Pseudophedrine-Derived Myers Enolates: Structures and Influence of Lithium Chloride on Reactivity and Mechanism

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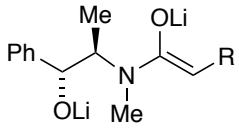
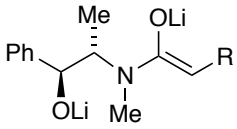
Chart 1. Substrates And Aggregates

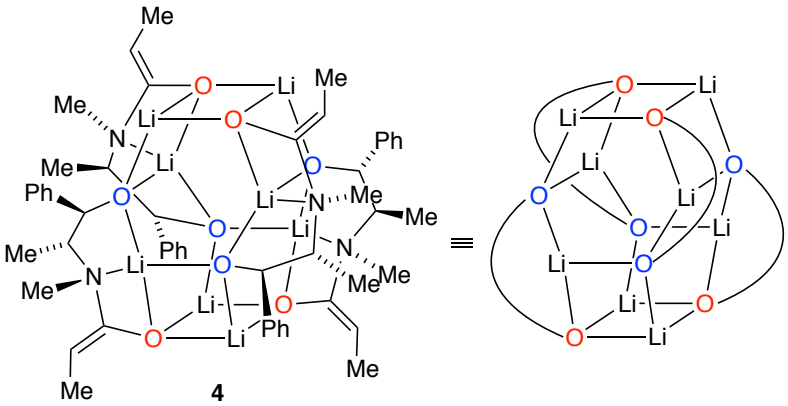


(*R,R*)



(*S,S*)

2; R = CH_3
7; R = H
8; R = *n*-Bu
9; R = *i*-Pr
10; R = *t*-Bu
11; R = $CH_2C_6H_5$
12; R = CH_2-*m*-C_6H_4F
13; R = C_6H_5
14; R = *o*-C_6H_4F
15; R = *m*-C_6H_4F
16; R = *p*-C_6H_4F
17; R = *m*-$C_6H_4CF_3$
18; R = 1-naphthalene
19; R = F
20; R = Cl
21; R = OMe
22; R = NH_2



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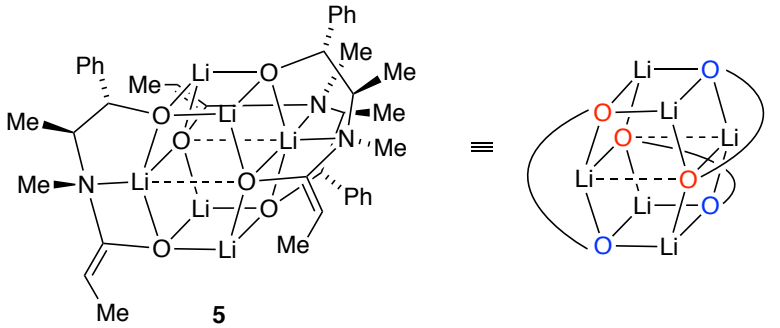

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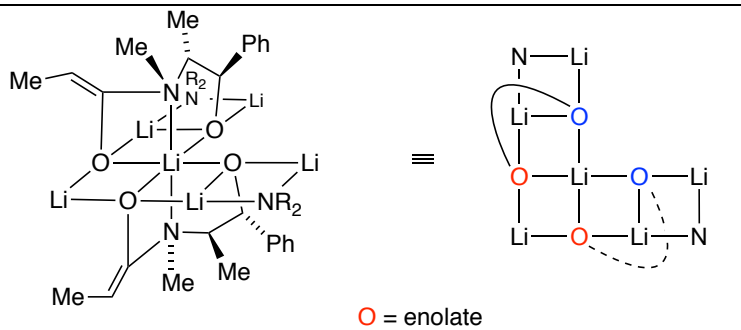
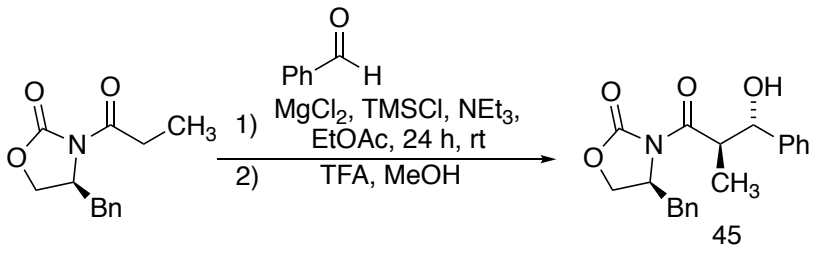


6

Part 1. Synthesis

Synthesis of 45



45

45 was synthesized using the procedure from Powell, S. A.; Tenenbaum, J. M.; Woerpel, K. A. *J. Am. Chem. Soc.* **2002**, *124*, 12648.

To a mixture of (*S*)-4-benzyl-3-propionyl-oxazolidin-2-one (2.0 g, 8.6 mmol) and $MgCl_2$ (0.092 g, 0.086 mmol) in 18.0 mL of EtOAc was added Et_3N (2.5 mL, 17.6 mmol), benzaldehyde (1.0 mL, 9.5 mmol), and $(CH_3)_3SiCl$ (1.62 mL, 13.2 mmol), respectively. The mixture was stirred for 24 h at 25 °C. The reaction mixture was filtered through a silica gel column with 200 mL of Et_2O. The solution was concentrated and dissolved in 150 mL MeOH. To the solution was added 2.0 mL of 1:9 TFA/MeOH and then concentrated to yield a white solid as a 24:1 mixture of diastereomers as determined by ^{1}H NMR spectroscopy. The solid was purified by flash chromatography (25% EtOAc in hexanes) to give a white solid (2.6 g, 92%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.44 (dd, J = 8.1, 1.5 Hz, 2H), 7.38 (dd, J = 8.4, 6.8 Hz, 2H), 7.35 – 7.23 (m, 4H), 7.18 – 7.13 (m, 2H), 4.83 (d, J = 8.0 Hz, 1H), 4.69 (ddt, J = 9.5, 7.7, 3.1 Hz, 1H), 4.36 (dq, 1H), 4.24 – 4.08 (m, 2H), 3.20 (dd, J = 13.6, 3.4 Hz, 1H), 2.67 (dd, J = 13.6, 9.3 Hz, 1H), 1.12 (d, J = 6.9 Hz, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 176.78, 153.67, 142.17, 135.32, 129.61, 129.09, 128.72, 128.20, 127.46, 126.78, 77.61, 66.11, 55.54, 44.46, 37.73, 15.02, 14.35.

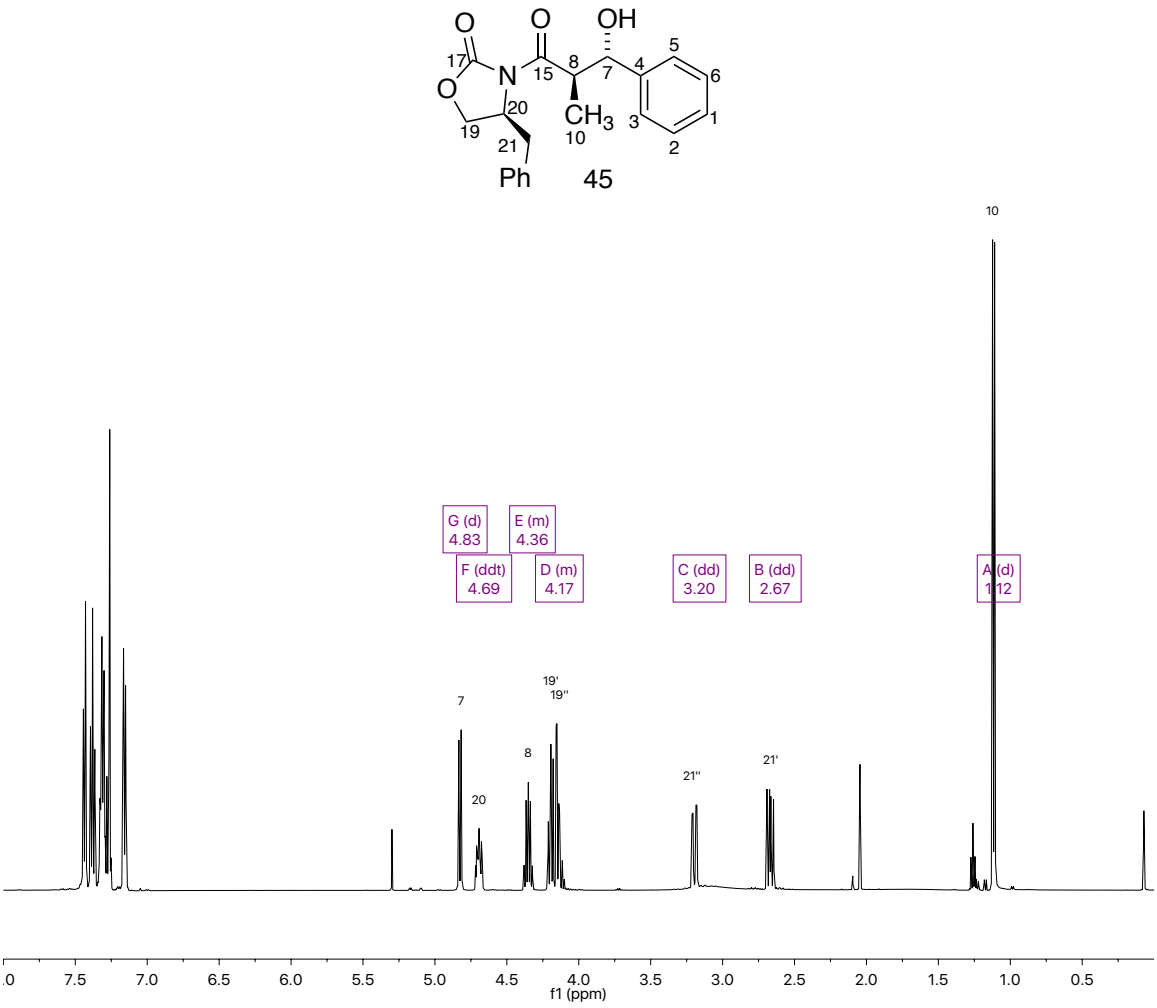


Figure 1. ^{1}H NMR spectrum of **45** in $CDCl_3$ at 25 °C.

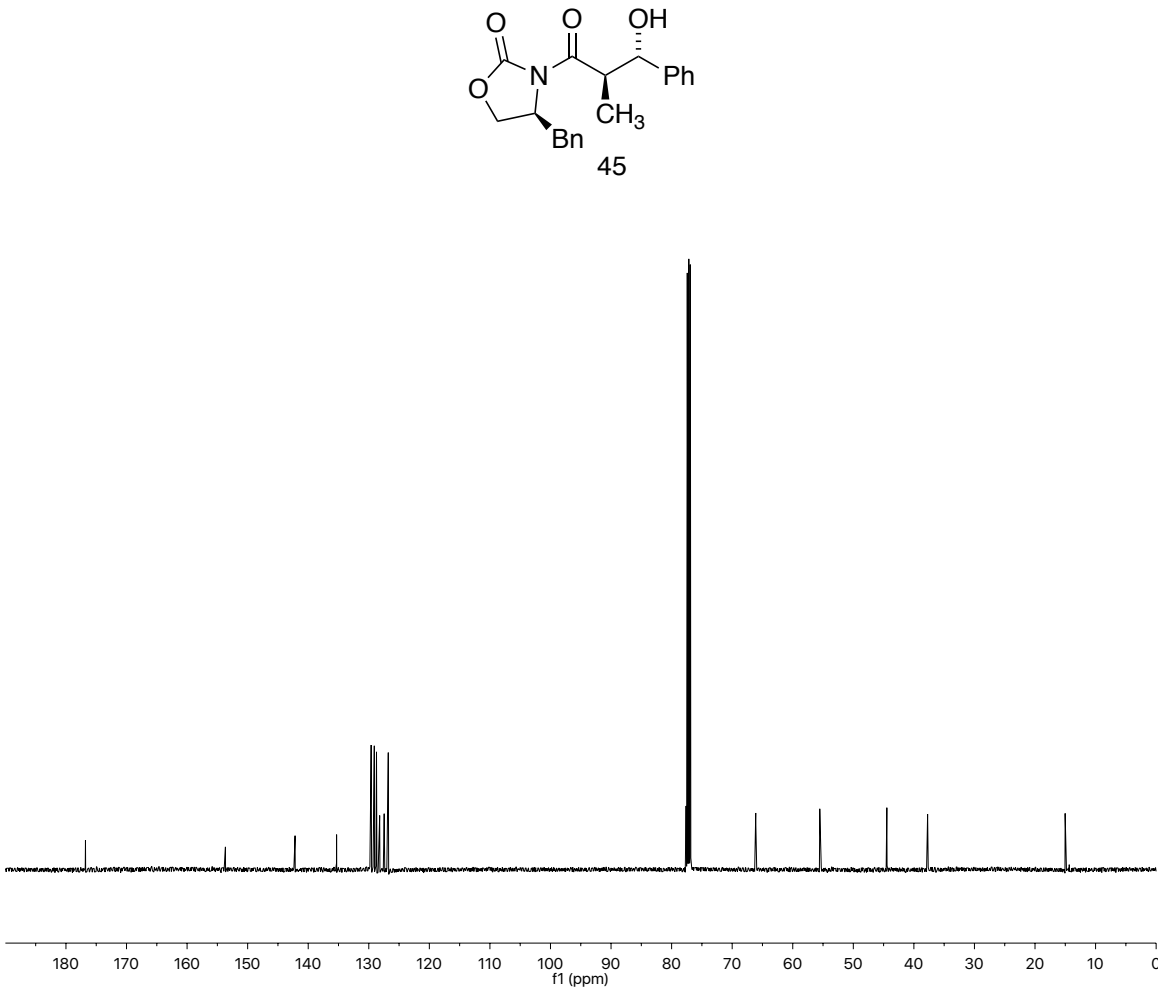
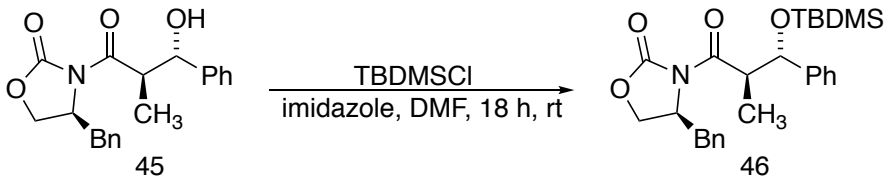


Figure 2. ^{13}C NMR spectrum of **45** in $CDCl_3$ at 25 °C.

Synthesis of 46



46 was synthesized using a slightly modified procedure Oishi, S.; Saito, S. *Angew. Chem. Int. Ed.* **2012**, *51*, 5395.

To a DMF solution of **45** (1.45 g, 4.3 mmol) and imidazole (292 mg, 4.3 mmol) was added *tert*-butyldimethylsilyl chloride (1.62 g, 10.8 mmol) at 25 °C, and the mixture was stirred for 24 h. Then the mixture was dissolved in EtOAc (100 mL) and washed with H_2O (30 mL × 3). The organic layer was dried over Na_2SO_4 and filtrated. The evaporation of the filtrate gave a colorless oil, which was purified by flash chromatography (28% EtOAc in hexanes) to yield **46** (1.79 g, 3.9 mmol, 92%). ^{1}H NMR (599 MHz, $CDCl_3$) δ 7.40 - 7.25 (m, 10H), 4.94 (d, J = 9.3 Hz, 1H), 4.70 (ddt, J = 10.7, 7.1, 3.4 Hz, 1H), 4.26 (dq, 1H), 4.19 – 4.08 (m, 2H), 3.48 (dd, J = 13.3, 3.4 Hz, 1H), 2.71 (dd, J = 13.4, 10.2 Hz, 1H), 0.85 (d, J = 6.9 Hz, 3H), 0.80 (d, J = 1.1 Hz, 9H), -0.00 (s, 3H), –0.28 (s, 3H).

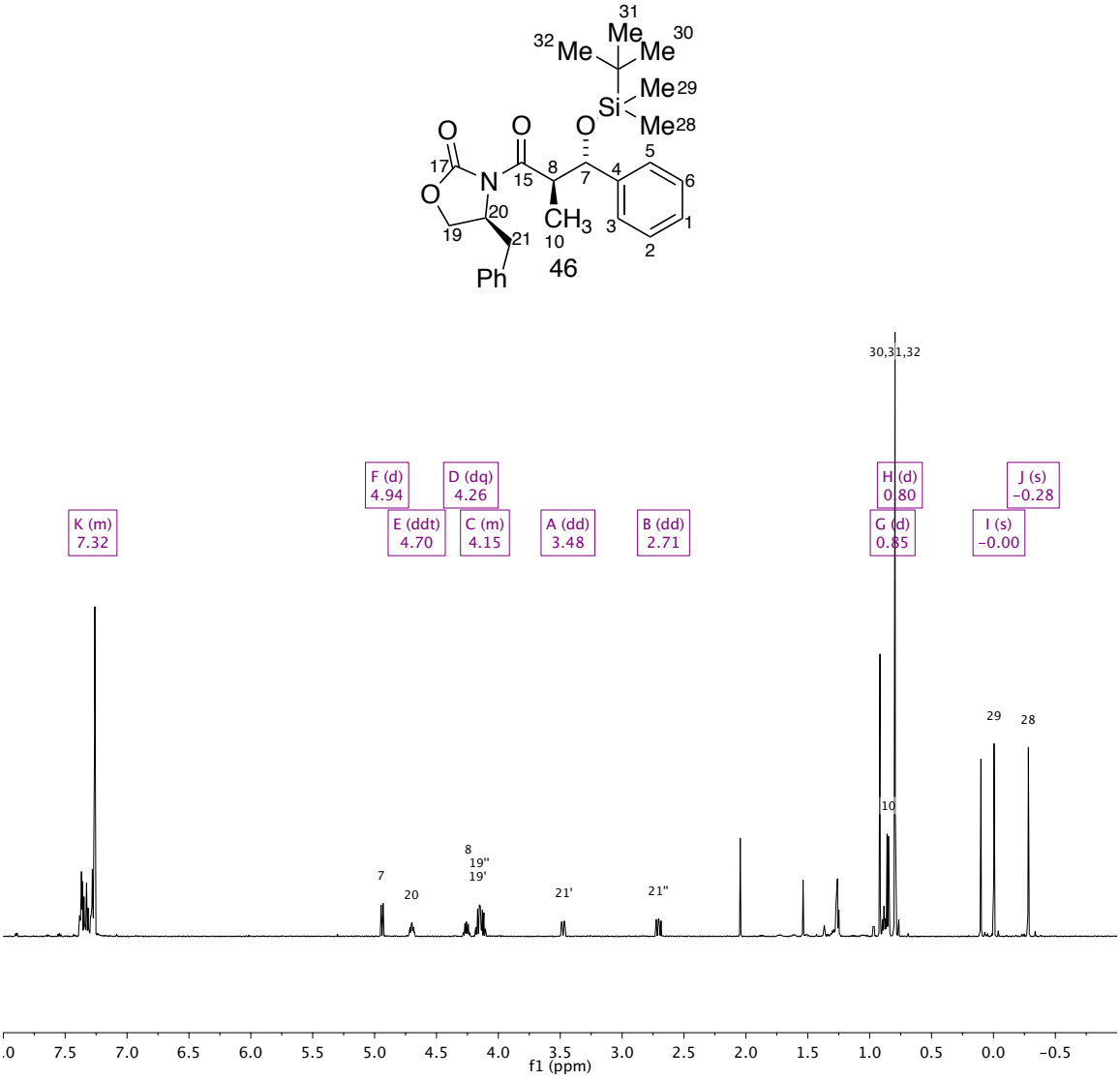
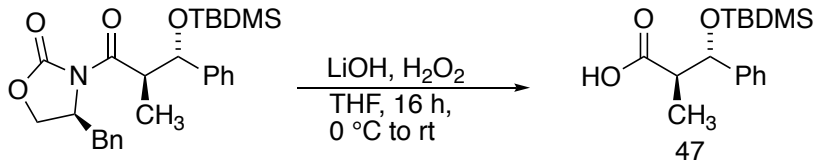


Figure 3. ^{1}H NMR spectrum of **46** in $CDCl_3$ at 25 °C.

Synthesis of 47



47 was synthesized using a slightly modified procedure from Hartung, I. V.; Rude. M. A.; Schnarr, N. A.; Hunziker, D.; Khosla, C. *J. Am. Chem. Soc.*,**2005**, *127*, 11202 and Hajra, S.; Mandal, A.; Hazra, S. *Tetrahedron Lett.* **2013**, *54*, 2171.

46 (1.23 g, 2.71 mmol, 1.0 equiv) were dissolved in 5.0 mL THF, cooled to 0 °C, and treated subsequently with H_2O_2 (30%, 3.8 mL, 37.9 mmol, 14.0 equiv.) and LiOH•H_2O (0.79 g, 19.0 mmol, 7.0 equiv.). The instantly formed yellowish-orange solution was warmed gradually to room temperature, and stirred for 16 h. The reaction was carefully quenched with aqueous sodium thiosulphate solution at 0 °C and stirred for 20 min, extracted with EtOAc. The aqueoust part was acidified with 10% HCl at ice-cold solution maintaining pH ~6 then extracted with EtOAc (50mL × 3). Organic part was washed with brine and dried over Na_2SO_4, and concentrated as a white solid, which was purified by flash chromatography (70 % EtOAc in hexanes) to yield **47** (0.583 g, 73%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.38 - 7.24 (m, 5H), 4.73 (d, J = 8.5 Hz, 1H), 2.77 (dq, 1H), 0.96 (d, J = 7.1 Hz, 3H), 0.84 (s, 9H), 0.03 (s, 3H), -0.26 (s, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 141.78, 128.28, 127.99, 126.95, 77.59, 48.94, 25.64, 18.01, 14.06, –3.57, –4.65, –5.40. DART calculated for $C_{16}H_{26}O_3Si$ $(M + H)^+$ m/z: 295.1724, found m/z: 295.1722.

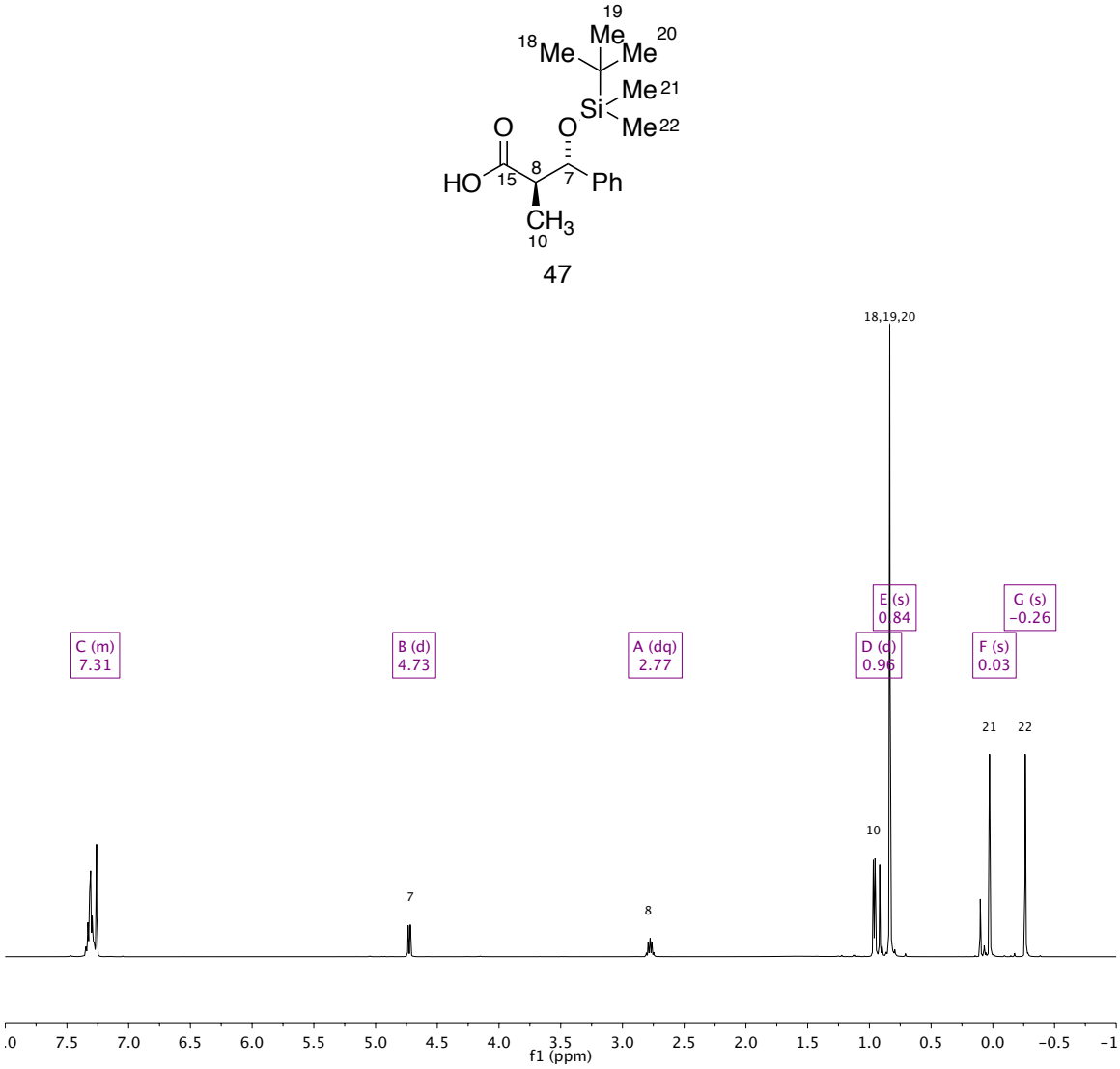


Figure 4. ^{1}H NMR spectrum of **47** in $CDCl_3$ at 25 °C.

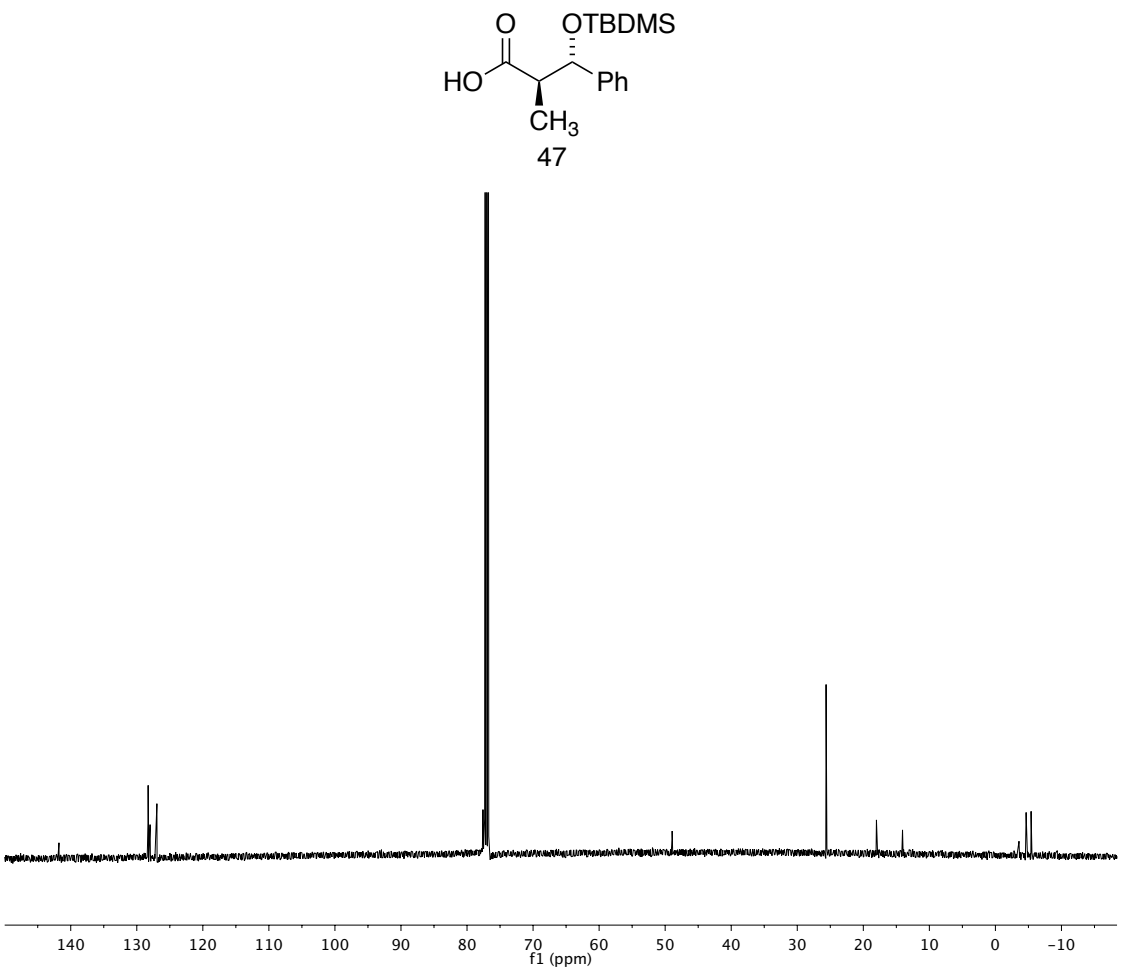
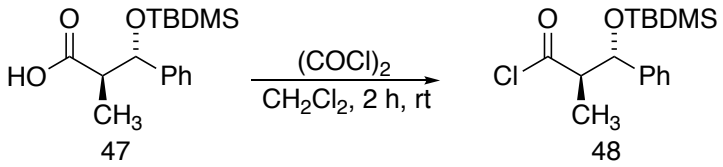


Figure 5. ^{13}C NMR spectrum of **47** in $CDCl_3$ at 25 °C.

Synthesis of 48



48 was synthesized using a slightly modified procedure from *SOSEI R and D LTD. - WO2008/71948, **2008**, A2*.

47 (0.50 g, 1.7 mmol) was dissolved in anhydrous dichloromethane (3.0 mL), and oxalyl chloride (0.30 ml, 3.5 mmol) was cautiously added. The mixture was stirred at room temperature for 16 h. The solvent was removed under reduced pressure to yield **48** as colorless oil (0.478 g, 90 %). This material was used without any further purification. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.37 – 7.28 (m, 5H), 4.77 (d, J = 9.2 Hz, 1H), 3.17 (dq, J = 9.2, 7.0 Hz, 1H), 0.97 (d, J = 7.0 Hz, 3H), 0.83 (s, 9H), 0.04 (s, 3H), -0.32 (s, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 176.04, 140.86, 128.58, 128.55, 127.33, 77.54, 60.56, 25.74, 18.13, 13.89, –4.44, –5.35.

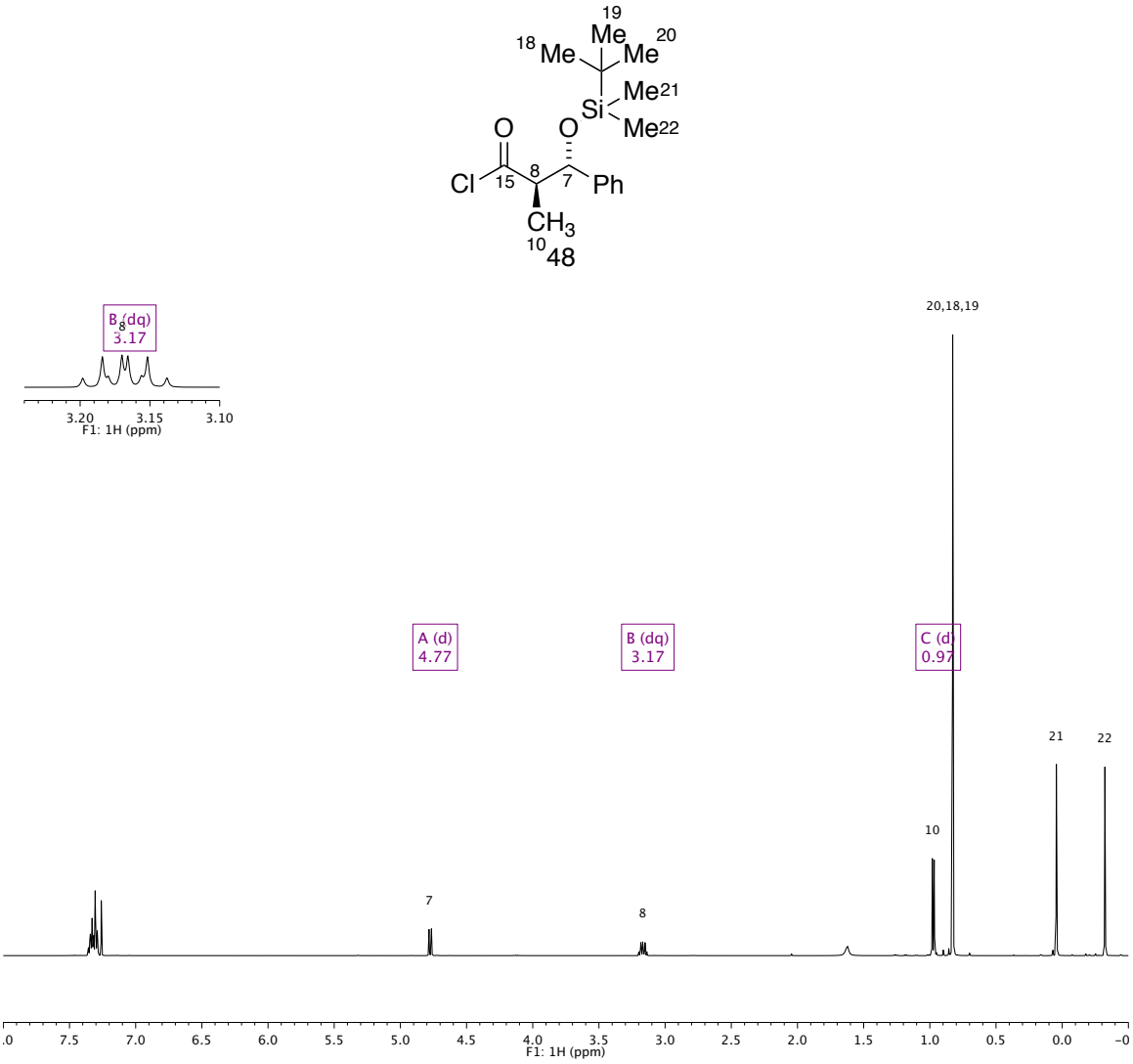


Figure 6. ^{1}H NMR spectrum of **48** in $CDCl_3$ at 25 °C.

