Supplementary Information

Electrophilic lithium carbazolide as an efficient trap for organolithium species. Complexes containing a monomeric *n*-BuLi, *t*-BuLi and Me_3SiCH_2Li units

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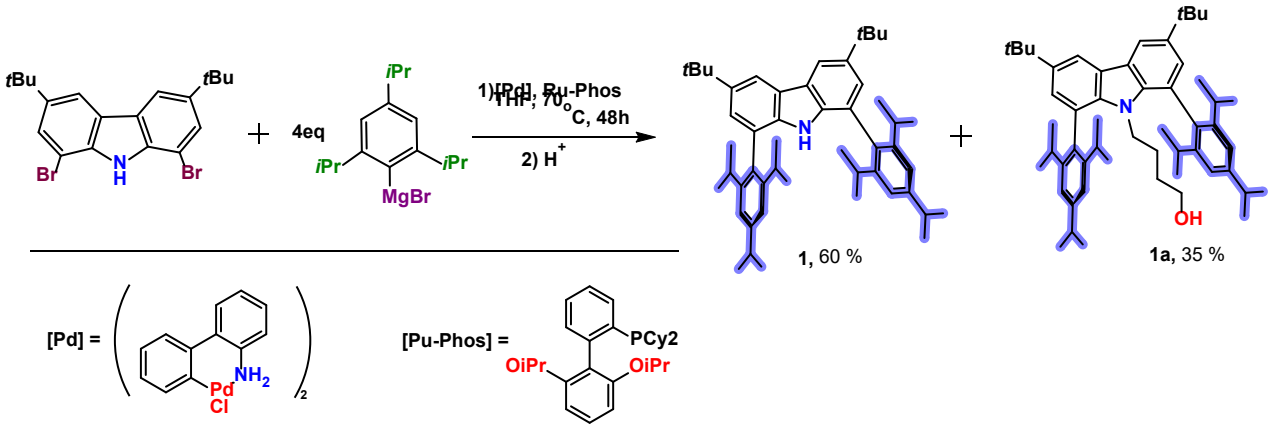
Table S1. The crystallographic data and structure refinement details for **2-4, 6**.

	2	**3**	**4**	**6**
Formula	$C_{54}H_{77}Li_2N$	$C_{54}H_{79}Li_2NSi$	$C_{54}H_{77}Li_2N$	$C_{57}H_{76}LiN$
Formula weight	754.04	784.15	754.04	782.12
Crystal system	Triclinic	Monoclinic	Monoclinic	Monoclinic
Space group	*P-1*	*P2₁/c*	*P2₁/c*	*P2₁/c*
T, K	100.0(2)	100.0(2)	100.0(2)	100.0(2)
a (Å)	13.0200(14)	38.6636(14)	22.7861(5)	12.7955(5)
b (Å)	13.5522(11)	13.1619(5)	19.6508(3)	21.3653(7)
c (Å)	26.710(2)	20.1069(9)	23.5221(5)	17.8574(5)
α (deg)	81.291(7)	90	90	90
β (deg)	89.485(9)	102.221(4)	113.266(2)	95.565(3)
γ (deg)	89.155(9)	90	90	90
V (Å^3)	4658.1(7)	10000.3(7)	9675.9(4)	4858.8(3)
Z	4	8	8	4
ρ_{calc} (g/cm^3)	1.075	1.042	1.035	1.069
μ (mm^{-1})	0.060	0.080	0.057	0.060
F_{000}	1656	3440	3312	1712
Crystal dimensions (mm)	0.61×0.40×0.17	0.36×0.31×0.19	0.50×0.36×0.28	0.58×0.31×0.22
θ range for data collection (deg)	2.17-26.21	2.07-26.02	2.07–27.10	2.10–26.06
Reflections collected / unique [$F^2 > 2\sigma(F^2)$]	75167 / 14402	101518 / 13337	179208 / 13620	42635 / 6512
R_{int}	0.0769	0.0724	0.0659	0.0402
Completeness, %	98.1	99.9	99.7	99.9
Data / restraints / parameters	26322 / 1528 / 1209	19695 / 1351 / 1137	21303 / 42 / 1111	9595 / 1070 / 758
Final *R* indices [$F^2 > 2\sigma(F^2)$]	R_1 = 0.0879	R_1 = 0.0732	R_1 = 0.0765	R_1 = 0.0897
	wR_2 = 0.2620	wR_2 = 0.1584	wR_2 = 0.1860	wR_2 = 0.2455
Final *R* indices (all data)	R_1 = 0.1449	R_1 = 0.1149	R_1 = 0.1267	R_1 = 0.1244
	wR_2 = 0.2837	wR_2 = 0.1784	wR_2 = 0.2214	wR_2 = 0.2762
$S(F^2)$	1.051	1.049	1.062	1.018
Larg. diff. peak and hole, e/Å^3	0.40 / -0.41	1.26 / -0.78	0.99 / -0.76	0.51 / -0.67

Synthesis of 3,6-di-*tert*-butyl-1,8-bis-(2,4,6-triisopropylphenyl)-9H-carbazole (1) and 4-(3,6-di-tert-butyl-1,8-bis(2,4,6-triisopropylphenyl)-9H-carbazol-9-yl)butan-1-ol (1a) via Kumada cross-coupling.



A solution of Grignard reagent in THF (50 ml), obtained from 1-bromo-2,4,6-triisopropylbenzene (10.36 g, 36.65 mmol) and magnesium (1.05 g, 44.93 mmol), was added to a solid mixture of 1,8-dibromo-3,6-di-*tert*-butylcarbazole (4.00 g, 9.15 mmol), palladium catalyst (0.06 g, 0.09 mmol, 1 mol %) and Ru-Phos (0.09 g, 0.09 mmol, 1 mol %) at room temperature. The reaction mixture was heated at 70 °C for 48 h. Afterwards, the brownish mixture was allowed to cool to ambient temperature and transferred into a separation funnel. Then 100 ml of deionized water and 100 ml of ether were added. Phases were separated, the aqueous phase extracted with 2 x 50 ml of diethyl ether and the combined organic phases were washed once with 50 ml of water. The organic phase was dried over $MgSO_4$ and then evaporated on a rotary evaporator, leaving a brown oil behind. The oil was evacuated at 100 °C, the excess triisopropylbenzene was separated in the receiver. The brown semi-solid was re-dissolved in hexane and purified by flash chromatography on silica gel. The fractions were combined and the hexane was evaporated to give carbazole **1** in 60% yield (3.76 g). Spectroscopic data are consistent with carbazole **1**. Then, the polarity of the eluent was increased by adding 10% ethyl acetate and carbazole **1a** was isolated from the chromatographic column as a beige substance with a yield of 35% (2.42 g).

Spectroscopic data for carbazole 1a.

^{1}H NMR (300 MHz, $CDCl_3$, 298 K): δ 8.16 (d, 2H, 4,5-CH-carbazolyl, $^{4}J_{HH}$= 1.9 Hz), 7.18 (d, 2H, 2,7-CH-carbazolyl, $^{4}J_{HH}$= 1.9 Hz), 7.05 (s, 4H, CH-Ar), 3.51-3.37 (m, 2H, NCH_2CH$_2$), 3.02-2.86 (m, 2H, *p*-CH(CH$_3$)$_2$), 2.82 (t, 2H, CH_2OH, $^{3}J_{HH}$= 6.7 Hz), 2.65-2.48 (m, 4H, *o*-CH(CH$_3$)$_2$), 1.45 (s, 18H, *t*Bu), 1.29 (d, 12H, *p*-CH(CH_3)$_2$, $^{3}J_{HH}$= 6.9 Hz), 1.11 (d, 12H, *o*-CH(CH_3)$_2$, $^{3}J_{HH}$= 6.9 Hz), 1.01 (d, 12H, *o*-CH(CH_3)$_2$, $^{3}J_{HH}$= 6.7 Hz), 0.95-0.82 (m, 2H, CH$_2$), 0.26 (p, 2H, CH$_2$, $^{3}J_{HH}$= 6.8 Hz).

^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$, 298 K): δ 148.59 (s, *ipso*-C-aryl), 147.41 (s, *ipso*-C-aryl), 140.95 (s, C-carbazolyl), 136.73 (s, C-carbazolyl), 135.49 (s, *ipso*-C-aryl), 128.49 (s, CH-carbazolyl), 123.21 (s, C-carbazolyl), 121.83 (s, C-carbazolyl), 120.41 (s, 3,5-CH-aryl), 114.32 (s, CH-carbazolyl), 61.74 (s, *C*H$_2$OH), 44.79 (s, N*C*H$_2$), 34.69 (s, *C*(CH$_3$)$_3$-carbazolyl), 34.42 (s, *p*-*C*H(CH$_3$)$_2$), 31.83 (s, C(*C*H$_3$)$_3$-carbazolyl), 30.86 (s, *o*-*C*H(CH$_3$)$_2$), 29.85 (s, CH$_2$), 26.94 (s, CH$_2$), 25.81 (s, *o*-CH(*C*H$_3$)$_2$), 24.17 (s, *p*-CH(*C*H$_3$)$_2$), 22.22 (s, *o*-CH(*C*H$_3$)$_2$).

IR (KBr): 3485 (s, OH), 1761 (m), 1605 (s), 1556 (s), 1304 (s), 1271 (s), 1235 (s), 1182 (m), 1053 (s), 1034 (s), 986 (m), 932 (s), 870 (s), 814 (w), 789 (w), 758 (s), 725 (s), 659 (m).

Anal. Calcd for $C_{54}H_{77}NO$ (756.22 g mol^{-1}) C, 85.77; H, 10.26; N 1.85. Found C, 85.65; H, 10.34; N 1.80.

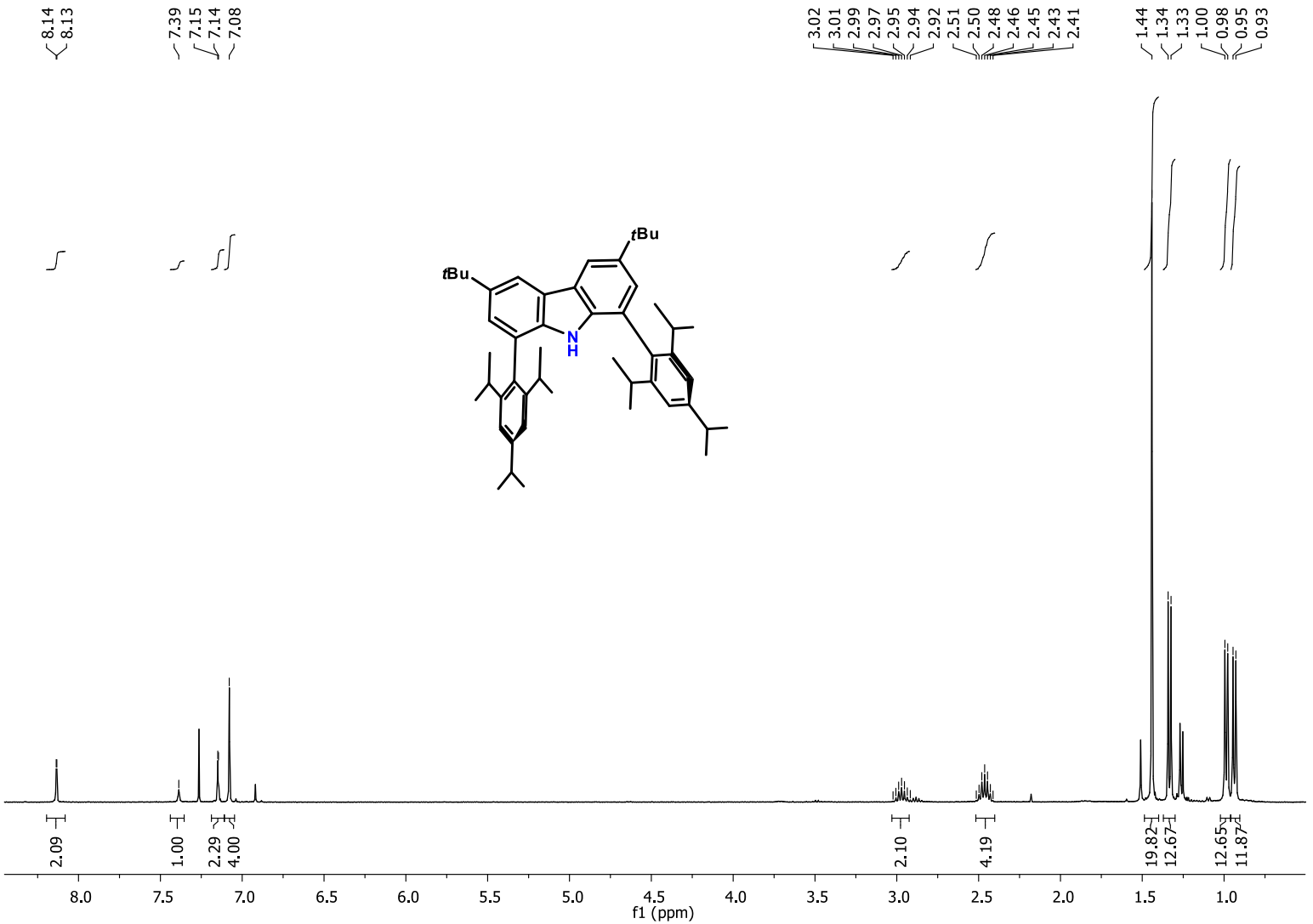


Figure S1. ^{1}H NMR spectrum of 3,6-di-*tert*-butyl-1,8-bis-(2,4,6-triisopropylphenyl)-9H-carbazole **(1)** (400 MHz, $CDCl_3$, 293 K).

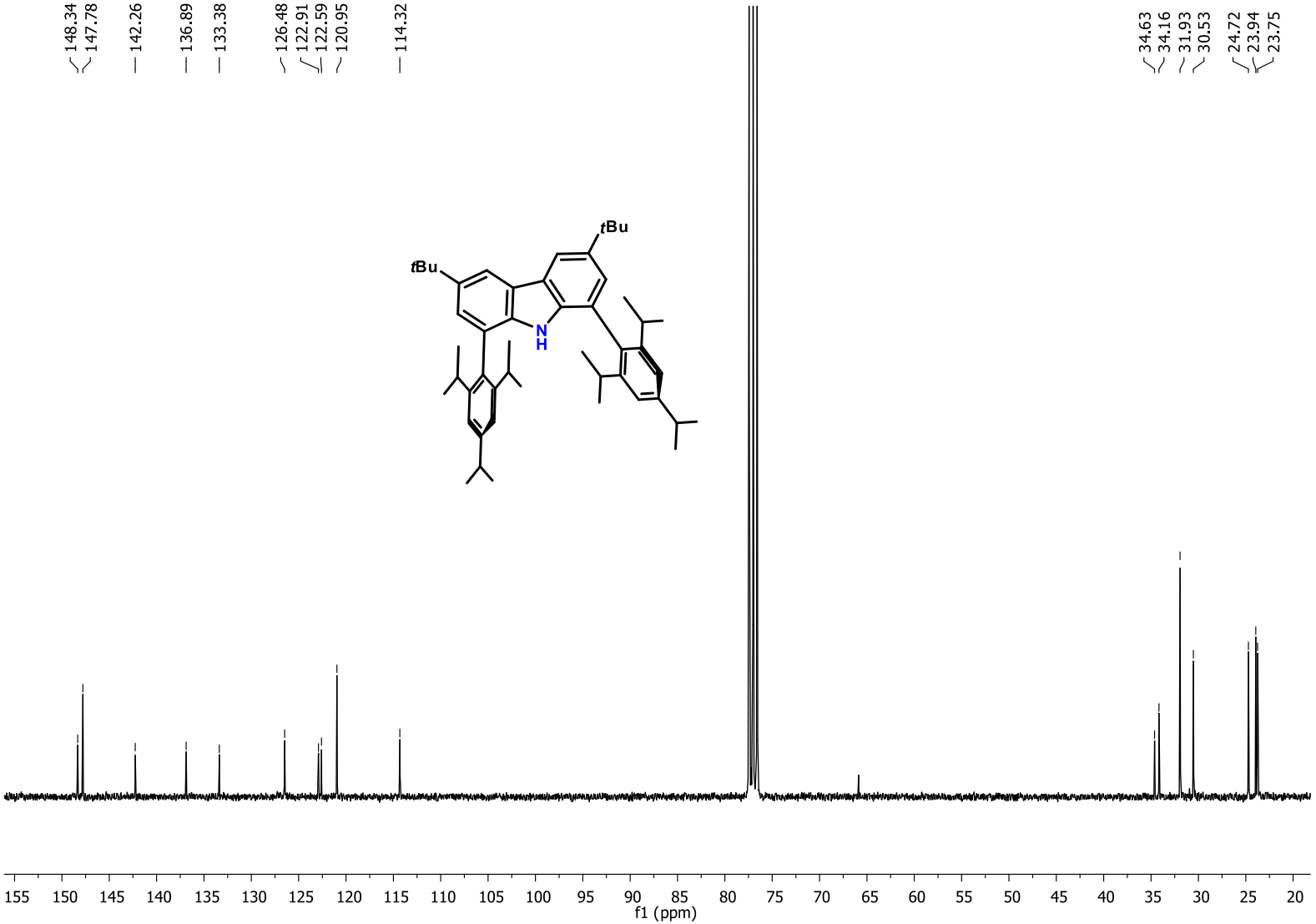


Figure S2. $^{13}C\{^{1}H\}$ NMR spectrum of 3,6-di-*tert*-butyl-1,8-bis-(2,4,6-triisopropylphenyl)-9H-carbazole **(1)** (100 MHz, $CDCl_3$, 293 K).

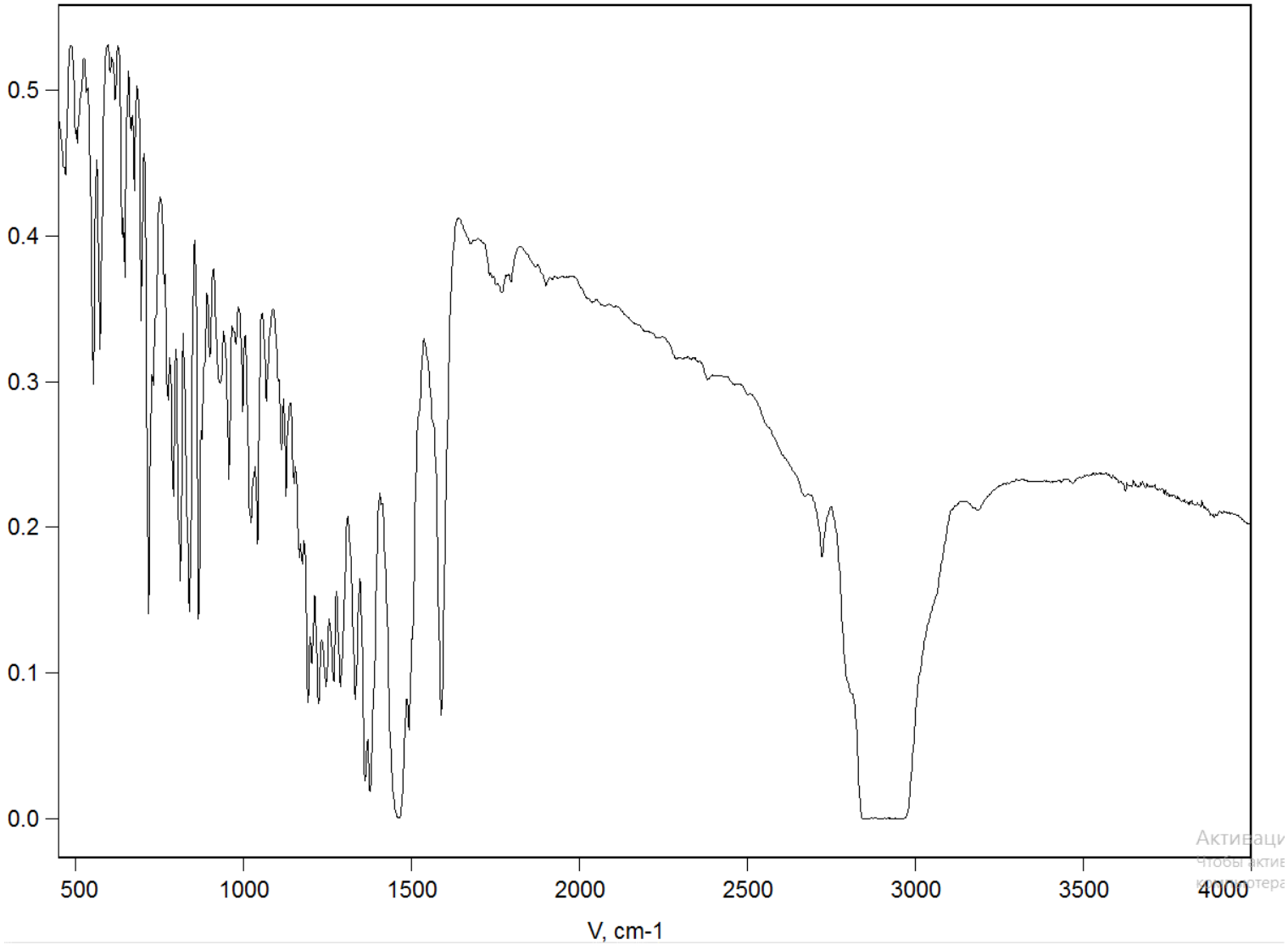


Figure S3. IR (KBr, Nujol) spectrum of 3,6-di-*tert*-butyl-1,8-bis-(2,4,6-triisopropylphenyl)-9H-carbazole (**1**).

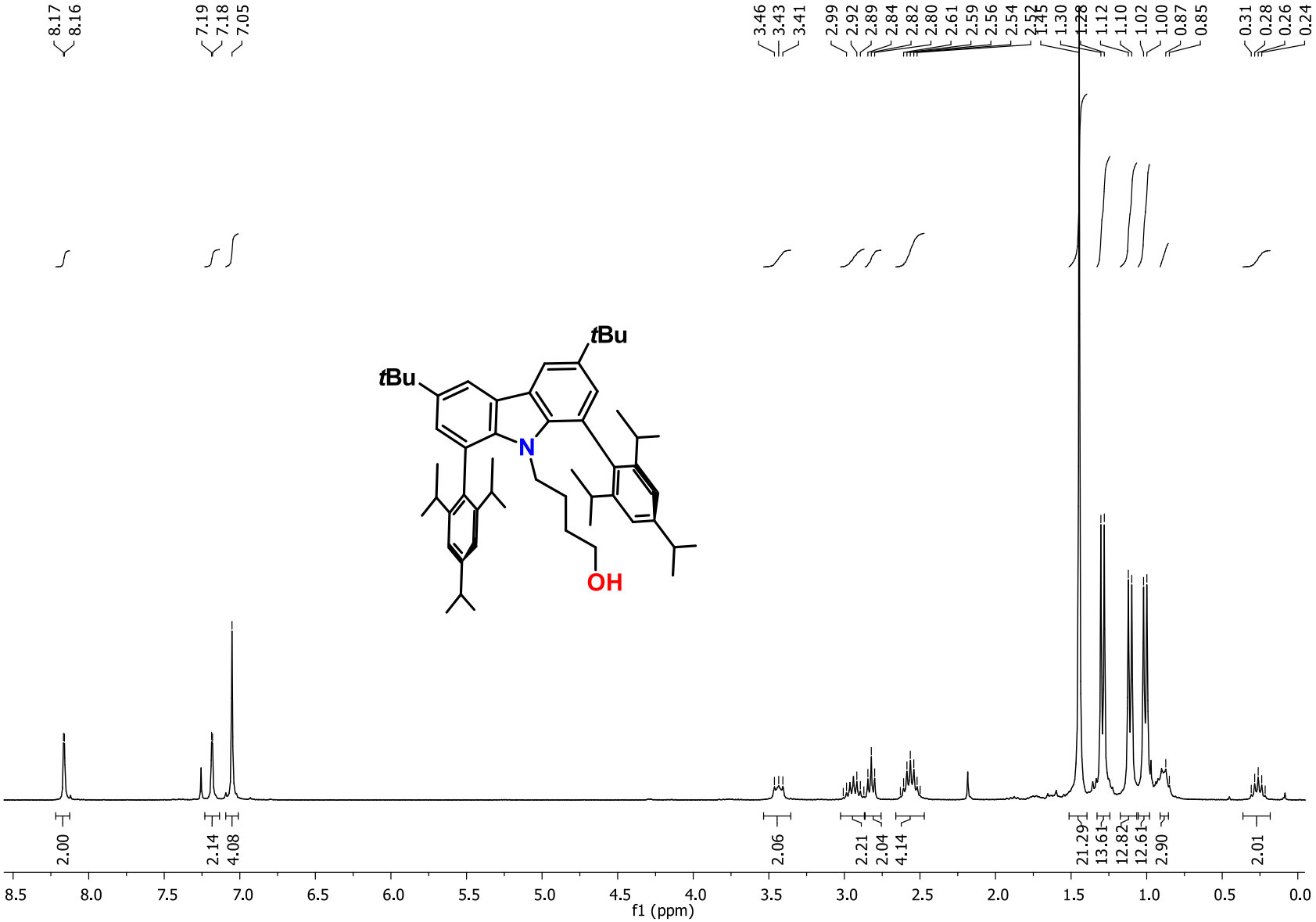


Figure S4. ^{1}H NMR spectrum of 4-(3,6-di-tert-butyl-1,8-bis(2,4,6-triisopropylphenyl)-9H-carbazol-9-yl)butan-1-ol (**1a**) (300 MHz, $CDCl_3$, 293 K).

