Electronic Supplementary Material (ESI) for ChemComm.

Supplementary Information

The importance of the Lewis base in lithium mediated metalation and bond cleavage reaction of allyl amines and allyl phosphines

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General Experimental:

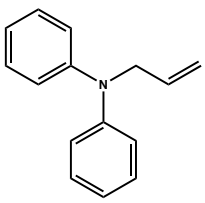
All reactions were performed under a nitrogen atmosphere and dry conditions. All synthesis and manipulations were undertaken with the use of air-sensitive Schleck line techniques. Hexane, tetrahydrofuran and diethylether were water and oxygen were removed from hexane, diethyl ether (Et_2O) and tetrahydrofuran (THF) using MBRAUN SPS-800 solvent purification system and stored over 4 Å molecular sieves under N_2.

Proton NMR were recorded on a BRUKER AVANCE DRX 400 (400 MHz) spectrometer. Chemical shifts were recorded on the δ scale in parts per million (ppm). Spectra were measuring in d-chloroform ($CDCl_3$) using the residual $CDCl_3$ (7.26 ppm) signal, d_6-benzene (C_6D_6) using the residual C_6D_6 (7.16 ppm) signal and d_8-tetrahydrofuran (d_8-THF) using the residual d_8-THF (1.73 and 3.58 ppm) signals. The residual signal of each solvent was used as an internal reference. The resonance was reported according to the following convention: chemical shift (δ ppm) [number of hydrogens, multiplicity, coupling constant, and assignment]. Multiplicities are designated as (s) = singlet, (bs) = broad singlet, (d) = doublet, (dd) = doublet of doublets, (t) = triple, (m) = multiplet. Coupling constants were recorded on Hz scale and are designated as $^2J_{HH}$ = germinal coupling constant, $^3J_{HH}$ = vicinal coupling constant, $^4J_{HH}$ = long range coupling constant.

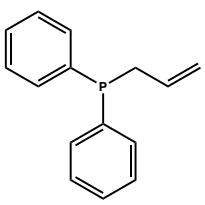
Carbon NMR were recorded at 100.6 MHz on a BRUKER AVANCE DRX 400 spectrometer. Chemical shifts were recorded on the δ scale in parts per million (ppm). Spectra were measuring in d-chloroform ($CDCl_3$) using the triplet carbon signal (77.16 ppm) signal, d_6-benzene (C_6D_6) using the triple carbon (128.06 ppm) signal and d_8-tetrahydrofuran (d_8-THF) using the pentent carbon (25.37 and 67.57 ppm) signals.

X-ray Crystallography: Crystallographic data for compounds **3, 5** and **6** were obtained on a Bruker X8 APEXII CCD diffractometer[1] equipped with an OXFORD Cryosystems 700 and cooled to 123(1) K. Data was collected with monochromatic (graphite) Mo Kα radiation (λ = 0.71073 Å) and processed using the Bruker Apex2 v2012.2.0 software; Lorentz, polarization and absorption corrections (multi-scan – SADABS)[2] were applied. Compounds **3, 5** and **6** were solved and refined with SHELX-97.[3] All non-hydrogen atoms were refined with anisotropic thermal parameters unless otherwise indicated and hydrogen atoms were placed in calculated positions using a riding model with C-H = 0.95-0.98 Å and U_{iso}(H)=xU_{iso}(C), x = 1.2 or 1.5. Data for **3, 5** and **6** has been deposited with the Cambridge Crystallographic Database with CCDC number 1452499, 1452498 and 1452869 respectively.

Compound Synthesis



Synthesis of $Ph_2NCH_2CH=CH_2$ 1: *n*BuLi (31.25 mL [1.6 M solution in hexane], 50 mmol) was added dropwise to a solution of diphenylamine (8.46g, 50 mmol) in THF (50 mL) at -78 °C. This solution was allowed to warm to room temperature overnight. Next, allyl bromide (4.3 mL, 50 mmol) was added at -78 °C and the solution stirred for 2 hours, warming to room temperature. The resulting solution was quenched with H_2O (30 mL), extracted with ethyl acetate (3 × 30 mL), washed with brine (30 mL) and dried with $MgSO_4$. All solvent was removed under vacuum to afford a yellow oil which was distilled under vacuum (B.p. 124 °C) to give the title compound as a colourless oil 7.3 g, 85 %. **^{1}H NMR (400.2 MHz, $CDCl_3$, 20 °C)** δ: 4.32 (2H, d, $^2J_{HH}$ = 4.8 Hz,N-C**H_2**), 5.20 (2H, dd, $^2J_{HH}$ = 8.8 Hz, CH=C**H_2**), 5.90 (1H, tt), 6.90 (2H, t, *para*-**H**), 7.0 (d, 4H *ortho*-**H**), 7.22 (4H, t, *meta*-**H**). **^{13}C NMR (100.6 MHz, $CDCl_3$, 20 °C)** δ**:** 53.75 (**C**H_2CH, s), 115.37 (**C**H=CH_2, s), 119.73 (*ortho*-**C**, s), 120.31 (*meta*-**C**, s), 128.17 (*para*-**C**, s), 133.28 (CH=**C**H_2, s), 146.84 (*quaternary*-**C**, s).



Synthesis of $Ph_2PCH_2CH=CH_2$ 2: *n*BuLi (31.25 mL [1.6 M solution in hexane], 50 mmol) was added dropwise to a solution of diphenylphosphine (8.75 mL, 50 mmol) in hexane (50 mL) at 0 °C to give the immediate formation of a bright yellow precipitate. The mother liquor was removed via cannular and the yellow solid washed with hexane (2 x 30 mL). The yellow solid was re-suspended in hexane, cooled to 0 °C and allyl bromine (4.23 mL, 50 mM) added. The solution was allowed to warm to room temperature overnight. The resulting solution was filtered (via filter canular) and the solid washed with hexane (2 x 20 mL). Removal of the solvent under vacuum, from the combined mother liquors, resulted in a colourless oil that was purified via vacuum distillation (b.p. 140 C) to give the title compound as a clear thick oil 9.4 g, 83 %. **^{1}H NMR (400.2 MHz, C_6D_6, 20 °C)** δ: 2.80 (2H, d, $^2J_{HH}$ = 7.6 Hz, P-C**H_2**), 4.99 (m, 2H, CH=C**H_2**), 5.85 (m, 1H, C**H**=CH_2), 7.14-7.16 (m, 6H, meta-H and para-H), 7.48 (m, 4H, ortho-H).**^{13}C NMR (100.6 MHz, $CDCl_3$, 20 °C)** δ: 32.61 (d, $J_{P,C}$ = 14.1 Hz,), 115.95 (d, $J_{P,C}$ = 10.1 Hz,), 127.2, 127.3 (d, $J_{P,C}$ = 14.1 Hz,), 131.8 (d, $J_{P,C}$ = 18.1 Hz,), 132.8 (d, $J_{P,C}$ = 17.1 Hz), 137.6 (d, $J_{P,C}$ = 16.1 Hz,). **^{31}P NMR (121.5 MHz, C_6D_6, 20 °C)** δ: -16.2

Attempted synthesis of **$[Ph_2NCHCH=CH_2Li(Et_2O)]$** and **$[Ph_2NCHCH=CH_2Li(THF)]$** resulted in the formation of bright red solutions that upon solvent removal under vacuum gave oily red residues. ^{1}H NMR spectroscopy of these oils showed multiple species that were difficult to characterize and rationally assign to chemically sensible products. All attempts to grow crystalline material failed using a variety and combination of solvent systems.

Synthesis of **$[Ph_2NCHCH=CH_2Li(TMEDA)]$ 5:** ^{n}BuLi (2.5 mL [1.6 M solution in hexane], 4 mmol) was added dropwise to a stirred solution of allyldiphenylamine (0.85g, 4 mmol) at -78 °C in 10 mL of hexane. The solution was allowed to warm slowly to room temperature. This resulted in a clear, yellow solution. After 2 hours of stirring at room temperature, TMEDA (0.4 mL, 4 mmol) was added dropwise at room temperature to give a red, oily solution. The volume was reduced by half and then placed in a freezer (-18°C). Crystals deposited of the title compound overnight 0.98 g, 62 %. **Microanalysis data:** Calculated for $C_{21}H_{30}LiN_3$: C, 75.64; H, 9.67; N, 12.07. Found: C, 75.69; H, 9.45; N, 12.07. **^{1}H NMR (400.2 MHz, C_6D_6, 20 °C)** δ: 1.662 (12 H, TMEDA-C**H_2**), 1.754 (4 H, TMEDA-C**H_3**), 1.96 (2H, d, $^2J_{HH}$ = 12.4 Hz, CH=C**H_2**), 4.58 (1H, d, $^2J_{HH}$ = 5.6 Hz, C**H**CH), 6.27 (1H, m, C**H**=CH_2), 6.77 (2H, t, $^3J_{HH}$ = 14 Hz, *para*-**H**), 7.14 (t, 4H, $^3J_{HH}$

= 7.8 Hz, *ortho*-**H**), 7.49 (4H, d, $^{3}J_{HH}$ = 8 Hz, *meta*-**H**). **^{13}C NMR (100.6 MHz, C_6D_6, 20 °C)** δ: 43.92 (TMEDA-**C**H_2), 45.9 (TMEDA-**C**H_3), 56.59 (C-C=**C**, s), 86.48 (C-**C**=C, s), 120.04 (*ortho*-**C**, s), 120.94 (*meta*-**C**, s), 128.79 (*para*-**C**,s), 133.4 (N-**C**, s), 148.62 (*quaternary*-**C**, s).**^{7}Li NMR (155.5 MHz, C_6D_6, 20 °C)**: δ 0.47 (s, br).

