CH_3)_2\underline{Cy}]NAl[CH_3]_3$, -0.92 (s, 9H) $_3[(CH_3)_2Cy]NAl[C\underline{H_3}]_3$. ^{13}C NMR (126 MHz, $cdcl_3$) δ 65.75, 41.08, 27.23 and 25.95, $_3[(CH_3)_2\underline{Cy}]NAl[CH_3]_3$ 25.91 $_3[(\underline{C}H_3)_2Cy]NAl[CH_3]_3$, -7.95 $_3[(CH_3)_2Cy]NAl[\underline{C}H_3]_3$.

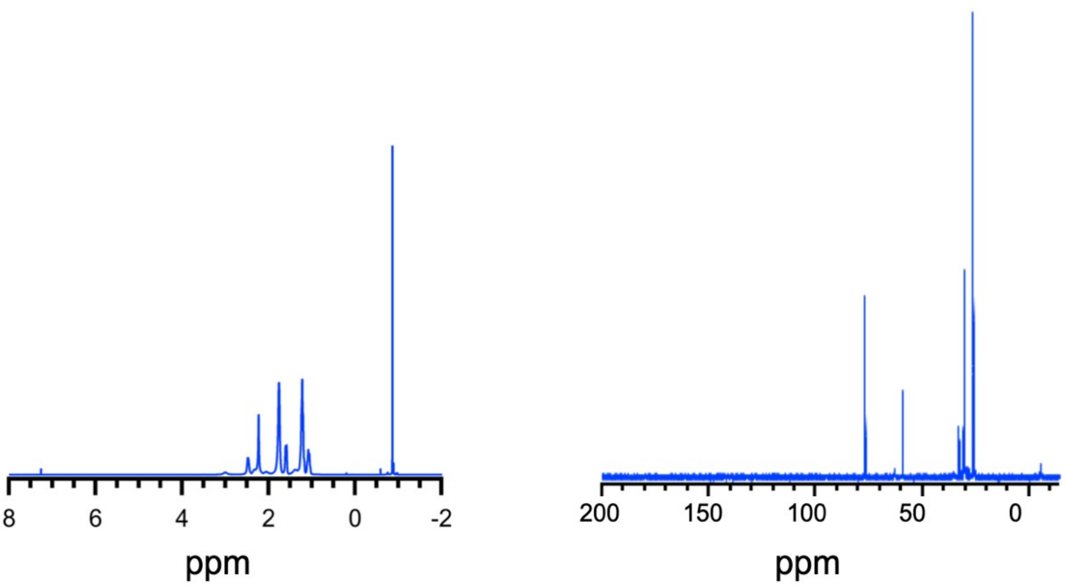


Figure S 4 ^{1}H NMR and ^{13}C NMR for $Cy_2MeNAlMe_3$: ^{1}H NMR (500 MHz, $cdcl_3$) δ 2.47 (m, 2H), 2.21 (s, 3H), and 1.98-1.03 (m, 12H) $_3[(CH_3)_2\underline{Cy}]NAl[CH_3]_3$, 0.87 (s, 9H) $_3[(CH_3)_2Cy]NAl[C\underline{H_3}]_3$. ^{13}C NMR

(126 MHz, cdcl$_3$) δ 63.13, 59.44, 32.68, and 30.70 $_3[(CH_3)_2\underline{Cy}]NAl[CH_3]_3$, 26.35 $_3[(\underline{C}H_3)_2Cy]NAl[CH_3]_3$, -5.05 $_3[(Cy)_2CH_3]NAl[\underline{C}H_3]_3$.

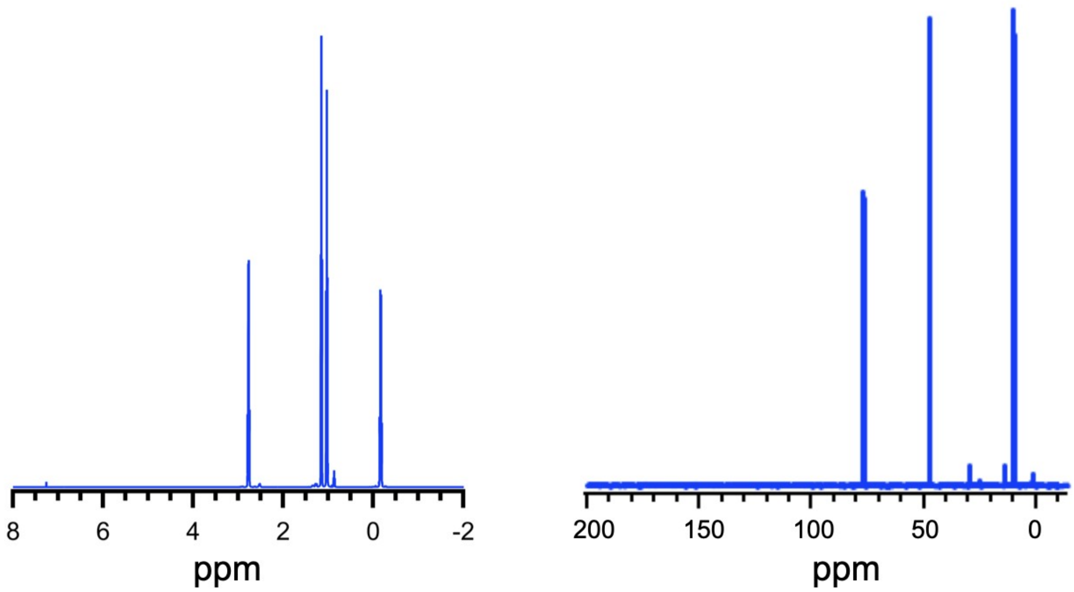


Figure S 5 ^{1}H NMR and ^{13}C NMR for Et_3NAlEt_3: ^{1}H NMR (500 MHz, cdcl$_3$) δ 2.77 (q, J = 7.3 Hz, 6H) $_3[CH_3C\underline{H_2}]NAl[CH_2CH_3]_3$, 1.15 (t, J = 7.3 Hz, 9H) $_3[C\underline{H_3}CH_2]NAl[CH_2CH_3]_3$, 1.03 (t, J = 8.1 Hz, 9H) $_3[CH_3CH_2]NAl[CH_2C\underline{H_3}]_3$, -0.17 (q, J = 8.1 Hz, 6H) $_3[CH_3CH_2]NAl[C\underline{H_2}CH_3]_3$. ^{13}C NMR (126 MHz, cdcl$_3$) δ 47.48 $_3[CH_3\underline{C}H_2]NAl[CH_2CH_3]_3$, 29.45 $[\underline{C}H_3CH_2]NAl[CH_2CH_3]_3$, 14.01 $[CH_3CH_2]NAl[CH_2\underline{C}H_3]_3$, 9.25 $[CH_3CH_2]NAl[\underline{C}H_2CH_3]_3$.

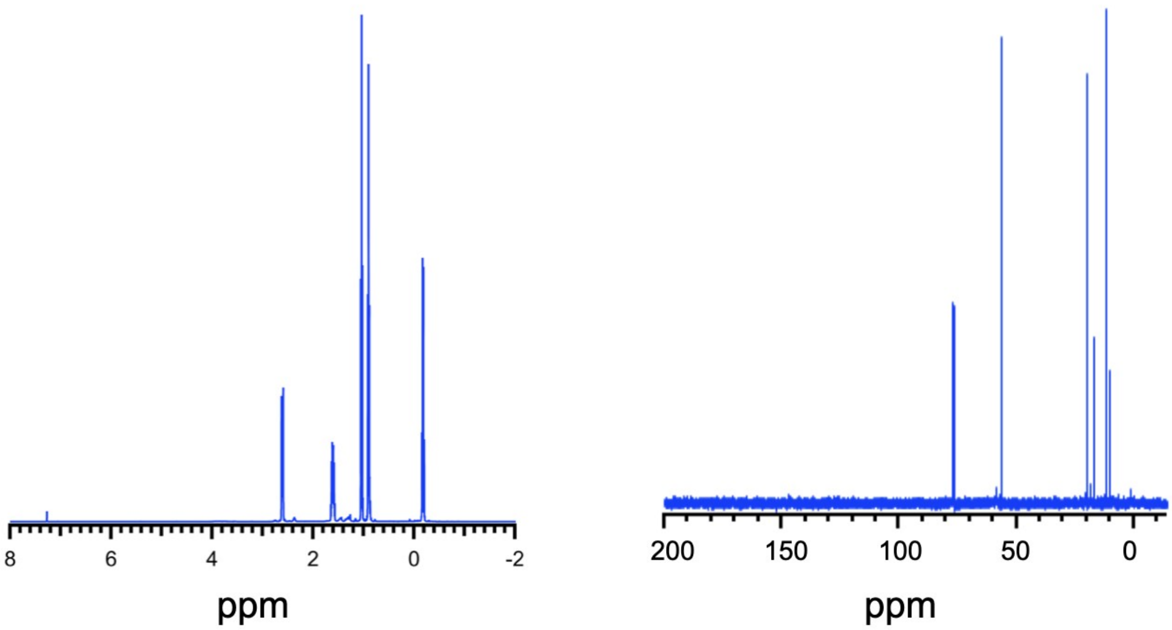


Figure S 6 ^{1}H NMR and ^{13}C NMR for Pr_3NAlEt_3: ^{1}H NMR (500 MHz, cdcl$_3$) δ 2.64 – 2.57 (m, 6H) $_3[CH_3CH_2C\underline{H_2}]NAl[CH_2CH_3]_3$, 1.66 – 1.55 (m, 6H) $_3[CH_3C\underline{H_2}CH_2]NAl[CH_2CH_3]_3$, 1.04 (t, *J* = 8.1 Hz, 9H) $_3[CH_3CH_2CH_2]NAl[CH_2C\underline{H_3}]_3$, 0.90 (m, 9H) $_3[C\underline{H_3}CH_2CH_2]NAl[CH_2CH_3]_3$, -0.18 (q, *J* = 8.1 Hz, 6H) $_3[CH_3CH_2CH_2]NAl[C\underline{H_2}CH_3]_3$. ^{13}C NMR (126 MHz, cdcl$_3$) δ 56.43 $_3[CH_3CH_2\underline{C}H_2]NAl[CH_2CH_3]_3$, 20.25 $_3[CH_3\underline{C}H_2CH_2]NAl[CH_2CH_3]_3$, 17.04 $_3[\underline{C}H_3CH_2CH_2]NAl[CH_2CH_3]_3$, 11.93 $_3[CH_3CH_2CH_2]NAl[\underline{C}H_2CH_3]_3$10.24 $CH_3CH_2CH_2NAl\underline{C}H_2CH_3$.

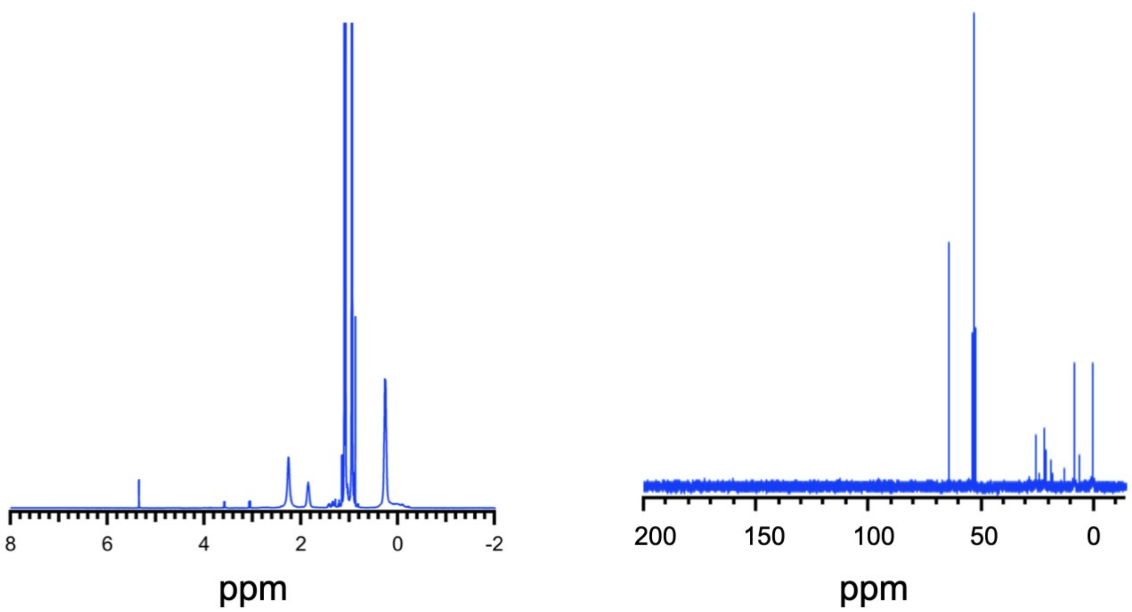


Figure S 7 ^{1}H NMR and ^{13}C NMR for iBu_3NAlEt_3: ^{1}H NMR (500 MHz, cd$_2$cl$_2$) δ 2.25 (b, 6H) $_3[(CH_3)_2CHC\underline{H_2}]NAl[CH_2CH_3]_3$, 1.86-1.83 (b, 3H) $_3[(CH_3)_2C\underline{H}CH_2]NAl[CH_2CH_3]_3$, 1.09 (t, *J* = 8.0 Hz, 9H) $_3[(CH_3)_2CHCH_2]NAl[CH_2C\underline{H_3}]_3$, 0.94 (d, *J* = 6.6 Hz, 18H) $_3[(C\underline{H_3})_2CHCH_2]NAl[CH_2CH_3]_3$, 0.26 (q, *J* = 8.0 Hz, 6H) $_3[(CH_3)_2CHCH_2]NAl[C\underline{H_2}CH_3]_3$. ^{13}C NMR (126 MHz, cd$_2$cl$_2$) δ 64.38 $_3[(CH_3)_2CH\underline{C}H_2]NAl[CH_2CH_3]_3$, 25.77 $_3[(CH_3)_2\underline{C}HCH_2]NAl[CH_2CH_3]_3$, 19.21 $_3[(CH_3)_2\underline{C}HCH_2]NAl[CH_2CH_3]_3$, 13.51 $_3[(\underline{C}H_3)_2CHCH_2]NAl[CH_2CH_3]_3$, 8.64 $_3[(CH_3)_2CHCH_2]NAl[CH_2\underline{C}H_3]_3$, 0.52 $_3[(CH_3)_2CHCH_2]NAl[\underline{C}H_2CH_3]_3$.

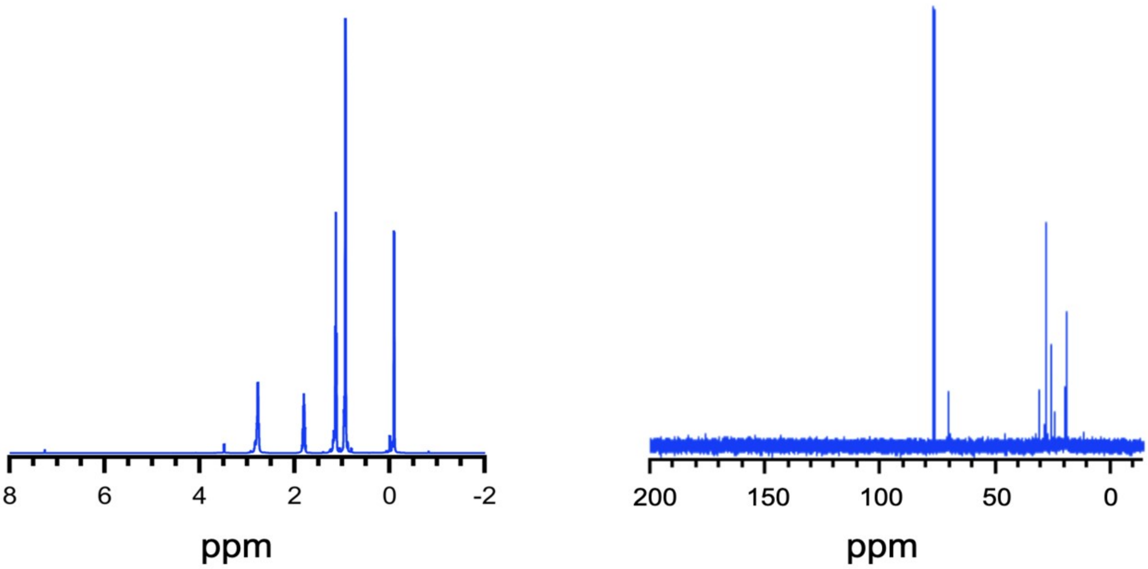


Figure S 8 ^{1}H NMR and ^{13}C NMR for $Et_3NAliBu_3$: ^{1}H NMR (500 MHz, $cdcl_3$) δ 2.80 (q, *J* = 7.3 Hz, 6H) $_3[CH_3C\underline{H_2}]NAl[CH_2CH(CH_3)_2]_3$, 1.80 (dq, *J* = 6.6, 6.8 Hz, 3H) $_3[CH_3CH_2]NAl[CH_2C\underline{H}(CH_3)_2]_3$, 1.13 (t, *J* = 7.3 Hz, 9H) $_3[C\underline{H_3}CH_2]NAl[CH_2CH(CH_3)_2]_3$, 0.93 (b, *J* = 6.5 Hz, 18H) $_3[CH_3CH_2]NAl[CH_2CH(C\underline{H_3})_2]_3$, -0.09 (d, *J* = 6.8 Hz, 6H) $_3[CH_3CH_2]NAl[C\underline{H_2}CH(CH_3)_2]_3$. ^{13}C NMR (126 MHz, $cdcl_3$) δ 47.90 $_3[CH_3\underline{C}H_2]NAl[CH_2CH(CH_3)_2]_3$, 30.96 $_3[CH_3CH_2]NAl[CH_2CH(\underline{C}H_3)_2]_3$, 28.37 $_3[CH_3CH_2]NAl[CH_2\underline{C}H(CH_3)_2]_3$, 25.51 $_3[CH_3CH_2]NAl[CH_2CH(CH_3)_2]_3$, 19.75 $_3[CH_3CH_2]NAl[\underline{C}H_2CH(CH_3)_2]_3$, 19.35 $_3[\underline{C}H_3CH_2]NAl[CH_2CH(CH_3)_2]_3$.

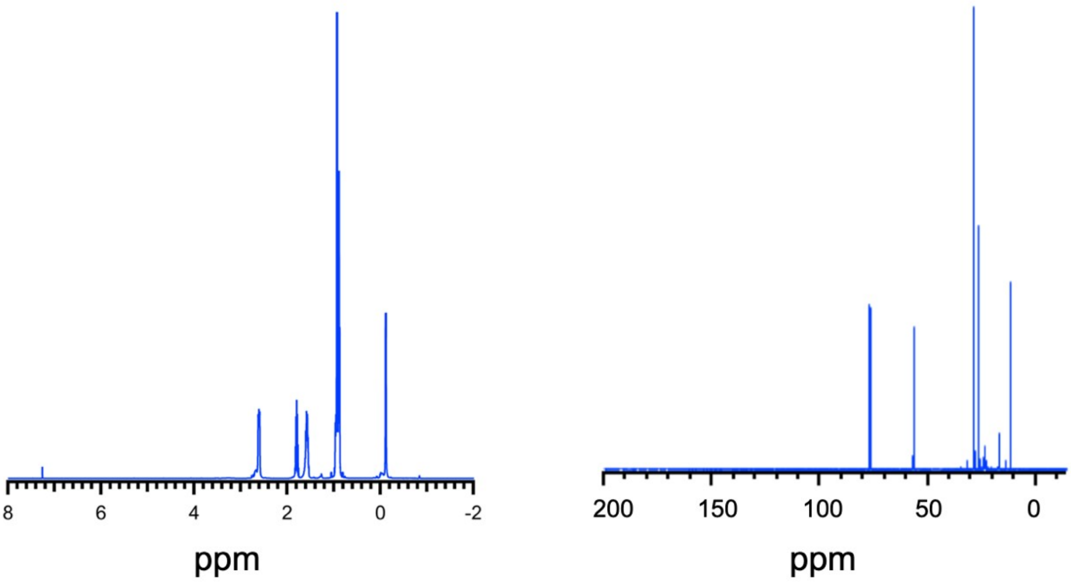


Figure S 9 ^{1}H NMR and ^{13}C NMR for $Pr_3NAliBu_3$: ^{1}H NMR (500 MHz, cdcl$_3$) δ 2.64–2.57 (m, 6H) ${}_3[CH_3CH_2C\underline{H_2}]NAl[CH_2CH(CH_3)_2]_3$, 1.79 (dh J = 13.1, 6.8 Hz, 3H) ${}_3[CH_3CH_2CH_2]NAl[CH_2C\underline{H}(CH_3)_2]_3$, 1.58 (m, 6H) ${}_3[CH_3C\underline{H_2}CH_2]NAl[CH_2CH(CH_3)_2]_3$, 0.93-0.91 (d, J = 13.1, 18H) ${}_3[CH_3CH_2CH_2]NAl[CH_2CH(C\underline{H_3})_2]_3$, 0.91-0.84 (d, J = 6.9 Hz, 9H) ${}_3[C\underline{H_3}CH_2CH_2]NAl[CH_2CH(CH_3)_2]_3$. -0.12 (d, J = 6.8 Hz, 6H) ${}_3[CH_3CH_2CH_2]NAl[C\underline{H_2}CH(CH_3)_2]_3$. ^{13}C NMR (126 MHz, cdcl$_3$) δ 56.74 ${}_3[CH_3CH_2CH_2]NAl[CH_2CH(\underline{C}H_3)_2]_3$, 29.05 ${}_3[CH_3CH_2\underline{C}H_2]NAl[CH_2CH(CH_3)_2]_3$, 26.61 ${}_3[CH_3CH_2CH_2]NAl[CH_2\underline{C}H(CH_3)_2]_3$, 24.02 ${}_3[CH_3CH_2CH_2]NAl[\underline{C}H_2CH(CH_3)_2]_3$, 17.12 ${}_3[CH_3\underline{C}H_2CH_2]NAl[CH_2CH(CH_3)_2]_3$, 11.76 ${}_3[\underline{C}H_3CH_2CH_2]NAl[CH_2CH(CH_3)_2]_3$.

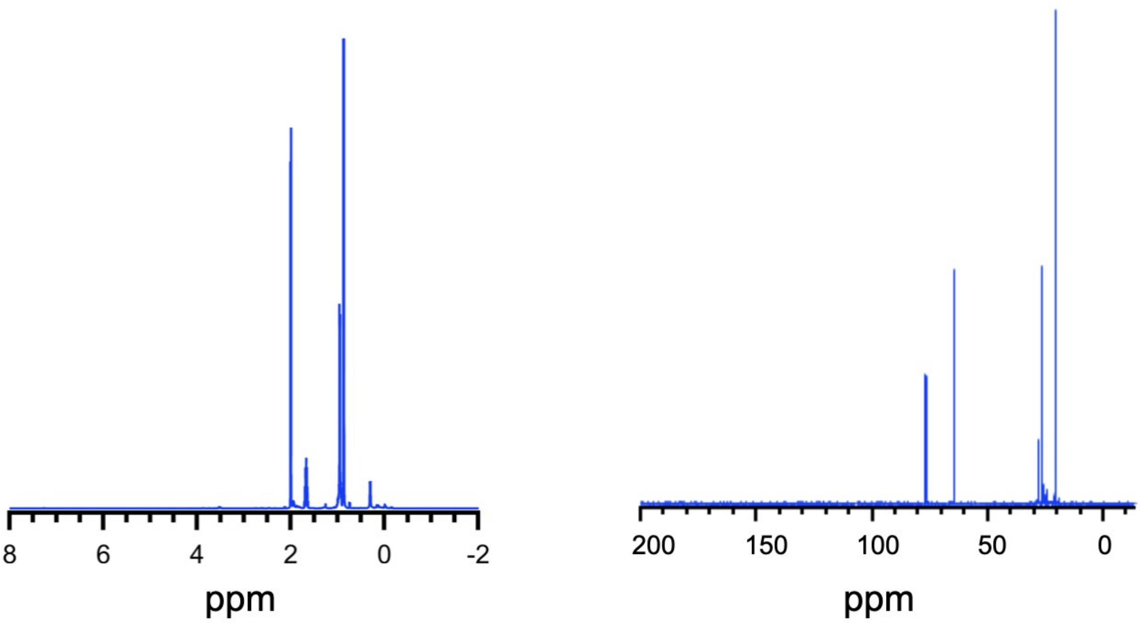


Figure S 10 ^{1}H NMR and ^{13}C NMR for $iBu_3NAliBu_3$: ^{1}H NMR (500 MHz, cdcl$_3$) δ 2.00 (d, J = 7.1 Hz, 6H) ${}_3[(CH_3)_2CHC\underline{H_2}]NAl[CH_2CH(CH_3)_2]_3$, 1.97–1.80 (m, 3H) ${}_3[(CH_3)_2C\underline{H}CH_2]NAl[CH_2CH(CH_3)_2]_3$, 1.68 (dq, J = 13.5, 6.6 Hz, 3H) ${}_3[(CH_3)_2CHCH_2]NAl[CH_2C\underline{H}(CH_3)_2]_3$, 1.04 – 0.91 (m, 18H) ${}_3[(C\underline{H_3})_2CHCH_2]NAl[CH_2CH(CH_3)_2]_3$, 0.87 (d, J = 6.6 Hz, 18H) ${}_3[(CH_3)_2CHCH_2]NAl[CH_2CH(C\underline{H_3})_2]_3$, 0.23 (d, J = 7.1 Hz, 6H) ${}_3[(CH_3)_2CHCH_2]NAl[C\underline{H_2}CH(CH_3)_2]_3$. ^{13}C NMR (126 MHz, cdcl$_3$) δ 64.90 ${}_3[(CH_3)_2CH\underline{C}H_2]NAl[CH_2CH(CH_3)_2]_3$, 28.30 ${}_3[(CH_3)_2\underline{C}HCH_2]NAl[CH_2CH(CH_3)_2]_3$, 26.66 ${}_3[(CH_3)_2CHCH_2]NAl[CH_2\underline{C}H(CH_3)_2]_3$, 21.14 ${}_3[(\underline{C}H_3)_2CHCH_2]NAl[CH_2CH(\underline{C}H_3)_2]_3$, 14.30 ${}_3[(CH_3)_2CHCH_2]NAl[\underline{C}H_2CH(CH_3)_2]_3$.