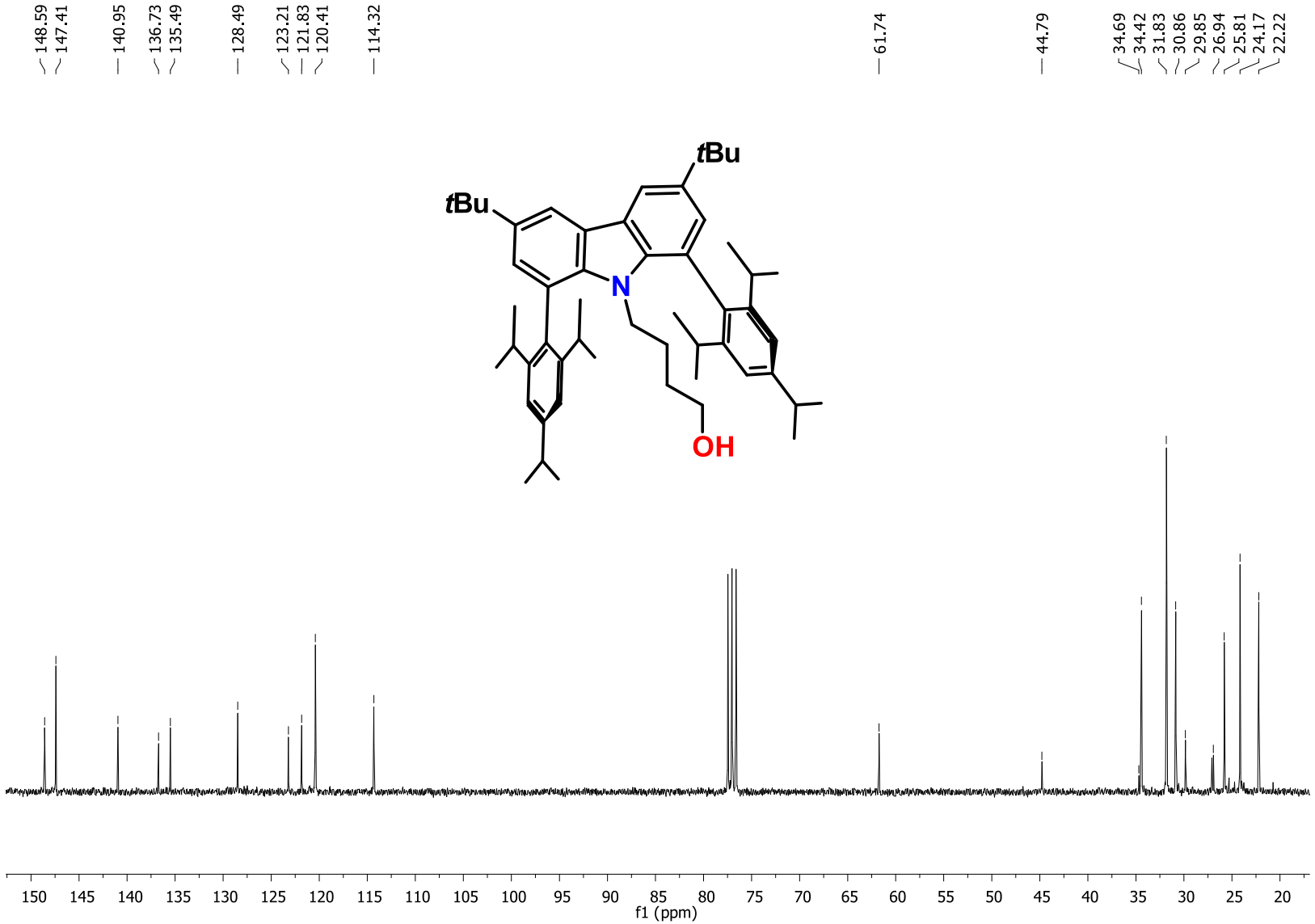


Figure S5. $^{13}C\{^{1}H\}$ NMR spectrum of 4-(3,6-di-tert-butyl-1,8-bis(2,4,6-triisopropylphenyl)-9H-carbazol-9-yl)butan-1-ol (**1a**) (75 MHz, $CDCl_3$, 293 K).

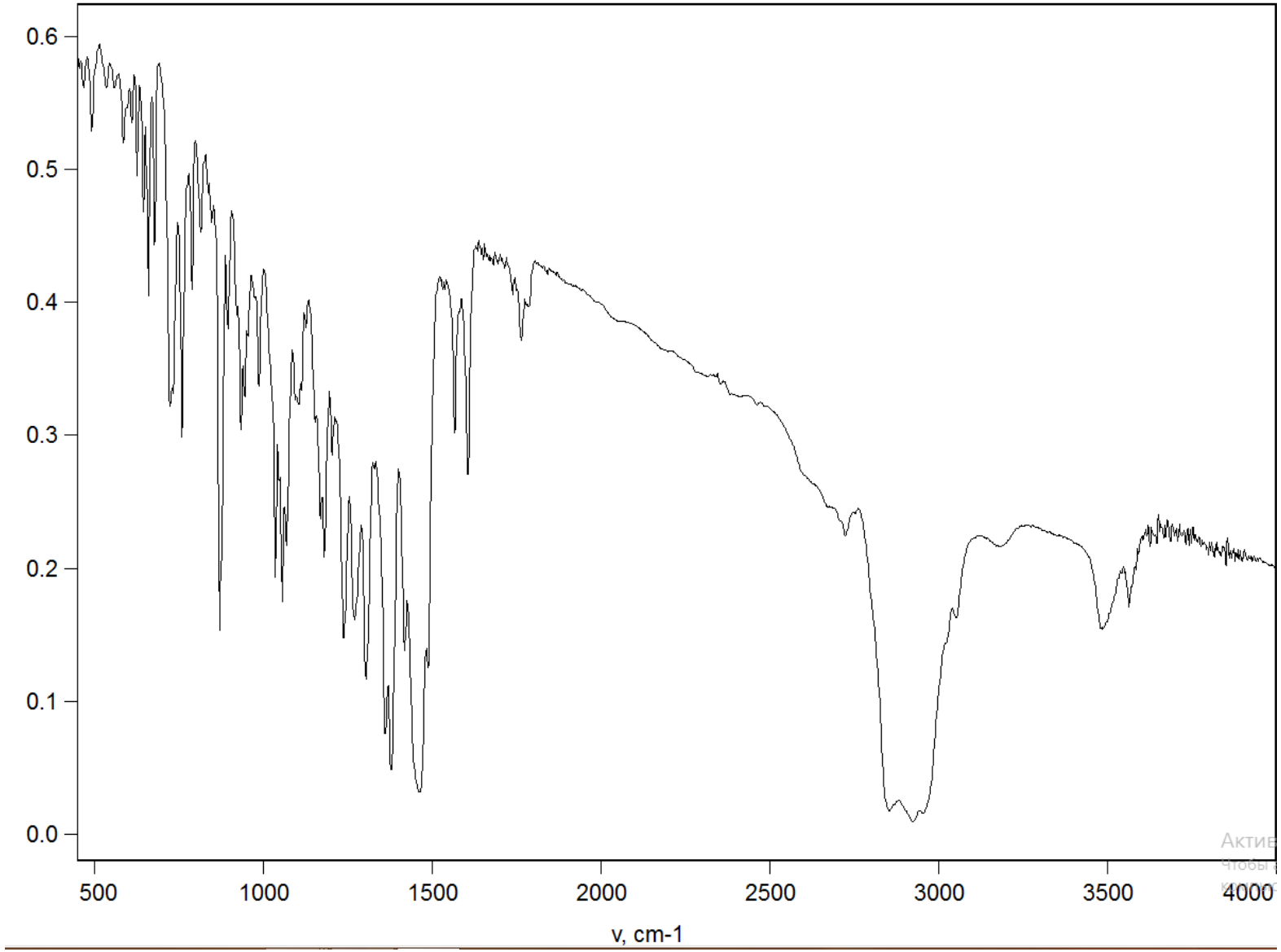


Figure S6. IR (KBr, Nujol) spectrum of 4-(3,6-di-tert-butyl-1,8-bis(2,4,6-triisopropylphenyl)-9H-carbazol-9-yl)butan-1-ol (**1a**).

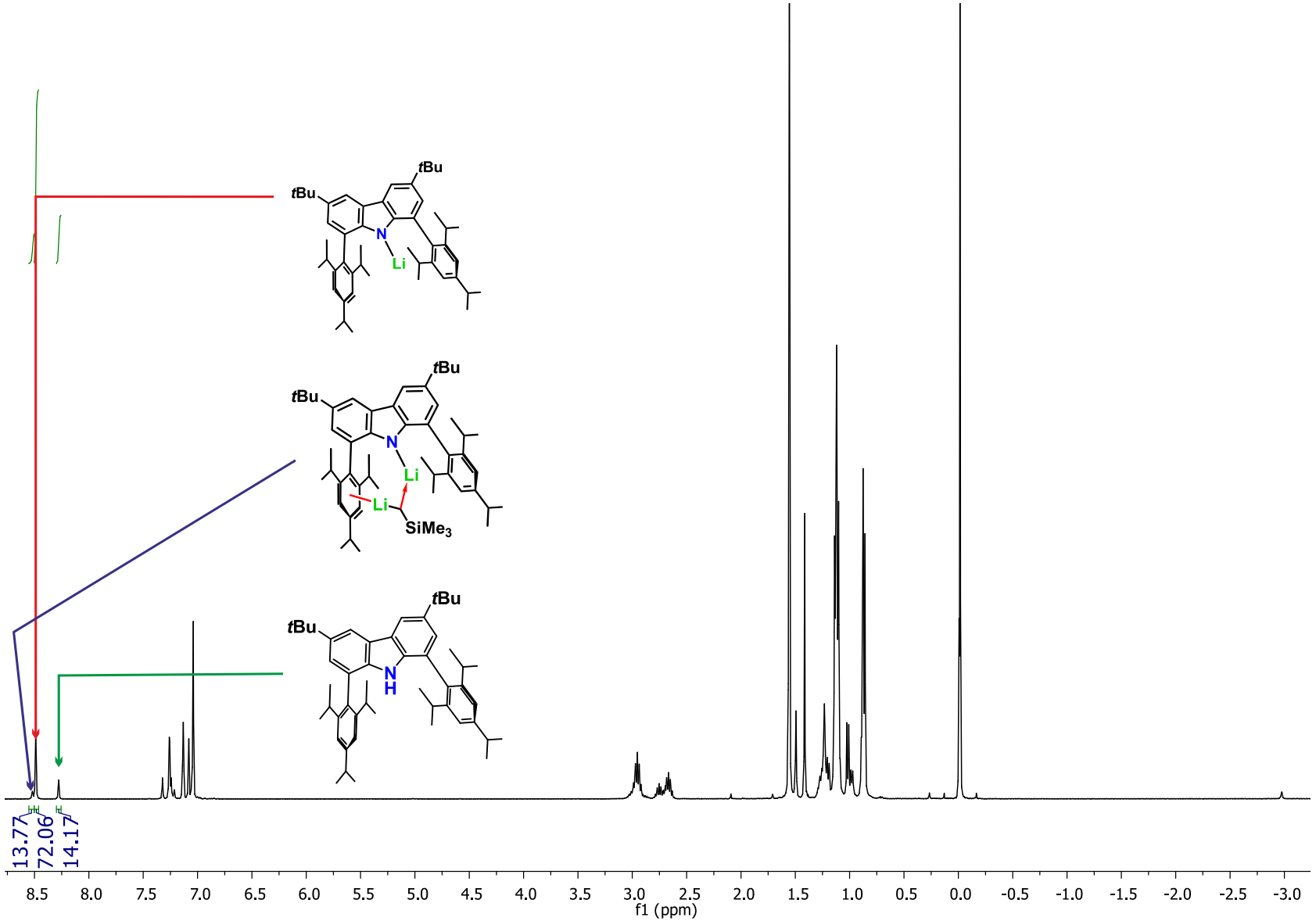


Figure S7. ^{1}H NMR spectrum of reaction of **1** with Me_3SiCH_2Li (1:1) (400 MHz, C_6D_6, 293 K).

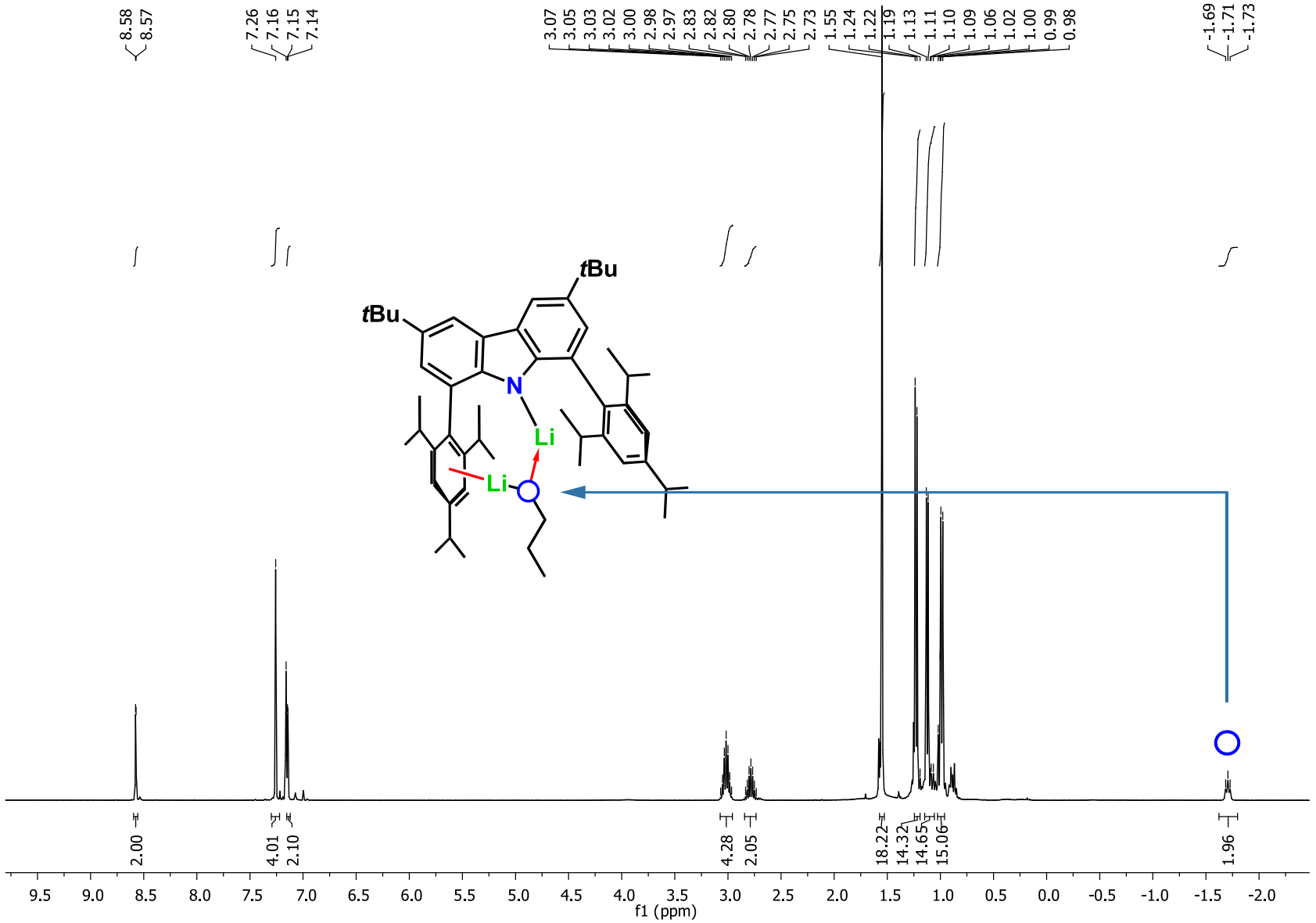


Figure S8. ^{1}H NMR spectrum of complex **2** (400 MHz, C_6D_6, 293 K).

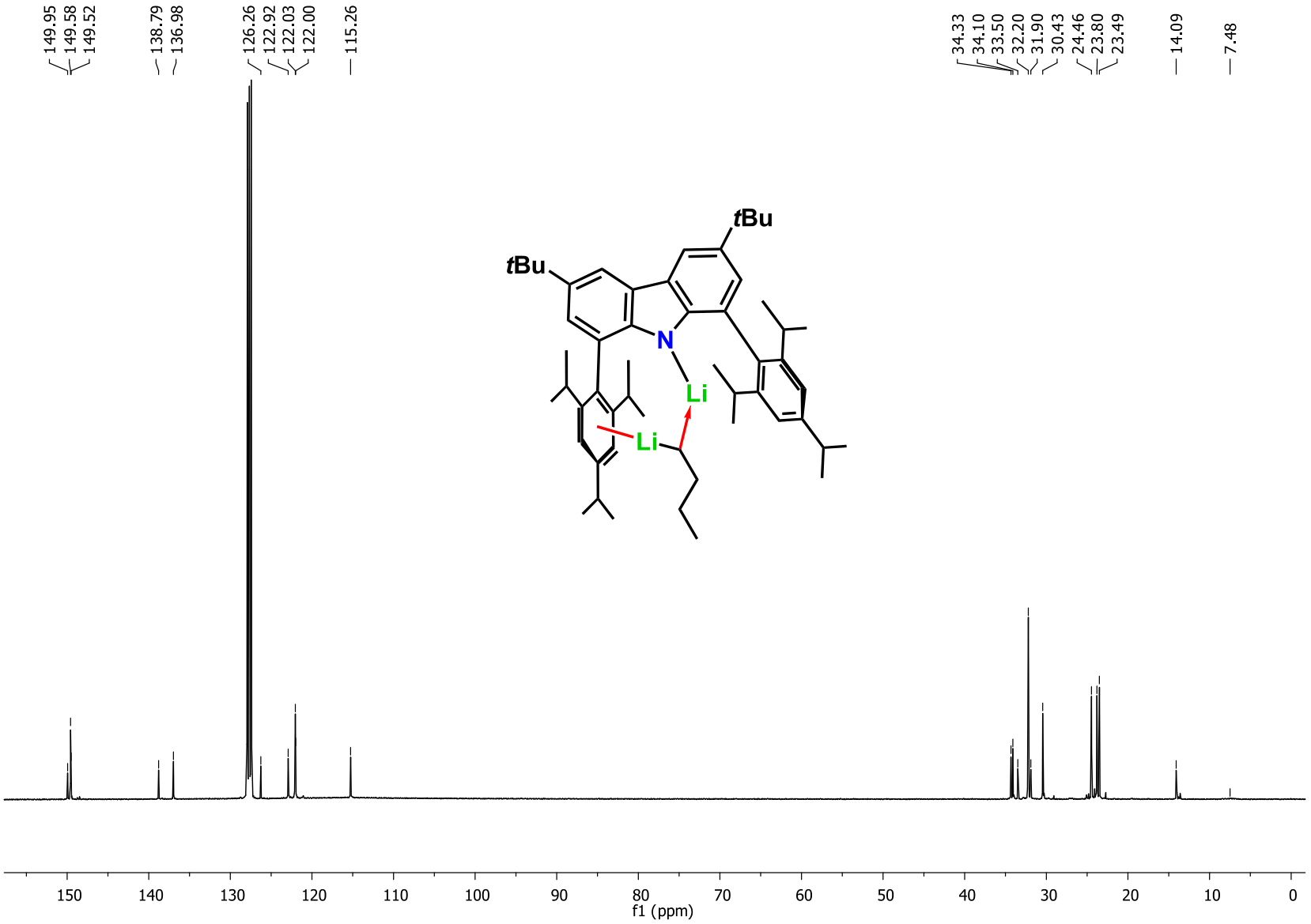


Figure S9. ^{13}C $\{^{1}H\}$ NMR spectrum of complex **2** (100 MHz, C_6D_6, 293 K).

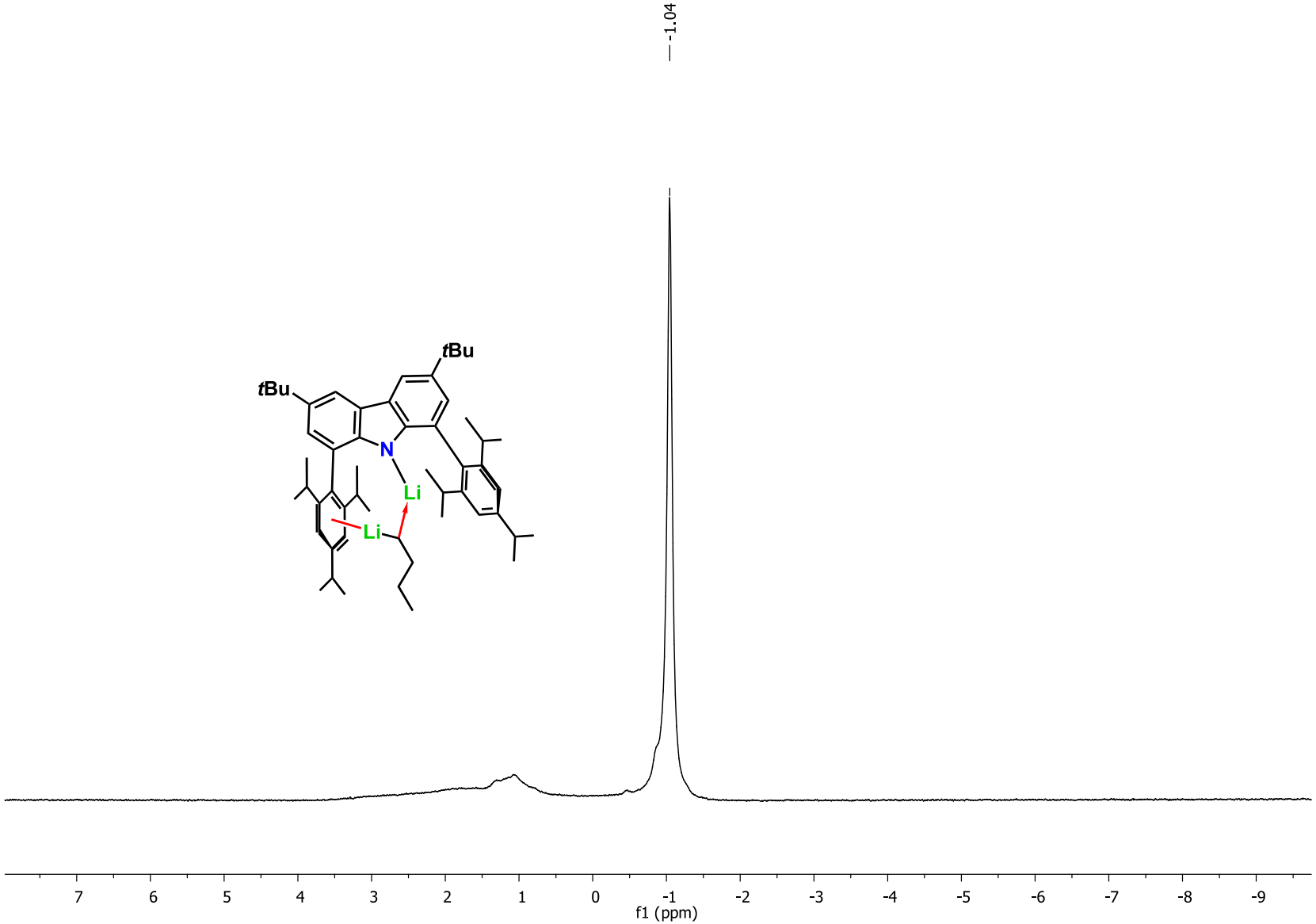


Figure S10. ^{7}Li NMR spectrum of complex **2** (100 MHz, C_6D_6, 293 K).

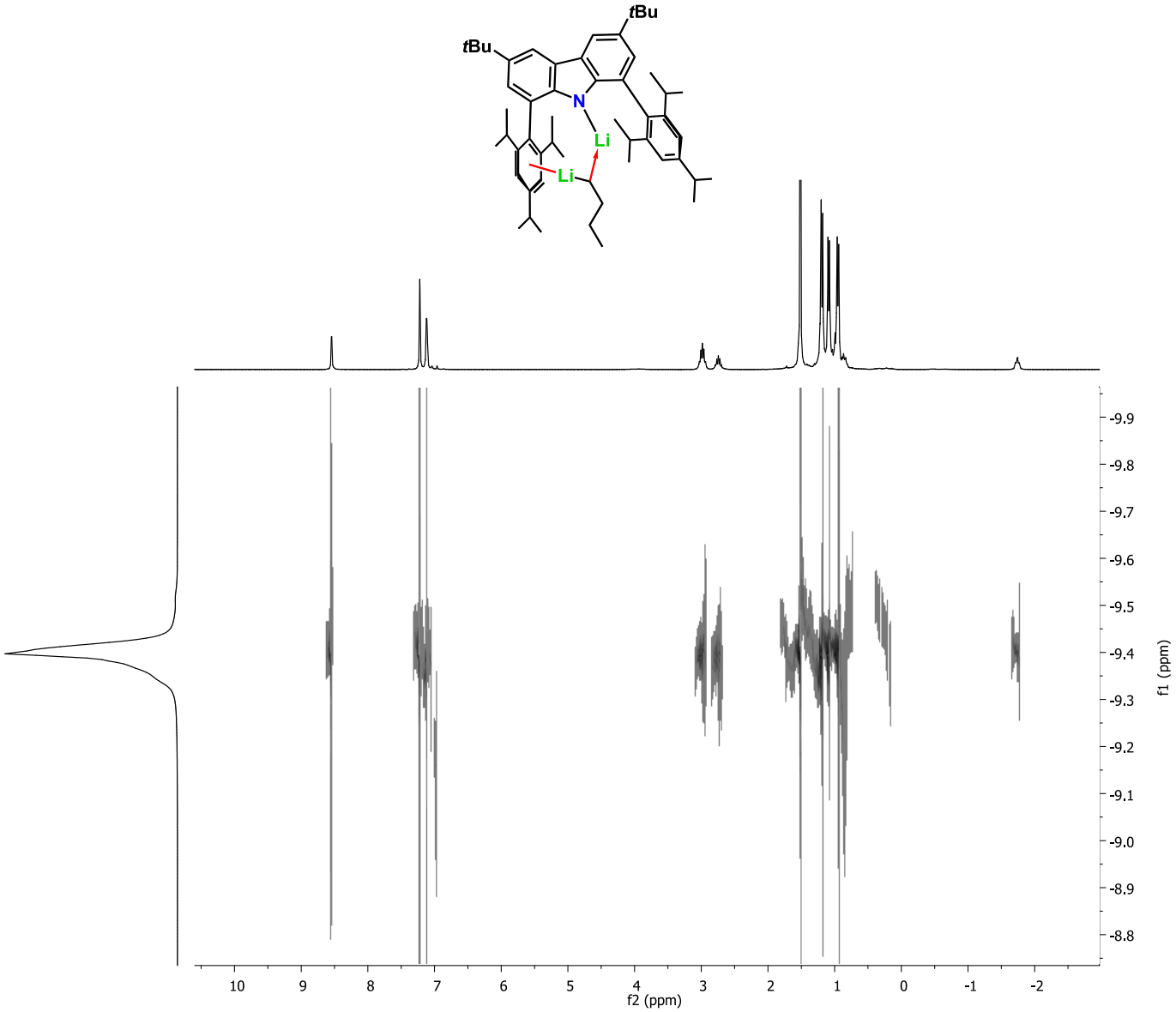


Figure S11. ^{1}H DOSY NMR spectrum of complex **2** (100 MHz, C_6D_6, 293 K).