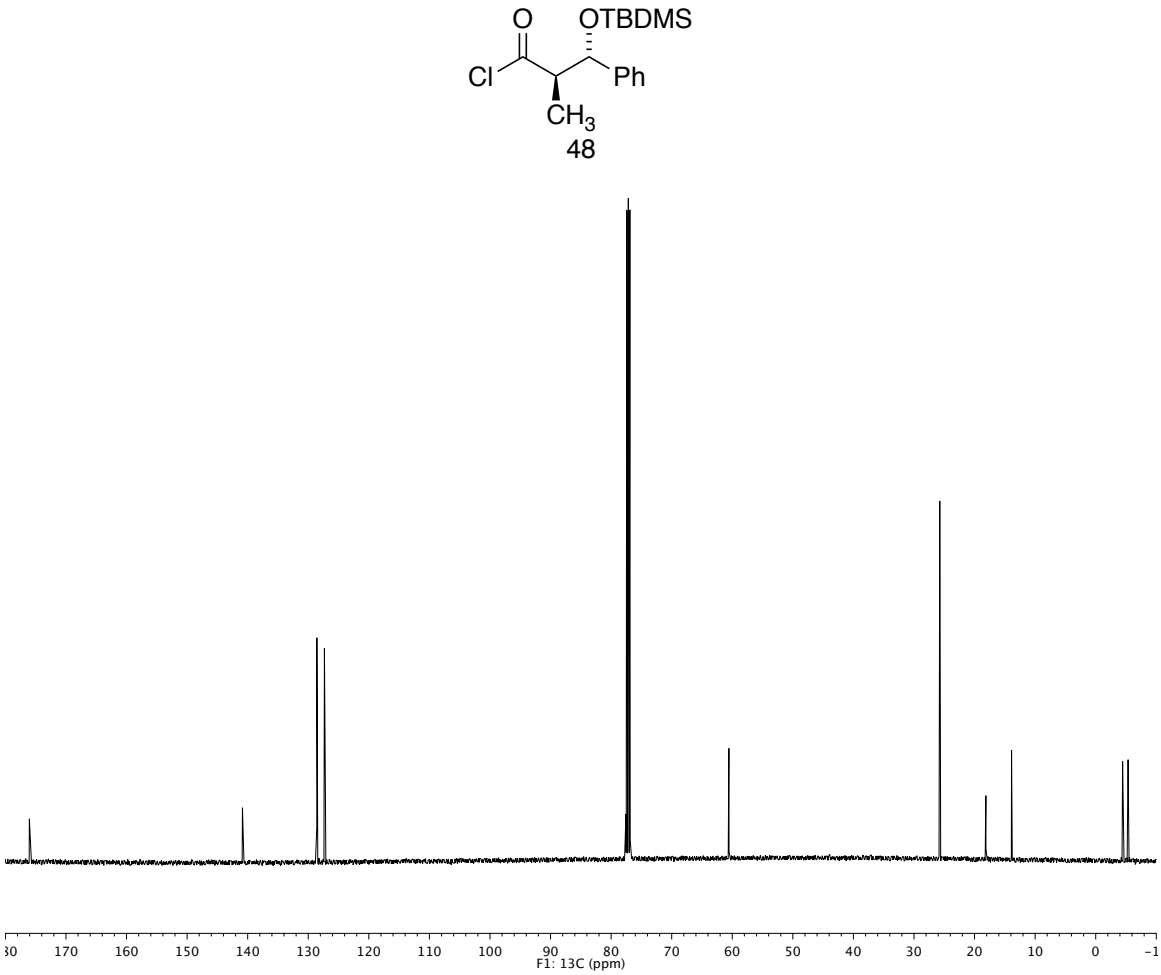
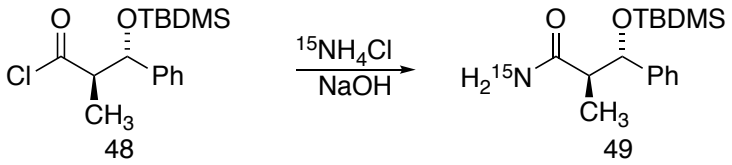


Figure 7. ^{13}C NMR spectrum of **48** in $CDCl_3$ at 25 °C.

Synthesis of 49



48 49

49 was synthesized using a slightly modified procedure from Zuend, S. J.; Ramirez, A.; Lobkovsky, E.; Collum, D. B. *J. Am. Chem. Soc.* **2006**, *128*, 5939.

A round bottom flask was charged with $^{15}NH_4Cl$ (20.0 mg, 0.37 mmol) and 1.0 mL of distilled water. **48** (100 mg, 0.32 mmol) in 1.0 mL Et_2O was layered on to the aqueous solution. The reaction mixture was cooled in an ice bath and 50 % aq NaOH (2.0 mL) was added via syringe with slow stirring to avoid mixing the layers. The reaction was warmed to room temperature and stirred for an additional 30 min. The reaction was then extracted with CH_2Cl_2 (2 mL × 10), washed with brine, dried over Na_2SO_4, and concentrated in vacuo. The resulting colorless oil was purified with flash chromatography (5% MeOH in CH_2Cl_2) to yield **49** (82.9 mg, 88 %) as a white solid. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.39 – 7.22 (m, 5H), 5.66 (dd, J = 235.4, 88.3 Hz, 2H), 4.69 (d, J = 7.8 Hz, 1H), 2.52 (p, J = 7.2 Hz, 1H), 0.95 (d, J = 7.0 Hz, 3H), 0.85 (s, 9H), 0.03 (s, 3H), -0.23 (s, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 177.67, 177.56, 142.58, 128.28, 127.78, 126.85, 77.62, 50.17, 50.12, 25.89, 18.21, 15.03, 14.31, 1.13, –4.38, –4.60, –4.83, –5.15. ^{15}N NMR (51 MHz, $CDCl_3$) δ 103.16. DART calculated for [^{15}N]-$C_{16}H_{27}NO_2Si$ ($M + H^+$) m/z: 295.1854, found m/z: 295.1854.

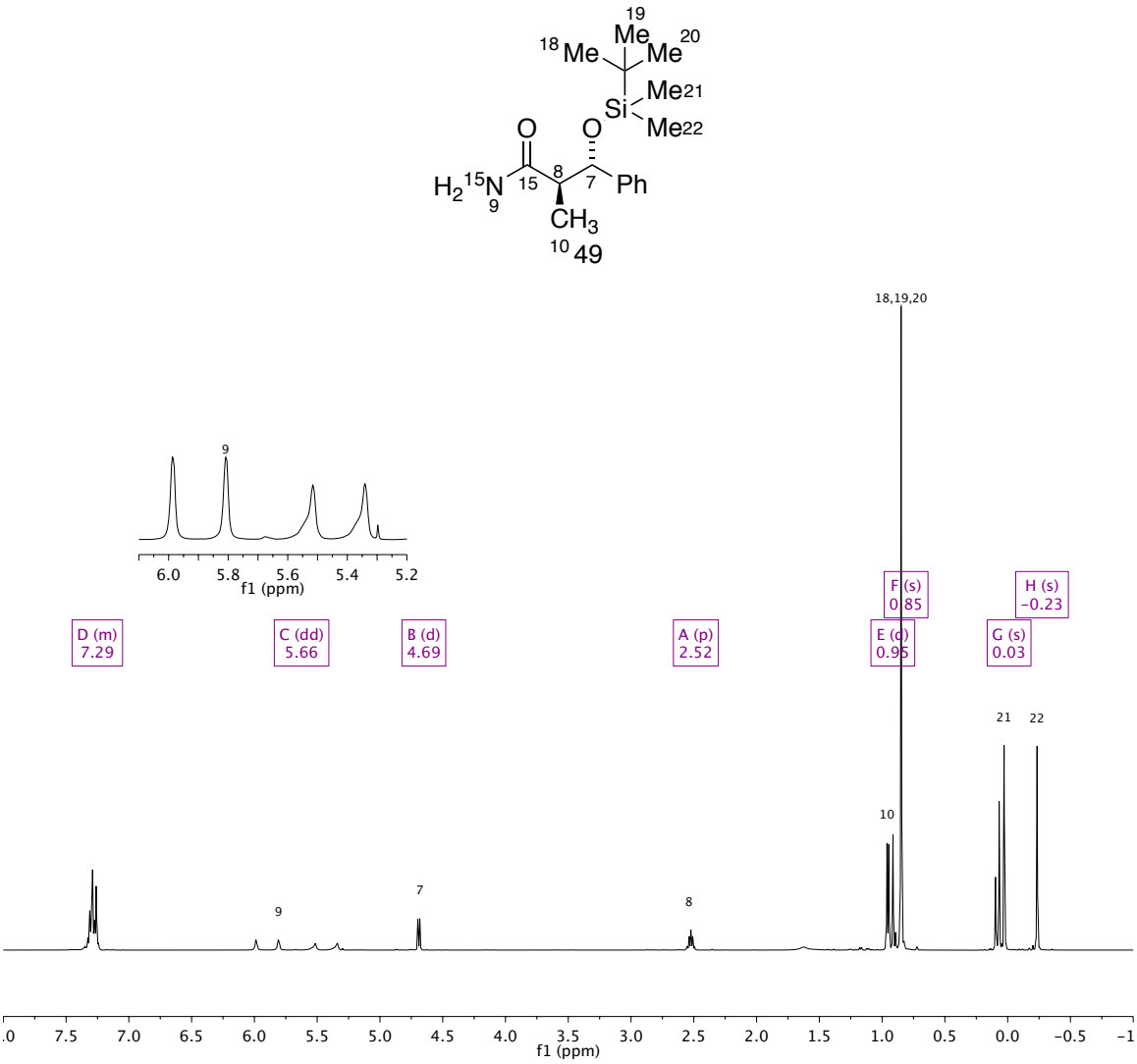


Figure 8. ^{1}H NMR spectrum of **49** in $CDCl_3$ at 25 °C.

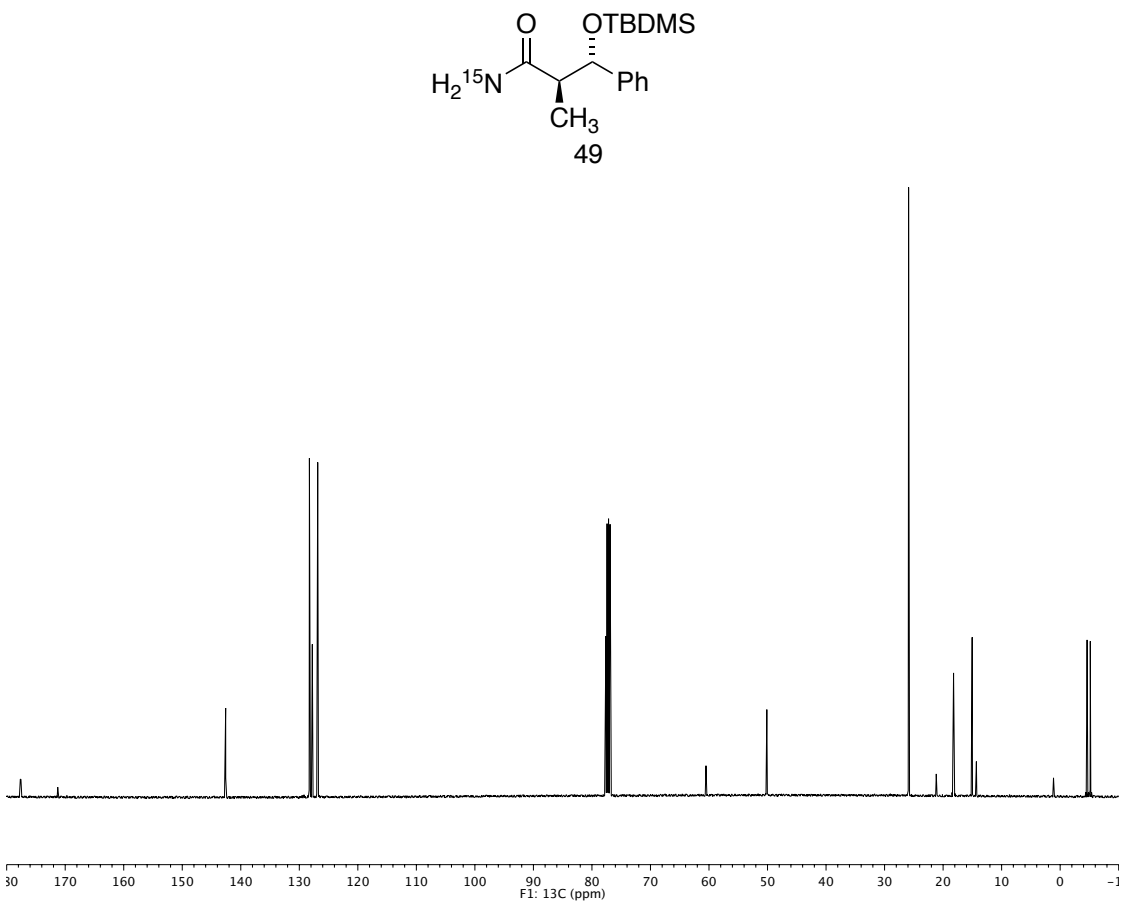


Figure 9. ^{13}C NMR spectrum of **49** in $CDCl_3$ at 25 °C.

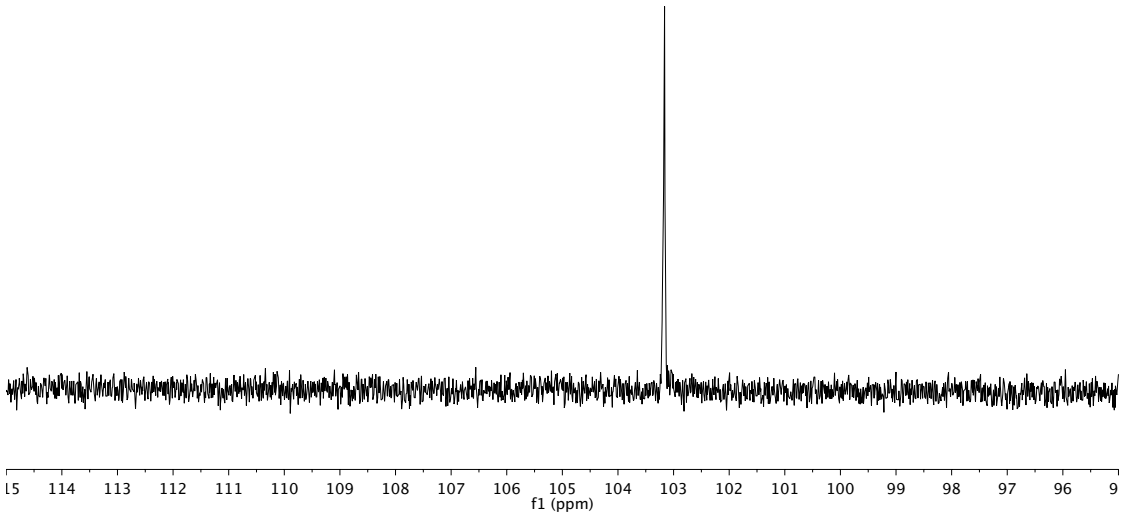
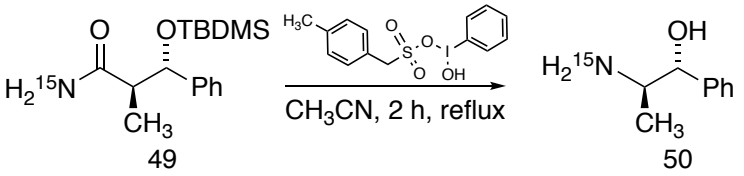


Figure 10. ^{15}N NMR spectrum of **49** in $CDCl_3$ at 25 °C.

Synthesis of 50



50 was synthesized using a slightly modified procedure from Liu, S. J.; Zhang, J. Z.; Tian, G. R.; Liu, P. *Synthetic communications,* **2005**, *35*, 823.

49 (117.6 mg, 0.40 mmol) was dissolved in hot CH_3CN (5.0 mL) and added to a 25 mL round bottom flask which was charged with [hydroxyl(tosyloxy)iodo]benzene (204 mg, 0.50 mmol). The mixture was heated at reflux for 2 h. The reaction was allowed to cool down and concentrated. The resulting product was treated with 1.0 M NaOH, extracted with DCM (5 mL × 3), and concentrated as a white solid which was purified with flash chromatography (3% MeOH in CH_2Cl_2) to yield **23** (40.8 mg, 67%) as a white solid. ^{1}H NMR (599 MHz, $CDCl_3$) δ 7.44 – 7.34 (m, 5H), 5.04 (dd, *J* = 7.2, 2.8 Hz, 1H), 3.87 – 3.80 (m, 1H), 1.39 (dd, *J* = 6.1, 3.1 Hz, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 137.79, 129.16, 129.03, 126.05, 85.54, 56.73, 20.08. ^{15}N NMR (51 MHz, $CDCl_3$) δ 91.48, 91.28. Only the dehydrated form was observed in DART, calculated for [15N]-$C_9H_{11}N$ (M – H_2O + H)+ m/z: 135.0935, found m/z: 135.0936.

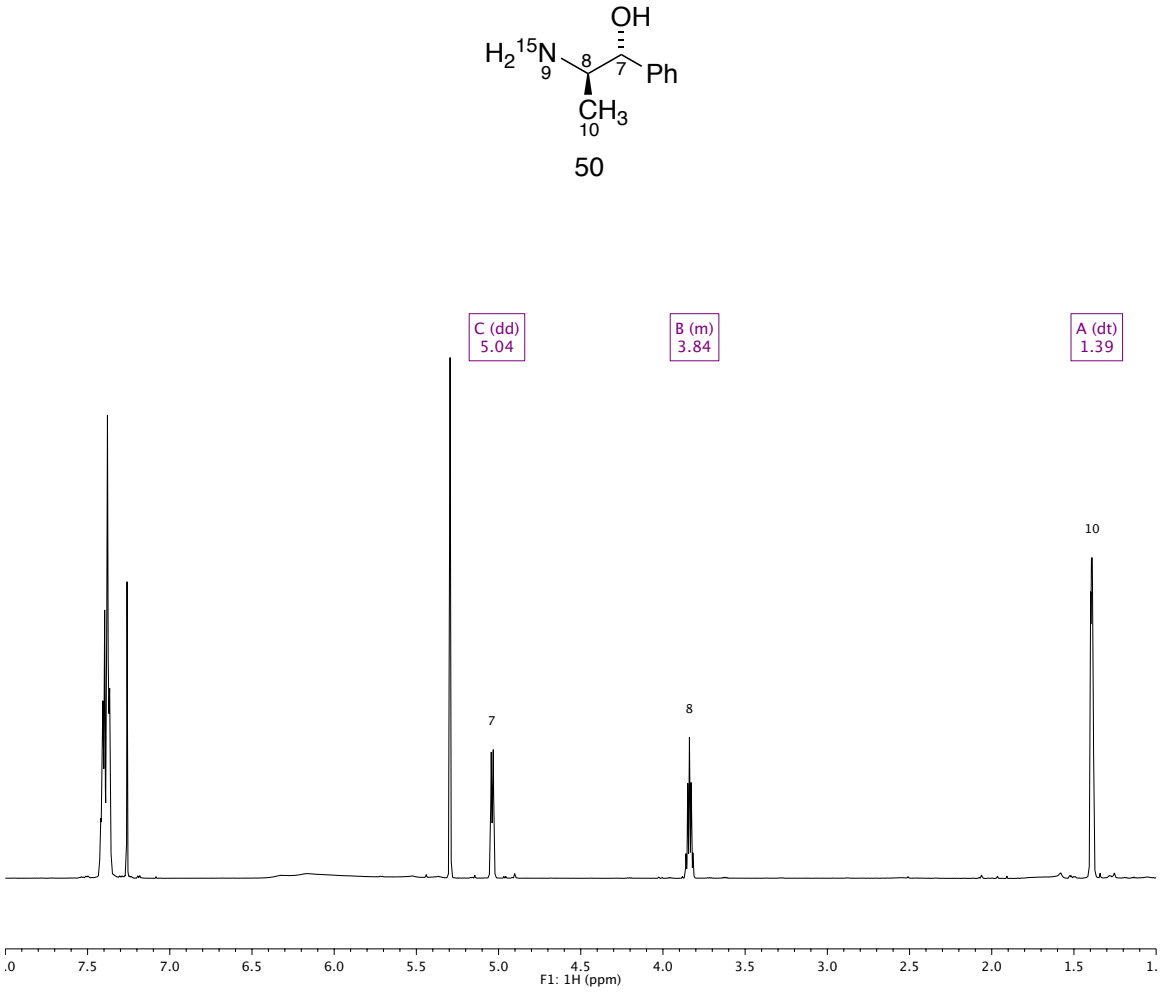


Figure 11. ^{1}H NMR spectrum of **50** in $CDCl_3$ at 25 °C.

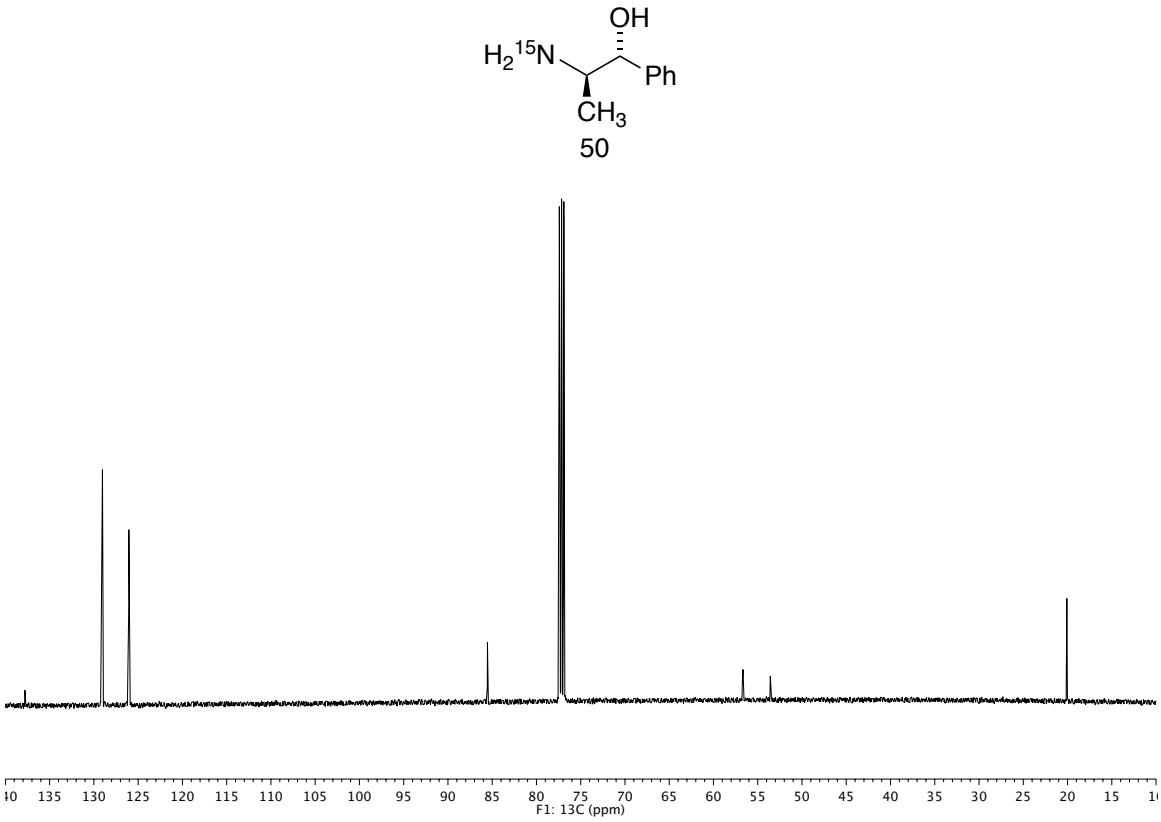


Figure 12. ^{13}C NMR spectrum of **50** in $CDCl_3$ at 25 °C.

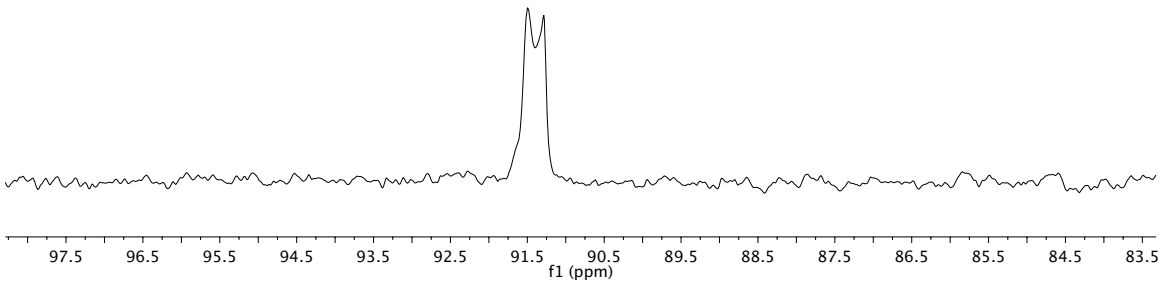
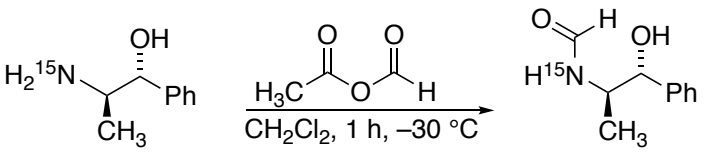


Figure 13. ^{15}N NMR spectrum of **50** in $CDCl_3$ at 25 °C.

Synthesis of 51



50 51

24 was synthesized using a slightly modified procedure from Effenberger, F.; Gutterer, B.; Jäger, J. *Tetrahedron: Asymmetry* **1997**, *8*, 459.

Acetic formic anhydride (95 µL, 1.20 mmol) was added dropwise at –30 °C to a solution of **23** (90.0 mg, 0.59 mmol) in 2.0 mL DCM. After stirring for 1 h the volatile compounds were removed in vacuo. This material was used without any further purification. ^{1}H NMR (500 MHz, $CDCl_3$) δ 9.09 (d, J = 1.9 Hz, 1H), 7.47 – 7.32 (m, 5H), 5.04 (dd, J = 7.4, 2.3 Hz, 1H), 3.88 – 3.79 (m, 1H), 1.42 – 1.36 (m, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 167.99, 156.20, 137.76, 129.17, 129.03, 126.04, 85.54, 56.65, 22.33, 21.36, 20.07. ^{15}N NMR (51 MHz, $CDCl_3$) δ 91.22.

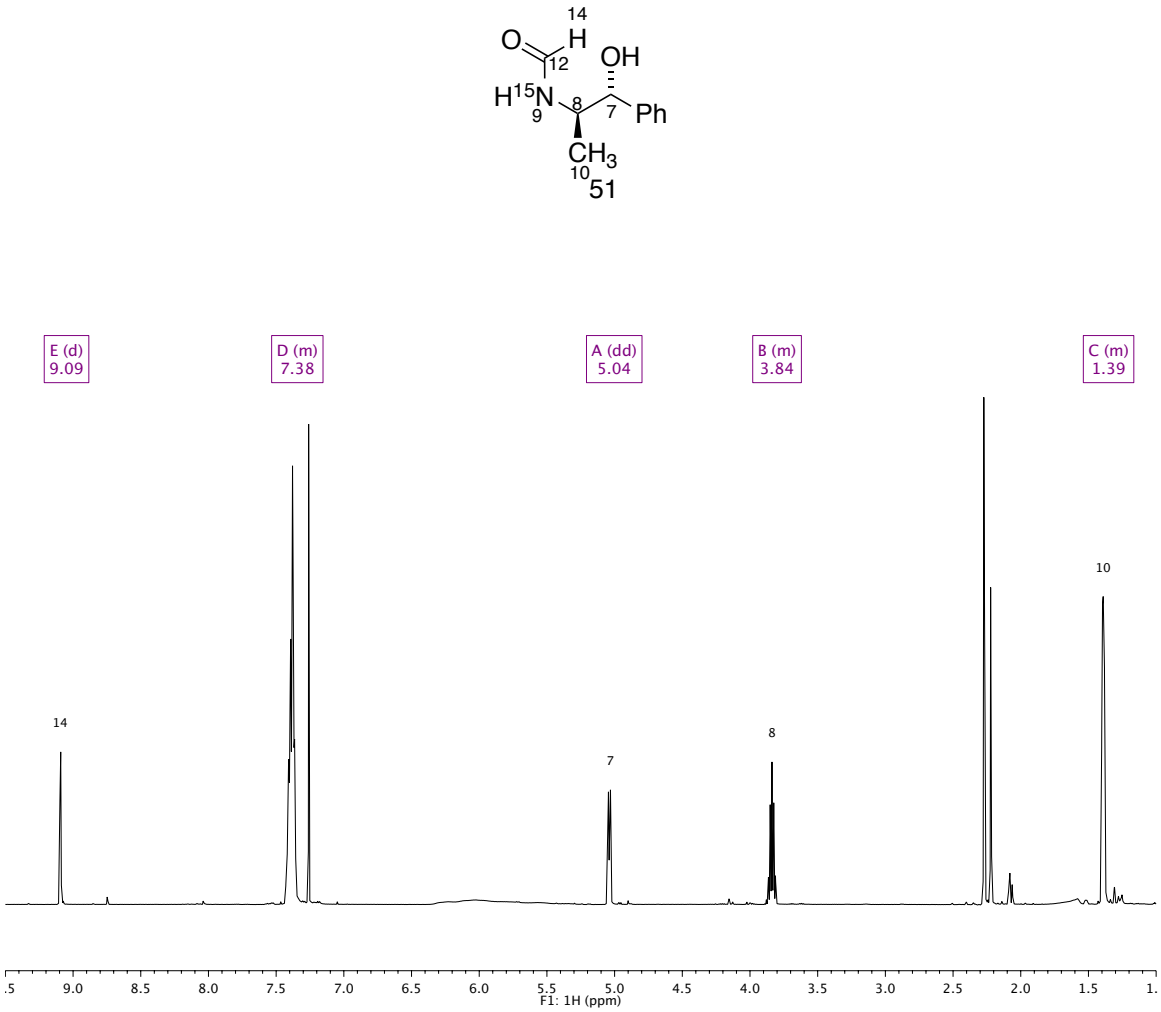


Figure 14. ^{1}H NMR spectrum of **51** in $CDCl_3$ at 25 °C.

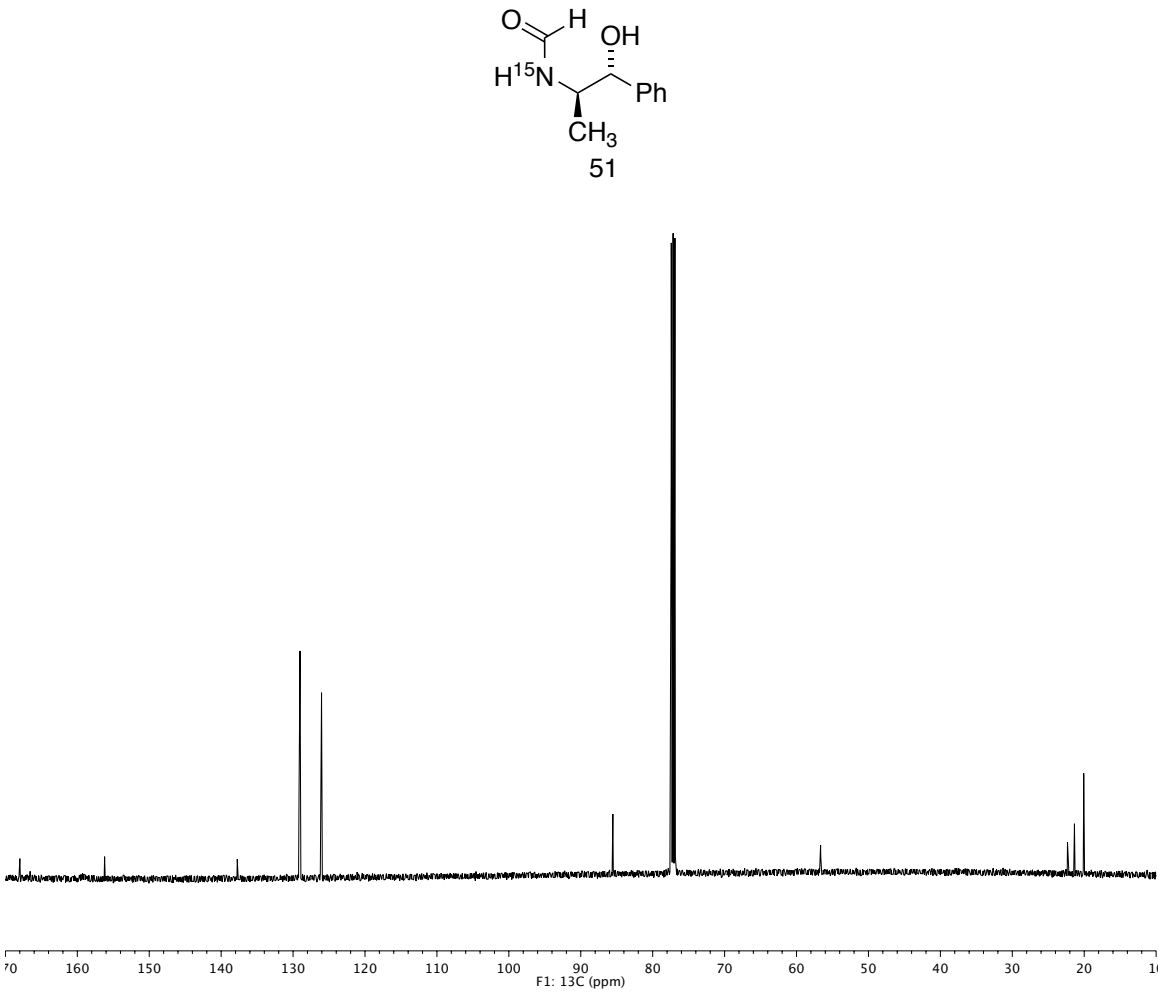


Figure 15. ^{13}C NMR spectrum of **51** in $CDCl_3$ at 25 °C.