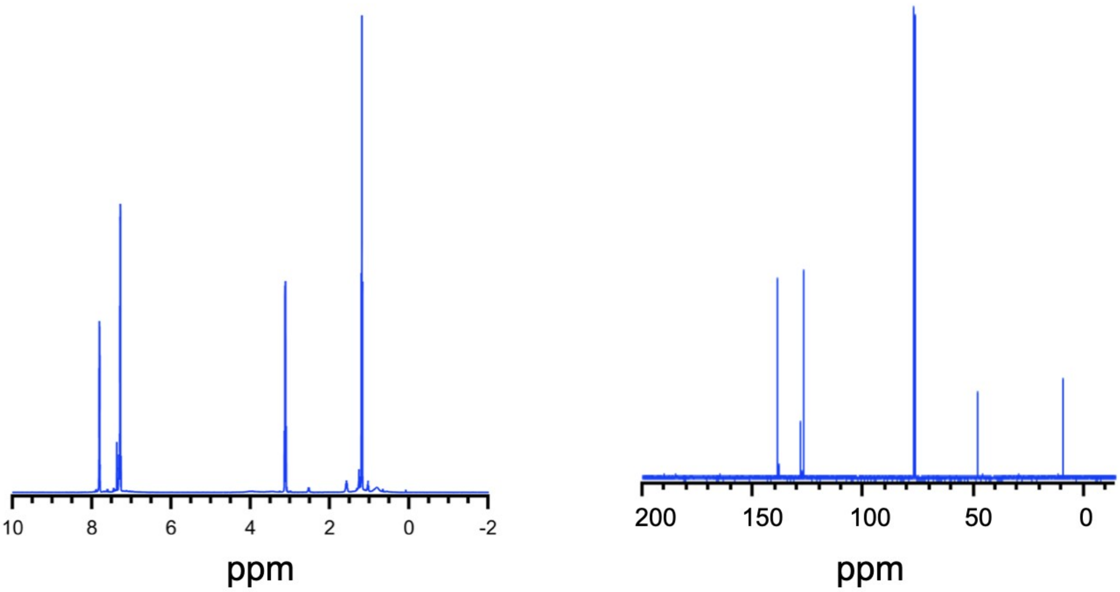


Figure S 11 ^{1}H NMR and ^{13}C NMR for Et_3NAlPh_3: ^{1}H NMR (500 MHz, cdcl$_3$) δ 6.25 – 6.20 (m, 6H) and 5.64 – 5.41 (m, 9H), 5.64 – 5.41 (m, 9H) $_3[CH_3CH_2]NAl[\underline{Ph}]_3$, 0.70 (q, *J* = 7.3 Hz, 6H) $_3[CH_3C\underline{H_2}]NAl[Ph]_3$, -1.22 (t, *J* = 7.3 Hz, 9H) $_3[C\underline{H_3}CH_2]NAl[Ph]_3$,. ^{13}C NMR (126 MHz, cdcl$_3$) δ 138.98, 128.33, 127.59, 127.31, 127.16, 127.06, 127.03 $_3[CH_3CH_2]NAl[\underline{Ph}]_3$, 47.90 $_3[CH_3\underline{C}H_2]NAl[Ph]_3$, 9.57 $_3[\underline{C}H_3CH_2]NAl[Ph]_3$.

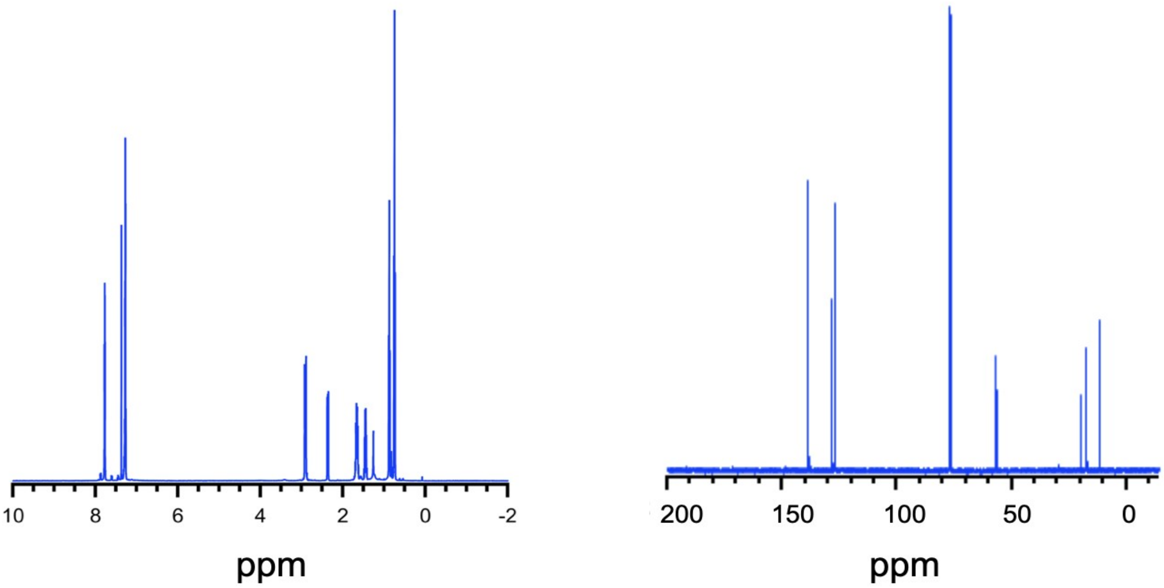


Figure S 12 ^{1}H NMR and ^{13}C NMR for Pr_3NAlPh_3: ^{1}H NMR (500 MHz, cdcl$_3$) δ 7.89 – 7.11 (m, 15H) $_3[CH_3CH_2CH_2]NAl[\underline{Ph}]_3$, 2.94 – 2.85 (m, 4H) and 2.44 – 2.31 (m, 2H) $_3[CH_3CH_2C\underline{H_2}]NAl[Ph]_3$, 1.73 – 1.60 (m, 4H), 1.50 – 1.39 (m, 2H) $_3[CH_3C\underline{H_2}CH_2]NAl[Ph]_3$, 0.95 – 0.80 (m, 3H) and 0.75 (t, *J* = 7.2 Hz, 6H) $_3[C\underline{H_3}CH_2CH_2]NAl[Ph]_3$. ^{13}C NMR (126 MHz, cdcl$_3$) δ 138.93, 138.29, 137.94, 128.33, 127.59, 127.31, 127.16, 127.06, 127.03 $_3[CH_3CH_2CH_2]NAl[\underline{Ph}]_3$, 47.90 $_3[CH_3CH_2\underline{C}H_2]NAl[Ph]_3$, 11.67$_3[CH_3\underline{C}H_2CH_2]NAl[Ph]_3$, 9.30 $_3[\underline{C}H_3CH_2CH_2]NAl[Ph]_3$.

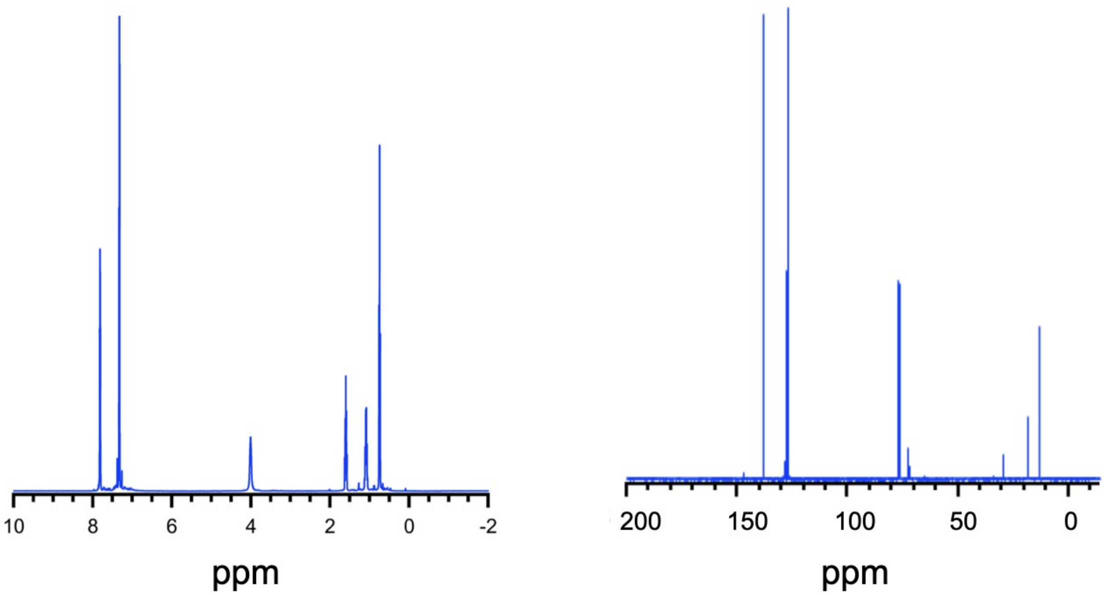


Figure S 13 ^{1}H NMR and ^{13}C NMR for iBu_3NAlPh_3: ^{1}H NMR (500 MHz, $cdcl_3$) δ 7.84 – 7.80 (m, 6H) and 7.38 – 7.29 (m, 9H) $_3[(CH_3)_2CHCH_2]NAl[\underline{Ph}]_3$, 4.01 (d, J = 10.5 Hz, 3H) $_3[(CH_3)_2C\underline{H}CH_2]NAl[Ph]_3$, 1.75 – 1.41 (m, 6H) $_3[(CH_3)_2CHC\underline{H_2}]NAl[Ph]_3$, 1.10-0.56 (m, 18H). ^{13}C NMR (126 MHz, $cdcl_3$) δ 138.29, 127.61, 127.46, 127.36, 127.17, 126.93 $_3[(CH_3)_2CHCH_2]NAl[\underline{Ph}]_3$, 72.41$_3[(CH_3)_2CH\underline{C}H_2]NAl[Ph]_3$, 29.76 $_3[(CH_3)_2\underline{C}HCH_2]NAl[Ph]_3$, 18.15 $_3[(\underline{C}H_3)_2CHCH_2]NAl[Ph]_3$.

Kinetic Data

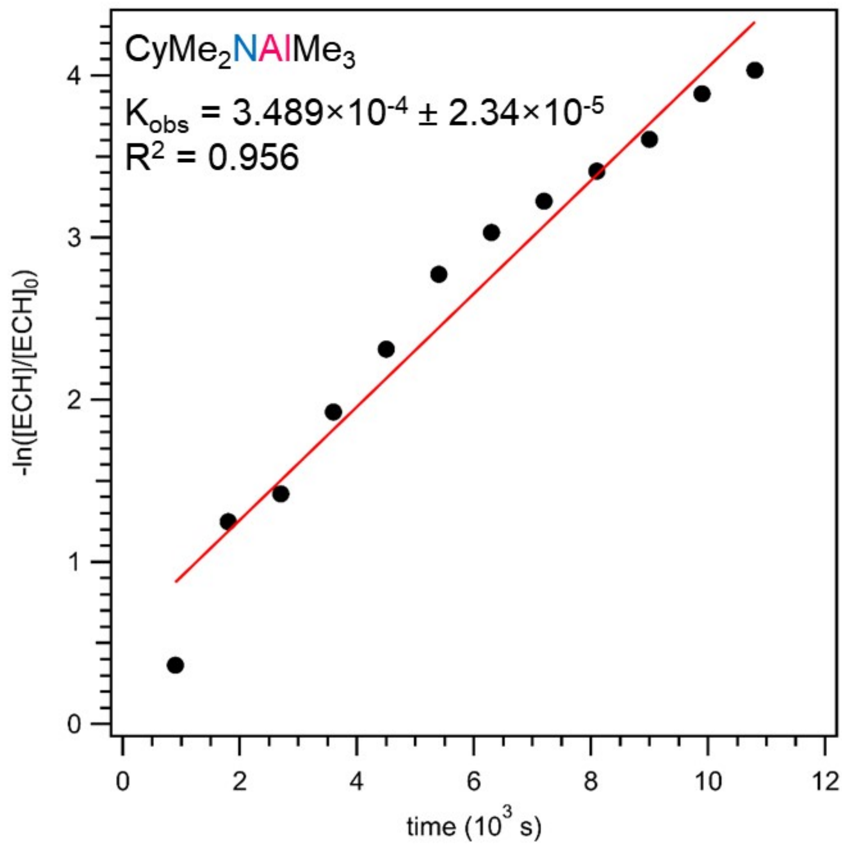


Figure S 14. Plot of $-\ln([ECH]/[ECH]_0)$ as a function of time for catalyst $CyMe_2NAlMe_3$. The reaction was monitored for three hours with ^1H NMR spectroscopy and conversion was determined from integration of the resonances associated with the monomer peaks compared to the total integral of the monomer and polymer. The slope of a linear fit to the data is the observed rate constant (k_{obs}). For this catalyst, k_{obs} was determined to be $3.489\times10^{-4}\pm2.34\times10^{-5}$ with an R^2 of 0.956 indicating a good fit to the data.

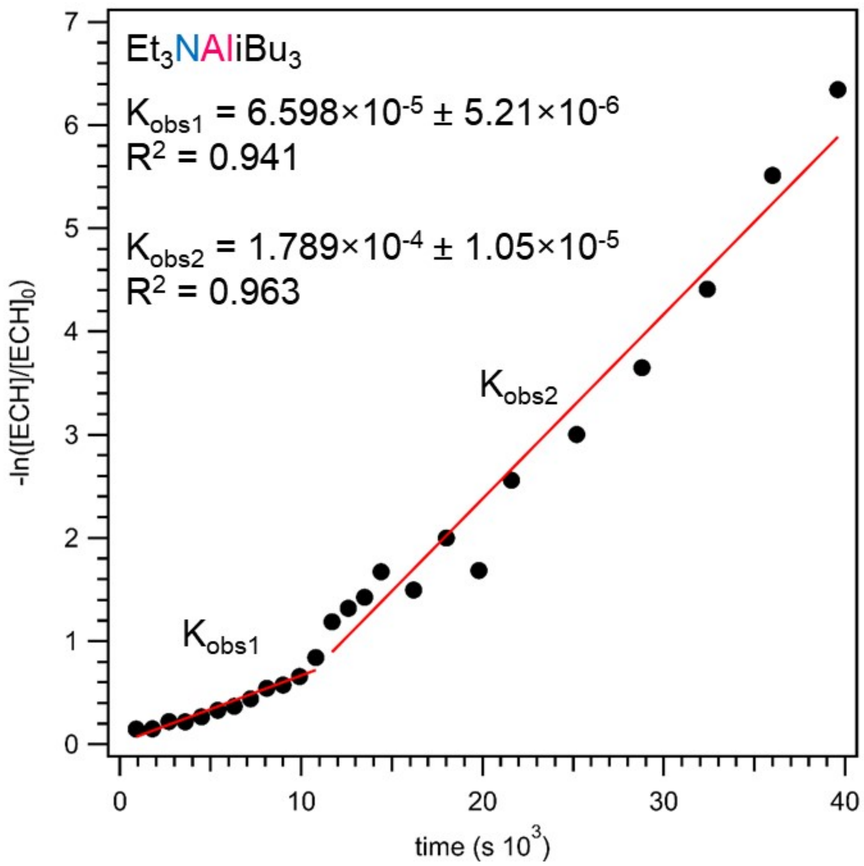


Figure S 15. Kinetic data for $Et_3NAliBu_3$.

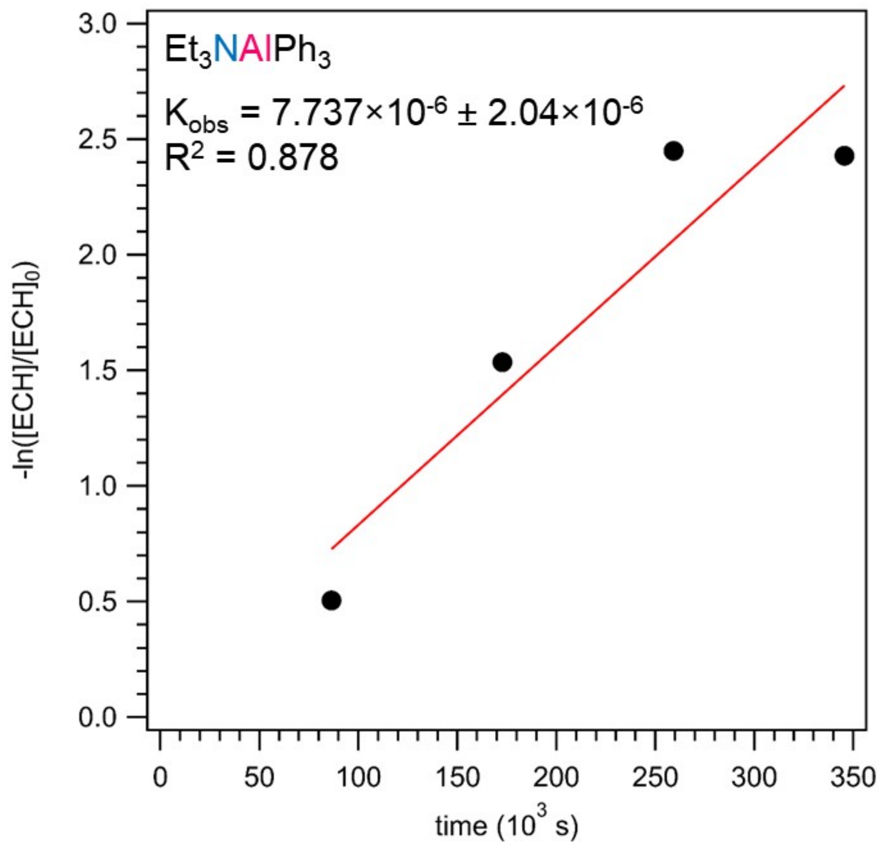


Figure S 16. Kinetic data for Et_3NAlPh_3

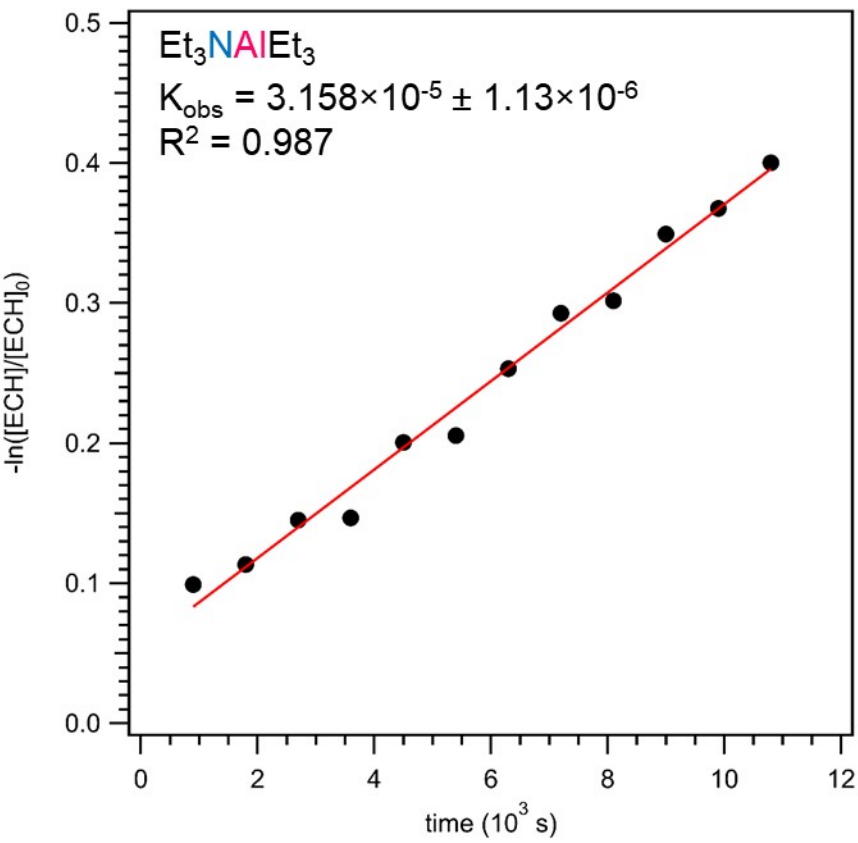


Figure S 17. Kinetic data for Et_3NAlEt_3.