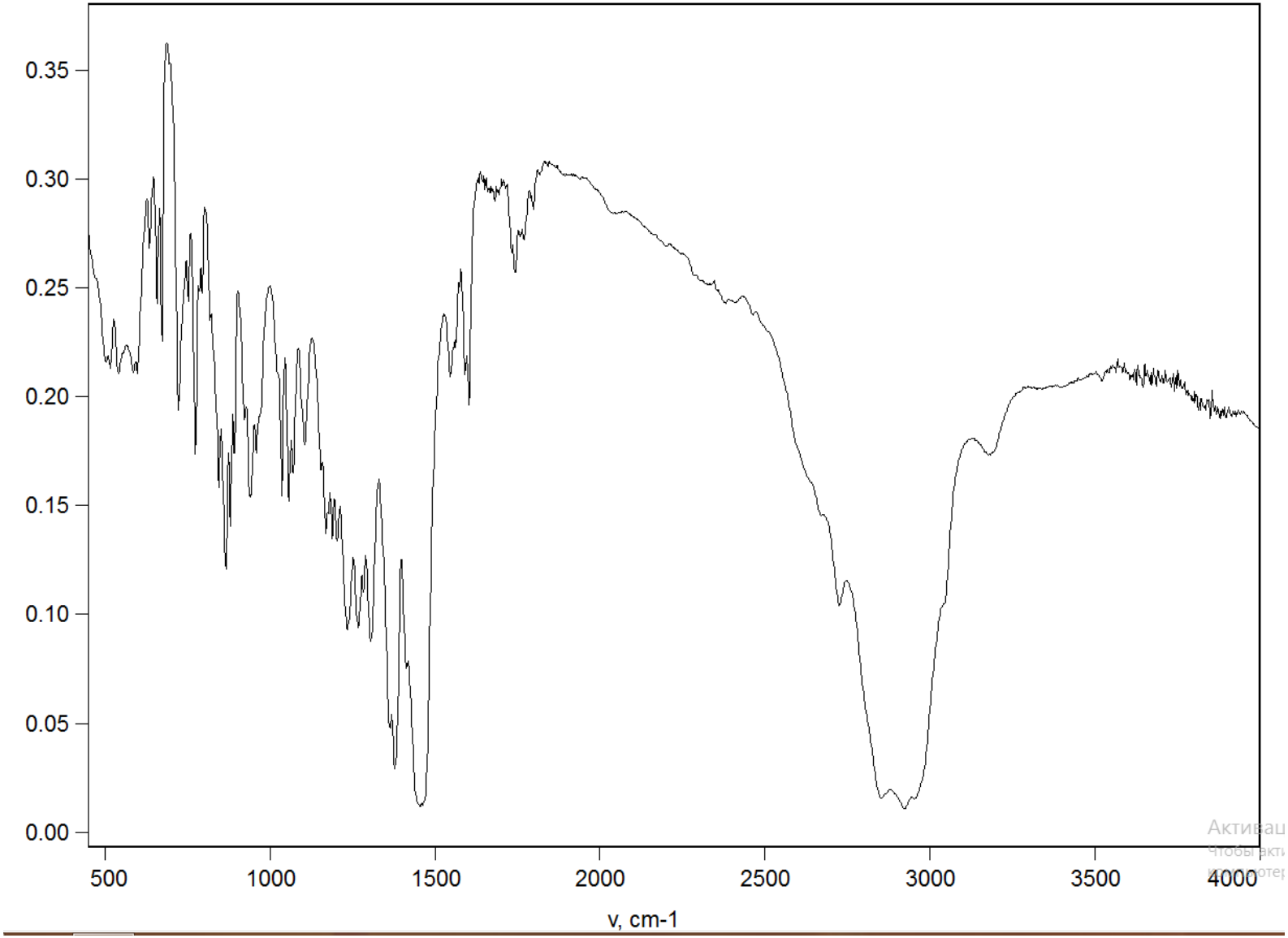


Figure S12. IR (KBr, Nujol) spectrum of complex **2**.

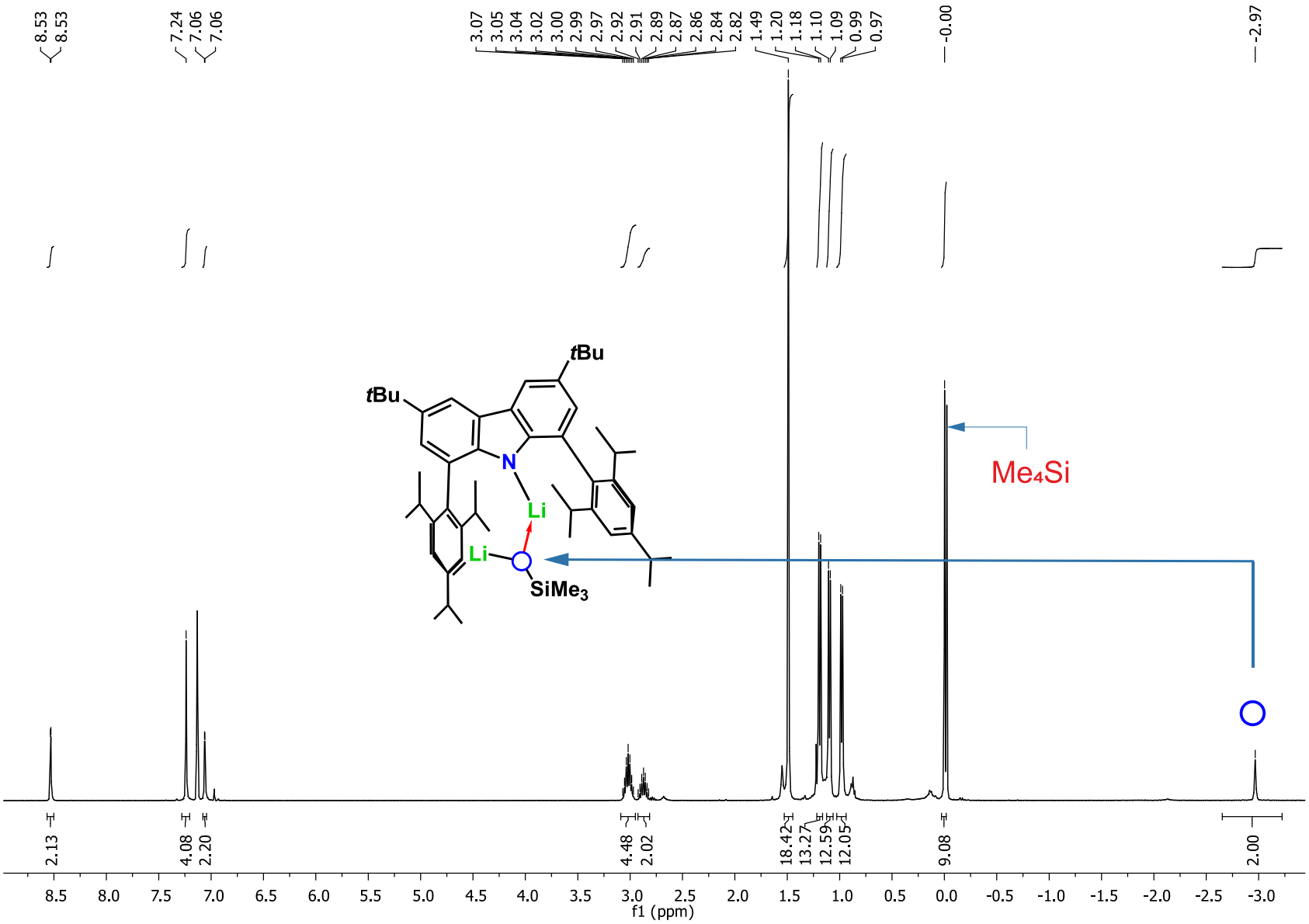


Figure S13. ^{1}H NMR spectrum of complex **3** (400 MHz, C_6D_6, 293 K).

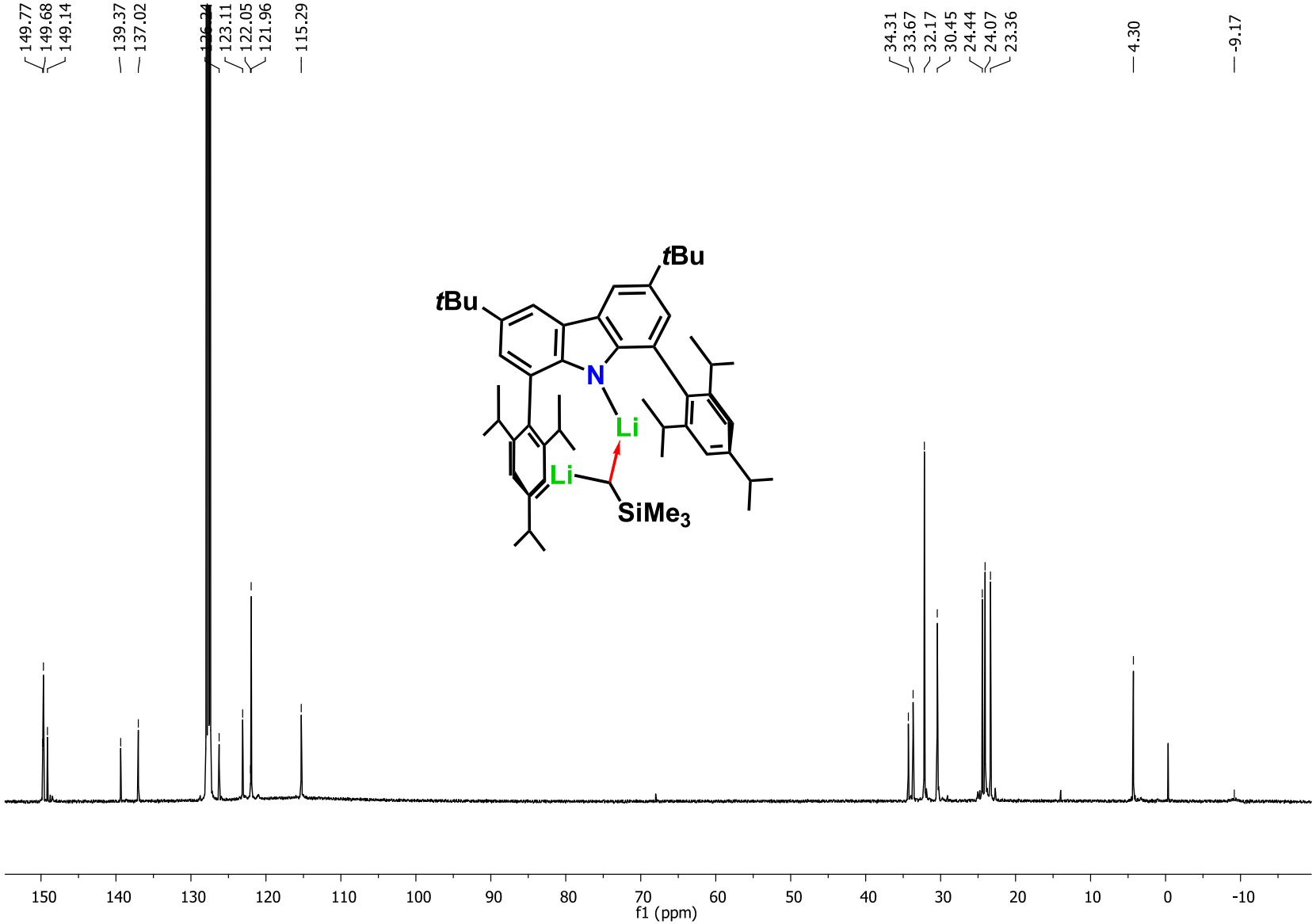


Figure S14. ^{13}C {^{1}H} NMR spectrum of complex **3** (100 MHz, C_6D_6, 293 K).

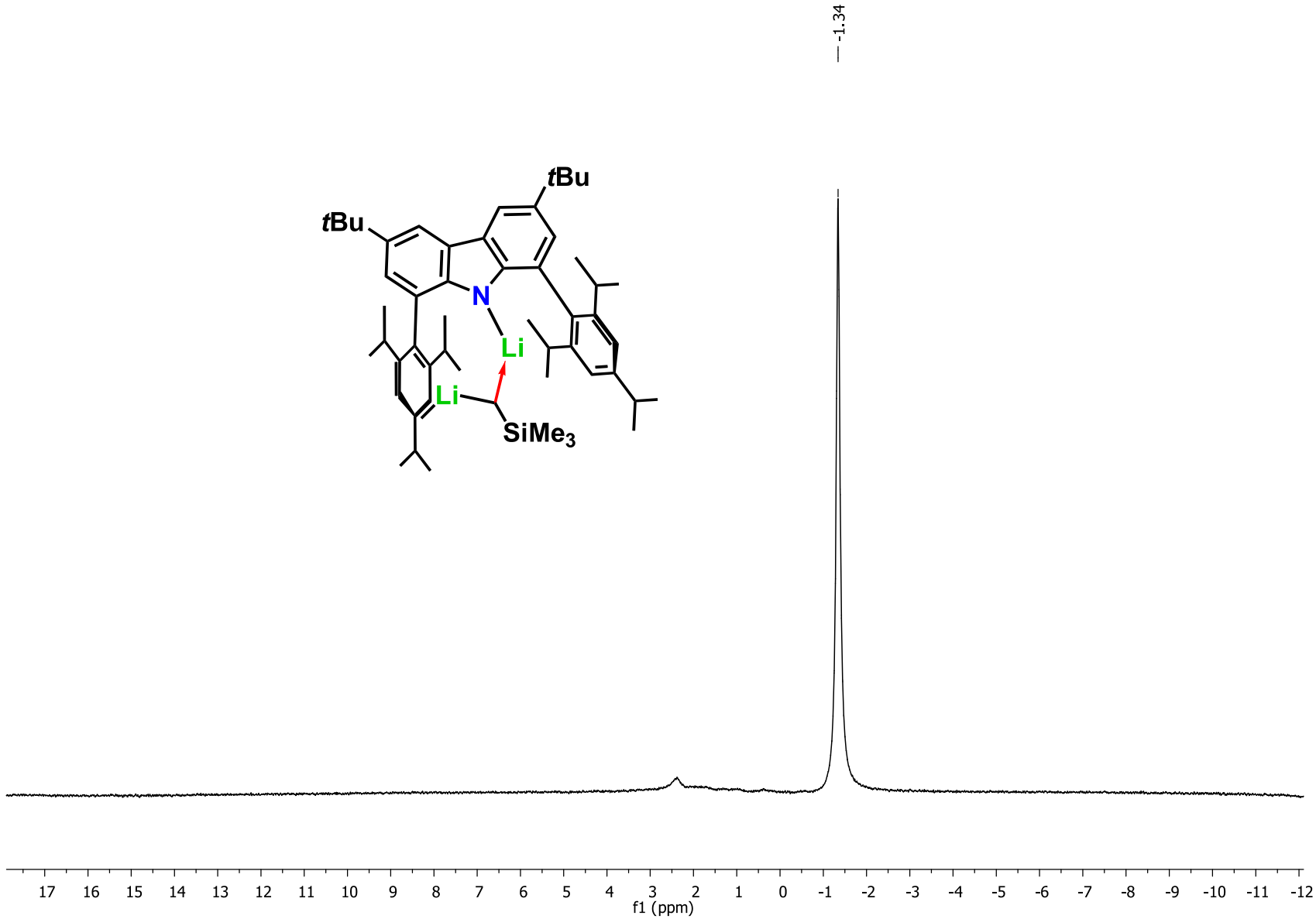


Figure S15. ^{7}Li NMR spectrum of complex **3** (100 MHz, C_6D_6, 293 K).

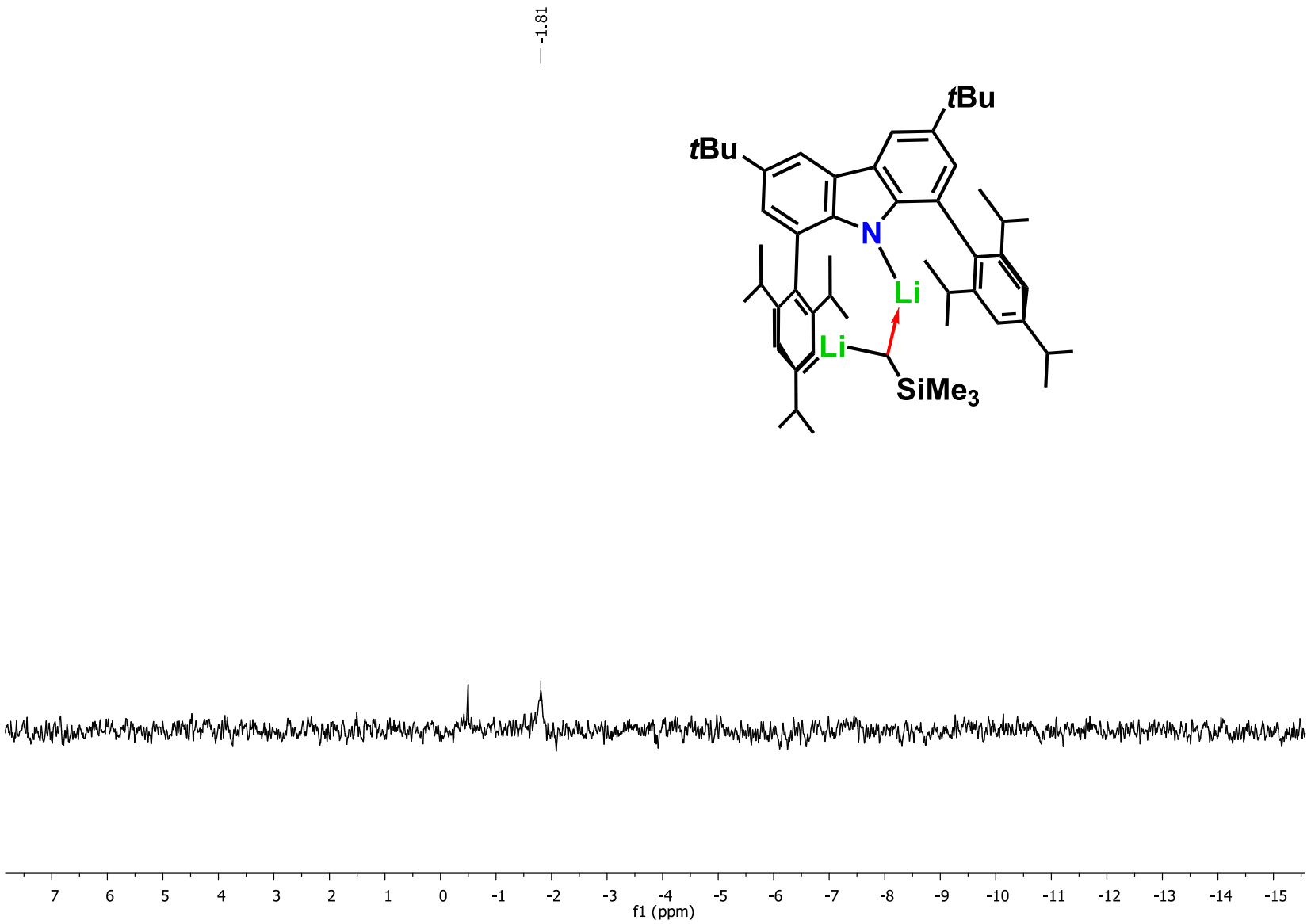


Figure S16. ^{29}Si NMR spectrum of **3** (79.5 MHz, C_6D_6, 293 K).

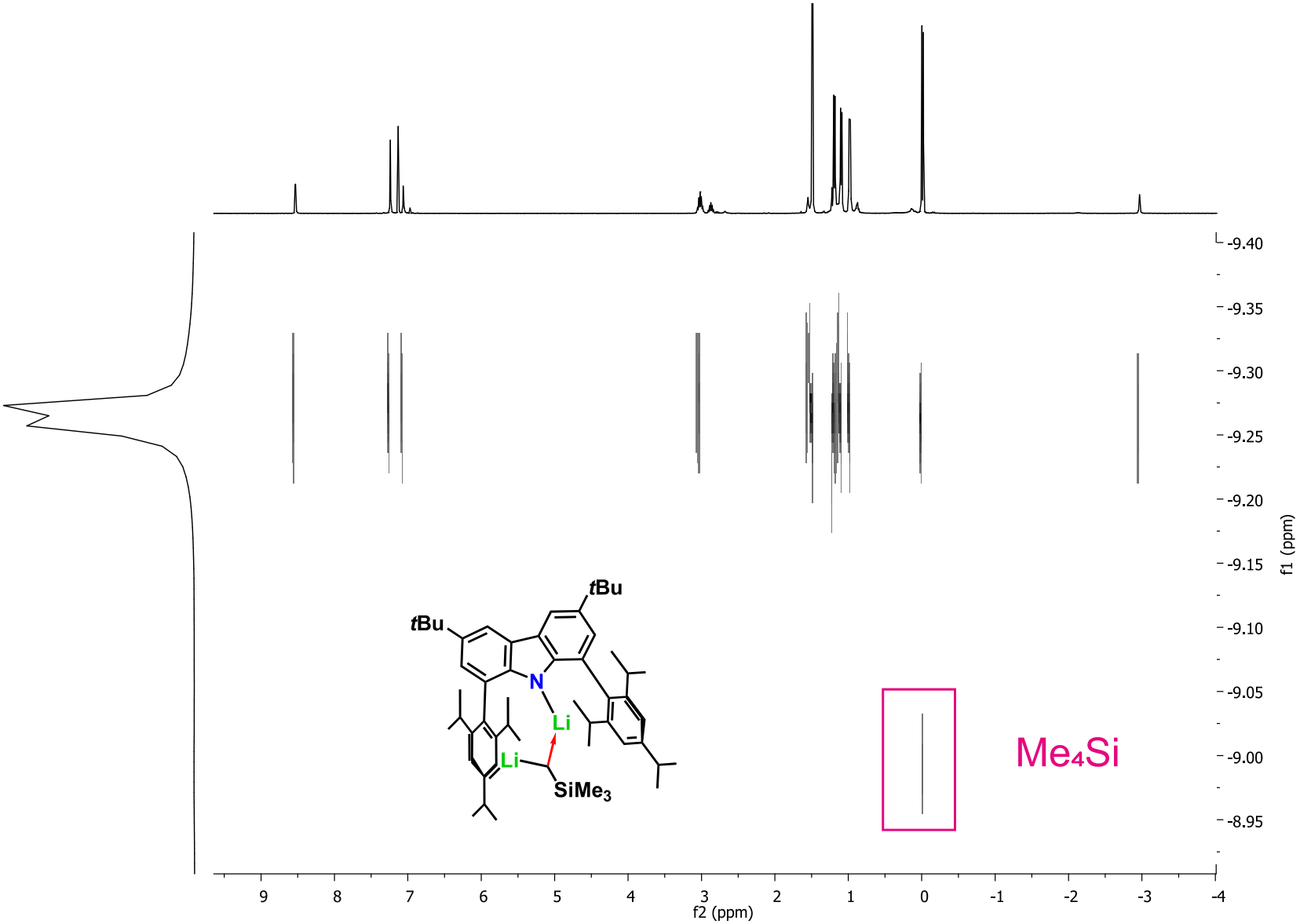


Figure S17. ^{1}H DOSY NMR spectrum of complex **3** (100 MHz, C_6D_6, 293 K).

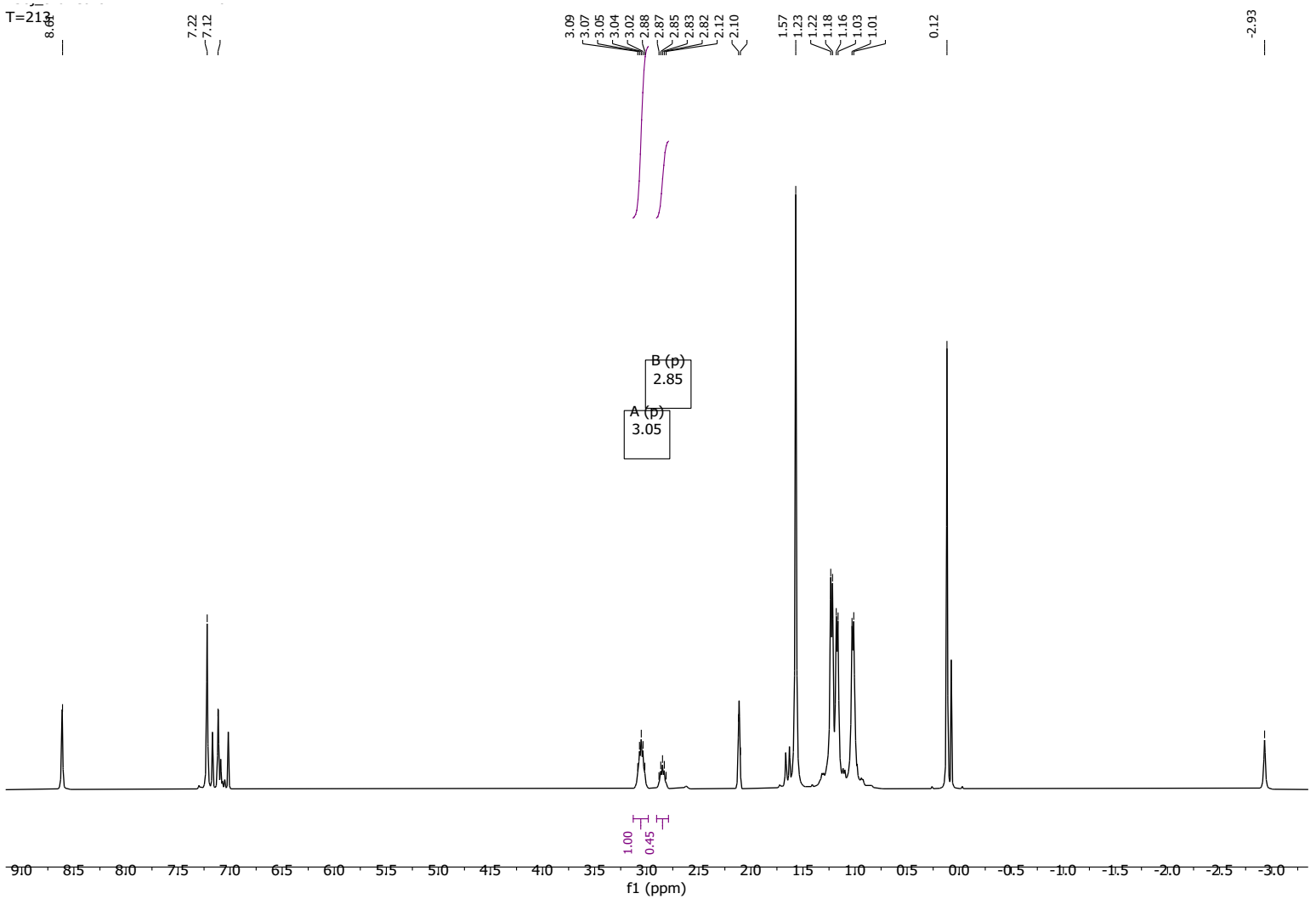


Figure S18. ^{1}H NMR spectrum of complex **3** (400 MHz, C_7D_8, 213 K).