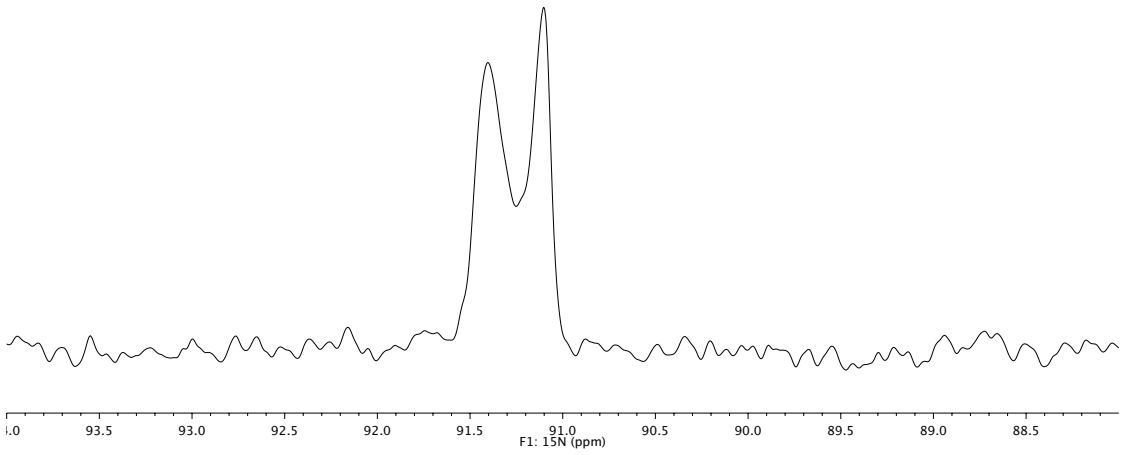
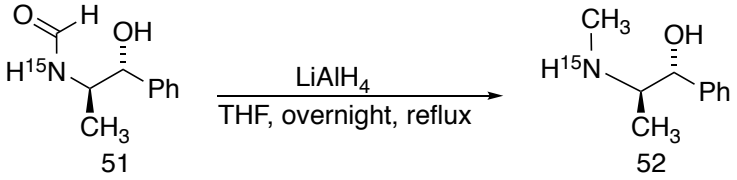


Figure 16. ^{15}N NMR spectrum of **51** in $CDCl_3$ at 25 °C.

Synthesis of 52



51 52

51 (95.0 mg, 0.53 mmol) was dissolved in THF (3.0 mL). $LiAlH_4$ (50.0 mg, 1.3mmol) was carefully added to the solution at –78 °C. The reaction was warmed till refluxing for 24 h. The reaction was cooled down to –78 °C and quenched with water (1.0 equiv), 2.0 M NaOH solution (2.0 equiv) and water (3.0 equiv). After the quenching was complete, the reaction was allowed to warm to room temperature with continued stirring. The salt by-products were separated from the reaction solution by filtration through a fritted funnel, and the solids were washed with diethyl ether (1.0 mL × 4). The filtrate and washes were combined and the combined liquid was concentrated to remove the organic solvents. The resulting concentrate was then partitioned between ethyl ether (4.0 mL) and water (1.0 mL). The layers were separated, and the organic phase was washed sequentially with water (1.0 mL) and saturated aqueous sodium chloride solution (1.0 mL). The organic solution was then dried over magnesium sulfate. The dried solution was filtered, and the filtrate was concentrated as a colorless oil which was purified with flash chromatography (10% MeOH in CH_2Cl_2) to yield **52** (77 mg, 88%) as a white solid. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.40 – 7.29 (m, 6H), 4.22 (d, J = 8.2 Hz, 1H), 2.65 (dq, J = 8.3, 6.5 Hz, 1H), 2.49 (s, 3H), 0.98 (dd, J = 6.5, 1.8 Hz, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 142.32, 128.44, 127.83, 127.14, 77.76, 61.58, 33.56, 15.78. ^{15}N NMR (51 MHz, $CDCl_3$) δ 31.93. DART calculated for [^{15}N]-$C_{10}H_{15}NO$ $(M + H)^+$ m/z: 167.1197, found m/z: 167.1198.

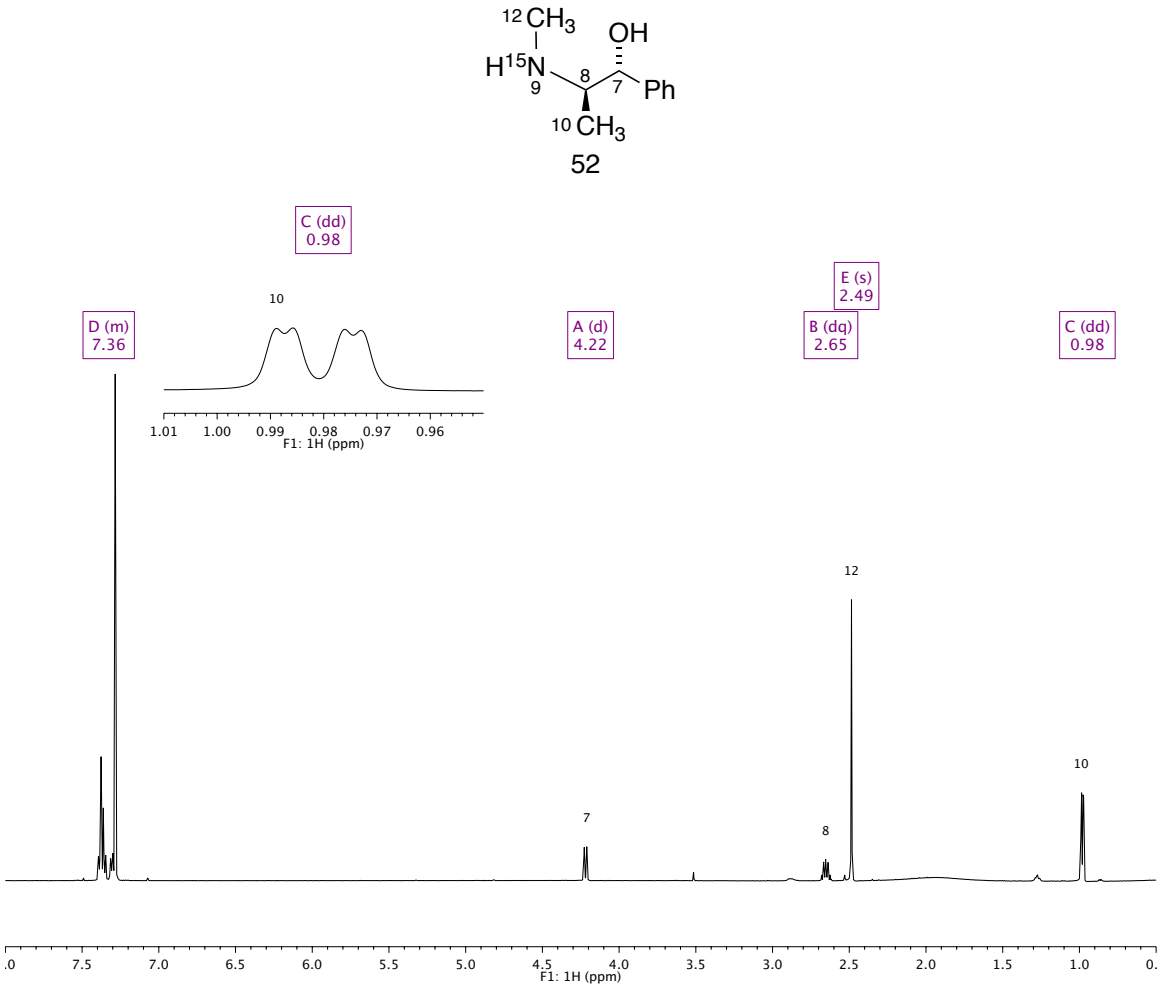


Figure 17. ^{1}H NMR spectrum of **52** in $CDCl_3$ at 25 °C.

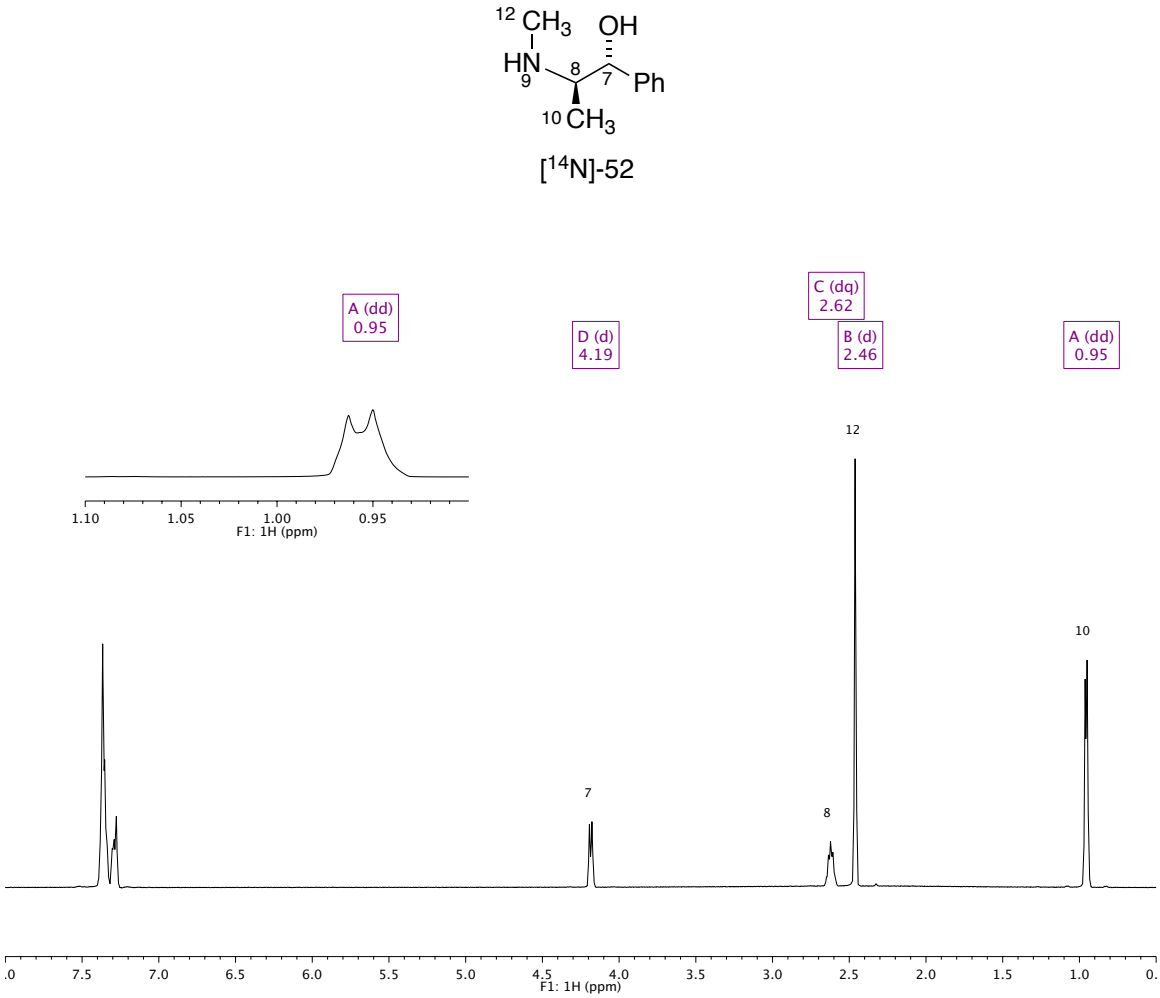


Figure 18. ^{1}H NMR spectrum of [^{14}N]-**52** in $CDCl_3$ at 25 °C.

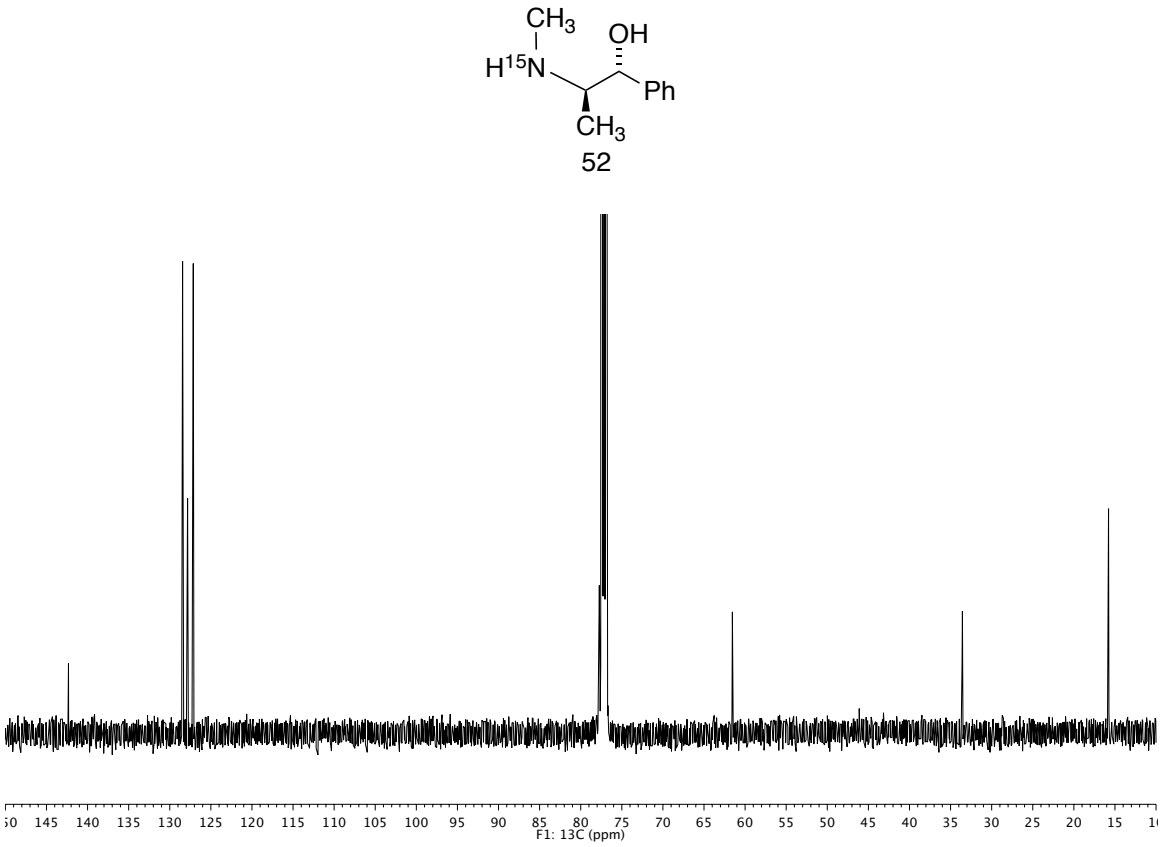


Figure 19. ^{13}C NMR spectrum of **52** in $CDCl_3$ at 25 °C.

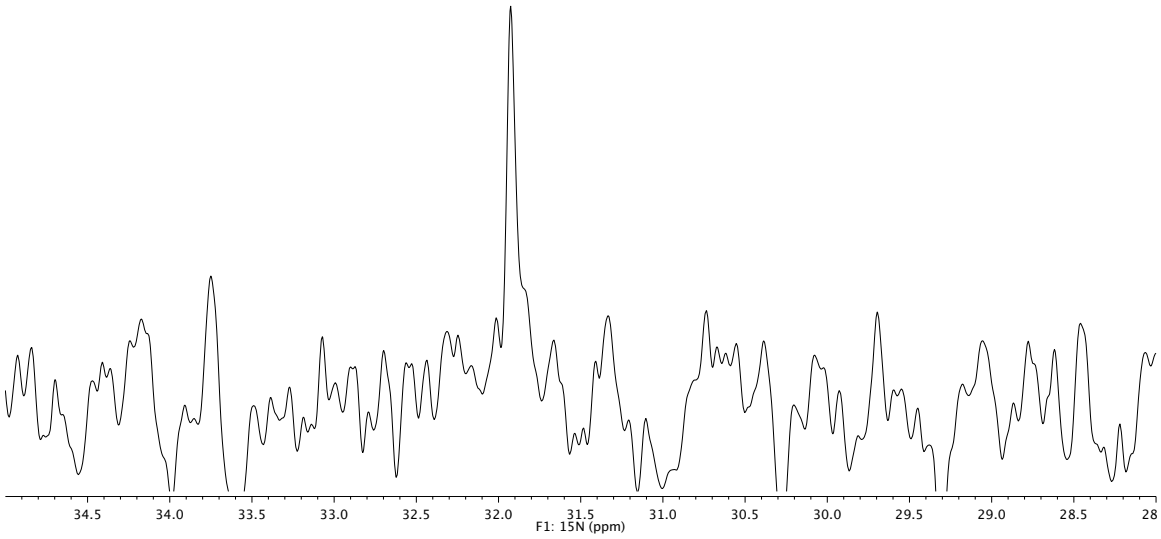
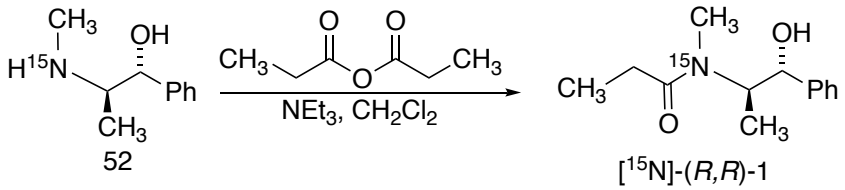


Figure 20. ^{15}N NMR spectrum of **52** in $CDCl_3$ at 25 °C.

Synthesis of [^{15}N]-(*R,R*)-1



[^{15}N]-(*R,R*)-**1** was synthesized using a slightly modified procedure Myers, A. G.; Yang, B. H.; Chen, H.; McKinstry, L.; Kopecky, D. J.; Gleason, J. L. *J. Am. Chem. Soc.* **1997**, *119*, 6496.

A 10 mL flask was charged with **52** (50.0 mg, 0.30 mmol), triethylamine (50 µL, 0.36 mmol), and CH_2Cl_2 1.0 mL. The flask was placed in a water bath at 25 °C, and propionic anhydride (42.0 mg, 0.32 mmol) was added to the solution. The reaction was stirred for 30 min, and then excess anhydride was quenched with distilled water (1.0 mL). The organic layer was separated and extracted with half-saturated aqueous sodium bicarbonate solution (1 mL × 2) and 1.0 M aqueous hydrochloric acid solution (1 mL × 2). The organic extract was dried over sodium sulfate and concentrated to furnish a white solid, which was purified with flash chromatography (70% EtOAc in hexanes) to yield [^{15}N]-(*R,R*)-**1** (59.0 mg, 89%) as a white solid. ^{1}H NMR (599 MHz, $CDCl_3$) δ 7.41 – 7.27 (m, 5H), 4.60 (t, *J* = 7.3 Hz, 1H), 4.58 – 4.55* (m, 1H), 4.44 (dq, 1H), 4.01* (dq, 1H), 2.93* (s, 1H), 2.81 (s, 3H), 2.53* (dq, 1H), 2.40* (dq, 1H), 2.32 (dq, 1H), 2.31 (dq, 1H), 1.17* (t, *J* = 7.4 Hz, 1H), 1.13 (t, *J* = 7.4 Hz, 3H), 1.12 (d, *J* = 7.0 Hz, 3H), 0.98* (d, *J* = 6.8 Hz, 1H). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.41 – 7.27 (m, 7H), 4.63 – 4.54 (m, 1H), 4.44* (s, 1H), 4.29 (s, 1H), 4.01* (p, *J* = 6.9 Hz, 1H), 2.93* (s, 3H), 2.81 (d, *J* = 1.0 Hz, 3H), 2.54* (dq, *J* = 15.0, 7.4 Hz, 1H), 2.45 – 2.37* (m, 1H), 2.32 (dq, *J* = 13.0, 7.8 Hz, 2H), 1.17* (t, *J* = 7.4 Hz, 3H), 1.13 (t, *J* = 7.5 Hz, 3H), 1.11 (dd, *J* = 7.3, 2.0 Hz, 3H), 0.98* (dd, *J* = 6.8, 2.4 Hz, 3H). (3:1 rotamer ratio, asterisk denotes minor rotamer peaks.) ^{13}C NMR (126 MHz, $CDCl_3$) δ 176.47, 176.36, 142.74, 142.65, 128.90, 128.64, 128.53, 127.81, 127.07, 126.52, 27.78, 27.73, 14.64, 9.35. DART calculated for [^{15}N]-$C_{13}H_{19}NO_2$ $(M + H)^+$ m/z: 223.1459, found m/z: 223.1450.

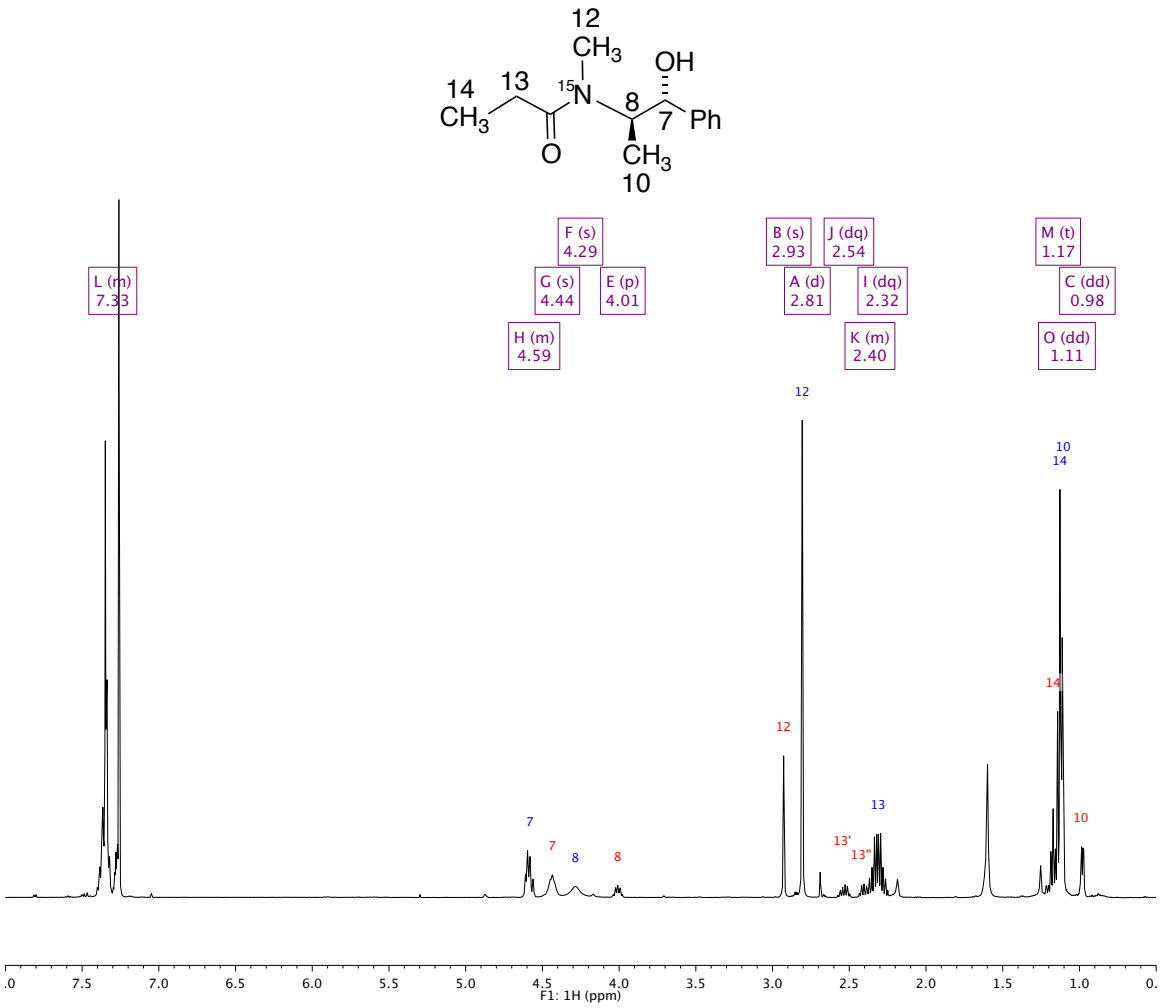


Figure 21. ^{1}H NMR spectrum of [^{15}N]-(*R,R*)-1 in in $CDCl_3$ at 25 °C.

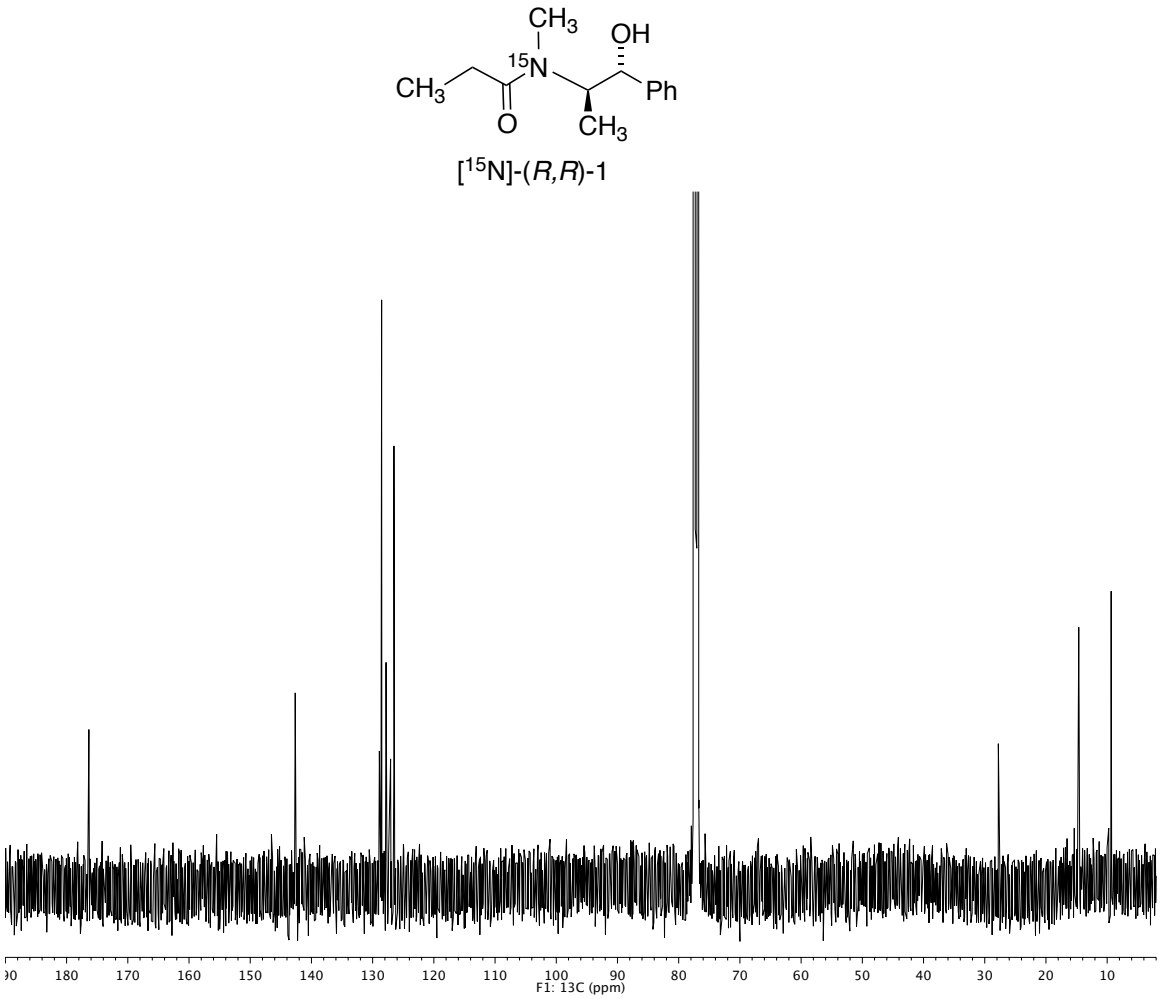


Figure 22. ^{13}C NMR spectrum of [^{15}N]-(*R,R*)-1 in in $CDCl_3$ at 25 °C.

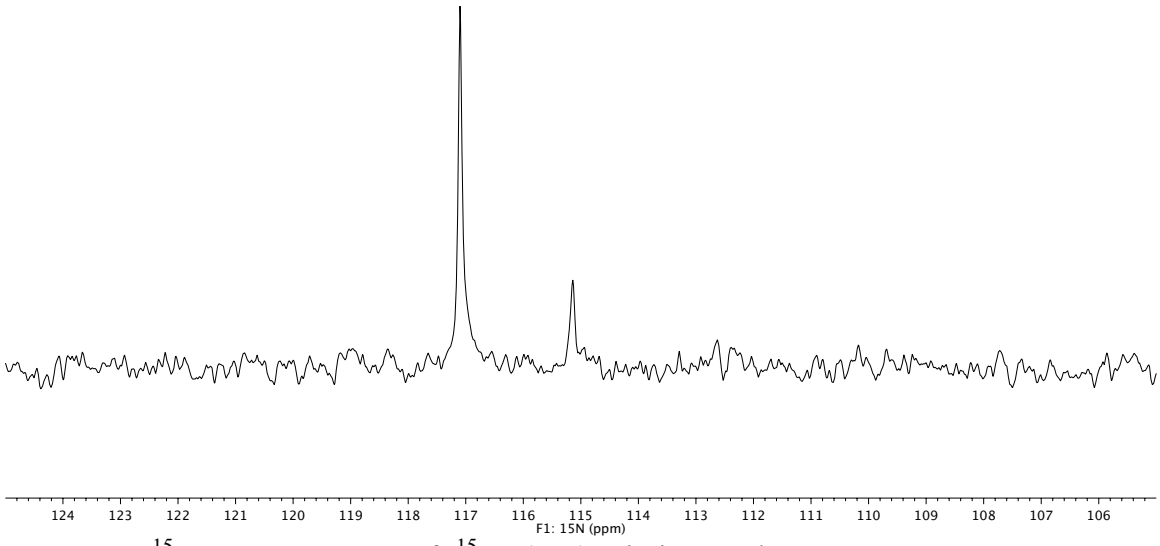
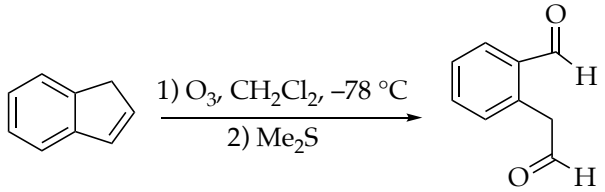


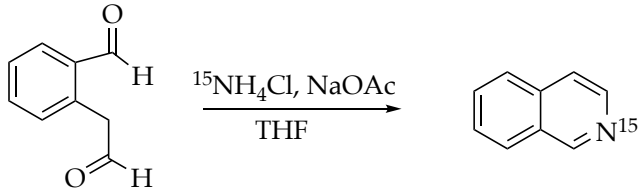
Figure 23. ^{15}N NMR spectrum of [^{15}N]-(*R,R*)-1 in in $CDCl_3$ at 25 °C.

Synthesis of [^{15}N]-Isoquinoline

Homophthalaldehyde was synthesized using a slightly modified procedure from Garratt, P. J.; Vollhardt, K. P. C. *Synthesis* **1971**, *8*, 423. [^{15}N]-Isoquinoline was synthesized using a slightly modified procedure from Huang, X.; Tanaka, K. S.; Bennet, A. J. *J. Am. Chem. Soc.* **1997**, *119*, 11147-11154.