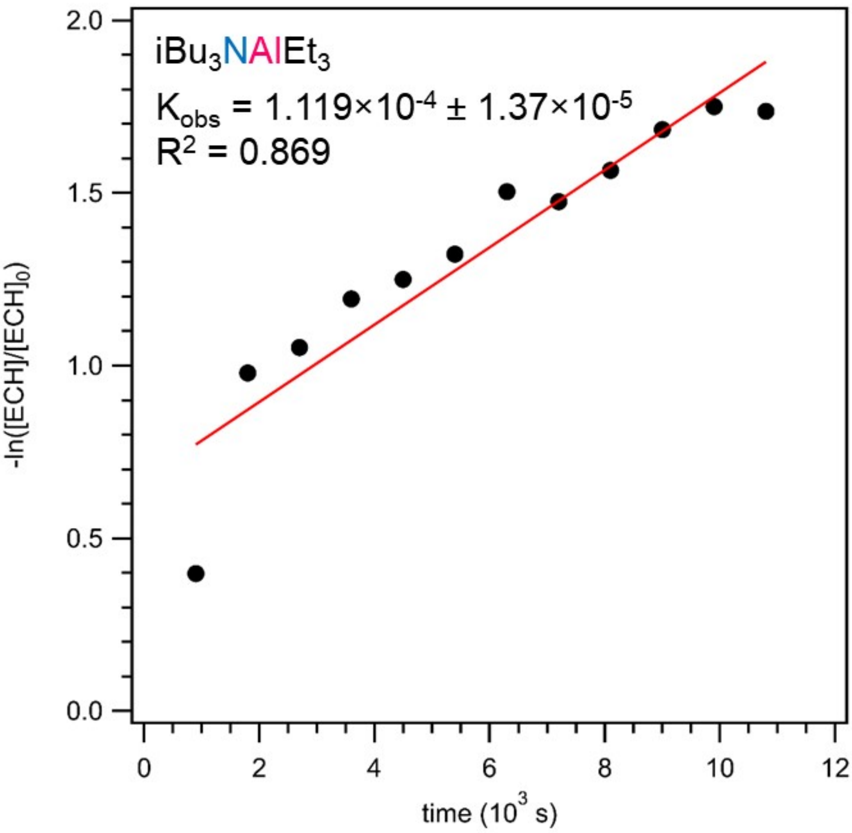


Figure S 18. Kinetic data for iBu_3NAlEt_3

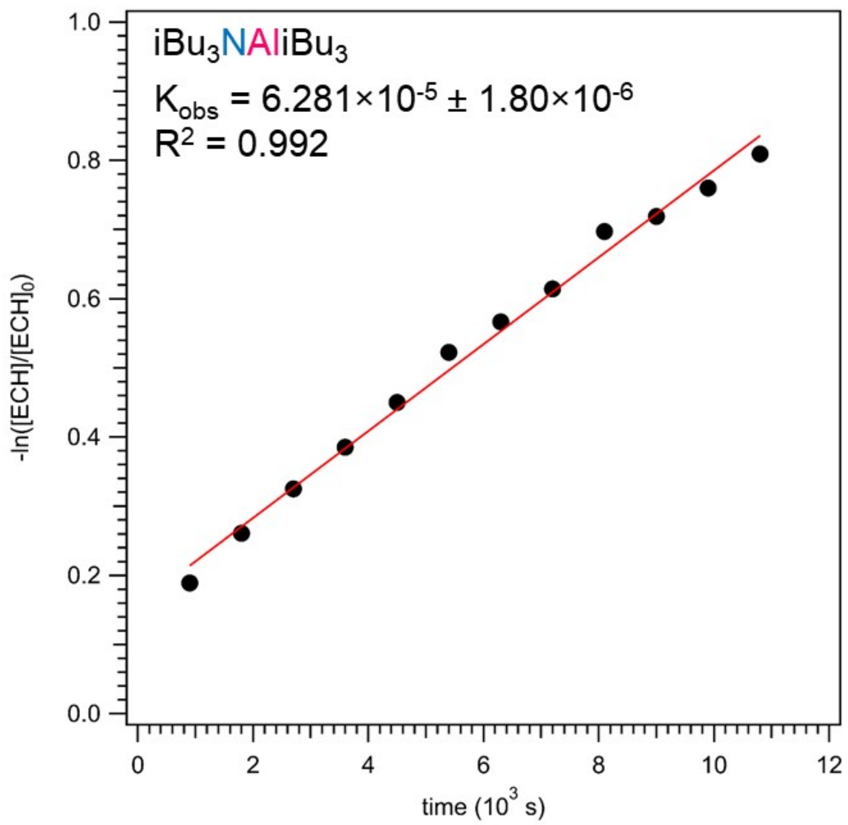


Figure S 19. Kinetic data for $iBu_3NAliBu_3$

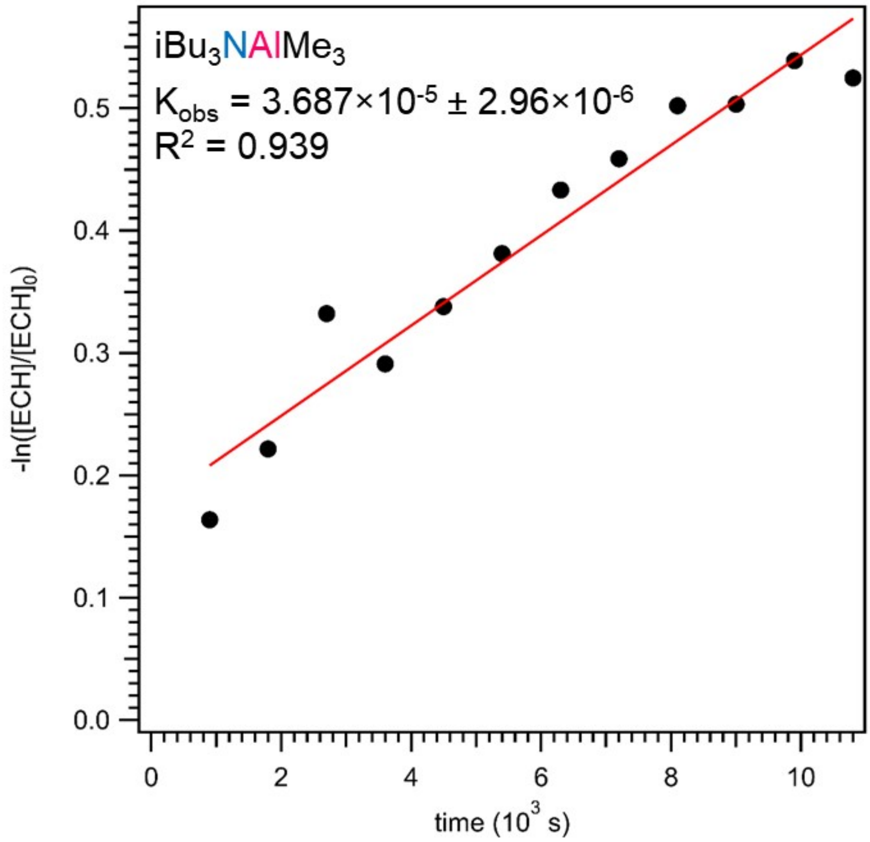


Figure S 20. Kinetic data for iBu_3NAlMe_3**.**

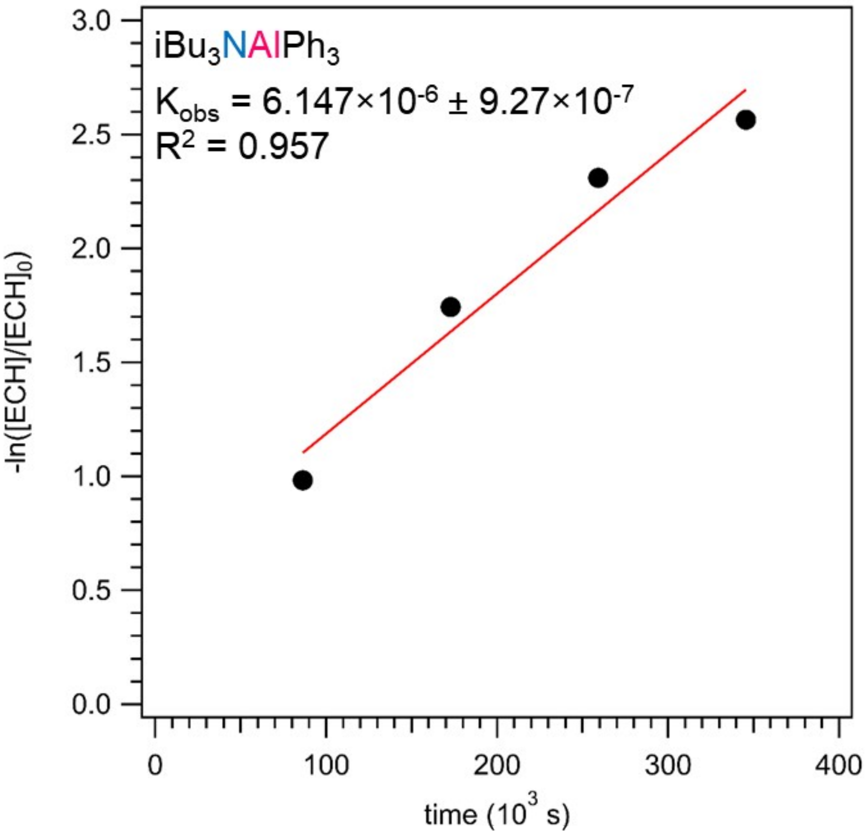


Figure S 21. Kinetic data for iBu_3NAlPh_3

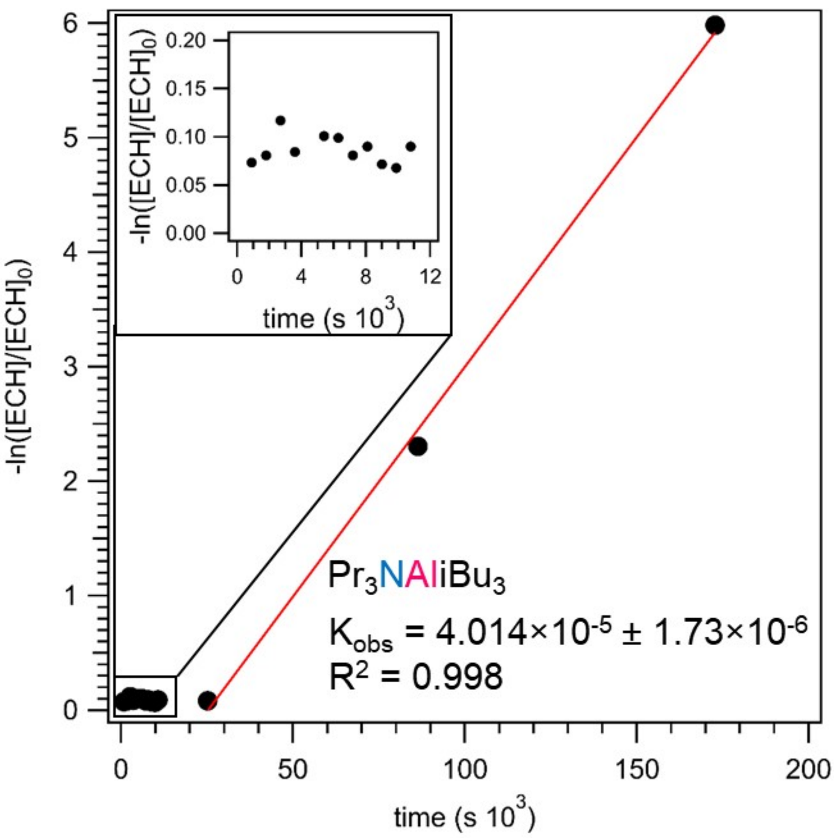


Figure S 22. Kinetic data for $Pr_3NAliBu_3$

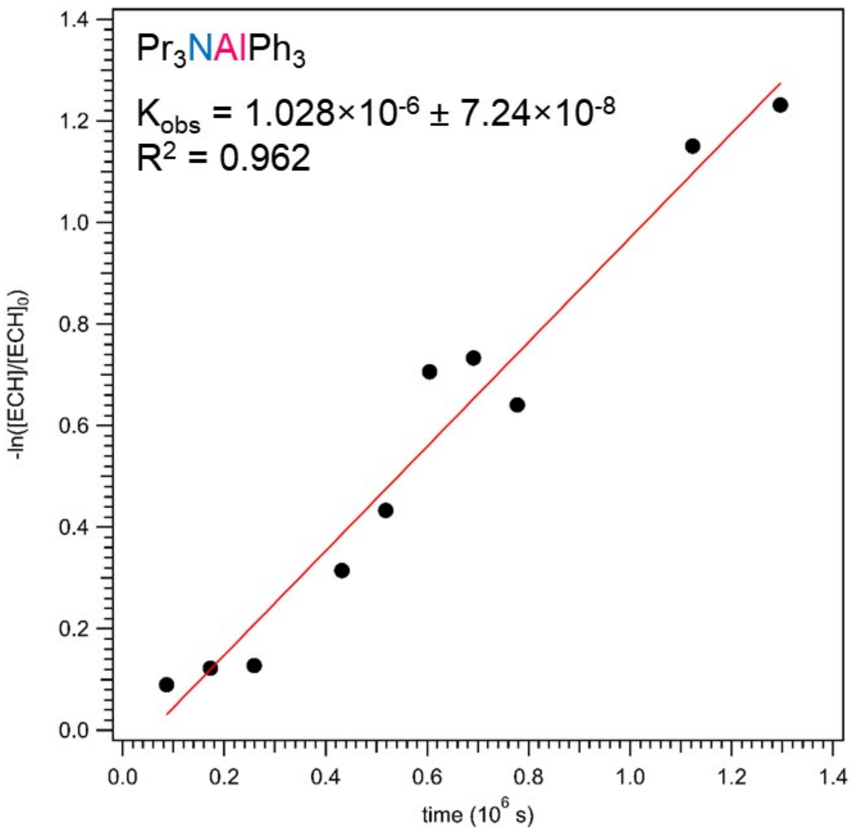


Figure S 23. Kinetic data for Pr_3NAlPh_3

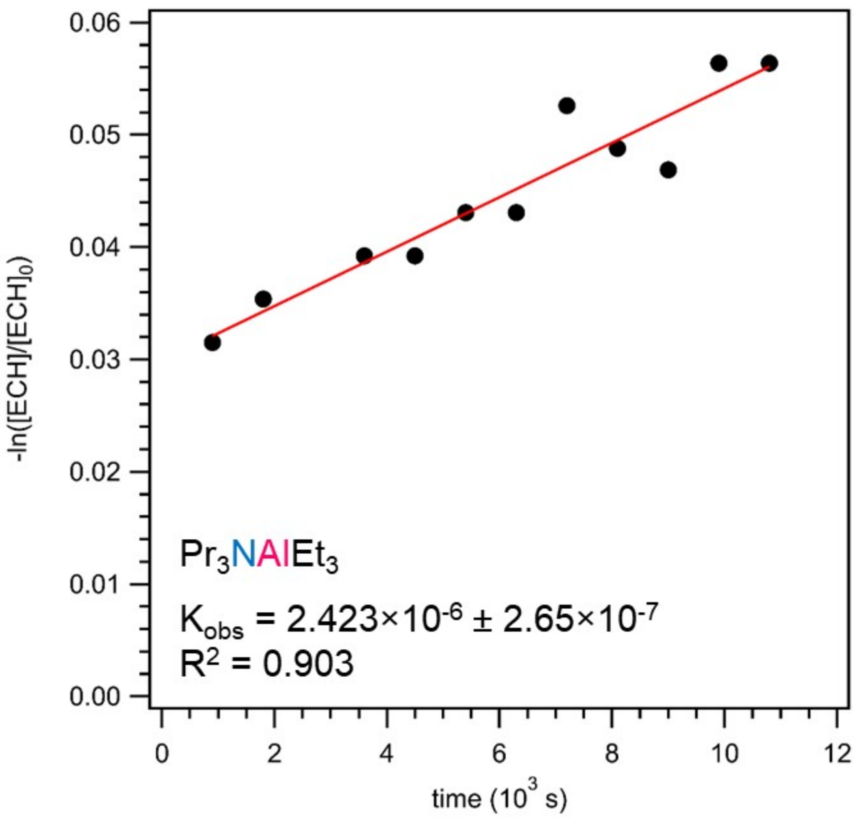


Figure S 24. Kinetic data for Pr_3NAlEt_3

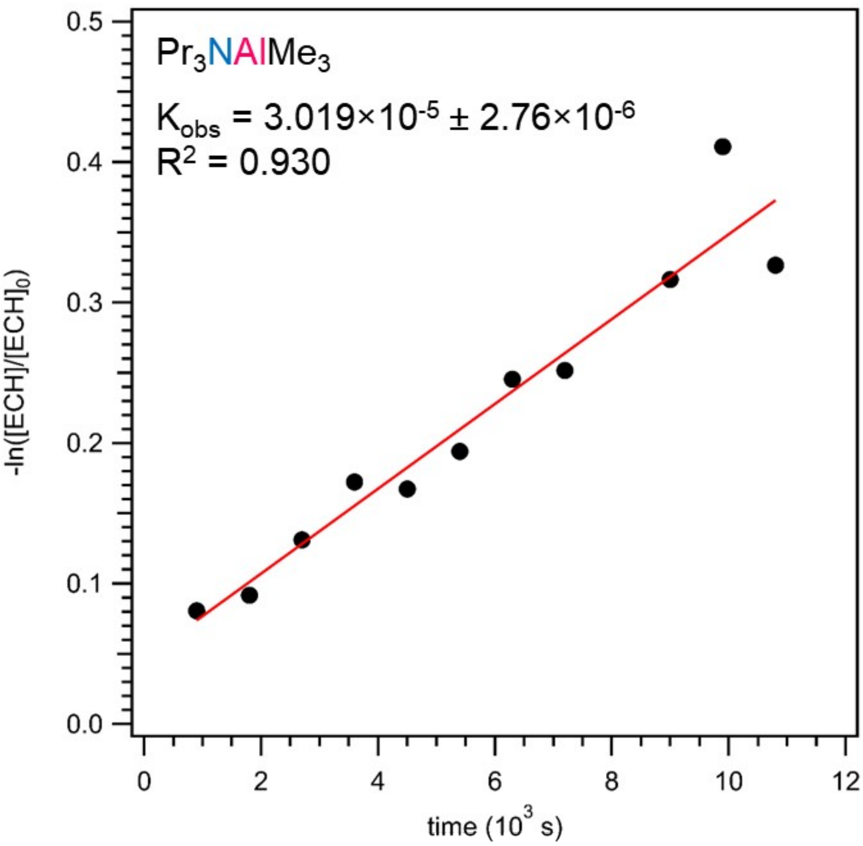


Figure S 25. Kinetic data for Pr_3NAlMe_3.

Size exclusion chromatography data.

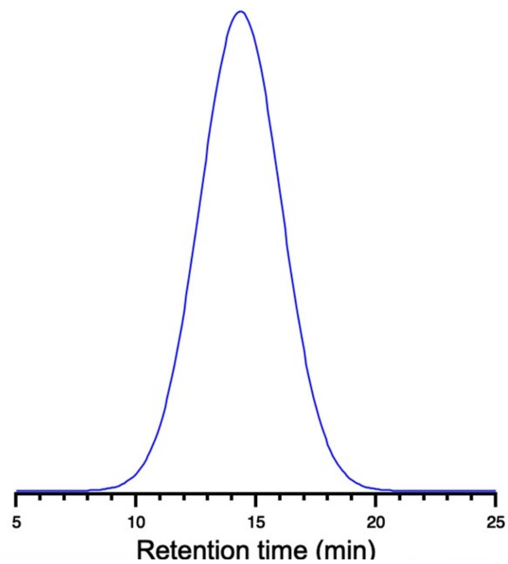


Figure S 26 SEC trace of targeted 30k BnSPECH. the M_n is determined to be 30.1 kg/mol with Đ of 3.30 using Pr_3NAlMe_3

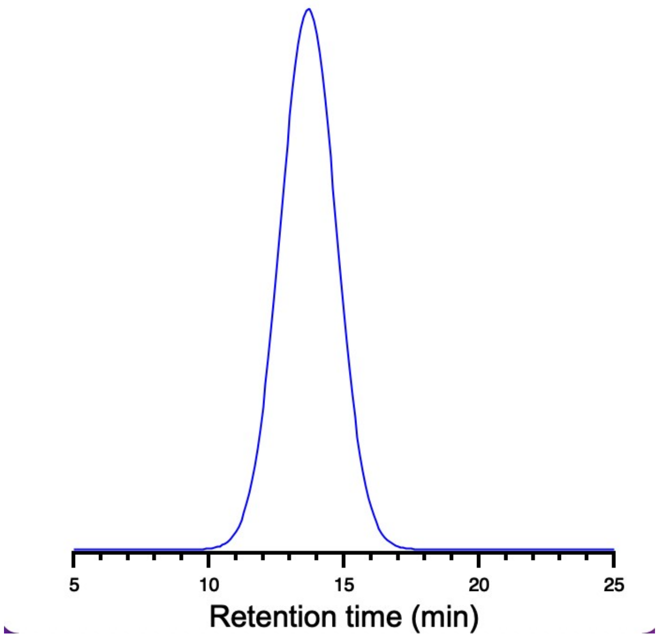


Figure S 27 SEC trace of targeted 30k BnSPECH. the M_n is determined to be 36.6 kg/mol with Đ of 1.51 using Pr_3NAlMe_3

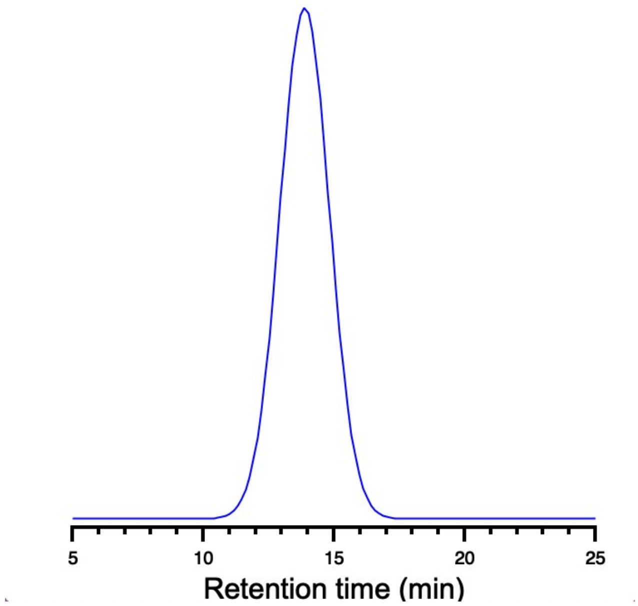


Figure S 28 SEC trace of targeted 30k BnSPECH. the M_n is determined to be 32.9 kg/mol with Đ of 2.52 using $CyMe_2NAlMe_3$

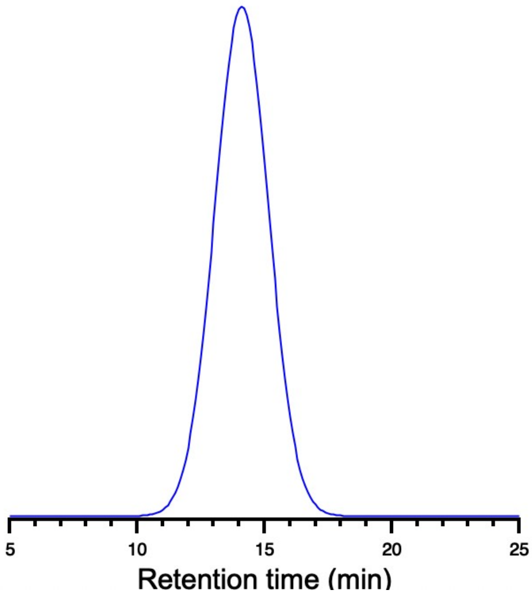


Figure S 29 SEC trace of targeted 30k BnSPECH. the M_n is determined to be 27.8 kg/mol with Đ of 1.21 using Et_3NAlEt_3

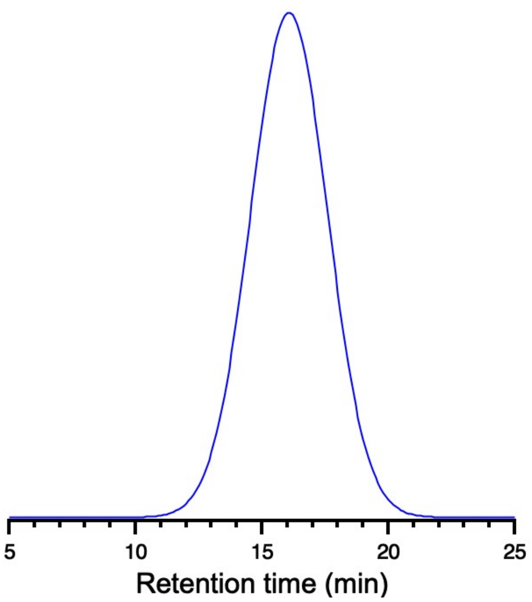


Figure S 30 SEC trace of targeted 30k BnSPECH. the M_n is determined to be 28.4 kg/mol with Đ of 2.78 using $(Pr)_3NAl(Et)_3$

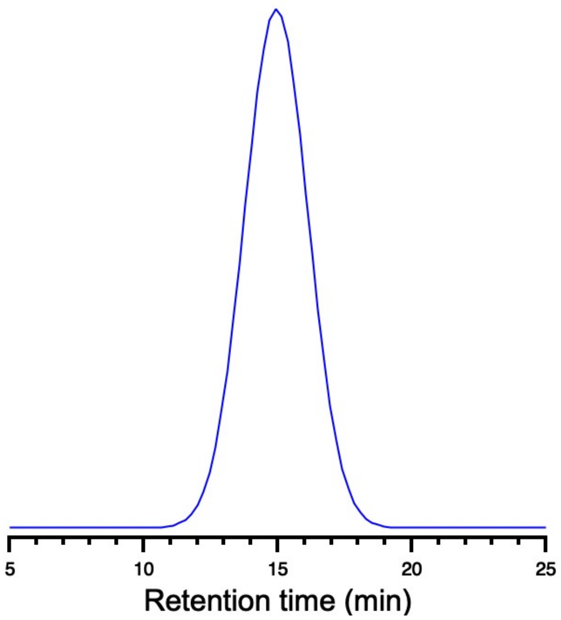


Figure S 31 SEC trace of targeted 30k BnSPECH. the M_n is determined to be 35.9 kg/mol with Đ of 2.47 using $(iBu)_3NAl(Et)_3$

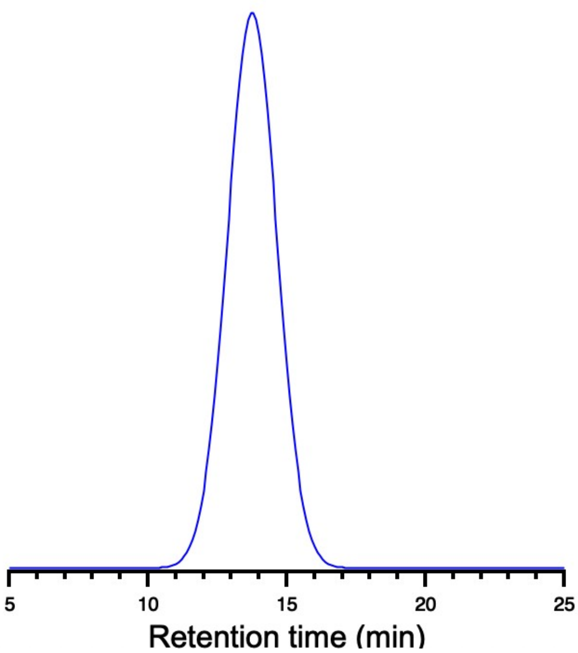


Figure S 32 SEC trace of targeted 30k BnSPECH. the M_n is determined to be 36.1 kg/mol with Đ of 2.66 using $(Et)_3NAl(iBu)_3$

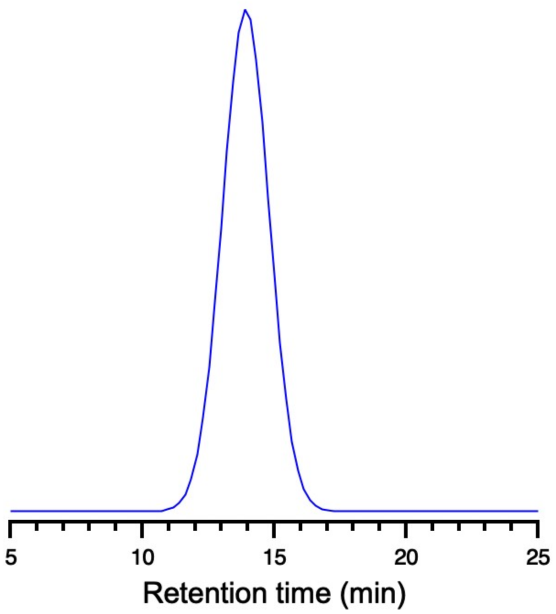


Figure S 33 SEC trace of targeted 30k BnSPECH. the M_n is determined to be 33.2 kg/mol with Đ of 1.18 using $(Pr)_3NAl(iBu)_3$

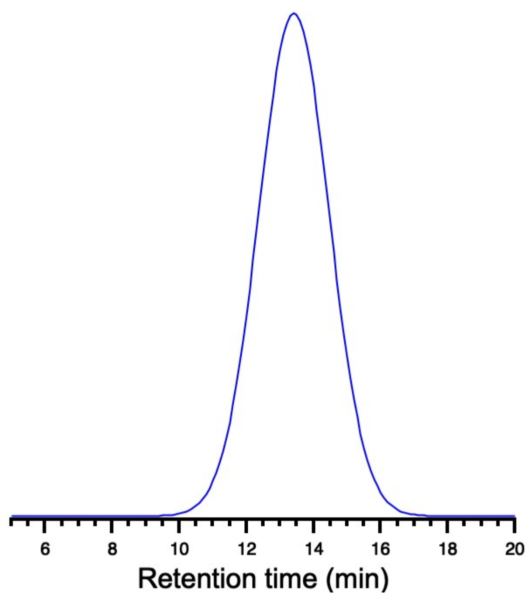


Figure S 34 SEC trace of targeted 30k BnSPECH. the M_n is determined to be 27.3 kg/mol with Đ of 1.82 using $(iBu)_3NAl(iBu)_3$

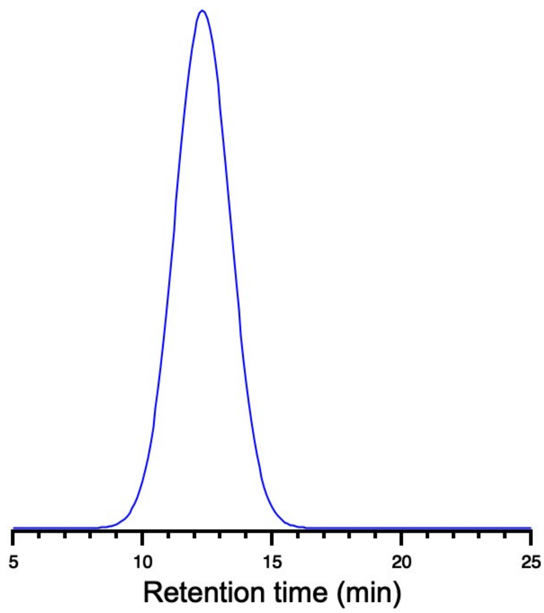


Figure S 35 SEC trace of targeted 30k BnSPECH. the M_n is determined to be 37.9 kg/mol with Đ of 1.66 using $(Et)_3NAl(ph)_3$

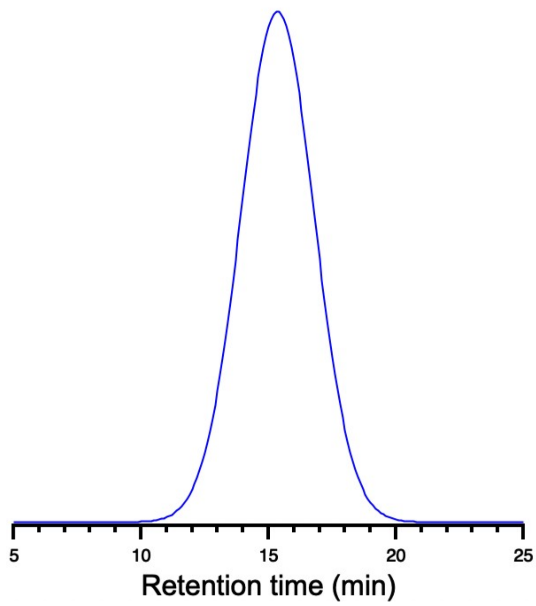


Figure S 36 SEC trace of targeted 30k BnSPECH. the M_n is determined to be 26.5 kg/mol with Đ of 1.45 using $(Pr)_3NAl(ph)_3$

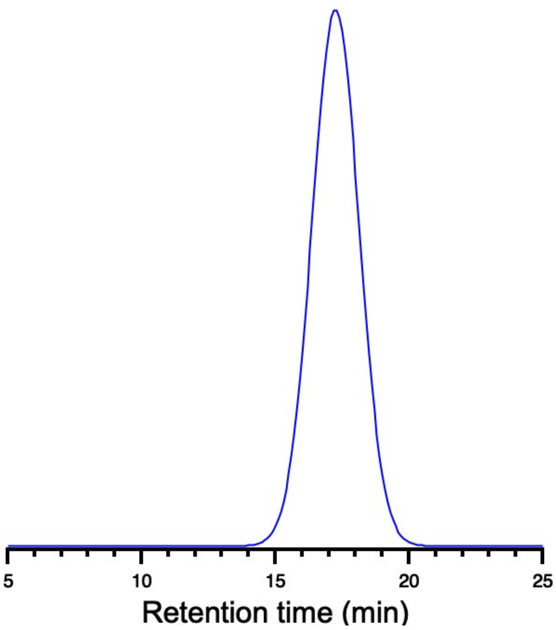


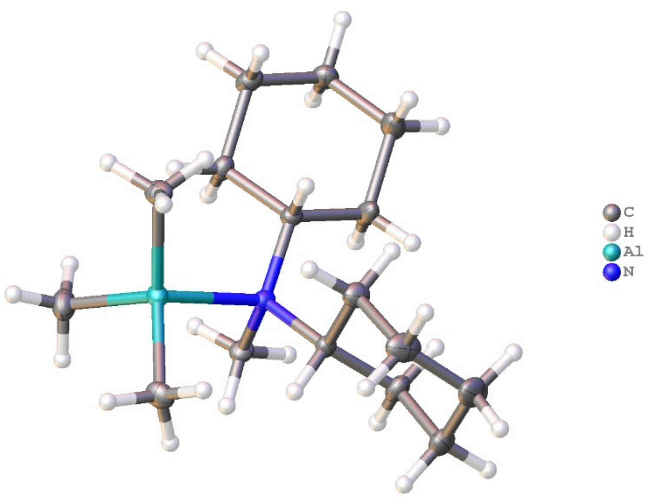
Figure S 37 SEC trace of targeted 30k BnSPECH. the M_n is determined to be 22.4 kg/mol with Đ of 1.09 using $(iBu)_3NAl(ph)_3$

Crystallography Data

$MeCy_2NAlMe_3$

Crystal structure from crystal mounted from the cold stage and glove bag.

Crystal Data and Experimental



Experimental. Single colourless block crystals of **MeCy2NAlMe3** used as received. A suitable crystal with dimensions 0.40 × 0.28 × 0.15 mm^3 was selected and solvent frozen at liquid nitrogen on nylon loop on a XtaLAB Synergy, Dualflex, HyPix diffractometer. The crystal was kept at a steady T = 100.00(10) K during data collection. The structure was solved with the **ShelXT** (Sheldrick, 2015) solution program using dual methods and by using **Olex2** (Dolomanov et al., 2009) as the graphical interface. The model was refined with **ShelXL** 2018/3 (Sheldrick, 2015) using full matrix least squares minimisation on $\boldsymbol{F}^2$.

Crystal Data. $C_{16}H_{34}AlN$, M_r = 267.42, orthorhombic, $P2_12_12_1$ (No. 19), a = 7.25651(12) Å, b = 14.5203(2) Å, c = 16.1412(2) Å, α = β = γ = 90°, V = 1700.75(5) Å^3, T = 100.00(10) K, Z = 4, Z' = 1, μ(Cu Kα) = 0.906, 6653 reflections measured, 3177 unique (R_{int} = 0.0565) which were used in all calculations. The final wR_2 was 0.0976 (all data) and R_1 was 0.0375 (I > 2(I)).