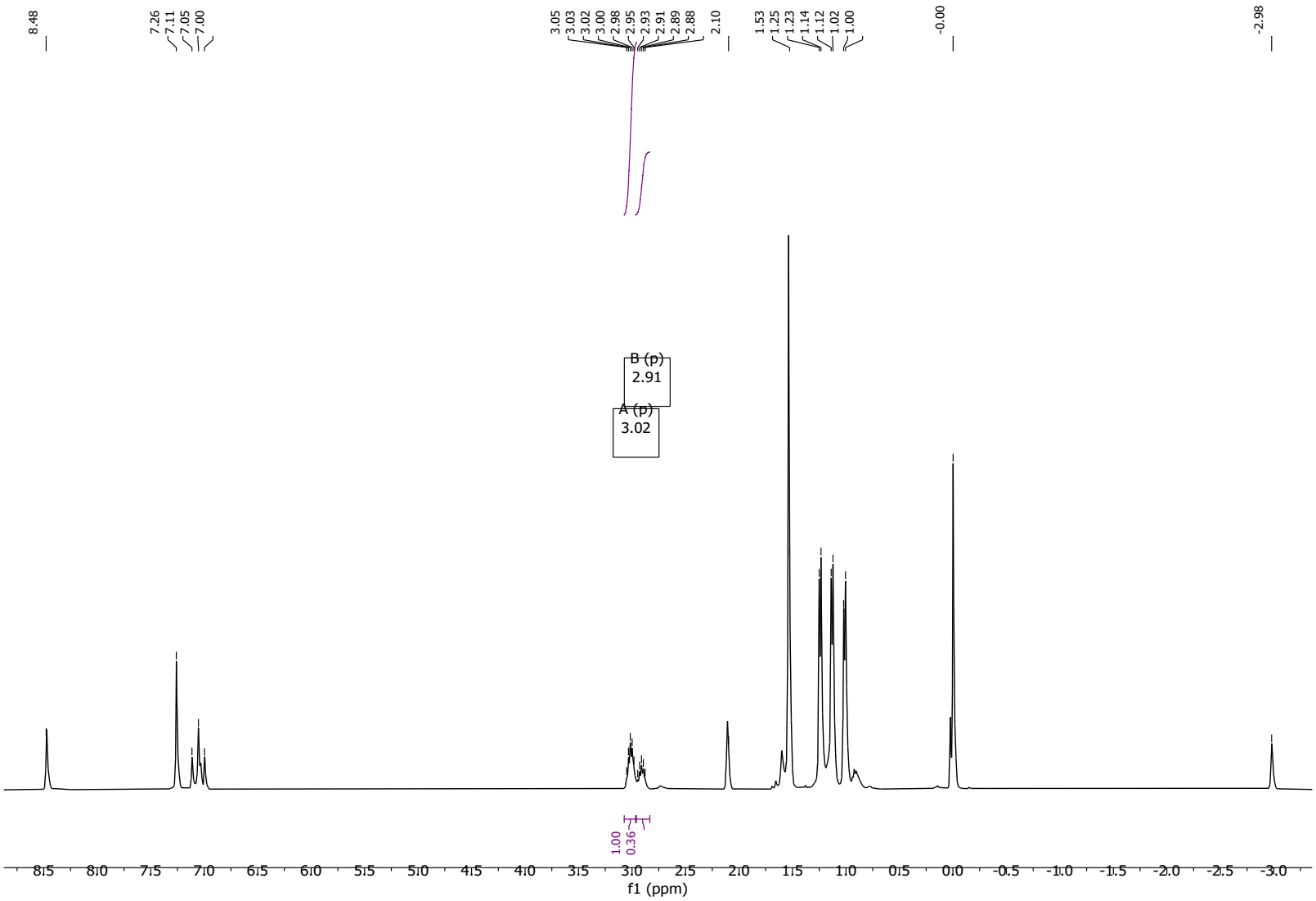


Figure S19. ^{1}H NMR spectrum of complex **3** (400 MHz, C_7D_8, 293 K).

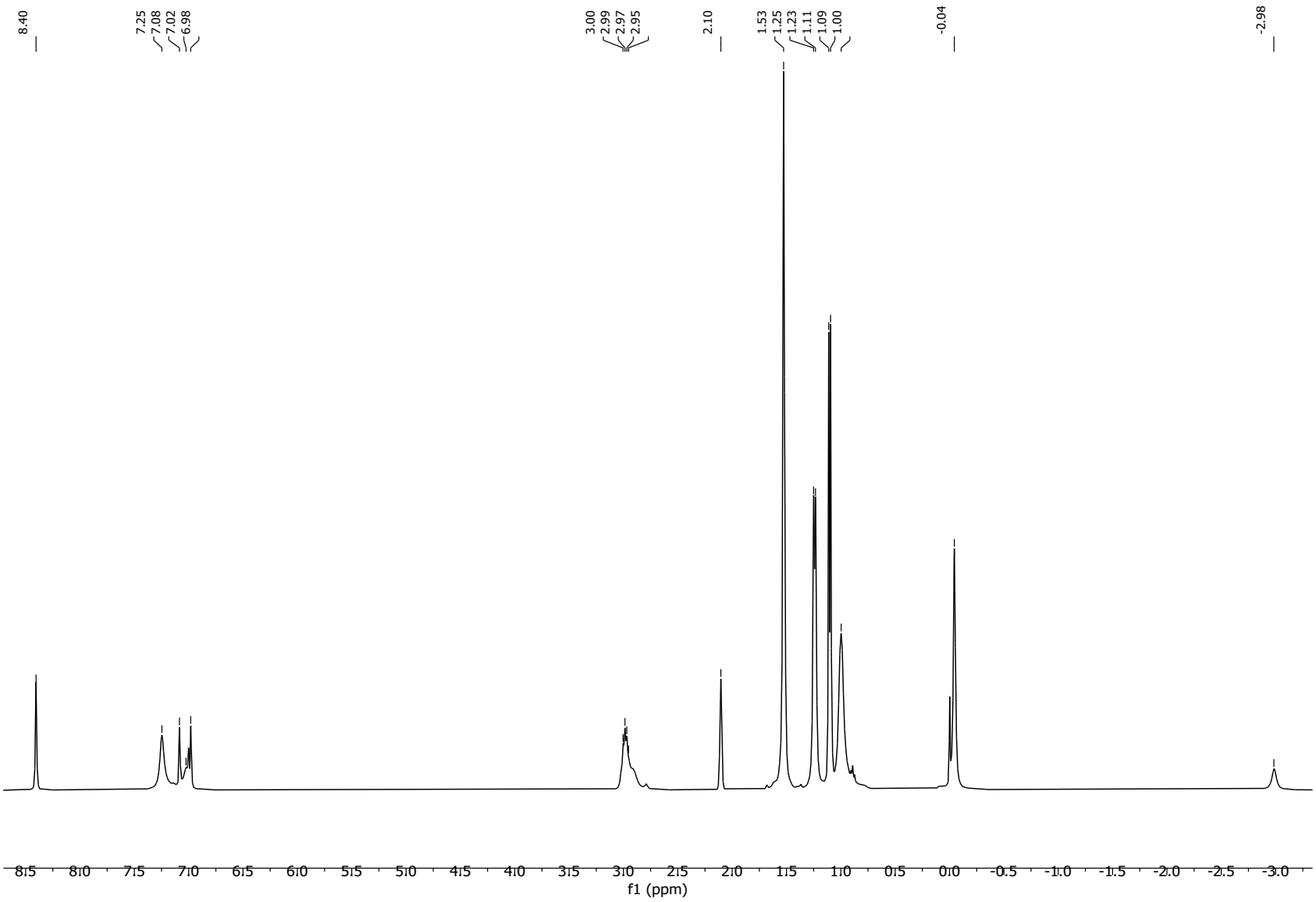


Figure S20. ^{1}H NMR spectrum of complex **3** (400 MHz, C_7D_8, 343 K).

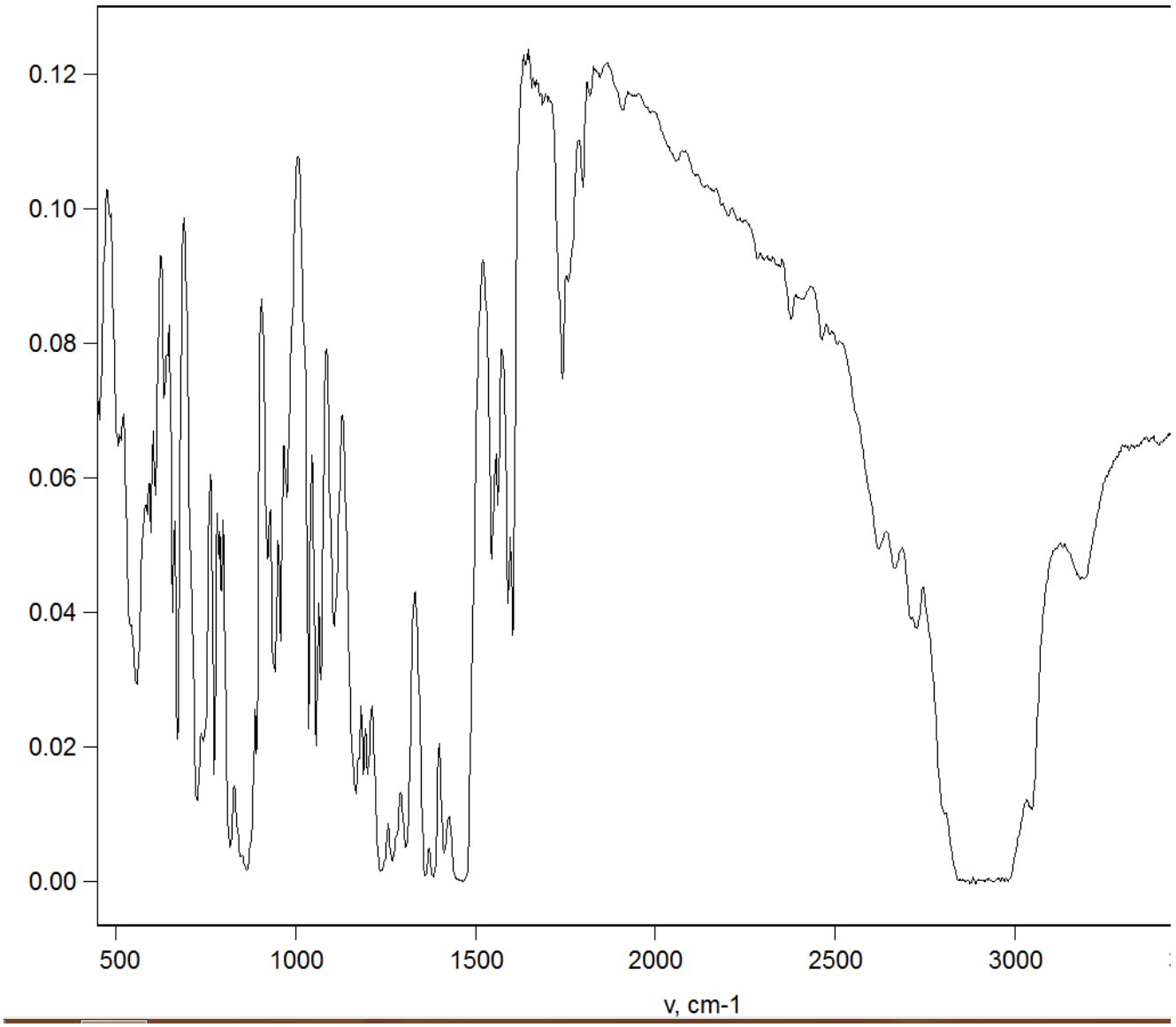


Figure S21. IR (KBr, Nujol) spectrum of complex **3**.

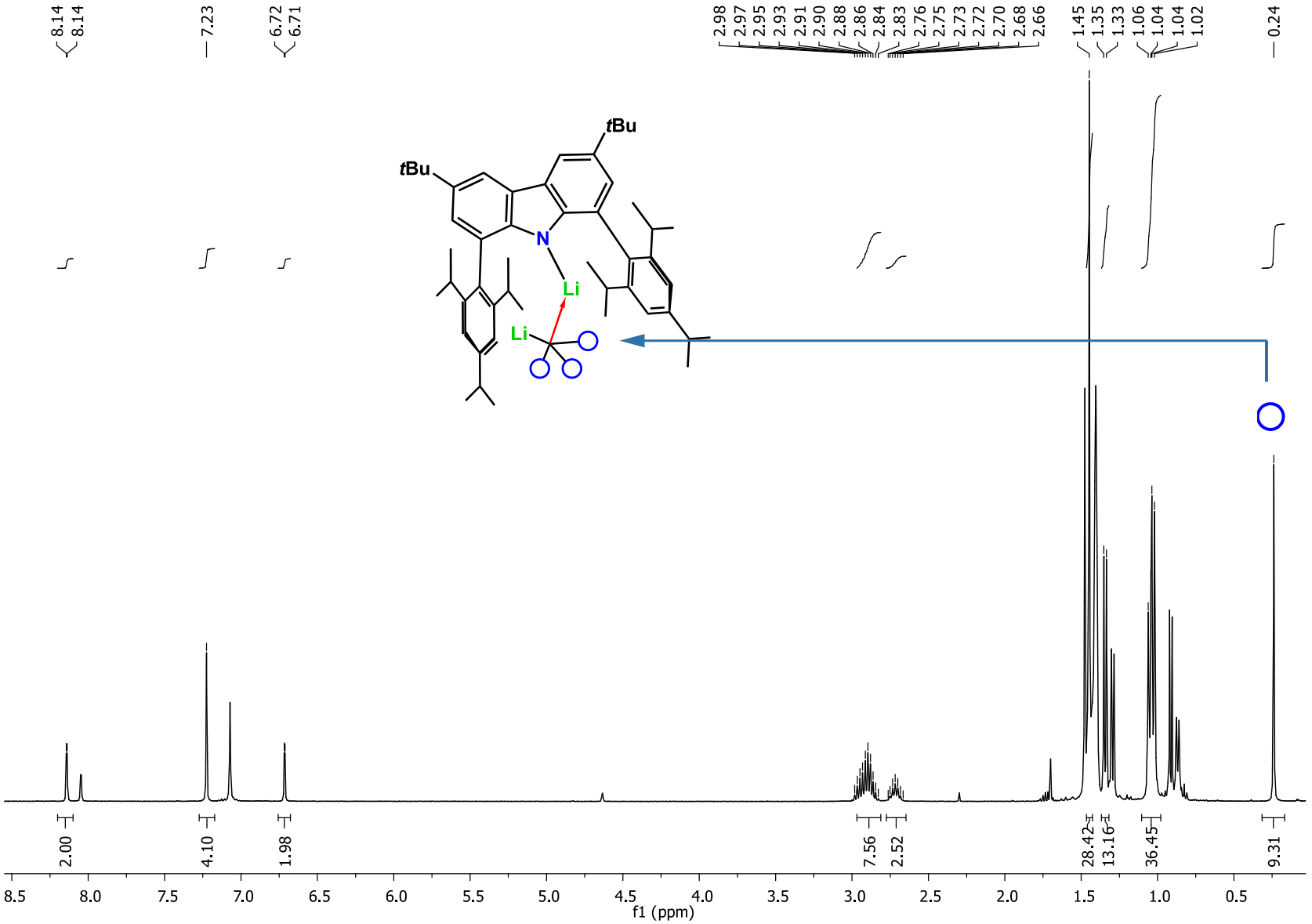


Figure S22. ^{1}H NMR spectrum of complex **4** (400 MHz, C_6D_{12}, 293 K).

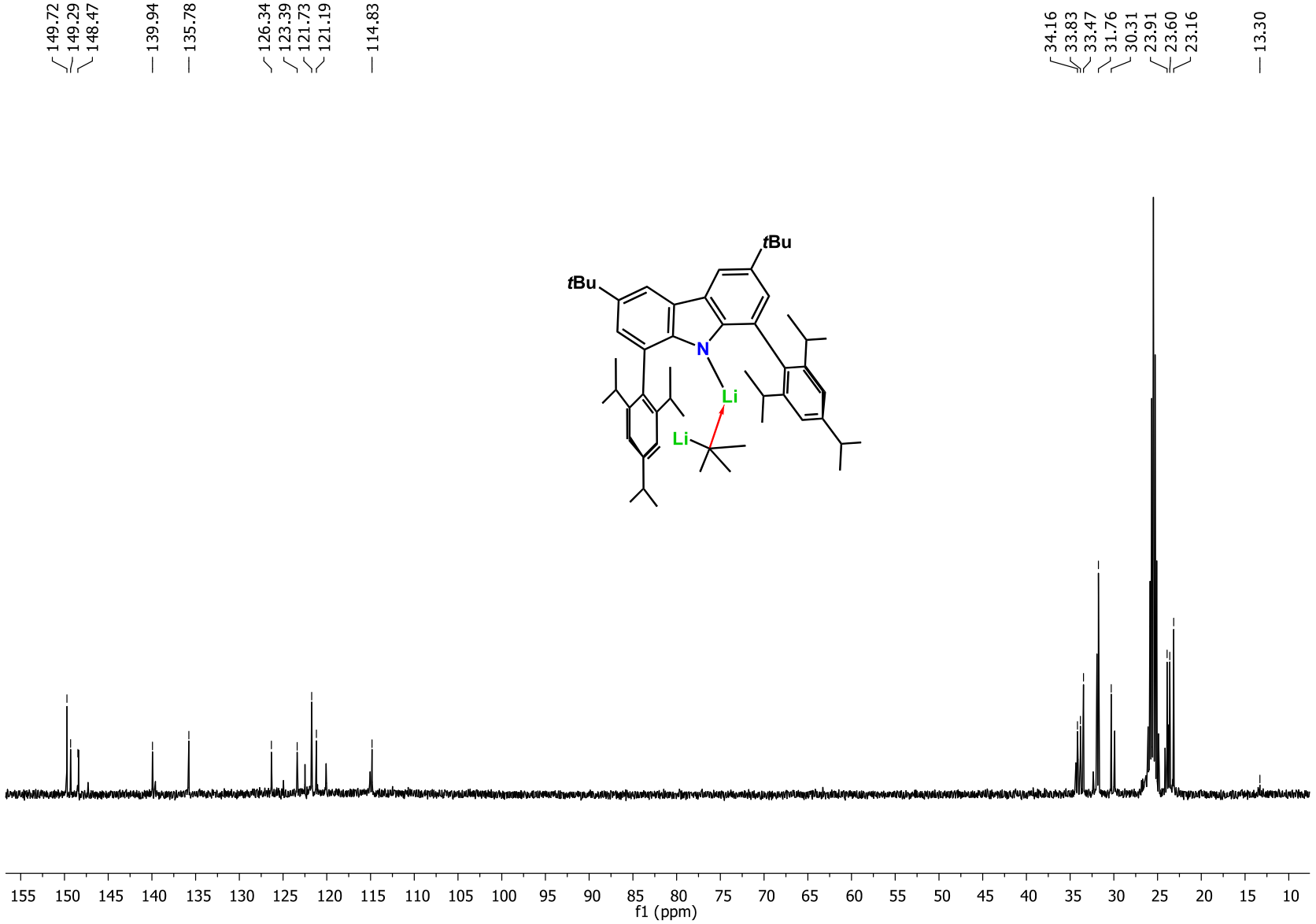


Figure S23. ^{13}C $\{^{1}H\}$ NMR spectrum of complex **4** (100 MHz, C_6D_{12}, 293 K).

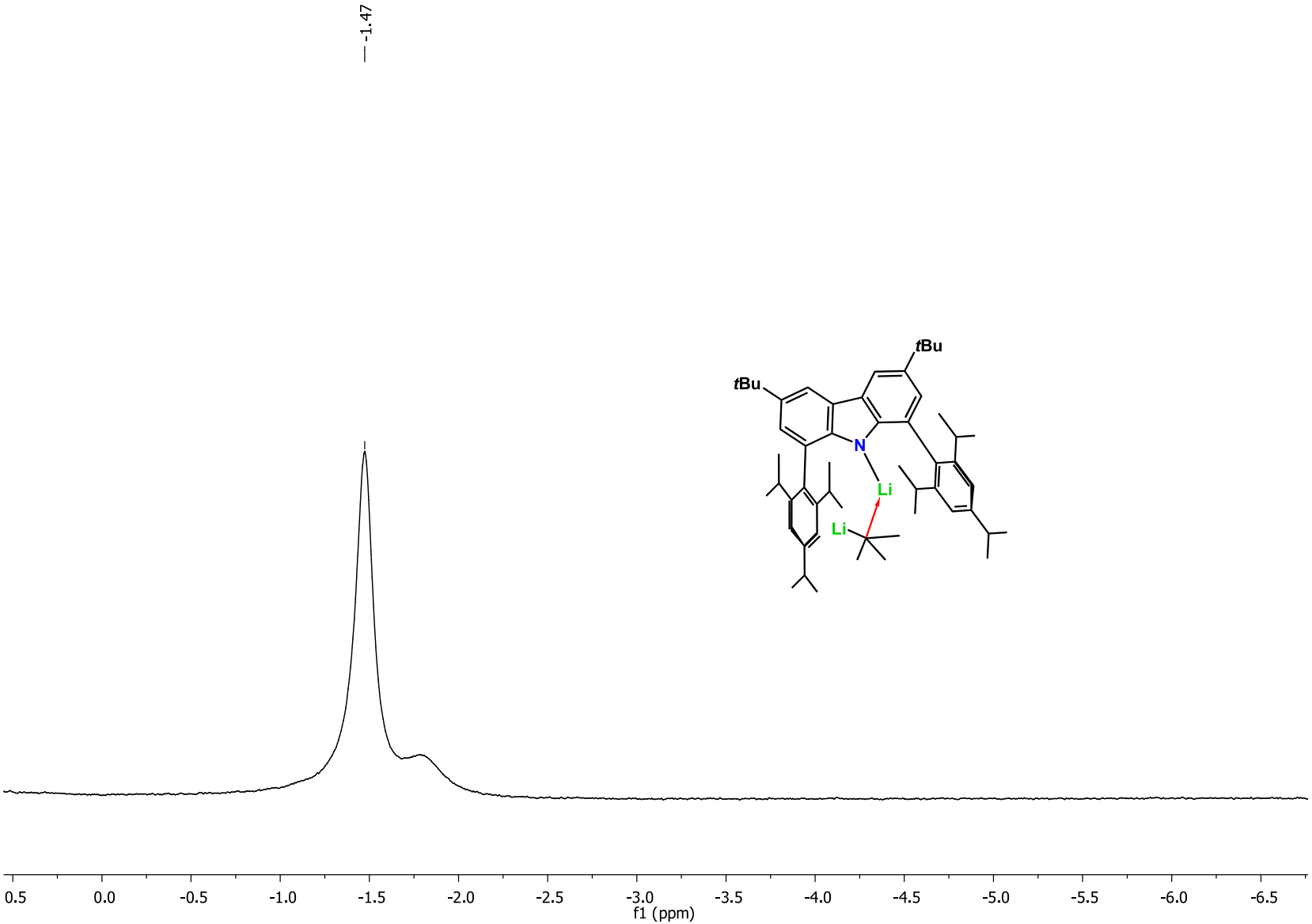


Figure S24. ^{7}Li NMR spectrum of complex **4** (100 MHz, C_6D_{12}, 293 K).

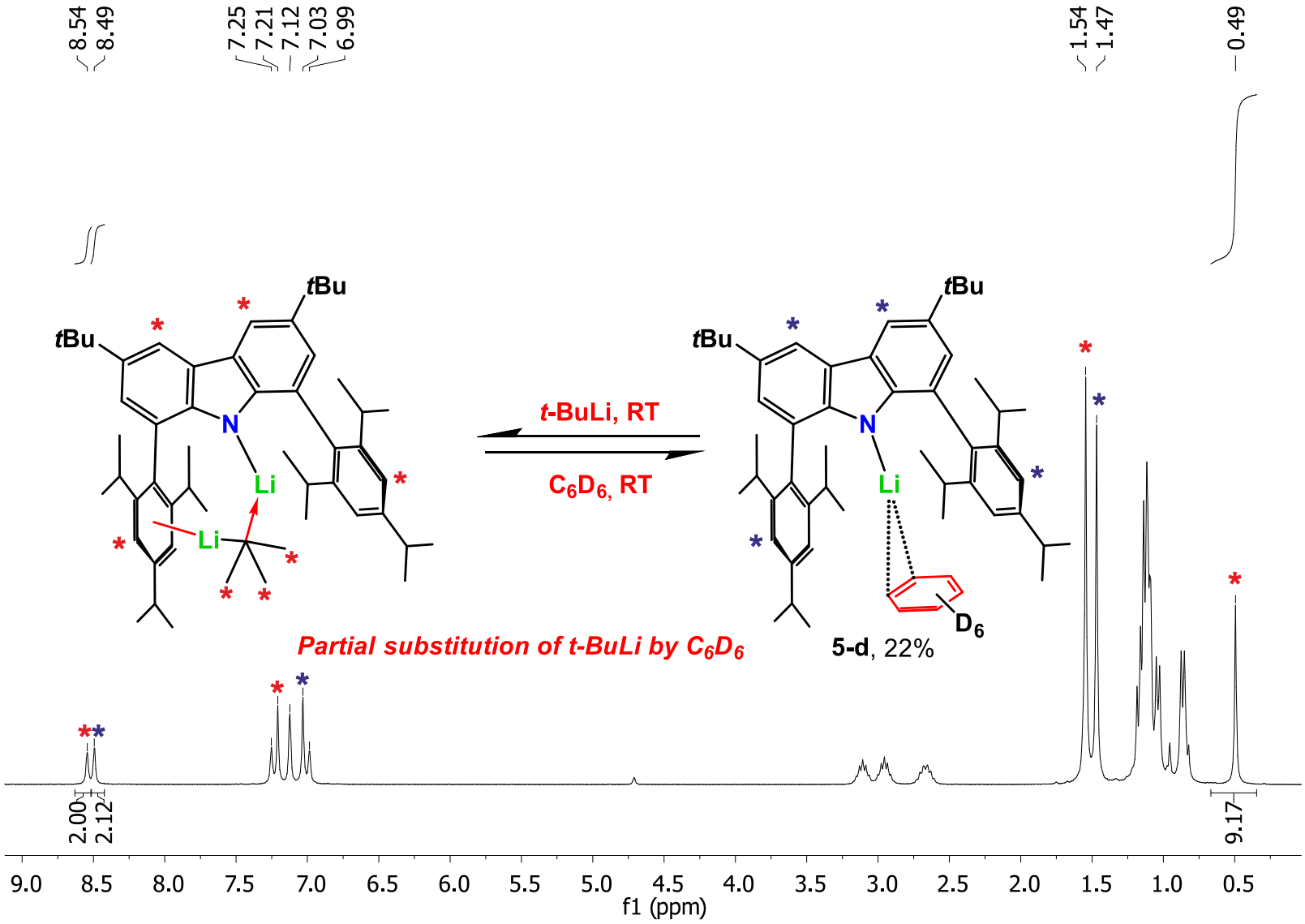


Figure S25. ^{1}H NMR spectrum of **4**, showing partial substitution of *t*BuLi by C_6D_6 at room temperature.