Homophthalaldehyde: Indene (5.0 g, 43.0 mmol) was added to dry CH_2Cl_2 (30 mL). The solution was cooled to –78 °C, and ozone in oxygen was bubbled through for 2 h. The resulting blue solution was treated with dimethyl sulfide (20 mL, 272 mmol) gradually until the blue color disappeared. The reaction was stirred for 30 min at room temperature to ensure the completion of quenching. The reaction mixture was extracted with brine (30 mL × 3), dried over Na_2SO_4, and concentrated as a pale-yellow oil (5.59 g, 87.6%). The product was purified with flash chromatography (25% EtOAc in hexanes) to give a colorless liquid. The product was directed subjected to the following reaction. The product was suspected to react exothermically with DMSO, caution!



[^{15}N]-Isoquinoline: A solution of ^{15}N ammonium chloride (2.0 g; 36.7 mmol) and sodium acetate (3.28 g) in water (30 mL) was added to a solution containing homophthalaldehyde (5.92 g; 40 mmol) in tetrahydrofuran (30 mL). The resulting mixture was stirred for 60 min at room temperature, the volume was reduced (30 mL) using an aspirator, and the pH of the solution was adjusted to 2. Following extraction of the acidic solution with ether (30 mL × 2), the aqueous phase was adjusted to pH 8. Dichloromethane (50 mL × 3) was utilized to extract the labeled isoquinoline. The organic layers were combined, dried with Na_2SO_4, filtered, and concentrated at aspirator pressure to give a brown oil. Dry HCl gas was passed into an ice-cold ether (50 mL) solution of the isoquinoline to give the hydrochloride salt as a pale-yellow solid (2.4 g; yield from $^{15}NH_4Cl$ 40%) which was filtered, rinsed with ice-cold ether and dried over aspirator. The resulting solid (0.50 g, 3.2 mmol) was treated with diethyl ether (6.0 mL) and 1.0 M NaOH aqueous solution (3.0 mL, 0.9 equiv, 2.9 mmol). The reaction mixture was stirred for 10 min, extracted with diethyl ether (10 mL × 3), dried over Na_2SO_4, and concentrated as a brown oil (0.34 g, 90%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 9.29 (d, J = 10.6 Hz, 1H), 8.55 (dd, J = 10.5, 5.8 Hz, 1H), 8.00 (dd, J = 8.3, 1.2 Hz, 1H), 7.85 (dd, J = 8.3, 1.1 Hz, 1H), 7.73 (ddd, J = 8.2, 6.8, 1.3 Hz, 1H), 7.70 – 7.67 (m, 1H), 7.64 (ddd, J = 8.0, 6.8, 1.2 Hz, 1H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 152.68, 143.16, 135.94, 135.92, 130.48, 128.84, 128.82, 127.78, 127.77, 127.38, 126.62, 120.61, 120.59. ^{15}N NMR (51 MHz, $CDCl_3$) δ 305.54. DART calculated for [^{15}N]-C9H7N·HCl $(M + H)^+$ m/z: 131.0622, found m/z: 131.0618 .

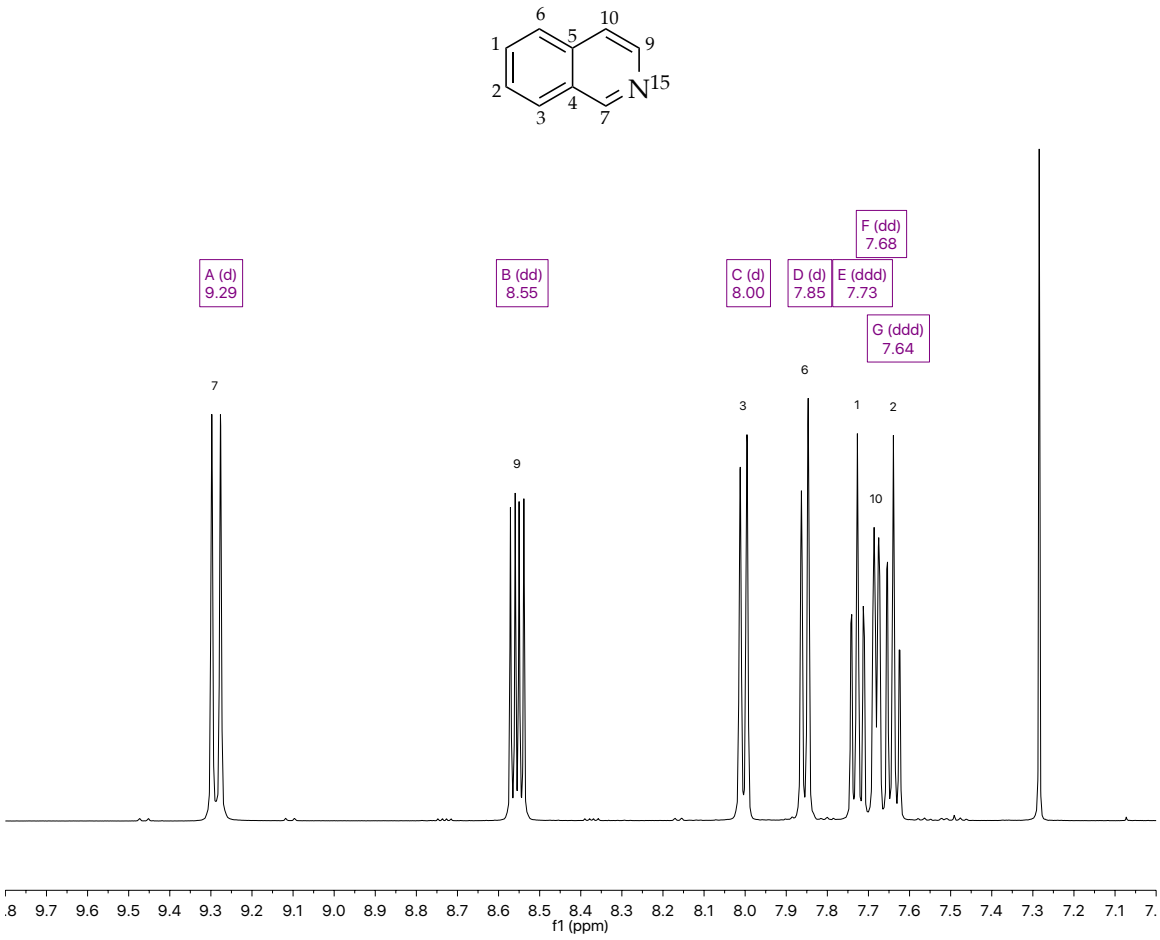


Figure 24. ^{1}H NMR spectrum of [^{15}N]-isoquinoline in $CDCl_3$ at 25 °C.

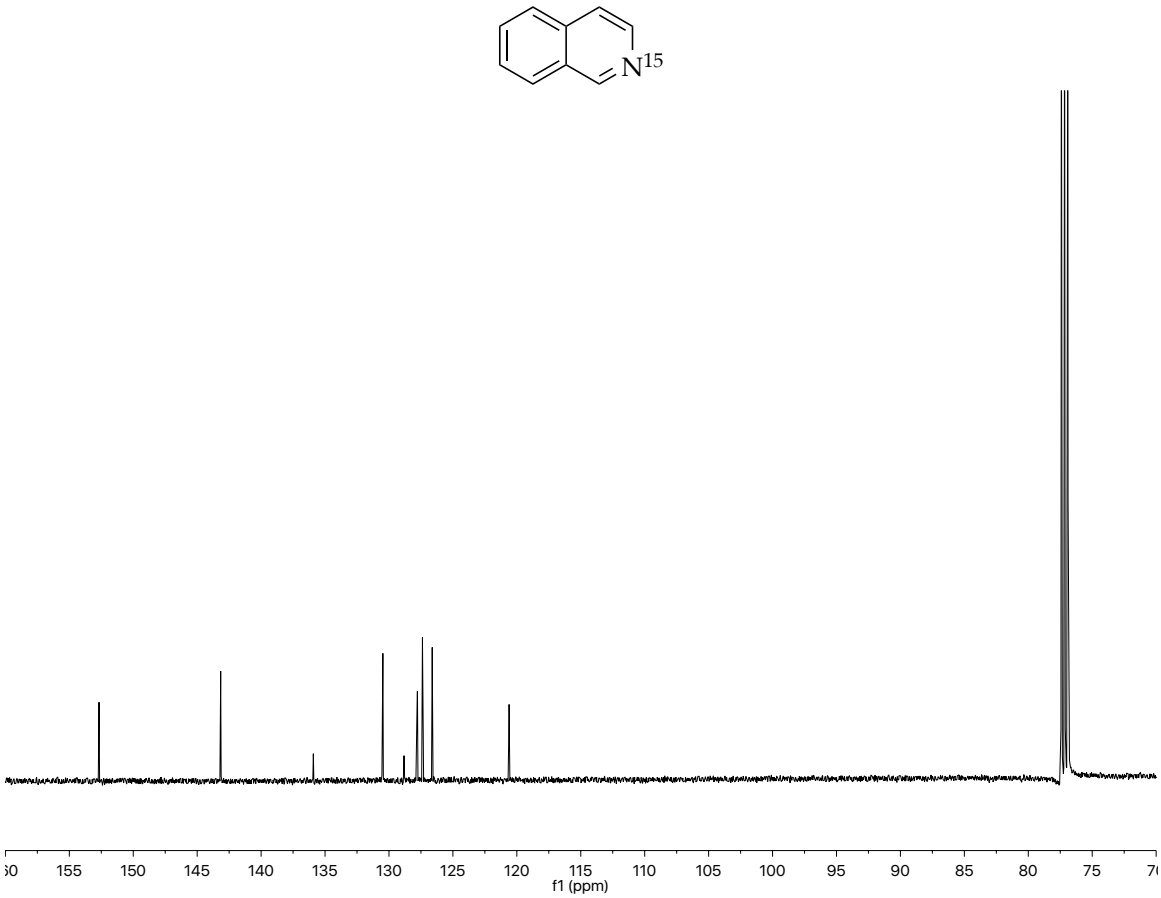


Figure 25. ^{13}C NMR spectrum of [^{15}N]-isoquinoline in $CDCl_3$ at 25 °C.

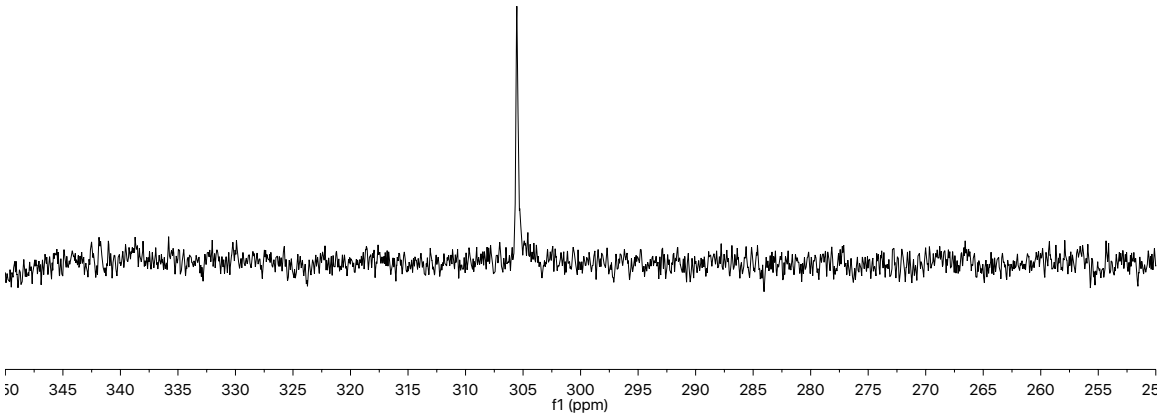
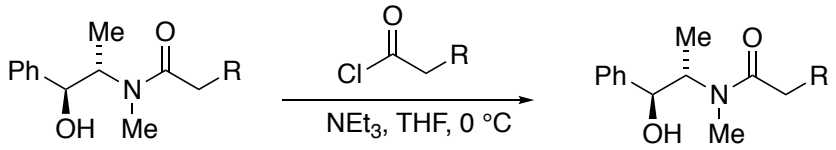
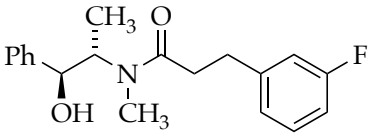


Figure 26. ^{15}N NMR spectrum of [^{15}N]-isoquinoline in $CDCl_3$ at 25 °C.



Substrates **12, 14, 15, 18** was synthesized using the procedure from Myers, A. G.; Yang, B. H.; Chen, H.; McKinstry, L.; Kopecky, D. J.; Gleason, J. L. *J. Am. Chem. Soc.* **1997**, *119*, 6496.



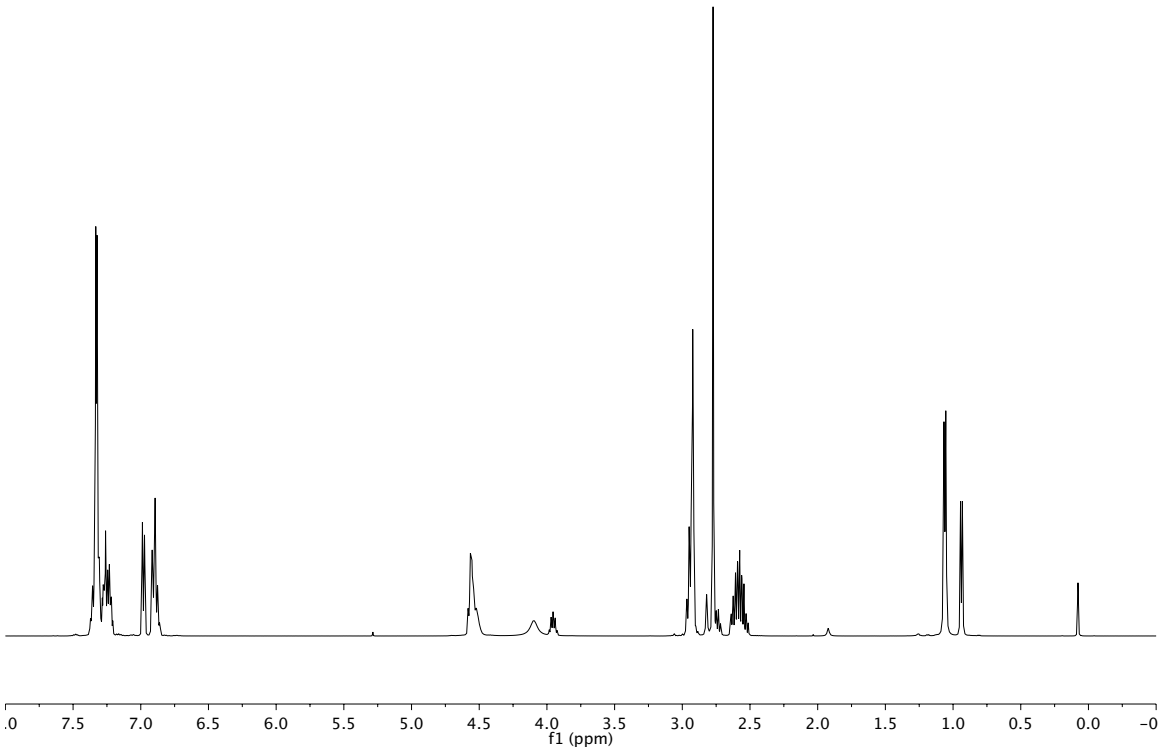


Figure 27. ^{1}H NMR spectrum of (*S,S*)-**12** in $CDCl_3$ at 25 °C.

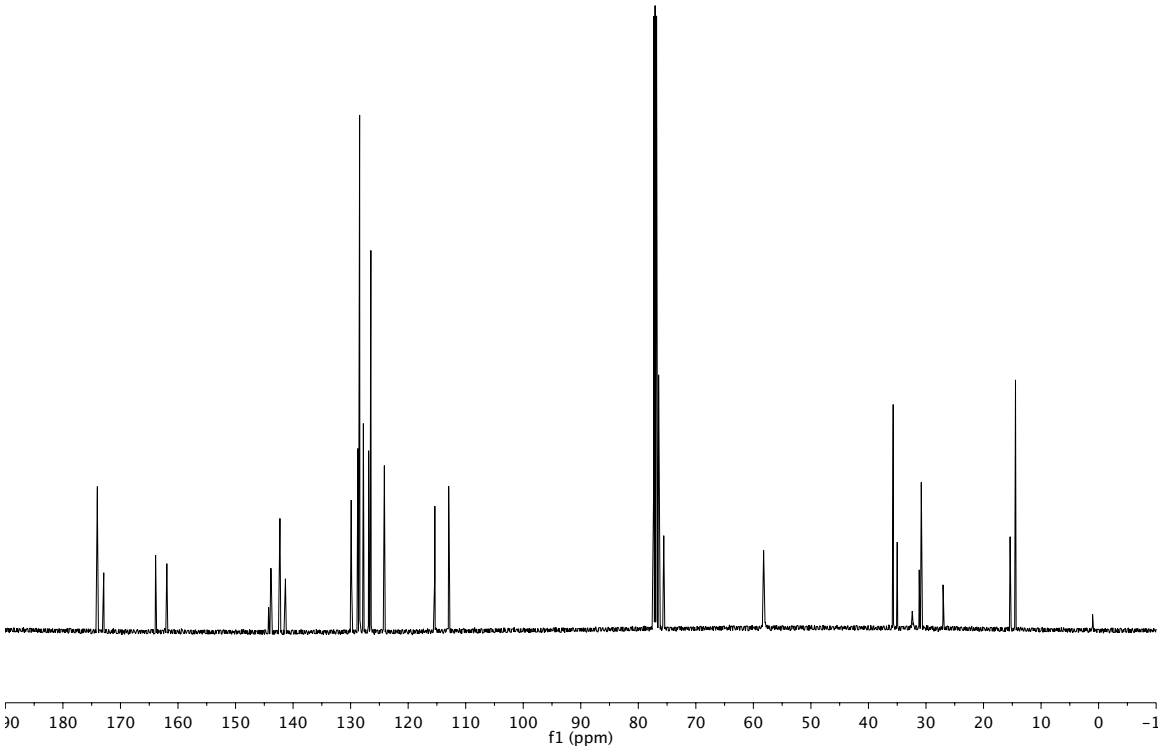


Figure 28. ^{13}C NMR spectrum of (*S,S*)-**12** in $CDCl_3$ at 25 °C.

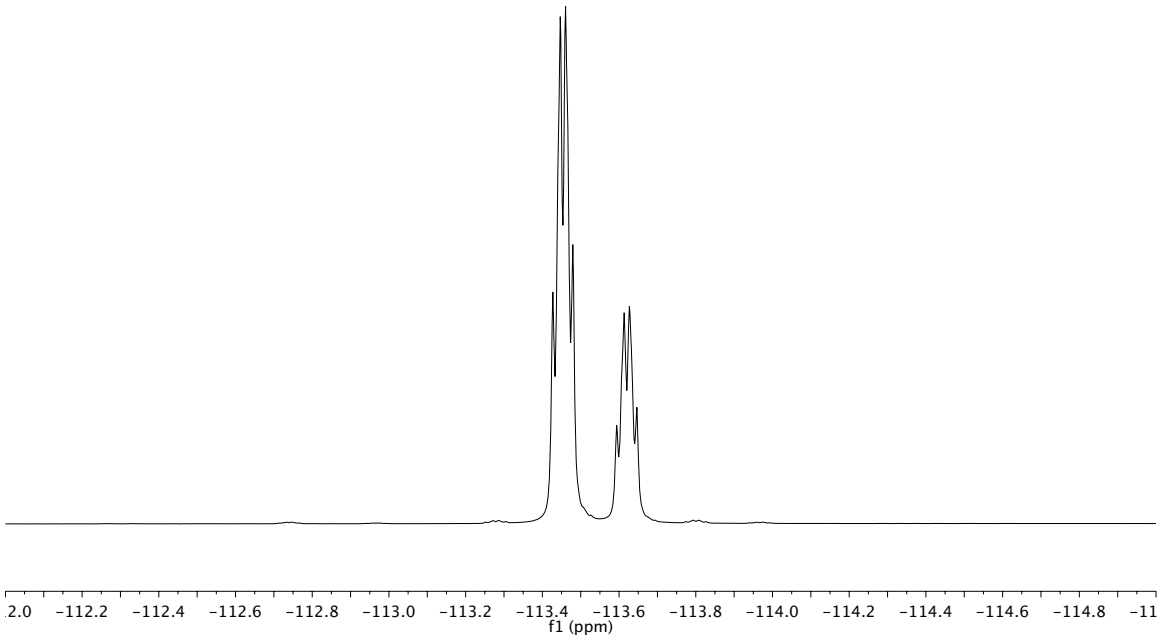


Figure 29. ^{19}F NMR spectrum of (*S,S*)-**12** in $CDCl_3$ at 25 °C.

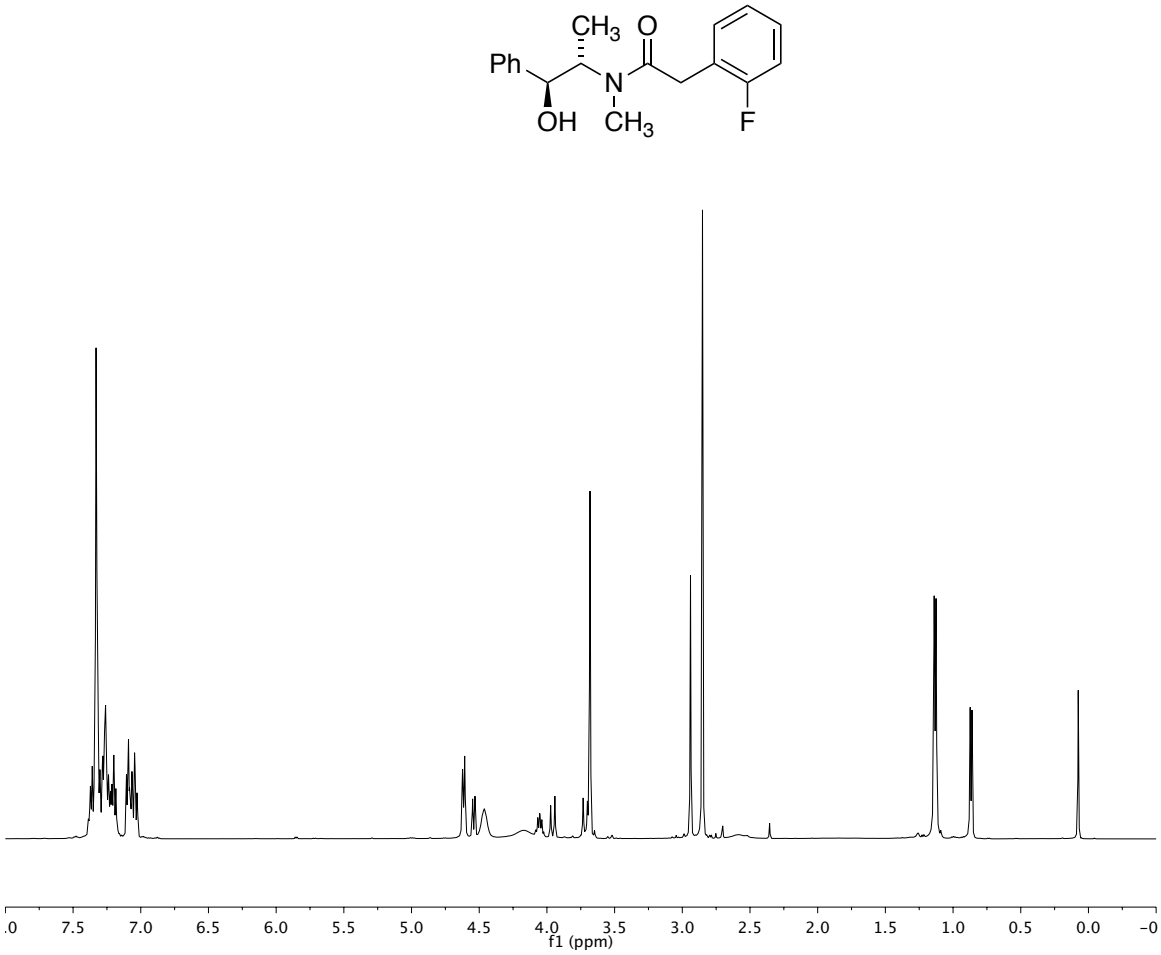


Figure 30. ^{1}H NMR spectrum of (*S,S*)-**14** in $CDCl_3$ at 25 °C.

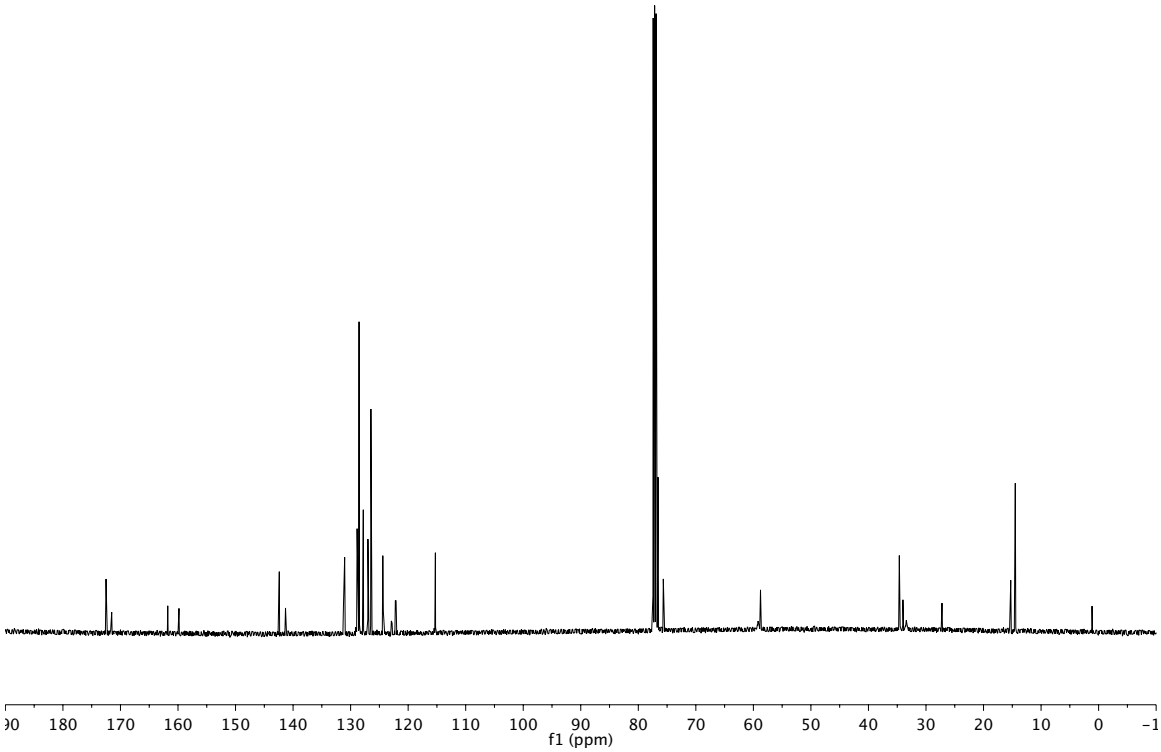


Figure 31. ^{13}C NMR spectrum of (*S,S*)-**14** in $CDCl_3$ at 25 °C.

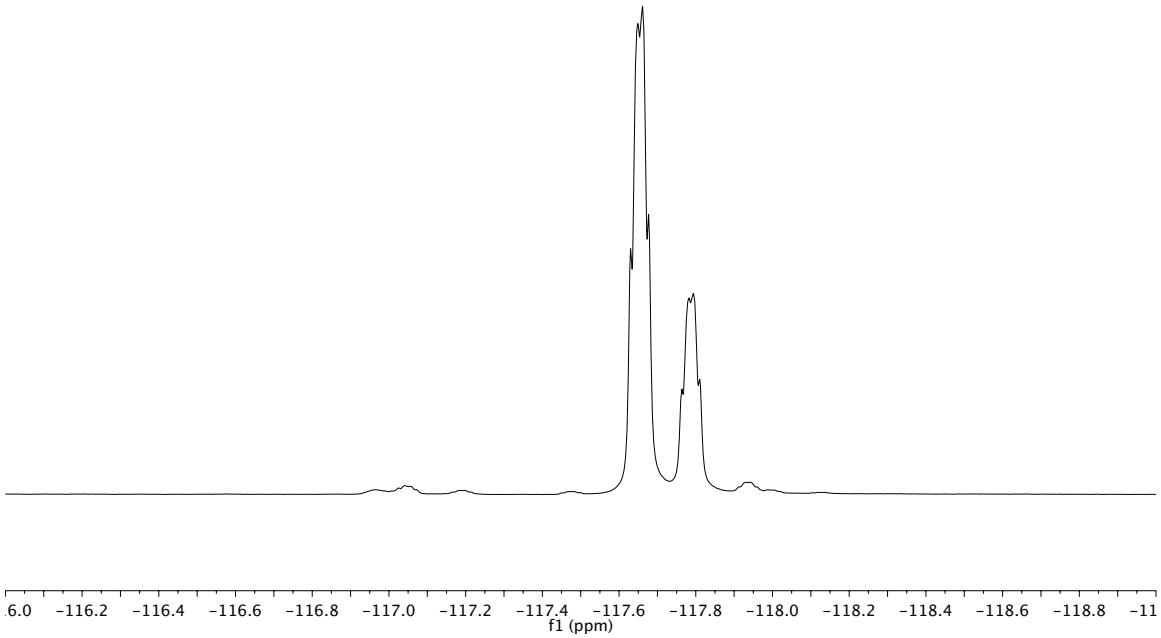


Figure 32. ^{19}F NMR spectrum of (*S,S*)-**14** in $CDCl_3$ at 25 °C.

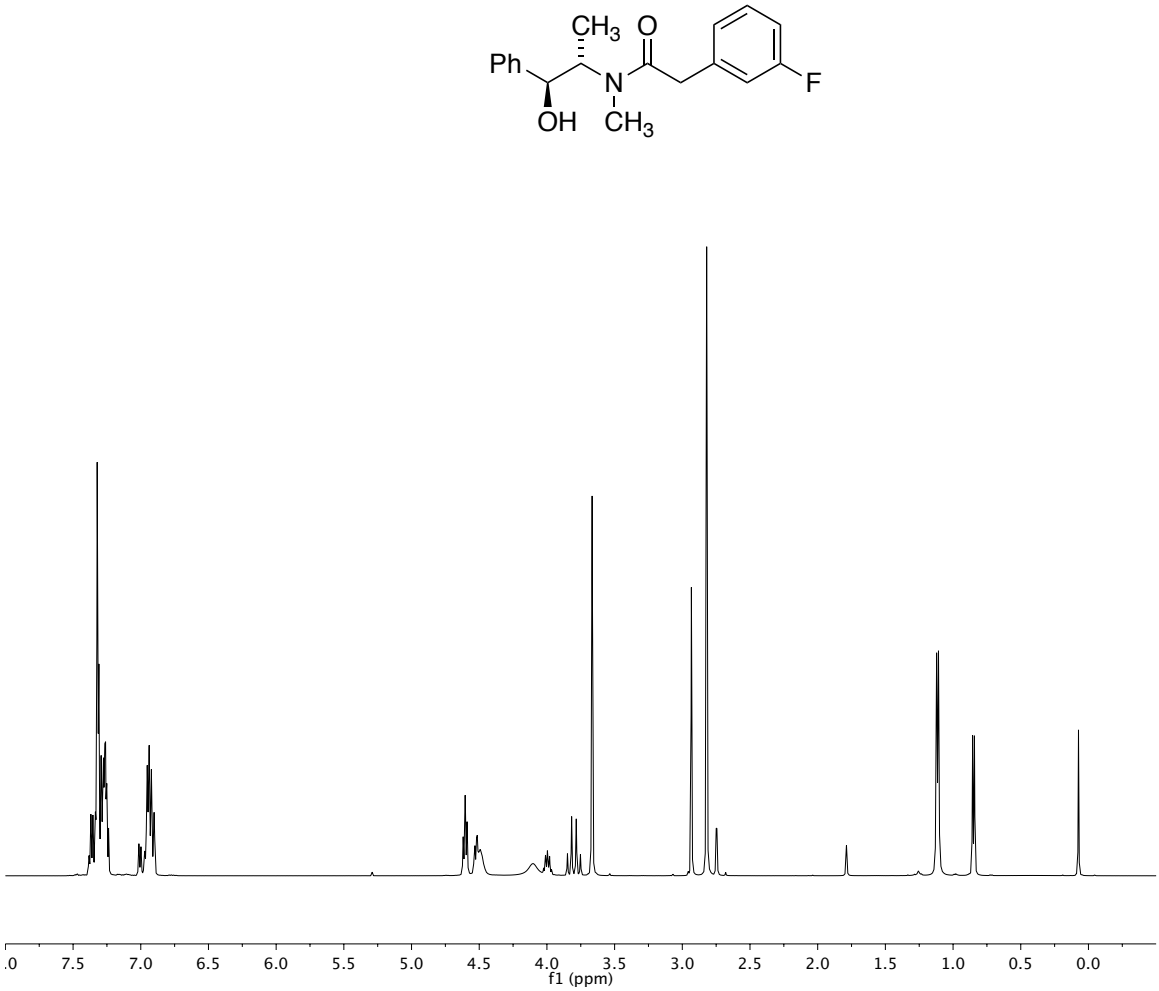


Figure 33. ^{1}H NMR spectrum of (*S,S*)-**15** in $CDCl_3$ at 25 °C.

