Supporting Information for:

Synthesis and Characterization of Two "Tied-back" Lithium Ketimides and Isolation of a Ketimide-bridged $[Cr_2]^{6+}$ Dimer with Strong Antiferromagnetic Coupling

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Experimental

General Methods

All reactions and subsequent manipulations were performed under anaerobic and anhydrous conditions either under high vacuum or an atmosphere of nitrogen. Hexanes, pentane, and diethyl ether were dried using a Vacuum Atmospheres DRI-SOLV solvent purification system. Tetrahydrofuran (THF) was first distilled from calcium hydride then distilled from sodium benzophenone, collected, and stored over 3Å sieves for 24 h prior to use. C_6D_6 and THF-d_8 were dried over activated 3Å molecular sieves for 24 h before use. All reagents were purchased from commercial suppliers and used as received.

^{1}H, ^{13}C{^{1}H}, and ^{7}Li{^{1}H} NMR spectra were recorded on a Varian UNITY INOVA 400 MHz, Varian UNITY INOVA 500 MHz spectrometer, or Varian UNITY INOVA 600 MHz spectrometer. ^{1}H and ^{13}C{^{1}H} NMR spectra are referenced using the residual protio solvent peaks as internal standards (^{1}H NMR experiments) or the characteristic resonances of the solvent nuclei (^{13}C NMR experiments).[1, 2] ^{7}Li{^{1}H} spectra were referenced to a saturated LiCl solution in D_2O. Elemental analyses were performed by the Microanalytical Laboratory at UC Berkeley.

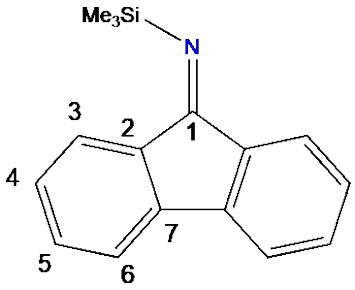
X-ray Crystallography. Data for **2**, **3**·Et_2O, **6**, and **7**·C_6H_6 were collected on a Bruker KAPPA APEX II diffractometer equipped with an APEX II CCD detector using a TRIUMPH monochromater with a Mo Kα X-ray source (α = 0.71073 Å). The crystals of **2**, **3**·Et_2O, **6**, and **7**·C_6H_6 were mounted on a cryoloop under Paratone-N oil, and all data were collected at 100(2) K using an Oxford nitrogen gas cryostream system. A hemisphere of data was collected using ω scans with 0.5º frame widths. Frame exposures of 10, 10, 15, and 20 s were used for **2**, **3**·Et_2O, **6**, and **7**·C_6H_6, respectively. Data collection and cell parameter determinations were conducted using the SMART program.[3] Integration of the data frames and final cell parameter refinements were performed using SAINT software.[4] Absorption corrections were carried out using the multi-scan method SADABS.[5] Subsequent calculations were carried out using SHELXTL[6] Structure determination was done using direct or Patterson methods and difference Fourier techniques. All hydrogen atom positions were idealized and rode on the atom of attachment. Structure solution, refinement, graphics, and creation of publication materials were performed using SHELXTL.

Further crystallographic details can be found in Tables S1. Complexes **2**, **3**·Et_2O, **6**, and **7**·C_6H_6 have been deposited in the Cambridge Structural Database (**2**: CCDC 2054150; **3**·Et_2O: CCDC 2054151; **6**: CCDC 2054152; **7**·C_6H_6: CCDC 2054153).

SQUID Magnetometry. The magnetic properties of **7** were recorded using a Quantum Design Magnetic Property Measurement System SQUID vibrating sample magnetometer (MPMS3 SQUID-VSM). 10.1 mg

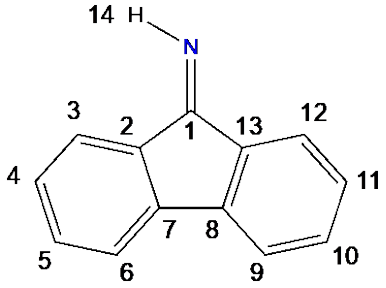
of polycrystalline **7**·C_6H_6 was loaded into a polypropylene capsule under inert atmosphere, which was subsequently sealed with vacuum grease to prevent exposure to air. The magnetic susceptibility of **7**·C_6H_6 was corrected for the sample holder and the sample diamagnetism (χ_{dia} = -8.759 × 10^{-4} $cm^3 \cdot mol^{-1}$) using Pascal's constants.[7] Magnetism data was modeled using julX.[8]

Synthesis of $(Me_3Si)N=C_{13}H_8$ (1). The synthesis of **1** is a modification of a previously reported procedure.[9] To a yellow stirring solution of 9-fluorenone (1.13 g, 6.2 mmol) in Et_2O (5 mL) was added $KN(SiMe_3)_2$ (1.25 g, 6.2 mmol), dropwise, as an Et_2O solution (5 mL). After the addition of $KN(SiMe_3)_2$, the solution began to warm and slowly turned deep yellow-orange in color. After 15 min of stirring, the volatiles were removed *in vacuo* to provide an oily-solid. This material was extracted into hexanes (10 mL) to provide a cloudy yellow-orange solution. The solution was then filtered through a Celite column supported on a medium porosity glass frit, leaving behind a large plug of tan solid on the Celite pad, which was discarded. The volatiles were removed from the filtrate *in vacuo* to yield a deep yellow-orange oil. The oil was extracted into hexanes (5 mL) and filtered through a Celite column supported on glass wool (0.5 cm × 2 cm). The volatiles were the removed in vacuo affording the product as a deep yellow-orange oil (1.56 g, 91% yield). ^{1}H NMR (600 MHz, 25 °C, benzene-d_6): δ 7.73 (d, J = 8.2 Hz, 2H, **3**), 7.25 (d, J = 7.1 Hz, 2H, **6**), 7.09 (t, J = 7.3 Hz, 2H, **5**), 7.00 (t, J = 7.5 Hz, 2H, **4**), 0.46 (s, 9H, $((CH_3)_3Si)$).^{13}C{^{1}H} NMR (C_6D_6, 25 °C, 150 MHz): δ 169.9 (**1**), 143.9 (**7**), 136.9 (**2**), 131.7 (**5**), 128.3 (**4**), 123.7 (**3**), 120.0 (**6**), 1.36 ($(CH_3)_3Si$)).

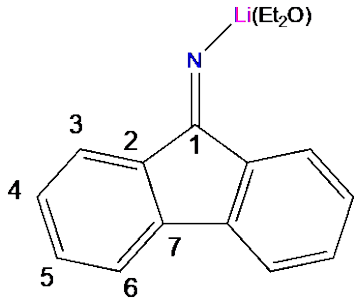


Synthesis of $HN=C_{13}H_8$ (2). To a stirring solution of 9-fluorenone (2.70 g, 14.9 mmol) in Et_2O (10 mL) was added $KN(SiMe_3)_2$ (2.98 g, 14.9 mmol) as a solid. After addition of $KN(SiMe_3)_2$, the solution began to warm and slowly turned deep yellow-orange in color. After 30 min, the volatiles were removed *in vacuo* and the resulting oily-solid was extracted into hexanes (10 mL) to yield a cloudy yellow-orange solution. The solution was filtered through a Celite column supported on a medium porosity glass frit, leaving behind a large plug of tan solid on the Celite pad, which was discarded. The volatiles were removed from the filtrate *in vacuo* and the resulting oil was extracted into hexanes (5 mL) and filtered through a Celite column supported on glass wool (0.5 cm × 2 cm). To the filtrate was added phenol (1.40 g, 14.9 mmol) as a 10:1 pentane/Et_2O solution, which resulted in a color change to bright yellow, concomitant with the deposition of a yellow powder. The yellow power was collected on a medium porosity glass frit and

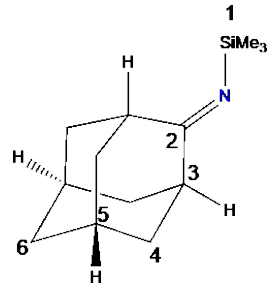
rinsed with additional hexanes (5 mL). Dissolution of the solid in warm Et_2O/THF (4:1, 20 ml), followed by storage at -25 °C for 24 h, afforded pale yellow crystalline blocks of **2** (2.23 g, 83% yield). ^{1}H NMR (THF-d_8, 25 °C, 500 MHz): δ 11.04 (s, 1H, **14**), 7.90 (d, J = 7.4 Hz, 1H, **3** or **12**), 7.72 (d, J = 7.5 Hz, 1H, **3** or **12**), 7.66-7.64 (m, 2H, **6** and **9**), 7.41 (t, J = 7.2 Hz, 2H, **5** and **10**), 7.33 (t, J = 7.5 Hz, 2H, **4** and **11**). ^{13}C{^{1}H} NMR (THF-d_8, 25 °C, 125 MHz): δ 172.7 (**1**), 143.7 (**7**), 142.7 (**8**), 139.0 (**2**), 134.5 (**13**), 132.7 (**5**), 132.6 (**10**), 129.1 (**4**), 128.9 (**11**), 123.8 (**3**), 122.8 (**12**), 121.0 (**6**), 120.9 (**9**). TOF-MS (THF, positive ion mode, 1.3 kV): *m/z* 180.1 $[M+H]^+$ (Calcd *m/z* 180.08). IR (KBr pellet, cm^{-1}): 3191 (m), 1639 (m), 1610 (w), 1598 (w), 1475 (w), 1454 (m), 1440 (w), 1346 (m), 1263 (m), 1214 (w), 1178 (w), 1170 (w), 1151 (w), 1101 (w), 960 (w), 948 (w), 925 (w), 885(m), 877 (m), 798 (s), 744 (s), 738 (s), 692 (w), 651 (m), 632 (m).



Synthesis of $[Li(Et_2O)]_4[N=C_{13}H_8]_4$ (3). To a yellow, stirring solution of **2** (0.405 g, 2.6 mmol) in Et_2O (2 mL) was added LiN^iPr_2 (0.243 g, 2.6 mmol), dropwise, as a Et_2O solution (4 mL). After addition, the solution slowly turned deep blue-green, concomitant with the deposition of a deep blue-green solid. After 30 min, the deep blue-green solid was isolated by decanting off the supernatant and then dried *in vacuo* (341.2 mg, 58% yield). Subsequent storage of the supernatant at -25 °C for 24 h afforded deep blue crystals of **3**. The crystals were isolated by decanting off the supernatant, dried *in vacuo*, and then combined with the previously isolated deep blue-green solid (total yield: 0.447 g, 76%). Anal. Calcd for $C_{17}H_{18}NLiO$: C, 78.75; H, 7.00; N, 5.40. Found: C, 78.12; H, 6.66; N, 5.53. ^{1}H NMR (THF-d_8, 25 °C, 400 MHz): δ 7.73 (d, J = 7.5 Hz, 2H, **3**), 7.62 (d, J = 7.4 Hz, 2H, **6**), 7.22 (t, J = 7.4 Hz, 2H, **5**), 7.06 (t, J = 7.4 Hz, 2H, **4**), 3.35 (q, 4H, Et_2O), 1.08 (t, 6H, Et_2O). ^{13}C{^{1}H} NMR (THF-d_8, 25 °C, 150 MHz): δ 166.4 (**1**), 144.2 (**7**), 138.0 (**2**), 129.2 (**5**), 128.3 (**4**), 121.5 (**3**), 119.7 (**6**), 66.5 (Et_2O), 15.9 (Et_2O). ^{7}Li{^{1}H} NMR (THF-d_8, 25 °C, 155 MHz): δ 2.99. IR (KBr pellet, cm^{-1}): 3196 (m), 3051 (w), 2976 (w), 2931 (w), 2868 (w), 1641 (s), 1612 (m), 1601 (m), 1454 (m), 1383 (w), 1348 (w), 1281 (w), 1263 (w), 1178 (w), 1151 (w), 1120 (w), 1103 (w), 1051 (w), 949 (w), 926 (w), 887 (m), 798 (m), 775 (w), 739 (s), 652 (m), 633 (w), 617 (w), 602 (w), 440 (s).