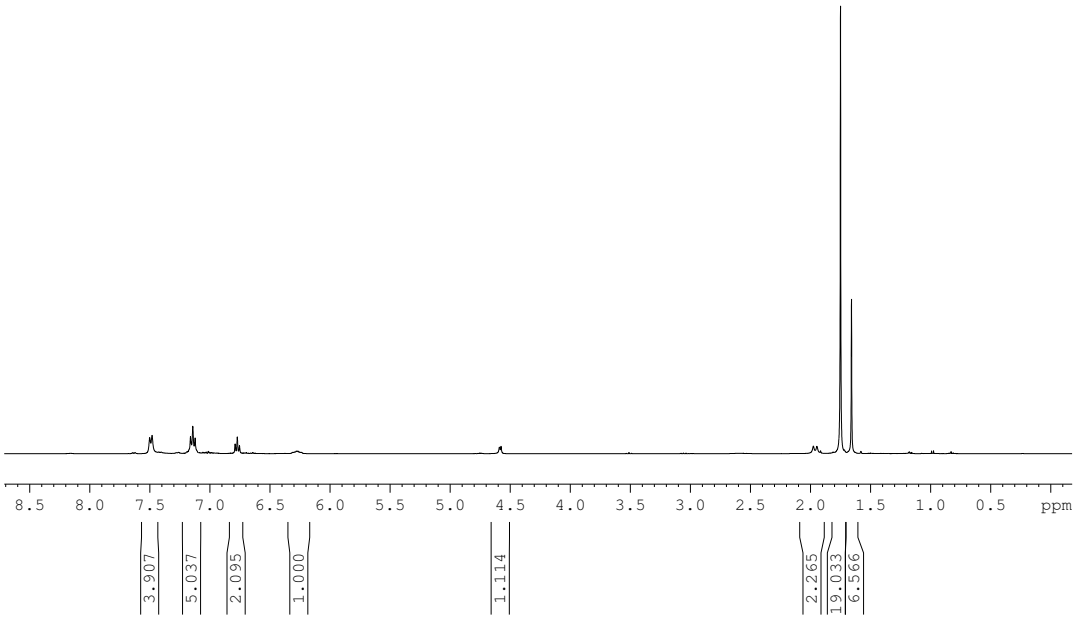


Figure S1 1H NMR of **[Ph_2NCHCH=CH_2Li(TMEDA)] 5 in C_6D_6**

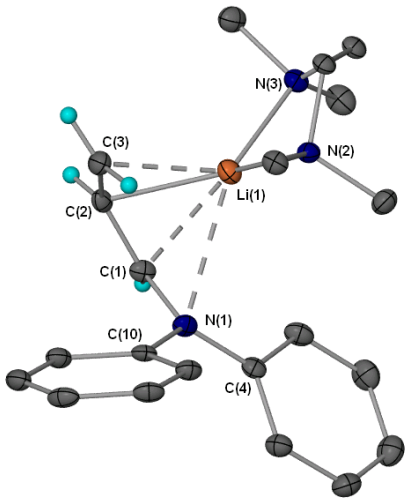


Figure S2 Molecular structure of **5** Hydrogen atoms (except allyl ones) omitted for clarity. Thermal ellipsoids show at 45%. Selected bond lengths (Å) and angles (°): N1-Li1, 2.599(3); N2-Li1, 2.0272(3); N3-Li1, 2.109(3); C1-Li1, 2.325(3); C2-Li1, 2.175(3); C3-Li1, 2.241(3); C4-N1-

C1, 117.26(14); N1-C1, 1.439(2); C1-C2, 1.384(2); C2-C3, 1.374(2); C10-N1-C1, 119.25(13); N2-Li1-N3, 87.50(13).

Crystallographic data for $C_{21}H_{30}LiN_3$ **5**: *M* = 331.42, orange/red crystals, 0.34 × 0.21 × 0.19 mm, monoclinic, space group P21, a = 10.1048(8) Å, b = 12.9834(8) Å, c = 15.3410(10) Å, α = 90°, β = 102.567(4)°, γ = 90°, V = 1964.4(2) $Å^3$, Z = 4, D_c = 1.121 mg/m^3, F_{000} = 720, *T* = 123(2) K, 14246 reflections collected, 8649 unique (R_{int} = 0.0284), Final F^2 = 1.021, R1 = 0.0417, wR2 = 0.1051, 459 parameters, 1 restraint. Lp and absorption corrections applied, μ = 0.065 mm^{-1}.

Synthesis of **[$Ph_2NCHCH{=}CH_2Li(PMDETA)$] 6:** ^{n}BuLi (2.5 mL [1.6 M solution in hexane], 4 mmol) was added dropwise to a stirred solution of allyldiphenylamine (0.85g, 4 mmol) at -78 °C in 10 mL of hexane. The solution was allowed to warm slowly to room temperature overnight resulting in a pale yellow solution. Next, PMDETA (0.82 mL, 4 mmol) was added dropwise at room temperature resulting in a red, oily solution. Storage of the solution overnight at room temperature deposited a crop of red needle crystals from the oil 0.65 g, 42 % (crystalline yield). **^{1}H NMR (400.2 MHz, C_6D_6, 20 °C)**: δ 1.51 (2H, dd, CH=C**H_2**), 5.057 (1H, d, $^2J_{HH}$ = 6.52 Hz, N-C**H**), 6.434 (1H, bs, CH-C**H**=CH_2), 6.813 (2H, t, $^3J_{HH}$ = 7.2 Hz, *para*-**H**), 7.239 (t, 4H, $^3J_{HH}$ = 7.8 Hz, *ortho*-**H**), 7.746 (4H, d, $^2J_{HH}$ = 6.4 Hz, *meta*-**H**). **^{13}C NMR (100.6 MHz, C_6D_6, 20 °C)** δ: 44.5 (PMDETA-CH_3), 45.6 (PMDETA-CH_3), 53.5 (PMDETA-CH_2), 57.10 (C-C=**C**, s), 93.9 (N-**C**, s), 118.62 (*ortho*-**C**, s), 120.80 (*meta*-**C**, s), 128.57 (*para*-**C**,s), 139.41 (C-**C**=C, s), 148.62 (*Quaternary*-**C**, s).**^{7}Li NMR (155.5 MHz, C_6D_6, 20 °C)** δ: 1.00 (s).

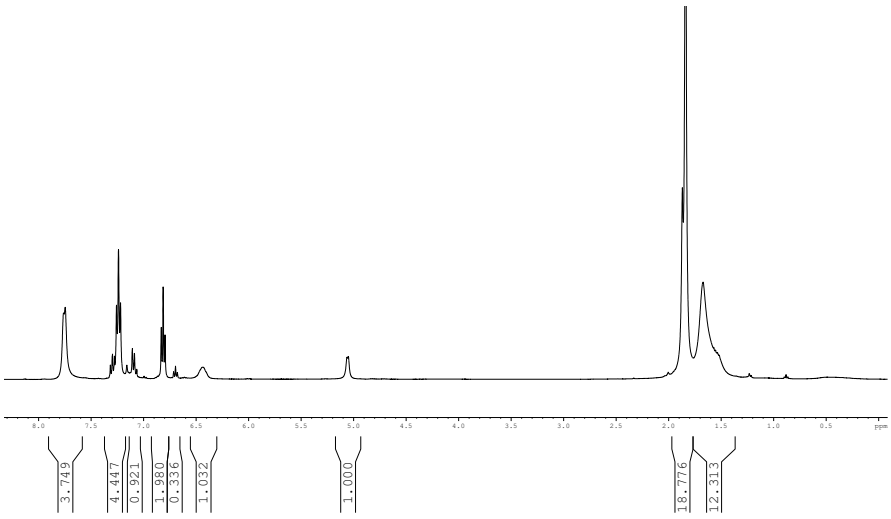


Figure S3 ^{1}H NMR of **[$Ph_2NCHCH{=}CH_2Li(PMDETA)$] 6 in C_6D_6**

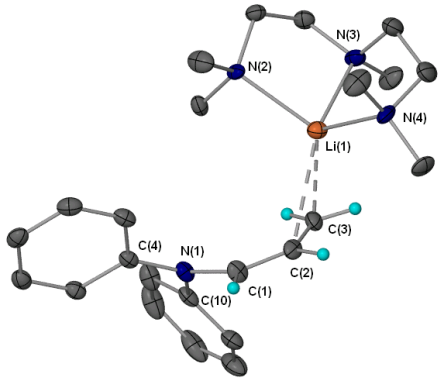


Figure S4 Molecular structure of **6** Hydrogen atoms (except allyl ones) and one disordered PMDETA molecule omitted for clarity. Thermal ellipsoids show at 45%. Selected bond lengths (Å) and angles (°): N1-C1, 1.433(2); N2-Li1, 2.199(7); N3-Li1, 2.133(7); N2-Li1, 2.128(10); C1-C2, 1.360(2); C2-C3, 1.391(2); C2-Li1, 2.690(3); C3-Li1, 2.197(2); N3-Li1-N2, 83.5(3); N4-Li1-N3, 88.3(3).

Crystallographic data for $C_{24}H_{37}LiN_4$ **6**: *M* = 388.52, orange/red needle-like crystals, 0.41 × 0.32 × 0.23 mm, monoclinic, space group P21/c, a = 10.1275(4) Å, b = 8.6095(3) Å, c = 27.5008(12) Å, α = 90°, β = 91.558(3)°, γ = 90°, V = 2396.98(16) $Å^3$, Z = 4, D_c = 1.077 mg/m^3, F_{000} = 848, *T* = 123(2) K, 13075 reflections collected, 4754 unique (R_{int} = 0.0481), Final F^2 = 1.005, R1 = 0.0478, wR2 = 0.0979, 371 parameters, 18 restraints. Lp and absorption corrections applied, μ = 0.063 mm^{-1}.