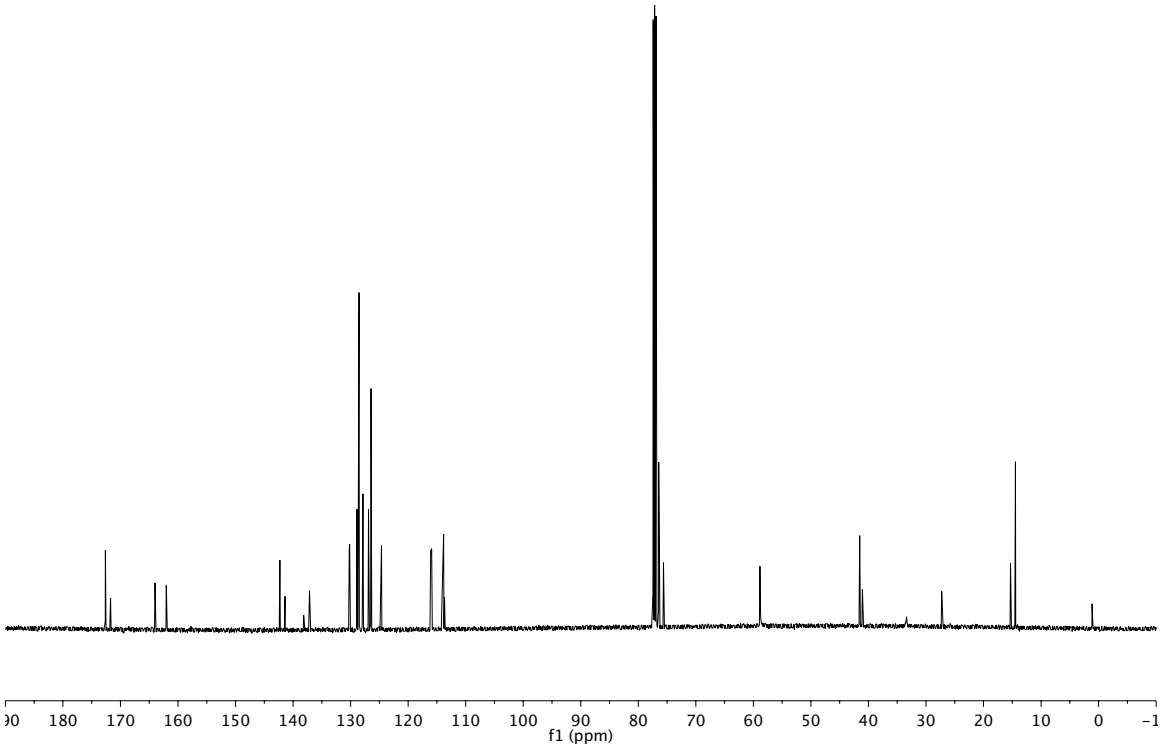


Figure 34. ^{13}C NMR spectrum of (*S,S*)-**15** in $CDCl_3$ at 25 °C.

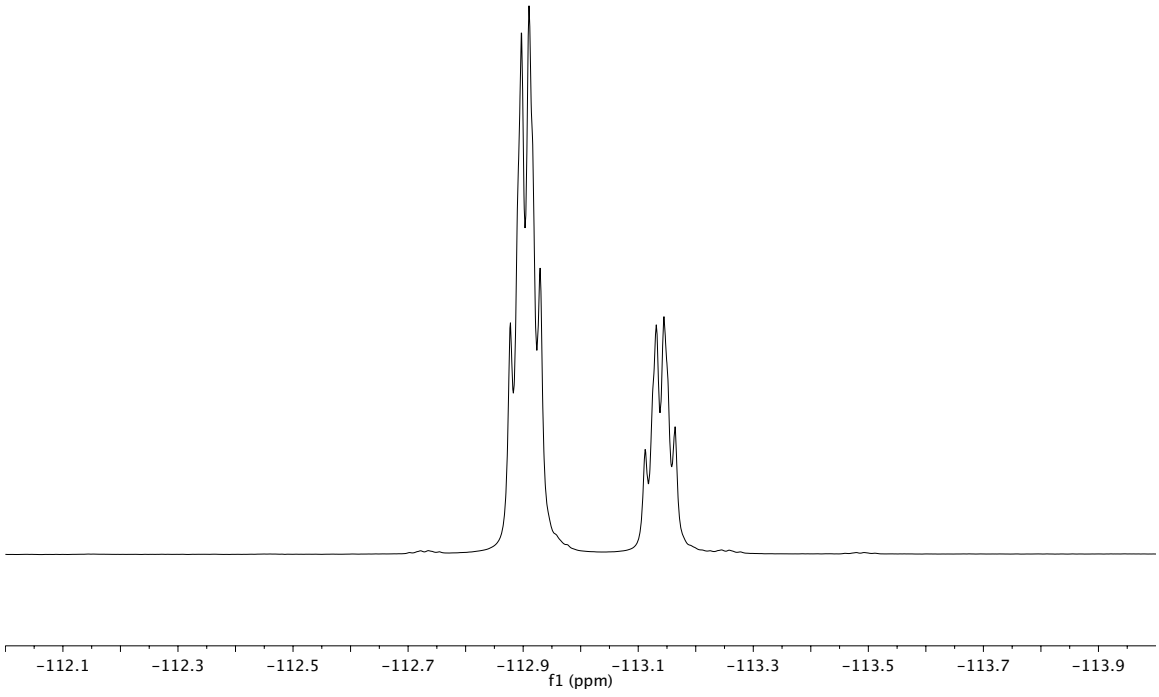


Figure 35. ^{19}F NMR spectrum of (*S,S*)-**15** in $CDCl_3$ at 25 °C.

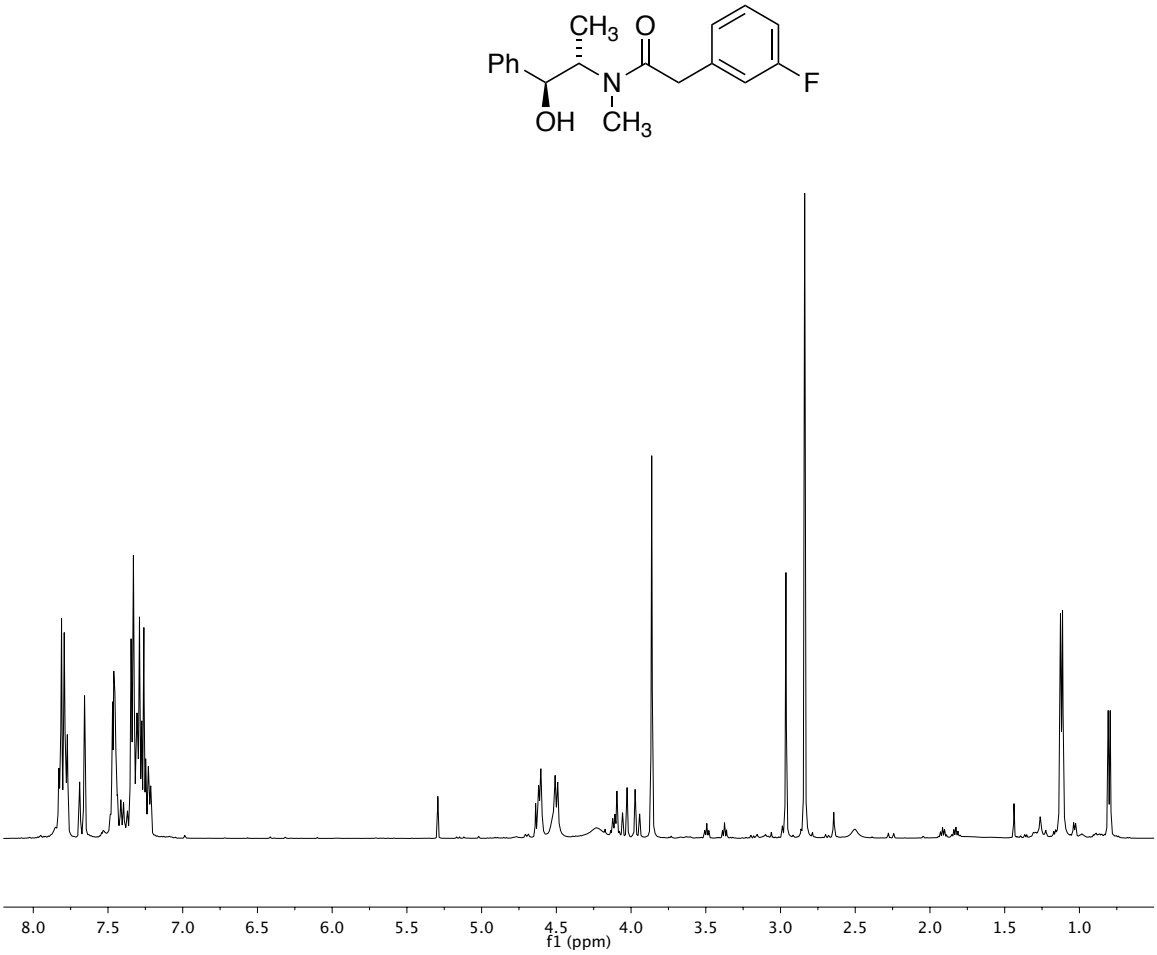


Figure 36. ^{1}H NMR spectrum of (*S,S*)-**18** in $CDCl_3$ at 25 °C.

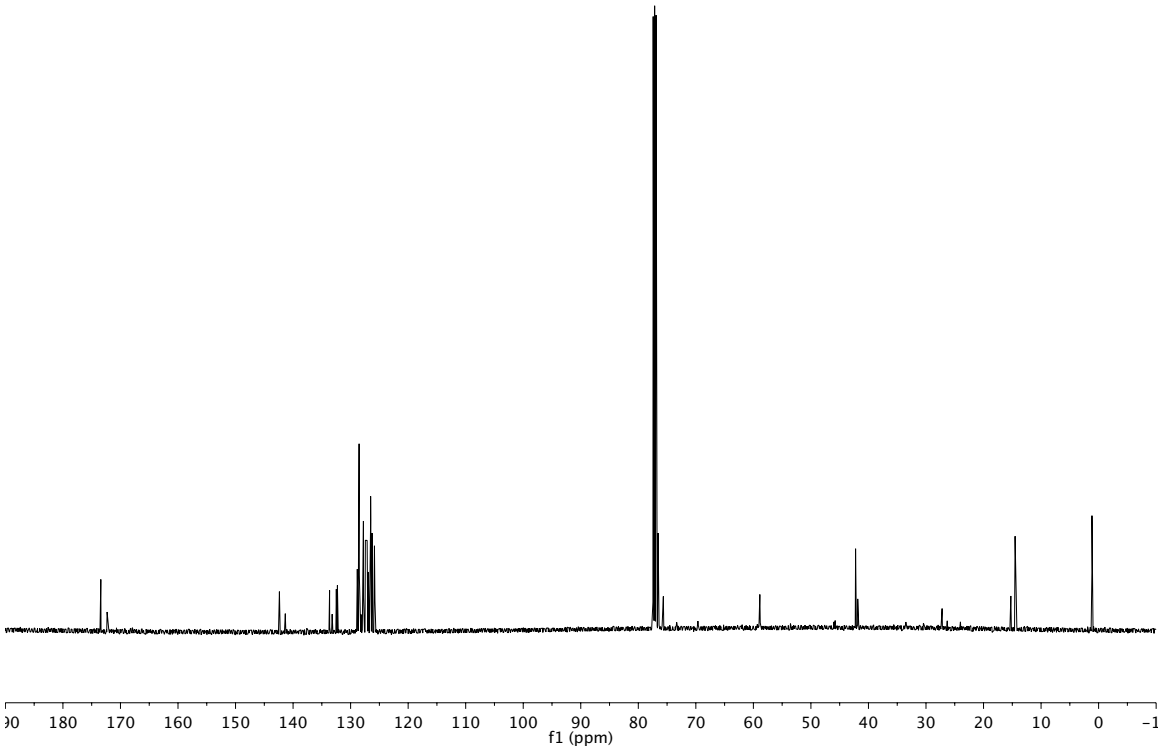


Figure 37. ^{13}C NMR spectrum of (*S,S*)-**18** in $CDCl_3$ at 25 °C.

Part 2 Homoaggregate 4 Characterization

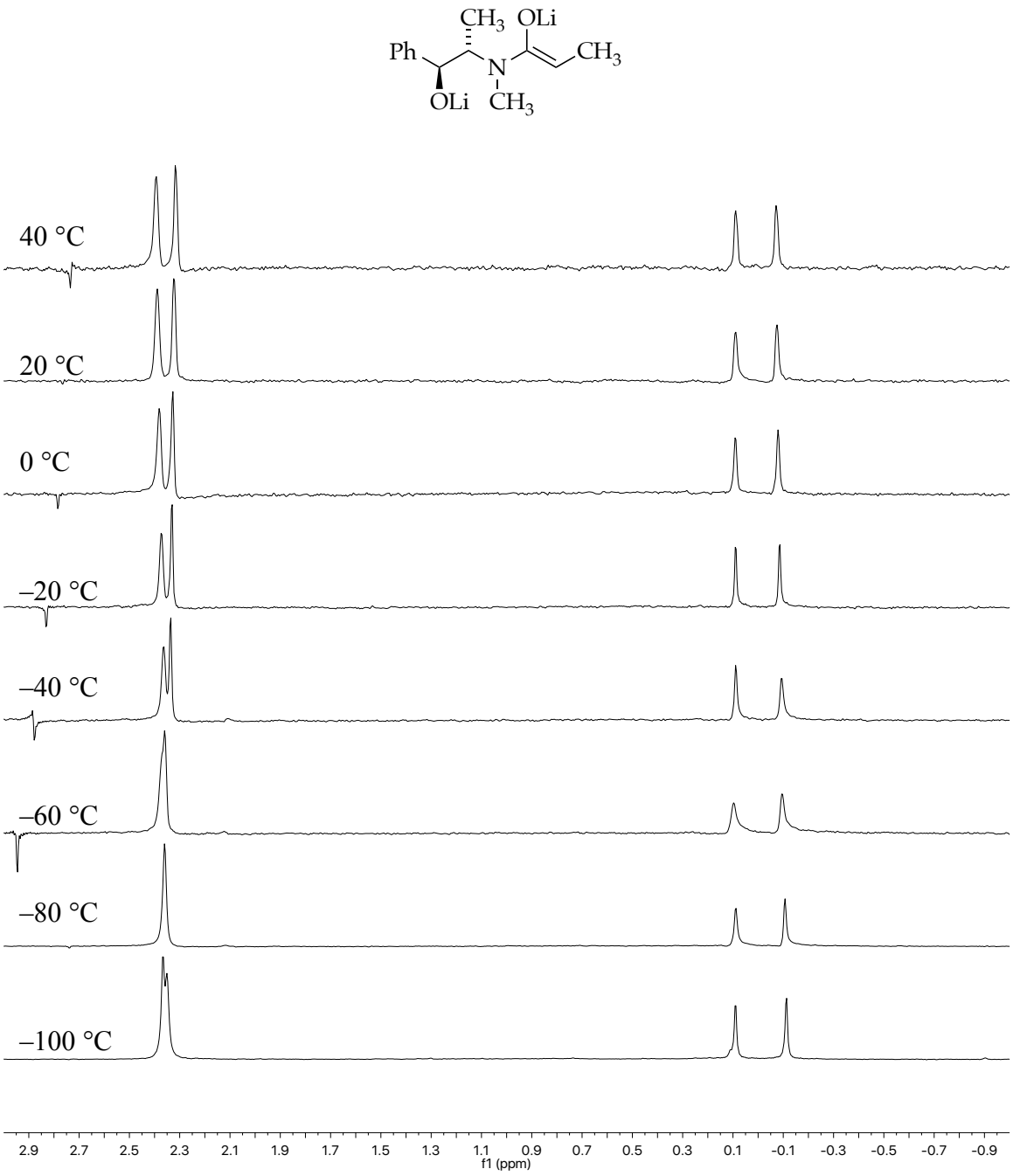


Figure 38. ^{6}Li NMR spectra of an aged solution of 0.10 M [^{6}Li]-(*S,S*)-**2** in 12.3 M THF at varying temperature showing temperature-dependent resolution. T1 relaxation was not optimized for integration.

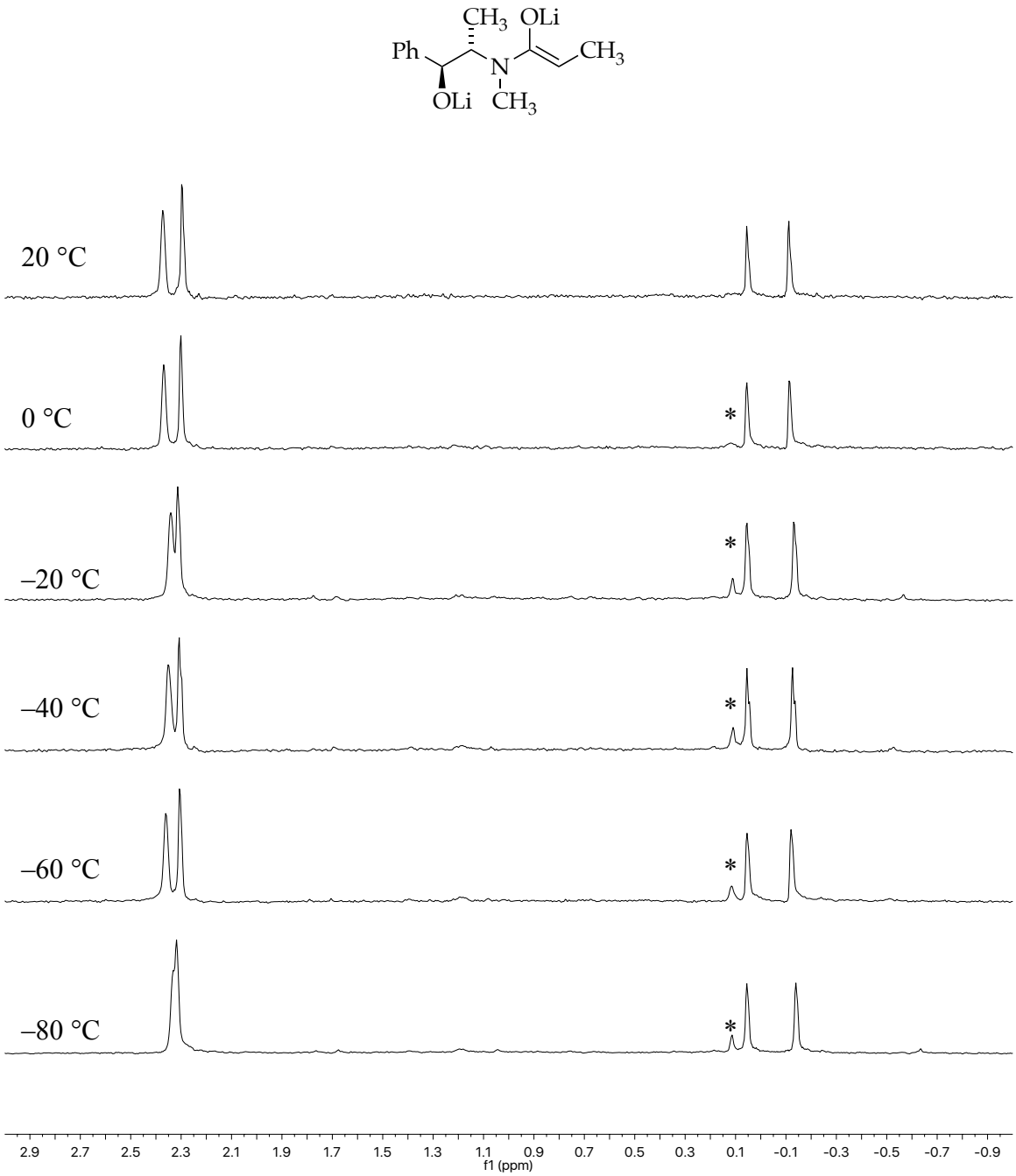


Figure 39. ^{6}Li NMR spectra of an aged solution of 0.10 M [^{6}Li]-(*S,S*)-**2** in 6.1 M THF and 4.7 M toluene showing temperature-dependent resolution. The peak at 0.055 ppm (*) corresponds to alkoxides owing to a slight deficiency of LDA. T1 relaxation was not optimized for integration.

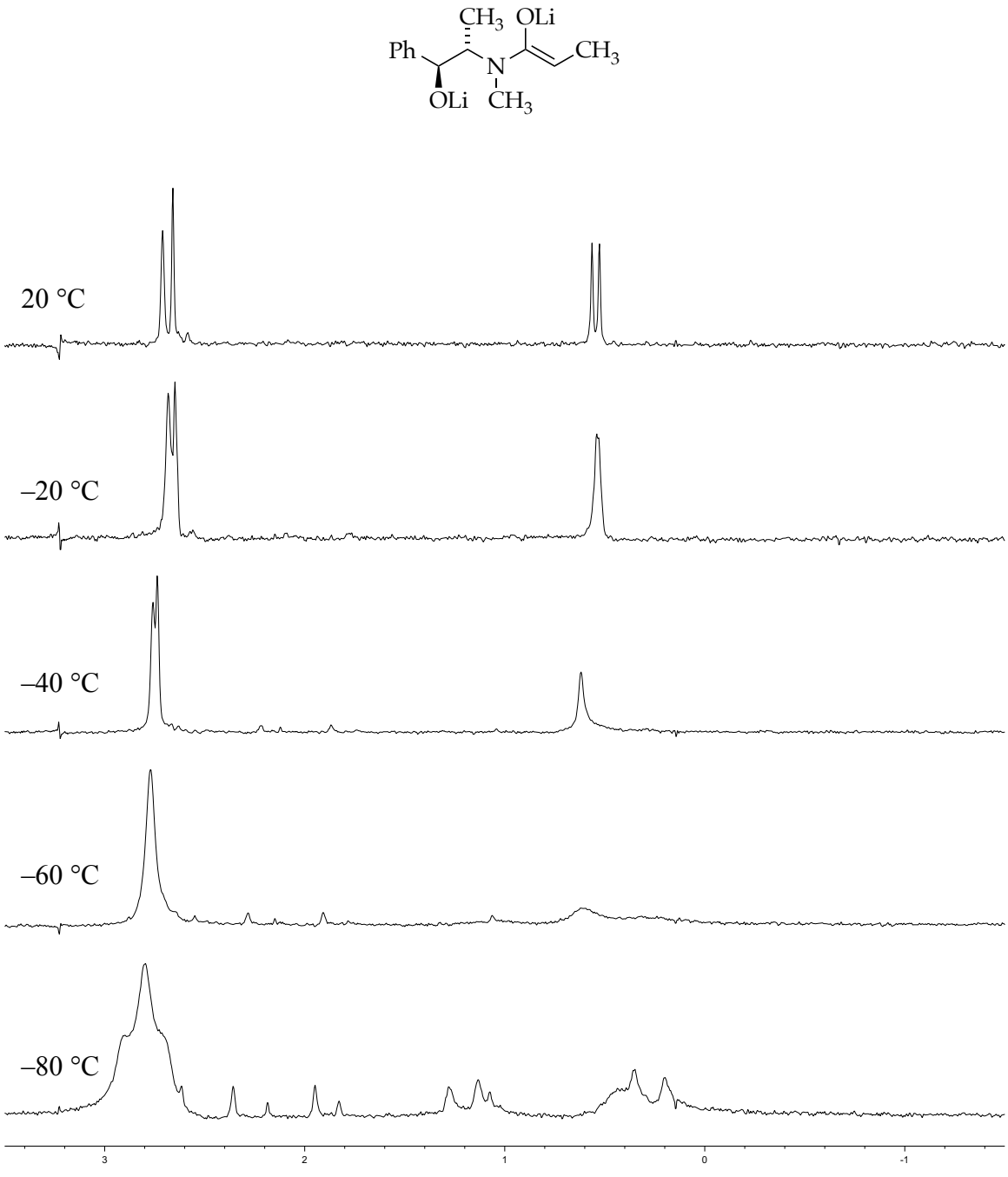


Figure 40. ^{6}Li NMR spectra of an aged solution of 0.10 M [^{6}Li]-(*S,S*)-**2** in 2.0 M THF, 0.20 M pyridine/toluene at varying temperature showing poor resolution of pyridine-solvated resonances. T1 relaxation was not optimized for integration.

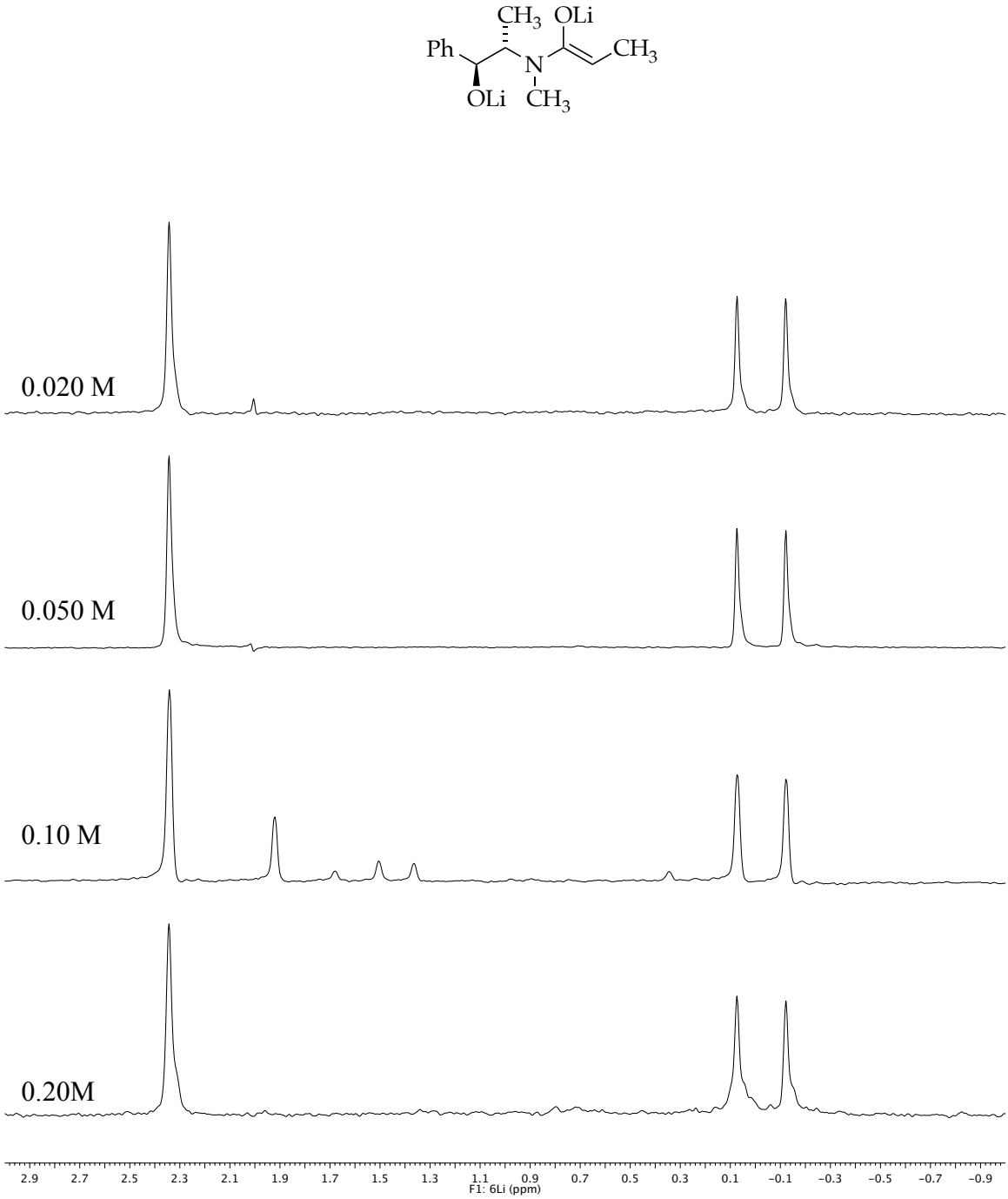


Figure 41. ^{6}Li NMR spectra of aged solutions of [^{6}Li]-(*S,S*)-**2** in 12.3 M THF at –80 °C temperature with varying enolate concentrations showing no change in relative integration of the four peaks.

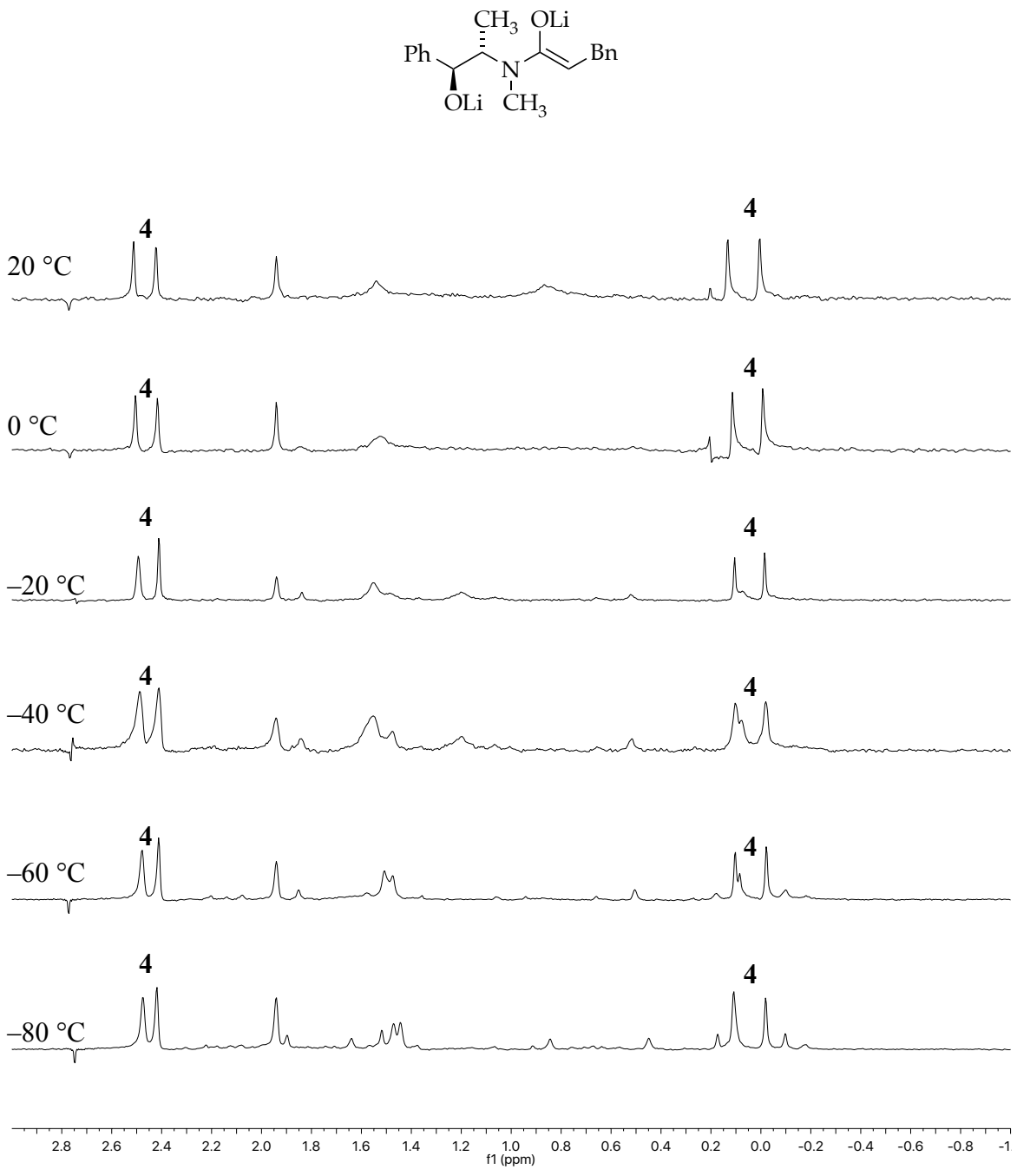


Figure 42. ^{6}Li NMR spectra of an aged solution of 0.10 M [^{6}Li]-(*S,S*)-**11** in 12.3 M THF at varying temperature showing resonances(*) characteristic of octalithiated homoaggregate (**4**). Resonances in the 0.40–2.0 ppm range are LDA-mixed aggregates owing to excess LDA.