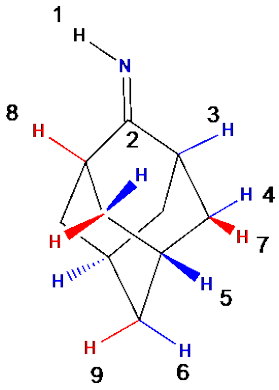


Synthesis of $(Me_3Si)N=C_{10}H_{14}$ (4). To a colorless, stirring solution of 2-adamantanone (1.03 g, 6.6 mmol) in pentane (5 mL) was added $KN(SiMe_3)_2$ (1.31 g, 6.6 mmol) as a solid. After 7 d, the solution was filtered through a Celite column supported on a medium porosity glass frit, leaving behind a large plug of tan solid on the Celite pad, which was discarded. The volatiles were removed *in vacuo* and the resulting pale yellow oil was extracted into hexanes (5 mL), and filtered through a Celite column supported on glass wool (0.5 cm × 2 cm). The volatiles were then removed *in vacuo*, which afforded the colorless oil (1.33 g, 89% yield). ^{1}H NMR (C_6D_6, 25 °C, 500 MHz): δ 2.59 (m, 2H, **3**), 1.77 (m, 8H, **4**), 1.70 (s, 2H, **6**), 1.62 (s, 2H, **5**), 0.31 (s, 9H, **1**). ^{13}C{^{1}H} NMR (C_6D_6, 25 °C, 150 MHz): δ 190.7 (**2**), 46.6 (**3**), 39.4 (**4**), 36.9 (**5**), 28.0 (**6**), 1.45 (**1**). IR (KBr pellet, cm^{-1}): 2904 (m), 2850 (m), 1697 (s), 1670 (s), 1450 (m), 1348 (w), 1288 (w), 1245 (s), 1224 (w), 1151 (w), 1097 (w), 1054 (s), 1035 (m), 997 (w), 952 (w), 898 (m), 856 (s), 835 (s), 748 (s), 686 (s), 624 (m), 615 (w), 561 (m).

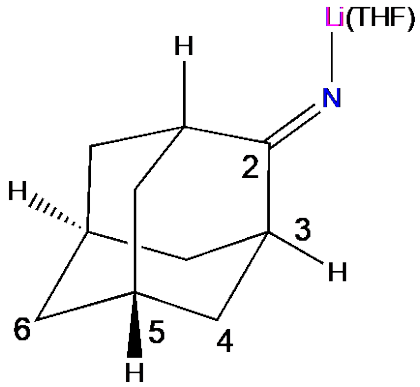


Synthesis of $HN=C_{10}H_{14}$ (5). To a colorless, stirring sample of **4** (1.28 g, 5.0 mmol) was added methanol (0.5 mL, 12.3 mmol), whereupon the solution warmed and became cloudy. After 1 min, the volatiles were removed *in vacuo* to yield a white oily-solid. This material was and triturated with pentane (3 × 2 mL). The resulting white solid was extracted into Et_2O (2 mL) and filtered through a Celite column supported on glass wool (0.5 cm × 2 cm). Storage of this solution at -25 °C for 2 h resulted in the deposition of a white crystalline solid. (0.77 g, 88% yield). ^{1}H NMR (C_6D_6, 25 °C, 500 MHz): δ 8.63 (s, 1H, **1**), 2.85 (s, 1H, **3**), 1.92 (s, 1H, **8**), 1.75 (m, 4H, **4**), 1.63 (s, 2H, **5**), 1.58 (m, 4H, **7**), 1.58-1.51 (s, 2H, **6** and **9**). ^{13}C{^{1}H} NMR (C_6D_6, 25 °C, 125 MHz): δ 187.5 (**2**), 46.6 (**3**), 41.6 (**8**), 38.65 (**4**), 38.59 (**7**), 36.3 (**6**/**9**), 27.6 (**5**). TOF-MS (THF, positive ion mode, 1.6 kV): *m/z* 150.1 $[M+H]^+$ (Calcd *m/z* 150.12). IR (KBr pellet, cm^{-1}): 3201 (w), 3183 (w), 2910 (vs), 2850 (s), 1681 (m), 1648 (vs), 1450 (s), 1388 (m),

1349 (m), 1322 (m), 1311 (m), 1286 (w), 1164 (m), 1151 (m), 1097 (w), 1049 (s), 1031 (w), 993 (m), 950 (m), 923 (m), 879 (m), 867 (s), 835 (w), 800 (w), 746 (w), 719 (w), 628 (w).



Synthesis of [Li(THF)]$_4$[N=C$_{10}$H$_{14}$]$_4$ (6). To a colorless, stirring solution of **5** (472.6 mg, 3.17 mmol) in Et_2O (4 mL) was added LiN^iPr_2 (339.2 mg, 3.17 mmol), dropwise, as an Et_2O solution (2 mL), whereupon a fine white precipitate began to form. After 30 min, the volatiles were removed *in vacuo* to provide a white solid. The solid was dissolved in THF (2 mL), filtered through a Celite column supported on glass wool (0.5 cm × 2 cm), and then the filtrate was layered with hexanes (5 mL). Storage of this solution at -25 °C for 24 h resulted in the deposition of **6** as a white crystalline solid. (521.9 mg, 72.5% yield). Single crystals suitable for X-ray diffraction can be obtained by storage of a THF solution layered with hexanes at -25 °C for 24 h. Anal. Calcd for $C_{14}H_{22}NLiO$: C, 73.99; H, 9.76; N, 6.16. Found: C, 74.51; H, 9.58; N, 6.68. ^{1}H NMR (500 MHz, 25 °C, THF-d_8): δ 3.58 (4H, THF), 1.97 (s, 2H, **3**), 1.83 (m, 8H, **4**), 1.80 (s, 2H, **6**), 1.76 (s, 2H, **5**), 1.74 (4H, THF). ^{7}Li{^{1}H} NMR (THF-d_8, 25 °C, 155 MHz): δ 0.16. ^{13}C{^{1}H} NMR (126 MHz, 25 °C, THF-d_8): δ 68.40 (THF) 53.02 (**3**), 40.40 (**4**), 38.98 (**5**), 30.04 (**6**), 26.55 (THF). The imine *C*=N resonance could not be located. IR (KBr pellet, cm^{-1}): 2902 (s), 2846 (s), 1660 (s), 1630 (s), 1448 (s), 1350 (w), 1321 (w), 1282 (w), 1201 (w), 1171 (w), 1061 (s), 1034 (s), 1012 (s), 987 (s), 951 (m), 910 (m), 876 (m), 839 (m), 798 (w), 781 (w), 748 (w), 721 (w), 669 (m), 621 (m), 606 (m), 555 (s).



Synthesis of [Li][$Cr_2(N{=}C_{10}H_{14})_7$] (7). To a stirring slurry of $CrCl_3$ (49.3 mg, 0.311 mmol) in cold THF (2 mL) was added **6** (247.6 mg, 1.089 mmol), dropwise, as a THF solution (2 mL). Upon addition, the stirring suspension immediately became dark brown and the purple $CrCl_3$ flakes began to dissolve. After 5 min, no $CrCl_3$ flakes remained visible, whereupon the volatiles were removed *in vacuo* to yield a dark brown oily-solid. The resulting oil was extracted into pentane (4 mL) and filtered through a Celite column supported on glass wool (0.5 cm × 2 cm). Benzene (0.25 mL) was then added to the filtrate. Storage of this solution at -25 °C for 24 h resulted in the deposition of **7** as dark brown crystals (76.1 mg, 43 % yield). Anal. Calcd for $Cr_2LiC_{70}H_{98}N_7 \cdot C_6H_6$: C, 74.42; H, 8.55; N, 7.99. Anal. Calcd for $Cr_2LiC_{70}H_{98}N_7$: C, 73.20; H, 8.60; N, 8.54. Found: C, 72.78; H, 8.92; N, 7.88. ^{1}H NMR (600 MHz, 25 °C, THF-d_8): δ 6.59, 6.05, 5.80, 5.42, 4.81, 4.71, 4.55, 4.09, 3.72, 3.27, 2.96, 1.08, 0.66, 0.15. ^{7}Li{^{1}H} NMR (THF-d_8, 25 °C, 155 MHz): δ -5.74. IR (KBr pellet, cm^{-1}): 2904 (s), 2846 (s), 1649 (s), 1450 (m), 1342 (w), 1321 (w), 1203 (w), 1171 (w), 1092 (w), 1059 (w), 1047 (w), 995 (w), 953 (w), 924 (w), 881 (w), 800 (w), 683 (w), 652 (w), 636 (w), 619 (w), 538 (w).

Table S1. X-ray Crystallographic Data for Complexes **2**, **3**·Et_2O, **6**, and **7**·C_6H_6

	2	**3**·Et_2O	**6**	**7**·C_6H_6
empirical formula	$NC_{13}H_9$	$Li_4N_4C_{72}H_{82}O_5$	$N_4C_{56}H_{88}O_4Li_4$	$Cr_2N_7C_{76}H_{104}Li$
Crystal habit, color	Block, Yellow	Block, Green	Block, Colorless	Block, Brown
crystal size (mm)	0.40 × 0.15 × 0.15	0.40 × 0.30 × 0.20	0.20 × 0.15 × 0.10	0.2 × 0.1 × 0.05
crystal system	Orthorhombic	Triclinic	Tetragonal	Orthorhombic
space group	$P2_12_12_1$	$P\bar{1}$	$I4_1/a$	$Pna2_1$
vol (Å^3)	914.39(9)	3162.9(3)	5026.0(4)	6537.9(8)
a (Å)	5.3877(2)	13.2825(8)	20.3399(7)	24.3613(17)
b (Å)	11.1900(7)	13.4420(5)	20.3399(7)	12.4342(9)
c (Å)	15.1670(10)	19.2746(9)	12.1486(5)	21.5833(17)
α (deg)	90.00	102.399(3)	90.00	90.00
β (deg)	90.00	108.620(3)	90.00	90.00
γ (deg)	90.00	92.330(3)	90.00	90.00
Z	4	2	4	4
fw (g/mol)	179.21	1111.17	909.06	1226.60
density (calcd) (Mg/m^3)	1.302	1.167	1.201	1.246
abs coeff (mm^{-1})	0.076	0.071	0.073	0.382
F_{000}	376	1188	1984	2640
Total no. reflections	4296	25397	10773	20547
Unique reflections	1890	12959	2150	10719
R_{int}	0.0351	0.0499	0.0511	0.1234
final R indices [$I > 2\sigma(I)$]	R_1 = 0.0423 wR_2 = 0.0902	R_1 = 0.0511 wR_2 = 0.1170	R_1 = 0.0604, wR_2 = 0.1270	R_1 = 0.0702, wR_2 = 0.1172
largest diff peak and hole (e$^-$Å^{-3})	0.457 and -0.273	0.932 and -0.321	0.595 and -0.532	0.628 and -0.641
GOF	1.060	1.106	1.003	1.006

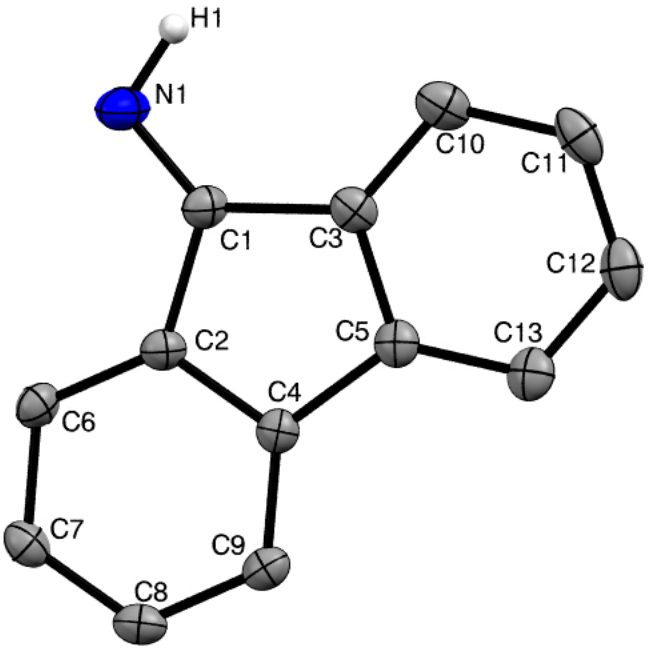


Figure S1. Solid-state structure of $HN{=}C_{13}H_8$ (**2**) with 50% probability ellipsoids. Aryl hydrogen atoms omitted for clarity. Selected bond lengths (Å) and angles (°): N1–C1 = 1.290(3), N1–C1–C2 = 123.51(18), N1–C1–C3 = 131.1(19), C2–C1–C3 = 105.47(16).