Compound	**RF220c**
CCDC	1986283
Formula	$C_{16}H_{34}AlN$
$D_{calc.}$/ g cm^{-3}	1.044
μ/mm^{-1}	0.906
Formula Weight	267.42
Colour	colourless
Shape	block
Size/mm^3	0.40×0.28×0.15
T/K	100.00(10)
Crystal System	orthorhombic
Flack Parameter	-0.04(2)
Hooft Parameter	-0.04(2)
Space Group	$P2_12_12_1$
a/Å	7.25651(12)
b/Å	14.5203(2)
c/Å	16.1412(2)
α/°	90
β/°	90
γ/°	90
V/Å^3	1700.75(5)
Z	4
Z'	1
Wavelength/Å	1.54184
Radiation type	Cu K_α
Θ_{min}/°	4.095
Θ_{max}/°	77.052
Measured Refl's.	6653
Ind't Refl's	3177
Refl's with I > 2(I)	3041
R_{int}	0.0565
Parameters	168
Restraints	0
Largest Peak	0.290
Deepest Hole	-0.431
GooF	1.030
wR_2 (all data)	0.0976
wR_2	0.0962
R_1 (all data)	0.0433
R_1	0.0375

Structure Quality Indicators

Reflections:	d min (Cu) 0.79	I/σ 15.8	Rint 5.65%	complete 100% (IUCr) 94%
Refinement:	Shift -0.001	Max Peak 0.3	Min Peak -0.4	GooF 1.030
	Flack -.04(2)			

A colourless block-shaped crystal with dimensions 0.40×0.28×0.15 mm^3 was solvent frozen at liquid nitrogen on nylon loop. Data were collected using a a XtaLAB Synergy, Dualflex, HyPix diffractometer equipped with an Oxford Cryosystems low-temperature device, operating at T = 100.00(10) K.

Data were measured using □ scans of 0.5° per frame for 0.1 s using Cu Kα radiation (micro-focus sealed X-ray tube, 50 kV, 1 mA). The total number of runs and images was based on the strategy calculation from the program **CrysAlisPro** (Rigaku, V1.171.40.69a, 2020). The actually achieved resolution was Θ = 77.052.

Cell parameters were retrieved using the **CrysAlisPro** (Rigaku, V1.171.40.69a, 2020) software and refined using **CrysAlisPro** (Rigaku, V1.171.40.69a, 2020) on 4459 reflections, 67 % of the observed reflections. Data reduction was performed using the **CrysAlisPro** (Rigaku, V1.171.40.69a, 2020) software which corrects for Lorentz polarization. The final completeness is 100.00 out to 77.052 in Θ CrysAlisPro 1.171.40.69a (Rigaku Oxford Diffraction, 2020) Numerical absorption correction based on gaussian integration over a multifaceted crystal model Empirical absorption correction using spherical harmonics, implemented in SCALE3 ABSPACK scaling algorithm.

The structure was solved in the space group $P2_12_12_1$ (# 19) by using dual methods using the ShelXT (Sheldrick, 2015) structure solution program. The structure was refined by Least Squares using version 2014/6 of **XL** (Sheldrick, 2008) incorporated in **Olex2** (Dolomanov et al., 2009). All non-hydrogen atoms were refined anisotropically. Hydrogen atom positions were calculated geometrically and refined using the riding model, except for the hydrogen atom on the non-carbon atom(s) which were found by difference Fourier methods and refined isotropically when data permits.

CCDC 1986283 contains the supplementary crystallographic data for this paper. The data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/structures.

There is a single molecule in the asymmetric unit, which is represented by the reported sum formula. In other words: Z is 4 and Z' is 1.

The Flack parameter was refined to -0.04(2). Determination of absolute structure using Bayesian statistics on Bijvoet differences using the Olex2 results in -0.04(2). Note: The Flack parameter is used to determine chirality of the crystal studied, the value should be near 0, a value of 1 means that the stereochemistry is wrong and the model should be inverted. A value of 0.5 means that the crystal consists of a racemic mixture of the two enantiomers.

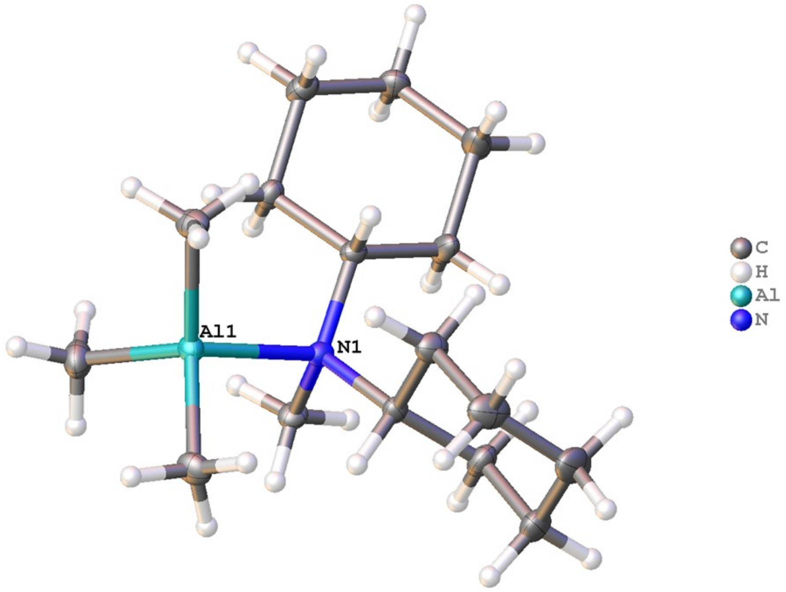


Figure S 38

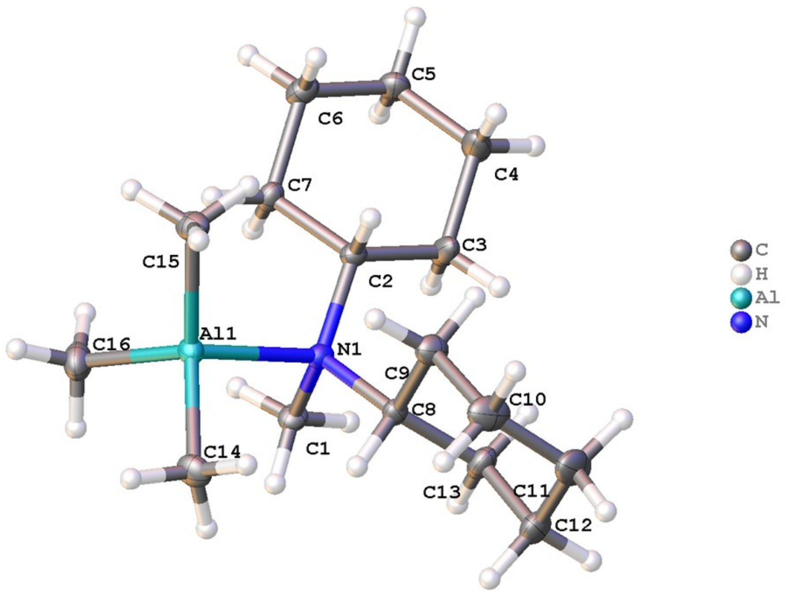


Figure S 39:

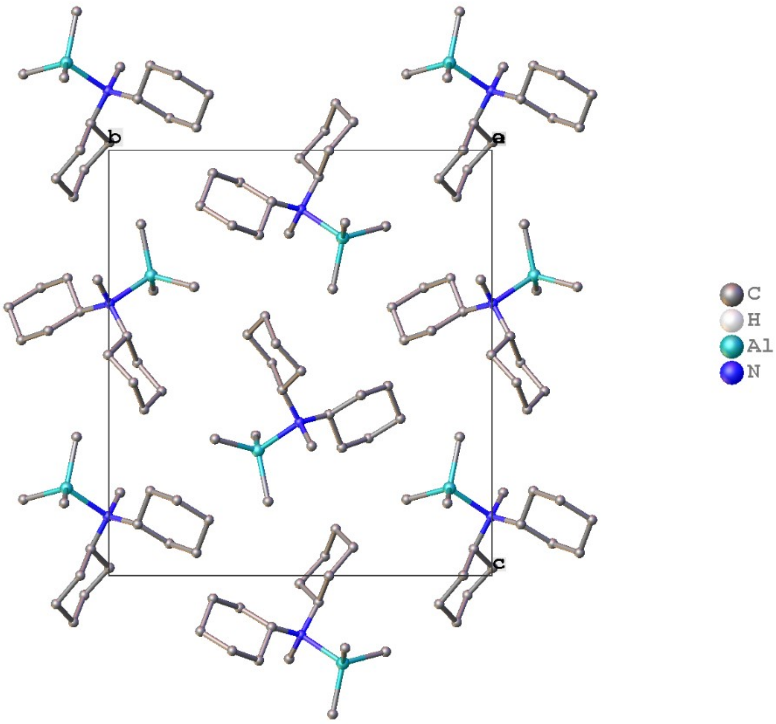
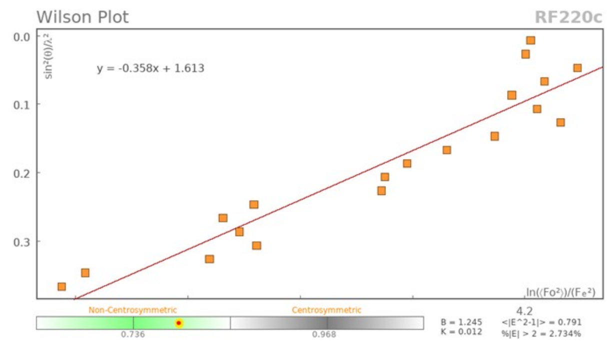
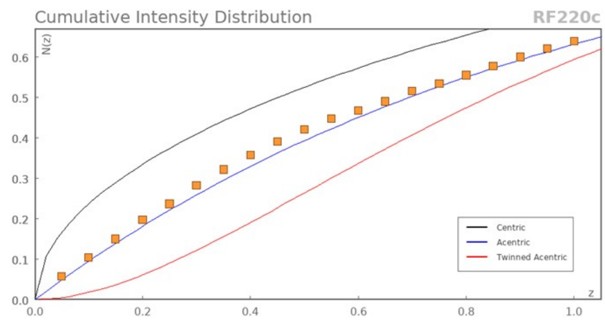
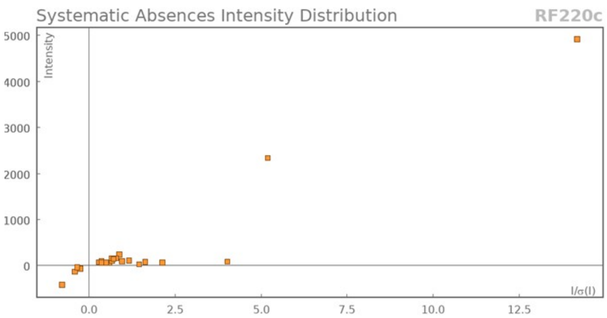


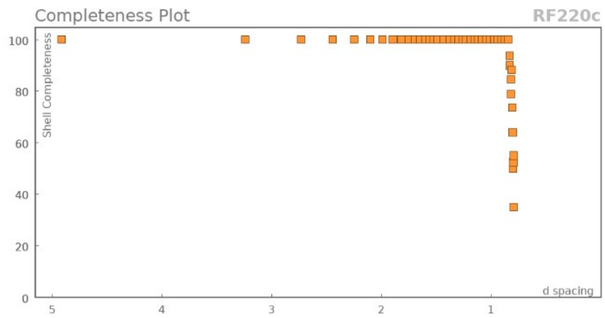
Figure S 40: Packing diagram of **MeCy2NAlMe3**.

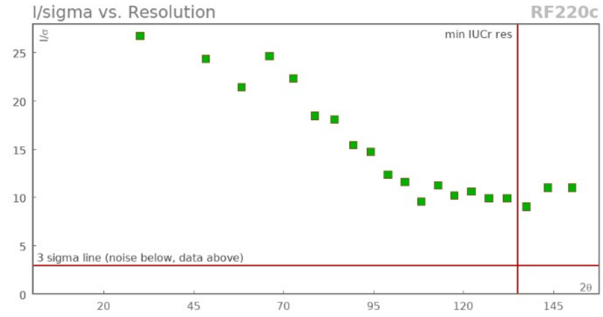
Data Plots: Diffraction Data



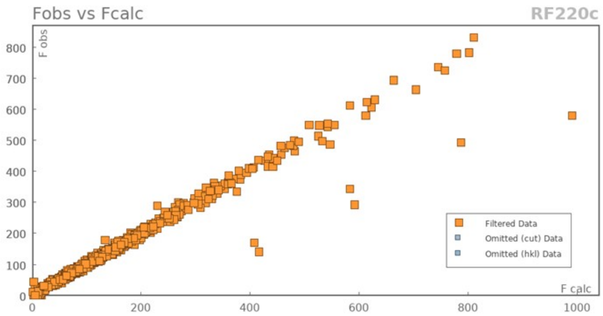


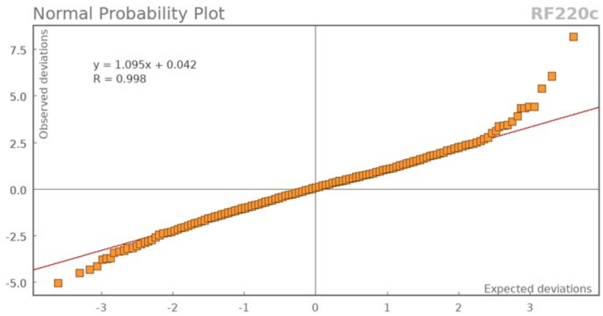






Data Plots: Refinement and Data





Reflection Statistics

Total reflections (after filtering)	6679	Unique reflections	3177
Completeness	0.885	Mean I/σ	15.66
hkl_{max} collected	(8, 17, 17)	hkl_{min} collected	(-3, -18, -20)
hkl_{max} used	(8, 18, 20)	hkl_{min} used	(-8, 0, 0)
Lim d_{max} collected	100.0	Lim d_{min} collected	0.77
d_{max} used	16.14	d_{min} used	0.79
Friedel pairs	479	Friedel pairs merged	0
Inconsistent equivalents	9	R_{int}	0.0565
R_{sigma}	0.0634	Intensity transformed	0
Omitted reflections	0	Omitted by user (OMIT hkl)	0
Multiplicity	(3899, 946, 230, 47, 2)	Maximum multiplicity	8
Removed systematic absences	26	Filtered off (Shel/OMIT)	0

Images of the Crystal on the Diffractometer

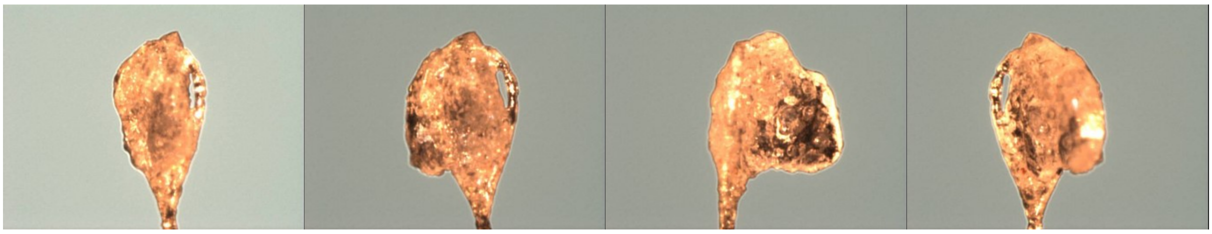


Table 1: Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for **MeCy2NAlMe3**. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{ij}.

Atom	x	y	z	U_{eq}
Al1	3151.1(8)	6107.2(4)	7057.3(4)	15.80(18)

Atom	x	y	z	U_{eq}
N1	4428(2)	5021.2(12)	6396.5(10)	13.9(4)
C1	5944(3)	4706.6(15)	6953.4(13)	16.9(4)
C2	3088(3)	4247.5(14)	6209.3(12)	14.8(4)
C3	3903(3)	3418.1(16)	5756.0(15)	26.0(5)
C4	2410(4)	2715.8(18)	5539.1(15)	28.6(6)
C5	1376(3)	2391.6(16)	6308.7(14)	21.8(5)
C6	587(3)	3220.0(16)	6767.9(14)	20.7(5)
C7	2088(3)	3917.0(15)	6990.7(12)	17.5(4)
C8	5266(3)	5471.5(14)	5627.4(13)	15.3(4)
C9	3788(3)	5746.9(17)	5005.0(13)	21.9(5)
C10	4599(4)	6374.7(19)	4334.4(15)	30.5(6)
C11	6239(4)	5922(2)	3906.3(15)	33.8(6)
C12	7684(3)	5640.3(19)	4541.4(14)	26.4(5)
C13	6879(3)	4985.5(16)	5187.3(13)	22.5(5)
C14	4603(3)	7227.0(15)	6788.4(15)	22.7(5)
C15	529(3)	6164.2(16)	6704.3(14)	21.3(5)
C16	3460(3)	5841.9(18)	8257.3(14)	26.8(5)

Table 2: Anisotropic Displacement Parameters (×10[4]) for **MeCy2NAlMe3**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2} \times U_{11}+ ... +2hka^* \times b^* \times U_{12}]$

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Al1	14.5(3)	17.3(3)	15.6(3)	-2.4(3)	-0.4(2)	0.9(3)
N1	13.3(8)	15.1(8)	13.2(7)	2.1(7)	-0.4(7)	0.0(7)
C1	13.1(10)	20.7(10)	17.0(10)	1.6(8)	-1.3(8)	1.9(8)
C2	13.0(9)	16.9(9)	14.6(9)	0.5(8)	0.1(8)	-2.0(8)
C3	24.7(12)	21.0(12)	32.2(12)	-12.4(10)	13.4(10)	-7.8(10)
C4	34.3(13)	25.3(12)	26.3(11)	-9.6(10)	10.0(11)	-13.6(11)
C5	22.9(11)	18.7(10)	23.8(11)	-1.6(9)	2.8(9)	-6.4(9)
C6	17.2(11)	19.5(10)	25.4(10)	1.6(9)	5.5(9)	-1.5(9)
C7	19.6(10)	16.3(9)	16.6(9)	0.6(9)	4.8(8)	-1.3(9)
C8	17.0(10)	15.9(10)	13.0(9)	0.2(8)	2.0(8)	-3.1(8)
C9	22.1(11)	27.1(11)	16.6(10)	4.6(9)	-1.5(8)	-4.6(9)
C10	31.1(13)	38.1(14)	22.2(10)	12.6(10)	-5.4(10)	-9.2(11)
C11	37.1(14)	47.7(16)	16.7(11)	5.2(11)	5.0(10)	-16.6(13)
C12	25.7(12)	32.8(13)	20.7(10)	-0.3(10)	8.0(9)	-7.4(10)
C13	22.3(11)	23.4(11)	21.8(10)	-0.7(9)	8.8(9)	-2.7(10)
C14	24.5(12)	15.2(10)	28.2(11)	-3.6(9)	-2.2(9)	0.0(9)
C15	15.5(10)	20.9(11)	27.4(10)	-3.2(10)	-0.6(9)	2.5(9)
C16	27.5(13)	35.3(13)	17.6(10)	-4.6(10)	0.8(9)	2.8(11)

Table 3: Bond Lengths in Å for **MeCy2NAlMe3**.

Atom	Atom	Length/Å
Al1	N1	2.1172(18)
Al1	C14	1.986(2)
Al1	C15	1.988(2)
Al1	C16	1.988(2)
N1	C1	1.492(3)
N1	C2	1.516(3)
N1	C8	1.529(2)
C2	C3	1.528(3)
C2	C7	1.532(3)
C3	C4	1.528(3)

Atom	Atom	Length/Å
C4	C5	1.526(3)
C5	C6	1.524(3)
C6	C7	1.530(3)
C8	C9	1.523(3)
C8	C13	1.540(3)
C9	C10	1.533(3)
C10	C11	1.525(4)
C11	C12	1.522(4)
C12	C13	1.527(3)

Table 4: Bond Angles in ° for **MeCy2NAlMe3**.

Atom	Atom	Atom	Angle/°
C14	Al1	N1	105.52(8)
C14	Al1	C15	114.28(10)
C14	Al1	C16	108.17(11)
C15	Al1	N1	107.79(8)
C16	Al1	N1	107.30(9)
C16	Al1	C15	113.28(10)
C1	N1	Al1	104.30(12)
C1	N1	C2	111.46(16)
C1	N1	C8	109.07(15)
C2	N1	Al1	111.82(12)
C2	N1	C8	114.22(15)
C8	N1	Al1	105.34(12)
N1	C2	C3	115.55(18)
N1	C2	C7	111.84(16)

Atom	Atom	Atom	Angle/°
C3	C2	C7	109.31(17)
C4	C3	C2	111.18(19)
C5	C4	C3	111.6(2)
C6	C5	C4	109.71(19)
C5	C6	C7	111.65(18)
C6	C7	C2	110.56(17)
N1	C8	C13	118.73(17)
C9	C8	N1	111.58(16)
C9	C8	C13	110.56(18)
C8	C9	C10	110.59(19)
C11	C10	C9	111.3(2)
C12	C11	C10	110.4(2)
C11	C12	C13	111.3(2)
C12	C13	C8	108.68(19)

Table 5: Torsion Angles in ° for **MeCy2NAlMe3**.

Atom	Atom	Atom	Atom	Angle/°
Al1	N1	C2	C3	-178.20(15)
Al1	N1	C2	C7	-52.30(19)
Al1	N1	C8	C9	-72.57(18)
Al1	N1	C8	C13	157.09(16)
N1	C2	C3	C4	-175.55(18)
N1	C2	C7	C6	173.23(17)
N1	C8	C9	C10	167.86(18)
N1	C8	C13	C12	-170.21(18)
C1	N1	C2	C3	-61.9(2)
C1	N1	C2	C7	64.0(2)
C1	N1	C8	C9	175.97(18)
C1	N1	C8	C13	45.6(2)
C2	N1	C8	C9	50.5(2)
C2	N1	C8	C13	-79.8(2)
C2	C3	C4	C5	-57.2(3)
C3	C2	C7	C6	-57.5(2)
C3	C4	C5	C6	55.5(3)
C4	C5	C6	C7	-56.1(3)
C5	C6	C7	C2	58.0(2)
C7	C2	C3	C4	57.3(3)
C8	N1	C2	C3	62.3(2)
C8	N1	C2	C7	-171.81(16)
C8	C9	C10	C11	55.7(3)
C9	C8	C13	C12	59.0(2)
C9	C10	C11	C12	-55.3(3)
C10	C11	C12	C13	57.8(3)
C11	C12	C13	C8	-59.2(3)
C13	C8	C9	C10	-57.7(2)

Table 6: Hydrogen Fractional Atomic Coordinates (×10⁴) and Equivalent Isotropic Displacement Parameters (Å²×10³) for **MeCy2NAlMe3**. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{ij}.

Atom	**x**	**y**	**z**	U_{eq}
H1A	6816.16	5212.59	7040.77	25
H1B	6585.16	4184.84	6698.1	25
H1C	5425.67	4515.76	7487.18	25
H2	2123.85	4511.7	5836.04	18
H3A	4515.66	3628.54	5241.66	31
H3B	4844.91	3122.13	6110.9	31
H4A	1527.38	2996.85	5145.86	34
H4B	2984.43	2178.82	5262.98	34
H5A	364.47	1971.59	6144.96	26
H5B	2224.64	2049.46	6677.1	26
H6A	-28.32	3007.68	7280.97	25
H6B	-351.75	3523.24	6416.11	25
H7A	2984.3	3628.31	7373.13	21
H7B	1526.07	4450.5	7277.18	21
H8	5791.89	6067.14	5829.49	18
H9A	2778.68	6072.73	5295.27	26
H9B	3266.84	5187.61	4744.09	26
H10A	3637.92	6515.82	3918.2	37
H10B	4997.96	6962.18	4588.84	37
H11A	5817.74	5371.34	3597.66	41
H11B	6788.81	6357.57	3504.73	41
H12A	8165.63	6196.99	4821.45	32
H12B	8724.86	5335.13	4255.35	32
H13A	7837.75	4815.33	5595.87	27
H13B	6436.77	4415.77	4915.26	27
H14A	5916.57	7102.08	6874.82	34
H14B	4216.17	7734.21	7149.15	34
H14C	4394.2	7397.46	6208.5	34
H15A	305.86	6742.94	6408.43	32
H15B	-269.76	6133.97	7193.24	32
H15C	257.42	5643.9	6337.4	32
H16A	3049.38	5212.08	8373.67	40
H16B	2720.98	6277.21	8581.27	40
H16C	4761.49	5905.68	8408.71	40

Citations

CrysAlisPro Software System, Rigaku Oxford Diffraction, 2020.

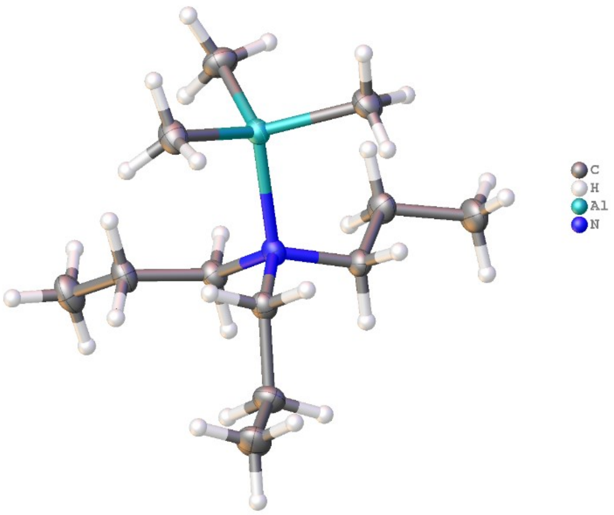
O.V. Dolomanov and L.J. Bourhis and R.J. Gildea and J.A.K. Howard and H. Puschmann, *J. Appl. Cryst.*, 2009, **42**, 339-341.

G.M. Sheldrick, *Acta Cryst.*, 2008, **A64**, 339-341.

Pr2NAlMe3

Crystal structure of crystals grown and mount on cold stage in glove bag.

Crystal Data and Experimental



Experimental. Single colourless block crystals of **Pr2NAlMe3** used as received. A suitable crystal with dimensions 0.16 × 0.12 × 0.12 mm^3 was selected and mounted on a nylon loop with paratone oil on a XtaLAB Synergy, Dualflex, HyPix diffractometer. The crystal was kept at a steady T = 100.01(10) K during data collection. The structure was solved with the **ShelXT** 2018/2 (Sheldrick, 2018) solution program using dual methods and by using **Olex2** (Dolomanov et al., 2009) as the graphical interface. The model was refined with **XL** (Sheldrick, 2008) using full matrix least squares minimisation on $\boldsymbol{F}^2$.

Crystal Data. $C_{12}H_{30}AlN$, M_r = 215.35, orthorhombic, $P2_12_12_1$ (No. 19), a = 7.5824(2) Å, b = 12.9289(3) Å, c = 15.4855(3) Å, α = β = γ = 90°, V = 1518.08(6) Å^3, T = 100.01(10) K, Z = 4, Z' = 1, μ(Cu Kα) = 0.920, 6059 reflections measured, 2769 unique (R_{int} = 0.0371) which were used in all calculations. The final wR_2 was 0.1047 (all data) and R_1 was 0.0396 (I > 2(I)).

Compound	**Pr2NAlMe3**
CCDC	1986516
Formula	$C_{12}H_{30}AlN$
$D_{calc.}$/ g cm^{-3}	0.942
μ/mm^{-1}	0.920
Formula Weight	215.35
Colour	colourless
Shape	block
Size/mm^3	0.16×0.12×0.12
T/K	100.01(10)
Crystal System	orthorhombic
Flack Parameter	0.03(3)
Hooft Parameter	0.02(2)
Space Group	$P2_12_12_1$
a/Å	7.5824(2)
b/Å	12.9289(3)
c/Å	15.4855(3)
α/°	90
β/°	90
γ/°	90
V/Å^3	1518.08(6)
Z	4
Z'	1
Wavelength/Å	1.54184
Radiation type	Cu K□
Θ_{min}/°	4.455
Θ_{max}/°	77.060
Measured Refl's.	6059
Ind't Refl's	2769
Refl's with I > 2(I)	2643
R_{int}	0.0371
Parameters	133
Restraints	0
Largest Peak	0.215
Deepest Hole	-0.283
GooF	1.026
wR_2 (all data)	0.1047
wR_2	0.1027
R_1 (all data)	0.0413
R_1	0.0396

Structure Quality Indicators

Reflections:		I/σ 22.8	Rint 3.71%	complete 100% (IUCr) 93%	
Refinement:	Shift 0.000	Max Peak 0.2	Min Peak -0.3	GooF 1.026	Flack .03(3)

A colourless block-shaped crystal with dimensions 0.16×0.12×0.12 mm³ was mounted on a nylon loop with paratone oil. Data were collected using a a XtaLAB Synergy, Dualflex, HyPix diffractometer equipped with an Oxford Cryosystems low-temperature device, operating at T = 100.01(10) K.