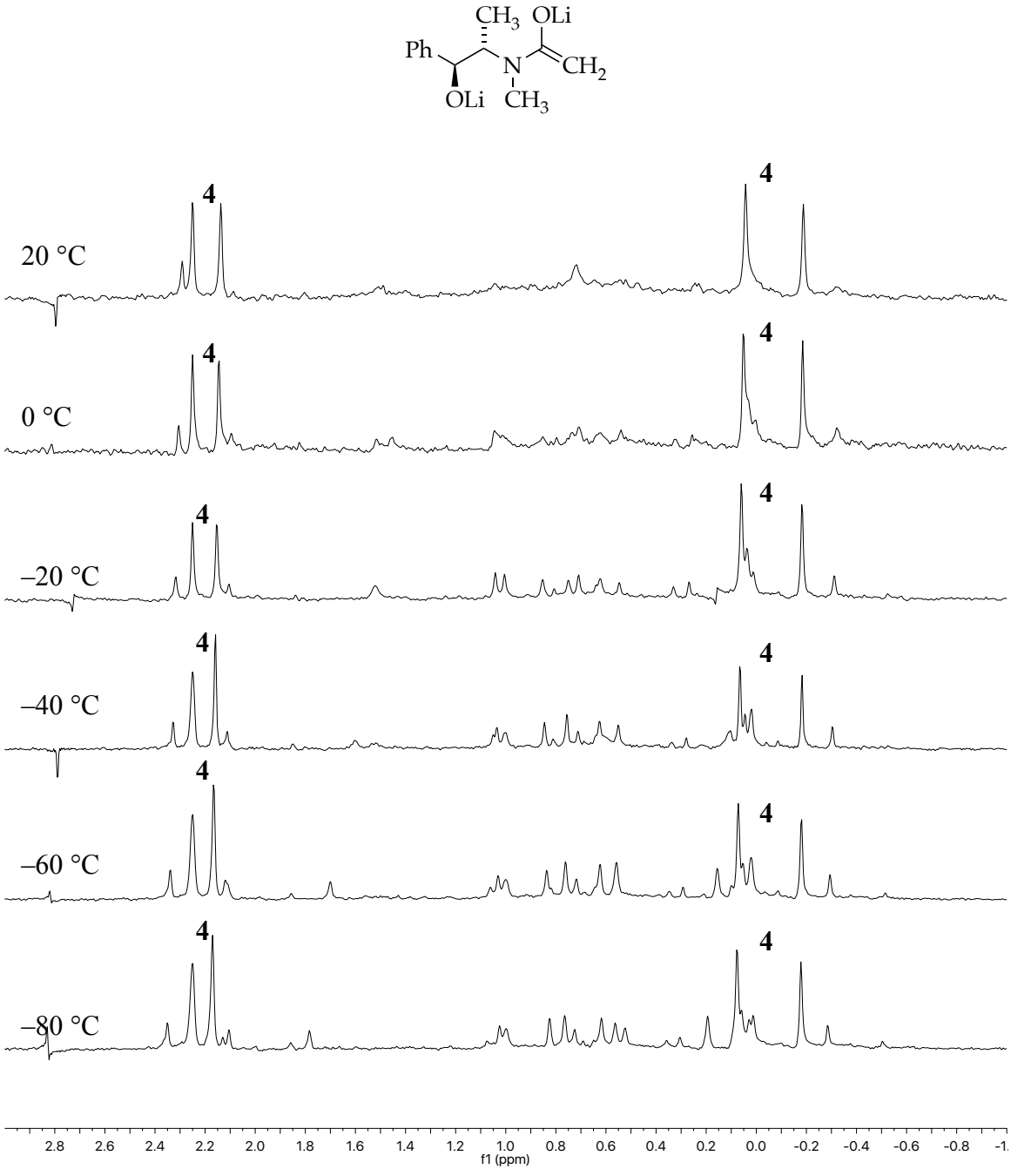


Figure 43. ^{6}Li NMR spectra of an aged solution of 0.10 M (*S,S*)-**7** in 12.3 M THF at varying temperature. Minor resonances are reproducible, appearing to be isomers instead of impurities. This experiment shows that (*S,S*)-**7** is not sterically hindered enough to produce structurally stabilized enolates.

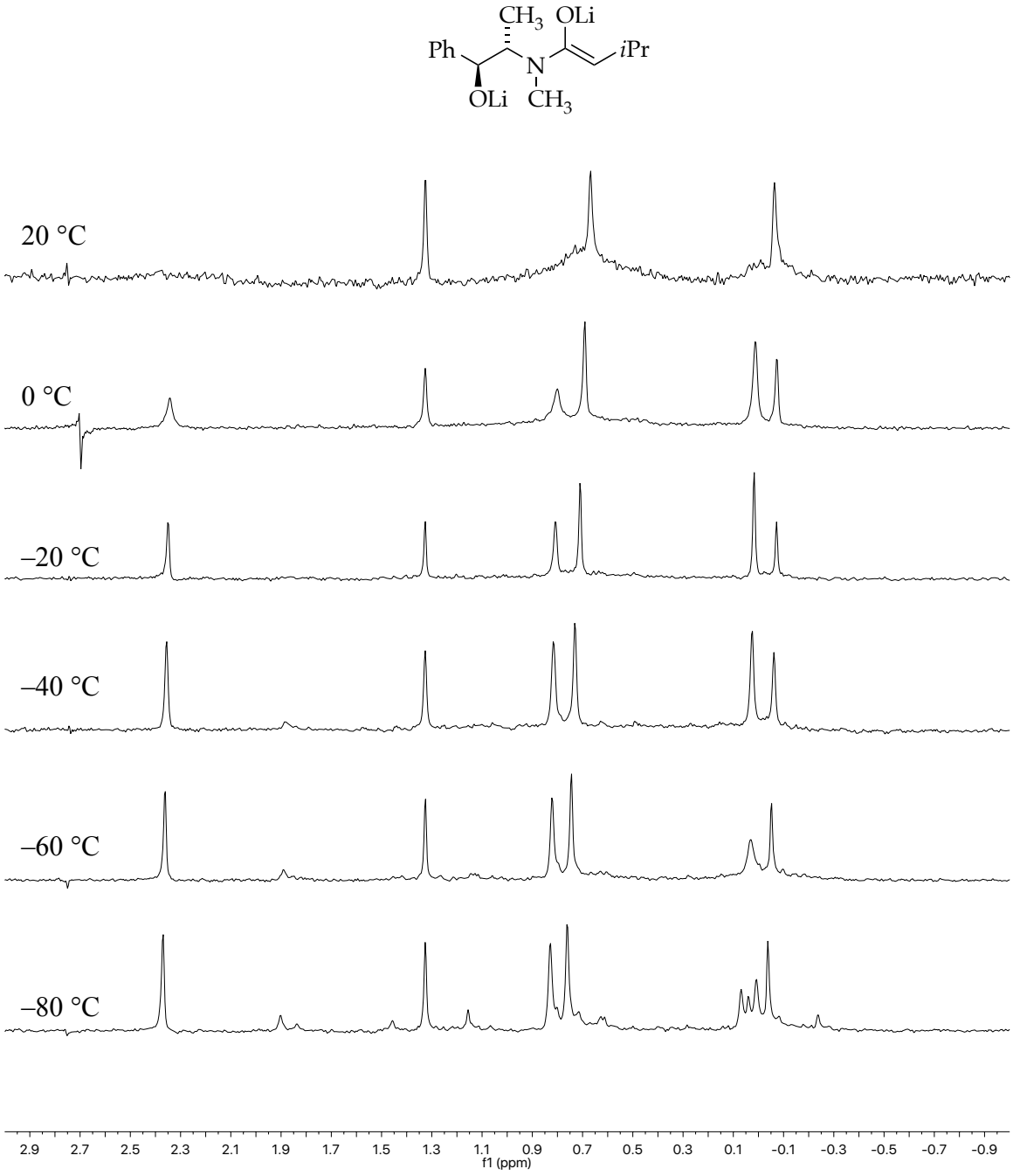


Figure 44. ^{6}Li NMR spectra of an aged solution of 0.10 M [^{6}Li]-(*S,S*)-**9** in 12.3 M THF at varying temperature showing a complex mixture.

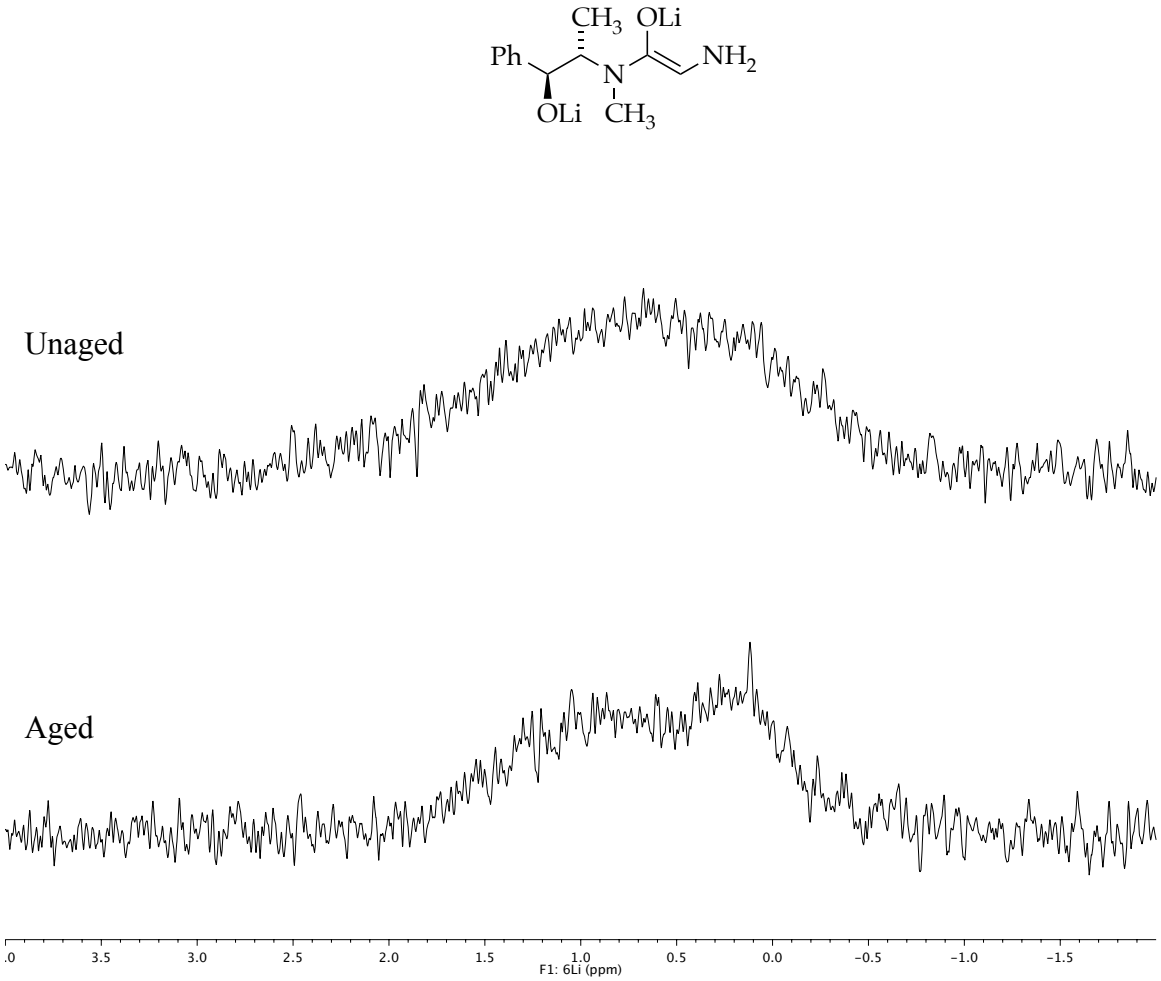


Figure 45. ^{6}Li NMR spectra of a solution of 0.10 M [^{6}Li]-(*S,S*)-**22** in 12.3 M THF at –80 °C showing hopelessly broad resonancest.

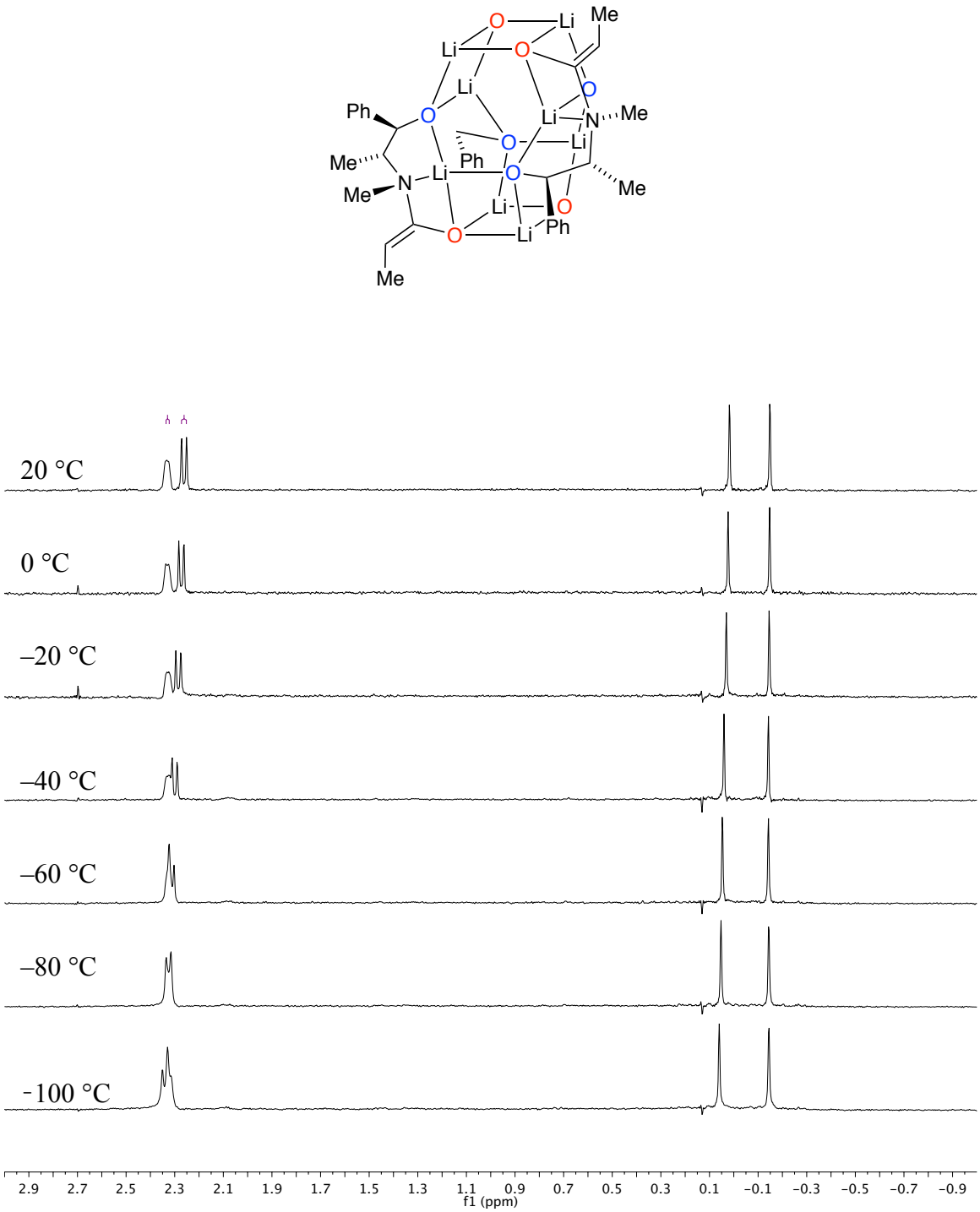


Figure 46. ^{6}Li NMR spectra of an aged solution of 0.10 M [^{6}Li,^{15}N]-(*S,S*)-**2** in 12.3 M THF at varying temperature. This experiment shows Li–N contacts (20 °C, δ 2.33 ppm (d, J = 0.89 Hz), 2.26 ppm (d, J = 1.5 Hz)), two of the four kinds of lithium atoms are coupled to nitrogen.

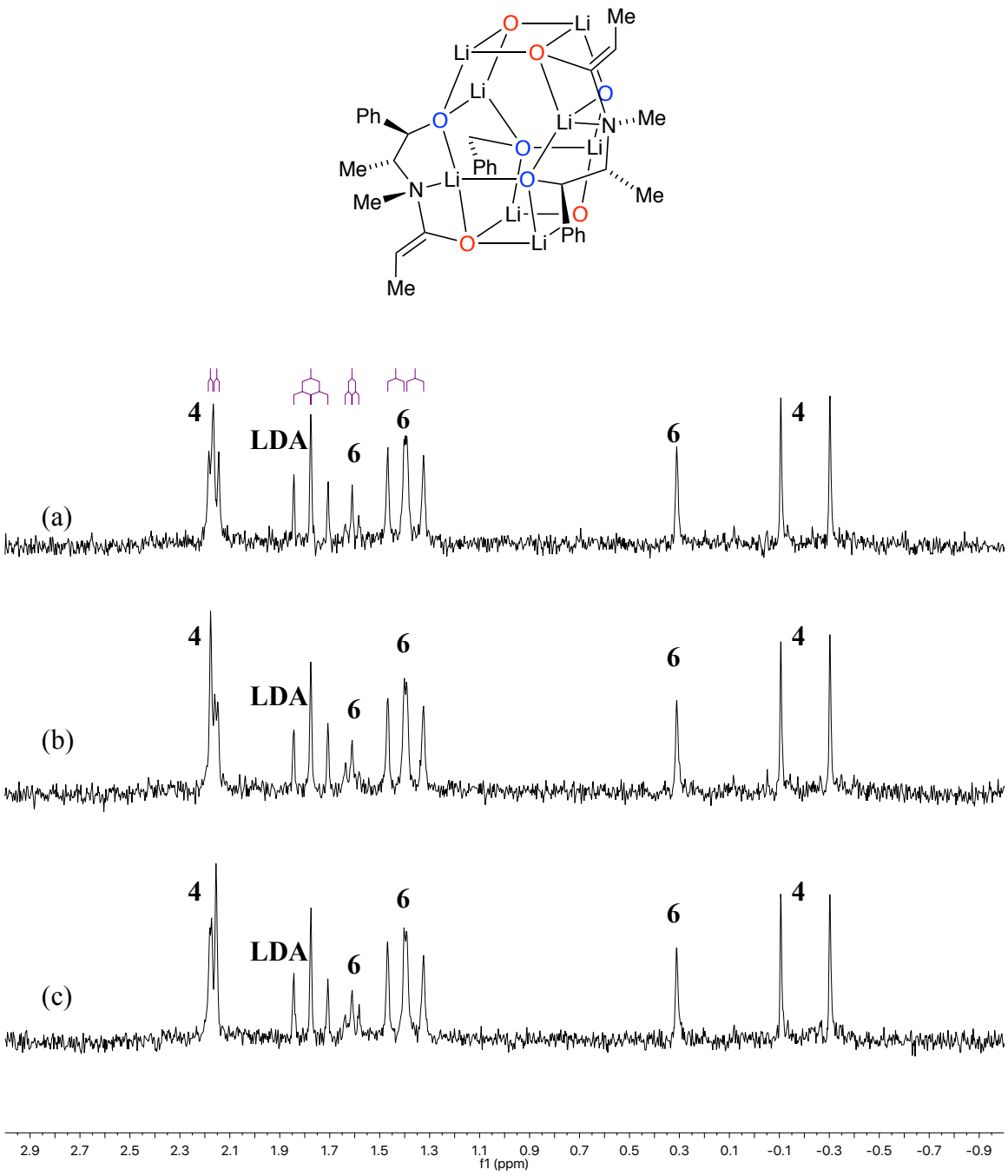


Figure 47. ^{6}Li NMR spectra of 0.050 M [^{6}Li,^{15}N]-(*S,S*)-**2** in 2.0 M THF and 7.9 M toluene at –80 °C, (a) no decoupling; (b) selective ^{15}N decoupling at 56.2 ppm; (c) selective ^{15}N decoupling at 55.8 ppm(–80 °C, δ 2.20 ppm (d, J = 0.51 Hz), 2.16 ppm (d, J = 0.95 Hz)). Resonances in the 0.3 – 2.1 ppm range are from LDA-mixed aggregates.

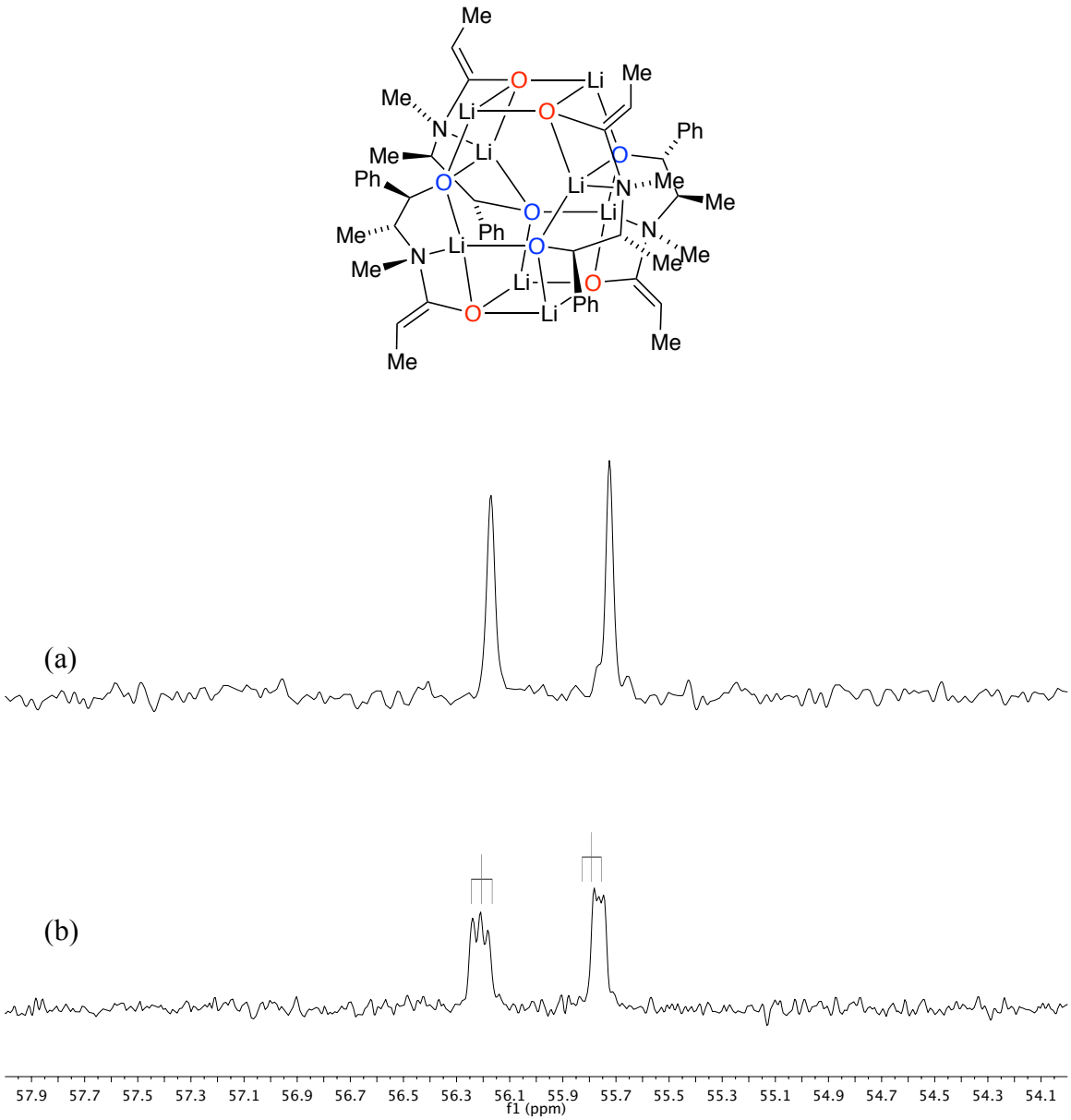


Figure 48. ^{15}N NMR spectra of an aged solution of 0.050 M [^{6}Li,^{15}N]-(*S,S*)-**2** in 2.0 M THF and 7.9 M toluene at –80 °C, (δ 56.2 ppm (d, J = 1.3 Hz), 55.7 ppm (d, J = 0.85 Hz)), (a) broadband decoupling; (b) no decoupling.

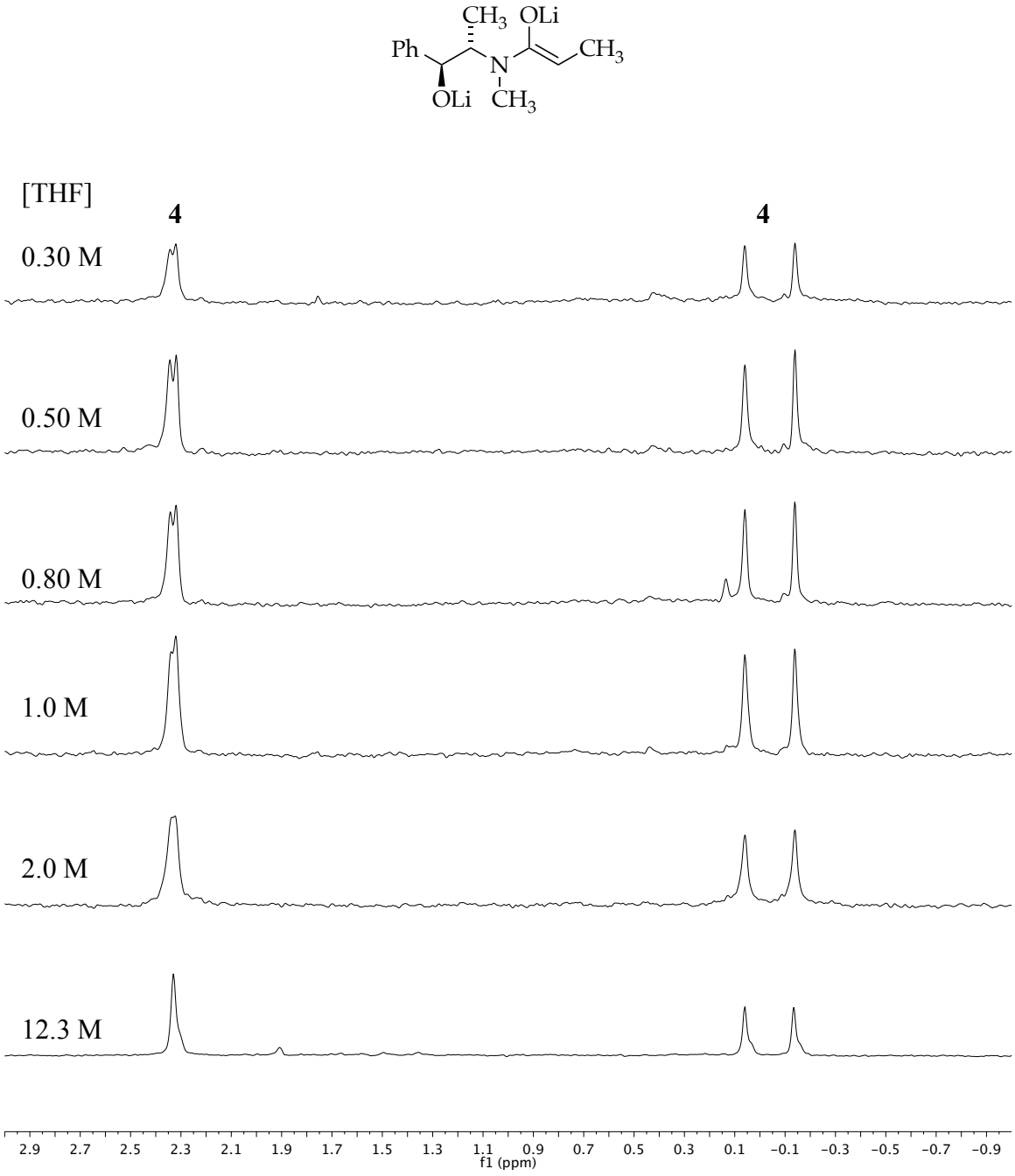
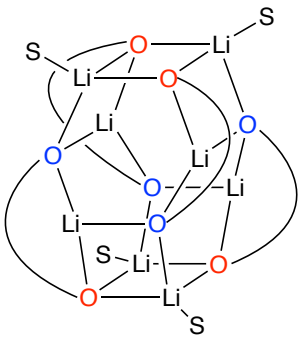


Figure 49. ^{6}Li NMR spectra of an aged solution of 0.10 M [^{6}Li]-(*S,S*)-**2** in toluene at –80 °C. This experiment shows that peaks at 2.3 ppm can be resolved by adding toluene.



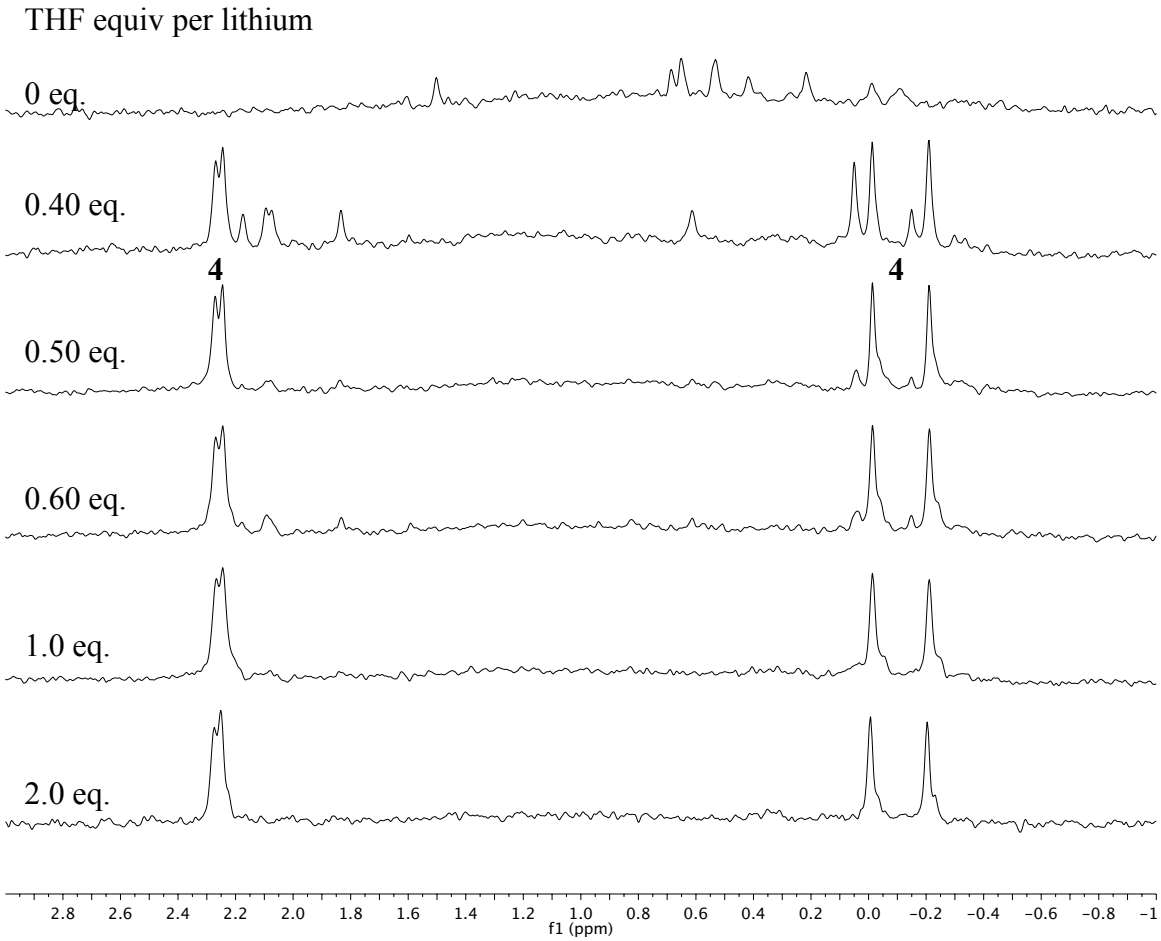


Figure 50. ^{6}Li NMR spectra of an aged solution of 0.050 M [^{6}Li]-(*S,S*)-**2** in toluene at –80 °C and varying THF concentration, confirming octalithiated homotetramer (**4**) contains four coordinated THF ligands.

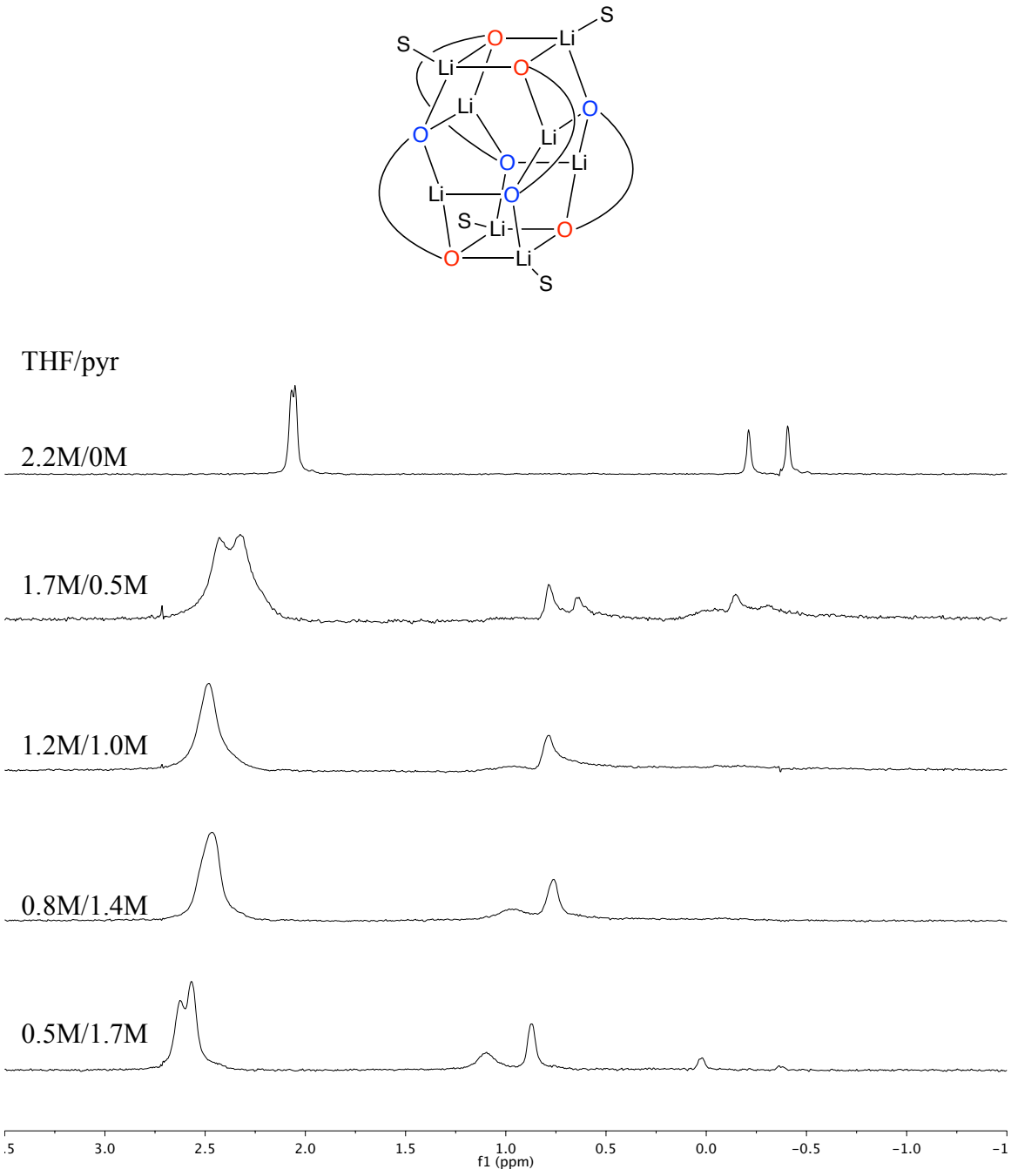


Figure 51. ^{6}Li NMR spectra of an aged solution of 0.10 M [^{6}Li]-(*S,S*)-**2** in 6.4 M toluene at –80 °C with varying THF and pyridine concentrations. T1 relaxation was not optimized for integration. All four peaks from the homotetramers are shifted by pyridine. However, the upfield peaks show a greater shift than downfield peaks owing to direct coordination by pyridine.