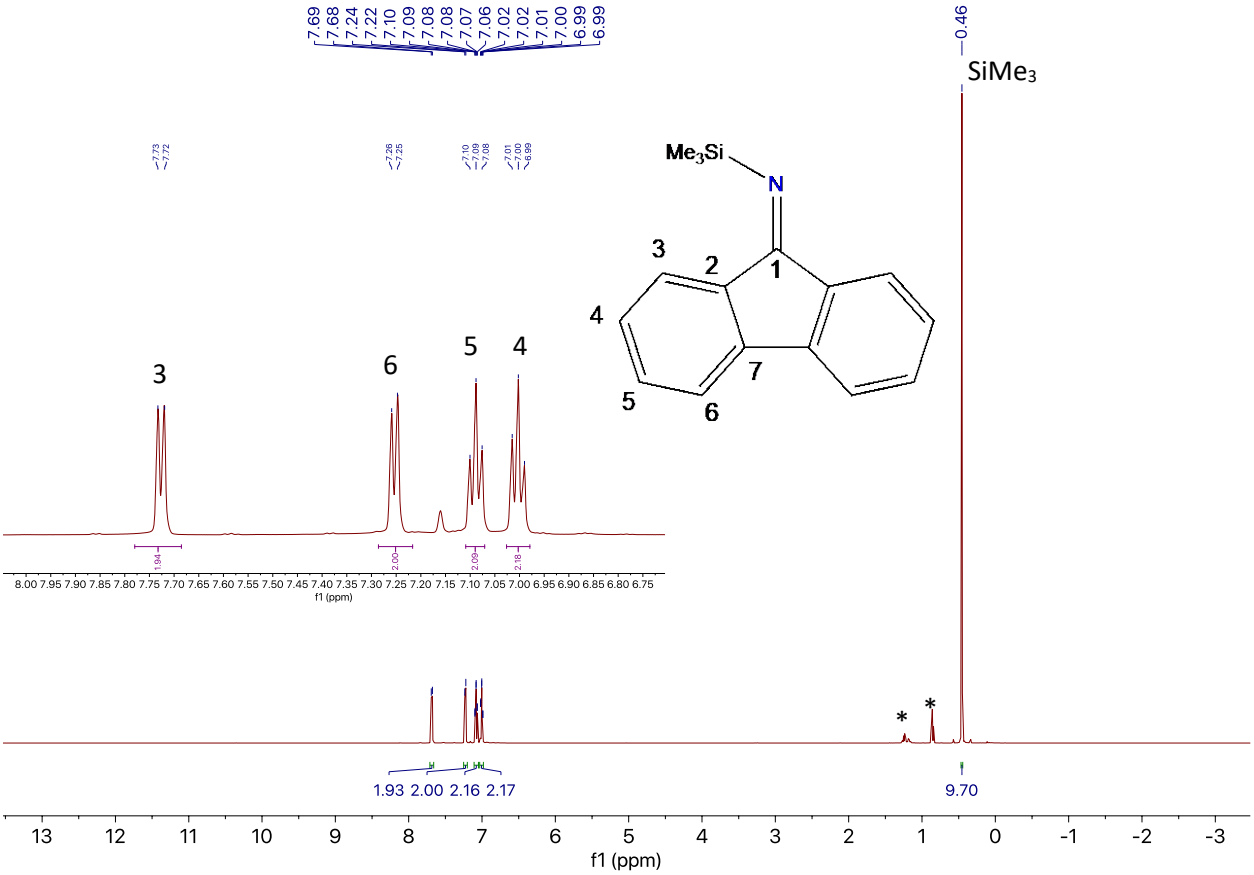


Figure S2. ^{1}H NMR spectrum at 25 °C in C_6D_6 of **1**. (*) indicates the presence of *n*-pentane.

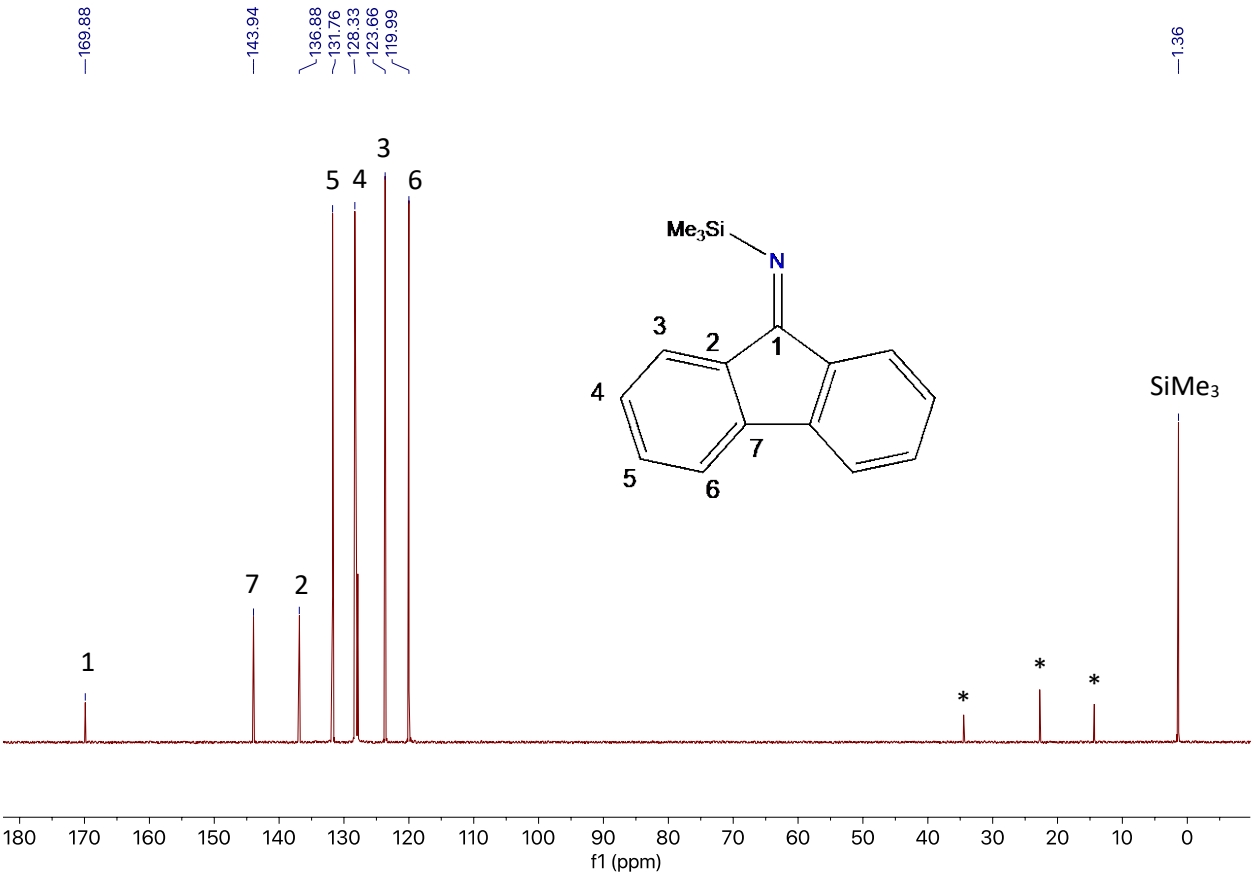


Figure S3. $^{13}C\{^{1}H\}$ NMR spectrum at 25 °C in C_6D_6 of **1**. (*) indicates the presence of *n*-pentane.

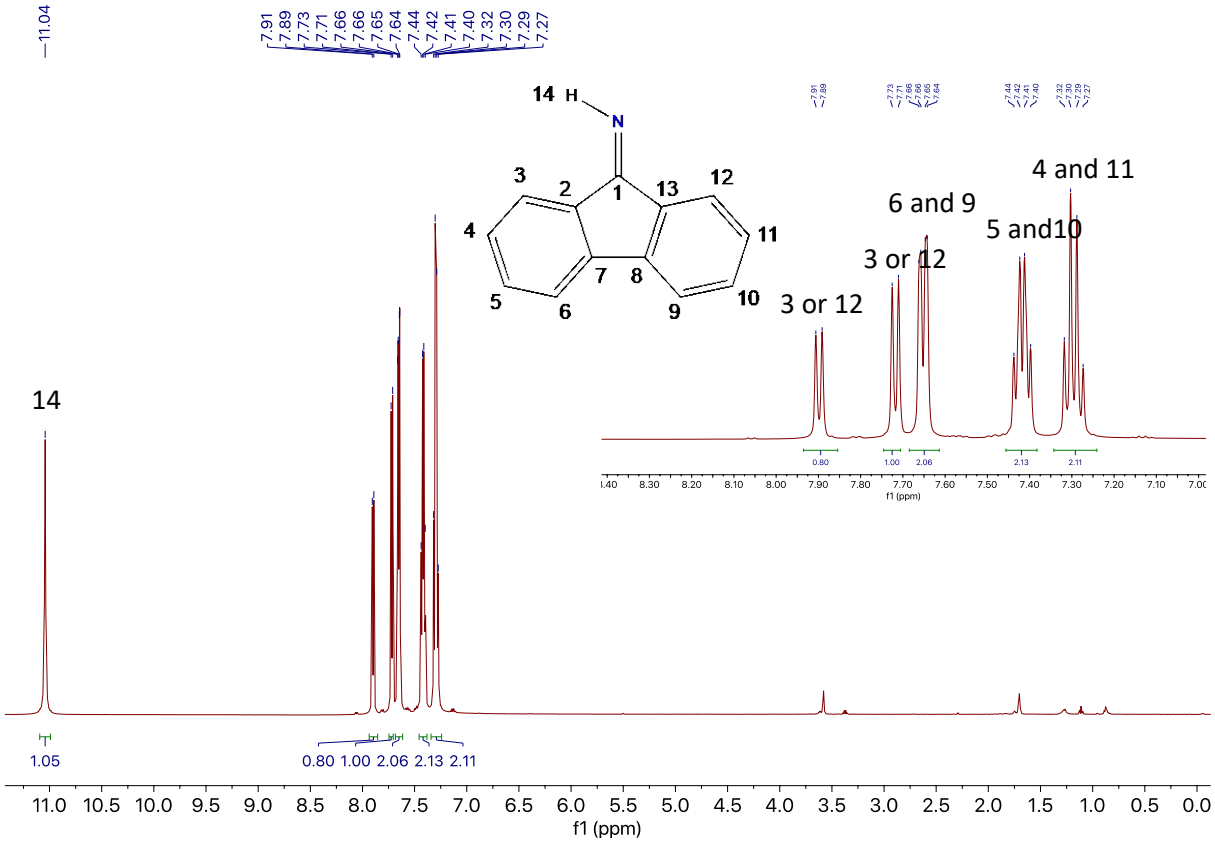


Figure S4. ^{1}H NMR spectrum at 25 °C in THF-d_8 of **2**.

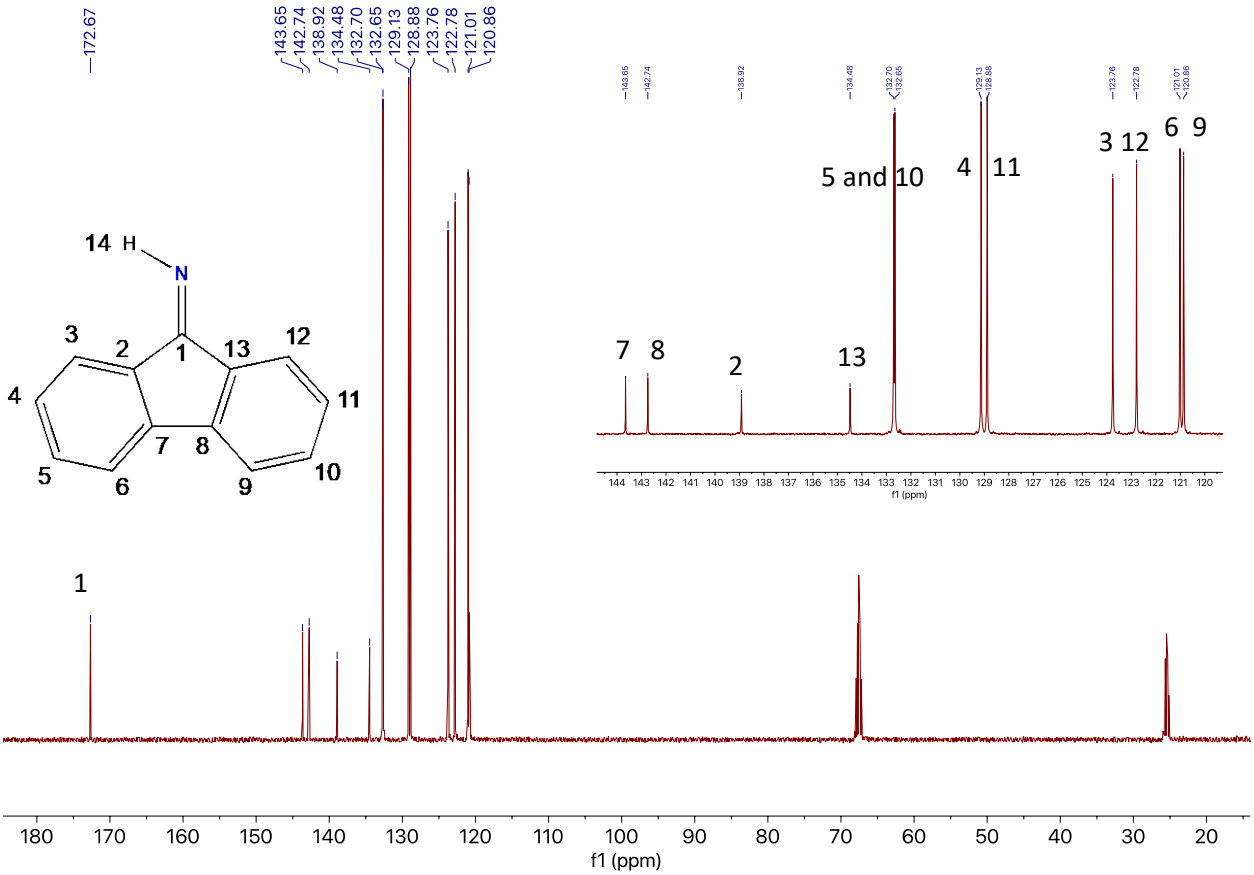


Figure S5. $^{13}C\{^{1}H\}$ NMR spectrum at 25°C in THF-d_8 of **2**.