Data were measured using ω scans of 0.5° per frame for 0.1 s using Cu Kα radiation (micro-focus sealed X-ray tube, 50 kV, 1 mA). The total number of runs and images was based on the strategy calculation from the program **CrysAlisPro** (Rigaku, V1.171.40.69a, 2020). The actually achieved resolution was Θ = 77.060.

Cell parameters were retrieved using the **CrysAlisPro** (Rigaku, V1.171.40.69a, 2020) software and refined using **CrysAlisPro** (Rigaku, V1.171.40.69a, 2020) on 3673 reflections, 61 % of the observed reflections. Data reduction was performed using the **CrysAlisPro** (Rigaku, V1.171.40.69a, 2020) software which corrects for Lorentz polarization. The final completeness is 99.60 out to 77.060 in Θ CrysAlisPro 1.171.40.69a (Rigaku Oxford Diffraction, 2020) Empirical absorption correction using spherical harmonics, implemented in SCALE3 ABSPACK scaling algorithm.

The structure was solved in the space group $P2_12_12_1$ (# 19) by using dual methods using the ShelXT 2018/2 (Sheldrick, 2018) structure solution program. The structure was refined by Least Squares using version 2014/6 of **XL** (Sheldrick, 2008) incorporated in **Olex2** (Dolomanov et al., 2009). All non-hydrogen atoms were refined anisotropically. Hydrogen atom positions were calculated geometrically and refined using the riding model, except for the hydrogen atom on the non-carbon atom(s) which were found by difference Fourier methods and refined isotropically when data permits.

CCDC 1986516 contains the supplementary crystallographic data for this paper. The data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/structures.

There is a single molecule in the asymmetric unit, which is represented by the reported sum formula. In other words: Z is 4 and Z' is 1.

The Flack parameter was refined to 0.03(3). Determination of absolute structure using Bayesian statistics on Bijvoet differences using the Olex2 results in 0.02(2). Note: The Flack parameter is used to determine chirality of the crystal studied, the value should be near 0, a value of 1 means that the stereochemistry is wrong and the model should be inverted. A value of 0.5 means that the crystal consists of a racemic mixture of the two enantiomers.

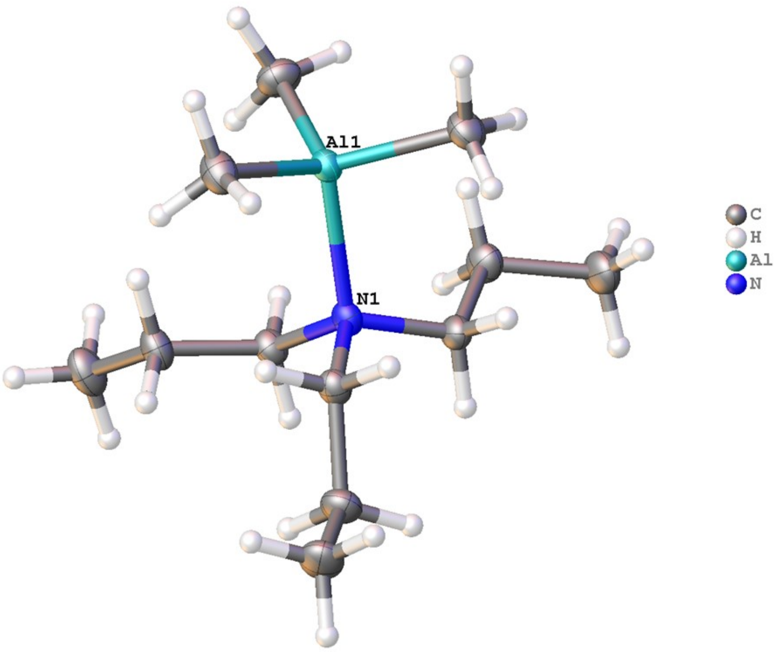


Figure S 41:

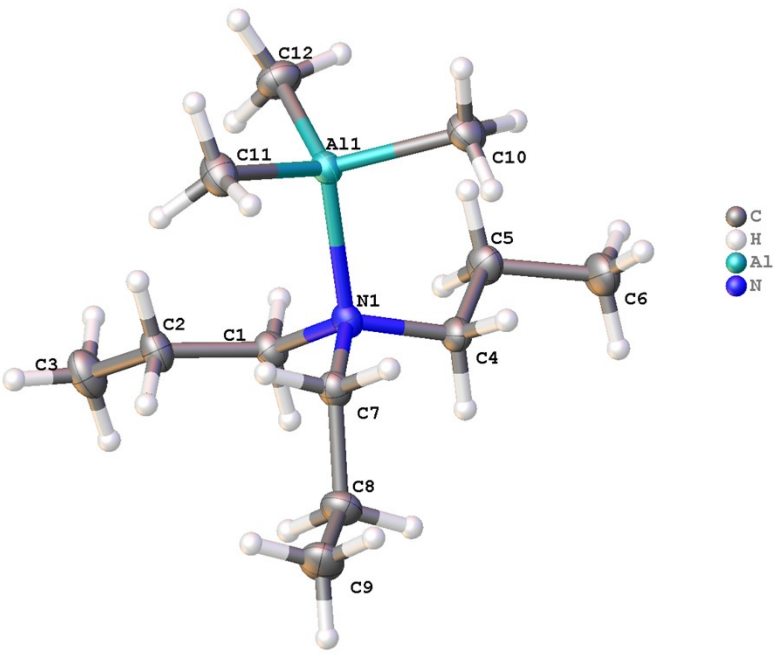


Figure S 42:

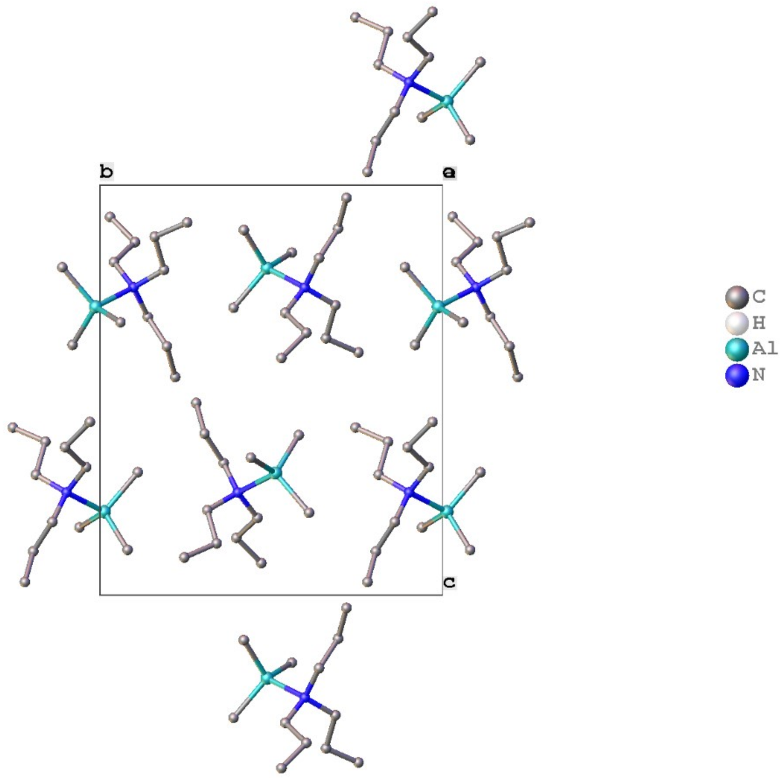
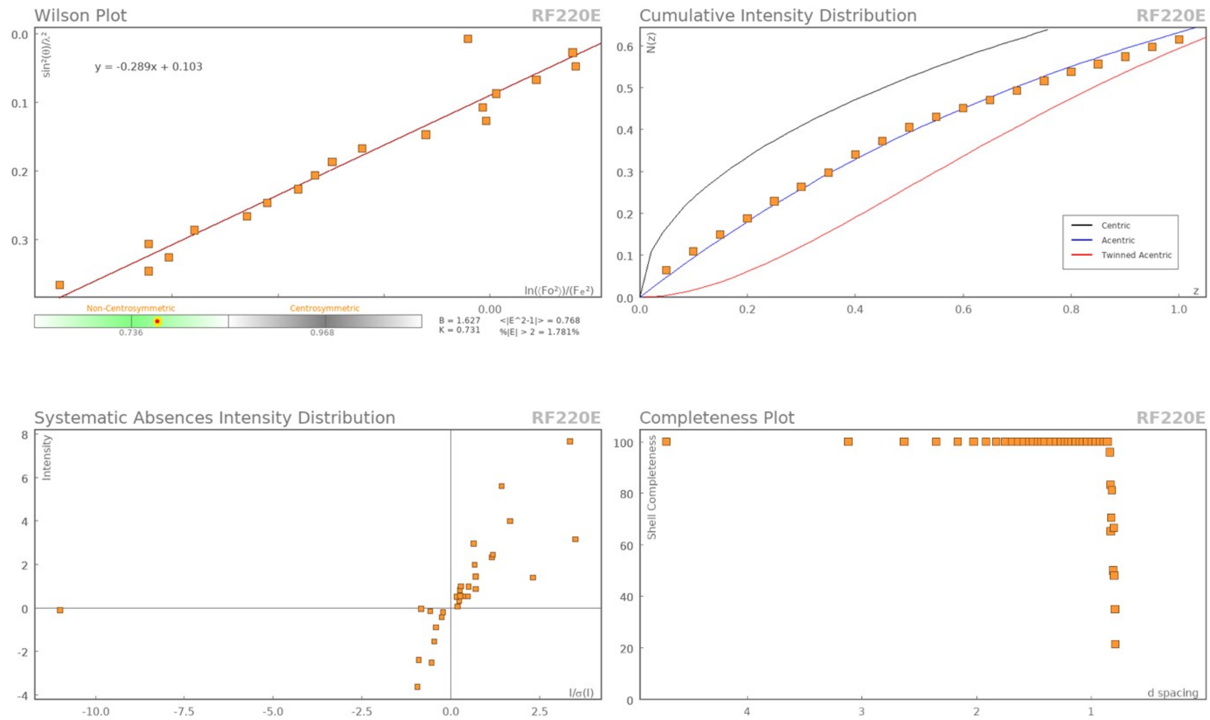
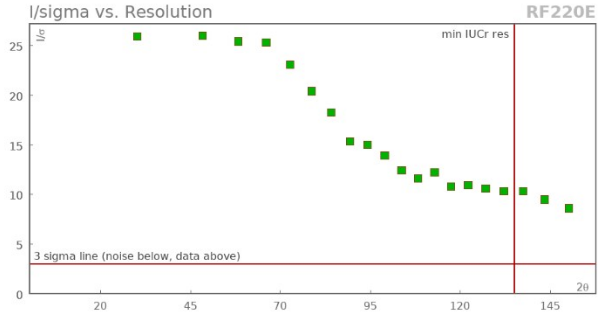


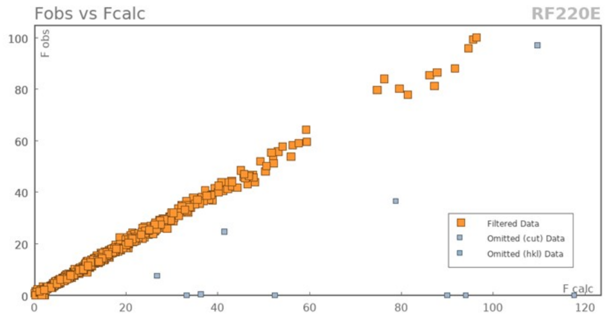
Figure S 43: Packing diagram of **Pr2NAlMe3**.

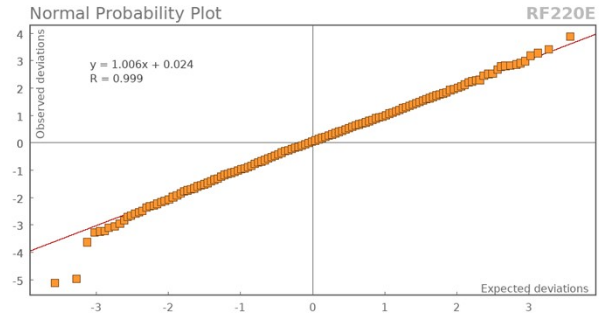
Data Plots: Diffraction Data





Data Plots: Refinement and Data





Reflection Statistics

Total reflections (after filtering)	6103	Unique reflections	2769
Completeness	0.863	Mean I/σ	16.63
hkl_{max} collected	(9, 15, 13)	hkl_{min} collected	(-8, -16, -19)
hkl_{max} used	(9, 16, 19)	hkl_{min} used	(-9, 0, 0)
Lim d_{max} collected	100.0	Lim d_{min} collected	0.77
d_{max} used	15.49	d_{min} used	0.79
Friedel pairs	261	Friedel pairs merged	0
Inconsistent equivalents	3	R_{int}	0.0371
R_{sigma}	0.0439	Intensity transformed	0
Omitted reflections	0	Omitted by user (OMIT hkl)	13
Multiplicity	(3188, 1023, 209, 53, 6)	Maximum multiplicity	7
Removed systematic absences	31	Filtered off (Shel/OMIT)	0

Images of the Crystal on the Diffractometer

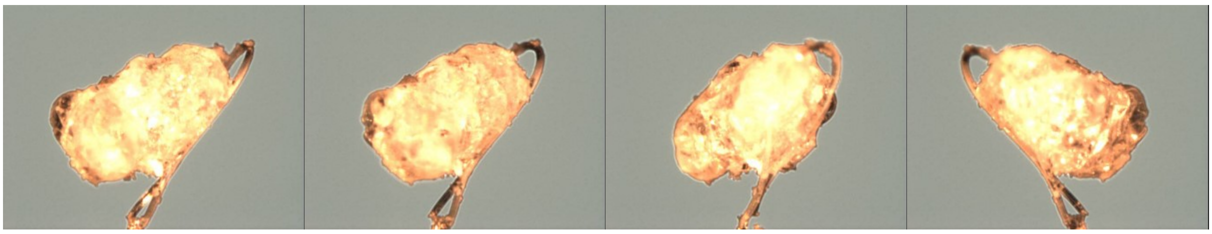


Table 7: Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for **Pr2NAlMe3**. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{ij}.

Atom	x	y	z	U_{eq}
Al1	7886.6(8)	4873.3(5)	7028.7(4)	20.43(19)

Atom	x	y	z	U_{eq}
N1	6132(2)	5977.2(14)	7501.6(11)	19.8(4)
C1	7043(3)	6869.1(15)	7932.4(13)	22.2(4)
C2	8086(3)	6595.1(18)	8739.2(13)	26.9(5)
C3	9038(4)	7543(2)	9084.0(16)	34.2(6)
C4	5004(3)	6392.9(18)	6782.7(13)	23.0(5)
C5	6008(3)	6949.2(19)	6064.2(14)	27.5(5)
C6	4762(3)	7194(2)	5317.1(15)	34.9(6)
C7	4958(3)	5405.2(17)	8118.7(12)	22.8(4)
C8	3559(3)	6022(2)	8605.6(15)	29.5(5)
C9	2585(3)	5294(2)	9221.0(15)	35.3(6)
C10	6506(3)	4197.2(18)	6099.6(15)	29.5(5)
C11	8376(3)	3898.2(18)	7992.7(15)	30.6(5)
C12	10054(3)	5598.3(19)	6649.4(16)	30.7(5)

Table 8. Anisotropic Displacement Parameters (×10^4) for **Pr2NAlMe3**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2} \times U_{11}+ ... +2hka^* \times b^* \times U_{12}]$

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Al1	22.6(3)	21.4(3)	17.3(3)	0.0(2)	-0.6(2)	0.4(2)
N1	23.2(8)	21.0(9)	15.2(8)	2.4(7)	-0.6(7)	-1.1(7)
C1	27.1(10)	19.3(9)	20.1(10)	-0.5(8)	-0.4(10)	-1.6(8)
C2	34.6(12)	27.2(11)	19.0(10)	0.3(8)	-3.8(9)	-4.4(10)
C3	43.0(14)	34.5(13)	25.0(11)	-2.1(10)	-3.6(11)	-10.9(12)
C4	23.7(10)	26.1(11)	19.3(10)	2.0(9)	-1.9(8)	4.1(9)
C5	29.1(11)	31.5(12)	22.1(10)	7.0(9)	0.2(10)	0.8(10)
C6	38.1(13)	45.8(15)	20.9(11)	6.5(11)	-2.1(11)	5.9(12)
C7	24.6(10)	25.1(10)	18.6(10)	2.4(8)	0.7(8)	-2.5(9)
C8	28.9(10)	36.1(13)	23.5(11)	0.1(10)	6.0(9)	1.0(10)
C9	31.0(12)	48.7(16)	26.2(11)	3.1(11)	8.3(9)	-2.2(11)
C10	35.4(12)	27.4(12)	25.6(11)	-4.2(9)	-1.4(10)	1.3(10)
C11	41.2(12)	24.3(11)	26.2(11)	1.6(10)	-4.9(10)	3.2(9)
C12	24.8(11)	32.5(13)	34.7(12)	3.2(11)	4.7(10)	-0.7(9)

Table 9: Bond Lengths in Å for **Pr2NAlMe3**.

Atom	Atom	Length/Å
Al1	N1	2.0841(18)
Al1	C10	1.982(2)
Al1	C11	1.989(2)
Al1	C12	1.981(2)
N1	C1	1.501(3)
N1	C4	1.503(3)
N1	C7	1.501(3)

Atom	Atom	Length/Å
C1	C2	1.520(3)
C2	C3	1.519(3)
C4	C5	1.528(3)
C5	C6	1.527(3)
C7	C8	1.527(3)
C8	C9	1.529(3)

Table 10: Bond Angles in ° for **Pr2NAlMe3**.

Atom	Atom	Atom	Angle/°
C10	Al1	N1	102.70(9)
C10	Al1	C11	111.34(10)
C11	Al1	N1	106.83(9)
C12	Al1	N1	108.05(9)
C12	Al1	C10	115.57(11)
C12	Al1	C11	111.56(11)
C1	N1	Al1	112.87(13)
C1	N1	C4	108.44(16)
C1	N1	C7	111.62(16)

Atom	Atom	Atom	Angle/°
C4	N1	Al1	110.35(13)
C7	N1	Al1	105.36(13)
C7	N1	C4	108.09(16)
N1	C1	C2	115.20(17)
C3	C2	C1	110.37(19)
N1	C4	C5	115.10(17)
C6	C5	C4	109.92(18)
N1	C7	C8	117.99(18)
C7	C8	C9	108.8(2)

Table 11: Torsion Angles in ° for **Pr2NAlMe3.**

Atom	Atom	Atom	Atom	Angle/°
Al1	N1	C1	C2	-63.8(2)
Al1	N1	C4	C5	-62.0(2)
Al1	N1	C7	C8	177.58(15)
N1	C1	C2	C3	176.44(19)
N1	C4	C5	C6	171.84(19)
N1	C7	C8	C9	-177.51(18)
C1	N1	C4	C5	62.1(2)
C1	N1	C7	C8	54.7(2)
C4	N1	C1	C2	173.64(18)
C4	N1	C7	C8	-64.4(2)
C7	N1	C1	C2	54.7(2)
C7	N1	C4	C5	-176.70(18)

Table 12: Hydrogen Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for **Pr2NAlMe3**. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{ij}.

Atom	x	y	z	U_{eq}
H1A	6144.07	7392.38	8088.27	27
H1B	7854.62	7191.96	7510.62	27
H2A	7276.02	6323.28	9186.5	32
H2B	8955.38	6048.61	8600.94	32
H3A	9893.54	7784.71	8654.76	51
H3B	9654.88	7363.73	9619.54	51
H3C	8179.3	8092.39	9200.16	51
H4A	4134.01	6879.2	7032.16	28
H4B	4339.43	5810.99	6524.4	28
H5A	6521.96	7598.62	6291.12	33
H5B	6984.89	6506.04	5856.46	33
H6A	5414.6	7548.92	4858.41	52
H6B	3805.92	7640.7	5523	52
H6C	4264.1	6549.11	5090.48	52
H7A	5720.12	5061.6	8551.37	27
H7B	4349.5	4852.69	7791.36	27
H8A	2715.36	6332.24	8191.94	35
H8B	4122.82	6587.59	8936.33	35
H9A	2041.85	4731.76	8890	53
H9B	1667.54	5679.06	9529.44	53
H9C	3422.46	5003.79	9637.94	53
H10A	7107.81	3563.49	5915.9	44
H10B	6399.54	4669.37	5607.3	44
H10C	5327.83	4024.4	6316.28	44
H11A	8637.01	4290.81	8518.78	46
H11B	9391.33	3464.15	7844.07	46
H11C	7341.52	3459.28	8090.24	46
H12A	9896.14	5851.17	6057.91	46
H12B	11053.98	5118.25	6667.95	46
H12C	10285.43	6184.02	7034.86	46

Citations

CrysAlisPro Software System, Rigaku Oxford Diffraction, (2020).

O.V. Dolomanov and L.J. Bourhis and R.J. Gildea and J.A.K. Howard and H. Puschmann, Olex2: A complete structure solution, refinement and analysis program, *J. Appl. Cryst.*, (2009), **42**, 339-341.

Sheldrick, G.M., A short history of ShelX, *Acta Cryst.*, (2008), **A64**, 339-341.

Computationally Estimated Parameters.

Table 13. Triad binding energies.

Triad	Binding Energy (kT)
I-M + LA	3.943
I-M + LB	8.484
LA-LB + M	8.733
LA-LB + I	-8.461
LA-M + LB	5.728
LA-M + I	6.874
I-LA + LB	-4.358
I-LA + M	13.983
LB-I + M	12.894
LB-I + LA	-9.988
LB-M + LA	-12.283
LB-M + I	-6.596

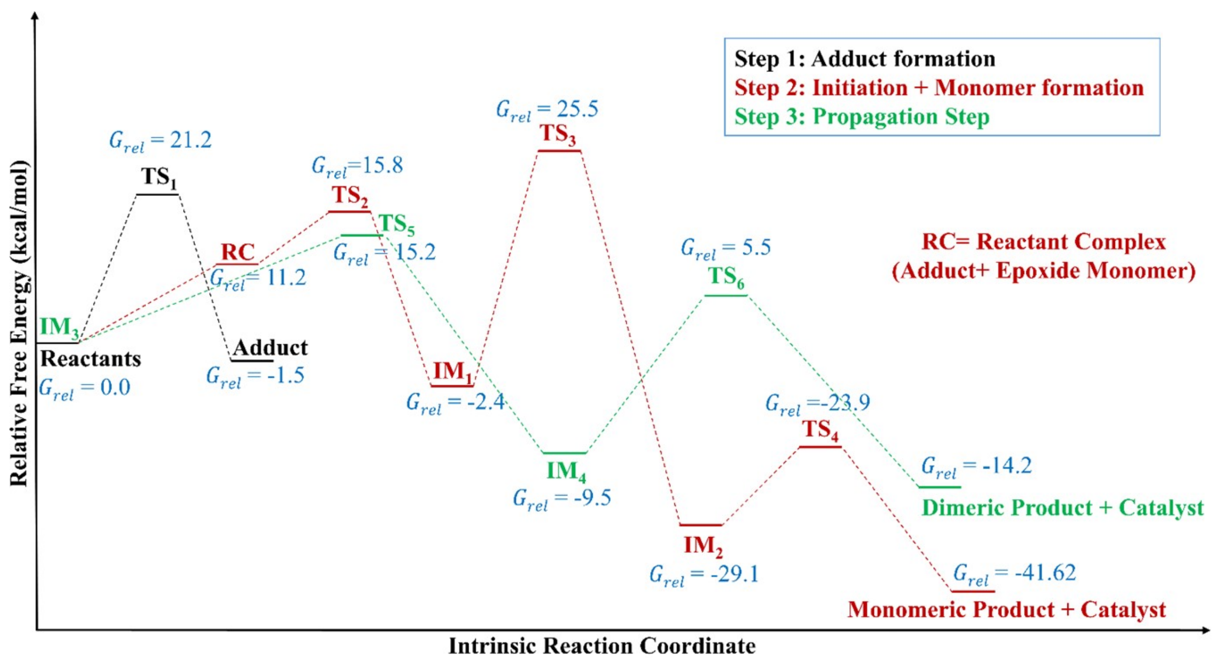


Figure S44. The relative free energy plot for reactants, reactant complex (RC), intermediates (IMs), transition states (TSs) and products are provided for all three steps in a same graph. Different color lines are used to represent different steps. The relative free energies given here are computed at B3LYP-D3/Def2-TZVP level.

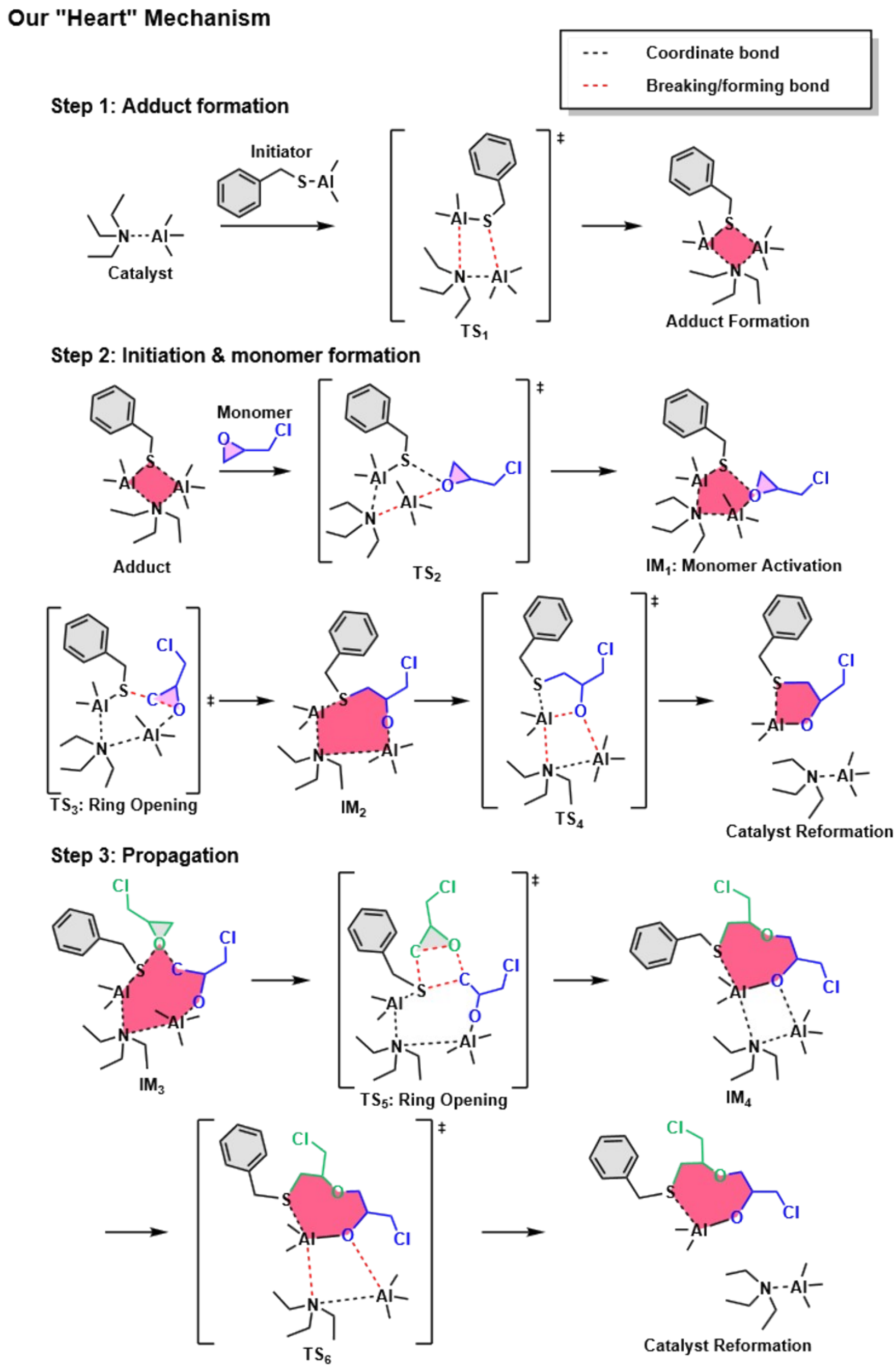


Figure S45. Overview of the adduct formation, initiation, and propagation steps including transition states.