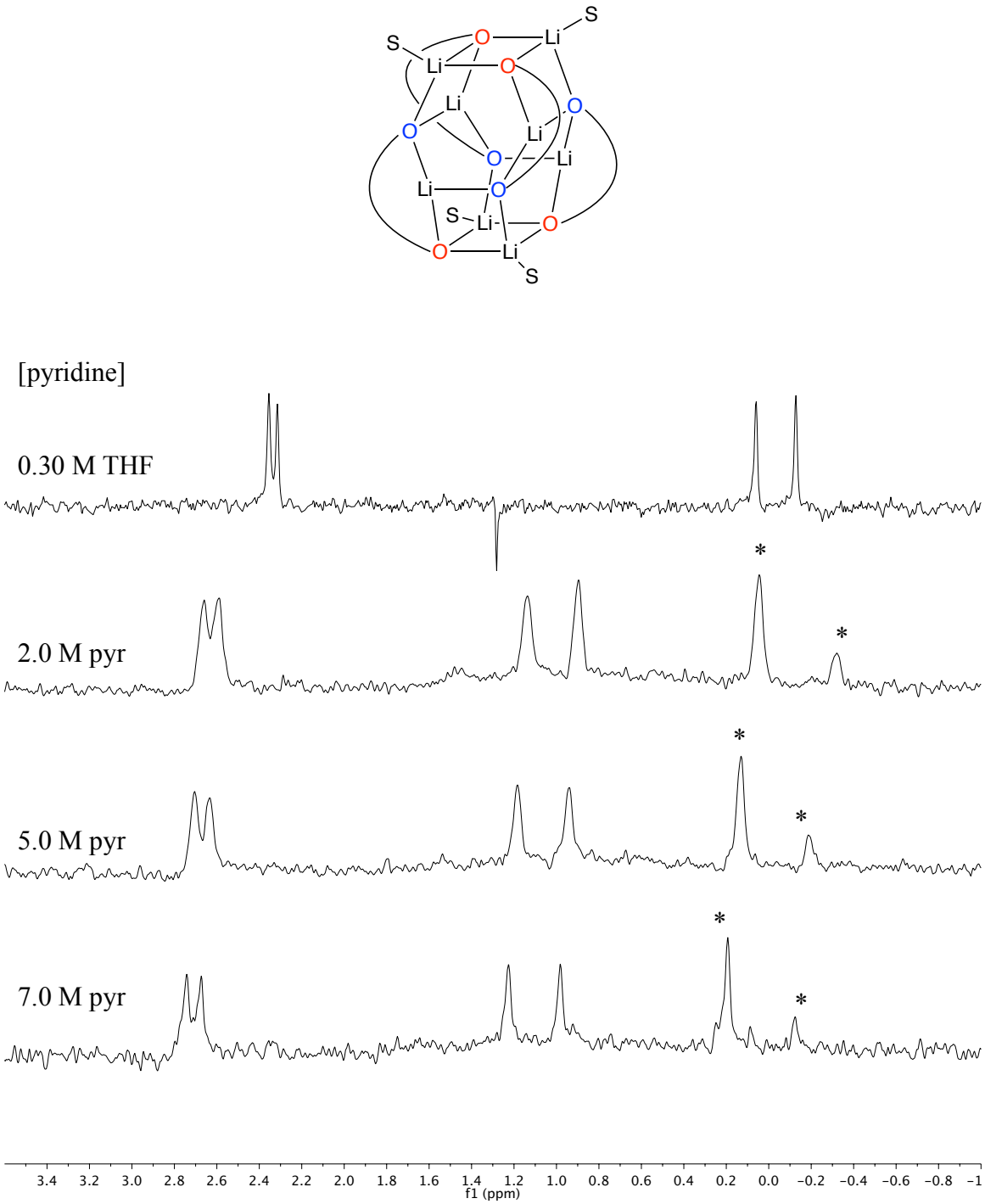


Figure 52. ^{6}Li NMR spectra of an aged solution of 0.10 M [^{6}Li]-(*S,S*)-**2** at –80 °C in toluene with varying pyridine concentration. T1 relaxation was not optimized for integration. Peaks labeled as asterisks (*) are not characterized. The upfield peaks are shifted markedly downfield indicative of direct coordination by pyridine.

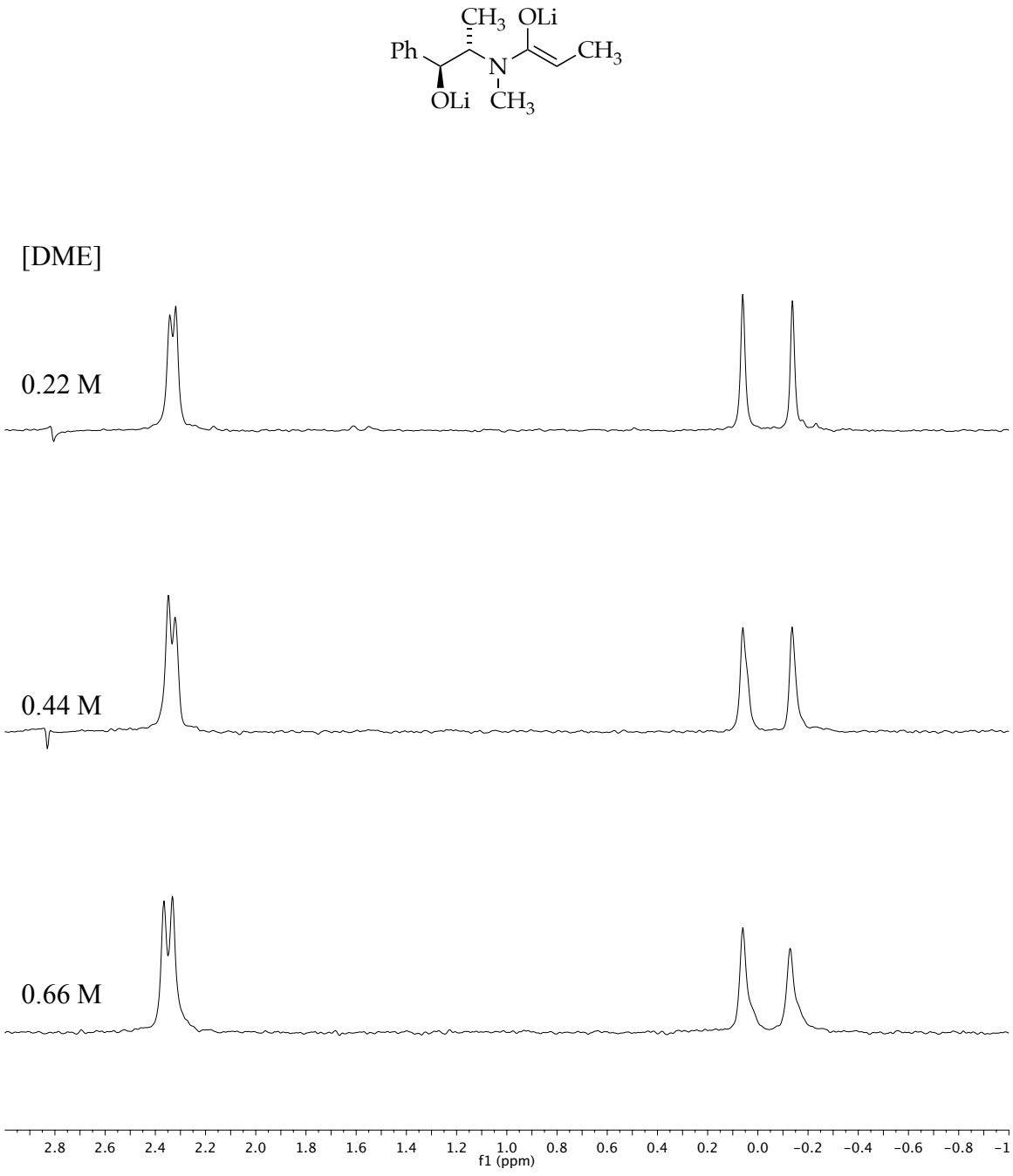


Figure 53. ^{6}Li NMR spectra of an aged solution of 0.10 M [^{6}Li]-(*S,S*)-**2** in 0.30 M THF/toluene at –80 °C with varying dimethoxyethane (DME) concentration showing no significant structural changes.

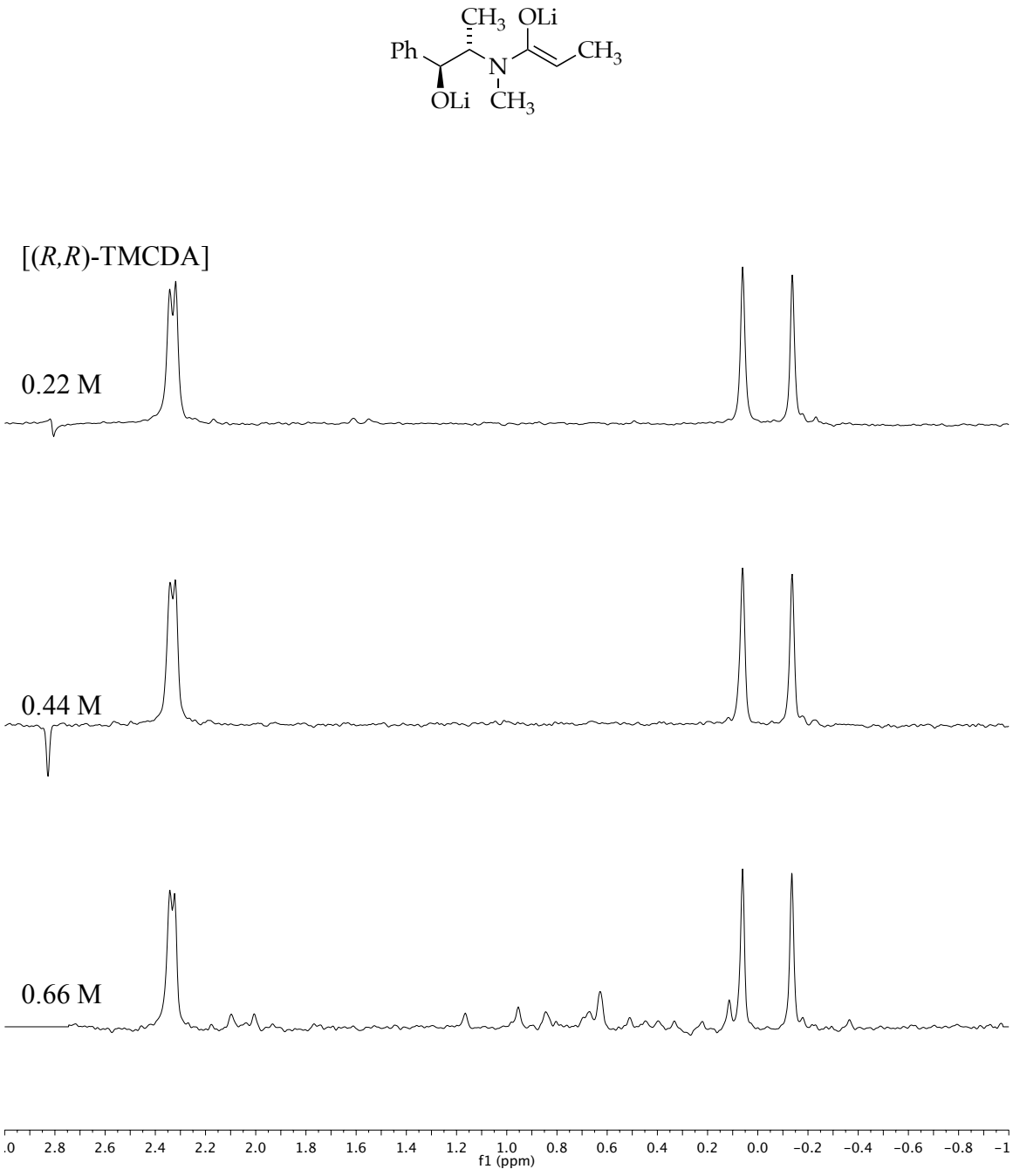


Figure 54. ^{6}Li NMR spectra of an aged solution of 0.10 M [^{6}Li]-(*S,S*)-**2** in 0.30 M THF/toluene at –80 °C with varying (*R,R*)-*trans*-*N,N,N′,N′*-tetramethyl-cyclohexanediamine ((*R,R*)-TMCDA) concentration showing no significant structural changes..

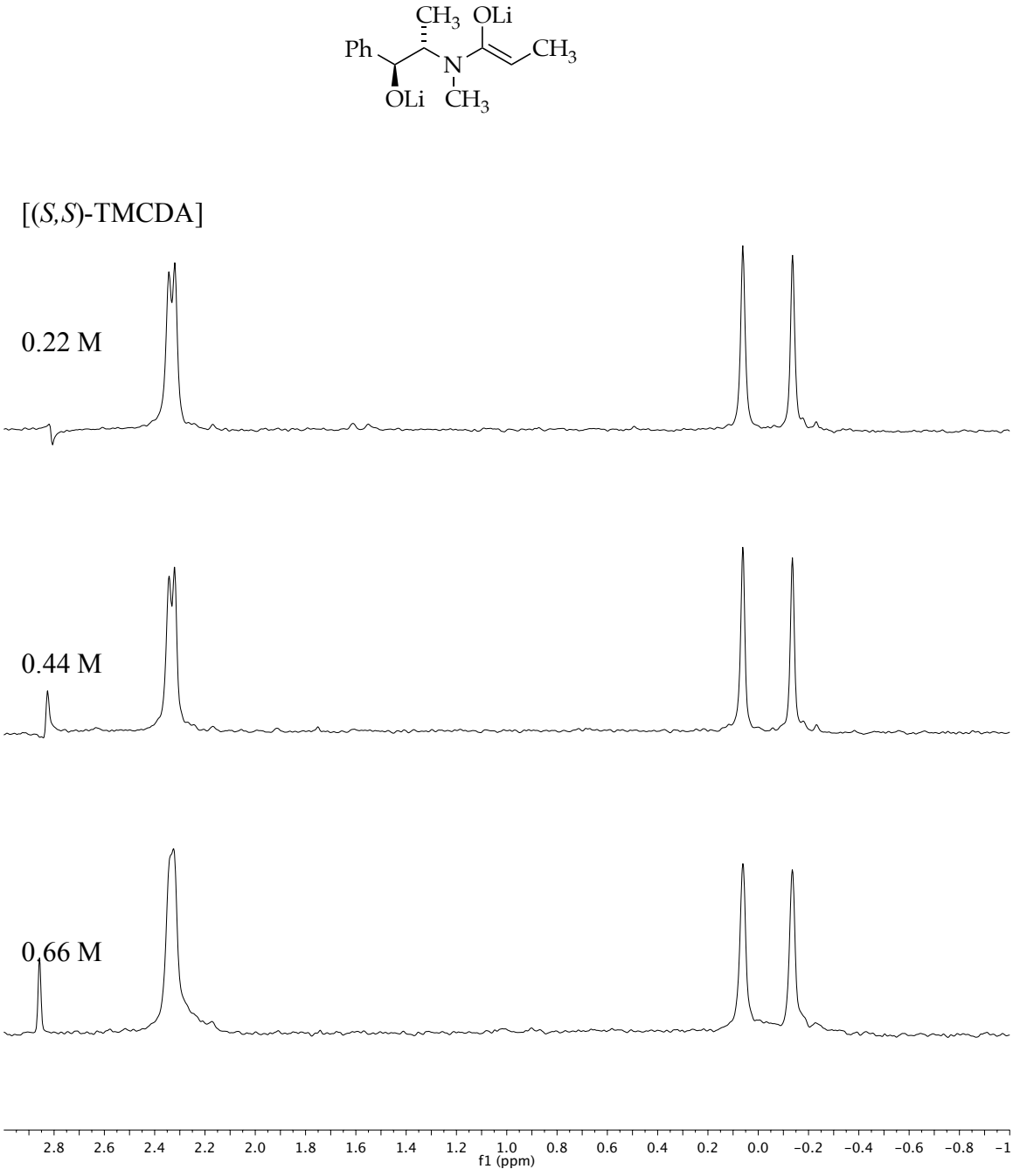


Figure 55. ^{6}Li NMR spectra of an aged solution of 0.10 M [^{6}Li]-(*S,S*)-**2** in 0.30 M THF/toluene at –80 °C with varying (*S,S*)-*trans*-*N,N,N′,N′*-tetramethylcyclohexanediamine ((*S,S*)-TMCDA) concentrations showing no significant structural changes.

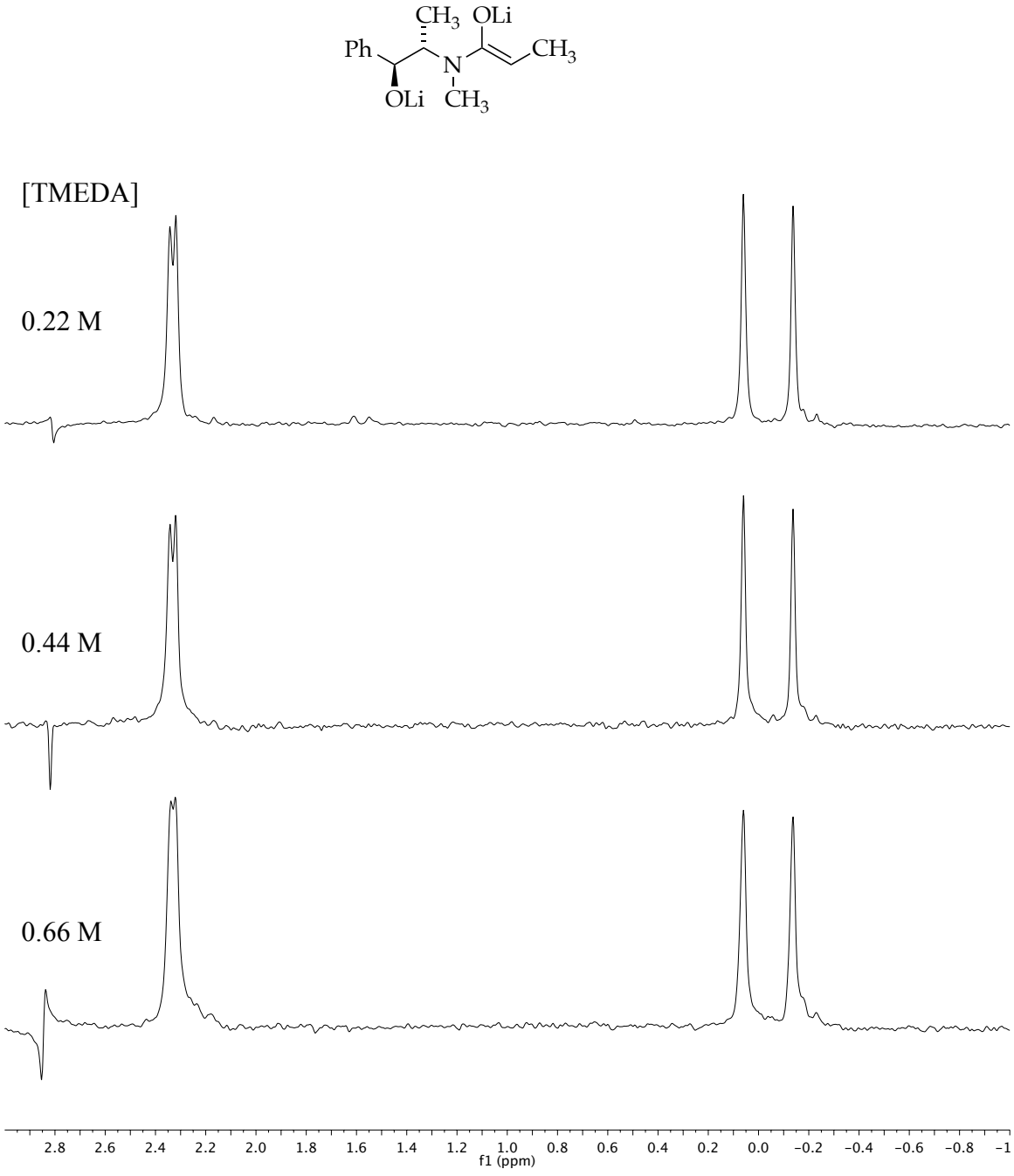


Figure 56. ^{6}Li NMR spectra of an aged solution of 0.10 M [^{6}Li]-(*S,S*)-**2** in 0.30 M THF/toluene at –80 °C with varying *N,N,N′,N′*-tetramethylethylenediamine (TMEDA) concentrations showing no significant structural changes.

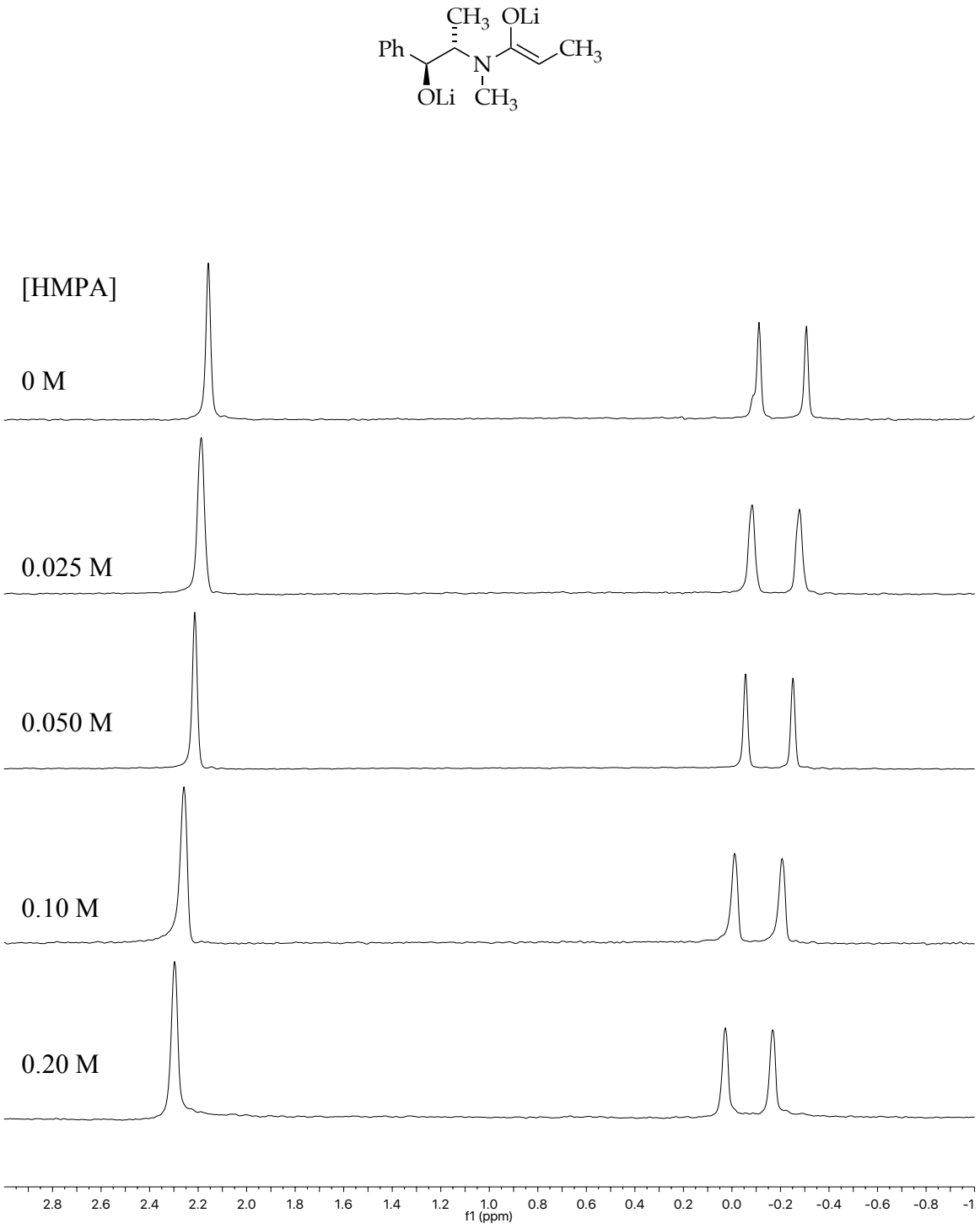


Figure 57. ^{6}Li NMR spectra of an aged solution of 0.10 M [^{6}Li]-(*S,S*)-**2** in THF at –80 °C with varying hexamethylphosphoramide (HMPA) concentrations showing no significant structural changes because HMPA does not compete with THF as a ligand.

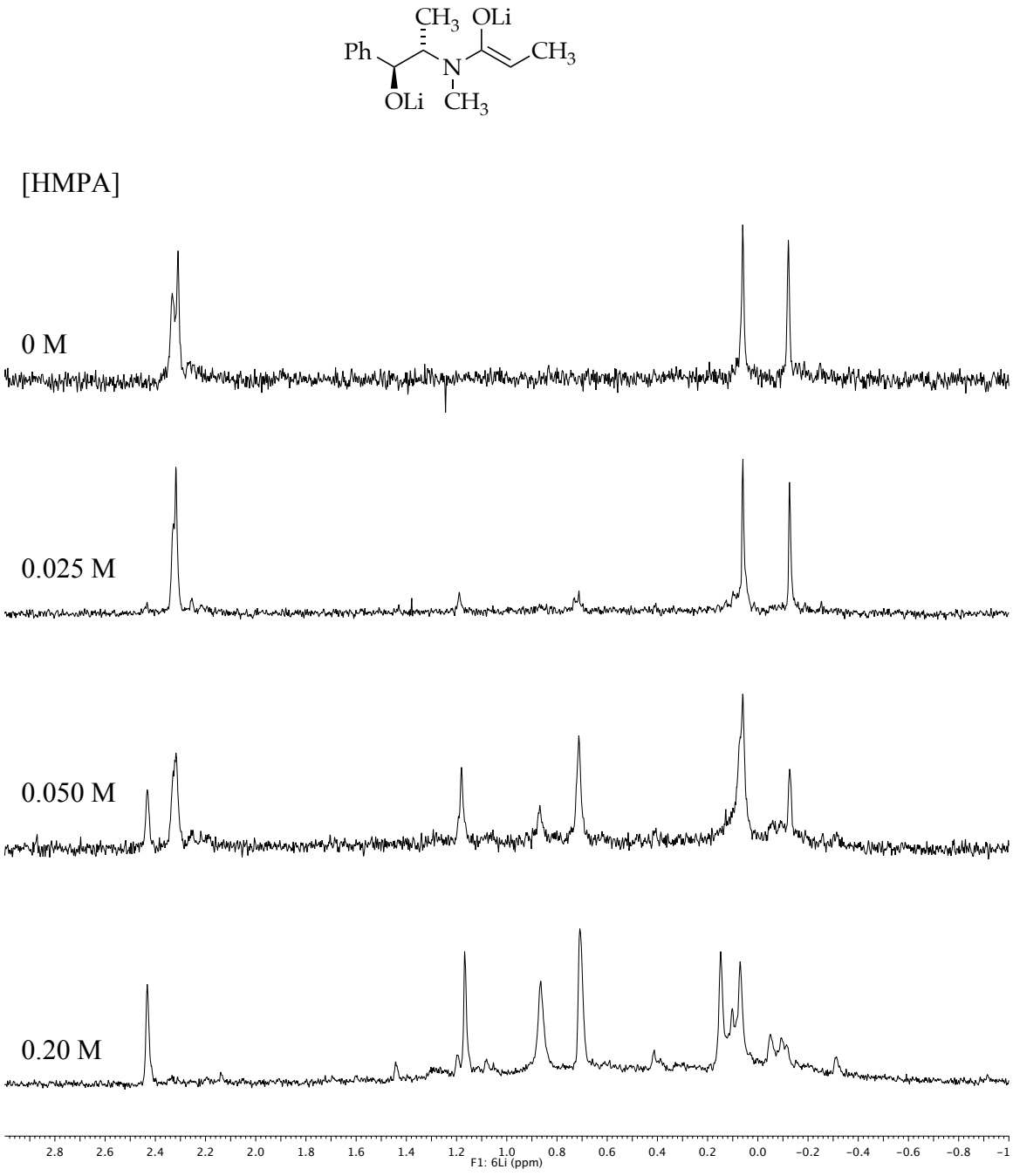


Figure 58. ^{6}Li NMR spectra of an aged solution of 0.05 M [^{6}Li]-(*S,S*)-**2** in 0.22 M THF/pentane at –80 °C at varying HMPA concentrations. Spectra became broadened and more complex with increasing amount of HMPA.

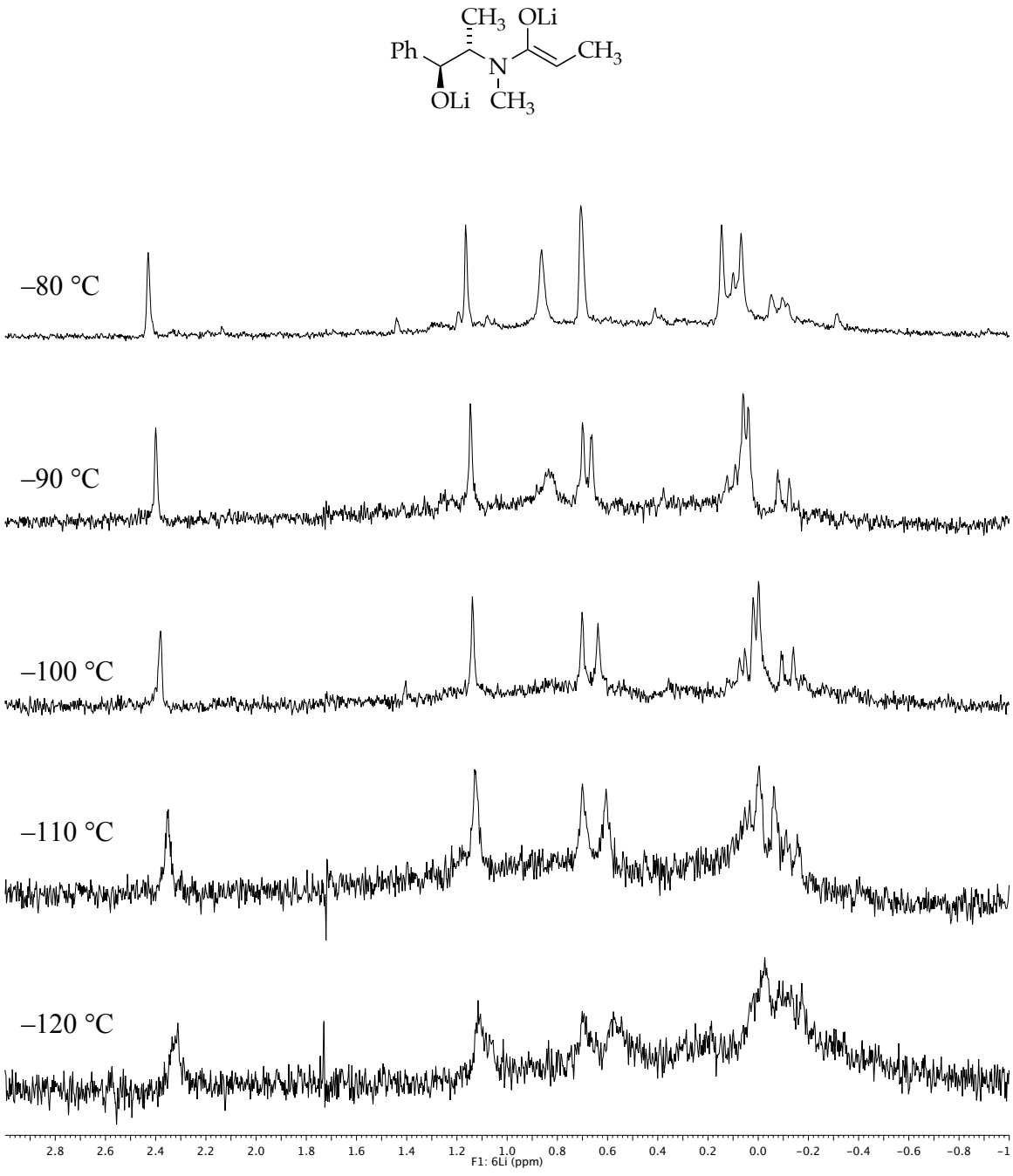


Figure 59. ^{6}Li NMR spectra of an aged solution of 0.05 M [^{6}Li]-(*S,S*)-**2** in 0.22 M THF/pentane at –80 °C with 0.20 M HMPA and varying temperature. Spectra became broad with lowering temperature.