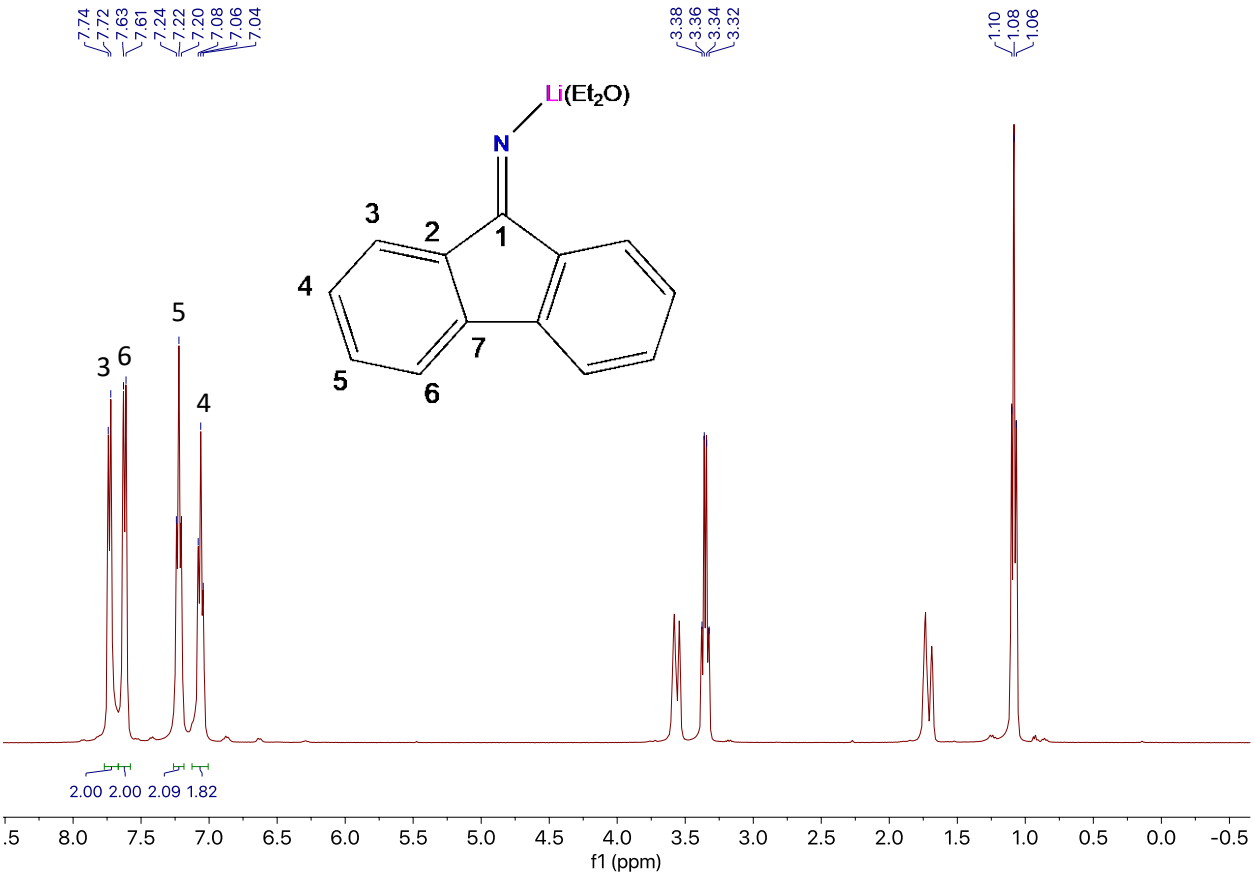


Figure S6. ^{1}H NMR spectrum at 25 °C in THF-d_8 of **3**.

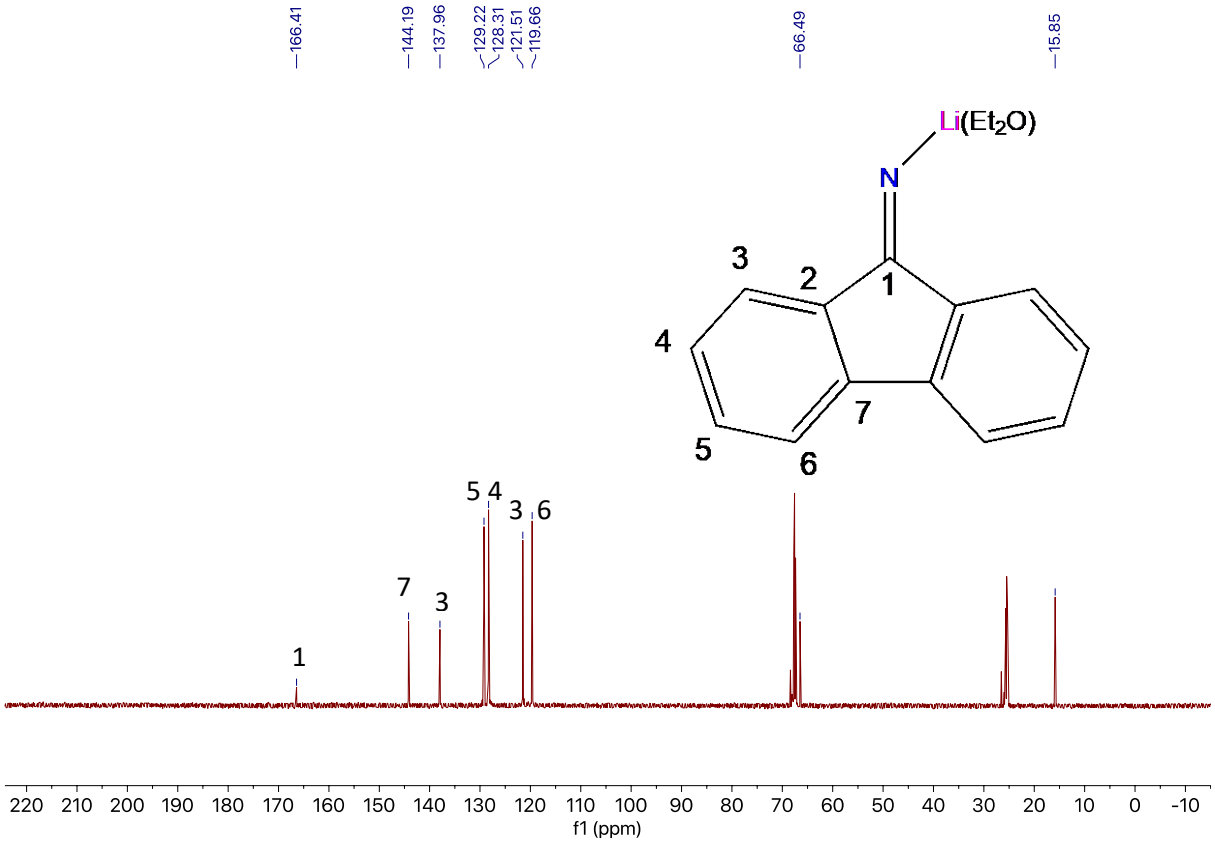


Figure S7. $^{13}C\{^{1}H\}$ NMR spectrum at 25 °C in THF-d_8 of **3**.

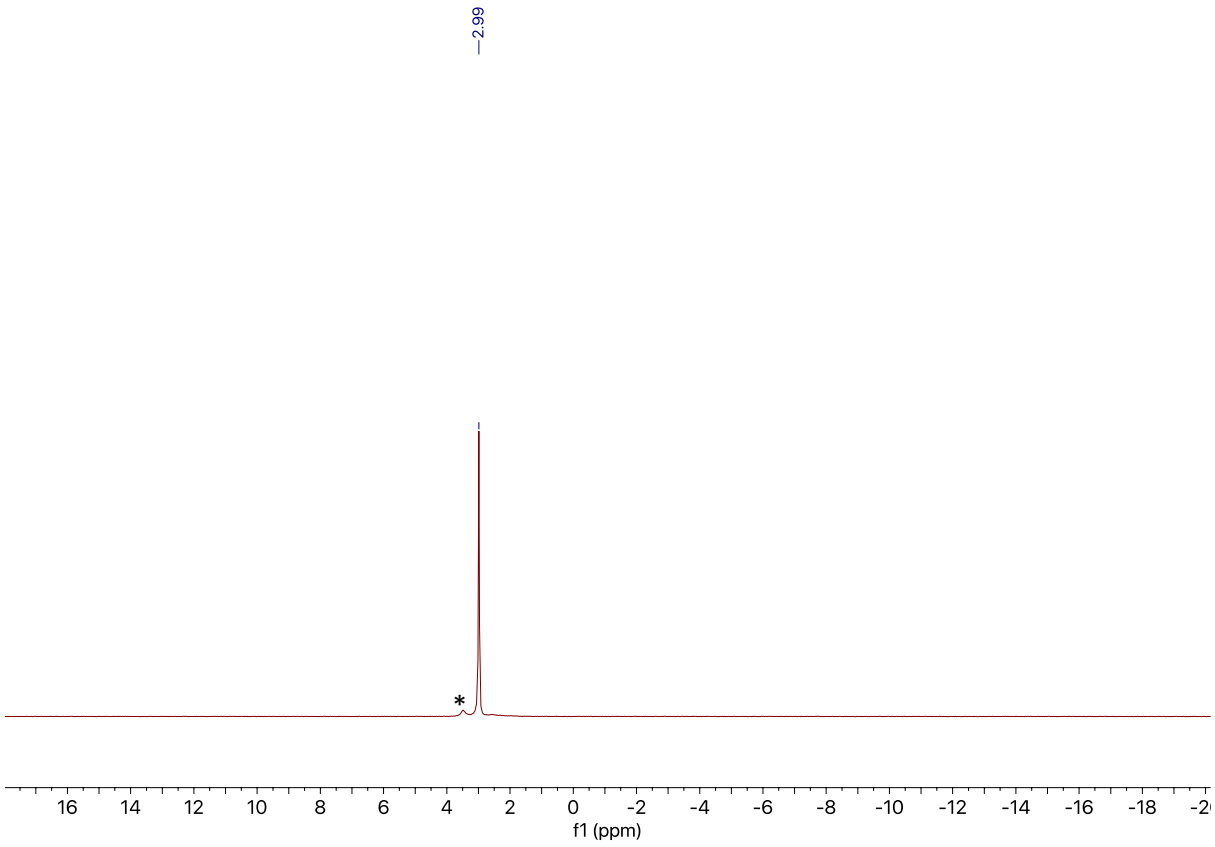


Figure S8. $^{7}Li\{^{1}H\}$ NMR spectrum at 25 °C THF-d_8 of **3**. (*) indicates the presence of an unidentified impurity.

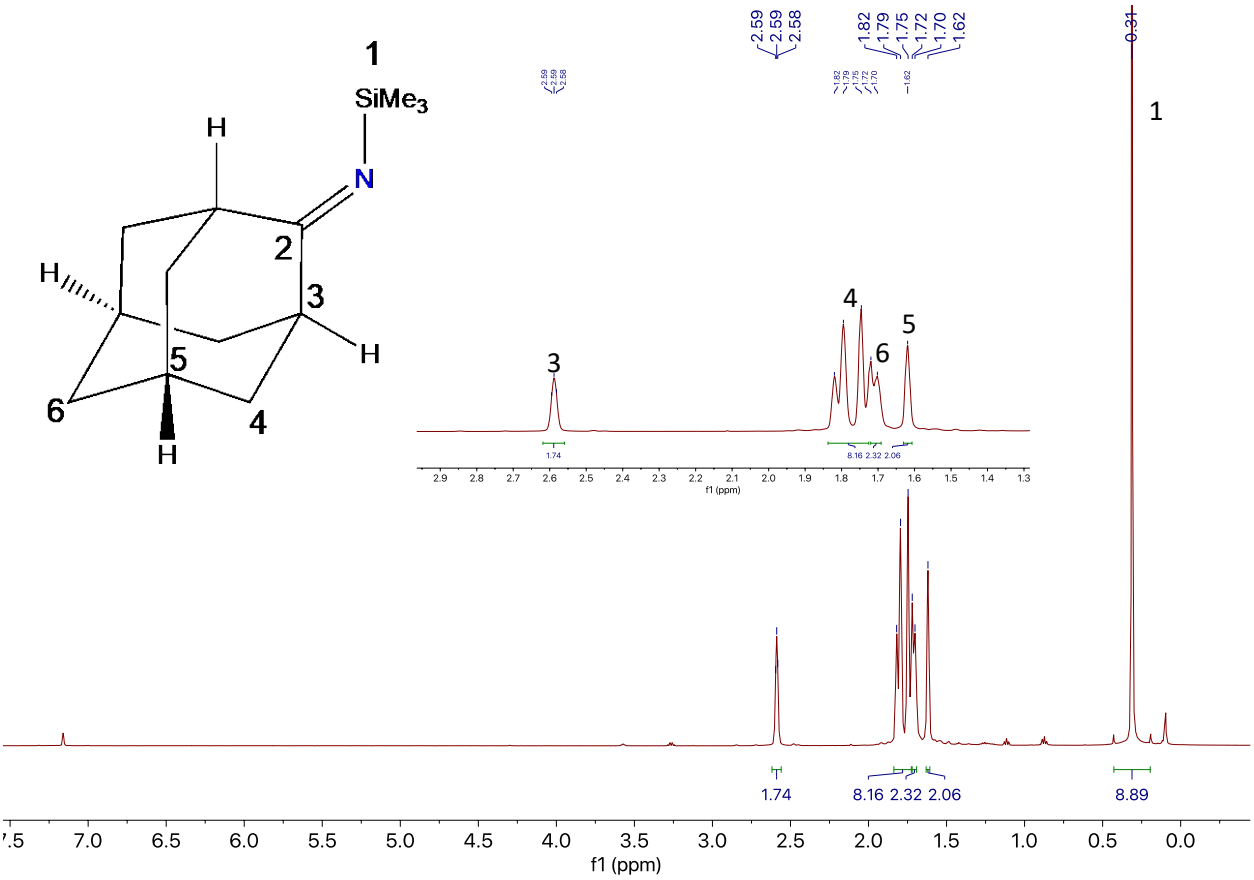


Figure S9. ^{1}H NMR spectrum at 25 °C of **4** in C_6D_6.