Deuterium quench: Complex **5** or **6** was synthesised according to the above proceedures and quenched with an excess of D_2O. After stirring at room temperature for over 1 hr, ethyl acetate (10mL) was added and the organic layer separated from the aqueous layer. The organic layer was dried (MgSO4), concentrated in vacuo to afford a light brown/yellow oil. Inspection by 1H NMR spectroscopy was consistent with the formation of the known monodeutero-enamine [Ph_2**N**CH=CHCH_2D] ($CDCl_3$) δ 1.19 (m, 2H, C**H**$_2$D), 4.82 (q, 1H, C**H**CH_2D), 5.90 (d, 1H, NC**H**) 7.10-7.34 (10H, m, Ar).[5]

Synthesis **[Ph_2PCHCH=CH_2Li(Et_2O)]$_\infty$ 3:** ^{n}BuLi (1.25 mL [1.6 M solution in hexane], 2 mmol) was added dropwise to a stirred solution of allyldiphenylphosphine (0.40 g, 2 mmol) at -50 °C in 10 mL of hexane. The yellow solution was allowed to warm slowly to room temperature overnight. Addition of diethylether (1 mL) at room temperature and storage of the solution in the freezer (-18°C) overnight deposited a crop of yellow plate crystals 0.46 g, 75 %. Storage

of the solution at room temperature results in the title compound as a yellow precipitate 0.51 g, 84%. **Microanalysis data:** Calculated for $C_{19}H_{24}LiOP$: C, 74.50; H, 7.90. Found: C, 74.37; H, 7.64. **^{1}H NMR (400.2 MHz, C_6D_6 , 20 °C)** δ: 1.09 (6H, t, C**H**$_3$-Et$_2$O), 3.25 (4H, q, C**H**$_2$-Et$_2$O), 3.63 (1H, d, br, $J_{P,C}$ = 11.6 Hz, C=C**H**$_2$), 3.67 (1H, dd, $J_{P,C}$ = 5.2 Hz, C**H**CH=CH$_2$), 3.83 (1H, d, br, $J_{P,C}$ = 15.6 Hz, C=C**H**$_2$), 7.14 (2H, m, para-Ar**H**), 7.26 (4H, m, meta-Ar**H**), 7.34 (1H, m, CHC**H**=CH$_2$), 7.88 (4H, m, ortho-Ar**H**). **^{13}C NMR (100.6 MHz, C_6D_6, 20 °C)** δ: 15.42 (s, **C**H$_3$-Et$_2$O), 56.1 (d, P**C**H, $J_{P,C}$ = 10.12 Hz), 65.86 (s, **C**H$_2$-Et$_2$O), 67.0 (d, br, PCHCH=**C**H$_2$, $J_{P,C}$ = 22.25 Hz), 126.34 (s, para-Ar**C**), 127.87 (s, meta-Ar**C**), 132.33 (s, ortho-Ar**C**), 132.51 (s, ortho-Ar**C**) 149.0 (d, CH**C**H=CH$_2$, $J_{P,C}$ = 9 Hz), 150.58 (s, br, q-Ar**C**), 151.05 (s, br, q-Ar**C**). **^{7}Li NMR (155.5 MHz, C_6D_6, 20 °C)** δ: -0.06 (s). **^{31}P NMR (121.5 MHz, C_6D_6, 20 °C)** δ: -3.08 (s, br)

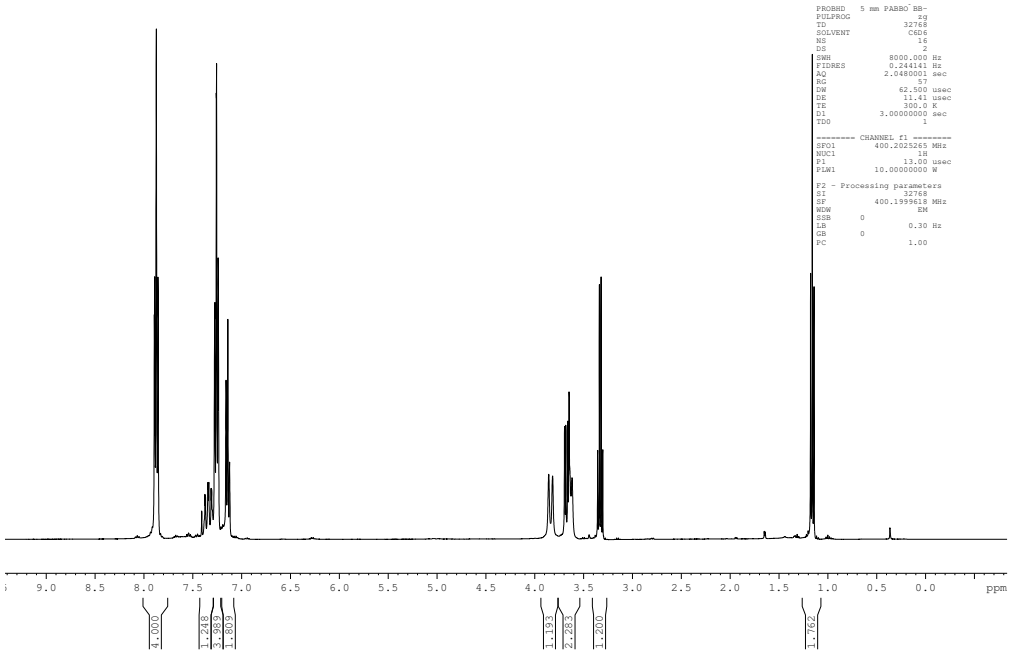


Figure S5 ^{1}H NMR of **[$Ph_2PCHCH=CH_2Li(Et_2O)]_\infty$ 3 in C_6D_6**

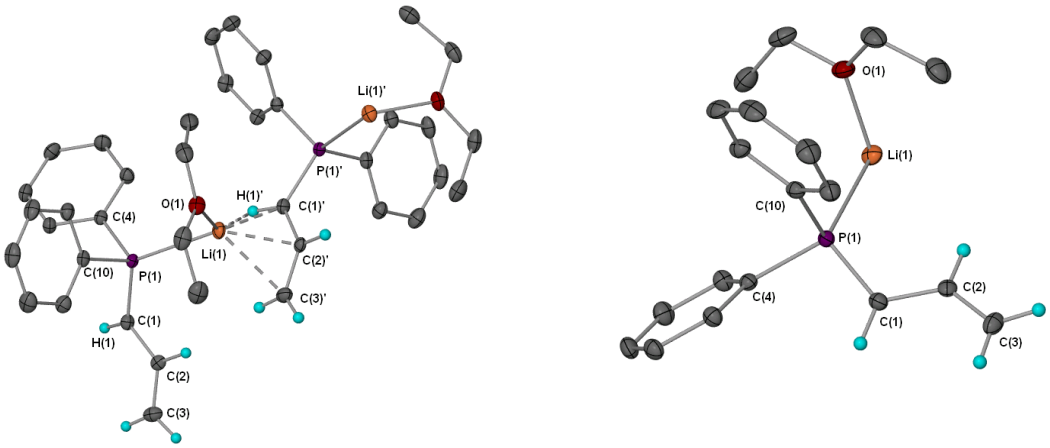


Figure S6 Molecular structure of **3**. ASU of **3** on LHS polymeric section on RHS. Hydrogen atoms (except allyl ones) have been omitted for clarity. Selected bond lengths (Å) and angles (°); Li1-P1, 2.592(3); Li1-O1, 1.962(3); P1-C1, 1.7614(17); C1-C2, 1.417(2); C2-C3, 1.369(2); Li1-C1', 2.270(3); Li(1)-C2', 2.203(3); Li1-C3', 2.432(3).

Crystallographic data for $C_{38}H_{48}Li_2iO_2P_2$ **3**: *M* = 612.58, yellow crystals, 0.09 × 0.02 × 0.02 mm, monoclinic, space group Cc, a = 10.592(2) Å, b = 18.626(4) Å, c = 9.1190(18) Å, α = 90°, β = 95.24(3)°, γ = 90°, V = 1791.5(6) Å^3, Z = 2, D_c = 1.136 mg/m^3, F_{000} = 656, *T* = 123(2) K, 14517 reflections collected, 4215 unique (R_{int} = 0.0392), Final F^2 = 1.046, R1 = 0.0343, wR2 = 0.0908, 4215 parameters, 2 restraint. Lp and absorption corrections applied, μ = 0.065 mm^{-1}.