XYZ coordinates of the optimized catalysts.

$Cy_2MeNAlMe_3$

```
52
Cy2MeNAlMe3
Al        -0.16344        2.33239        -0.21493
N         -0.03434        0.28870         0.62076
C         -0.21866        0.44911         2.08320
H          0.62097        1.01538         2.48460
H         -0.27257       -0.50963         2.60082
H         -1.12214        1.01193         2.28714
C         -1.12934       -0.55233        -0.00188
H         -0.99142       -0.43462        -1.07683
C         -1.09812       -2.05754         0.30766
H         -0.13677       -2.48802         0.04258
H         -1.24011       -2.22416         1.37988
C         -2.18943       -2.79739        -0.47858
H         -1.96354       -2.72130        -1.54837
H         -2.15741       -3.86105        -0.23009
C         -3.58262       -2.22643        -0.22063
H         -4.32280       -2.73636        -0.84212
H         -3.86381       -2.41383         0.82203
C         -3.60359       -0.72100        -0.48329
H         -4.58248       -0.30197        -0.23938
H         -3.43809       -0.53034        -1.54904
C         -2.52449       -0.00458         0.33223
H         -2.73650       -0.15541         1.39445
H         -2.57010        1.06579         0.14761
C          1.38658       -0.17974         0.33742
H          1.98508        0.70392         0.56087
C          1.61579       -0.50051        -1.14219
H          1.21938        0.30027        -1.76484
H          1.08468       -1.41476        -1.42002
C          3.10868       -0.68883        -1.43048
H          3.24763       -0.93770        -2.48506
H          3.62816        0.25998        -1.26104
C          3.72039       -1.76919        -0.53818
H          3.27681       -2.74004        -0.78838
H          4.79315       -1.85679        -0.72699
C          3.46376       -1.46409         0.93794
H          3.99214       -0.54437         1.21280
H          3.86980       -2.25755         1.57005
C          1.96693       -1.29331         1.23180
H          1.84131       -1.04908         2.28643
H          1.46436       -2.24589         1.06685
C          1.71383        2.99500        -0.25006
H          2.21450        2.99725         0.72444
H          1.67339        4.04411        -0.56810
H          2.37548        2.48585        -0.95751
C         -0.97862        2.11515        -2.01999
H         -0.40242        1.49857        -2.71683
H         -1.02964        3.11284        -2.47317
H         -2.00209        1.72871        -2.02253
C         -1.26200        3.36321         1.08789
H         -2.27452        2.99484         1.27724
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H          -1.37668          4.37634          0.68328
H          -0.77317          3.47987          2.06079
```

$CyMe_2NAlMe_3$

```
39
CyMe2NAlMe3
Al         -2.06677         -0.53009         -0.18122
N          -0.47330          0.87992          0.19534
C          -0.55683          1.28688          1.61713
H          -1.57862          1.59533          1.83365
H           0.11226          2.12289          1.83571
H          -0.31305          0.44880          2.26290
C           0.88483          0.32508         -0.18210
H           0.79599          0.11943         -1.25180
C           2.05735          1.29884          0.01868
H           1.87072          2.25234         -0.47576
H           2.18411          1.50875          1.08502
C           3.35891          0.69768         -0.52722
H           3.26532          0.56636         -1.61101
H           4.18054          1.40023         -0.36850
C           3.67221         -0.65128          0.12010
H           4.57479         -1.08285         -0.31939
H           3.88216         -0.49977          1.18511
C           2.49226         -1.61137         -0.02942
H           2.69531         -2.55241          0.48655
H           2.35570         -1.85921         -1.08776
C           1.19455         -1.00286          0.51284
H           1.29900         -0.84512          1.59031
H           0.37517         -1.70250          0.37256
C          -3.67275          0.64341         -0.28308
H          -3.79196          1.32244          0.56927
H          -4.56087          0.00048         -0.27633
H          -3.73817          1.24870         -1.19267
C          -1.48929         -1.32147         -1.91225
H          -2.29252         -1.95346         -2.30784
H          -0.60097         -1.95782         -1.84838
H          -1.29138         -0.56912         -2.68429
C          -2.14961         -1.71758          1.41424
H          -1.33653         -2.43933          1.52851
H          -3.07425         -2.30335          1.34488
H          -2.22061         -1.16141          2.35541
C          -0.78839          2.05639         -0.65345
H          -0.74776          1.76879         -1.70308
H          -1.79224          2.40406         -0.42844
H          -0.09036          2.87716         -0.47905
```

Et_3NAlEt_3

```
44
Et3NAlEt3
Al          0.92763          0.15069         -0.21317
N          -1.21865          0.00393         -0.01761
C          -1.62401         -0.95382          1.05870
H          -2.69537         -0.83124          1.25419
H          -1.09843         -0.64790          1.96036
```

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C          -1.31811        -2.41850         0.78411
H          -1.90435        -2.82266        -0.04073
H          -0.26448        -2.57803         0.56766
C          -1.79259         1.35590         0.28559
H          -2.88328         1.29040         0.23930
H          -1.46908         2.01754        -0.51678
C          -1.40236         1.95368         1.63023
H          -1.81815         1.39564         2.46867
H          -0.32468         2.01487         1.75617
C          -1.69573        -0.42950        -1.37220
H          -1.18244        -1.35627        -1.61273
H          -1.32927         0.31615        -2.07906
C          -3.20056        -0.61771        -1.55350
H          -3.76014         0.31182        -1.45569
H          -3.61545        -1.34183        -0.85169
C           1.20642         1.90319        -1.13800
H           2.16925         1.74386        -1.64471
H           0.49639         2.02916        -1.96708
C           1.46407        -1.34698        -1.43161
H           1.07304        -2.32431        -1.12620
H           1.05922        -1.17661        -2.43747
C           1.72306         0.00002         1.61527
H           1.27757         0.69069         2.33960
H           2.73968         0.39272         1.46445
H          -3.37903        -0.99982        -2.55998
H          -1.56517        -2.99472         1.67697
H          -1.80201         2.96765         1.68186
C           2.99966        -1.44550        -1.53450
H           3.45586        -1.65888        -0.56359
H           3.32888        -2.23180        -2.22198
H           3.44002        -0.50928        -1.89043
C           1.29614         3.21496        -0.34142
H           1.97478         3.12106         0.51109
H           1.65633         4.05375        -0.94653
H           0.32688         3.51724         0.06315
C           1.83845        -1.39404         2.25591
H           2.25671        -2.12601         1.55946
H           2.47640        -1.39881         3.14595
H           0.86501        -1.78114         2.56869
```

$Et_3NAliBu_3$