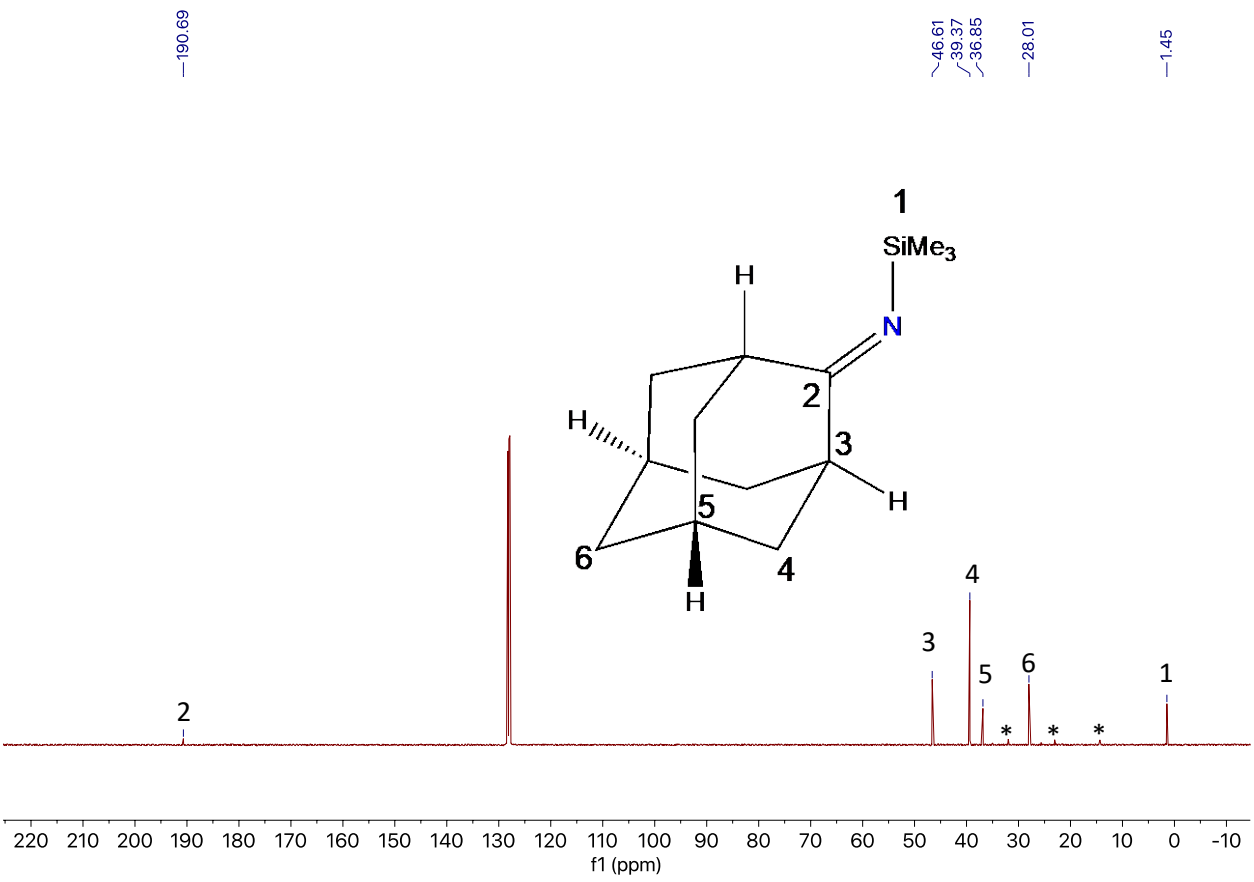


Figure S10. $^{13}C\{^{1}H\}$ NMR spectrum at 25 °C of **4** in C_6D_6. (*) denotes resonances assignable to hexanes.

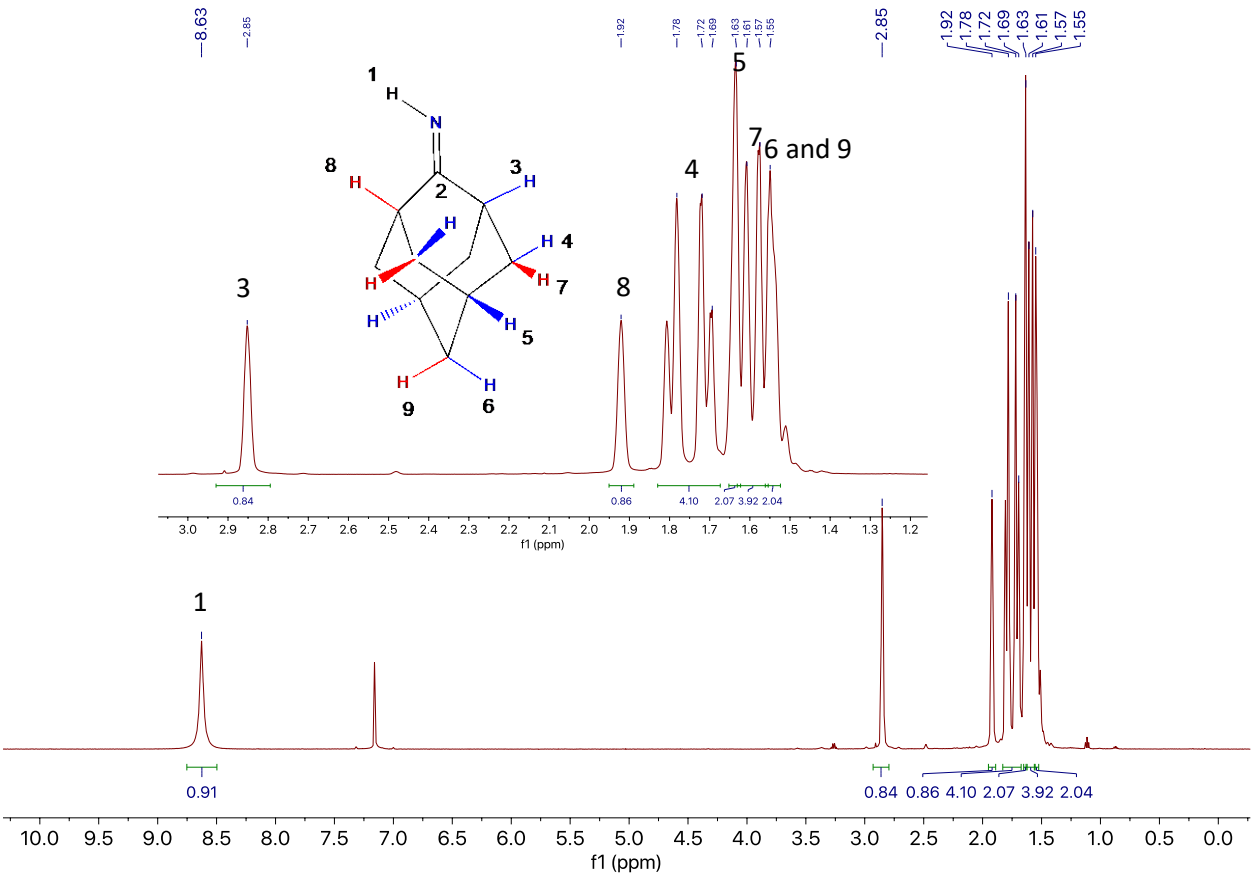


Figure S11. ^{1}H NMR spectrum at 25 °C of **5** in C_6D_6.

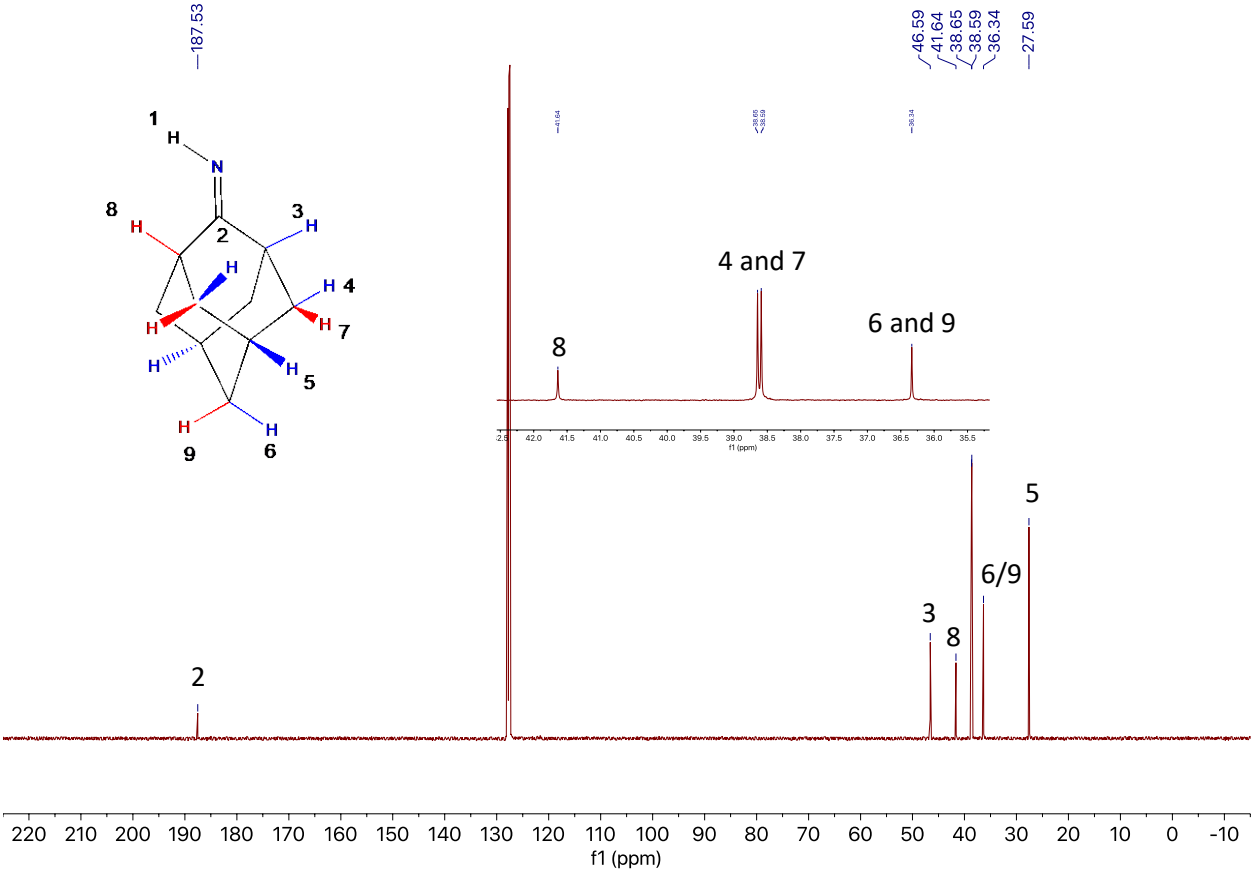


Figure S12. $^{13}C\{^{1}H\}$ NMR spectrum at 25 °C of **5** in C_6D_6.