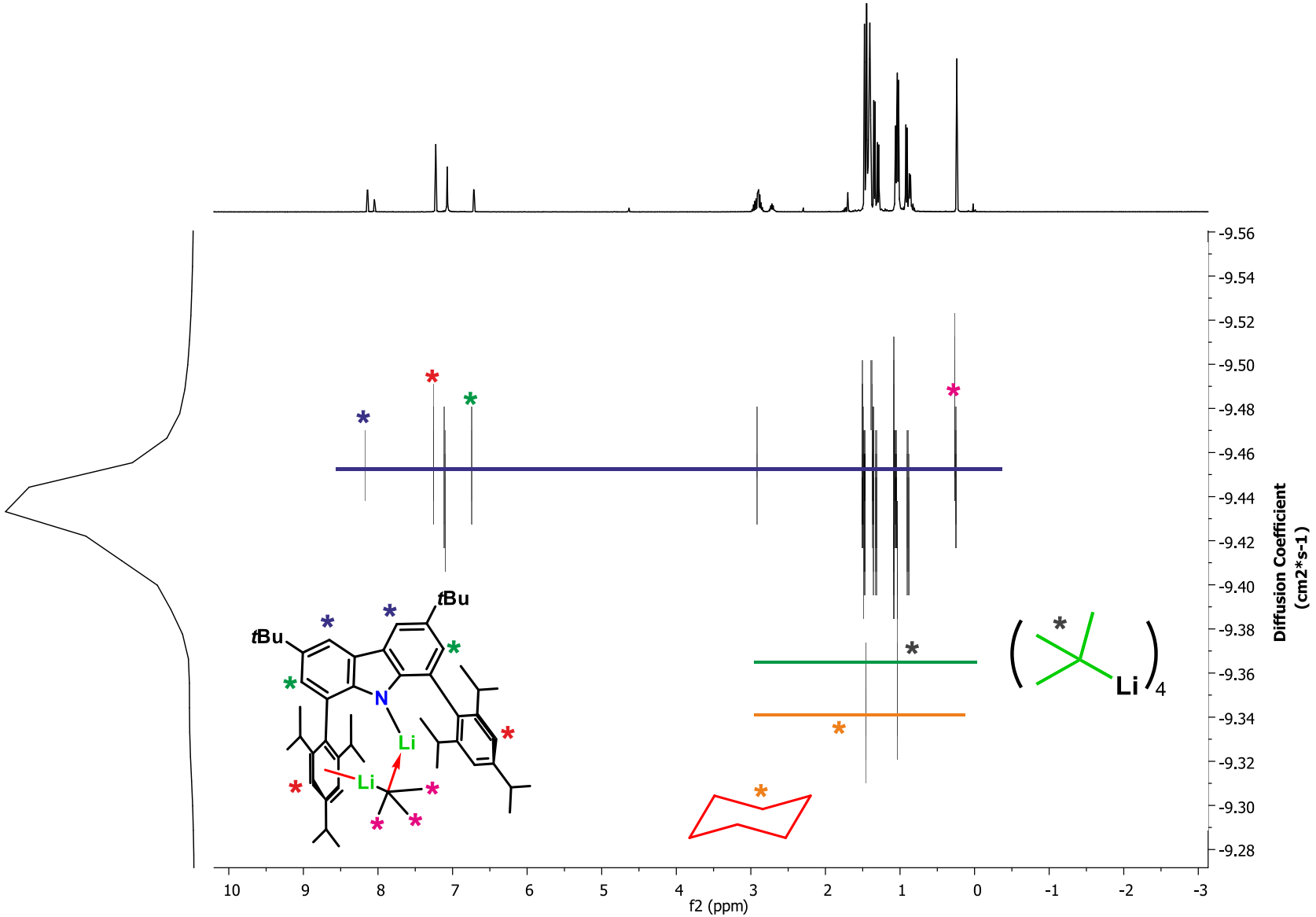


Figure S26. ^{1}H DOSY NMR spectrum of complex **4** (100 MHz, C_6D_{12}, 293 K).

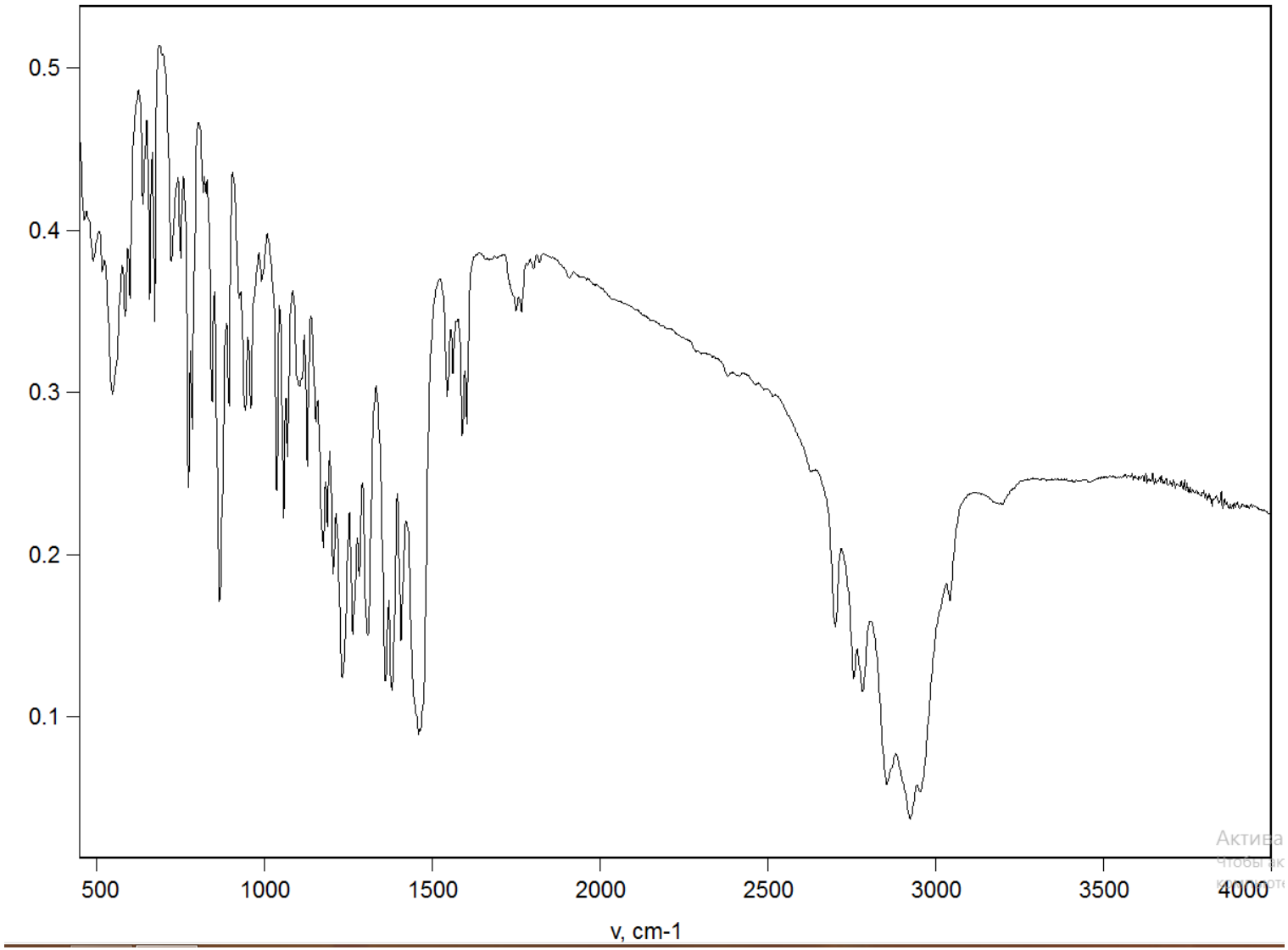


Figure S27. IR (KBr, Nujol) spectrum of complex **4**.

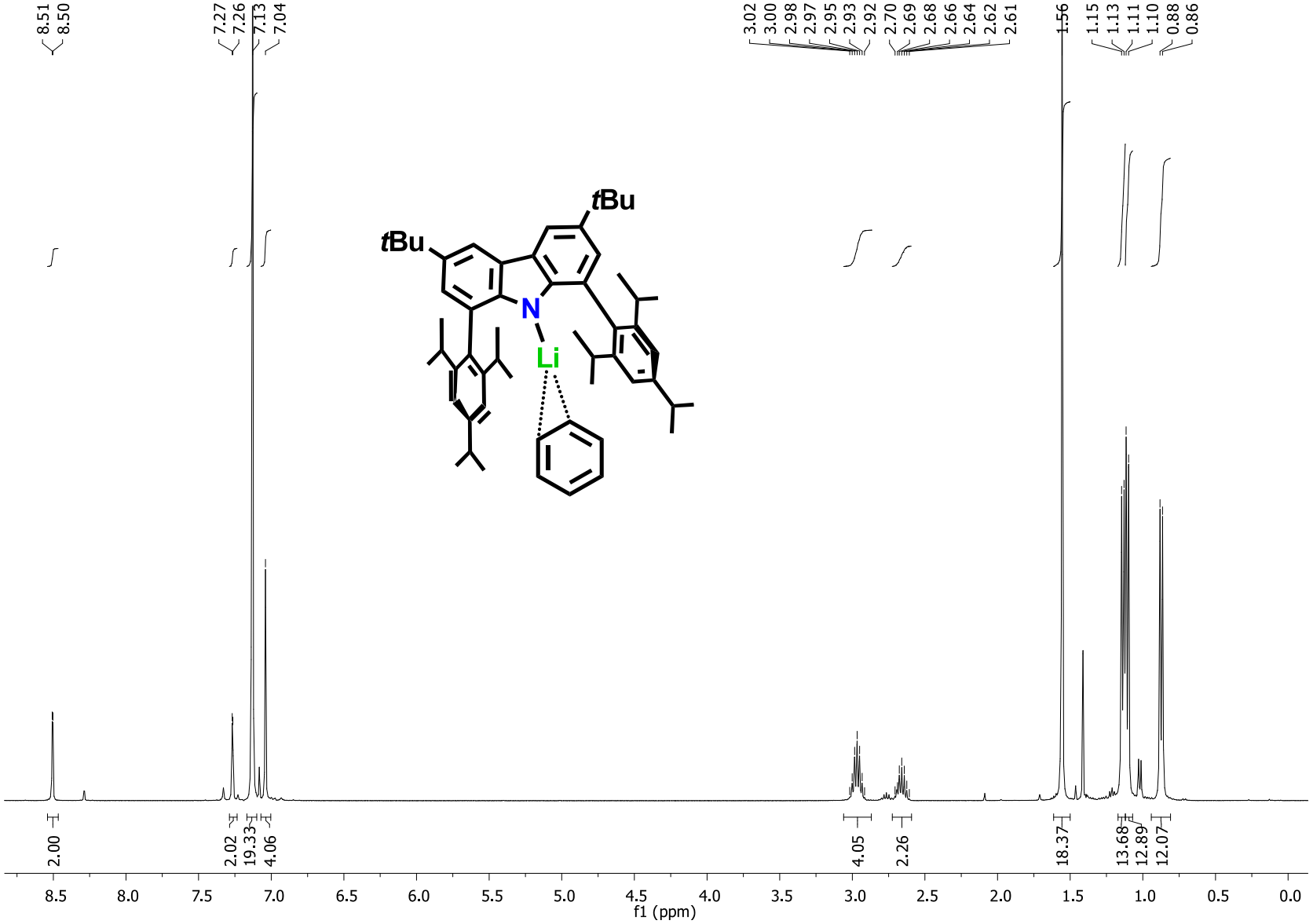


Figure S28. ^{1}H NMR spectrum of complex **5** (400 MHz, C_6D_6, 293 K).

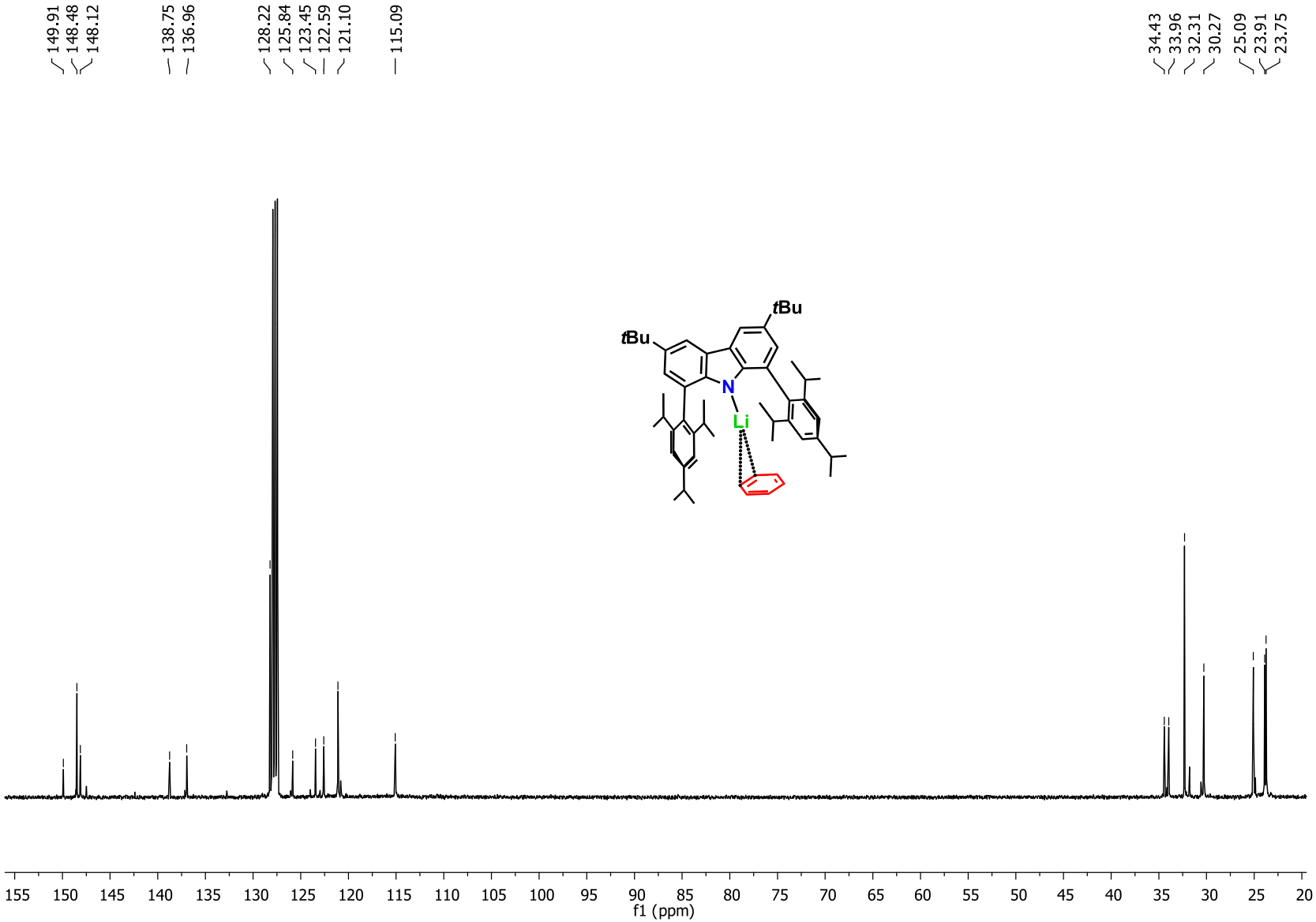


Figure S29. ^{13}C {^{1}H} NMR spectrum of complex **5** (100 MHz, C_6D_6, 293 K).

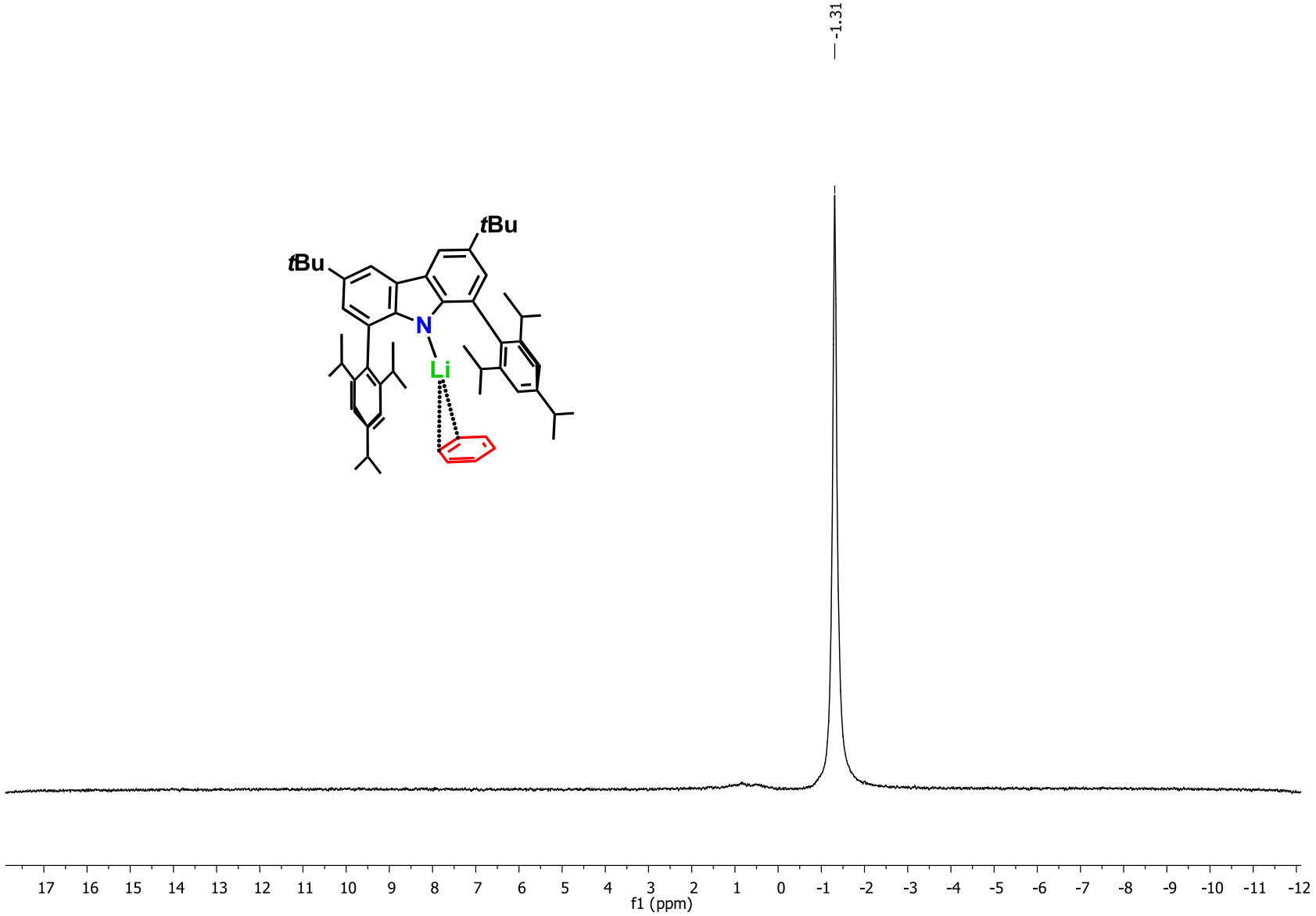


Figure S30. ^{7}Li NMR spectrum of complex **5** (100 MHz, C_6D_6, 293 K).

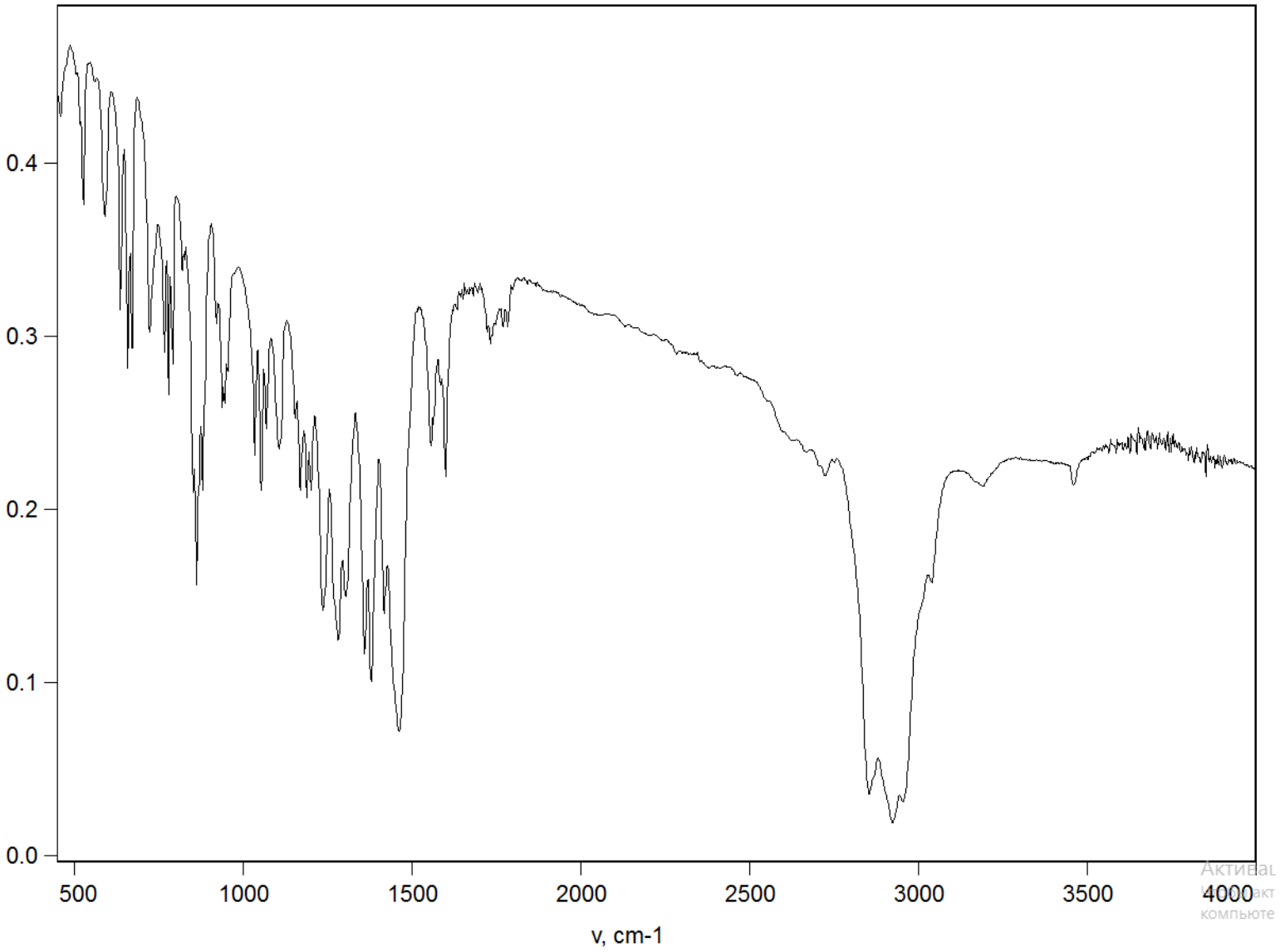


Figure S31. IR (KBr, Nujol) spectrum of complex **5**.

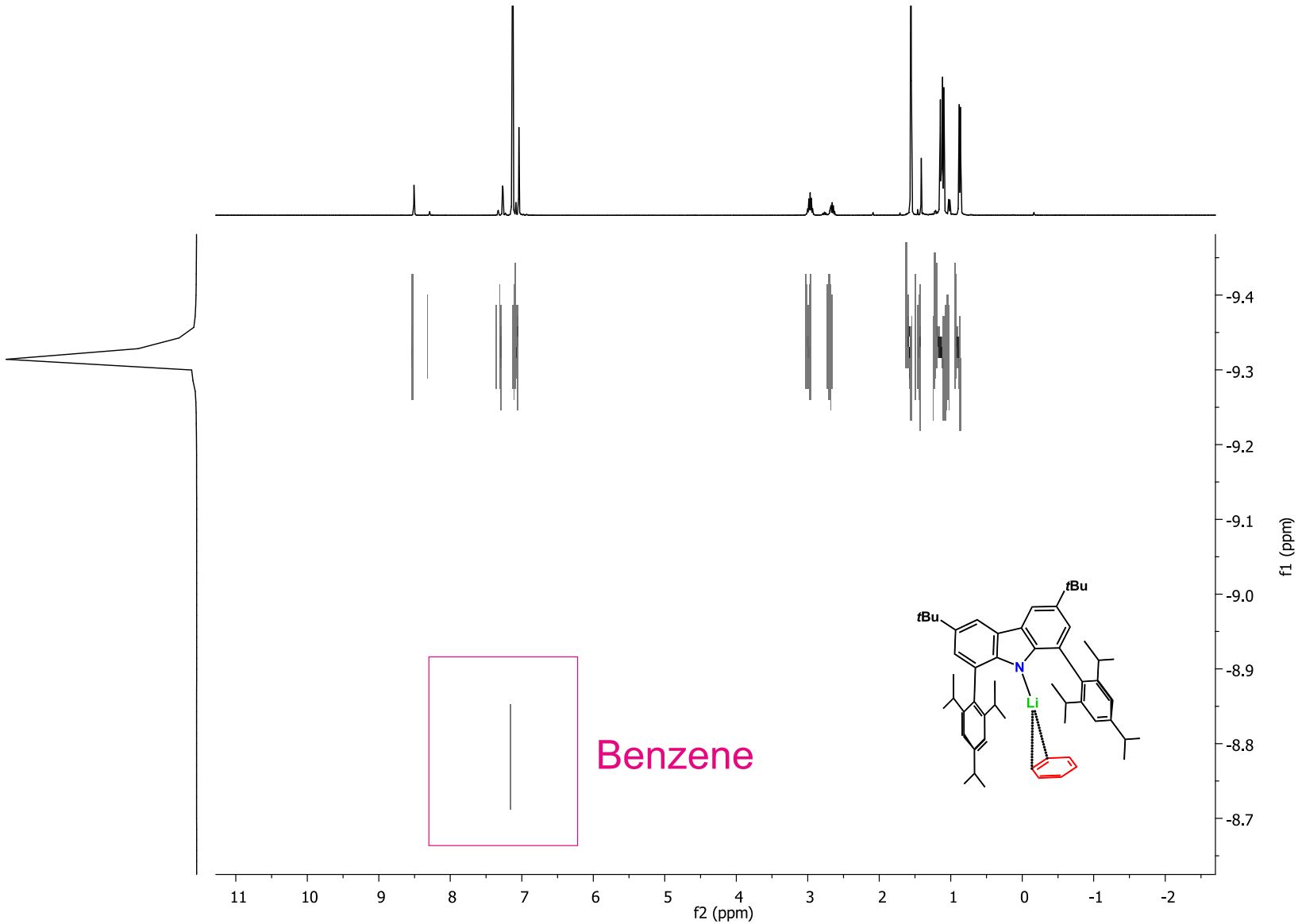


Figure S32. ^{1}H DOSY NMR spectrum of complex **5** (100 MHz, C_6D_6, 293 K).