Synthesis **[$Ph_2PCHCH{=}CH_2Li(TMEDA)$] 4:** ^{n}BuLi (1.25 mL [1.6 M solution in hexane], 2 mmol) was added dropwise to a stirred solution of allyldiphenylphosphine (0.40 g, 2 mmol) at -50 °C in 10 mL of hexane. The yellow solution was allowed to warm slowly to room temperature overnight. Addition of TMEDA (0.31 mL, 2 mmol) at room temperature resulted in the formation of an orange oily solution. Storage of the solution in the refrigerator (-4°C) overnight deposited a crop of yellow plate crystals 0.52 g, 75 %. **Microanalysis data:** Calculated for $C_{21}H_{30}LiN_2P$: C, 72.40; H, 8.68; N, 8.04. Found: C, 72.27; H, 8.49; N, 7.83.**^{1}H NMR (400.2 MHz, C_6D_6 , 20 °C)** δ: 1.65 (4H, s, C**H**$_2$-TMEDA), 1.78 (9H, s, br, C**H**$_3$-TMEDA), 3.52 (1H, d, br, P-C**H**), 3.55 (1H, dd, $J_{P,C}$ = 6.4 Hz, CH=C**H**$_2$), 3.67 (1H, dd, br, $J_{P,C}$ = 14.4 Hz, C=C**H**$_2$), 7.14 (2H, m, para-Ar**H**), 7.25 (4H, m, meta-Ar**H**), 7.31 (1H, m, CHC**H**=CH$_2$), 7.85 (4H, m, ortho-Ar**H**).**^{13}C NMR (100.6 MHz, C_6D_6, 20 °C)** δ: 45.64 (TMEDA-**C**H$_3$), 56.63 (TMEDA-**C**H$_2$), 56.40 d, br, CH=**C**H$_2$), 67.3 (d, $J_{P,C}$ = 21.1 Hz, P-**C**H), 126.37 (s, para-Ar**C**), 127.82 (s, meta-ArC), 132.65

(d, ortho-ArC), 149.21 (s, br, q-ArC), 150.47 (d, $J_{P,C}$ = 47.3 Hz, CH**C**H=CH_2) **^{7}Li NMR (155.5 MHz, C_6D_6, 20 °C)** δ: 0.50 (s). **^{31}P NMR (121.5 MHz, C_6D_6, 20 °C)** δ: -2.16 (s, br)

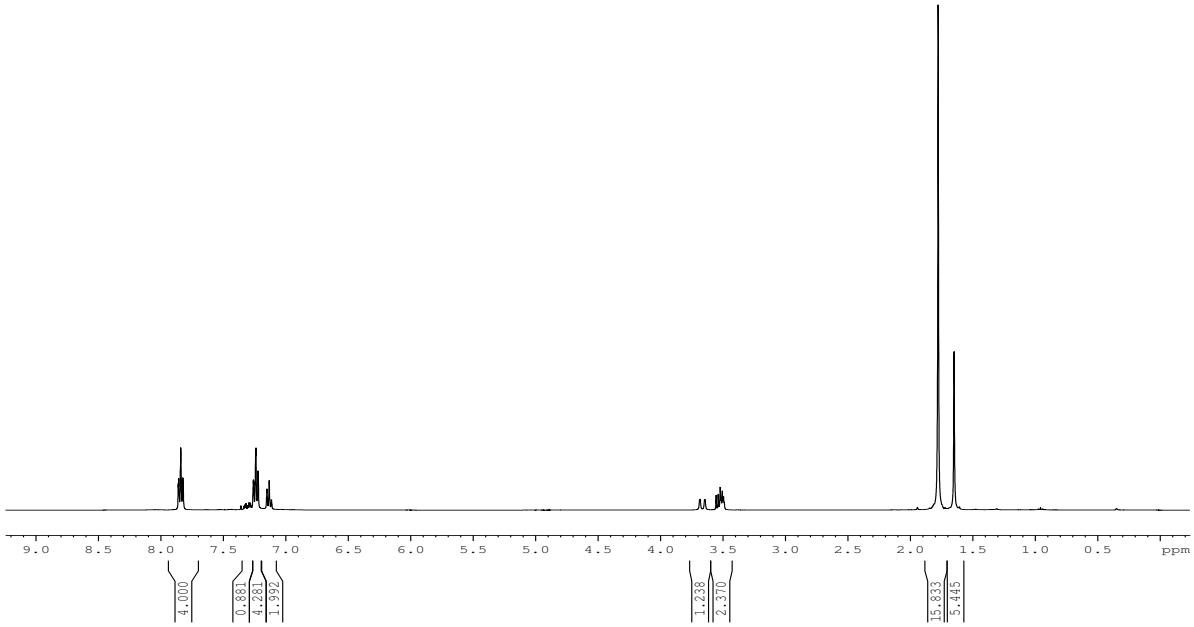


Figure S7 ^{1}H NMR of **[Ph_2PCHCH=CH_2Li(TMEDA)] 4 in C_6D_6**

Deuterium quench: Complex **3** or **4** was synthesised according to the above procedures and quenched with an excess of degassed D_2O allowing to stir for 1 hr. Keeping under an inert atmosphere, dry ethyl acetate (10mL) was added and the organic layer separated from the aqueous layer. The organic layer was dried ($MgSO_4$), concentrated *in vacuo* to afford a light yellow oil. Inspection by ^{1}H NMR spectroscopy was consistent with the formation of the monodeutero-phosphine [Ph_2PCHDCH=CH_2] ($CDCl_3$) δ 2.78 (d, 2H, PC**H**D), 4.85 (m, 2H,CH=C*H_2*), 5.68 (m, 1H, C**H=**CH_2).

Synthesis of **[Ph_2PLi(PMDETA)] 7:** ^{n}BuLi (1.25 mL [1.6 M solution in hexane], 2 mmol) was added dropwise to a stirred solution of allyldiphenylphosphine (0.40 g, 2 mmol) at -50 °C in 10 mL of hexane. The yellow solution was allowed to warm slowly to room temperature overnight. Addition of PMDETA (0.40 mL, 2 mmol) at room temperature resulted in the formation of an orange oily solution. Storage of the solution at room temperature overnight deposited a crop of orange needle crystals 0.53 g, 73%. ^{1}H, ^{13}C, ^{7}Li and ^{31}P NMR was consistent

with reported literature values.[6] X-ray diffraction studies confirmed the formation of the title compound by collecting multiple unit cells.

^{1}H NMR Reaction monitor: A sample of complex **3** (approx 80 mg, 0.26 mM) was put in a Youngs tap NMR tube and dissolved in the minimum amount of C_6D_6. A ^{1}H NMR spectrum was conducted to ensure the complex was stable and pure in solution. The sample was cooled to -10°C and PMDETA (0.06 mL, 0.27mM) was added. As quickly as possible the sample was then monitored via ^{1}H NMR at room temperature. This revealed the following species;

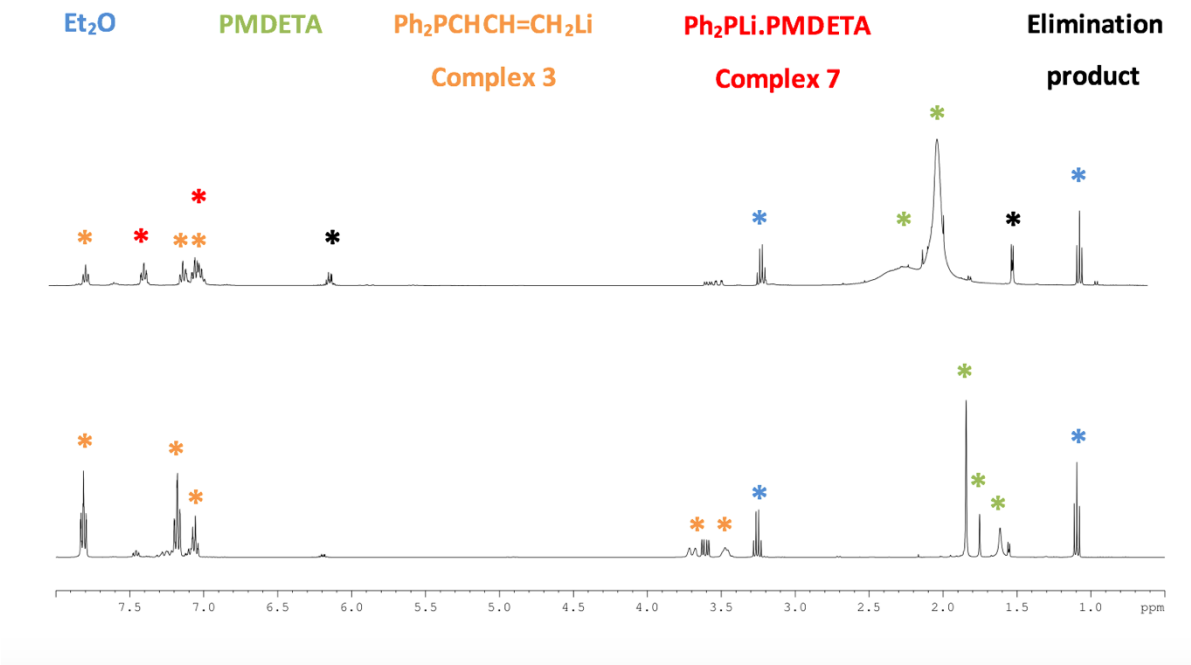


Figure S8 ^{1}H NMR spectrum of complex 3 in C_6D_6 (bottom) at approx. 10 minutes after PMDETA addition. Top spectrum after 1hr.

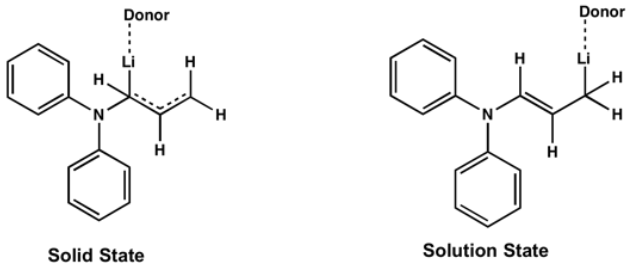


Figure S9 Two isomeric allylic metal derivatives of compounds 5 and 6 in both the solid and solution state.

^{1}H and ^{7}Li NMR temperature study of Compound 5 in d_8-toluene

Compound **5** was dissolved in d_8-toluene and monitored by both ^{1}H and ^{7}Li NMR spectroscopy over the temperature range 30°C to -60°C. Below -60°C the compound began to crash out of solution so no lower temperature NMR could be collected. The spectra were observed to show broadening of the allylic and Lewis donor (TMEDA) signals as temperature decreased in the ^{1}H NMR, while the ^{7}Li signal got gradually broader and shifted slightly upfield. Unfortunately the low temperature NMR spectra did not conclusively give a coalescence point or show any additional species forming in solution.