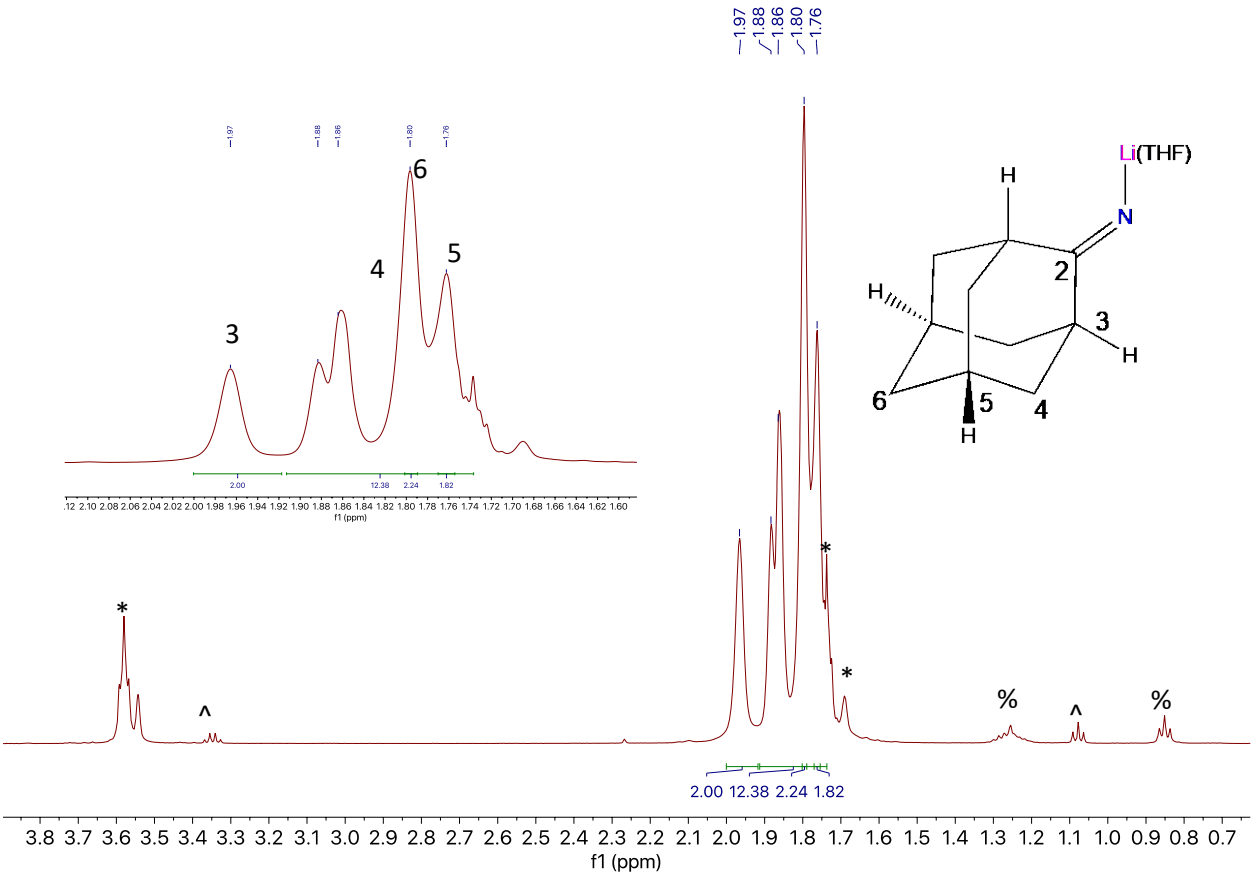


Figure S13. ^{1}H NMR spectrum at 25 °C of **6** in THF-d_8. (*) denotes THF, (^) denotes Et_2O, (%) denotes hexanes.

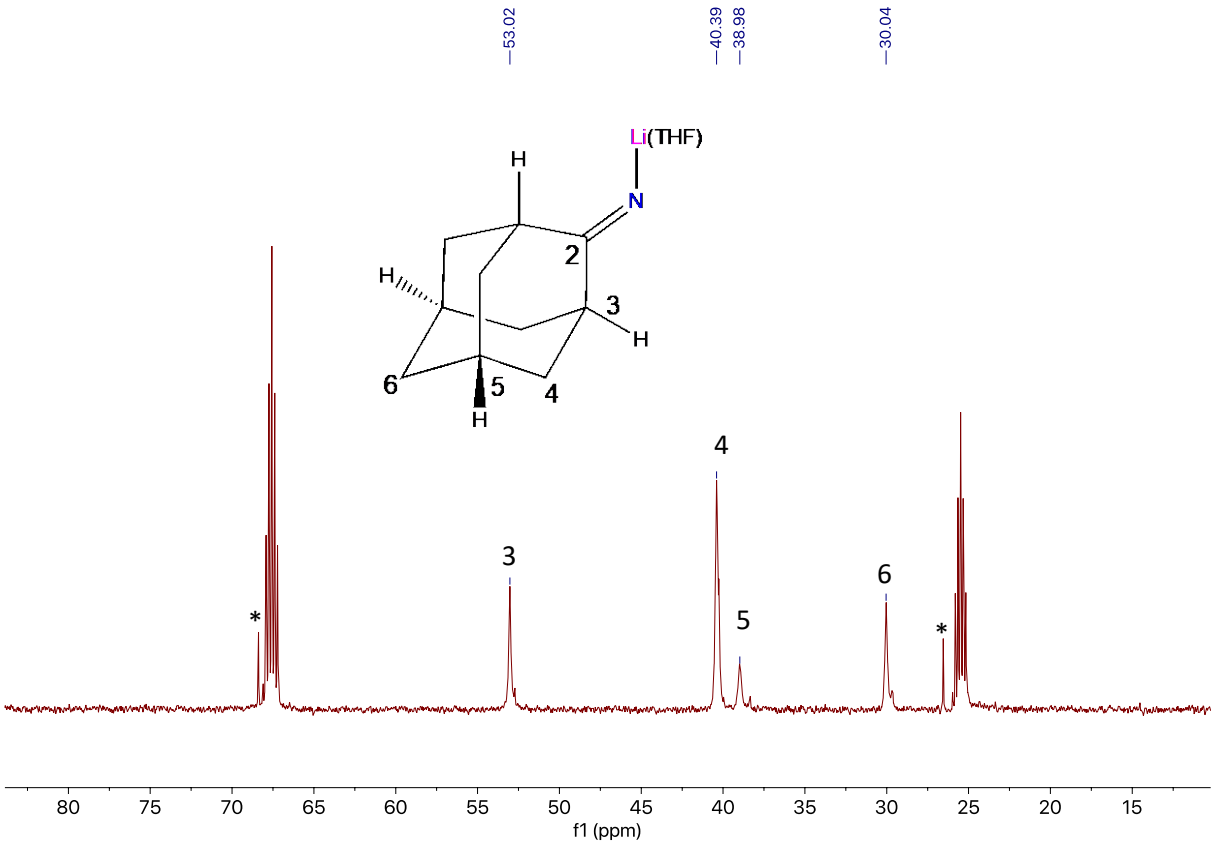


Figure S14. $^{13}C\{^{1}H\}$ NMR spectrum at 25 °C of **6** in THF-d_8. (*) denotes THF.

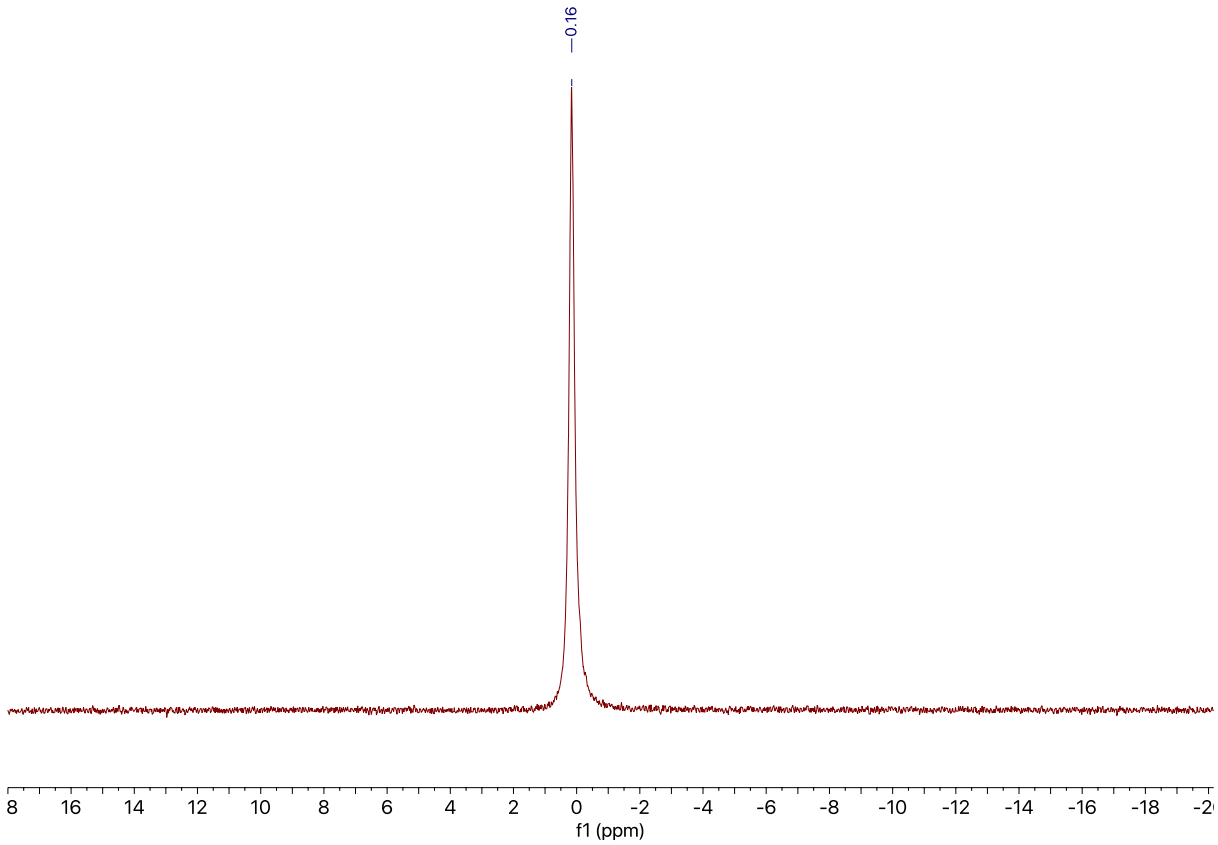


Figure S15. $^{7}Li\{^{1}H\}$ NMR spectrum at 25 °C of **6** in THF-d_8.

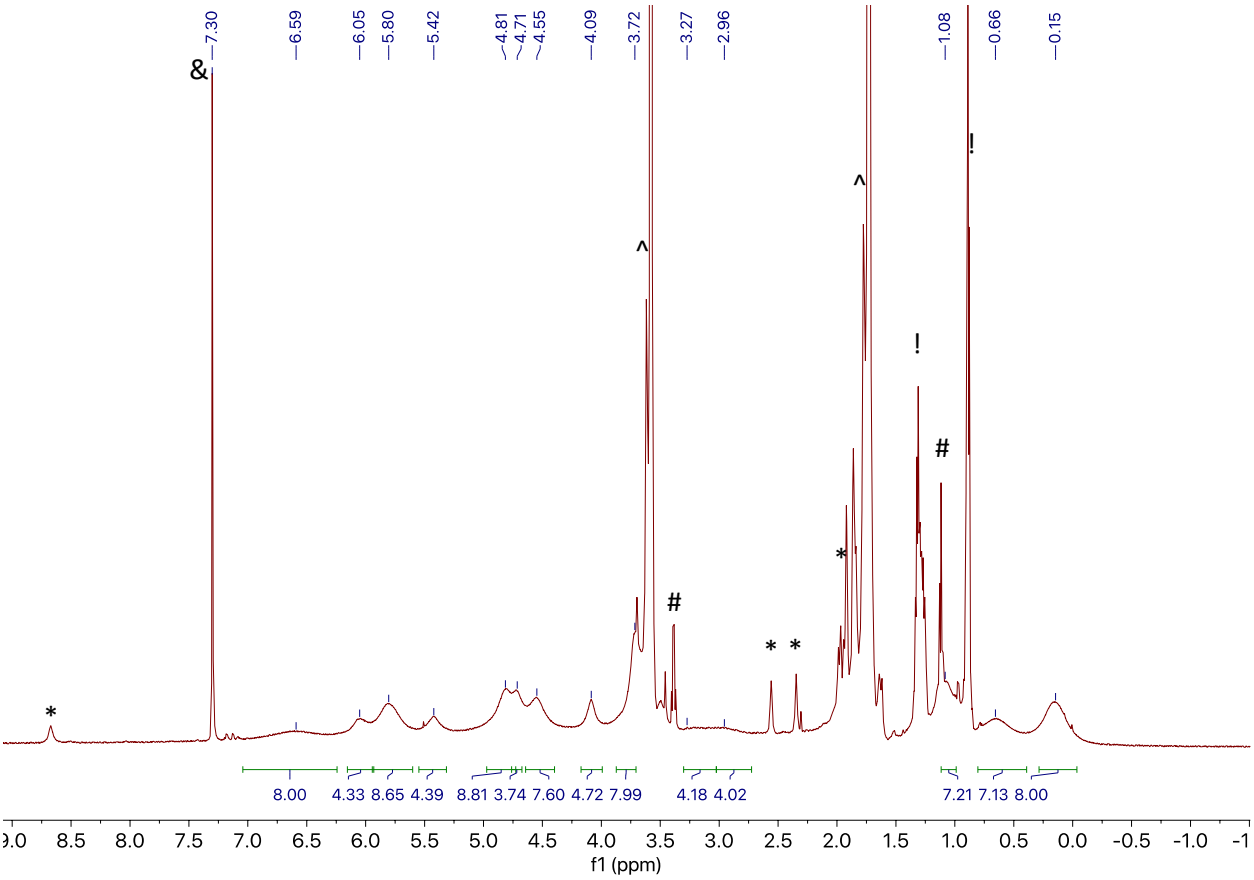


Figure S16. ^{1}H NMR spectrum at 25 °C of **7** in THF-d_8. (*) denotes free HN=$C_{10}H_{14}$, (^) denotes THF, (#) denotes diethyl ether, (!) denotes hexanes, (&) denotes benzene.