```
62
Et3NAliBu3
Al          0.05672         0.12721         0.00368
C           0.54249        -1.04964         1.55586
H           0.00080        -0.81562         2.48129
H           0.21331        -2.06092         1.28761
C           0.59349         2.06547         0.08607
H          -0.27607         2.70641        -0.10058
H           0.90321         2.31927         1.10881
C           0.46958        -0.74126        -1.76513
H           1.19334        -0.05756        -2.22843
H          -0.37402        -0.74265        -2.46769
C           1.71048         2.51457        -0.87745
H           1.40685         2.25746        -1.90060
```

C	2.04943	-1.11449	1.89810
H	2.63551	-1.04967	0.97209
C	1.08322	-2.15694	-1.77138
H	1.83206	-2.22329	-0.97270
C	1.92303	4.03277	-0.83843
H	2.69412	4.35382	-1.54517
H	1.00018	4.56501	-1.08168
H	2.23323	4.34867	0.16221
C	3.03305	1.79389	-0.59887
H	3.38579	2.01658	0.41169
H	2.93240	0.70949	-0.68003
H	3.81170	2.10570	-1.29945
C	2.42456	-2.44166	2.56726
H	2.18925	-3.28818	1.91791
H	3.49088	-2.48736	2.80838
H	1.86315	-2.57014	3.49782
C	2.47106	0.05867	2.78701
H	2.22611	1.01778	2.33175
H	1.95516	0.00616	3.75103
H	3.54611	0.04489	2.98335
C	1.80171	-2.45831	-3.09237
H	2.59255	-1.72940	-3.28285
H	2.25385	-3.45472	-3.09182
H	1.09813	-2.40915	-3.92935
C	0.03014	-3.23390	-1.49721
H	-0.43677	-3.10250	-0.52044
H	-0.75817	-3.19885	-2.25668
H	0.46612	-4.23578	-1.51968
N	-2.11422	0.24006	0.07593
C	-2.58857	1.35262	0.95741
H	-3.68168	1.39508	0.90930
H	-2.21858	2.27833	0.52656
C	-2.13590	1.27612	2.40734
H	-2.51798	0.39388	2.92064
H	-1.05077	1.27881	2.49121
C	-2.67386	0.44342	-1.30080
H	-3.76148	0.53584	-1.22495
H	-2.46438	-0.46780	-1.85900
C	-2.12969	1.63856	-2.07159
H	-2.36498	2.58851	-1.59346
H	-1.05224	1.58198	-2.21074
C	-2.56796	-1.09783	0.58449
H	-2.05735	-1.27958	1.52569
H	-2.18672	-1.83525	-0.12129
C	-4.06918	-1.29951	0.77608
H	-4.63404	-1.18748	-0.14899
H	-4.48785	-0.62071	1.51962
H	-4.23272	-2.31648	1.13643
H	-2.51446	2.15371	2.93379
H	-2.59396	1.64620	-3.05936

Et_3NAlMe_3

35
Et3NAlMe3

Al	1.42754	-0.32425	-0.21542

N	-0.65281	0.23436	-0.00721
C	-1.18533	-0.12201	1.34490
H	-2.17656	0.32968	1.46460
H	-0.52879	0.34820	2.07274
C	-1.25828	-1.61157	1.64592
H	-1.97993	-2.13330	1.01761
H	-0.28979	-2.09343	1.52899
C	-0.81186	1.70955	-0.22548
H	-1.87760	1.95420	-0.19172
H	-0.45960	1.91422	-1.23554
C	-0.07595	2.61065	0.75680
H	-0.46029	2.52258	1.77251
H	0.99264	2.41202	0.77309
C	-1.36730	-0.49438	-1.10630
H	-1.14332	-1.55110	-0.99153
H	-0.89424	-0.18205	-2.03849
C	-2.87895	-0.29999	-1.20275
H	-3.16192	0.72770	-1.42810
H	-3.39436	-0.60493	-0.29141
C	2.06490	0.95833	-1.59796
H	3.08608	0.67972	-1.88320
H	2.10704	2.00693	-1.28920
H	1.47646	0.91720	-2.52194
C	1.41142	-2.19793	-0.89019
H	0.86676	-2.92367	-0.27842
H	2.45055	-2.54779	-0.92045
H	1.03153	-2.28769	-1.91324
C	2.16384	-0.14082	1.62427
H	2.07577	0.85360	2.07128
H	3.23595	-0.36833	1.59270
H	1.72684	-0.85090	2.33460
H	-3.25398	-0.92605	-2.01411
H	-1.57261	-1.73883	2.68299
H	-0.21984	3.64569	0.44188

Et_3NAlPh_3

56
Et3NAlPh3

Al	-0.03022	-0.00882	-0.22371
N	-0.03867	-0.19265	1.92355
C	0.70327	0.91639	2.60742
H	0.49430	0.86149	3.68116
H	0.26922	1.84604	2.24821
C	2.20769	0.94358	2.38010
H	2.71764	0.10477	2.85350
H	2.46595	0.93685	1.32278
C	-1.44737	-0.22386	2.44686
H	-1.41090	-0.47741	3.50920
H	-1.95048	-1.04069	1.93242
C	-2.24715	1.06239	2.28792
H	-1.87797	1.86086	2.93100
H	-2.25015	1.43238	1.26551
C	0.59250	-1.53124	2.18097
H	1.58052	-1.50611	1.73164
H	0.00642	-2.25835	1.61591

C	0.71369	-1.98124	3.63482
H	-0.25067	-2.16405	4.10684
H	1.26564	-1.26648	4.24593
H	1.26749	-2.92136	3.65324
H	2.60434	1.85985	2.82039
H	-3.27887	0.85803	2.57909
C	-0.48094	1.89277	-0.60008
C	-1.62772	2.20238	-1.35093
C	0.30687	2.98619	-0.20173
C	-1.97980	3.51212	-1.66627
H	-2.26691	1.40104	-1.70593
C	-0.03286	4.30096	-0.50635
H	1.22486	2.81936	0.35280
C	-1.18473	4.56892	-1.23819
H	-2.87251	3.70751	-2.24915
H	0.60284	5.11568	-0.17889
H	-1.45429	5.59002	-1.47926
C	1.81294	-0.48476	-0.82540
C	2.58178	0.49873	-1.47215
C	2.40739	-1.75465	-0.72181
C	3.86023	0.24429	-1.96209
H	2.17332	1.49443	-1.60483
C	3.68334	-2.02512	-1.20660
H	1.86546	-2.57069	-0.25511
C	4.41902	-1.02077	-1.82633
H	4.41785	1.03320	-2.45358
H	4.10199	-3.01993	-1.10567
H	5.41301	-1.22502	-2.20544
C	-1.42300	-1.32983	-0.75971
C	-1.05438	-2.51634	-1.41625
C	-2.80328	-1.13872	-0.56907
C	-1.99068	-3.45804	-1.83669
H	-0.00848	-2.71106	-1.62367
C	-3.75102	-2.06851	-0.98506
H	-3.16300	-0.23494	-0.08895
C	-3.34529	-3.23853	-1.61831
H	-1.66231	-4.35988	-2.34043
H	-4.80555	-1.87870	-0.82071
H	-4.07821	-3.96621	-1.94515

iBu_3NAlEt_3

62
iBu3NAlEt3

Al	1.22636	-0.48570	-0.74423
N	-0.54675	0.38503	0.14683
C	-1.04298	-0.30751	1.38316
H	-1.99547	0.14682	1.67919
H	-0.33042	-0.04684	2.15671
C	-1.19182	-1.83660	1.40955
H	-0.28428	-2.27887	0.99937
C	-0.31213	1.83406	0.48891
H	-1.12179	2.16905	1.14468
H	-0.41495	2.38010	-0.44502
C	1.02466	2.26258	1.11576

H	1.83502	1.86028	0.50842
C	-1.51464	0.29524	-1.00412
H	-1.50759	-0.74264	-1.31557
H	-1.06796	0.85858	-1.82581
C	-2.98354	0.73432	-0.84054
H	-3.37792	0.32582	0.09248
C	1.75661	0.94247	-2.05612
H	1.47490	0.58204	-3.05412
H	1.19164	1.87394	-1.92951
C	0.63477	-2.15237	-1.69089
H	0.02856	-2.83406	-1.08522
H	0.00605	-1.89152	-2.55178
C	2.62289	-0.87019	0.63282
H	2.99614	0.03572	1.12015
H	3.46021	-1.18962	-0.00555
C	1.86847	-2.92124	-2.20706
H	2.50302	-3.25972	-1.38328
H	1.60155	-3.80762	-2.79215
H	2.49441	-2.29460	-2.85043
C	3.25881	1.28203	-2.06079
H	3.86999	0.39574	-2.25238
H	3.52501	2.02470	-2.82049
H	3.58712	1.67980	-1.09581
C	2.39146	-1.95829	1.69111
H	2.03631	-2.89025	1.24166
H	3.29829	-2.20252	2.25448
H	1.63906	-1.65839	2.42536
C	-2.39616	-2.40001	0.64932
H	-3.32493	-1.93022	0.98390
H	-2.31818	-2.27385	-0.42717
H	-2.48457	-3.47155	0.83751
C	-3.21317	2.25023	-0.84235
H	-2.81660	2.74312	0.04244
H	-2.74945	2.71075	-1.71892
H	-4.28240	2.46777	-0.88375
C	1.09494	3.79275	1.01677
H	2.03620	4.15997	1.42811
H	1.02900	4.13016	-0.01949
H	0.28194	4.26237	1.57866
C	-1.29119	-2.25412	2.88421
H	-1.37116	-3.33857	2.97096
H	-0.41721	-1.93809	3.45551
H	-2.17765	-1.81772	3.35424
C	1.24365	1.82444	2.56565
H	0.40081	2.11930	3.19763
H	1.38845	0.75011	2.65949
H	2.14042	2.29990	2.96753
C	-3.77672	0.09729	-1.99075
H	-4.83153	0.37042	-1.93143
H	-3.39896	0.44028	-2.95804
H	-3.71000	-0.99160	-1.97329

$iBu_3NAliBu_3$

80

iBu3NAliBu3

Al	0.80534	0.02771	-0.34258
N	-1.35009	0.28541	0.09637
C	-1.92822	-0.65837	1.11146
H	-3.01001	-0.49055	1.16688
H	-1.52410	-0.33103	2.06156
C	-1.66802	-2.16868	1.01020
H	-0.60751	-2.32287	0.81823
C	-1.63485	1.68756	0.56792
H	-2.65006	1.71436	0.97604
H	-1.63780	2.30657	-0.32503
C	-0.69074	2.36008	1.57634
H	0.32957	2.24706	1.21655
C	-1.94426	0.09606	-1.27429
H	-1.59144	-0.86821	-1.61827
H	-1.47262	0.83756	-1.92191
C	-3.47063	0.14902	-1.49463
H	-3.96712	-0.43169	-0.71396
C	1.16240	1.76314	-1.30734
H	1.44201	1.50638	-2.33839
H	0.22030	2.31456	-1.41939
C	0.85550	-1.58201	-1.54590
H	0.23415	-2.38575	-1.13453
H	0.40058	-1.34541	-2.51838
C	1.82159	-0.15693	1.37506
H	1.81004	0.81895	1.87404
H	2.86478	-0.26248	1.03820
C	2.25830	-2.16812	-1.82320
H	2.79884	-2.25747	-0.87379
C	2.21772	2.74829	-0.76130
H	2.05611	2.88755	0.31514
C	1.57455	-1.24894	2.43229
H	0.50724	-1.27316	2.67750
C	-2.47250	-2.91093	-0.06131
H	-3.54328	-2.72378	0.05527
H	-2.18819	-2.63995	-1.07444
H	-2.31483	-3.98663	0.03553
C	-4.07754	1.55732	-1.51463
H	-4.06258	2.04433	-0.54226
H	-3.54122	2.19894	-2.21909
H	-5.11910	1.51215	-1.83927
C	-1.01395	3.86048	1.56289
H	-0.35452	4.40028	2.24388
H	-0.88555	4.28793	0.56663
H	-2.04411	4.04559	1.88170
C	-1.98683	-2.77855	2.38340
H	-1.79237	-3.85188	2.37966
H	-1.38349	-2.33378	3.17593
H	-3.04058	-2.63302	2.63914
C	-0.75586	1.82563	3.00887
H	-1.78530	1.80783	3.37819
H	-0.33779	0.82545	3.10102
H	-0.17752	2.47039	3.67339
C	-3.75745	-0.54425	-2.83472
H	-4.82678	-0.53973	-3.05207
H	-3.25029	-0.02676	-3.65388
H	-3.41901	-1.58139	-2.83514

C	2.17286	-3.57510	-2.42619
H	3.16471	-3.99724	-2.61386
H	1.63805	-4.25627	-1.75969
H	1.63280	-3.54993	-3.37775
C	3.08359	-1.25629	-2.73576
H	2.58608	-1.13283	-3.70275
H	3.21718	-0.26320	-2.30747
H	4.07587	-1.67476	-2.92254
C	2.09608	4.13126	-1.41278
H	1.10398	4.55845	-1.24569
H	2.83553	4.83407	-1.01728
H	2.24655	4.05778	-2.49398
C	3.64240	2.21467	-0.93232
H	3.77550	1.25015	-0.44036
H	3.87709	2.08409	-1.99271
H	4.37778	2.90555	-0.51226
C	2.32067	-0.95366	3.73929
H	2.01780	0.01011	4.15546
H	2.13553	-1.72214	4.49601
H	3.39881	-0.91120	3.55967
C	1.95617	-2.64106	1.92149
H	1.43782	-2.89622	0.99697
H	3.02877	-2.68564	1.71218
H	1.72901	-3.41291	2.66128

iBu_3NAlMe_3

53
iBu3NAlMe3

Al	-0.87810	-1.04769	1.53537
N	0.01338	0.17765	-0.01765
C	0.42809	-0.65777	-1.18859
H	0.78535	-0.00077	-1.99083
H	-0.49097	-1.11322	-1.53973
C	1.44627	-1.79077	-0.96156
H	1.34155	-2.15395	0.06158
C	-0.96054	1.22013	-0.48412
H	-0.48328	1.80724	-1.27369
H	-1.10581	1.88003	0.36817
C	-2.34621	0.77234	-0.99536
H	-2.64168	-0.13620	-0.47056
C	1.15747	0.84596	0.68860
H	1.80941	0.04266	1.01746
H	0.74287	1.28498	1.59917
C	2.01105	1.91687	-0.02871
H	2.16128	1.61750	-1.07029
C	-2.09326	0.22897	2.45806
H	-2.32403	-0.18545	3.44643
H	-1.65741	1.21705	2.64346
C	0.62236	-1.60659	2.72210
H	1.44848	-2.14484	2.24715
H	1.06041	-0.77776	3.28743
C	-1.73335	-2.57040	0.57824
H	-2.48662	-3.01145	1.24184
H	-1.01870	-3.36893	0.35615
C	1.10211	-2.94873	-1.90728

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H          1.81273       -3.76867       -1.78991
H          0.10183       -3.33690       -1.71411
H          1.14491       -2.62186       -2.95076
C          2.89993       -1.36647       -1.18910
H          3.03827       -1.00714       -2.21285
H          3.22211       -0.57774       -0.51524
H          3.57122       -2.21478       -1.04353
C          1.41932        3.33384        0.00118
H          0.50494        3.43818       -0.57675
H          1.19813        3.63081        1.02997
H          2.14049        4.04977       -0.39833
C          3.38385        1.95874        0.66023
H          4.03076        2.70214        0.19169
H          3.27282        2.23260        1.71316
H          3.89736        0.99756        0.62346
C         -2.39824        0.51270       -2.50682
H         -2.11152        1.41261       -3.05869
H         -1.74518       -0.29532       -2.83076
H         -3.41407        0.25157       -2.80914
C         -3.35990        1.87051       -0.64604
H         -4.35670        1.60425       -1.00171
H         -3.41648        2.03499        0.42989
H         -3.08264        2.81699       -1.12034
H         -2.25280       -2.33764       -0.35611
H          0.20340       -2.29521        3.46642
H         -3.05255        0.38719        1.95873
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iBu_3NAlPh_3

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74
iBu3NAlPh3
Al         0.09452        0.01759       -0.86544
N         -0.06184        0.26262        1.27244
C         -0.23337       -1.01035        2.04603
H         -0.38401       -0.76352        3.10243
H          0.72596       -1.51193        1.97519
C         -1.28295       -2.04566        1.60712
H         -1.19182       -2.18988        0.53127
C          1.18074        0.99077        1.75113
H          0.95572        1.45969        2.70539
H          1.32628        1.79868        1.03822
C          2.49229        0.19142        1.91716
H          2.46794       -0.68453        1.27089
C         -1.23329        1.20147        1.39452
H         -2.00069        0.80417        0.73802
H         -0.91424        2.14834        0.95631
C         -1.90946        1.47941        2.75277
H         -2.16530        0.53015        3.22350
C          1.68050       -1.15983       -1.08814
C          2.83996       -0.69296       -1.72751
C          1.72839       -2.48243       -0.61381
C          3.98313       -1.47742       -1.86026
H          2.85714        0.31003       -2.13930
C          2.86269       -3.27810       -0.73646
H          0.85749       -2.91614       -0.13444
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C	4.00129	-2.77239	-1.35602
H	4.85909	-1.07820	-2.35843
H	2.85882	-4.29239	-0.35394
H	4.88883	-3.38574	-1.45351
C	-1.59118	-0.83408	-1.52419
C	-1.48261	-2.07581	-2.17619
C	-2.88787	-0.29718	-1.45236
C	-2.58622	-2.74667	-2.69573
H	-0.50793	-2.53899	-2.28324
C	-4.00190	-0.95547	-1.96427
H	-3.05242	0.67119	-0.99094
C	-3.85525	-2.19052	-2.58527
H	-2.45443	-3.70258	-3.18947
H	-4.98334	-0.50256	-1.88257
H	-4.71839	-2.70835	-2.98559
C	0.30094	1.89441	-1.51618
C	-0.77215	2.50690	-2.18730
C	1.46852	2.66869	-1.40344
C	-0.69782	3.80348	-2.68931
H	-1.69251	1.95622	-2.34048
C	1.56079	3.96502	-1.90130
H	2.34577	2.25668	-0.91946
C	0.47091	4.54143	-2.54365
H	-1.55086	4.23496	-3.20031
H	2.48390	4.52266	-1.79219
H	0.53537	5.54993	-2.93389
C	-0.91977	-3.37167	2.29095
H	-1.61651	-4.15745	1.99582
H	0.08779	-3.70050	2.02876
H	-0.96844	-3.27731	3.37994
C	-1.09800	2.30184	3.75968
H	-0.27511	1.73711	4.19707
H	-0.68563	3.20171	3.29633
H	-1.73995	2.61882	4.58436
C	3.67655	1.05035	1.46131
H	4.61899	0.53628	1.65682
H	3.62931	1.25299	0.39224
H	3.69979	2.00619	1.99288
C	-3.22902	2.20033	2.43943
H	-3.78339	2.40557	3.35648
H	-3.04273	3.15567	1.94116
H	-3.86934	1.60256	1.78786
C	-2.74554	-1.70848	1.90216
H	-2.90972	-1.56843	2.97391
H	-3.09003	-0.82137	1.37759
H	-3.38233	-2.53222	1.57566
C	2.71760	-0.26048	3.36605
H	2.82286	0.60688	4.02441
H	1.90079	-0.86945	3.75259
H	3.63409	-0.84810	3.44490

Ph_3NAlMe_3

47
Ph3NAlMe3

Al	-0.02308	0.04396	2.84689
N	0.00466	-0.01008	-0.64604
C	1.65951	-0.96796	2.94497
H	1.67884	-1.58828	3.84828
H	2.54842	-0.33281	2.96590
H	1.75586	-1.65763	2.10090
C	-1.74194	-0.90795	2.91163
H	-2.36062	-0.66533	2.04231
H	-2.31750	-0.59617	3.79063
H	-1.63601	-1.99455	2.95928
C	0.00962	2.00902	2.88740
H	0.53584	2.36376	3.78090
H	-0.98633	2.45883	2.89499
H	0.55764	2.41404	2.03138
C	-1.39544	0.20019	-0.79647
C	-2.17019	-0.62689	-1.61238
C	-2.01739	1.24995	-0.11365
C	-3.53975	-0.41926	-1.72206
H	-1.70141	-1.43717	-2.15306
C	-3.38180	1.45992	-0.24021
H	-1.42552	1.89997	0.51504
C	-4.15510	0.62319	-1.03957
H	-4.12507	-1.07384	-2.35568
H	-3.84489	2.27430	0.30260
H	-5.22172	0.78242	-1.12851
C	0.89064	1.09490	-0.79214
C	0.58227	2.16724	-1.63138
C	2.09493	1.11698	-0.08204
C	1.45141	3.24628	-1.73808
H	-0.34141	2.15964	-2.19303
C	2.96383	2.19009	-0.20526
H	2.34569	0.28781	0.56425
C	2.64608	3.26643	-1.02854
H	1.19328	4.07107	-2.39049
H	3.88818	2.19063	0.35855
H	3.32082	4.10796	-1.11510
C	0.52267	-1.33087	-0.76984
C	1.61524	-1.60737	-1.59405
C	-0.06467	-2.37702	-0.05205
C	2.12047	-2.89910	-1.67821
H	2.07380	-0.80927	-2.16105
C	0.43552	-3.66603	-0.15301
H	-0.91565	-2.17421	0.58262
C	1.53612	-3.93611	-0.96097
H	2.97142	-3.09392	-2.31888
H	-0.02973	-4.46088	0.41626
H	1.93156	-4.94101	-1.03004

Pr_3NAlEt_3

53
Pr3NAlEt3

Al	1.31324	0.24037	-0.38235
N	-0.73847	-0.16721	0.14427
C	-0.85195	-0.99684	1.38892

H	-1.89887	-1.00567	1.71560
H	-0.29048	-0.45642	2.14625
C	-0.32268	-2.43457	1.34220
H	0.58781	-2.47834	0.74609
C	-1.47728	1.11901	0.35660
H	-2.53571	0.88798	0.51380
H	-1.40055	1.68100	-0.57423
C	-1.01017	2.00064	1.51045
H	-1.11340	1.47615	2.46170
H	0.04489	2.24320	1.39700
C	-1.29097	-0.84737	-1.07375
H	-0.72428	-1.76462	-1.19428
H	-1.02509	-0.21519	-1.92264
C	-2.80332	-1.14290	-1.11158
H	-3.20040	-1.23809	-0.09878
C	1.19284	1.83622	-1.58551
H	2.06825	1.70065	-2.23666
H	0.34210	1.75591	-2.27582
C	1.93231	-1.34351	-1.44540
H	1.76481	-2.30680	-0.95000
H	1.37383	-1.40445	-2.38811
C	2.34459	0.50654	1.30890
H	1.87380	1.22071	1.99332
H	3.24980	1.02651	0.96191
H	-2.93397	-2.12873	-1.56347
H	-0.01185	-2.66881	2.36320
C	3.43421	-1.22243	-1.77443
H	4.04506	-1.20346	-0.86733
H	3.80145	-2.05063	-2.38970
H	3.65361	-0.30059	-2.32132
C	1.24280	3.25909	-1.00634
H	2.06038	3.37224	-0.28887
H	1.38315	4.02557	-1.77601
H	0.32370	3.51707	-0.47540
C	2.77808	-0.73906	2.10072
H	3.23108	-1.49360	1.45189
H	3.50802	-0.50980	2.88425
H	1.93097	-1.22186	2.59435
C	-1.30979	-3.51514	0.89666
H	-2.23901	-3.45679	1.46888
H	-1.56767	-3.45013	-0.15889
H	-0.88162	-4.50497	1.06359
C	-3.63097	-0.13566	-1.91238
H	-3.58453	0.86842	-1.49058
H	-3.27131	-0.07494	-2.94205
H	-4.68045	-0.43422	-1.94558
C	-1.83526	3.28646	1.56058
H	-1.50763	3.92541	2.38145
H	-1.73657	3.85825	0.63542
H	-2.89683	3.07187	1.70795

$Pr_3NAliBu_3$

71
Pr3NAliBu3

Al	-0.49260	-0.40098	-0.26893
N	1.39676	0.69784	-0.04587
C	1.32643	1.80887	0.95159
H	2.33509	2.21018	1.10748
H	1.01714	1.36427	1.89403
C	0.37411	2.95004	0.62151
H	0.68704	3.46332	-0.28993
H	-0.62203	2.55506	0.43146
C	2.49761	-0.23700	0.35828
H	3.45027	0.29926	0.30805
H	2.53155	-1.02802	-0.38929
C	2.37897	-0.86303	1.74416
H	2.47384	-0.09905	2.51804
H	1.39698	-1.31634	1.87015
C	1.68150	1.20641	-1.42876
H	0.81475	1.77920	-1.74872
H	1.72602	0.33087	-2.07830
C	2.93827	2.05353	-1.63661
H	3.83787	1.48397	-1.39714
H	2.92899	2.92039	-0.97198
C	0.17910	-2.08711	-1.13103
H	-0.58067	-2.35541	-1.87745
H	1.05347	-1.82623	-1.74424
C	-1.54249	0.67923	-1.59888
H	-1.46314	1.75768	-1.41423
H	-1.08588	0.52994	-2.58911
C	-1.30964	-0.62368	1.54875
H	-0.68289	-1.32481	2.11392
H	-2.21942	-1.20690	1.33203
C	-3.04333	0.33735	-1.72423
H	-3.51927	0.51328	-0.75371
C	0.50817	-3.35501	-0.31990
H	1.11390	-3.08125	0.55158
C	-1.72369	0.52198	2.49207
H	-0.86263	1.17914	2.65793
C	0.31515	3.95347	1.77221
H	-0.35876	4.77721	1.53418
H	-0.04809	3.48174	2.68759
H	1.30031	4.37784	1.98188
C	3.01677	2.53121	-3.08719
H	3.90974	3.13514	-3.25393
H	3.05091	1.68659	-3.77920
H	2.14776	3.13886	-3.35002
C	3.46662	-1.91747	1.94711
H	3.40038	-2.35687	2.94318
H	3.37310	-2.72582	1.21910
H	4.46446	-1.48444	1.83994
C	-2.84537	1.38041	1.90200
H	-2.57518	1.79626	0.93131
H	-3.74673	0.77813	1.75673
H	-3.10320	2.20962	2.56578
C	-2.14540	-0.00530	3.86963
H	-1.33885	-0.57571	4.33627
H	-2.42233	0.80703	4.54853
H	-3.00790	-0.67129	3.77355
C	-3.74371	1.24439	-2.74324
H	-3.31683	1.09975	-3.74057

H	-4.81591	1.03487	-2.80422
H	-3.62052	2.29789	-2.48052
C	-3.27839	-1.13365	-2.08322
H	-2.76879	-1.38967	-3.01687
H	-2.90528	-1.80912	-1.31075
H	-4.34305	-1.34227	-2.21590
C	1.32888	-4.36133	-1.13556
H	2.26961	-3.91974	-1.47516
H	1.56784	-5.25777	-0.55528
H	0.77287	-4.67419	-2.02426
C	-0.76463	-4.02341	0.20855
H	-1.34593	-3.34599	0.83457
H	-1.40168	-4.33639	-0.62419
H	-0.53207	-4.91184	0.80143

Pr_3NAlMe_3

44
Pr3NAlMe3

Al	1.00601	1.14563	1.03653
N	-0.11143	-0.32082	-0.09457
C	-0.65509	0.26730	-1.35699
H	-1.05329	-0.53870	-1.98498
H	0.18893	0.69922	-1.89054
C	-1.71654	1.34690	-1.18221
H	-2.62439	0.92676	-0.74406
H	-1.35746	2.10909	-0.49080
C	-2.05409	1.98994	-2.52664
H	-1.17650	2.47364	-2.96110
H	-2.82999	2.74790	-2.41213
H	-2.41633	1.24824	-3.24322
C	0.77087	-1.48389	-0.43035
H	0.17053	-2.25095	-0.93006
H	1.11113	-1.90150	0.51721
C	1.98347	-1.17975	-1.30453
H	1.66586	-0.87549	-2.30384
H	2.54962	-0.34925	-0.88606
C	2.88299	-2.41058	-1.41291
H	3.73716	-2.21219	-2.06152
H	2.34216	-3.26548	-1.82719
H	3.26830	-2.70143	-0.43313
C	-1.19597	-0.78676	0.82833
H	-1.74971	0.09251	1.14824
H	-0.69814	-1.17291	1.72035
C	-2.17804	-1.83371	0.30041
H	-1.66168	-2.76399	0.05704
H	-2.64648	-1.48383	-0.62255
C	-3.26135	-2.11645	1.34172
H	-2.82611	-2.48698	2.27275
H	-3.96652	-2.86691	0.98176
H	-3.82664	-1.21204	1.57831
C	2.29761	0.00959	2.03907
H	2.83669	0.64469	2.75168
H	3.06012	-0.48778	1.43227
H	1.80826	-0.76482	2.64112

C	-0.31719	2.01363	2.24586
H	-1.17641	2.48289	1.75650
H	0.20231	2.81797	2.78096
H	-0.71072	1.34151	3.01541
C	1.74034	2.37333	-0.34822
H	2.39376	1.91057	-1.09359
H	2.34311	3.13933	0.15393
H	0.96231	2.91528	-0.89685

Pr_3NAlPh_3

65
Pr3NAlPh3

Al	-0.11417	0.00842	-0.56680
N	0.12064	-0.17918	1.59080
C	0.88962	0.97747	2.15176
H	0.82954	0.94588	3.24530
H	0.37822	1.88115	1.82968
C	2.34714	1.07349	1.72170
H	2.93541	0.26706	2.16509
H	2.41739	0.96628	0.64011
C	-1.22149	-0.23892	2.26017
H	-1.07428	-0.44532	3.32380
H	-1.74795	-1.09018	1.83207
C	-2.09382	1.00480	2.12896
H	-1.70253	1.81138	2.75259
H	-2.08694	1.35903	1.10044
C	0.82618	-1.48510	1.82099
H	1.74592	-1.46643	1.24334
H	0.20660	-2.25949	1.36439
C	1.15125	-1.87684	3.26279
H	0.24004	-2.00947	3.84850
H	1.72758	-1.08801	3.75147
C	0.37454	1.89767	-0.97472
C	-0.31346	3.03462	-0.51866
C	1.49030	2.14436	-1.79345
C	0.08905	4.32891	-0.83506
H	-1.19485	2.92318	0.10339
C	1.90669	3.43274	-2.11826
H	2.05333	1.30895	-2.19493
C	1.20854	4.53284	-1.63432
H	-0.47149	5.17771	-0.46038
H	2.77418	3.57735	-2.75182
H	1.52805	5.53769	-1.88262
C	1.13234	-1.32971	-1.36490
C	2.53507	-1.28500	-1.28448
C	0.59662	-2.38736	-2.11877
C	3.35030	-2.23145	-1.89639
H	3.02182	-0.48811	-0.73202
C	1.39901	-3.34356	-2.73768
H	-0.47779	-2.46878	-2.23797
C	2.78176	-3.27105	-2.62529
H	4.42823	-2.15660	-1.80913
H	0.94307	-4.14285	-3.31056
H	3.41083	-4.01128	-3.10474

C	-2.02354	-0.46655	-0.86802
C	-2.91729	0.48287	-1.38884
C	-2.56201	-1.73364	-0.58862
C	-4.26385	0.19790	-1.60030
H	-2.55636	1.47630	-1.63560
C	-3.90554	-2.03432	-0.79222
H	-1.91886	-2.52032	-0.20362
C	-4.76417	-1.06331	-1.29695
H	-4.92225	0.95881	-2.00319
H	-4.28235	-3.02412	-0.56139
H	-5.81113	-1.29005	-1.45779
C	2.93485	2.42708	2.11731
H	3.99117	2.48476	1.85206
H	2.41543	3.23619	1.60010
H	2.85096	2.60054	3.19336
C	1.95612	-3.17722	3.28216
H	1.39922	-3.99237	2.81451
H	2.89676	-3.06687	2.73804
H	2.19231	-3.47713	4.30403
C	-3.53523	0.68929	2.52539
H	-4.15219	1.58813	2.49440
H	-3.96953	-0.03924	1.83818
H	-3.59152	0.28092	3.53798

XYZ coordinatesof the structures involved in the “Heart” mechanism

Catalyst

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Et3NAlMe3

Al	1.42754	-0.32425	-0.21542
N	-0.65281	0.23436	-0.00721
C	-1.18533	-0.12201	1.34490
H	-2.17656	0.32968	1.46460
H	-0.52879	0.34820	2.07274
C	-1.25828	-1.61157	1.64592
H	-1.97993	-2.13330	1.01761
H	-0.28979	-2.09343	1.52899
C	-0.81186	1.70955	-0.22548
H	-1.87760	1.95420	-0.19172
H	-0.45960	1.91422	-1.23554
C	-0.07595	2.61065	0.75680
H	-0.46029	2.52258	1.77251
H	0.99264	2.41202	0.77309
C	-1.36730	-0.49438	-1.10630
H	-1.14332	-1.55110	-0.99153
H	-0.89424	-0.18205	-2.03849
C	-2.87895	-0.29999	-1.20275
H	-3.16192	0.72770	-1.42810
H	-3.39436	-0.60493	-0.29141
C	2.06490	0.95833	-1.59796
H	3.08608	0.67972	-1.88320
H	2.10704	2.00693	-1.28920
H	1.47646	0.91720	-2.52194
C	1.41142	-2.19793	-0.89019
H	0.86676	-2.92367	-0.27842
H	2.45055	-2.54779	-0.92045
H	1.03153	-2.28769	-1.91324

C	2.16384	-0.14082	1.62427
H	2.07577	0.85360	2.07128
H	3.23595	-0.36833	1.59270
H	1.72684	-0.85090	2.33460
H	-3.25398	-0.92605	-2.01411
H	-1.57261	-1.73883	2.68299
H	-0.21984	3.64569	0.44188

Initiator

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Initiator

S	-1.29920	1.51719	-0.31385
C	1.30551	0.44754	-0.56560
C	1.70059	-0.86928	-0.79489
C	1.98397	1.19018	0.40407
C	2.74598	-1.43619	-0.07157
H	1.18649	-1.45817	-1.54441
C	3.02779	0.62906	1.12527
H	1.67752	2.21068	0.60000
C	3.41215	-0.68920	0.89119
H	3.03851	-2.46106	-0.26359
H	3.54391	1.21924	1.87228
H	4.22567	-1.12753	1.45527
Al	-2.28086	-0.39071	0.15990
C	-1.66803	-2.06321	-0.65184
H	-0.79290	-2.44990	-0.12152
H	-2.44323	-2.83280	-0.61310
H	-1.37331	-1.93498	-1.69651
C	-3.79440	-0.26550	1.39076
H	-4.70281	-0.68024	0.94284
H	-3.60331	-0.84331	2.30093
H	-4.00703	0.76272	1.69014
C	0.17683	1.05755	-1.34850
H	-0.14122	0.39485	-2.15101
H	0.48786	1.99900	-1.80186

Epoxide

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Epoxide

C	2.14859	0.30310	-0.01844
H	2.31073	0.94292	-0.88195
H	2.98792	0.22164	0.66608
C	0.78626	0.09234	0.48297
H	0.64952	-0.15878	1.53201
C	-0.37508	0.77720	-0.16504
H	-0.19967	0.91134	-1.23024
H	-0.57161	1.73996	0.30448
Cl	-1.88832	-0.19944	0.00474
O	1.44573	-0.91282	-0.28350

TS_1

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TS-1

N	-3.02072	0.66730	-0.79893
C	-2.32275	1.70617	-0.05017
H	-2.49851	1.53180	1.01160

H	-1.25286	1.53888	-0.21506
C	-2.64656	3.16521	-0.39023
H	-3.69856	3.39330	-0.21315
H	-2.05180	3.83298	0.23619
H	-2.41994	3.39857	-1.43154
C	-2.71382	0.64087	-2.22904
H	-3.27273	-0.19658	-2.65123
H	-3.08113	1.54353	-2.74675
C	-1.23511	0.44449	-2.53875
H	-0.83557	-0.40602	-1.98476
H	-1.10200	0.25659	-3.60532
H	-0.63734	1.32232	-2.28720
C	-4.46850	0.64063	-0.57756
H	-4.85593	-0.19758	-1.15927
H	-4.95783	1.54389	-0.98058
C	-4.87092	0.45212	0.87938
H	-5.94810	0.28834	0.94254
H	-4.36587	-0.41190	1.31133
H	-4.64012	1.32474	1.49255
Al	-1.77199	-2.67704	0.40116
C	-1.97672	-1.91689	2.20351
H	-2.11926	-0.83432	2.13867
H	-2.85457	-2.31786	2.72119
H	-1.10194	-2.09321	2.83364
C	-3.31669	-2.80299	-0.81324
H	-3.09033	-2.38892	-1.80012
H	-3.57325	-3.85658	-0.97524
H	-4.20958	-2.30006	-0.43872
C	-0.19203	-3.71210	-0.16076
H	-0.44867	-4.77321	-0.26144
H	0.16184	-3.39340	-1.14717
H	0.64570	-3.63290	0.53466
Al	0.68193	1.57797	1.22896
C	1.29849	3.00134	0.03387
H	1.22718	2.72366	-1.02043
H	0.71552	3.91468	0.17822
H	2.34584	3.24910	0.22965
C	-0.16604	1.87734	2.96179
H	-0.89209	2.69405	2.91560
H	-0.68229	0.98379	3.31929
H	0.57354	2.15222	3.72053
S	0.95278	-0.53719	0.67944
C	1.96677	-0.53174	-0.87614
H	1.76737	-1.50366	-1.32706
H	1.58695	0.23263	-1.55028
C	3.43520	-0.35128	-0.62330
C	4.18452	-1.37551	-0.04010
C	4.07610	0.84105	-0.95607
C	5.53987	-1.20944	0.20636
H	3.69402	-2.30341	0.22906
C	5.43482	1.01136	-0.70852
H	3.50943	1.64238	-1.41382
C	6.17033	-0.01274	-0.12526
H	6.10733	-2.01397	0.65731
H	5.91734	1.94353	-0.97514
H	7.22773	0.11706	0.06757

Initiator and Catalyst Adduct

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59
Initiator & Catalyst Adduct
N          2.59082       0.69464       -0.35027
C          3.48855       1.87953       -0.14379
H          2.87115       2.76937       -0.24003
H          3.82060       1.85003        0.89327
C          4.68991       1.98394       -1.07734
H          4.39403       2.18627       -2.10635
H          5.31548       2.81482       -0.74791