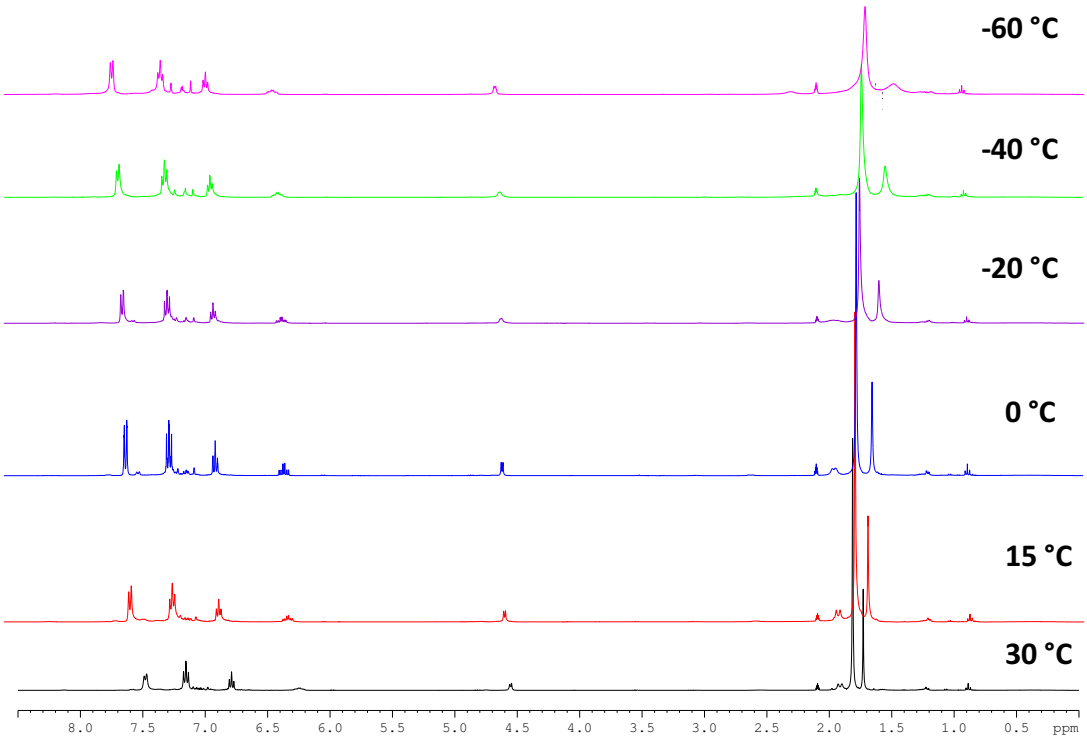


Figure S10 ^{1}H NMR of Compound 5 in d_8-toluene solution 30°C to -60°C

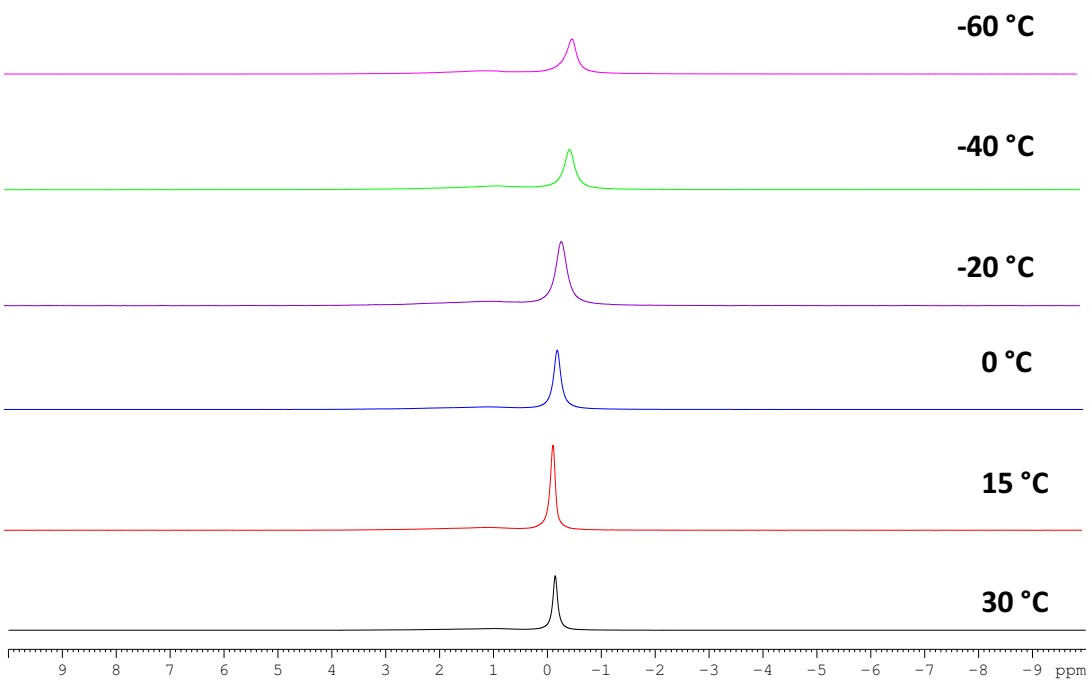


Figure S11 ^{7}Li NMR of Compound 5 in d_8-toluene solution 30°C to -60°C

DFT Calculations: Density functional calculations (DFT) using the Gaussian 09 suite of software.[4] Geometry optimisations and frequency calculations were performed at the B3LYP/6-31G(d) level and basis set, in order to compare ΔG values for the competing pathways, for each of the mono-, bi- and tri- dentate donors.

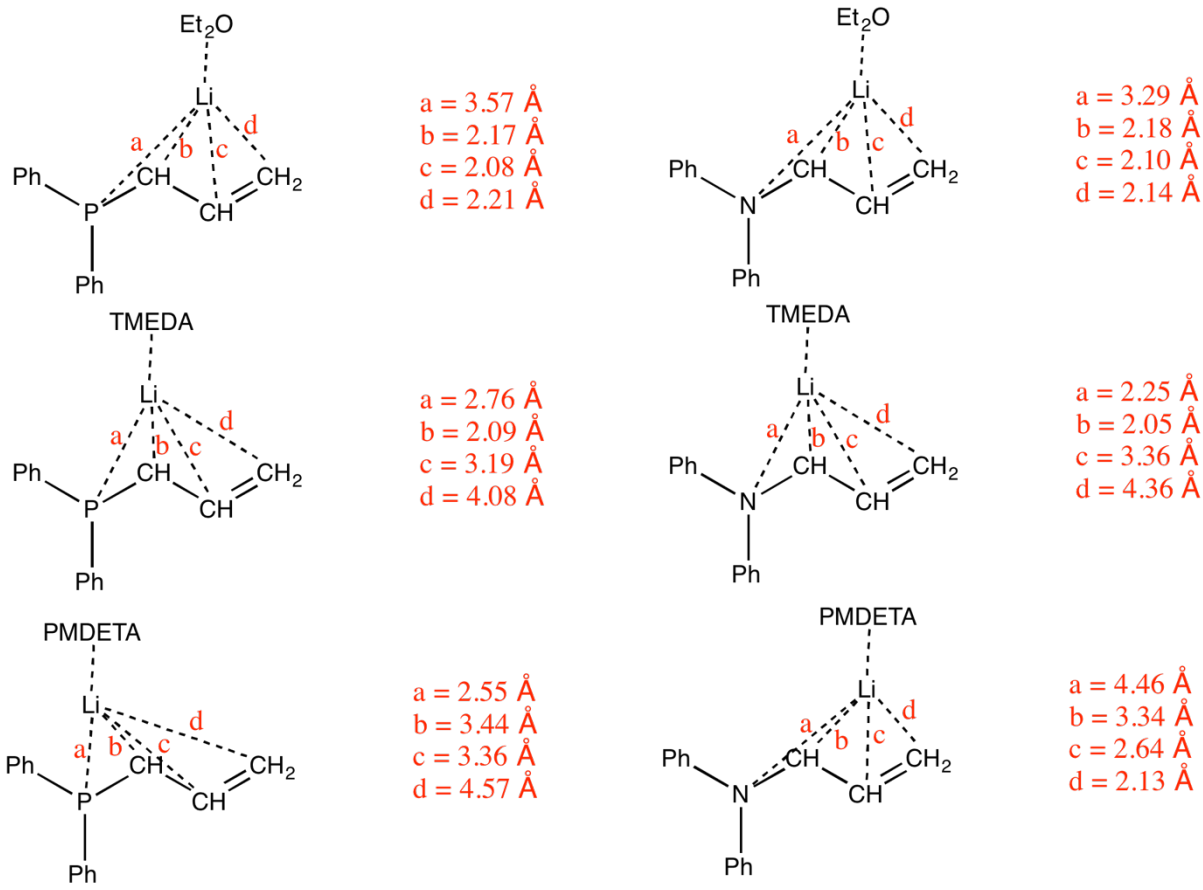


Figure S12 Comparative calculated bond lengths for all DFT generated complexes

DFT calculations were performed on the experimentally observed and theoretical species in the study. The following Cartesian coordinates represent the 12 relevant structures. Format: Atomic Number, x, y, z

Compound 3 [($Ph_2NCHCH=CH_2$)Li.Et_2O]

6	1.417165	2.241950	0.615615
6	0.725095	1.190086	-0.014937
6	-0.450815	1.504864	-0.722048
6	-0.919416	2.816483	-0.787393
6	-0.227768	3.852372	-0.153850