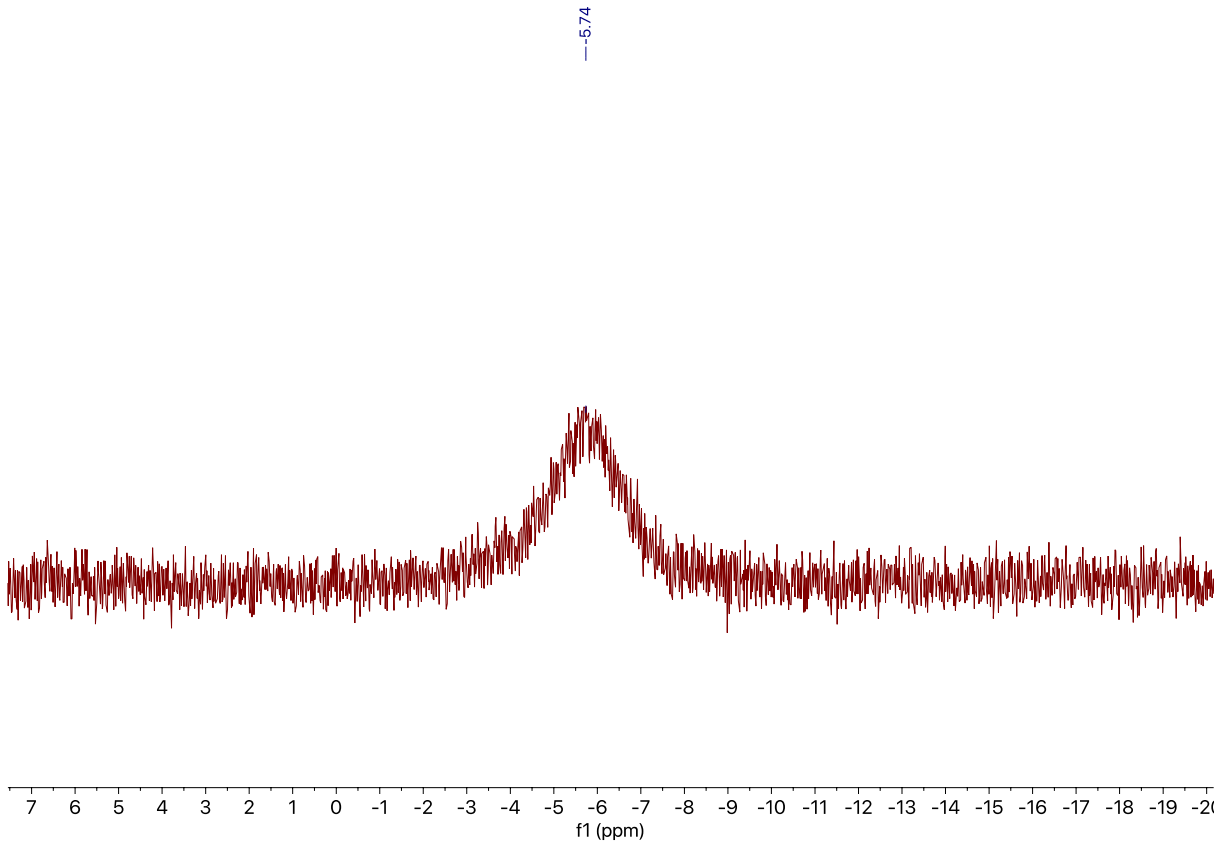


Figure S17. $^{7}Li\{^{1}H\}$ NMR spectrum of **7**.

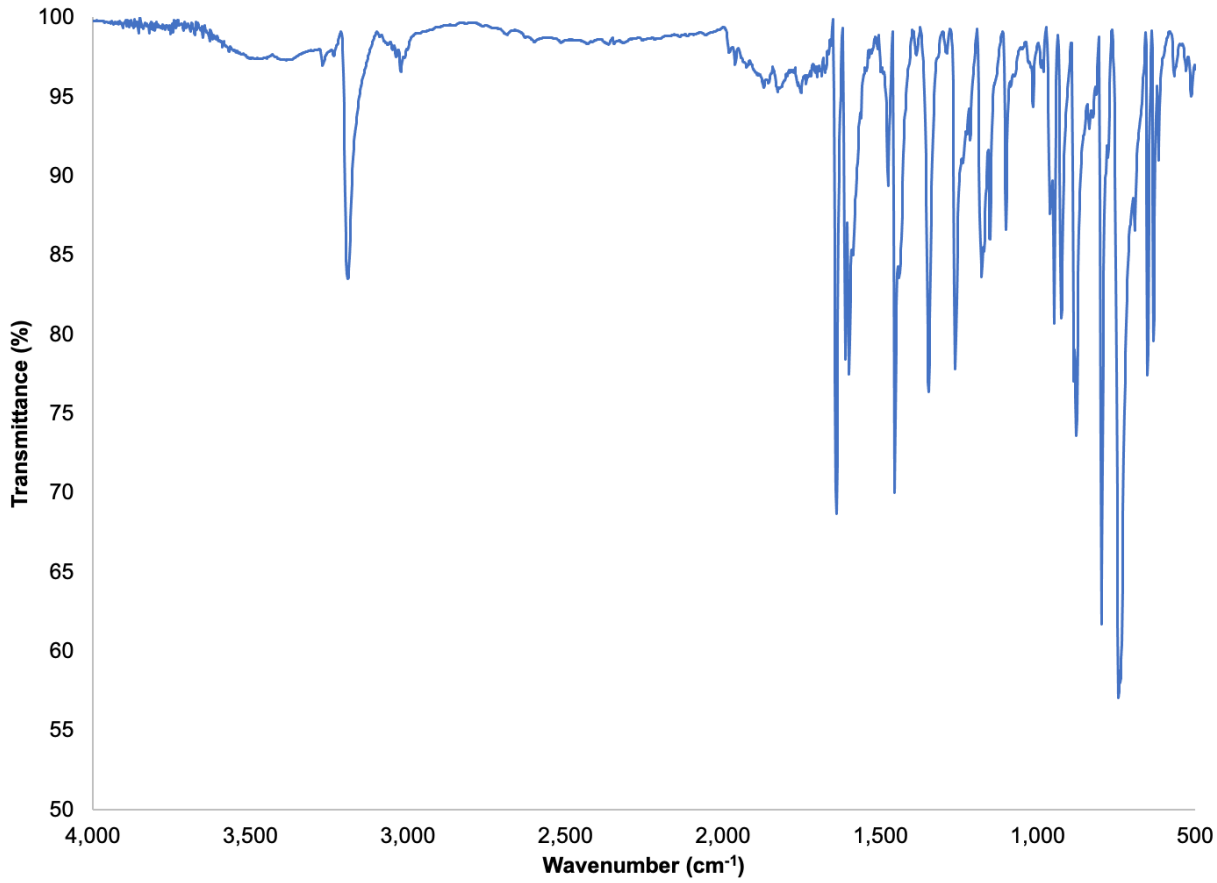


Figure S18. IR spectrum of **2** (KBr Pellet).

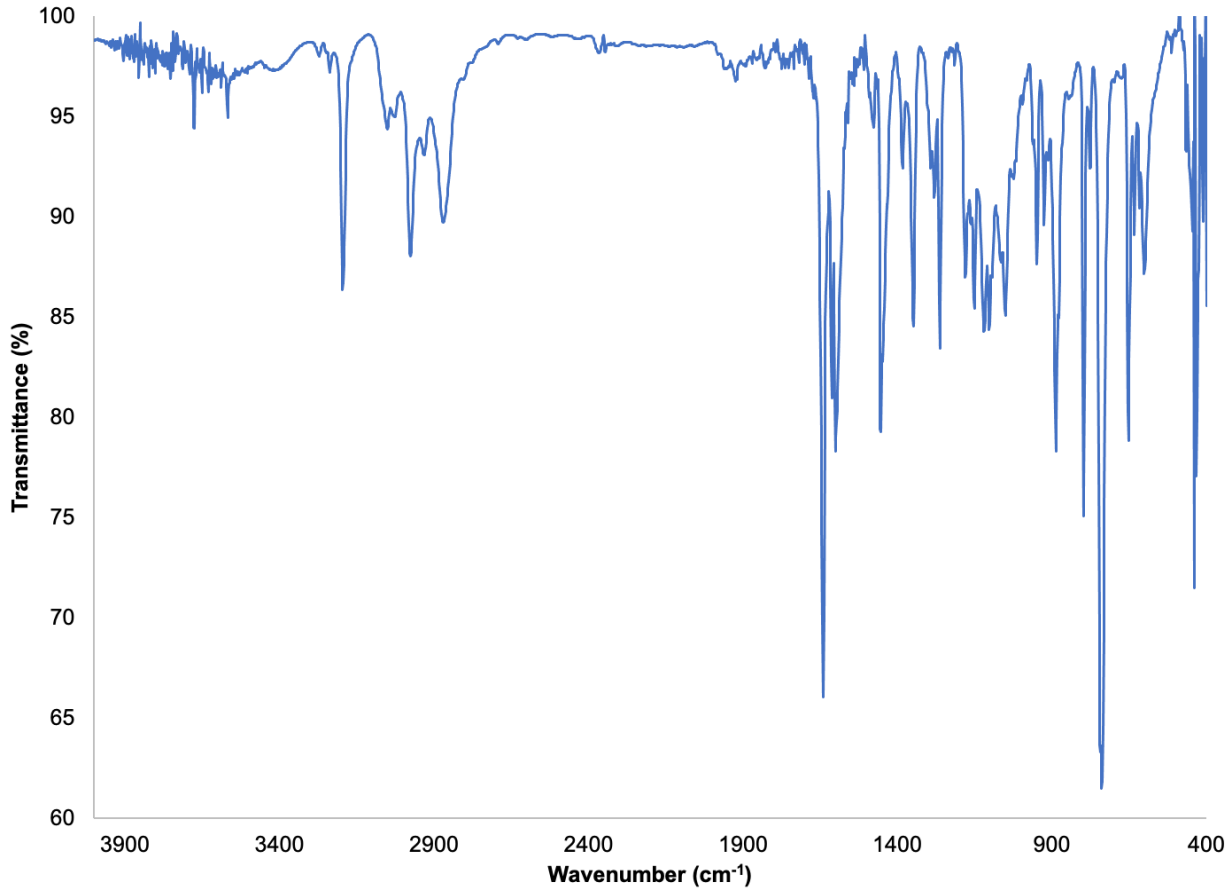


Figure S19. IR spectrum of **3** (KBr Pellet).