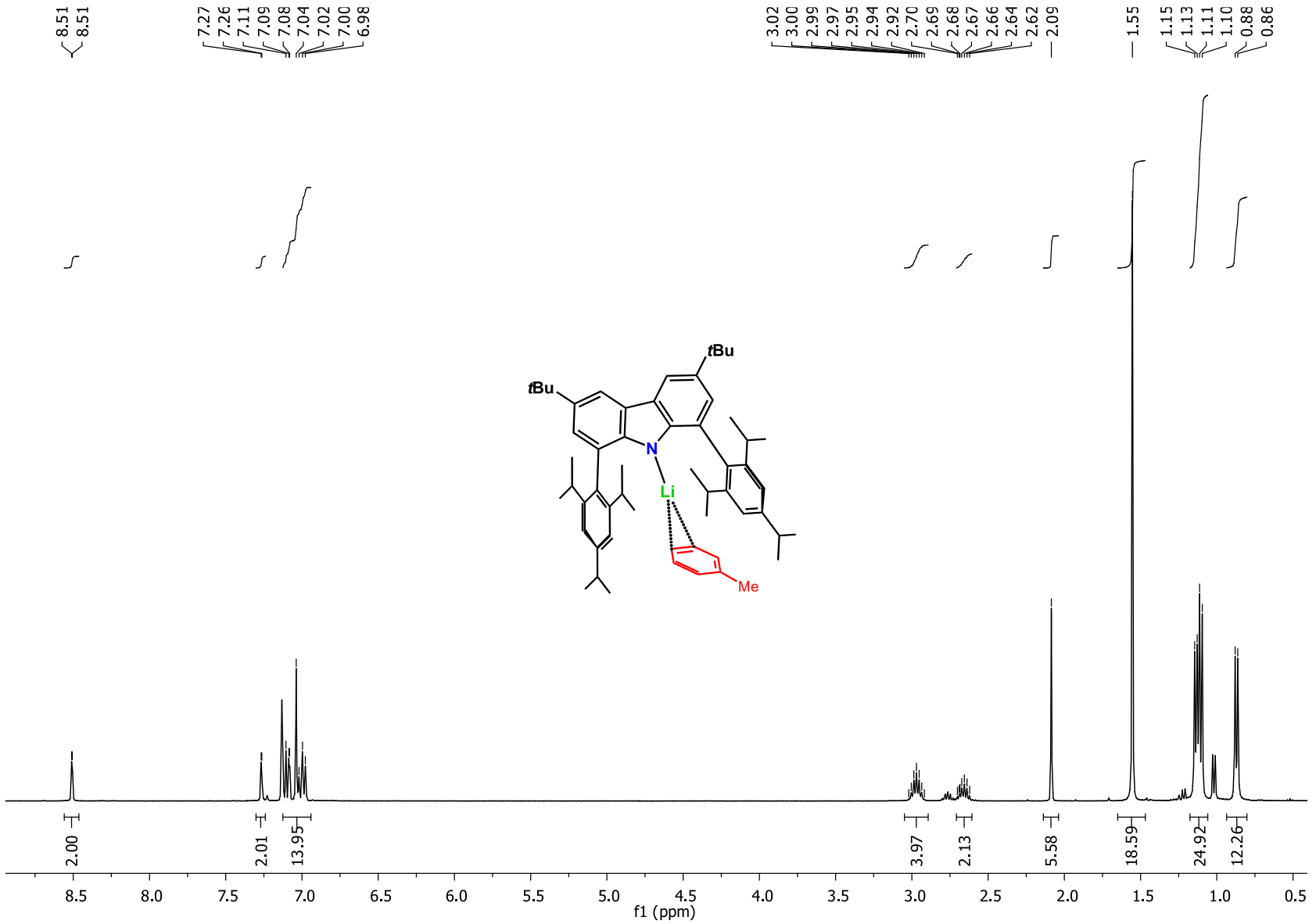


Figure S33. ^{1}H NMR spectrum of complex **6** (400 MHz, C_6D_6, 293 K).

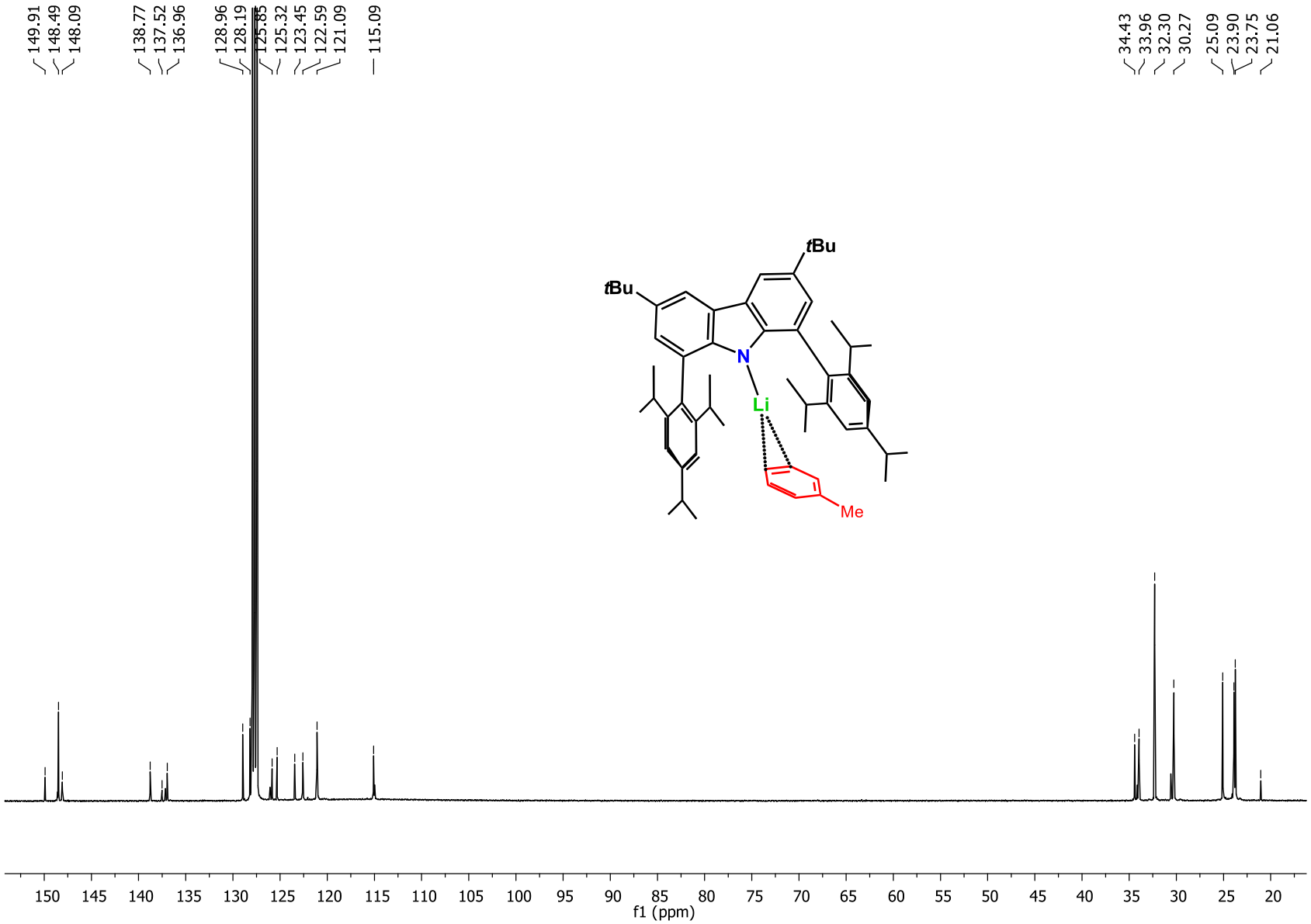


Figure S34. ^{13}C {^{1}H} NMR spectrum of complex **6** (100 MHz, C_6D_6, 293 K).

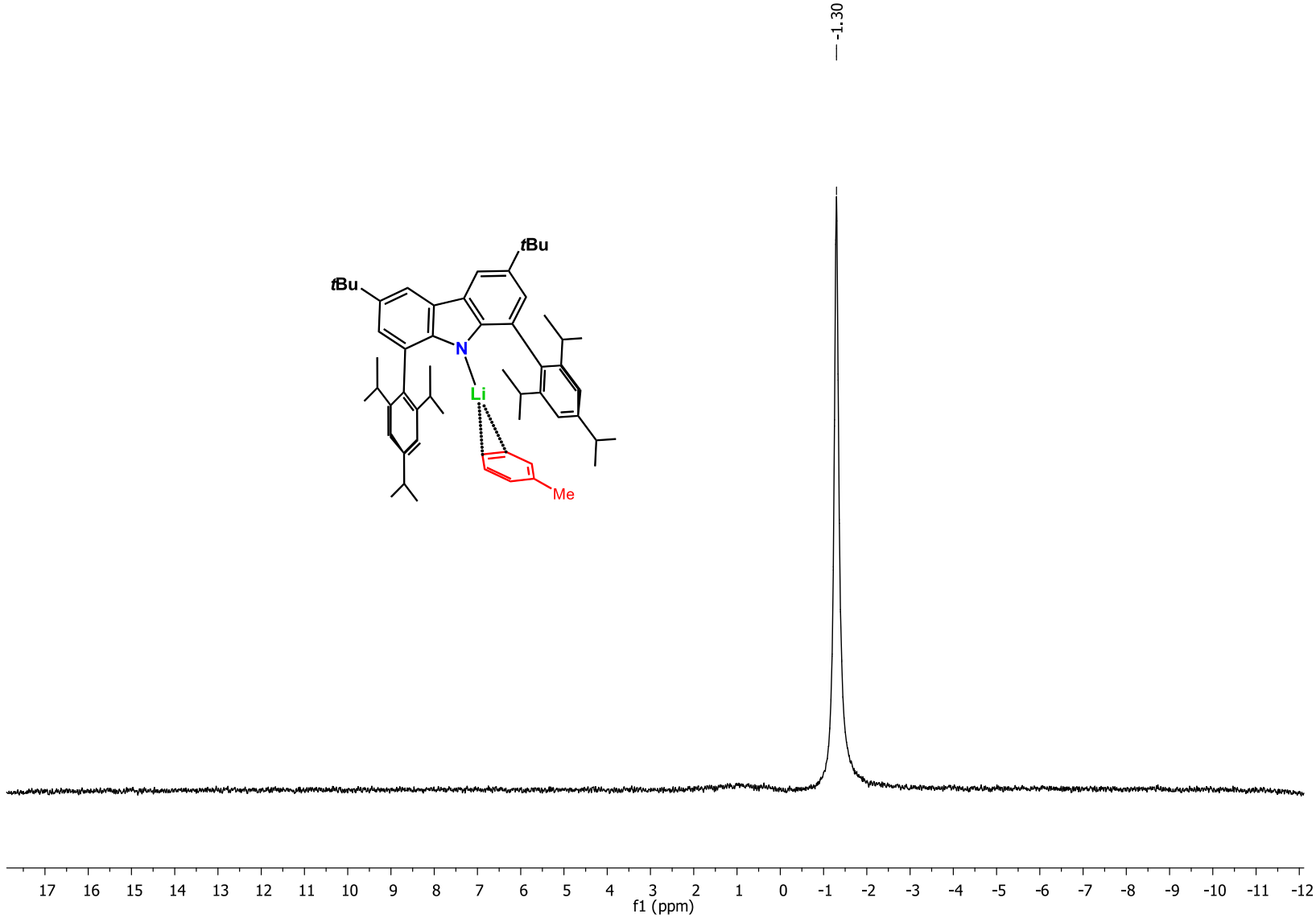


Figure S35. ^{7}Li NMR spectrum of complex **6** (100 MHz, C_6D_6, 293 K).

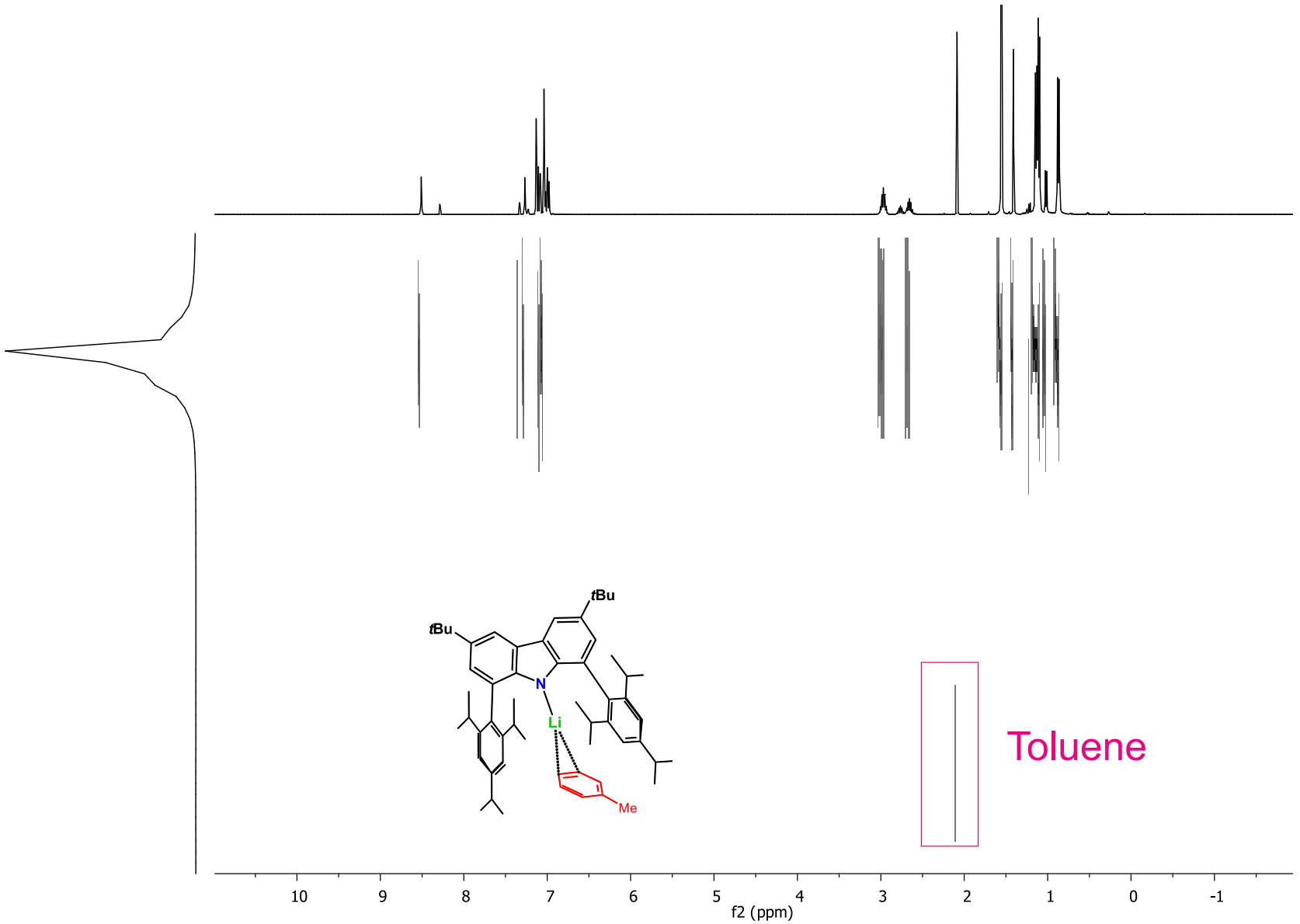


Figure S36. ^{1}H DOSY NMR spectrum of complex **6** (100 MHz, C_6D_6, 293 K).

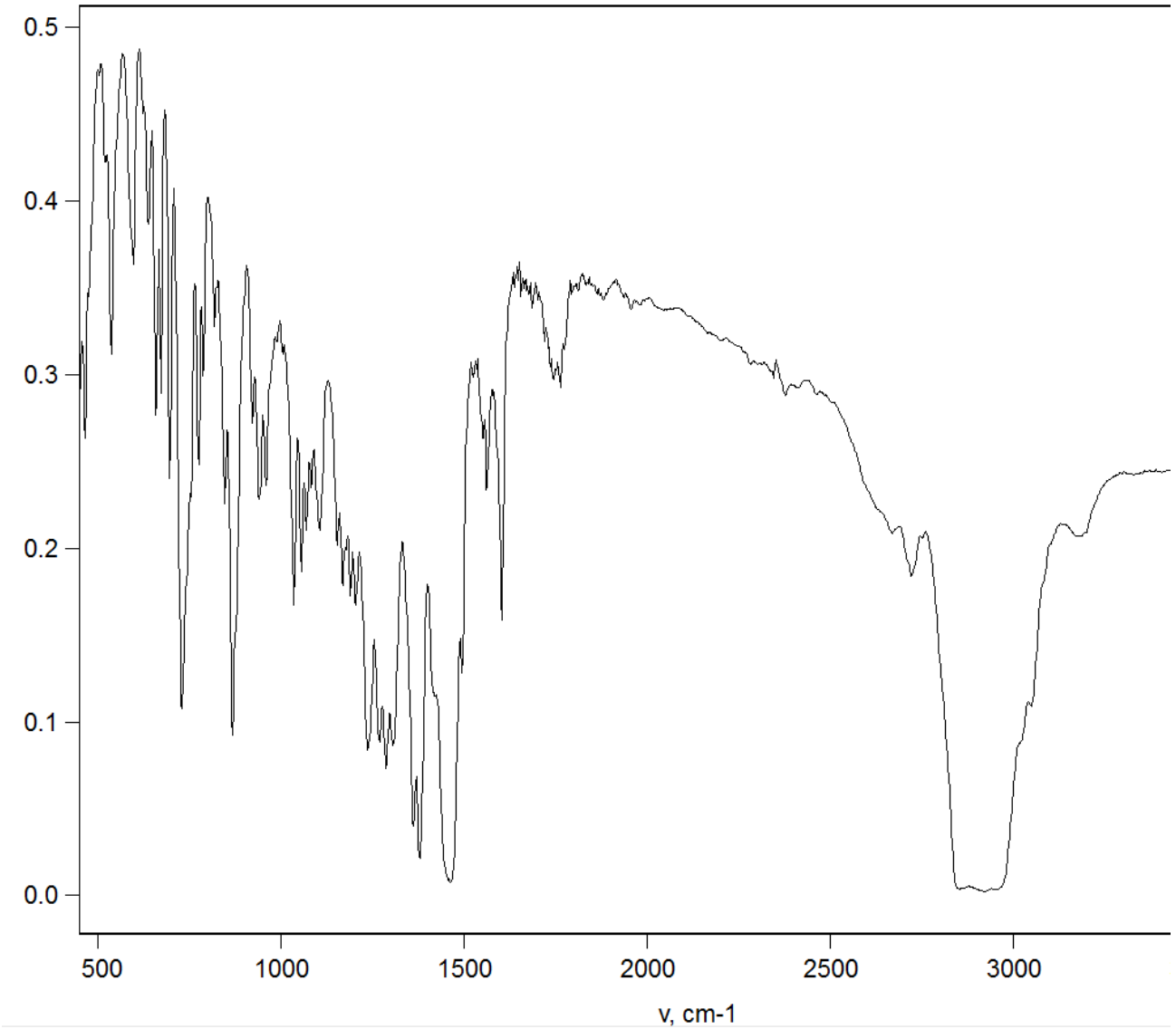


Figure S37. IR (KBr, Nujol) spectrum of complex **6**.

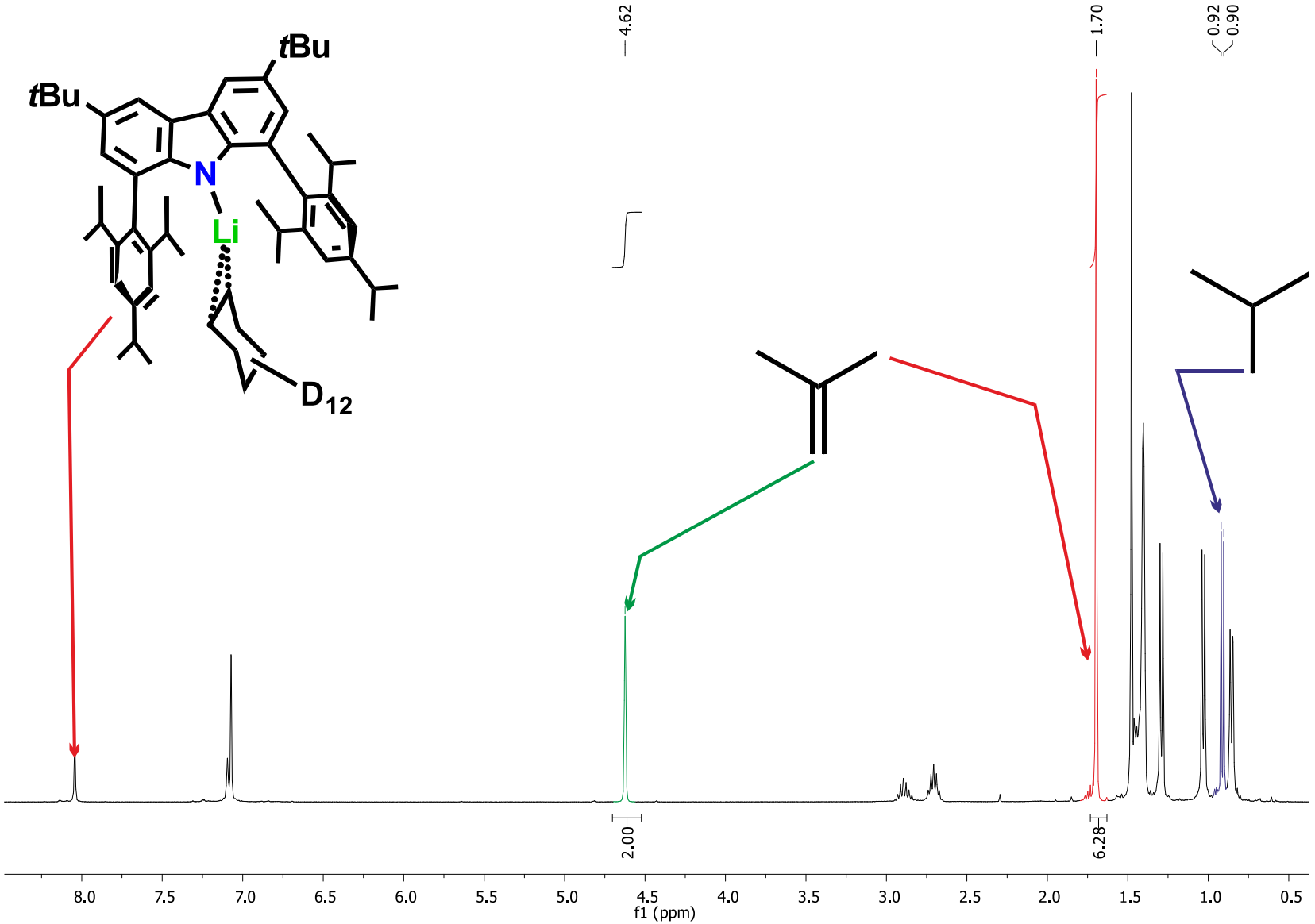


Figure S38. ^{1}H NMR spectrum of complex **4** after thermolysis (400 MHz, C_6D_{12}, 293 K).

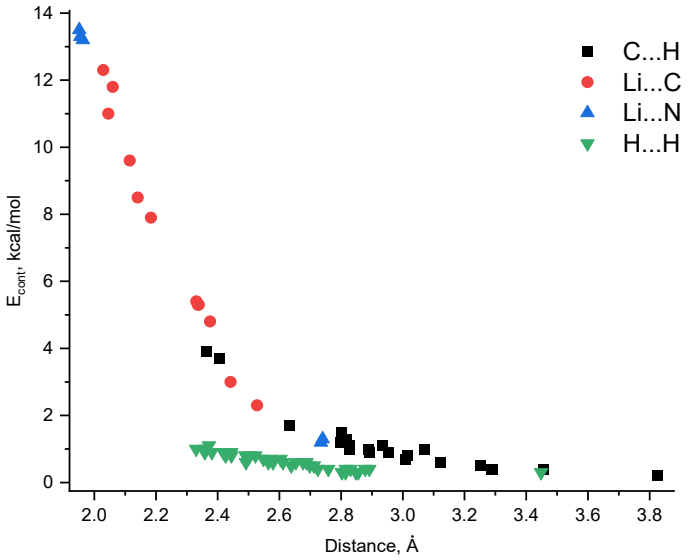


Figure. S39. Correlation of E_{cont} and interatomic distances for non-covalent interactions of different types in compounds **2**-**4**.