6	0.945718	3.551394	0.541558
7	1.172595	-0.147437	0.087834
6	0.220289	-1.186582	0.367656
6	-0.242540	-1.398970	1.677868
6	-1.218829	-2.307489	2.093880
6	2.535032	-0.477311	-0.071649
6	3.401555	0.312995	-0.856190
6	4.733074	-0.052642	-1.032401
6	5.241771	-1.217198	-0.451789
6	4.385869	-2.012791	0.311302
6	3.052315	-1.655380	0.501299
3	-1.959081	-1.071079	0.517810
8	-3.631541	-0.691619	-0.367533
6	-4.159824	-1.449529	-1.465068
6	-3.077145	-2.359531	-2.017334
6	-4.605486	0.160679	0.258050
6	-3.944050	0.939291	1.381728
1	-1.487618	-2.374118	3.142372
1	-1.426716	-3.199713	1.495406

1	0.040378	-0.624330	2.396703
1	0.223977	-2.018103	-0.343732
1	2.399684	-2.281930	1.098438
1	4.757601	-2.924948	0.772564
1	6.280674	-1.499984	-0.596490
1	5.375936	0.576366	-1.644055
1	3.024246	1.211431	-1.333126
1	-0.978462	0.707547	-1.237625
1	-1.820904	3.032557	-1.357004
1	-0.593231	4.874079	-0.205369
1	1.495412	4.341627	1.047315
1	2.323114	2.019983	1.170697
1	-5.427192	-0.463020	0.638256
1	-5.017268	0.838327	-0.503168
1	-3.544481	0.263007	2.147210
1	-4.681841	1.589757	1.863627
1	-3.131771	1.568988	1.002332
1	-4.518157	-0.751582	-2.235088
1	-5.021348	-2.034086	-1.111199

1	-2.212114	-1.782656	-2.361585
1	-3.467807	-2.925906	-2.869285
1	-2.742752	-3.081207	-1.262976

Compound 5 [($Ph_2NCHCH=CH_2$)Li.TMEDA]

6	-0.425076	2.357855	0.929346
6	0.571430	1.720797	0.148458
6	1.129828	2.467152	-0.916493
6	0.670284	3.746175	-1.215278
6	-0.347377	4.347698	-0.468554
6	-0.876129	3.639885	0.610666
7	0.973704	0.405732	0.446647
6	0.571482	-0.224677	1.740538
6	1.140877	0.340855	2.957910
6	1.486775	-0.315726	4.086621
6	2.045219	-0.205144	-0.273131
6	1.936686	-0.469085	-1.651494
6	2.960804	-1.125249	-2.335246
6	4.105981	-1.546850	-1.657162

6	4.213296	-1.301253	-0.284875
6	3.198562	-0.639319	0.403599
3	-1.097489	-0.465851	0.579067
7	-1.553309	-2.495925	0.048831
6	-2.598647	-2.372872	-0.982669
6	-3.575672	-1.231382	-0.685966
7	-2.892755	0.063406	-0.490766
6	-3.780131	1.015648	0.197355
6	-0.418699	-3.291974	-0.444644
6	-2.073234	-3.092809	1.289663
6	-2.452841	0.642579	-1.772804
1	1.045552	-0.147575	-2.184970
1	2.856743	-1.314903	-3.401112
1	4.901129	-2.062657	-2.188384
1	5.099635	-1.623535	0.256244
1	3.279268	-0.457936	1.470613
1	1.937359	2.047728	-1.503702
1	1.128130	4.284719	-2.042010
1	-0.693158	5.350188	-0.703284

1	-1.636229	4.097530	1.240949
1	-0.816038	1.846733	1.800629
1	0.798361	-1.292721	1.641225
1	1.251921	1.428822	2.965534
1	1.803096	0.214325	4.980491
1	0.016755	-2.815435	-1.327191
1	0.354129	-3.336729	0.326872
1	-0.717379	-4.322328	-0.703968
1	-2.441084	-4.121070	1.127184
1	-1.277527	-3.112857	2.038433
1	-2.892436	-2.491871	1.694163
1	-2.097736	-2.193187	-1.939666
1	-3.169155	-3.311918	-1.098164
1	-4.320237	-1.172973	-1.499446
1	-4.133199	-1.451368	0.230364
1	-1.772310	-0.041269	-2.288051
1	-3.307469	0.848704	-2.440129
1	-1.916147	1.574974	-1.582830
1	-4.700070	1.214301	-0.378932

1	-3.247381	1.957585	0.345211
1	-4.060933	0.617112	1.177364
1	1.424886	-1.401133	4.161349

Compound 6 [($Ph_2NCHCH=CH_2$)Li.PMDETA]

6	3.714945	1.897261	1.287121
6	3.443052	0.925831	0.306607
6	4.225436	0.923975	-0.863874
6	5.256261	1.847218	-1.032101
6	5.525014	2.803093	-0.050937
6	4.741364	2.819902	1.106700
7	2.374640	0.009562	0.477921
6	1.171811	0.446365	1.130266
6	0.429879	1.503234	0.673928
6	-0.774433	2.085626	1.188179
6	2.505924	-1.342047	0.122806
6	1.356208	-2.119724	-0.130834
6	1.456037	-3.473734	-0.445089
6	2.699332	-4.104373	-0.513635

6	3.844448	-3.346194	-0.251115
6	3.758330	-1.994528	0.067455
3	-2.032890	0.668804	0.225790
7	-2.805293	-1.008960	1.525968
6	-2.634546	-0.504732	2.898211
6	-2.169091	-2.330014	1.416570
6	-4.228266	-1.100007	1.156320
6	-4.883091	0.265126	0.923731
7	-4.174402	1.073594	-0.082444
6	-4.430381	0.626765	-1.464025
6	-3.254637	0.944281	-2.392789
7	-2.005271	0.280391	-1.976709
6	-2.005810	-1.142662	-2.343371
6	-4.476616	2.501500	0.081297
6	-0.842333	0.938075	-2.595892
1	4.662274	-1.436978	0.285829
1	4.824615	-3.817019	-0.280278
1	2.775889	-5.160422	-0.756503
1	0.547856	-4.041533	-0.640027

1	0.388915	-1.633896	-0.072511
1	3.099178	1.923040	2.179555
1	4.934134	3.556848	1.882981
1	6.324676	3.525884	-0.187935
1	5.843409	1.825474	-1.947469
1	4.016494	0.196777	-1.642441
1	-1.106867	-2.247323	1.658789
1	-2.258690	-2.702648	0.391602
1	-2.627206	-3.070136	2.096285
1	-3.134039	-1.156612	3.637278
1	-3.032997	0.507588	2.989754
1	-1.568550	-0.457553	3.131505
1	-4.810480	-1.642100	1.924761
1	-4.291498	-1.701801	0.242670
1	-5.943851	0.109562	0.656253
1	-4.883355	0.834775	1.857852
1	-5.553923	2.716187	-0.034931
1	-3.925973	3.087799	-0.658157
1	-4.147502	2.833735	1.069057

1	-5.347230	1.089353	-1.870089
1	-4.610000	-0.451951	-1.457409
1	-3.526910	0.675274	-3.429876
1	-3.071294	2.023562	-2.386208
1	0.073679	0.455322	-2.247774
1	-0.809168	1.987130	-2.290986
1	-0.876943	0.884870	-3.698147
1	-2.096959	-1.286261	-3.434912
1	-2.835327	-1.667285	-1.860705
1	-1.071035	-1.603001	-2.012056
1	0.942178	-0.062802	2.067964
1	0.800378	1.940776	-0.258588
1	-0.940069	3.125486	0.895176
1	-0.965874	1.929934	2.255990

[$Ph_2NLi.Et_2O$]

6	2.048404	1.787812	-0.363949
6	1.918107	0.472744	0.141864
6	3.117757	-0.249079	0.353475

6	4.358738	0.310027	0.056546
6	4.463574	1.606618	-0.452998
6	3.291257	2.341084	-0.654643
7	0.656009	0.008763	0.478143
6	0.307437	-1.324030	0.422504
6	-0.815763	-1.737963	1.201049
6	-1.377146	-3.012745	1.074409
6	-0.834412	-3.941742	0.190184
6	0.292491	-3.569505	-0.560809
6	0.854558	-2.305189	-0.456789
3	-1.140544	0.447714	0.259697
8	-2.709398	1.425598	-0.171135
6	-3.109666	2.634734	0.494988
6	-2.118493	2.949481	1.601599
6	-3.610290	1.010599	-1.212797
6	-3.049897	-0.224853	-1.895742
1	-1.105082	3.080313	1.206219
1	-2.099900	2.155070	2.356310
1	-2.406916	3.879651	2.102284

1	-4.122004	2.494714	0.899281
1	-3.148297	3.446593	-0.244596
1	-4.593239	0.806595	-0.765709
1	-3.726052	1.838319	-1.926213
1	-2.083335	-0.013441	-2.367562
1	-3.737460	-0.556447	-2.680847
1	-2.923826	-1.053337	-1.189287
1	-1.178331	-1.065172	1.981667
1	-2.225071	-3.284274	1.700316
1	-1.258182	-4.937396	0.097647
1	0.734781	-4.284895	-1.251722
1	1.711219	-2.042304	-1.068821
1	3.066281	-1.248147	0.776374
1	5.258504	-0.274834	0.237488
1	5.434653	2.036500	-0.682473
1	3.345402	3.355340	-1.045476
1	1.141675	2.369930	-0.525245

[$Ph_2NLi.TMEDA$]