H          5.30534       1.08463       -1.07095
C          3.31034      -0.61625       -0.11049
H          2.53611      -1.37282        0.00260
H          3.85836      -0.86766       -1.02181
C          4.26463      -0.67038        1.07258
H          3.79678      -0.36424        2.00337
H          4.58525      -1.70623        1.19268
H          5.15898      -0.06797        0.91548
C          2.09285       0.63297       -1.77468
H          1.48513      -0.26559       -1.85403
H          2.95938       0.47237       -2.42013
C          1.30287       1.83414       -2.26543
H          1.03715       1.65491       -3.30833
H          0.37687       1.96949       -1.71208
H          1.87640       2.76038       -2.22676
Al        -0.23387      -2.80732       -0.30930
C          0.80885      -2.88825       -2.00780
H          1.86959      -2.63477       -1.91972
H          0.77311      -3.91792       -2.38345
H          0.38244      -2.26036       -2.79731
C          0.72751      -3.36335        1.34007
H          0.23254      -3.01038        2.25022
H          0.75003      -4.45799        1.40075
H          1.76869      -3.02993        1.39446
C         -2.10801      -3.44876       -0.45733
H         -2.10711      -4.51808       -0.69908
H         -2.68864      -3.34476        0.46479
H         -2.66073      -2.94531       -1.25627
Al         1.00984       0.87564        0.99954
C          1.42514       0.07756        2.74820
H          2.18972       0.62784        3.30566
H          0.51222       0.13640        3.35215
H          1.70823      -0.97501        2.72098
C          0.49828       2.78103        1.09929
H          1.30726       3.39425        1.51046
H          0.17625       3.24517        0.16543
H         -0.33288       2.87825        1.80587
S         -0.62268      -0.35870       -0.09825
C         -2.00895      -0.19205        1.14109
H         -2.24648      -1.19820        1.47691
H         -1.63905       0.36929        1.99746
C         -3.20237       0.48068        0.53090
C         -4.21295      -0.27369       -0.06506
C         -3.30975       1.87191        0.52981
C         -5.30973       0.35039       -0.64763
H         -4.13480      -1.35345       -0.07805
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C	-4.40511	2.49729	-0.05194
H	-2.52698	2.46816	0.98252
C	-5.40921	1.73742	-0.64358
H	-6.08751	-0.24843	-1.10488
H	-4.47623	3.57787	-0.04182
H	-6.26412	2.22344	-1.09660

TS_2

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TS-2

N	3.77765	-0.36995	0.35837
C	4.83096	-1.13199	-0.35074
H	4.62560	-2.19036	-0.19833
H	4.69422	-0.95880	-1.41534
C	6.28005	-0.82174	0.03277
H	6.46438	-0.94859	1.10021
H	6.94640	-1.50182	-0.50109
H	6.56704	0.19538	-0.23675
C	3.94243	1.09383	0.17783
H	3.10710	1.57272	0.68687
H	4.84584	1.43135	0.70449
C	4.00578	1.58043	-1.26309
H	3.16102	1.23198	-1.85229
H	3.99310	2.67159	-1.26861
H	4.91904	1.26196	-1.76626
C	3.75853	-0.62803	1.82292
H	2.79138	-0.27481	2.18846
H	4.51895	-0.00730	2.31736
C	3.96910	-2.07446	2.25205
H	3.73789	-2.16241	3.31503
H	3.32206	-2.76171	1.71474
H	5.00153	-2.39601	2.11593
Al	1.39736	-1.09796	-0.61232
C	2.21587	-1.53789	-2.36248
H	2.94987	-2.34357	-2.26681
H	1.45084	-1.89949	-3.05496
H	2.72326	-0.70557	-2.85637
C	0.96018	-2.47815	0.73856
H	1.15850	-2.17415	1.76829
H	-0.11023	-2.69499	0.68356
H	1.48175	-3.42462	0.56824
C	0.74295	0.75886	-0.17418
H	-0.34427	0.71981	-0.25365
H	1.02155	1.04274	0.83817
H	1.19014	1.43161	-0.90738
Al	-0.34755	3.05661	-0.38709
C	0.38319	3.80662	1.27668
H	1.47741	3.81249	1.25079
H	0.05990	4.84354	1.41286
H	0.08399	3.25854	2.17354
C	0.33044	3.54654	-2.16769
H	-0.06666	4.51675	-2.48125
H	1.42195	3.62219	-2.18665
H	0.04114	2.82320	-2.93602
S	-2.53328	2.59213	-0.47665
C	-3.03728	2.34444	1.29569

H	-2.42855	2.98689	1.92938
H	-4.06660	2.69547	1.35549
C	-2.94116	0.91110	1.72964
C	-1.77643	0.41867	2.32191
C	-4.00081	0.02871	1.51329
C	-1.66802	-0.91896	2.67910
H	-0.94445	1.08934	2.49603
C	-3.90010	-1.30888	1.87721
H	-4.90518	0.38953	1.03876
C	-2.73091	-1.78892	2.45775
H	-0.75277	-1.28585	3.12406
H	-4.73148	-1.97701	1.69282
H	-2.64670	-2.83153	2.73733
C	-1.45343	-0.75347	-2.47497
C	-1.99652	-1.31694	-1.24318
O	-0.61483	-1.54491	-1.60325
H	-1.67099	-1.22417	-3.42719
H	-1.21706	0.30376	-2.50174
H	-2.14383	-0.65309	-0.39965
C	-2.83595	-2.55849	-1.25908
H	-2.80069	-3.06468	-0.29776
H	-2.51350	-3.23291	-2.04903
Cl	-4.56036	-2.12957	-1.57054

IM_1

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IM-1

N	4.18529	-0.43394	0.42933
C	5.22927	-0.88996	-0.49343
H	5.07697	-1.95503	-0.66836
H	5.05323	-0.41103	-1.45703
C	6.68012	-0.64673	-0.06106
H	6.91046	-1.14568	0.88207
H	7.36355	-1.03646	-0.81825
H	6.89434	0.41640	0.06220
C	4.16127	1.01603	0.63045
H	3.29558	1.23422	1.26227
H	5.03772	1.36234	1.20483
C	4.05757	1.82341	-0.65798
H	3.27539	1.42734	-1.30579
H	3.81502	2.86147	-0.42565
H	4.99279	1.82425	-1.21893
C	4.18158	-1.11916	1.72464
H	3.27196	-0.80299	2.24339
H	5.02260	-0.78955	2.35939
C	4.19602	-2.63959	1.63061
H	3.97916	-3.06874	2.61018
H	3.44015	-2.99631	0.93147
H	5.16679	-3.02272	1.31340
Al	0.91505	-1.38450	-0.71367
C	2.00154	-1.90806	-2.26761
H	3.06620	-1.74951	-2.08380
H	1.87010	-2.96431	-2.52298
H	1.74342	-1.32730	-3.16008
C	0.67352	-2.51217	0.88896
H	1.22726	-2.13508	1.75299

H	-0.37977	-2.54190	1.18501
H	0.99297	-3.54596	0.72903
C	0.67243	0.59085	-0.41955
H	-0.30782	0.70589	0.04322
H	1.46292	0.96542	0.22400
H	0.73138	1.02281	-1.42135
Al	-0.06515	2.96827	-0.54276
C	0.69313	3.61228	1.15362
H	1.78659	3.58938	1.11558
H	0.40187	4.65013	1.34440
H	0.39030	3.02939	2.02664
C	0.67747	3.49456	-2.28604
H	0.51772	4.56260	-2.46409
H	1.75484	3.31416	-2.34233
H	0.21100	2.96279	-3.12089
S	-2.29478	2.71864	-0.66812
C	-2.85157	2.62392	1.10356
H	-2.17991	3.22475	1.71407
H	-3.83234	3.09723	1.12363
C	-2.93680	1.21971	1.62737
C	-1.85405	0.63130	2.28549
C	-4.09632	0.46212	1.45067
C	-1.92317	-0.67754	2.74688
H	-0.94783	1.20397	2.43657
C	-4.17404	-0.84403	1.91977
H	-4.94144	0.89765	0.93151
C	-3.08560	-1.42069	2.56646
H	-1.06928	-1.11804	3.24442
H	-5.08181	-1.41354	1.76897
H	-3.14309	-2.43805	2.93272
C	-1.76350	-0.84553	-2.33195
C	-2.24017	-1.39663	-1.06903
O	-0.89711	-1.71502	-1.54561
H	-2.07571	-1.29112	-3.26847
H	-1.46454	0.19473	-2.35486
H	-2.26134	-0.74038	-0.20811
C	-3.15357	-2.58452	-1.03201
H	-3.14099	-3.05733	-0.05353
H	-2.87833	-3.30397	-1.79981
Cl	-4.84536	-2.05640	-1.35433

TS_3

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TS-3

N	4.16420	-0.18261	0.40267
C	5.23405	-0.35801	-0.58094
H	5.06614	-1.30766	-1.08943
H	5.10879	0.40585	-1.34925
C	6.66978	-0.31140	-0.04369
H	6.84700	-1.09070	0.69996
H	7.37974	-0.46282	-0.85948
H	6.89748	0.65049	0.41974
C	4.13683	1.12986	1.04553
H	3.24146	1.15409	1.67429
H	4.98763	1.26872	1.73564
C	4.08576	2.30134	0.07241

H	3.30976	2.14986	-0.67918
H	3.86106	3.22121	0.61360
H	5.03364	2.44814	-0.44661
C	4.07243	-1.24187	1.40880
H	3.13659	-1.07727	1.95233
H	4.87784	-1.15903	2.16015
C	4.06761	-2.65556	0.84120
H	3.80243	-3.36345	1.62793
H	3.33798	-2.75797	0.03857
H	5.04488	-2.94699	0.45401
Al	0.54518	-1.78645	-1.08656
C	1.75363	-2.26502	-2.56710
H	2.79688	-2.05707	-2.30793
H	1.69413	-3.32333	-2.83887
H	1.53374	-1.68884	-3.47241
C	0.36923	-2.92476	0.52665
H	1.11479	-2.66601	1.28495
H	-0.60905	-2.82348	1.00591
H	0.50642	-3.98495	0.29252
C	0.76364	0.20346	-0.57174
H	-0.12792	0.40792	0.02556
H	1.68940	0.33675	-0.01860
H	0.82134	0.67643	-1.55376
Al	0.03031	2.52347	-0.57074
C	0.68791	3.31208	1.10586
H	1.26715	2.60683	1.70630
H	1.35143	4.14950	0.87127
H	-0.11003	3.70438	1.74134
C	0.62518	3.13221	-2.34288
H	0.36764	4.18560	-2.49007
H	1.70949	3.04308	-2.45777
H	0.16617	2.57743	-3.16713
S	-2.27310	2.27820	-0.73271
C	-2.93012	2.22077	1.01001
H	-2.46058	3.05520	1.52979
H	-3.99222	2.43841	0.91541
C	-2.71943	0.93457	1.75561
C	-1.47744	0.61405	2.31030
C	-3.76462	0.02321	1.89861
C	-1.27297	-0.60449	2.94279
H	-0.66272	1.32182	2.24343
C	-3.56568	-1.19587	2.53797
H	-4.73623	0.25901	1.48754
C	-2.31541	-1.51993	3.05070
H	-0.29750	-0.84461	3.34517
H	-4.38939	-1.89287	2.62992
H	-2.15243	-2.47443	3.53391
C	-2.02239	-0.08020	-2.03408
C	-2.23055	-1.14863	-1.06285
O	-1.21811	-1.79449	-1.82064
H	-2.66021	-0.02991	-2.90729
H	-1.09617	0.44237	-2.06813
H	-1.96781	-0.93205	-0.02996
C	-3.53237	-1.92828	-1.17992
H	-3.62491	-2.63998	-0.36429
H	-3.54731	-2.45266	-2.13222
Cl	-4.99078	-0.86766	-1.14598

IM_2

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69
IM-2
N          3.69624      -0.21854      -0.32954
C          3.98797       1.24245      -0.14497
H          3.06371       1.78577      -0.34459
H          4.20002       1.39687       0.91450
C          5.12662       1.79746      -0.99221
H          5.00067       1.58254      -2.05705
H          5.13487       2.88424      -0.87868
H          6.10713       1.42610      -0.68123
C          4.93121      -1.04422      -0.11436
H          4.64442      -2.08716      -0.27050
H          5.65067      -0.79040      -0.90058
C          5.59046      -0.88241       1.24811
H          4.91732      -1.11699       2.07685
H          6.43219      -1.57709       1.30682
H          5.98240       0.12554       1.40199
C          3.21595      -0.52846      -1.72471
H          2.74514      -1.51789      -1.67420
H          4.09776      -0.64437      -2.36611
C          2.27382       0.48672      -2.35979
H          1.87097       0.04914      -3.27739
H          1.42850       0.76436      -1.72949
H          2.79161       1.40710      -2.63696
Al        -1.21665       2.78532      -0.49121
C          0.77519       3.04177      -0.18650
H          1.19475       2.13751       0.28056
H          1.34303       3.24138      -1.10812
H          0.97561       3.86935       0.50790
C         -2.21863       4.50631      -0.42545
H         -1.88628       5.20705      -1.20541
H         -3.29768       4.35441      -0.56576
H         -2.09026       5.01558       0.53986
C         -1.55981       1.75254      -2.19676
H         -2.54857       1.27070      -2.20324
H         -1.54384       2.44509      -3.05093
H         -0.81495       0.97134      -2.40964
Al         2.33827      -0.87402       1.09257
C          2.58938      -2.82580       1.22214
H          3.52684      -3.10068       1.71963
H          1.78286      -3.25532       1.83110
H          2.56994      -3.35204       0.25922
C          2.33380       0.35217       2.61843
H          3.33839       0.53726       3.01738
H          1.89641       1.32665       2.37086
H          1.74432      -0.06727       3.44323
S          0.17954      -0.62847       0.08628
C         -0.25401      -2.29406      -0.58371
H          0.35596      -2.38871      -1.48647
H          0.06227      -3.05396       0.13310
C         -1.72217      -2.39538      -0.88772
C         -2.26569      -1.74409      -1.99741
C         -2.57045      -3.08108      -0.01533
C         -3.63828      -1.75728      -2.21599
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H	-1.62226	-1.17937	-2.66537
C	-3.94581	-3.09693	-0.23479
H	-2.15593	-3.59986	0.84593
C	-4.48182	-2.42717	-1.33135
H	-4.04991	-1.22183	-3.06488
H	-4.59744	-3.62274	0.45560
H	-5.55471	-2.41956	-1.49218
C	-0.99426	-0.43815	1.47631
C	-2.16851	0.47032	1.02256
O	-1.73271	1.75343	0.93373
H	-0.45482	0.07663	2.27486
H	-1.28242	-1.44110	1.80530
H	-2.55897	0.07494	0.06797
C	-3.28231	0.30863	2.06355
H	-3.52254	-0.74353	2.23654
H	-2.99478	0.79428	2.99849
Cl	-4.80494	1.08747	1.51645

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Al	0.32670	-1.21166	1.31726
C	-0.10081	-2.90860	0.23815
H	0.87683	-3.32137	0.09535
H	-0.66474	-3.54523	0.88705
H	-0.59721	-2.83130	-0.70649
C	0.85293	-2.19143	2.88895
H	1.83310	-1.91118	3.21436
H	0.14067	-1.94380	3.64820
H	0.82558	-3.24546	2.70499
S	-1.79811	-1.24852	0.80647
C	-2.16638	-1.01942	-0.92031
H	-1.70887	-0.11579	-1.26617
H	-1.78473	-1.84853	-1.47871
C	-3.69162	-0.92895	-1.11401
C	-4.33290	0.31603	-1.05943
C	-4.43830	-2.09212	-1.34631
C	-5.72017	0.39779	-1.23984
H	-3.76352	1.20351	-0.88055
C	-5.82607	-2.01031	-1.52561
H	-3.94893	-3.04305	-1.38687
C	-6.46689	-0.76555	-1.47235
H	-6.20989	1.34837	-1.20084
H	-6.39575	-2.89822	-1.70365
H	-7.52627	-0.70289	-1.60922
C	-2.26147	0.14594	1.74505
C	-1.20233	1.16403	1.28763
O	0.09891	0.60126	1.54087
H	-2.18320	-0.03022	2.79738
H	-3.26425	0.45172	1.53145
H	-1.26669	1.26193	0.22418
C	-1.42173	2.54243	1.93736
H	-0.66710	3.22104	1.59815
H	-1.36404	2.44828	3.00163
Cl	-3.00826	3.15650	1.48720
N	3.80010	-0.61029	-0.20499

C	3.75639	-1.74452	0.72496
H	3.75030	-1.33006	1.73477
H	2.79771	-2.25346	0.59985
C	4.84941	-2.81763	0.61922
H	4.82825	-3.31809	-0.34997
H	5.85009	-2.41550	0.76646
H	4.67486	-3.57880	1.38255
C	3.96461	-0.97466	-1.61158
H	4.00210	-0.04519	-2.18409
H	4.92003	-1.48592	-1.80502
C	2.82171	-1.83566	-2.13794
H	1.86042	-1.35093	-1.96503
H	2.93875	-1.99375	-3.21158
H	2.79141	-2.81681	-1.66324
C	4.64148	0.50685	0.22709
H	4.26524	0.84769	1.19496
H	4.47010	1.32852	-0.47343
C	6.15823	0.28881	0.32171
H	6.65331	1.24464	0.50790
H	6.42185	-0.38220	1.13898
H	6.56433	-0.12192	-0.60419
Al	2.09893	2.42007	-1.37776
C	2.06791	3.24268	0.39880
H	1.71547	2.51825	1.13782
H	3.04316	3.62240	0.71277
H	1.37307	4.09092	0.42230
C	3.51518	2.85564	-2.67416
H	3.70368	2.05251	-3.39156
H	3.19752	3.72530	-3.26379
H	4.46701	3.12665	-2.21048
C	0.58938	1.30686	-1.96442
H	0.71711	0.87131	-2.95744
H	0.46347	0.48998	-1.25005
H	-0.34647	1.87599	-1.96778

Reformed Catalyst and Monomeric Species

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Monomeric Species and Catalyst

Al	0.62549	-2.49797	0.00103
C	0.71246	-2.69717	1.95773
H	-0.15944	-3.24856	2.32279
H	1.59320	-3.25923	2.28496
H	0.71950	-1.73789	2.48289
C	0.13019	-4.00296	-1.15589
H	-0.95274	-4.16817	-1.12685
H	0.39337	-3.82655	-2.20265
H	0.59972	-4.94229	-0.84981
S	2.97216	-1.73179	-0.61695
C	3.60126	-1.04074	0.98159
H	2.75369	-0.68222	1.56023
H	4.00946	-1.91281	1.49185
C	4.63215	0.02772	0.77768
C	4.28218	1.37300	0.89210
C	5.94633	-0.30341	0.44225
C	5.22738	2.36984	0.67655
H	3.26494	1.64531	1.14516

C	6.89178	0.69019	0.23074
H	6.22573	-1.34586	0.34333
C	6.53347	2.03074	0.34587
H	4.93935	3.40940	0.76503
H	7.90890	0.42042	-0.02376
H	7.27053	2.80573	0.17871
C	2.25471	-0.25120	-1.40560
C	0.94571	0.15793	-0.71584
O	0.08907	-0.93934	-0.62316
H	2.04984	-0.55785	-2.43297
H	3.00008	0.54135	-1.41581
H	1.18160	0.56560	0.27787
C	0.21828	1.25195	-1.48752
H	-0.71598	1.49043	-0.99143
H	0.02406	0.94338	-2.51331
Cl	1.18138	2.78127	-1.54807
N	-4.08054	-0.18077	0.10657
C	-3.23374	-0.52499	-1.07757
H	-3.18881	0.36293	-1.70397
H	-2.22038	-0.68753	-0.71760
C	-3.69102	-1.71504	-1.91619
H	-4.62819	-1.52100	-2.43918
H	-2.92860	-1.92186	-2.66866
H	-3.81657	-2.62138	-1.32334
C	-4.12701	-1.29806	1.11624
H	-4.49953	-0.85676	2.04140
H	-4.88051	-2.02174	0.78909
C	-2.82632	-2.03942	1.38506
H	-2.01408	-1.37334	1.65313
H	-2.99023	-2.72063	2.22177
H	-2.51529	-2.64327	0.53300
C	-5.50902	0.07130	-0.27972
H	-6.03794	0.30873	0.64257
H	-5.93213	-0.86601	-0.65421
C	-5.74783	1.17330	-1.29929
H	-6.82173	1.24066	-1.48239
H	-5.40569	2.14275	-0.94639
H	-5.26485	0.96744	-2.25458
Al	-3.28847	1.58513	1.04812
C	-2.93946	2.90447	-0.41531
H	-2.88376	2.51679	-1.43680
H	-3.70738	3.68566	-0.42796
H	-1.98807	3.41624	-0.23121
C	-4.78318	2.08257	2.26515
H	-5.10707	1.28748	2.94563
H	-4.44660	2.90667	2.90528
H	-5.67575	2.44624	1.74515
C	-1.60991	1.05846	1.97813
H	-1.10110	1.98801	2.26184
H	-1.76228	0.49359	2.90280
H	-0.90766	0.49330	1.36034

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N	-5.15054	-0.59185	-0.13047

C	-5.99920	-0.93534	-1.27552
H	-6.06862	-0.05493	-1.91446
H	-5.47030	-1.68172	-1.86887
C	-7.40940	-1.44494	-0.95502
H	-7.98853	-0.70815	-0.39532
H	-7.94749	-1.65579	-1.88146
H	-7.38516	-2.36581	-0.36960
C	-4.83031	-1.72881	0.73453
H	-4.13148	-1.36367	1.49245
H	-5.71515	-2.07629	1.29516
C	-4.20487	-2.91156	0.00481
H	-3.40100	-2.58349	-0.65433
H	-3.78793	-3.61406	0.72802
H	-4.93399	-3.45595	-0.59630
C	-5.64637	0.52677	0.67589
H	-4.85274	0.77674	1.38595
H	-6.51727	0.23095	1.28652
C	-6.00261	1.77080	-0.12803
H	-6.15571	2.61260	0.54923
H	-5.20135	2.03453	-0.81783
H	-6.92160	1.64082	-0.70106
Al	-2.02385	0.82263	-1.19119
C	-2.76398	0.25525	-2.92315
H	-3.77504	-0.14292	-2.81495
H	-2.81596	1.08269	-3.63784
H	-2.16045	-0.53270	-3.38707
C	-2.48362	2.52619	-0.30514
H	-3.13460	2.38405	0.56169
H	-1.58194	3.02542	0.06316
H	-2.98960	3.22697	-0.97538
C	-1.39943	-0.64373	0.03646
H	-0.57004	-0.22434	0.60616
H	-2.21368	-0.94978	0.68659
H	-1.09792	-1.45019	-0.63614
Al	-0.14887	-2.44026	1.13319
C	-1.14524	-2.53325	2.82606
H	-2.16488	-2.88938	2.64982
H	-0.67563	-3.23901	3.51875
H	-1.22506	-1.57725	3.34878
C	-0.26319	-3.85650	-0.22654
H	0.19158	-4.78075	0.14353
H	-1.29957	-4.08778	-0.48896
H	0.26010	-3.59637	-1.15163
S	1.78550	-1.29178	0.85153
C	1.83398	-0.24843	2.37684
H	1.19162	-0.72611	3.11438
H	2.85959	-0.31230	2.73739
C	1.43859	1.18567	2.17363
C	0.11316	1.59578	2.33684
C	2.38606	2.13970	1.79702
C	-0.25784	2.91761	2.12287
H	-0.63545	0.87193	2.63292
C	2.02171	3.46534	1.59194
H	3.41632	1.83736	1.65346
C	0.69675	3.85886	1.75019
H	-1.29185	3.21224	2.24422
H	2.77239	4.18706	1.29742

H	0.40985	4.89075	1.59086
C	1.48931	0.41182	-1.26156
C	0.80259	1.73463	-1.07943
O	-0.29308	1.49232	-1.89366
H	2.47678	0.33880	-1.70785
H	0.82871	-0.41805	-1.41220
H	0.53643	1.90353	-0.03875
C	1.57837	3.05531	-1.55508
H	1.19894	3.85963	-0.93042
H	1.34905	3.25185	-2.59996
Cl	3.37104	3.03564	-1.37975
C	4.95082	-0.82600	0.76930
C	5.14776	-0.87331	-0.66890
O	4.15224	-0.02804	-0.12806
H	4.41905	-1.63685	1.25287
H	5.64647	-0.26548	1.38525
H	6.00186	-0.31584	-1.04943
C	4.95603	-2.09651	-1.58550
H	5.20341	-1.67947	-2.55974
H	4.12126	-2.78659	-1.68615
Cl	6.39542	-3.04404	-1.03951

TS_5

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N	-5.11939	-0.62319	-0.14244
C	-5.96098	-0.96677	-1.29268
H	-6.03826	-0.08208	-1.92475
H	-5.42222	-1.70252	-1.89043
C	-7.36639	-1.49436	-0.98038
H	-7.95516	-0.76849	-0.41650
H	-7.89951	-1.70366	-1.91004
H	-7.33369	-2.41959	-0.40227
C	-4.78913	-1.76348	0.71437
H	-4.09651	-1.39680	1.47723
H	-5.67168	-2.12514	1.26962
C	-4.14867	-2.93341	-0.02295
H	-3.34659	-2.59126	-0.67710
H	-3.72608	-3.63708	0.69583
H	-4.87006	-3.48091	-0.63052
C	-5.62976	0.48341	0.67139
H	-4.84094	0.73636	1.38573
H	-6.49909	0.17316	1.27708
C	-5.99737	1.72987	-0.12360
H	-6.16164	2.56447	0.55993
H	-5.19711	2.00790	-0.80892
H	-6.91326	1.59443	-0.70033
Al	-2.00544	0.83396	-1.18268
C	-2.73438	0.27242	-2.92127
H	-3.74131	-0.13767	-2.81921
H	-2.79343	1.10495	-3.62948
H	-2.12091	-0.50511	-3.38972
C	-2.48642	2.52520	-0.28439
H	-3.13824	2.36898	0.57937
H	-1.59133	3.03133	0.09053
H	-2.99816	3.22576	-0.95048

C	-1.36842	-0.63527	0.03503
H	-0.54531	-0.21140	0.61048
H	-2.18110	-0.95544	0.68030
H	-1.05617	-1.43295	-0.64312
Al	-0.10130	-2.42682	1.12102
C	-1.10137	-2.54427	2.81016
H	-2.11654	-2.91013	2.62810
H	-0.62599	-3.25031	3.49856
H	-1.19320	-1.59338	3.34026
C	-0.19619	-3.83319	-0.25032
H	0.26766	-4.75532	0.11365
H	-1.22923	-4.07370	-0.51762
H	0.32679	-3.55989	-1.17180
S	1.87175	-1.24439	0.86275
C	1.85364	-0.22310	2.38791
H	1.21461	-0.71390	3.11974
H	2.87901	-0.27890	2.75097
C	1.44329	1.20794	2.19505
C	0.11294	1.60215	2.35766
C	2.38124	2.17528	1.82882
C	-0.27196	2.92151	2.15317
H	-0.62850	0.86778	2.64574
C	2.00293	3.49845	1.63330
H	3.41517	1.88543	1.68587
C	0.67329	3.87614	1.79082
H	-1.30949	3.20379	2.27385
H	2.74647	4.23070	1.34675
H	0.37551	4.90606	1.63890
C	1.51224	0.46226	-1.24601
C	0.81042	1.77591	-1.05516
O	-0.28014	1.52822	-1.87474
H	2.50169	0.40374	-1.69004
H	0.86119	-0.37352	-1.40542
H	0.53958	1.93361	-0.01415
C	1.57302	3.10886	-1.51823
H	1.18302	3.90393	-0.88822
H	1.34454	3.31125	-2.56212
Cl	3.36532	3.10745	-1.33777
C	4.41564	-1.50689	0.79011
C	4.90703	-0.93475	-0.47154
O	4.03054	0.08063	-0.62774
H	4.16252	-2.54755	0.92852
H	4.50974	-0.88834	1.66904
H	5.94900	-0.58543	-0.32125
C	5.00731	-2.00542	-1.58003
H	5.25279	-1.57771	-2.55008
H	4.18024	-2.70344	-1.68856
Cl	6.45536	-2.94122	-1.03733

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N	4.85848	-1.34597	-0.50593
C	3.56609	-1.86361	0.03422
H	3.62584	-1.79068	1.11693
H	2.80339	-1.14923	-0.27236

C	3.12859	-3.26866	-0.36399
H	3.88695	-4.02023	-0.14044
H	2.23321	-3.52127	0.20505
H	2.87216	-3.33426	-1.42033
C	4.86803	-1.27508	-2.00790
H	3.87008	-0.96332	-2.31013
H	5.54237	-0.46171	-2.27875
C	5.28673	-2.51800	-2.79490
H	4.70219	-3.40211	-2.55061
H	5.13953	-2.30558	-3.85565
H	6.34099	-2.75717	-2.65782
C	6.04561	-2.11130	-0.02313
H	6.91594	-1.64722	-0.48779
H	5.99182	-3.13719	-0.39454
C	6.24011	-2.14286	1.48540
H	7.14978	-2.70586	1.70167
H	6.35443	-1.14571	1.90314
H	5.41811	-2.63943	2.00110
Al	4.92201	0.71922	0.09926
C	4.18596	0.77905	1.94713
H	3.12058	0.52987	1.98388
H	4.69017	0.15005	2.68577
H	4.27389	1.80791	2.31852
C	6.85450	1.13844	-0.11939
H	7.24503	0.91961	-1.11955
H	7.00809	2.21255	0.03529
H	7.50619	0.62913	0.59795
C	3.70336	1.57188	-1.22549
H	3.45010	2.58493	-0.89408
H	4.13759	1.67449	-2.22465
H	2.75004	1.04609	-1.34634
Al	-0.09572	-0.70035	0.62008
C	-0.01656	-1.18876	-1.29058
H	0.98608	-1.03108	-1.70092
H	-0.26665	-2.23896	-1.47111
H	-0.69013	-0.56999	-1.88845
C	0.38303	-2.00940	2.01166
H	1.46766	-2.08322	2.13228
H	-0.01898	-1.72017	2.98679
H	0.01509	-3.01778	1.79356
S	-2.61647	-0.78040	1.13137
C	-3.26701	-1.93115	-0.15237
H	-2.93393	-1.58647	-1.12901
H	-2.74580	-2.86435	0.06355
C	-4.75643	-2.09347	-0.08249
C	-5.58090	-1.46600	-1.01465
C	-5.34143	-2.84923	0.93594
C	-6.96388	-1.59033	-0.93447
H	-5.14420	-0.87193	-1.80765
C	-6.72048	-2.97828	1.01533
H	-4.70913	-3.33135	1.67218
C	-7.53640	-2.34677	0.07980
H	-7.59009	-1.09215	-1.66333
H	-7.16102	-3.57094	1.80698
H	-8.61249	-2.44523	0.14371
C	0.35052	2.11395	0.36279
O	0.33248	0.91455	1.07930

H	0.82887	1.99449	-0.61692
C	1.18078	3.09299	1.18586
H	2.16130	2.66507	1.36481
H	0.69996	3.30940	2.13825
Cl	1.43806	4.67281	0.33820
C	-3.46442	0.77778	0.72519
C	-3.07821	1.42150	-0.60844
O	-1.69396	1.65587	-0.74189
H	-3.23766	1.43659	1.56329
H	-4.53493	0.57740	0.74608
H	-3.31276	0.72643	-1.41621
C	-3.86440	2.70958	-0.86931
H	-3.48960	3.17933	-1.77528
H	-3.79021	3.40983	-0.03961
Cl	-5.62052	2.37961	-1.12536
C	-1.06872	2.60954	0.12456
H	-1.07159	3.59616	-0.34427
H	-1.57887	2.67290	1.09097

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N	3.66021	-1.80759	-1.37813
C	2.99602	-3.10431	-1.51150
H	2.48868	-3.33010	-0.56934
H	2.20255	-2.98337	-2.25003
C	3.85968	-4.31735	-1.88726
H	4.60907	-4.53219	-1.12319
H	3.22391	-5.20137	-1.97624
H	4.37985	-4.17974	-2.83473
C	3.76503	-1.00824	-2.59374
H	2.76877	-0.94766	-3.03854
H	4.02393	0.00978	-2.28713
C	4.76371	-1.46393	-3.66803
H	4.46778	-2.41144	-4.11935
H	4.81726	-0.71888	-4.46561
H	5.76759	-1.58220	-3.25570
C	4.85909	-1.79323	-0.55187
H	5.28425	-0.79062	-0.61689
H	5.64116	-2.47521	-0.92093
C	4.57463	-2.11469	0.91089
H	5.48617	-2.02836	1.50552
H	3.81092	-1.44052	1.31018
H	4.19621	-3.12926	1.04473
Al	4.84466	0.94939	2.28229
C	3.06106	1.02289	3.09385
H	2.26846	0.84828	2.36188
H	2.94337	0.30161	3.90683
H	2.87977	2.01669	3.52206
C	6.37111	0.21834	3.28307
H	6.81672	0.99167	3.92038
H	6.07904	-0.60077	3.94609
H	7.16850	-0.14377	2.62815
C	5.15111	1.75719	0.51223
H	5.04838	2.84777	0.54989
H	6.14819	1.54460	0.11812

H	4.42215	1.40511	-0.22372
Al	0.14421	-0.75285	0.11245
C	-0.21050	-1.35559	-1.72899
H	0.64812	-1.13209	-2.36791
H	-0.38492	-2.43348	-1.79666
H	-1.06418	-0.84058	-2.17470
C	0.69296	-2.00003	1.53082
H	0.71374	-1.50798	2.50719
H	0.01364	-2.85595	1.61173
H	1.69004	-2.40794	1.35370
S	-2.26392	-0.56098	1.09094
C	-3.16587	-1.84972	0.13131
H	-3.00070	-1.67175	-0.92917
H	-2.64285	-2.76898	0.39676
C	-4.62412	-1.91695	0.47385
C	-5.57649	-1.36332	-0.38036
C	-5.04830	-2.50489	1.66743
C	-6.92765	-1.39622	-0.05179
H	-5.26359	-0.89800	-1.30688
C	-6.39597	-2.54327	1.99497
H	-4.31431	-2.92783	2.34320
C	-7.34024	-1.98676	1.13568
H	-7.65392	-0.95757	-0.72394
H	-6.71194	-3.00681	2.92091
H	-8.39139	-2.01467	1.39279
C	0.68429	2.02142	-0.39216
O	0.73018	0.86240	0.38161
H	1.04671	1.84076	-1.41381
C	1.60995	3.02908	0.28412
H	2.58927	2.58553	0.41631
H	1.21840	3.32838	1.25466
Cl	1.84266	4.53465	-0.69494
C	-3.11828	0.96178	0.58206
C	-2.87353	1.41274	-0.85965
O	-1.50780	1.56821	-1.18378
H	-2.78627	1.71606	1.29513
H	-4.18426	0.80959	0.74676
H	-3.22180	0.63140	-1.53750
C	-3.64215	2.69344	-1.19595
H	-3.36517	3.02584	-2.19329
H	-3.44366	3.48833	-0.47936
Cl	-5.42659	2.42069	-1.20017
C	-0.74136	2.55219	-0.48840
H	-0.77198	3.50304	-1.02634
H	-1.11298	2.70938	0.52897

Dimeric Species

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Dimeric Species

Al	1.42416	2.25477	0.35990
C	1.09716	2.07124	2.29314
H	1.94564	2.46459	2.86396
H	0.21810	2.63217	2.62612
H	0.96918	1.02840	2.59268
C	1.19678	3.99392	-0.52860
H	1.94607	4.71319	-0.18157

H	1.30281	3.91708	-1.61437
H	0.21764	4.44198	-0.32713
S	-0.68436	1.20946	-0.69800
C	-1.94632	1.42684	0.62706
H	-1.55156	1.01296	1.55254
H	-1.99793	2.50953	0.74593
C	-3.27720	0.83993	0.26145
C	-3.69741	-0.36460	0.82266
C	-4.10208	1.47533	-0.66937
C	-4.91854	-0.92570	0.46397
H	-3.06807	-0.87264	1.54263
C	-5.32250	0.91986	-1.02537
H	-3.77902	2.40674	-1.11924
C	-5.73361	-0.28474	-0.45995
H	-5.22780	-1.86422	0.90569
H	-5.95482	1.42537	-1.74416
H	-6.68480	-0.71913	-0.73979
C	3.30970	0.12320	0.04511
O	2.69351	1.30630	-0.36029
H	3.58888	0.15107	1.10786
C	4.58193	-0.00628	-0.78862
H	5.18264	0.89043	-0.66717
H	4.34419	-0.13956	-1.84259
Cl	5.61217	-1.40890	-0.28538
C	-0.58184	-0.60175	-0.84018
C	0.00002	-1.33685	0.36930
O	1.28025	-0.87912	0.74885
H	0.01796	-0.77232	-1.73412
H	-1.58690	-0.96733	-1.04731
H	-0.62550	-1.13371	1.23981
C	0.02037	-2.85376	0.16041
H	0.52621	-3.32328	1.00045
H	0.51937	-3.13212	-0.76589
Cl	-1.64659	-3.54141	0.08832
C	2.37432	-1.06338	-0.15249
H	2.87994	-2.00810	0.06157
H	2.04386	-1.06623	-1.19605