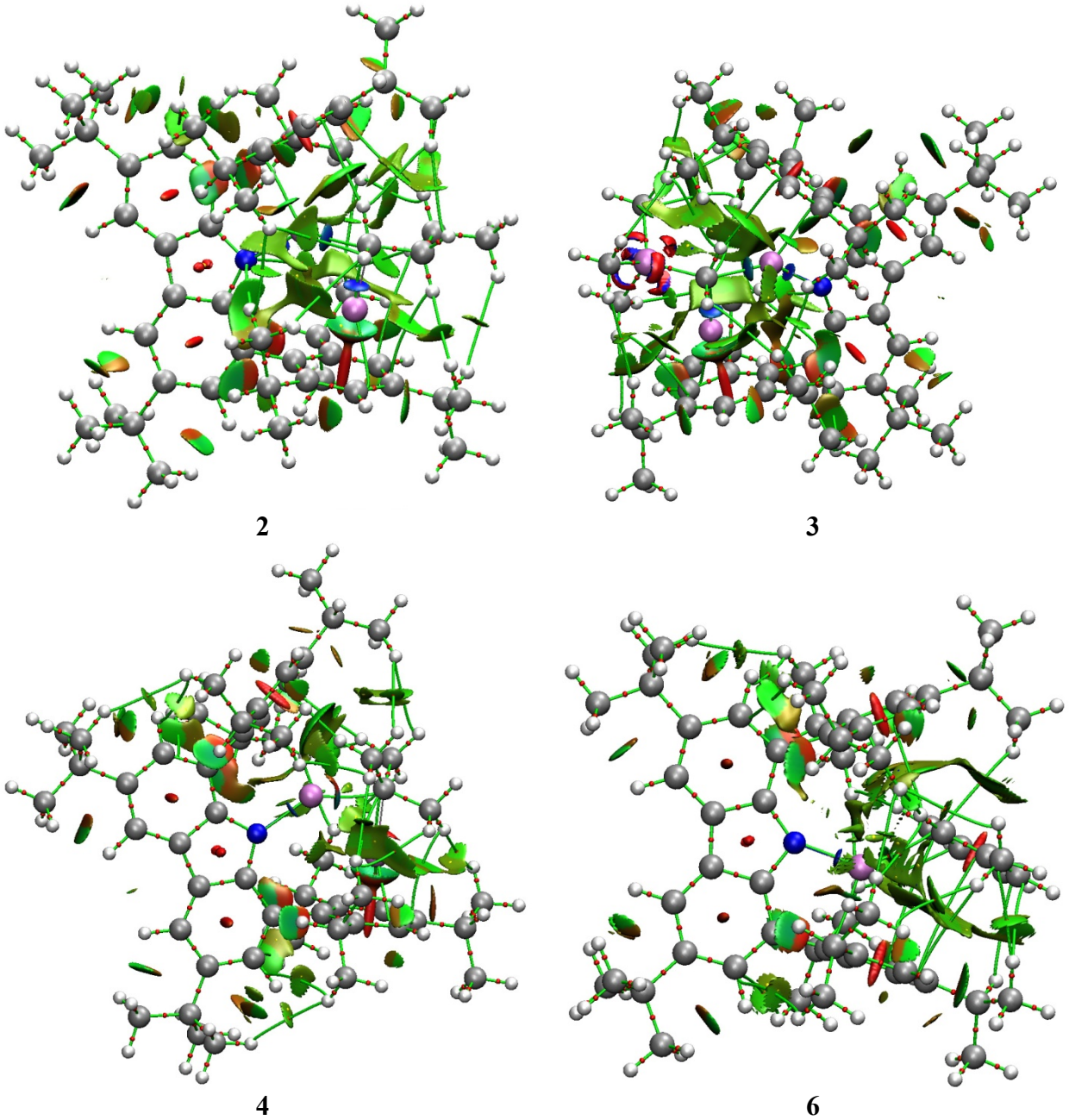


Figure S40. The RDG isosurface (isovalue is 0.5 a.u) combined with QTAIM molecular graph at the DLPNO-CCSD(T)/Def2-TZVP for the complexes **2–4** and **6** optimized at the r^2-SCAN-3c/Def2-TZVP //CPCM(hexane) level. *The standard color mapping by λ^2 correspond to that green areas are VdW interactions, red areas are steric repulsions*.

Table S2. QTAIM parameters at the DLPNO-CCSD(T)/Def2-TZVP level for the complexes **2-4** and **6** optimized at the r^2-SCAN-3c/Def2-TZVP //CPCM(hexane) level

Connected atoms	Distance	ρ, a.u.	Δρ, a.u.	V(r), a.u.	H(r), a.u.	Econt, kcal/mol
2 (R = Bu)						
131(H)... 37(H)	2.856	0.00183	0.00645	-0.00084	0.00039	0.3
49(H)... 1(N)	3.448	0.00227	0.00744	-0.00098	0.00044	0.3
128(H)... 23(C)	3.292	0.00315	0.00952	-0.00137	0.00051	0.4
127(H)... 84(C)	3.286	0.00266	0.00824	-0.00115	0.00045	0.4
122(H)... 34(H)	2.831	0.00290	0.00995	-0.00127	0.00061	0.4
122(H)...113(H)	2.878	0.00236	0.00891	-0.00118	0.00052	0.4
14(C)...118(H)	3.122	0.00385	0.01424	-0.00195	0.00080	0.6
94(H)...127(H)	2.653	0.00348	0.01279	-0.00181	0.00070	0.6
33(H)...113(H)	2.688	0.00334	0.01303	-0.00178	0.00074	0.6
127(H)...104(H)	2.604	0.00392	0.01456	-0.00209	0.00078	0.7
124(H)...105(H)	2.567	0.00374	0.01398	-0.00212	0.00069	0.7
121(H)...105(H)	2.548	0.00418	0.01450	-0.00226	0.00069	0.7
125(H)... 45(H)	2.490	0.00442	0.01484	-0.00242	0.00065	0.8
22(C)...125(H)	2.953	0.00587	0.01610	-0.00282	0.00060	0.9
49(H)... 94(H)	2.381	0.00516	0.01728	-0.00281	0.00075	0.9
49(H)...128(H)	2.418	0.00534	0.01737	-0.00290	0.00072	0.9
97(H)... 14(C)	2.797	0.00671	0.02231	-0.00367	0.00096	1.2
1(N)... 33(H)	2.735	0.00718	0.02381	-0.00389	0.00103	1.2
121(H)... 87(C)	2.819	0.00778	0.02290	-0.00413	0.00080	1.3
133(Li)...82(C)	2.442	0.01089	0.05998	-0.00945	0.00277	3.0
47(H)...3(C)	2.363	0.01672	0.06181	-0.01246	0.00150	3.9
134(Li)... 20(C)	2.336	0.01594	0.09751	-0.01705	0.00366	5.3
133(Li)...120(C)	2.115	0.02938	0.14833	-0.03066	0.00321	9.6
134(Li)...120(C)	2.029	0.03514	0.18266	-0.03916	0.00325	12.3
1(N)...133(Li)	1.955	0.03418	0.22923	-0.04236	0.00747	13.3
3 (R = CH_2SiMe_3)						
54(H)...123(C)	3.825	0.00156	0.00446	0.00028	-0.00057	0.2
137(H)...111(H)	2.803	0.00201	0.00721	0.00043	-0.00094	0.3
46(H)...129(H)	2.758	0.00235	0.00851	0.00049	-0.00116	0.4
43(H)...125(H)	2.892	0.00274	0.01053	0.00067	-0.00130	0.4
54(H)...121(H)	2.815	0.00254	0.01002	0.00062	-0.00127	0.4
124(H)... 98(H)	2.698	0.00308	0.01012	0.00053	-0.00147	0.5
122(H)...133(H)	2.492	0.00389	0.01207	0.00051	-0.00201	0.6
26(C)...129(H)	3.008	0.00443	0.01458	0.00071	-0.00224	0.7
23(C)...125(H)	3.014	0.00516	0.01586	0.00068	-0.00261	0.8
54(H)...128(H)	2.522	0.00472	0.01799	0.00094	-0.00261	0.8
37(H)... 98(H)	2.445	0.00456	0.01548	0.00072	-0.00243	0.8
43(H)...129(H)	2.358	0.00549	0.01817	0.00078	-0.00299	0.9
132(H)...111(H)	2.444	0.00488	0.01779	0.00084	-0.00277	0.9
34(H)... 7(C)	2.887	0.00571	0.01935	0.00090	-0.00305	1.0
132(H)... 90(C)	3.071	0.00597	0.01957	0.00089	-0.00312	1.0
43(H)...136(H)	2.360	0.00585	0.02029	0.00091	-0.00326	1.0
17(C)...101(H)	2.827	0.00671	0.02202	0.00095	-0.00360	1.1
132(H)...104(H)	2.372	0.00598	0.02152	0.00093	-0.00353	1.1

4(N)...121(H)	2.740	0.00727	0.02595	0.00116	-0.00418	1.3
121(H)... 19(C)	2.801	0.00778	0.02786	0.00113	-0.00471	1.5
21(C)... 1(Li)	2.528	0.00893	0.04875	0.00240	-0.00739	2.3
2(Li)... 90(C)	2.375	0.01477	0.08865	0.00346	-0.01524	4.8
1(Li)...123(C)	2.141	0.02680	0.13596	0.00338	-0.02724	8.5
123(C)... 2(Li)	2.046	0.03180	0.17009	0.00376	-0.03500	11.0
1(Li)...4(N)	1.952	0.03473	0.23205	0.00747	-0.04308	13.5
tBu(R = **4**)						
58(H)... 33(H)	2.814	0.00201	0.00730	-0.00095	0.00044	0.3
131(H)... 49(H)	2.848	0.00208	0.00765	-0.00098	0.00047	0.3
31(H)...120(C)	3.456	0.00257	0.00776	-0.00114	0.00040	0.4
73(H)... 97(H)	2.725	0.00245	0.00875	-0.00120	0.00049	0.4
33(H)... 4(C)	3.253	0.00322	0.01267	-0.00161	0.00078	0.5
122(H)...109(H)	2.638	0.00322	0.01078	-0.00160	0.00055	0.5
31(H)...128(H)	2.712	0.00324	0.01239	-0.00167	0.00071	0.5
97(H)... 15(H)	2.611	0.00367	0.01452	-0.00196	0.00084	0.6
31(H)...123(H)	2.564	0.00337	0.01128	-0.00179	0.00052	0.6
109(H)...132(H)	2.677	0.00353	0.01302	-0.00178	0.00074	0.6
127(H)... 39(H)	2.580	0.00352	0.01229	-0.00188	0.00060	0.6
93(H)...123(H)	2.504	0.00469	0.01669	-0.00253	0.00082	0.8
117(H)... 49(H)	2.426	0.00473	0.01604	-0.00254	0.00074	0.8
4(C)... 54(H)	2.892	0.00572	0.01889	-0.00300	0.00086	0.9
87(C)...130(H)	2.826	0.00627	0.01727	-0.00311	0.00061	1.0
130(H)...117(H)	2.330	0.00596	0.01908	-0.00327	0.00075	1.0
127(H)... 22(C)	2.932	0.00673	0.01929	-0.00339	0.00072	1.1
14(C)...113(H)	2.805	0.00704	0.02288	-0.00379	0.00097	1.2
84(C)...124(H)	2.632	0.00990	0.03040	-0.00553	0.00103	1.7
91(H)... 16(C)	2.405	0.01580	0.05903	-0.01172	0.00152	3.7
134(Li)... 20(C)	2.339	0.01587	0.09823	-0.01702	0.00377	5.3
134(Li)... 23(C)	2.331	0.01609	0.09906	-0.01722	0.00377	5.4
133(Li)...120(C)	2.184	0.02524	0.12471	-0.02523	0.00297	7.9
120(C)...134(Li)	2.060	0.03409	0.17475	-0.03774	0.00298	11.8
1(N)...133(Li)	1.963	0.03419	0.22585	-0.04192	0.00727	13.2
6						
130(C) -- 21(C)	3.962	0.00328	0.00883	0.00052	-0.00118	0.4
123(C) -- 23(C)	3.794	0.00345	0.01031	0.00064	-0.0013	0.4
128(C) -- 32(H)	3.127	0.00357	0.01278	0.00072	-0.00175	0.5
124(C) -- 38(H)	2.983	0.00519	0.01706	0.00082	-0.00263	0.8
132(C) -- 40(H)	2.85	0.00484	0.01877	0.0009	-0.0029	0.9
124(C) -- 40(H)	2.958	0.00506	0.01855	0.00094	-0.00275	0.9
88(C) -- 122(H)	2.841	0.00757	0.02373	0.00096	-0.00402	1.3
84(C) -- 131(H)	2.656	0.00864	0.02773	0.0011	-0.00474	1.5
135(H) -- 24(C)	3.328	0.00255	0.00955	0.0006	-0.0012	0.4
104(H) -- 121(C)	3.067	0.00467	0.01713	0.00091	-0.00247	0.8
122(H) -- 50(H)	2.965	0.00175	0.00659	0.00044	-0.00076	0.2
114(H) -- 134(H)	2.852	0.00211	0.0082	0.00053	-0.00099	0.3
135(H) -- 51(H)	2.673	0.00324	0.01203	0.00067	-0.00167	0.5
94(H) -- 131(H)	2.38	0.00503	0.01783	0.00081	-0.00283	0.9
114(H) -- 122(H)	2.228	0.00626	0.02015	0.00081	-0.00341	1.1
1(Li) -- 19(C)	2.377	0.01303	0.07317	0.0032	-0.01189	3.7

2(N) -- 1(Li)	1.915	0.0383	0.25921	0.00781	-0.04919	15.4
130(C) -- 1(Li)	2.384	0.01286	0.07145	0.00324	-0.01137	3.6

Table S3. QTAIM atomic charges (e) for the complexes **2-4** optimized at the r^2-SCAN-3c/Def2-TZVP //CPCM(hexane) level

Atom Molecule	N	C	Li^1	Li^2
Carb-N anion	-1.61		0.92	
Ate-complexes				
2 R=nBu	-1.55	-0.53	0.90	0.89
3 R=tBu	-1.55	-0.40	0.91	0.89
4 R=CH_2SiMe_3	-1.56	-1.45	0.90	0.90
$(R\text{-}Li)_n$				
R=nBu (n=6)		-0.51	0.89	
R=tBu (n=4)		-0.38	0.90	
R= CH_2SiMe_3 (n=6)		-1.44	0.90	

Table S4. Dissociation energy (kcal/mol) of associated $(RLi)_n$ calculated at DLPNO-CCSD(T)/Def2-TZVP//r^2-SCAN-3c/Def2-TZVP CPCM(hexane) level.

R	ΔE_{tot}	ΔH^o_{298}	ΔG^o_{298}
$(RLi)_n$ = n RLi			
nBu (n=6)	30.0	30.3	18.6
tBu (n=4)	29.8	30.1	19.0
CH_2SiMe_3 (n=6)	29.3	29.6	16.9
$(RLi)_n$ = n/2 $(RLi)_2$			
nBu (n=6)	25.5	25.8	14.9
tBu (n=4)	22.6	23.1	14.4
CH_2SiMe_3 (n=6)	22.8	22.9	11.6

Optimized Cartesian coordinates

120
Compound 1

N	3.217281000	1.308293000	10.850450000
C	3.551401000	0.485137000	11.904766000
C	3.588561000	-0.905066000	11.946669000
C	3.957996000	-1.482934000	13.161487000
H	3.993844000	-2.564927000	13.198645000
C	4.289473000	-0.730853000	14.302730000
C	4.251505000	0.662958000	14.218057000
H	4.506529000	1.274011000	15.077811000
C	3.883759000	1.282768000	13.026202000
C	3.745326000	2.657870000	12.604327000
C	3.939591000	3.891134000	13.231481000
H	4.265042000	3.911827000	14.264311000
C	3.715886000	5.071412000	12.527010000
C	3.283562000	4.986128000	11.186693000
H	3.088524000	5.897973000	10.630720000
C	3.071198000	3.781977000	10.525429000
C	3.322018000	2.621252000	11.257570000
C	3.299023000	-1.693962000	10.719821000
C	4.360058000	-2.216607000	9.959935000
C	4.069083000	-2.916509000	8.786338000
H	4.884458000	-3.325404000	8.195492000
C	2.766088000	-3.097008000	8.339558000
C	1.727592000	-2.566580000	9.105980000
H	0.704893000	-2.701509000	8.770872000
C	1.966723000	-1.868921000	10.286434000
C	5.807728000	-2.041169000	10.379871000
H	5.823540000	-1.376494000	11.248019000
C	6.416714000	-3.381172000	10.810425000
H	7.446087000	-3.241789000	11.155470000
H	6.431581000	-4.088713000	9.975006000
H	5.838841000	-3.831892000	11.622516000
C	6.650966000	-1.382067000	9.283125000
H	7.668144000	-1.204127000	9.645616000
H	6.221756000	-0.421801000	8.984449000
H	6.720641000	-2.013953000	8.392501000
C	2.483077000	-3.829296000	7.045280000
H	3.448484000	-4.168342000	6.649611000
C	1.851458000	-2.893151000	6.007341000
H	2.484571000	-2.019134000	5.829893000
H	0.874458000	-2.537615000	6.349942000
H	1.705539000	-3.414661000	5.056262000
C	1.606318000	-5.066212000	7.269844000
H	0.616354000	-4.782260000	7.640147000
H	2.059197000	-5.741715000	8.000924000
H	1.468193000	-5.613476000	6.332261000
C	0.810386000	-1.365778000	11.131924000
H	1.154787000	-0.474906000	11.668277000
C	-0.423329000	-0.968560000	10.319987000
H	-1.145021000	-0.462138000	10.967344000
H	-0.926190000	-1.841862000	9.893105000
H	-0.164157000	-0.289225000	9.502830000
C	0.442211000	-2.419702000	12.187069000
H	-0.366729000	-2.056158000	12.828730000
H	1.301593000	-2.659892000	12.818458000
H	0.107418000	-3.341076000	11.698785000
C	4.692177000	-1.394041000	15.624198000

C	4.688561000	-2.923736000	15.537407000
H	4.982280000	-3.341055000	16.504933000
H	5.397625000	-3.287544000	14.787470000
H	3.695413000	-3.312665000	15.293149000
C	3.704184000	-0.975037000	16.727856000
H	3.979528000	-1.442419000	17.679205000
H	2.686980000	-1.286967000	16.471965000
H	3.699770000	0.108337000	16.871950000
C	6.111214000	-0.941710000	16.013305000
H	6.411721000	-1.410040000	16.956483000
H	6.166899000	0.142153000	16.141679000
H	6.831549000	-1.228708000	15.241052000
C	3.911475000	6.456089000	13.149517000
C	2.576352000	7.222800000	13.124332000
H	1.813038000	6.684088000	13.694134000
H	2.206973000	7.355745000	12.104225000
H	2.702349000	8.215403000	13.569463000
C	4.388607000	6.377087000	14.602824000
H	3.664140000	5.858178000	15.237708000
H	4.514851000	7.389198000	14.997994000
H	5.351422000	5.863614000	14.683503000
C	4.963134000	7.237978000	12.341413000
H	5.114240000	8.230275000	12.779188000
H	4.654534000	7.371808000	11.301480000
H	5.921461000	6.709746000	12.345281000
C	2.557967000	3.677105000	9.133449000
C	3.438467000	3.349332000	8.080914000
C	2.922141000	3.168518000	6.800539000
H	3.597512000	2.917621000	5.989734000
C	1.559350000	3.294496000	6.532273000
C	0.710905000	3.627939000	7.581812000
H	-0.352061000	3.723013000	7.380217000
C	1.181596000	3.824035000	8.881966000
C	4.933266000	3.260669000	8.330126000
H	5.077206000	2.929065000	9.364132000
C	5.653527000	2.263776000	7.420914000
H	6.683383000	2.127197000	7.763026000
H	5.699640000	2.617593000	6.386326000
H	5.158683000	1.287988000	7.424800000
C	5.564000000	4.655594000	8.205476000
H	6.637126000	4.613835000	8.417344000
H	5.102343000	5.359071000	8.903372000
H	5.427816000	5.041765000	7.189709000
C	1.013989000	3.053854000	5.140667000
H	-0.066477000	3.239386000	5.182036000
C	1.618367000	4.020160000	4.116044000
H	1.163824000	3.869101000	3.132102000
H	2.696138000	3.859020000	4.015094000
H	1.458824000	5.060045000	4.414427000
C	1.225536000	1.597303000	4.708872000
H	0.776289000	1.417198000	3.727244000
H	0.776740000	0.905128000	5.427056000
H	2.292938000	1.364884000	4.638842000
C	0.200915000	4.110048000	10.004775000
H	0.768502000	4.525824000	10.841750000
C	-0.872361000	5.133013000	9.624463000
H	-1.465604000	5.393371000	10.506026000
H	-1.562309000	4.740562000	8.871613000
H	-0.423990000	6.049300000	9.229665000
C	-0.438666000	2.801271000	10.488442000
H	-1.117939000	2.989173000	11.326184000
H	0.323895000	2.089516000	10.818227000

H	-1.011248000	2.333827000	9.680355000
H	2.935485000	1.001040000	9.934283000

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Lithium carbozolide

Li	2.634306000	0.635421000	9.166648000
N	3.202743000	1.240661000	10.877518000
C	3.526332000	0.481744000	11.972596000
C	3.553003000	-0.917681000	12.031465000
C	3.859843000	-1.511358000	13.252884000
H	3.869497000	-2.594349000	13.297329000
C	4.178996000	-0.760116000	14.402714000
C	4.209779000	0.635017000	14.306394000
H	4.481001000	1.234281000	15.170869000
C	3.888263000	1.267318000	13.106385000
C	3.811633000	2.632390000	12.646406000
C	4.056355000	3.889462000	13.208103000
H	4.396059000	3.954281000	14.235471000
C	3.867039000	5.044311000	12.449583000
C	3.386376000	4.916605000	11.125270000
H	3.195053000	5.812033000	10.540821000
C	3.112735000	3.688667000	10.540546000
C	3.369352000	2.534668000	11.298107000
C	3.369551000	-1.622023000	10.735185000
C	4.494420000	-2.131142000	10.051262000
C	4.344001000	-2.578482000	8.739489000
H	5.209387000	-2.966989000	8.210546000
C	3.128812000	-2.517444000	8.061705000
C	2.018447000	-2.035046000	8.757457000
H	1.050275000	-2.023070000	8.270839000
C	2.113574000	-1.608862000	10.089135000
C	5.874430000	-2.103072000	10.682514000
H	5.740222000	-2.097242000	11.766353000
C	6.736843000	-3.315879000	10.328238000
H	7.650875000	-3.303960000	10.928921000
H	7.041288000	-3.311425000	9.277138000
H	6.209280000	-4.253244000	10.527415000
C	6.587085000	-0.796802000	10.303367000
H	7.554295000	-0.726436000	10.810786000
H	5.986399000	0.074255000	10.581419000
H	6.762884000	-0.762432000	9.222736000
C	3.077448000	-2.947398000	6.608330000
H	3.649966000	-3.882169000	6.538215000
C	3.790024000	-1.906305000	5.730810000
H	4.827625000	-1.764361000	6.043876000
H	3.283255000	-0.938466000	5.806678000
H	3.784886000	-2.214286000	4.680705000
C	1.670456000	-3.219797000	6.082784000
H	1.074447000	-2.302555000	6.043208000
H	1.140629000	-3.945088000	6.706868000
H	1.723390000	-3.619147000	5.066364000
C	0.865959000	-1.207129000	10.858977000
H	1.171825000	-0.488877000	11.625172000
C	-0.217075000	-0.546360000	10.004895000
H	-1.022545000	-0.184005000	10.648967000
H	-0.659750000	-1.243733000	9.287010000
H	0.157973000	0.321208000	9.446241000
C	0.302504000	-2.441681000	11.578794000
H	-0.571420000	-2.170466000	12.178943000
H	1.054176000	-2.879238000	12.241046000
H	0.000001000	-3.203177000	10.852023000
C	4.511245000	-1.427712000	15.742446000

C	4.435395000	-2.956553000	15.672388000
H	4.672082000	-3.376720000	16.654567000
H	5.152534000	-3.364606000	14.953413000
H	3.433895000	-3.298706000	15.394305000
C	3.514993000	-0.951760000	16.815430000
H	3.741695000	-1.418837000	17.780197000
H	2.491685000	-1.219374000	16.534479000
H	3.556014000	0.132514000	16.945933000
C	5.938667000	-1.042833000	16.172018000
H	6.188115000	-1.513457000	17.129389000
H	6.044094000	0.038548000	16.289204000
H	6.666622000	-1.374044000	15.424825000
C	4.129602000	6.448848000	13.000625000
C	2.823326000	7.264590000	12.979854000
H	2.059004000	6.778909000	13.594467000
H	2.427956000	7.365524000	11.965600000
H	2.996137000	8.271262000	13.375931000
C	4.647489000	6.421527000	14.442050000
H	3.923021000	5.963970000	15.122350000
H	4.826533000	7.445581000	14.783377000
H	5.590167000	5.871648000	14.520241000
C	5.182844000	7.157446000	12.129473000
H	5.377438000	8.165285000	12.512303000
H	4.850937000	7.248747000	11.092044000
H	6.123712000	6.598609000	12.135427000
C	2.446076000	3.466256000	9.230574000
C	3.151654000	2.851124000	8.168461000
C	2.447806000	2.408327000	7.044596000
H	2.991303000	1.938111000	6.230879000
C	1.066783000	2.596132000	6.921500000
C	0.402502000	3.244578000	7.955085000
H	-0.668977000	3.395414000	7.865217000
C	1.057888000	3.674357000	9.112482000
C	4.666417000	2.741722000	8.222895000
H	4.953164000	2.696315000	9.277359000
C	5.231666000	1.499982000	7.531599000
H	6.308491000	1.438323000	7.709465000
H	5.079015000	1.523612000	6.448253000
H	4.792239000	0.569555000	7.914336000
C	5.282414000	4.017413000	7.629313000
H	6.373857000	3.985253000	7.700550000
H	4.927669000	4.902700000	8.163851000
H	5.007477000	4.120383000	6.574143000
C	0.309886000	2.112141000	5.703589000
H	-0.731436000	2.433186000	5.827451000
C	0.845159000	2.737084000	4.410709000
H	0.236740000	2.426528000	3.556050000
H	1.875326000	2.420915000	4.219656000
H	0.830765000	3.828919000	4.466201000
C	0.324381000	0.582216000	5.616109000
H	-0.283484000	0.234737000	4.775029000
H	-0.065429000	0.130753000	6.533922000
H	1.344502000	0.216840000	5.465083000
C	0.249808000	4.258630000	10.256597000
H	0.934580000	4.835182000	10.882129000
C	-0.865010000	5.201391000	9.799146000
H	-1.308754000	5.694135000	10.669044000
H	-1.669864000	4.668483000	9.283736000
H	-0.482492000	5.974716000	9.126553000
C	-0.313933000	3.122981000	11.122615000
H	-0.837954000	3.529108000	11.993444000
H	0.485539000	2.464817000	11.475707000