6	3.426301	0.025642	-0.450405
6	2.144418	-0.570181	-0.336820
6	2.114469	-1.921684	0.089464
6	3.275654	-2.620827	0.402709
6	4.527667	-2.006941	0.302711
6	4.584093	-0.680126	-0.132358
7	0.955513	0.040518	-0.692775
6	0.755875	1.399345	-0.601963
6	-0.289709	1.960935	-1.394947
6	-0.701769	3.287063	-1.248519
6	-0.087122	4.126007	-0.319219
6	0.962155	3.606218	0.454347
6	1.380584	2.287707	0.325088
3	-0.898797	-0.240952	-0.362060
7	-2.452176	-1.542143	-0.981605
6	-3.447542	-1.400792	0.102383
6	-2.788763	-1.237291	1.477643
7	-1.855553	-0.096164	1.509892
6	-0.875294	-0.223717	2.600565

6	-3.038397	-1.213362	-2.289448
6	-1.876873	-2.897255	-1.022573
6	-2.560346	1.191450	1.621839
1	2.185328	1.914452	0.950232
1	1.460955	4.246649	1.179833
1	-0.396128	5.161742	-0.211824
1	-1.493639	3.671499	-1.888986
1	-0.718673	1.342508	-2.184757
1	3.504721	1.044877	-0.816813
1	5.548397	-0.186471	-0.237965
1	5.435268	-2.550802	0.549563
1	3.202967	-3.657032	0.728245
1	1.146790	-2.417351	0.157262
1	-3.419920	-0.187770	-2.277719
1	-2.265219	-1.284272	-3.060139
1	-3.864466	-1.892602	-2.560819
1	-2.641578	-3.659483	-1.251079
1	-1.097139	-2.936896	-1.787927
1	-1.415351	-3.147389	-0.063720

1	-4.054097	-0.517151	-0.120956
1	-4.139251	-2.260688	0.127709
1	-3.575917	-1.143900	2.246464
1	-2.218824	-2.139458	1.723737
1	-3.273636	1.311502	0.801979
1	-3.109056	1.273772	2.576200
1	-1.836457	2.007414	1.553894
1	-1.356487	-0.229971	3.593521
1	-0.178690	0.617167	2.550614
1	-0.300400	-1.146110	2.478070

[Ph_2NLi.PMDETA]

6	-0.693364	-2.355070	-1.211650
6	-1.453891	-1.512997	-0.360849
6	-2.427677	-2.158811	0.448067
6	-2.607190	-3.538634	0.408781
6	-1.833685	-4.348216	-0.430675
6	-0.874687	-3.736999	-1.241686
7	-1.139860	-0.163808	-0.294638

6	-2.123242	0.785218	-0.110592
6	-1.763599	2.069102	0.386803
6	-2.687879	3.102315	0.522712
6	-4.027436	2.914627	0.174930
6	-4.408709	1.663314	-0.322357
6	-3.492389	0.626871	-0.466448
3	0.757094	0.266884	-0.033935
7	2.774658	-0.740142	-0.282959
6	3.203898	-1.071451	1.089257
6	2.767800	-0.037660	2.131008
7	1.325048	0.246104	2.099691
6	1.023397	1.430383	2.915437
6	3.556426	0.369592	-0.867008
6	2.766093	1.118884	-1.943102
7	1.571274	1.784814	-1.392692
6	0.564212	2.023087	-2.442604
6	1.919089	3.057749	-0.747693
6	2.862972	-1.937431	-1.132789
6	0.529697	-0.896432	2.583789

1	-3.035183	-1.557351	1.118306
1	-3.359759	-3.991827	1.051725
1	-1.983010	-5.424081	-0.458074
1	-0.275044	-4.339416	-1.922364
1	0.024760	-1.884993	-1.880201
1	-3.821881	-0.321422	-0.879262
1	-5.443276	1.493031	-0.615743
1	-4.751568	3.716857	0.285318
1	-2.356815	4.064132	0.911895
1	-0.727426	2.239639	0.673508
1	-0.045336	1.649785	2.854134
1	1.576954	2.295369	2.535131
1	1.292872	1.285351	3.976499
1	0.799013	-1.168200	3.619856
1	0.669475	-1.768183	1.940883
1	-0.529157	-0.636331	2.540679
1	3.089168	-0.395728	3.127068
1	3.292495	0.909880	1.962612
1	4.300100	-1.195868	1.153125

1	2.769198	-2.044542	1.336157
1	3.887965	-2.347043	-1.160896
1	2.564390	-1.695758	-2.155940
1	2.177588	-2.703527	-0.762823
1	4.505112	0.001357	-1.295379
1	3.828073	1.066436	-0.069298
1	3.431219	1.838854	-2.452914
1	2.429880	0.410186	-2.706671
1	-0.321703	2.477245	-1.992735
1	0.260480	1.069360	-2.880614
1	0.948693	2.684653	-3.238103
1	2.355952	3.777310	-1.462739
1	2.640476	2.898431	0.059587
1	1.018156	3.502320	-0.316730

Compound 3 [($Ph_2PCHCH=CH_2$)Li.Et_2O]

6	0.263285	1.699264	0.679027
6	-0.721367	1.411003	-0.277106
6	-1.469753	2.485339	-0.791644

6	-1.245693	3.792889	-0.364219
6	-0.256981	4.062408	0.586637
6	0.496407	3.010338	1.106848
15	-1.035124	-0.285202	-0.972080
6	-2.705210	-0.633029	-0.213069
6	-3.552449	-1.515500	-0.902021
6	-4.800066	-1.868922	-0.385479
6	-5.229574	-1.334880	0.830535
6	-4.401974	-0.449460	1.524518
6	-3.152528	-0.102943	1.007832
6	0.103182	-1.370165	-0.102209
6	0.674511	-2.471958	-0.786261
6	1.559984	-3.409310	-0.273391
3	2.267846	-1.329507	-0.079910
8	3.911676	-0.342902	0.068782
6	4.963062	-0.732701	0.966014
6	4.388457	-1.605533	2.067396
6	4.358274	0.548376	-0.969887
6	3.201587	0.872220	-1.897490

1	1.955058	-4.199216	-0.903950
1	1.621741	-3.579930	0.803984
1	0.548277	-2.471518	-1.873565
1	0.048994	-1.439978	0.992180
1	-3.229324	-1.927159	-1.855778
1	-5.439741	-2.554307	-0.936521
1	-6.203441	-1.602758	1.232773
1	-4.730375	-0.026726	2.471393
1	-2.522939	0.592128	1.556902
1	0.848601	0.884938	1.098644
1	1.261403	3.206370	1.855294
1	-0.077479	5.082327	0.917064
1	-1.838522	4.605243	-0.777789
1	-2.237308	2.291608	-1.537997
1	5.181742	0.064774	-1.514888
1	4.751745	1.459728	-0.498663
1	2.821208	-0.028002	-2.394691
1	3.541774	1.560803	-2.678366
1	2.378840	1.350044	-1.356614

1	5.421386	0.175100	1.382689
1	5.734166	-1.271607	0.396878
1	3.637644	-1.060223	2.650462
1	5.186443	-1.914321	2.750825
1	3.931104	-2.512178	1.654202

Compound 4 [($Ph_2PCHCH=CH_2$)Li.TMEDA]

6	-2.623031	-0.895543	0.421675
6	-3.224337	-1.031518	1.683155
1	-2.653965	-0.781548	2.575982
6	-4.537374	-1.491287	1.810646
1	-4.987058	-1.582986	2.796857
6	-5.264554	-1.845086	0.673437
1	-6.284232	-2.210507	0.768009
6	-4.669670	-1.739704	-0.586660
1	-5.227910	-2.024572	-1.475635
6	-3.361383	-1.270288	-0.712818
1	-2.902290	-1.209910	-1.695230
15	-0.838937	-0.335247	0.324602

6	-1.078463	1.487128	0.019516
6	-2.012695	2.216073	0.778039
1	-2.669744	1.692175	1.466744
6	-2.125125	3.600476	0.656662
1	-2.861190	4.132558	1.254976
6	-1.305080	4.303299	-0.229455
1	-1.396576	5.381928	-0.327558
6	-0.376332	3.598892	-0.995269
1	0.253366	4.126712	-1.708835
6	-0.264555	2.210473	-0.871069
1	0.446424	1.675442	-1.493961
6	-0.015871	-0.959831	-1.145285
1	0.272448	-2.006235	-0.954962
6	-0.469534	-0.743519	-2.517049
1	-0.921612	0.231732	-2.716724
6	-0.363155	-1.581844	-3.571567
1	-0.679365	-1.285803	-4.567940
6	2.427331	-2.984613	1.193572
1	1.850862	-2.511865	1.993547

1	1.727276	-3.512854	0.540830
1	3.120779	-3.720227	1.635298
7	3.134496	-1.954515	0.415009
6	3.830341	-2.577000	-0.722738
1	4.587674	-3.308286	-0.391739
1	3.100763	-3.089775	-1.355558
1	4.328049	-1.818238	-1.333305
6	4.057380	-1.181785	1.269518
1	3.556409	-1.012796	2.227945
1	4.977620	-1.750638	1.490135
6	4.436479	0.162958	0.641592
1	5.121171	0.699360	1.321318
1	4.989341	-0.005798	-0.288678
7	3.252683	0.985195	0.314445
6	2.667690	1.602292	1.520998
1	2.351427	0.833976	2.231161
1	3.386786	2.272837	2.021544
1	1.781876	2.175296	1.237255
6	3.602194	2.035999	-0.655489

1	4.375999	2.719371	-0.266430
1	2.708850	2.620515	-0.888409
1	3.971533	1.580923	-1.579996
3	1.841801	-0.467385	-0.330809
1	0.042163	-2.588118	-3.467883

[($Ph_2PCHCH=CH_2$)Li.PMDETA]