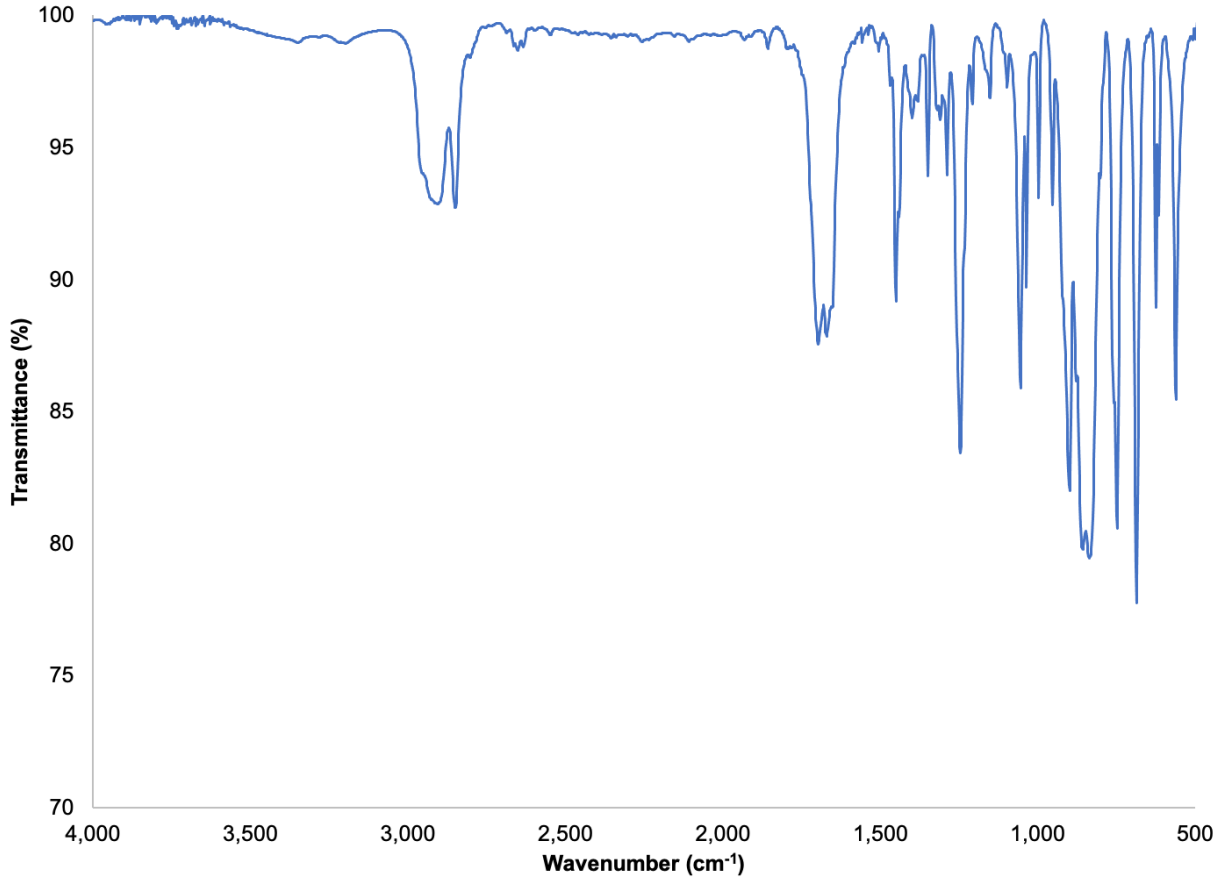


Figure S20. IR spectrum of **4** (KBr Pellet).

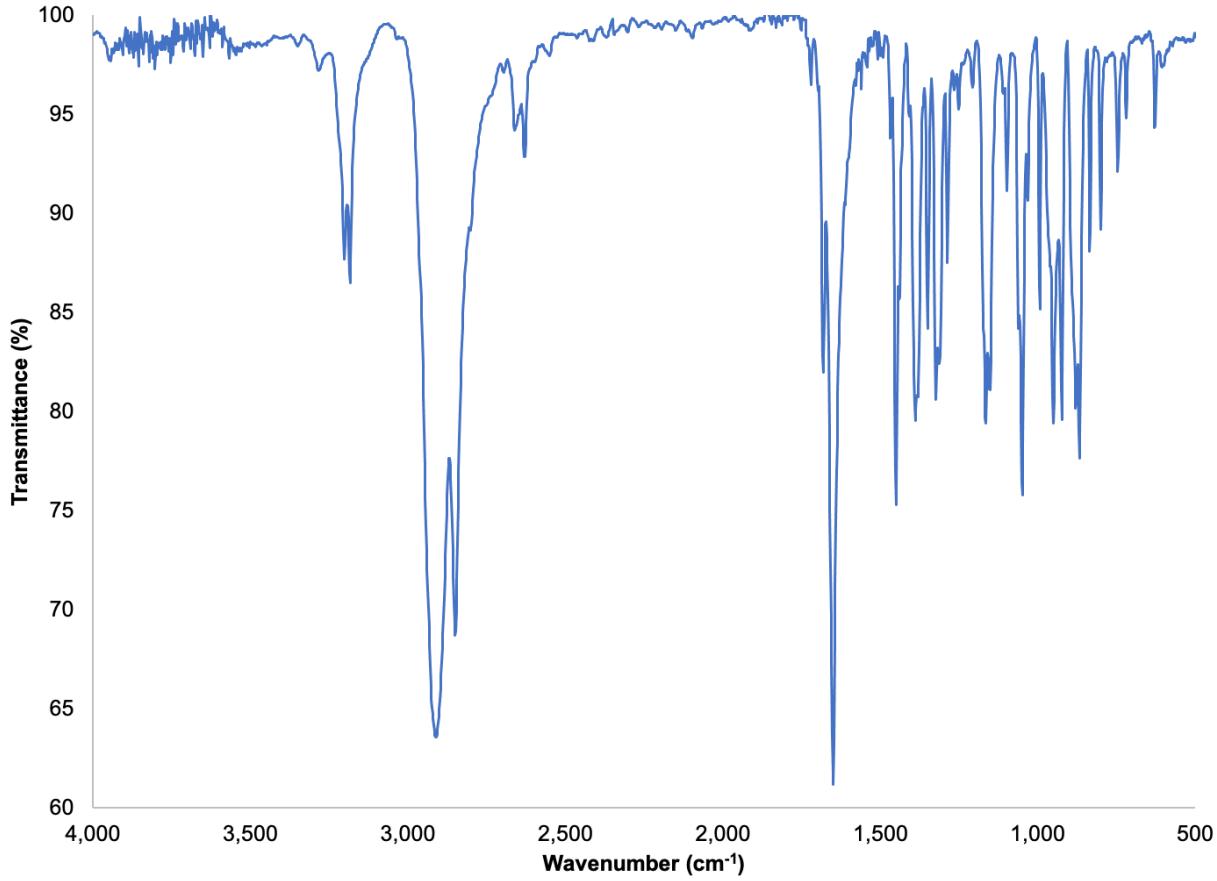


Figure S21. IR spectrum of **5** (KBr Pellet).

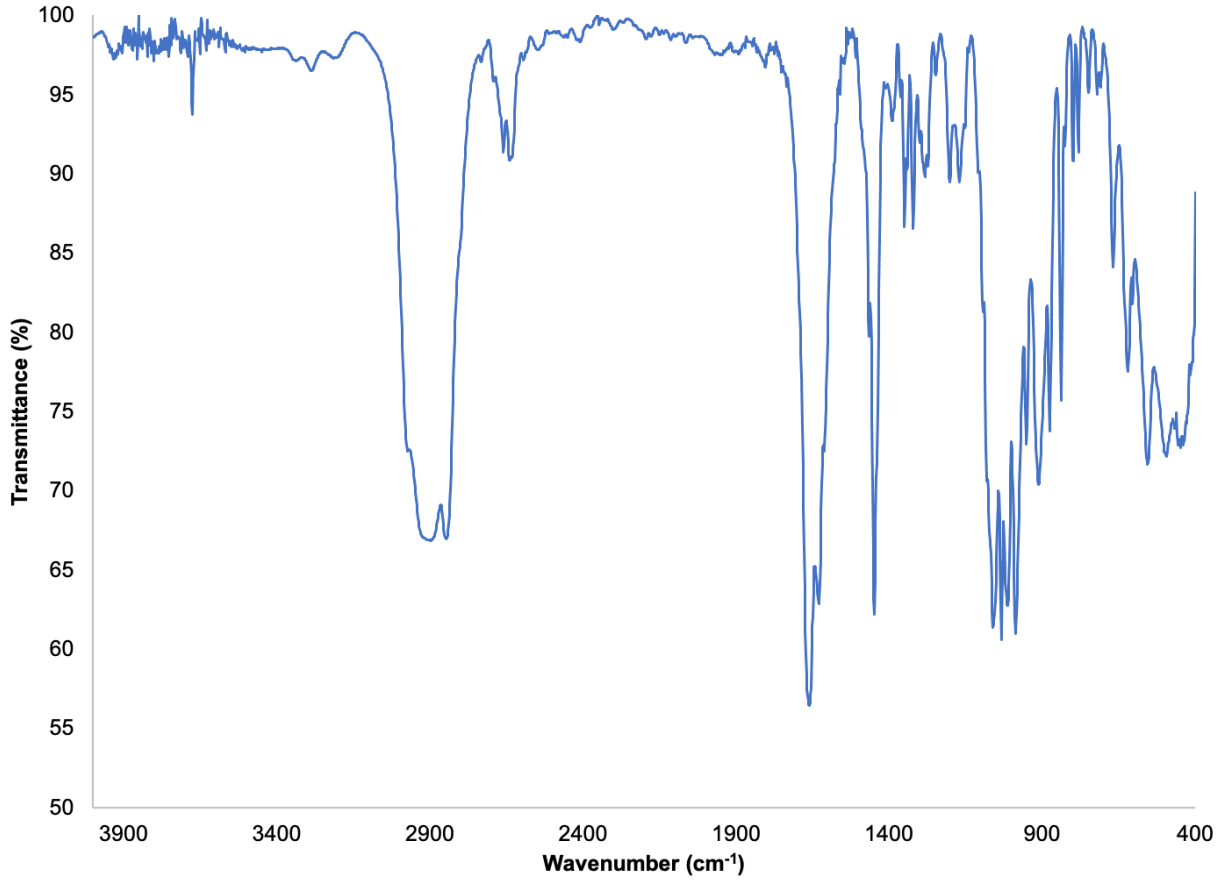


Figure S22. IR spectrum of **6** (KBr Pellet).

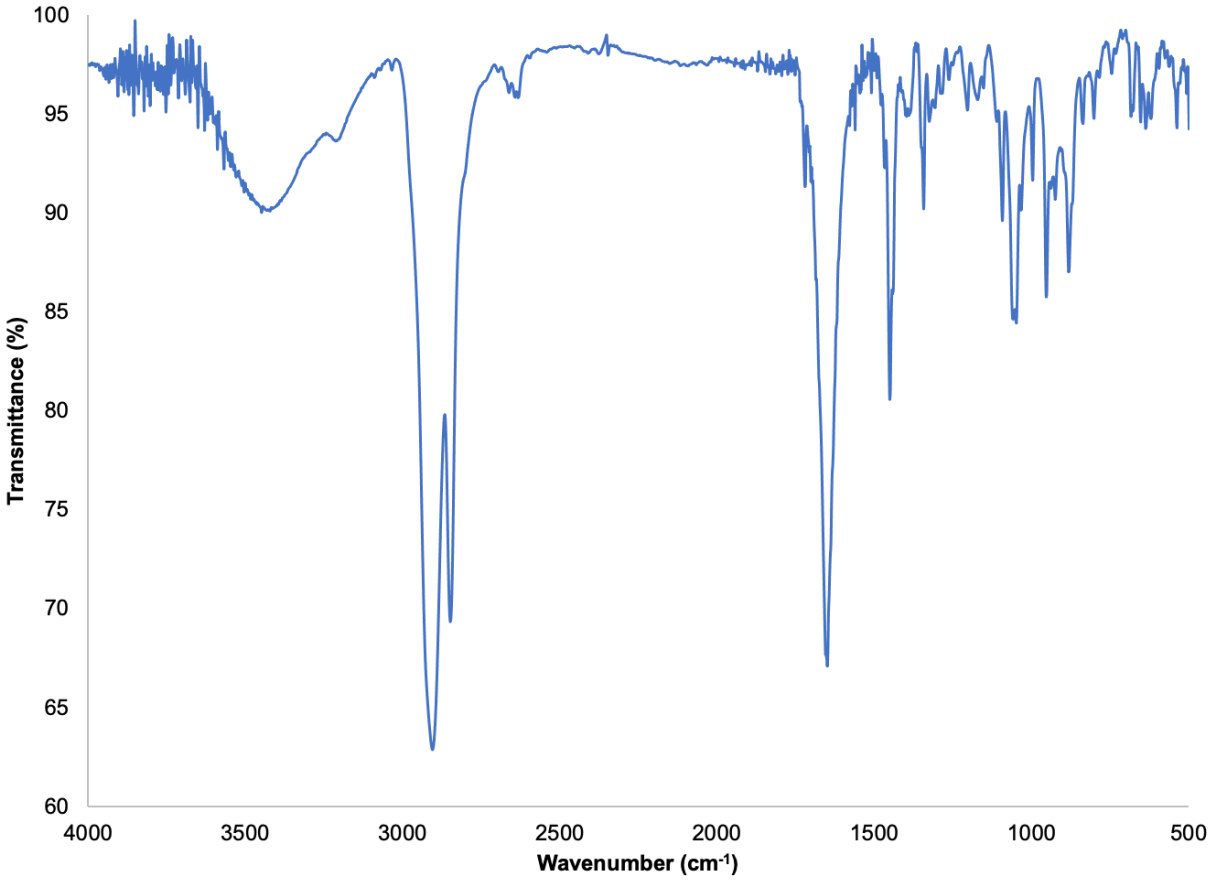


Figure S23. IR spectrum of **7** (KBr Pellet).

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