H	-1.024147000	2.522320000	10.544220000

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Compound 2

N	7.372717000	3.716672000	2.391447000
C	6.556989000	3.298954000	1.362838000
C	5.154641000	3.263010000	1.298038000
C	4.548838000	2.790414000	0.131981000
H	3.464742000	2.768735000	0.117850000
C	5.269747000	2.344444000	-0.988658000
C	6.662913000	2.372090000	-0.917232000
H	7.263001000	2.028963000	-1.755418000
C	7.301077000	2.837210000	0.228108000
C	8.679338000	2.983525000	0.595176000
C	9.889656000	2.733592000	-0.056960000
H	9.874578000	2.322450000	-1.060074000
C	11.094055000	3.019278000	0.578749000
C	11.046108000	3.567990000	1.879542000
H	11.974892000	3.818315000	2.383743000
C	9.862003000	3.823353000	2.559568000
C	8.653198000	3.521878000	1.910513000
C	4.288324000	3.642034000	2.443889000
C	3.644136000	4.900842000	2.485064000
C	2.795930000	5.200105000	3.561102000
H	2.309615000	6.166650000	3.590891000
C	2.560816000	4.288340000	4.595292000
C	3.209975000	3.050586000	4.536193000
H	3.034696000	2.333475000	5.333457000
C	4.058874000	2.704887000	3.478147000
C	3.908051000	5.931017000	1.402128000
H	4.077529000	5.373856000	0.475855000
C	2.744198000	6.893897000	1.168829000
H	2.941170000	7.490975000	0.274556000
H	2.617736000	7.592851000	2.001732000
H	1.801059000	6.359571000	1.021120000
C	5.198790000	6.703224000	1.715164000
H	6.048875000	6.023575000	1.820242000
H	5.088797000	7.267127000	2.648445000
H	5.421057000	7.412252000	0.911958000
C	1.599006000	4.570110000	5.731738000
H	2.021876000	4.096352000	6.627317000
C	0.251994000	3.892750000	5.435196000
H	-0.441206000	4.041296000	6.268188000
H	0.373740000	2.818574000	5.273274000
H	-0.196081000	4.323814000	4.534070000
C	1.398256000	6.054772000	6.029120000
H	0.799421000	6.171452000	6.936026000
H	0.861219000	6.555527000	5.217606000
H	2.350476000	6.571311000	6.180766000
C	4.655327000	1.312459000	3.416124000
H	5.369155000	1.302589000	2.589137000
C	5.414882000	0.929718000	4.686576000
H	6.222426000	1.640241000	4.881722000
H	5.860540000	-0.062146000	4.568512000
H	4.762022000	0.898286000	5.564917000
C	3.550964000	0.296947000	3.094211000
H	3.040567000	0.558084000	2.162702000
H	2.804737000	0.261738000	3.894981000
H	3.979266000	-0.703351000	2.983128000
C	4.580806000	1.829487000	-2.255970000
C	3.052800000	1.880401000	-2.155674000
H	2.680386000	1.255366000	-1.338191000

H	2.615505000	1.507407000	-3.086701000
H	2.692253000	2.902263000	-2.002366000
C	4.994313000	0.368317000	-2.508179000
H	6.075849000	0.275778000	-2.634784000
H	4.512331000	-0.013029000	-3.415061000
H	4.696890000	-0.265340000	-1.666847000
C	5.008064000	2.690421000	-3.458694000
H	4.525711000	2.331082000	-4.374318000
H	6.089775000	2.656692000	-3.610461000
H	4.721051000	3.735205000	-3.304533000
C	12.458641000	2.775872000	-0.070019000
C	12.333684000	2.177662000	-1.474675000
H	11.789922000	2.845426000	-2.149604000
H	11.819728000	1.211896000	-1.455970000
H	13.332197000	2.018645000	-1.892876000
C	13.222205000	4.108102000	-0.183965000
H	12.660230000	4.821535000	-0.794593000
H	14.199610000	3.947476000	-0.651970000
H	13.389112000	4.560662000	0.796967000
C	13.274513000	1.798084000	0.795292000
H	13.441110000	2.194629000	1.800306000
H	14.253058000	1.611948000	0.339366000
H	12.750919000	0.841891000	0.891436000
C	9.874923000	4.457940000	3.907513000
C	9.880032000	3.666352000	5.079523000
C	9.982993000	4.294236000	6.320309000
H	9.999529000	3.684929000	7.218079000
C	10.078759000	5.680809000	6.440684000
C	10.027710000	6.444944000	5.280441000
H	10.077285000	7.526704000	5.366303000
C	9.910412000	5.864100000	4.014942000
C	9.841155000	2.152069000	4.982876000
H	9.334772000	1.902441000	4.043392000
C	9.072381000	1.488949000	6.128403000
H	8.916078000	0.429730000	5.904848000
H	8.095434000	1.955481000	6.282238000
H	9.624912000	1.543955000	7.071636000
C	11.267550000	1.588407000	4.907647000
H	11.807342000	1.992807000	4.048613000
H	11.243447000	0.497855000	4.816238000
H	11.822733000	1.844818000	5.816403000
C	10.222281000	6.340150000	7.795867000
H	10.266122000	7.422292000	7.622496000
C	9.014760000	6.057137000	8.696710000
H	9.111077000	6.596314000	9.644232000
H	8.940544000	4.989159000	8.925169000
H	8.082666000	6.365403000	8.214971000
C	11.526293000	5.919381000	8.483647000
H	11.646776000	6.449399000	9.433400000
H	12.392531000	6.138152000	7.853020000
H	11.525171000	4.845528000	8.695441000
C	9.861676000	6.745875000	2.780901000
H	9.563901000	6.112316000	1.939637000
C	8.827717000	7.869631000	2.908148000
H	7.841896000	7.474406000	3.172469000
H	8.736311000	8.402533000	1.956952000
H	9.113306000	8.600013000	3.671138000
C	11.252116000	7.311851000	2.467811000
H	11.223243000	7.918838000	1.557609000
H	11.977226000	6.506630000	2.321332000
H	11.605265000	7.943904000	3.289529000
C	6.306200000	5.682853000	5.555577000

H	7.361052000	5.790799000	5.858117000
H	6.023396000	6.704498000	5.242279000
C	5.514709000	5.325231000	6.828274000
H	5.619762000	6.076508000	7.630827000
H	4.424911000	5.307779000	6.630602000
C	5.901030000	3.964050000	7.403133000
H	6.983503000	3.957750000	7.586019000
H	5.724980000	3.190630000	6.642235000
C	5.153954000	3.605804000	8.683342000
H	5.441842000	2.619207000	9.058640000
H	4.071071000	3.596628000	8.513639000
H	5.356878000	4.337234000	9.472521000
Li	7.448711000	4.645869000	4.109623000
Li	4.874343000	4.702793000	4.503739000

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Compound 3

Li	2.508953000	0.016279000	9.266126000
Li	1.702594000	1.936628000	7.503846000
Si	0.328106000	-0.351167000	6.271930000
N	3.094767000	1.166134000	10.730079000
C	3.475727000	0.437176000	11.841662000
C	3.536469000	-0.955289000	11.968519000
C	3.940274000	-1.488774000	13.192068000
H	3.969463000	-2.569147000	13.272665000
C	4.291542000	-0.695129000	14.299820000
C	4.223664000	0.692224000	14.160558000
H	4.481716000	1.340992000	14.992878000
C	3.822091000	1.257097000	12.953043000
C	3.639572000	2.602861000	12.490434000
C	3.806633000	3.844886000	13.090938000
H	4.140822000	3.893810000	14.123515000
C	3.550603000	5.015417000	12.374643000
C	3.132354000	4.883899000	11.041554000
H	2.940235000	5.772330000	10.449974000
C	2.957718000	3.652723000	10.401870000
C	3.202516000	2.478750000	11.131339000
C	3.144146000	-1.850926000	10.846857000
C	4.108545000	-2.291777000	9.912155000
C	3.739625000	-3.239947000	8.961518000
H	4.485989000	-3.613155000	8.265796000
C	2.445148000	-3.757346000	8.888258000
C	1.492742000	-3.261378000	9.772501000
H	0.476510000	-3.637651000	9.732871000
C	1.817168000	-2.313654000	10.749515000
C	5.542029000	-1.801655000	9.993565000
H	5.527040000	-0.854644000	10.544087000
C	6.400616000	-2.792166000	10.791591000
H	7.429031000	-2.426951000	10.876164000
H	6.422303000	-3.765793000	10.290353000
H	6.001809000	-2.933996000	11.799062000
C	6.162008000	-1.539236000	8.618943000
H	7.125710000	-1.034687000	8.734379000
H	5.515244000	-0.906142000	8.004856000
H	6.343749000	-2.469119000	8.071458000
C	2.141676000	-4.821879000	7.850721000
H	2.996788000	-5.511530000	7.860630000
C	2.063262000	-4.204547000	6.447928000
H	2.960677000	-3.626339000	6.212019000
H	1.203809000	-3.531762000	6.384065000
H	1.942905000	-4.983849000	5.688803000

C	0.882215000	-5.634446000	8.142268000
H	-0.018443000	-5.018924000	8.048003000
H	0.900694000	-6.061858000	9.148883000
H	0.793396000	-6.453909000	7.423747000
C	0.758073000	-1.856295000	11.736011000
H	1.193514000	-1.046921000	12.329452000
C	-0.487124000	-1.302986000	11.038274000
H	-1.192324000	-0.914127000	11.779220000
H	-1.002686000	-2.073220000	10.456773000
H	-0.227048000	-0.485941000	10.357357000
C	0.391947000	-2.992184000	12.698805000
H	-0.335463000	-2.646624000	13.439836000
H	1.277741000	-3.354059000	13.228543000
H	-0.048267000	-3.835725000	12.156796000
C	4.738485000	-1.304245000	15.632674000
C	4.743126000	-2.836105000	15.605116000
H	5.069485000	-3.215733000	16.578044000
H	5.430246000	-3.224508000	14.847076000
H	3.745342000	-3.239324000	15.406362000
C	3.784774000	-0.851132000	16.752726000
H	4.094697000	-1.278238000	17.712778000
H	2.762408000	-1.180537000	16.542736000
H	3.774449000	0.236988000	16.854243000
C	6.165807000	-0.829192000	15.960221000
H	6.500450000	-1.254694000	16.912699000
H	6.215784000	0.259760000	16.039298000
H	6.863593000	-1.143370000	15.177788000
C	3.741052000	6.378677000	13.045970000
C	2.817757000	6.479256000	14.273609000
H	3.035637000	5.694905000	15.002793000
H	1.769443000	6.380899000	13.975067000
H	2.946382000	7.448005000	14.768684000
C	5.204316000	6.527262000	13.500318000
H	5.483126000	5.745386000	14.211163000
H	5.355936000	7.497309000	13.986169000
H	5.881439000	6.461108000	12.643032000
C	3.413909000	7.545271000	12.108335000
H	3.563067000	8.490317000	12.639054000
H	2.373434000	7.512328000	11.770292000
H	4.063813000	7.550377000	11.227828000
C	2.566410000	3.672281000	8.968440000
C	3.543478000	3.450040000	7.971758000
C	3.195874000	3.603911000	6.623870000
H	3.953289000	3.437667000	5.867535000
C	1.912313000	3.986646000	6.230754000
C	0.948928000	4.172236000	7.228881000
H	-0.056518000	4.443122000	6.926753000
C	1.243676000	4.015400000	8.588620000
C	4.974316000	3.121831000	8.350675000
H	4.943885000	2.617719000	9.320204000
C	5.669121000	2.188849000	7.357704000
H	6.617322000	1.845643000	7.779917000
H	5.898203000	2.691514000	6.412635000
H	5.055968000	1.309748000	7.139010000
C	5.771284000	4.424165000	8.518753000
H	6.797295000	4.201091000	8.826127000
H	5.317827000	5.068570000	9.275854000
H	5.808350000	4.973119000	7.571491000
C	1.569621000	4.258831000	4.781596000
H	0.479749000	4.175848000	4.688607000
C	1.959834000	5.702158000	4.429542000
H	1.675173000	5.934293000	3.399154000

H	3.042176000	5.835944000	4.524996000
H	1.469061000	6.417698000	5.094718000
C	2.210234000	3.272058000	3.803327000
H	1.815918000	3.436515000	2.796990000
H	2.007838000	2.234035000	4.083711000
H	3.294944000	3.404618000	3.753963000
C	0.158464000	4.152634000	9.643336000
H	0.609930000	4.669837000	10.495496000
C	-1.056047000	4.959195000	9.189203000
H	-1.720696000	5.124750000	10.041037000
H	-1.634581000	4.428901000	8.425498000
H	-0.768693000	5.935352000	8.787617000
C	-0.272432000	2.760420000	10.133681000
H	-1.010596000	2.851476000	10.936005000
H	0.578554000	2.190068000	10.515182000
H	-0.734646000	2.193276000	9.316725000
C	1.897898000	-0.079525000	7.216702000
H	2.689413000	0.231511000	6.505921000
H	2.215017000	-1.090113000	7.527896000
C	-0.864619000	-1.436879000	7.245562000
H	-1.713792000	-1.738944000	6.623141000
H	-1.260203000	-0.893811000	8.109541000
H	-0.381492000	-2.342567000	7.623792000
C	-0.610543000	1.271171000	5.962614000
H	-1.542331000	1.048443000	5.430205000
H	-0.053063000	1.976249000	5.337351000
H	-0.890212000	1.785326000	6.889993000
C	0.565874000	-1.084516000	4.544804000
H	-0.392368000	-1.233702000	4.033949000
H	1.085590000	-2.046543000	4.575743000
H	1.169429000	-0.408847000	3.927651000

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Compound 4

N	6.038811000	5.792614000	14.070615000
C	6.637177000	6.228987000	15.235408000
C	6.454180000	7.428172000	15.949656000
C	7.185621000	7.627636000	17.118436000
H	7.018977000	8.560412000	17.649996000
C	8.113274000	6.701464000	17.633219000
C	8.303935000	5.523175000	16.921433000
H	9.008267000	4.772729000	17.262522000
C	7.586077000	5.290513000	15.747680000
C	7.579382000	4.201871000	14.822008000
C	8.286919000	2.999015000	14.764321000
H	8.998633000	2.767947000	15.548922000
C	8.074688000	2.121763000	13.707674000
C	7.137949000	2.496282000	12.722993000
H	6.958425000	1.830857000	11.883318000
C	6.413851000	3.684328000	12.748438000
C	6.628423000	4.563275000	13.825702000
C	5.525230000	8.518539000	15.557389000
C	4.251353000	8.608685000	16.164171000
C	3.459431000	9.735710000	15.918142000
H	2.479916000	9.808462000	16.382629000
C	3.881280000	10.774672000	15.081969000
C	5.122678000	10.643524000	14.452770000
H	5.460254000	11.420248000	13.777643000
C	5.952494000	9.534491000	14.674930000
C	3.734574000	7.508879000	17.070185000
H	4.476202000	6.705757000	17.055842000

C	2.409114000	6.932524000	16.561591000
H	1.608518000	7.678892000	16.579323000
H	2.098709000	6.095011000	17.192683000
H	2.510567000	6.564211000	15.535580000
C	3.609150000	8.008213000	18.513772000
H	4.567701000	8.383878000	18.882180000
H	3.285672000	7.193801000	19.168232000
H	2.873563000	8.815845000	18.588937000
C	2.998551000	11.993287000	14.909000000
H	1.961097000	11.633988000	14.915181000
C	3.229600000	12.753712000	13.604674000
H	3.166984000	12.094992000	12.733397000
H	4.208433000	13.242991000	13.594943000
H	2.473953000	13.535665000	13.494650000
C	3.178851000	12.925385000	16.117154000
H	2.509760000	13.786973000	16.037752000
H	4.209222000	13.292989000	16.159277000
H	2.965117000	12.406454000	17.055197000
C	7.309215000	9.453820000	14.005114000
H	7.615234000	8.403475000	14.030546000
C	7.281676000	9.904638000	12.543039000
H	6.492513000	9.394255000	11.982925000
H	8.238402000	9.672195000	12.067804000
H	7.124929000	10.983769000	12.449877000
C	8.335828000	10.265043000	14.807546000
H	9.324282000	10.185974000	14.345584000
H	8.406619000	9.901320000	15.835589000
H	8.052497000	11.322837000	14.832561000
C	8.859629000	7.033874000	18.926439000
C	7.848017000	7.246052000	20.067574000
H	7.165036000	8.071350000	19.849437000
H	8.370931000	7.479021000	21.001500000
H	7.249501000	6.343134000	20.222992000
C	9.680337000	8.322107000	18.732919000
H	9.039631000	9.172117000	18.483117000
H	10.406751000	8.196593000	17.924057000
H	10.224868000	8.568448000	19.650984000
C	9.819215000	5.914697000	19.342083000
H	10.326187000	6.195250000	20.270185000
H	10.585396000	5.738763000	18.581179000
H	9.287547000	4.975225000	19.520276000
C	8.808537000	0.786973000	13.565599000
C	7.786428000	-0.364296000	13.545447000
H	7.203254000	-0.376062000	14.471478000
H	8.299678000	-1.327187000	13.447939000
H	7.089452000	-0.267543000	12.708941000
C	9.609424000	0.775554000	12.250794000
H	10.142466000	-0.174831000	12.137911000
H	10.344377000	1.586428000	12.242108000
H	8.957190000	0.901573000	11.382584000
C	9.783733000	0.537939000	14.720261000
H	9.266380000	0.508087000	15.683926000
H	10.557166000	1.310433000	14.767338000
H	10.280981000	-0.425986000	14.575889000
C	5.459120000	3.960763000	11.642174000
C	4.262614000	3.222773000	11.542551000
C	3.458956000	3.384200000	10.411661000
H	2.541358000	2.807909000	10.325726000
C	3.789776000	4.265375000	9.389183000
C	4.962384000	5.010609000	9.517859000
H	5.239971000	5.695531000	8.723384000
C	5.810029000	4.869269000	10.615552000

C	3.832707000	2.247210000	12.623158000
H	4.588405000	2.275771000	13.412519000
C	2.492904000	2.649505000	13.250260000
H	2.555437000	3.642904000	13.702605000
H	2.213279000	1.935958000	14.031592000
H	1.690131000	2.666999000	12.506191000
C	3.775381000	0.812362000	12.086146000
H	4.733406000	0.518110000	11.648578000
H	3.006387000	0.709819000	11.313736000
H	3.537322000	0.112907000	12.893483000
C	2.912600000	4.395058000	8.161992000
H	2.062782000	3.715662000	8.302158000
C	3.660647000	3.957266000	6.896935000
H	4.044968000	2.938578000	6.999206000
H	4.508802000	4.619926000	6.698314000
H	2.996801000	3.991532000	6.027557000
C	2.359247000	5.814862000	8.003849000
H	1.693492000	5.871433000	7.136964000
H	3.168789000	6.536326000	7.854371000
H	1.799758000	6.121049000	8.891638000
C	7.163575000	5.561322000	10.635198000
H	7.457297000	5.684154000	11.682364000
C	8.207124000	4.655756000	9.962363000
H	8.261506000	3.683308000	10.457531000
H	9.198231000	5.118764000	10.002958000
H	7.944909000	4.494729000	8.911087000
C	7.169682000	6.944304000	9.983253000
H	6.390666000	7.590829000	10.395874000
H	7.023627000	6.886901000	8.900107000
H	8.136048000	7.427051000	10.154773000
C	2.981737000	7.713129000	12.323229000
C	2.313551000	6.346458000	12.181826000
H	1.459824000	6.374837000	11.473741000
H	1.917410000	5.978169000	13.136554000
H	2.974874000	5.564115000	11.777425000
C	1.894929000	8.672348000	12.836870000
H	1.028599000	8.702302000	12.147568000
H	2.235240000	9.719990000	12.906842000
H	1.500609000	8.387089000	13.822715000
C	3.384448000	8.203842000	10.931224000
H	4.082074000	7.519507000	10.433966000
H	3.864589000	9.191708000	10.959781000
H	2.506382000	8.293827000	10.257352000
Li	4.597054000	6.344493000	12.857924000
Li	3.904737000	8.751332000	13.844145000

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Compound 6

Li	0.153792000	-0.063055000	0.234003000
N	1.398535000	-1.415102000	-0.303322000
C	2.351755000	-0.867302000	-1.138805000
C	2.452422000	0.468892000	-1.543273000
C	3.493386000	0.826629000	-2.397005000
H	3.556141000	1.866079000	-2.697193000
C	4.441715000	-0.101366000	-2.871078000
C	4.325131000	-1.432894000	-2.465099000
H	5.037080000	-2.175222000	-2.815022000
C	3.295991000	-1.822491000	-1.609558000
C	2.888406000	-3.064419000	-1.017236000
C	3.388888000	-4.365874000	-1.096018000
H	4.266149000	-4.556804000	-1.703977000
C	2.759200000	-5.393738000	-0.403108000

C	1.624716000	-5.068309000	0.369305000
H	1.117163000	-5.856397000	0.918166000
C	1.099395000	-3.784895000	0.480616000
C	1.734364000	-2.752487000	-0.234442000
C	1.450067000	1.454338000	-1.057688000
C	0.235592000	1.635518000	-1.762342000
C	-0.674113000	2.586924000	-1.303512000
H	-1.599819000	2.741735000	-1.850642000
C	-0.424467000	3.375783000	-0.178500000
C	0.748756000	3.143941000	0.533087000
H	0.958351000	3.727586000	1.422362000
C	1.684972000	2.187509000	0.123682000
C	-0.037428000	0.865849000	-3.041840000
H	0.640164000	0.006434000	-3.053719000
C	-1.469046000	0.333835000	-3.134138000
H	-1.573683000	-0.299060000	-4.019992000
H	-2.202607000	1.141680000	-3.217324000
H	-1.725605000	-0.267770000	-2.257163000
C	0.300080000	1.741722000	-4.256007000
H	1.340097000	2.077033000	-4.218234000
H	-0.344458000	2.627028000	-4.280292000
H	0.151215000	1.182485000	-5.184759000
C	-1.404231000	4.477551000	0.175524000
H	-2.409075000	4.039030000	0.114217000
C	-1.222829000	5.056087000	1.575691000
H	-1.234157000	4.277134000	2.341604000
H	-2.029298000	5.761663000	1.793927000
H	-0.277758000	5.602874000	1.658720000
C	-1.319572000	5.600271000	-0.871145000
H	-1.502747000	5.222769000	-1.880131000
H	-0.323403000	6.054657000	-0.855613000
H	-2.055786000	6.380861000	-0.656136000
C	2.965086000	1.996211000	0.914727000
H	3.441706000	1.084008000	0.543103000
C	2.710532000	1.811894000	2.413180000
H	2.010113000	0.990878000	2.596804000
H	2.302870000	2.718121000	2.872177000
H	3.647293000	1.574938000	2.926022000
C	3.927526000	3.163100000	0.660150000
H	4.150292000	3.259052000	-0.406149000
H	4.868575000	3.007331000	1.196449000
H	3.490095000	4.106705000	1.003418000
C	5.580095000	0.305969000	-3.812905000
C	5.557475000	1.800822000	-4.148793000
H	5.667369000	2.417808000	-3.251578000
H	4.630049000	2.087360000	-4.654227000
H	6.389810000	2.034350000	-4.819553000
C	6.934089000	-0.012607000	-3.153216000
H	7.042422000	0.539260000	-2.214243000
H	7.757425000	0.271540000	-3.817754000
H	7.030079000	-1.078477000	-2.931618000
C	5.462808000	-0.479815000	-5.131622000
H	4.507865000	-0.265803000	-5.621776000
H	5.520772000	-1.557754000	-4.960952000
H	6.272121000	-0.200010000	-5.814996000
C	3.239067000	-6.846142000	-0.441053000
C	2.121856000	-7.744234000	-1.003328000
H	1.221231000	-7.697919000	-0.385523000
H	2.454212000	-8.787518000	-1.039029000
H	1.852849000	-7.432681000	-2.017464000
C	4.480460000	-7.022746000	-1.320895000
H	5.322077000	-6.428372000	-0.952575000

H	4.282566000	-6.735437000	-2.357975000
H	4.783827000	-8.074040000	-1.315701000
C	3.591937000	-7.311238000	0.983668000
H	4.384640000	-6.685968000	1.406227000
H	3.941646000	-8.349338000	0.969056000
H	2.726692000	-7.256303000	1.649583000
C	-0.106625000	-3.562987000	1.324265000
C	-1.381265000	-3.890843000	0.828950000
C	-2.492101000	-3.753733000	1.666396000
H	-3.478824000	-4.009801000	1.288754000
C	-2.378105000	-3.289794000	2.971111000
C	-1.105801000	-2.967192000	3.444848000
H	-1.000321000	-2.605278000	4.462609000
C	0.030940000	-3.096078000	2.650309000
C	-1.572886000	-4.409390000	-0.584999000
H	-0.609663000	-4.328987000	-1.096982000
C	-2.590052000	-3.582630000	-1.379344000
H	-2.290449000	-2.531712000	-1.430259000
H	-3.588513000	-3.631885000	-0.933811000
H	-2.663461000	-3.959851000	-2.404058000
C	-1.971295000	-5.890337000	-0.571250000
H	-1.227888000	-6.489896000	-0.038637000
H	-2.056385000	-6.275310000	-1.592425000
H	-2.936921000	-6.028793000	-0.073572000
C	-3.604176000	-3.115730000	3.842600000
H	-4.458260000	-3.509175000	3.277277000
C	-3.873456000	-1.632428000	4.126984000
H	-3.992449000	-1.067195000	3.198224000
H	-3.040435000	-1.189231000	4.683077000
H	-4.781967000	-1.513911000	4.726182000
C	-3.499405000	-3.910069000	5.148779000
H	-4.426634000	-3.824921000	5.723866000
H	-2.683867000	-3.532509000	5.773351000
H	-3.311201000	-4.969140000	4.951442000
C	1.411052000	-2.822277000	3.223753000
H	2.050088000	-2.504650000	2.392418000
C	1.444824000	-1.724802000	4.289493000
H	0.966160000	-0.802710000	3.947834000
H	2.482792000	-1.489322000	4.541971000
H	0.949403000	-2.040152000	5.213176000
C	2.003246000	-4.117359000	3.801519000
H	2.057822000	-4.899624000	3.041536000
H	1.380047000	-4.479639000	4.626417000
H	3.012904000	-3.939621000	4.185824000
C	-1.449373000	0.180578000	2.040349000
H	-0.605038000	-0.354090000	2.471058000
C	-1.908503000	1.346795000	2.663087000
C	-3.047967000	1.958906000	2.144046000
H	-3.433376000	2.855011000	2.621081000
C	-3.701762000	1.438221000	1.028097000
H	-4.586155000	1.935915000	0.644260000
C	-3.232662000	0.284262000	0.414369000
H	-3.746607000	-0.132587000	-0.444614000
C	-2.106646000	-0.352279000	0.934440000
H	-1.770492000	-1.297605000	0.512910000
C	-1.197098000	1.888010000	3.867730000
H	-1.766462000	2.689719000	4.341797000
H	-1.027720000	1.098426000	4.606154000
H	-0.213879000	2.284018000	3.590350000