6	2.264909	2.338224	-1.454593
6	2.245614	1.342364	-0.464677
6	3.051576	1.527190	0.671737
6	3.840774	2.670710	0.815898
6	3.845809	3.653954	-0.175519
6	3.056970	3.479244	-1.314341
15	1.059117	-0.088940	-0.676286
6	2.056429	-1.457280	0.146674
6	1.986817	-1.671411	1.533106
6	2.663354	-2.733926	2.139497
6	3.417285	-3.613650	1.361075
6	3.482578	-3.424830	-0.022227

6	2.803536	-2.362659	-0.620616
3	-1.320180	0.074885	0.232010
7	-1.524279	1.562040	1.796963
6	-1.088018	1.156299	3.140391
6	-2.965658	1.870483	1.796679
6	-3.539712	2.026368	0.385951
7	-3.264423	0.860537	-0.477037
6	-3.370649	1.243194	-1.897211
6	-4.160409	-0.278150	-0.170922
6	-3.505393	-1.630036	-0.465416
7	-2.297974	-1.863962	0.353907
6	-1.479020	-2.945766	-0.233026
6	-2.645105	-2.223445	1.736207
6	-0.723844	2.717496	1.348961
1	3.084244	0.762922	1.443424
1	4.461867	2.787501	1.701455
1	4.464349	4.541273	-0.065103
1	3.063060	4.230764	-2.100953
1	1.659883	2.190019	-2.346053

1	2.831186	-2.235511	-1.700317
1	4.061560	-4.111031	-0.636356
1	3.941243	-4.444832	1.826423
1	2.598296	-2.876968	3.216204
1	1.394111	-0.997317	2.151760
1	-0.025598	0.898642	3.113095
1	-1.650942	0.275644	3.465176
1	-1.232010	1.957049	3.886198
1	-0.908800	3.605002	1.978836
1	-0.955830	2.968278	0.311266
1	0.337138	2.464603	1.390260
1	-3.179815	2.792417	2.367807
1	-3.476259	1.054923	2.321666
1	-4.621912	2.231329	0.462164
1	-3.095704	2.902639	-0.094893
1	-4.374385	1.631229	-2.140893
1	-3.157969	0.388181	-2.540990
1	-2.626280	2.010192	-2.126819
1	-5.100855	-0.198509	-0.741500

1	-4.439007	-0.229463	0.885703
1	-4.249406	-2.433607	-0.319031
1	-3.200735	-1.667324	-1.515433
1	-0.568329	-3.068960	0.358072
1	-1.188427	-2.682831	-1.252416
1	-2.028793	-3.902290	-0.246300
1	-3.224947	-3.161703	1.784989
1	-3.235477	-1.433982	2.210675
1	-1.726779	-2.358231	2.315400
6	0.872247	-0.363445	-2.381591
6	-0.412050	-0.702299	-2.909816
1	1.741642	-0.433590	-3.036351
6	-0.790041	-1.131376	-4.145032
1	-1.230784	-0.584905	-2.189368
1	-1.835507	-1.305805	-4.387665
1	-0.071508	-1.290120	-4.945861

[$Ph_2PLi.Et_2O$]

6	0.608884	-3.316647	0.102643

6	-0.835100	-3.381117	0.564267
8	-1.582001	-2.299222	-0.023686
6	-2.990733	-2.362063	0.266871
6	-3.708194	-1.235147	-0.453523
1	-3.551674	-1.300123	-1.536436
1	-3.381392	-0.251048	-0.099710
1	-4.784894	-1.309450	-0.266621
1	-3.131412	-2.291494	1.354577
1	-3.365316	-3.340893	-0.062585
1	-0.909670	-3.306407	1.658544
1	-1.301446	-4.327070	0.256807
1	0.676455	-3.406814	-0.986683
1	1.171032	-4.144513	0.548156
1	1.101095	-2.385359	0.404274
6	-1.736257	2.269245	-1.021662
1	-1.716771	2.514652	-2.081529
6	-2.823443	2.663020	-0.250431
1	-3.640977	3.206483	-0.719508
6	-2.867642	2.387785	1.124725

1	-3.711352	2.711237	1.727826
6	-1.797957	1.704901	1.702118
1	-1.801774	1.488217	2.768629
6	-0.704293	1.298926	0.927243
1	0.127654	0.800174	1.420814
6	-0.625040	1.576430	-0.465319
15	0.655736	0.963433	-1.646758
6	2.106420	0.579590	-0.559659
6	2.540728	1.388957	0.512607
1	1.960745	2.265464	0.788902
6	3.709859	1.101812	1.216567
1	4.010387	1.746615	2.039881
6	4.506422	0.010703	0.858881
1	5.421432	-0.206761	1.403659
6	4.113737	-0.788260	-0.217053
1	4.726321	-1.635469	-0.518580
6	2.932352	-0.511946	-0.906445
1	2.642550	-1.146865	-1.742077
3	-0.766495	-0.685147	-0.626153

[$Ph_2PLi.TMEDA$]

6	-3.647163	0.129405	-0.368433
7	-2.722198	-0.994484	-0.593012
6	-2.917470	-1.532682	-1.949839
6	-2.901940	-2.031350	0.442285
6	-1.712352	-2.992495	0.513370
7	-0.434011	-2.287026	0.746294
6	-0.272069	-1.925674	2.165237
6	0.706550	-3.116447	0.317758
6	-0.163110	1.891786	-0.392725
6	-1.139516	2.802503	-0.879221
6	-2.019603	3.466864	-0.032057
6	-1.974780	3.261504	1.353857
6	-1.026328	2.375689	1.865773
6	-0.144532	1.700497	1.014193
15	0.824739	0.964842	-1.647184
6	2.354418	0.465707	-0.738058
6	3.025230	-0.702723	-1.165812

6	4.251337	-1.089744	-0.624989
6	4.852280	-0.329045	0.381483
6	4.213540	0.835237	0.815801
6	2.997288	1.231910	0.259416
3	-0.680910	-0.492451	-0.388528
1	0.605579	1.046694	1.453668
1	-0.957937	2.212897	2.940052
1	-2.650671	3.795597	2.016111
1	-2.736777	4.169819	-0.451432
1	-1.174783	3.002650	-1.948264
1	2.546503	2.163147	0.591089
1	4.675167	1.452804	1.583869
1	5.803704	-0.631667	0.811028
1	4.737759	-1.992763	-0.988913
1	2.574285	-1.309714	-1.949597
1	-3.449410	0.583278	0.606174
1	-3.477668	0.893441	-1.129923
1	-4.702066	-0.191451	-0.411671
1	-3.941562	-1.918575	-2.093800

1	-2.731782	-0.740678	-2.679965
1	-2.209935	-2.341303	-2.151426
1	-3.021320	-1.518343	1.402508
1	-3.827242	-2.610904	0.275993
1	-1.901472	-3.748788	1.294786
1	-1.622089	-3.537874	-0.431309
1	-1.080862	-1.265140	2.489384
1	-0.265031	-2.818285	2.814269
1	0.673587	-1.393053	2.296320
1	0.777243	-4.050321	0.900808
1	1.634259	-2.550993	0.432877
1	0.596949	-3.370824	-0.740499

Compound 7 [$Ph_2PLi.PMDETA$]

6	-2.169239	1.777489	0.853720
6	-1.646822	1.728291	-0.459975
6	-1.456691	2.974534	-1.100915
6	-1.730801	4.185721	-0.464018
6	-2.240846	4.203558	0.836017

6	-2.467481	2.985831	1.484345
15	-1.087522	0.209708	-1.355951
3	1.072921	-0.052322	-0.107293
7	2.621767	1.344756	-0.806112
6	3.264420	2.132156	0.254691
6	-2.232817	-1.126949	-0.828567
6	-3.542535	-0.944402	-0.331354
6	-4.372277	-2.026859	-0.037291
6	-3.941572	-3.339400	-0.242938
6	-2.659509	-3.547401	-0.760693
6	-1.827316	-2.466117	-1.040973
6	3.571860	0.410292	-1.439301
6	3.835928	-0.826871	-0.578327
7	2.605549	-1.612559	-0.350125
6	2.359084	-2.534702	-1.468187
6	2.626871	-2.331908	0.937959
6	2.346000	-1.409119	2.128916
7	1.087244	-0.658681	1.982410
6	-0.085748	-1.534884	2.154898

6	1.018686	0.444290	2.952557
6	2.053020	2.258866	-1.812558
1	-3.924432	0.061971	-0.188970
1	-5.373884	-1.839016	0.345278
1	-4.592006	-4.180025	-0.016039
1	-2.305601	-4.560022	-0.946988
1	-0.839702	-2.654706	-1.461094
1	-1.108013	2.982866	-2.131400
1	-1.570869	5.120569	-0.997977
1	-2.472571	5.144487	1.328312
1	-2.877638	2.976023	2.492702
1	-2.358149	0.849476	1.386848
1	0.107495	1.022334	2.775885
1	1.878676	1.108697	2.823635
1	1.011980	0.082924	3.995703
1	-0.091598	-2.007756	3.152822
1	-0.109162	-2.314238	1.391253
1	-0.996569	-0.947675	2.031339
1	2.352434	-2.014655	3.053794

1	3.155996	-0.677955	2.232944
1	3.588005	-2.849824	1.103353
1	1.860554	-3.110931	0.891018
1	3.158355	-3.289615	-1.569680
1	2.287168	-1.976776	-2.405231
1	1.405969	-3.047209	-1.317683
1	4.615127	-1.444527	-1.057004
1	4.241281	-0.519766	0.389732
1	4.531056	0.907650	-1.671180
1	3.138122	0.100209	-2.395469
1	1.333326	2.923900	-1.329802
1	1.516694	1.682089	-2.570022
1	2.834133	2.868204	-2.299841
1	4.082826	2.761993	-0.136838
1	3.678947	1.479556	1.028242
1	2.520913	2.783976	0.722254

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