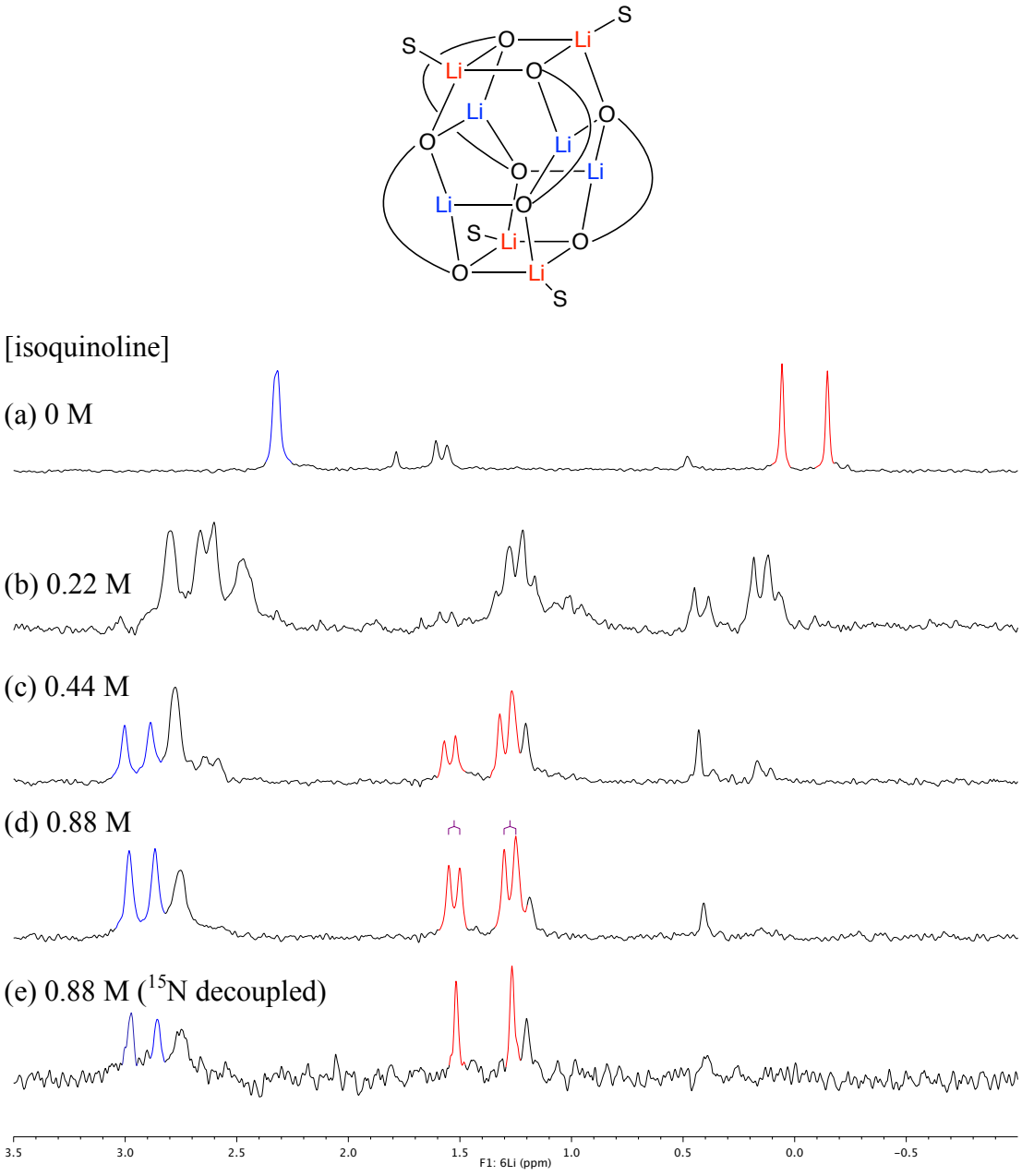
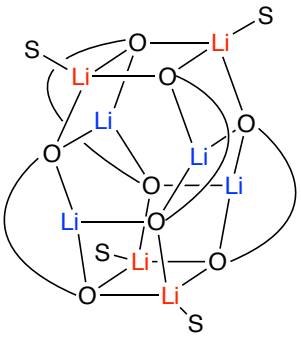


Figure 60. ^{6}Li NMR spectra of an aged solution of 0.050 M [^{6}Li]-(*S,S*)-**2** in 0.20 M THF/toluene at –95 °C with varying [^{15}N]-isoquinoline concentration showing upfield resonances as doublets (δ 1.53 ppm (d, J = 3.9 Hz), 1.28 ppm (d, J = 3.9 Hz)) (e) broadband decoupled. Poor signal to noise of (e) is caused by detecting through the lock channel.



4

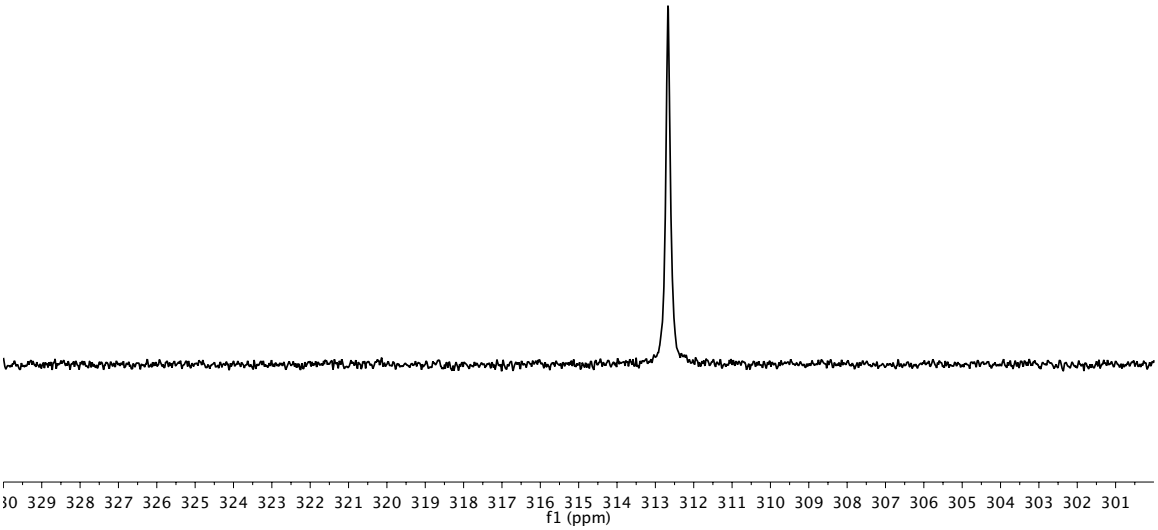
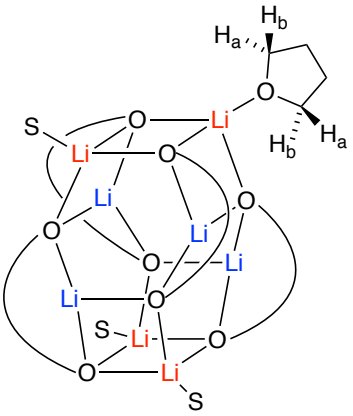


Figure 61. ^{15}N NMR spectrum of an aged solution of 0.050 M [^{6}Li]-(*S,S*)-**2** in 0.10 M [^{15}N]-isoquinoline and 12.3 M THF at –80 °C. Expected coupling is obscured by broadening. The peak width at half height is 6.5 Hz which is larger than the coupling constant (J = 3.8 Hz shown by ^{6}Li NMR spectroscopy).



4

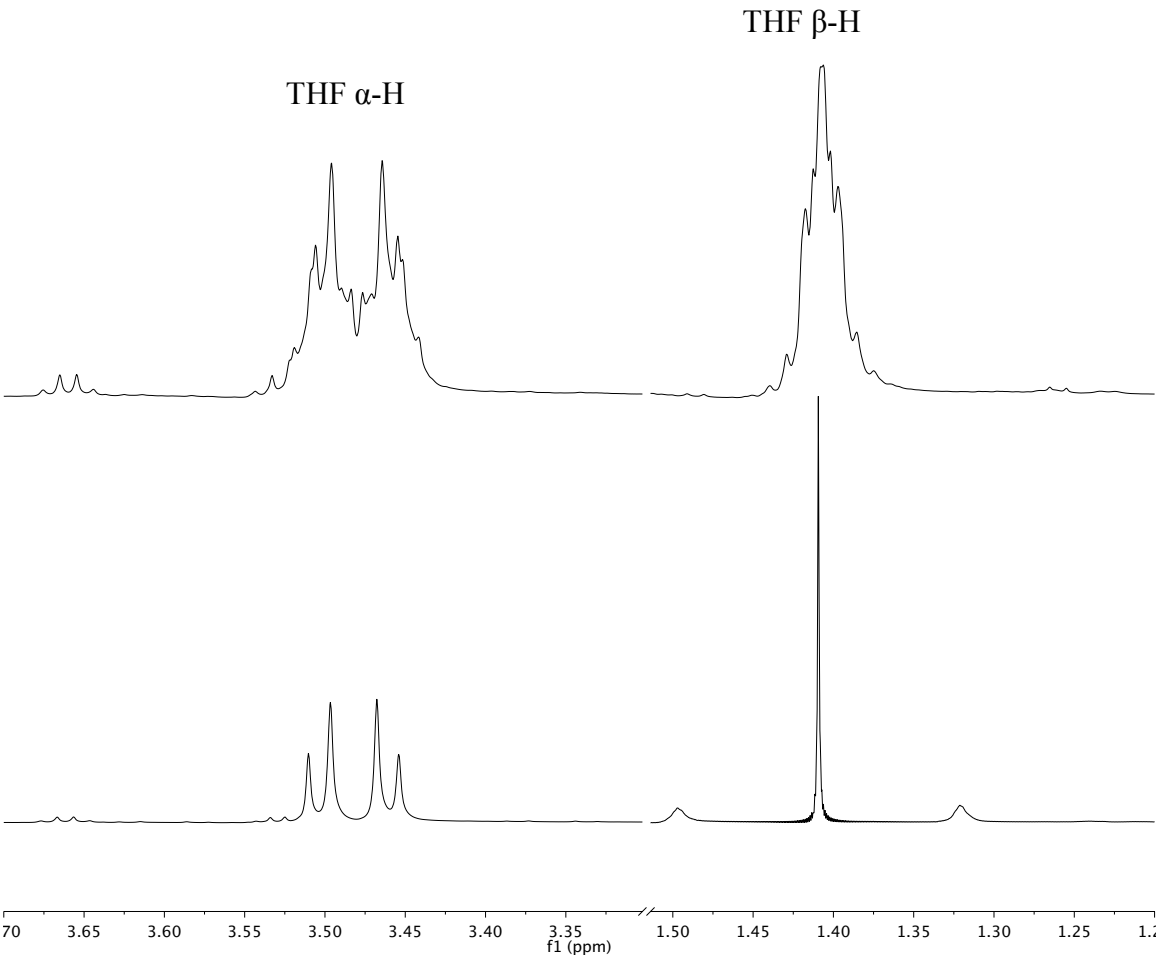


Figure 62. ^{1}H NMR spectra of an aged solution of 0.10 M (*S,S*)-**2** in 0.44 M THF and 9.1 M toluene-d_8 at 20 °C with single-frequency irradiation at 1.40 ppm. The two α-protons of bound THF couple to each other ($J_{H(a)–H(b)}$ = 8.3 Hz).

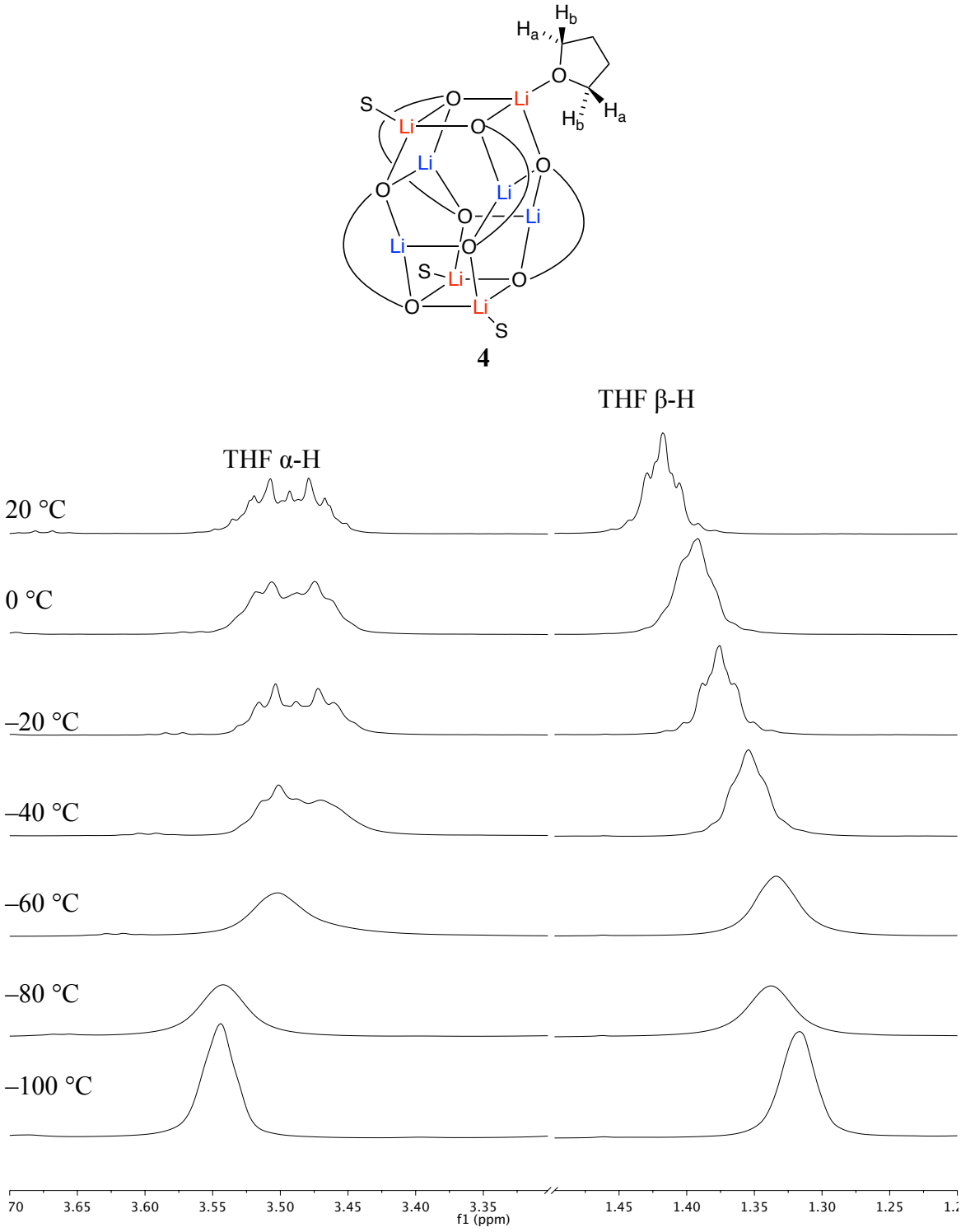


Figure 63. ^{1}H NMR spectra of an aged solution of 0.10 M (*S,S*)-**2** in 9.1 M toluene-d_8 and 0.44 M THF at varying temperature. As temperature drops, α-proton of THF goes from a doublet of triplet to a broad peak which may be caused by restricted rotation.

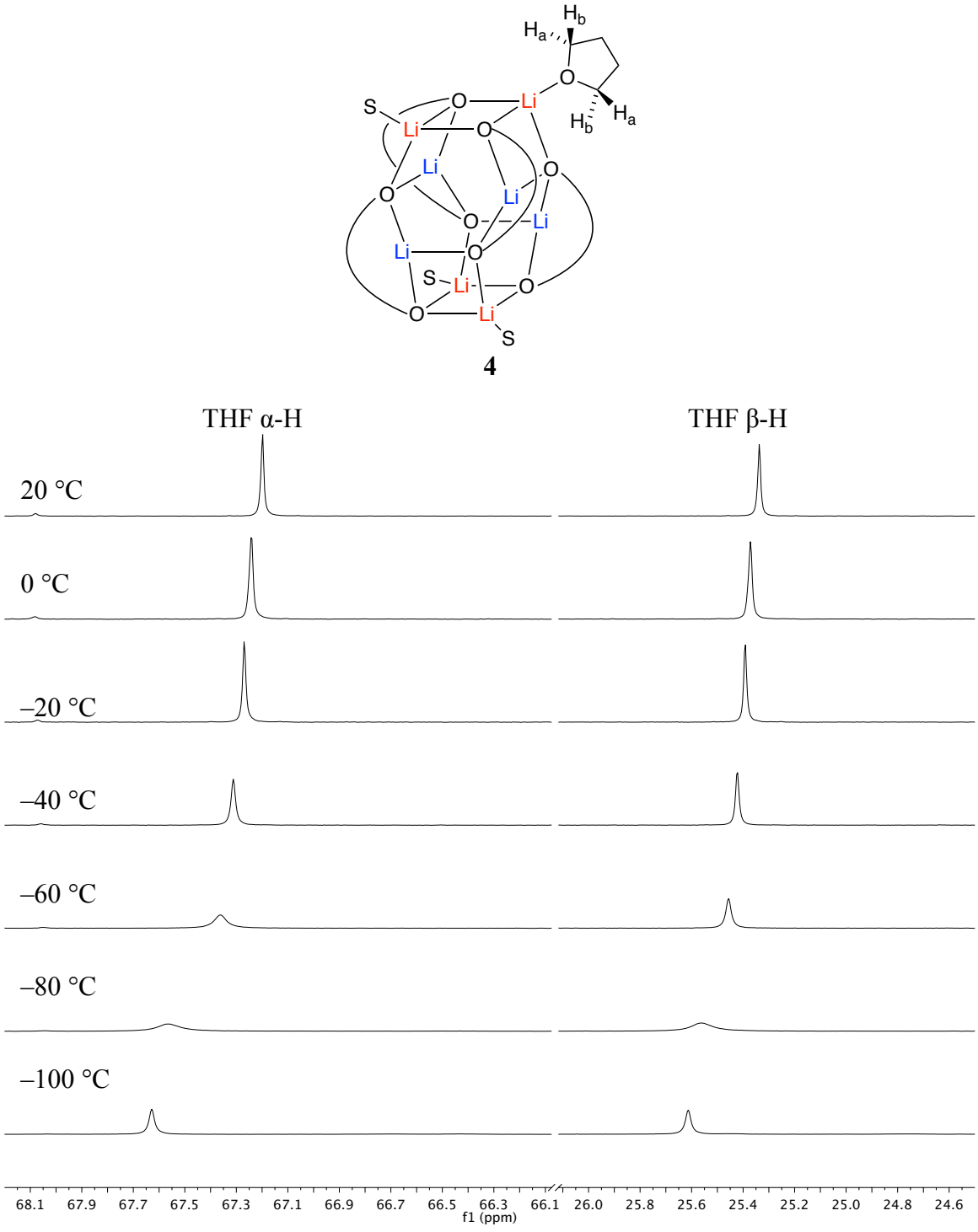
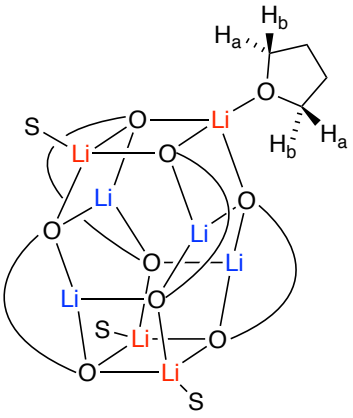


Figure 64. ^{13}C NMR spectra of an aged solution of 0.10 M (*S,S*)-**2** in 9.1 M toluene-d_8 and 0.44 M THF at varying temperature. As temperature drops, α-carbon of THF does not resolve to show free and bound THF. The origin of the temperature-dependent chemical shift is unknown.



4

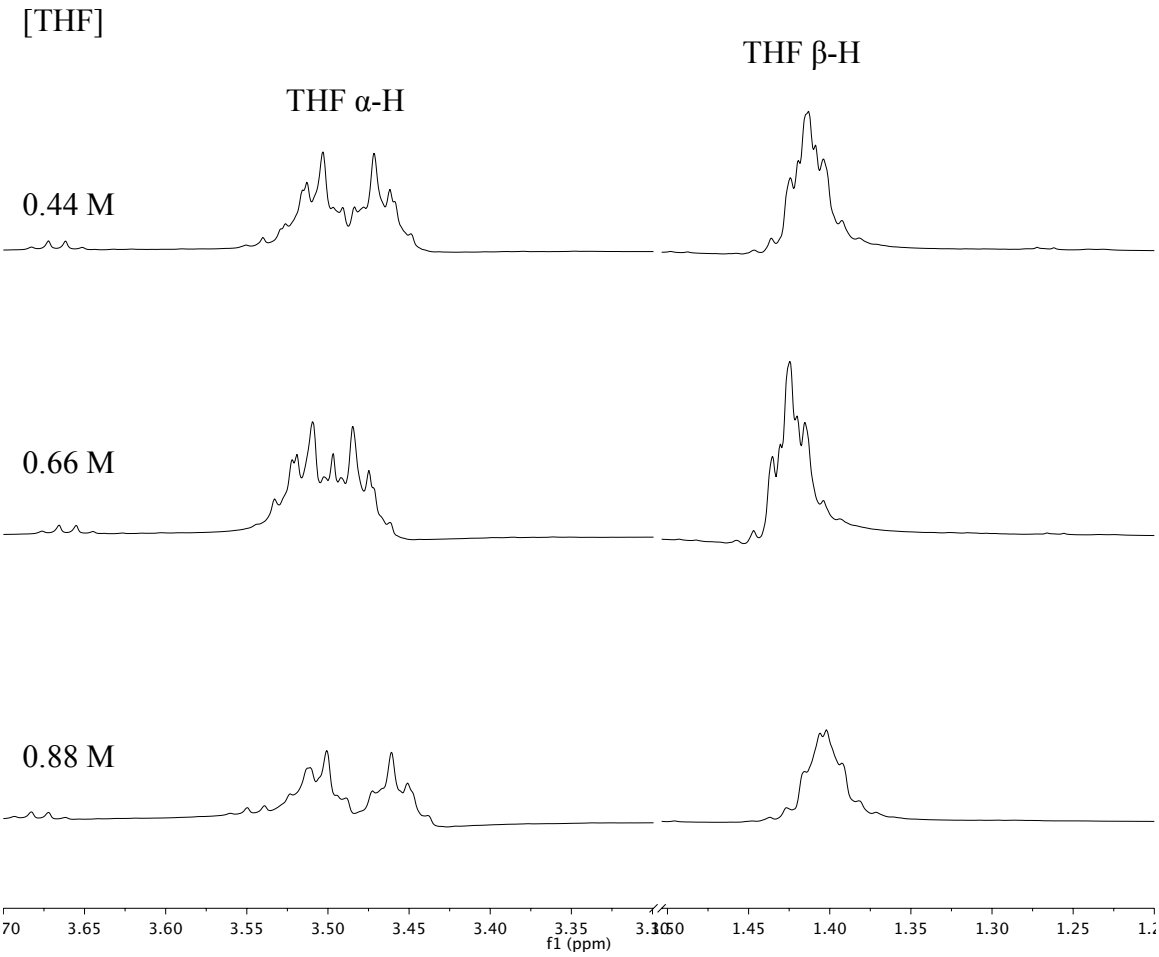
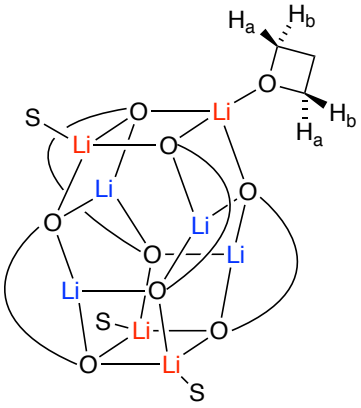


Figure 65. ^{1}H NMR spectra of an aged solution of 0.10 M (*S,S*)-**2** in toluene at 20 °C with varying THF concentrations. Increasing THF concentrations does not give resolved free and bound THF.



4

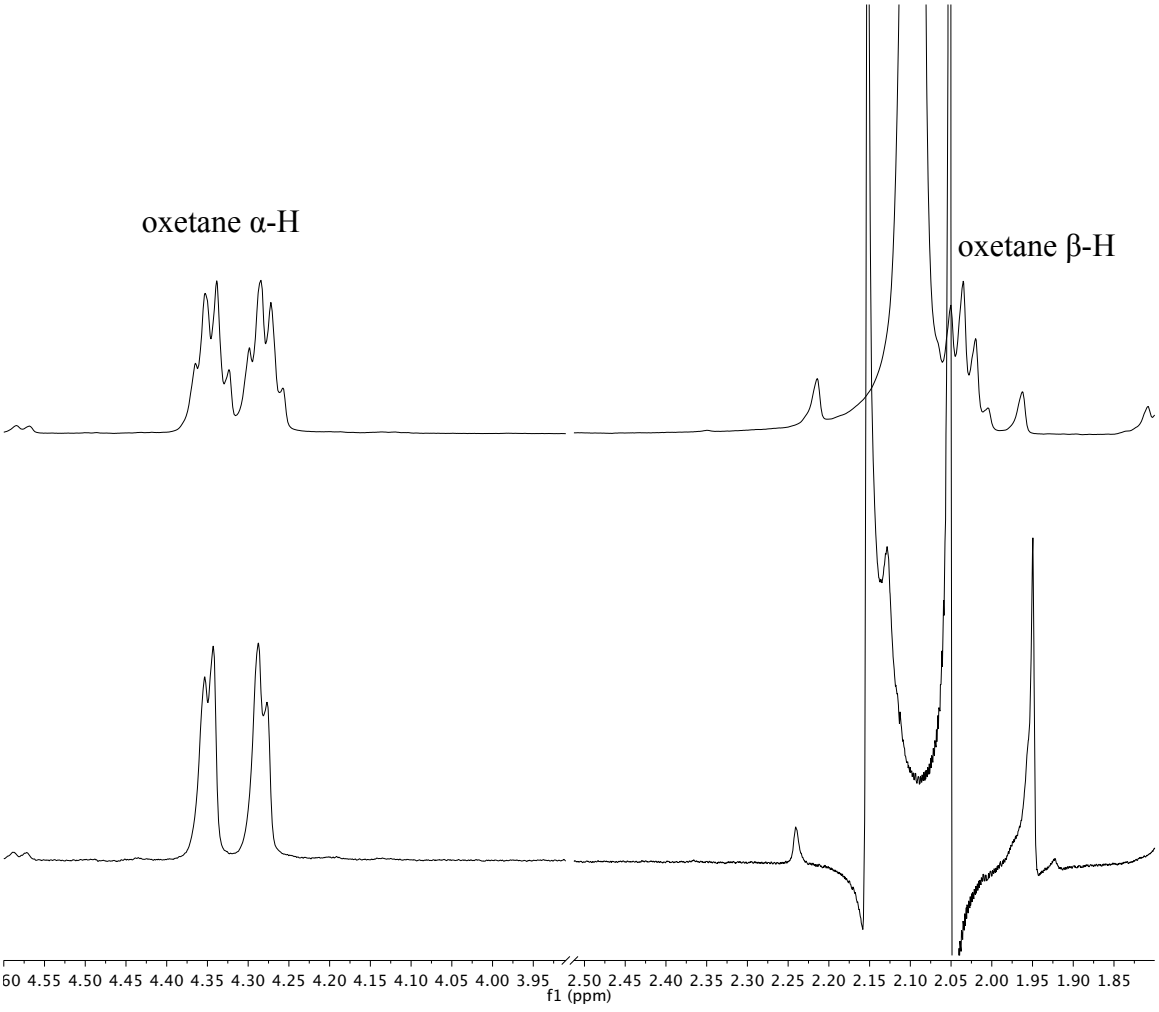


Figure 66. ^{1}H NMR spectra of an aged solution of 0.10 M [^{6}Li]-(*S,S*)-**2** in 0.22 M oxetane and 9.3 M toluene at 20 °C. Single frequency irradiated at 1.91 ppm β-proton of oxetane is under the toluene resonance at δ 2.10 ppm. The two α-protons appear as an AB quartet ($J_{H(a)–H(b)}$ = 5.2 Hz).

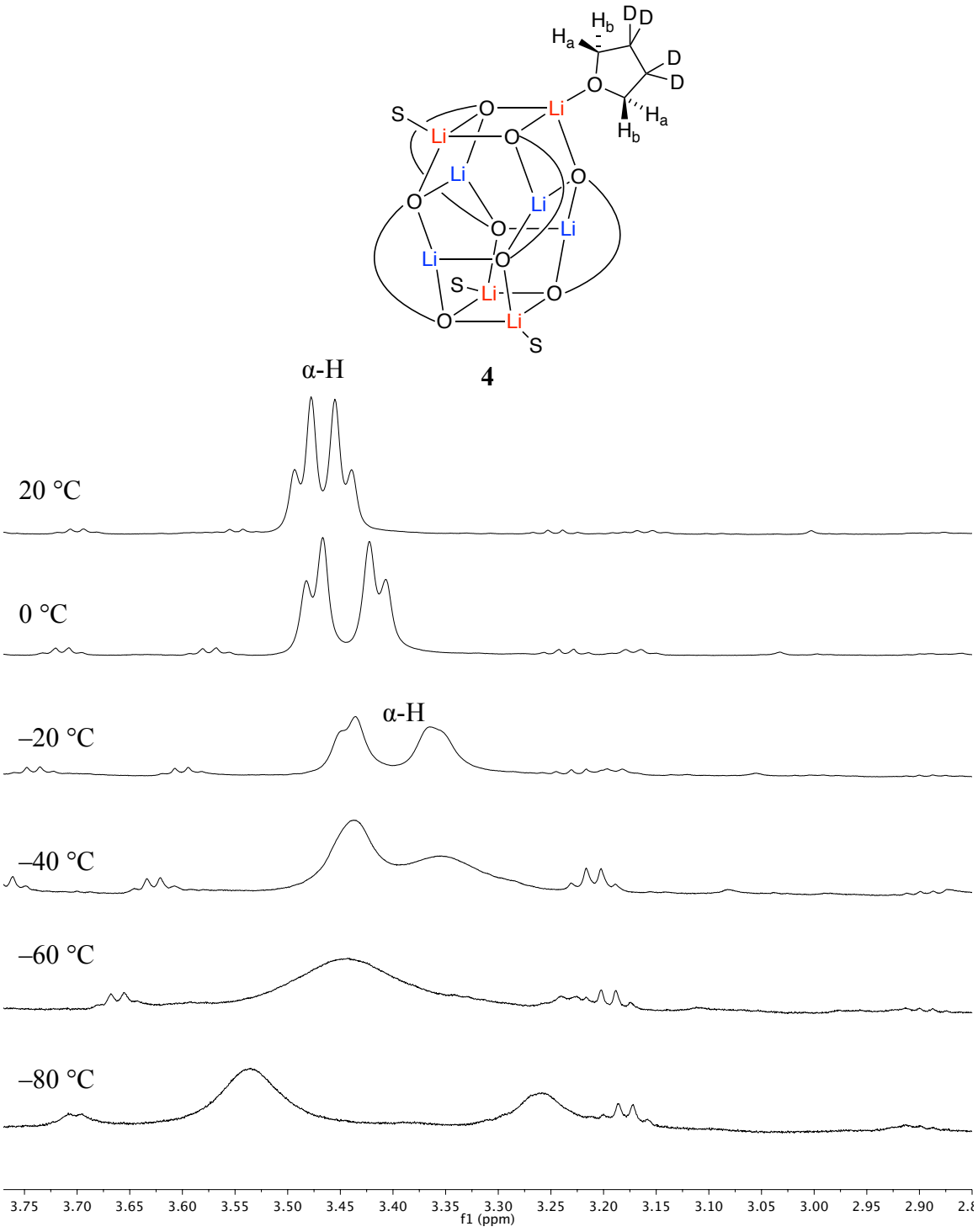


Figure 67. ^{1}H NMR spectra of an aged solution of 0.10 M [^{6}Li]-(*S,S*)-**2** in toluene and 0.20 M 3,3,4,4-tetradeuteriotetrahydrofuran at varying temperatures. Peaks that are not labeled are from homotetramers. This experiment gives similar results as THF. As temperature drops, α-proton of THF goes from two doublets (that are roofing to each other) to broad peaks because of restricted rotation.

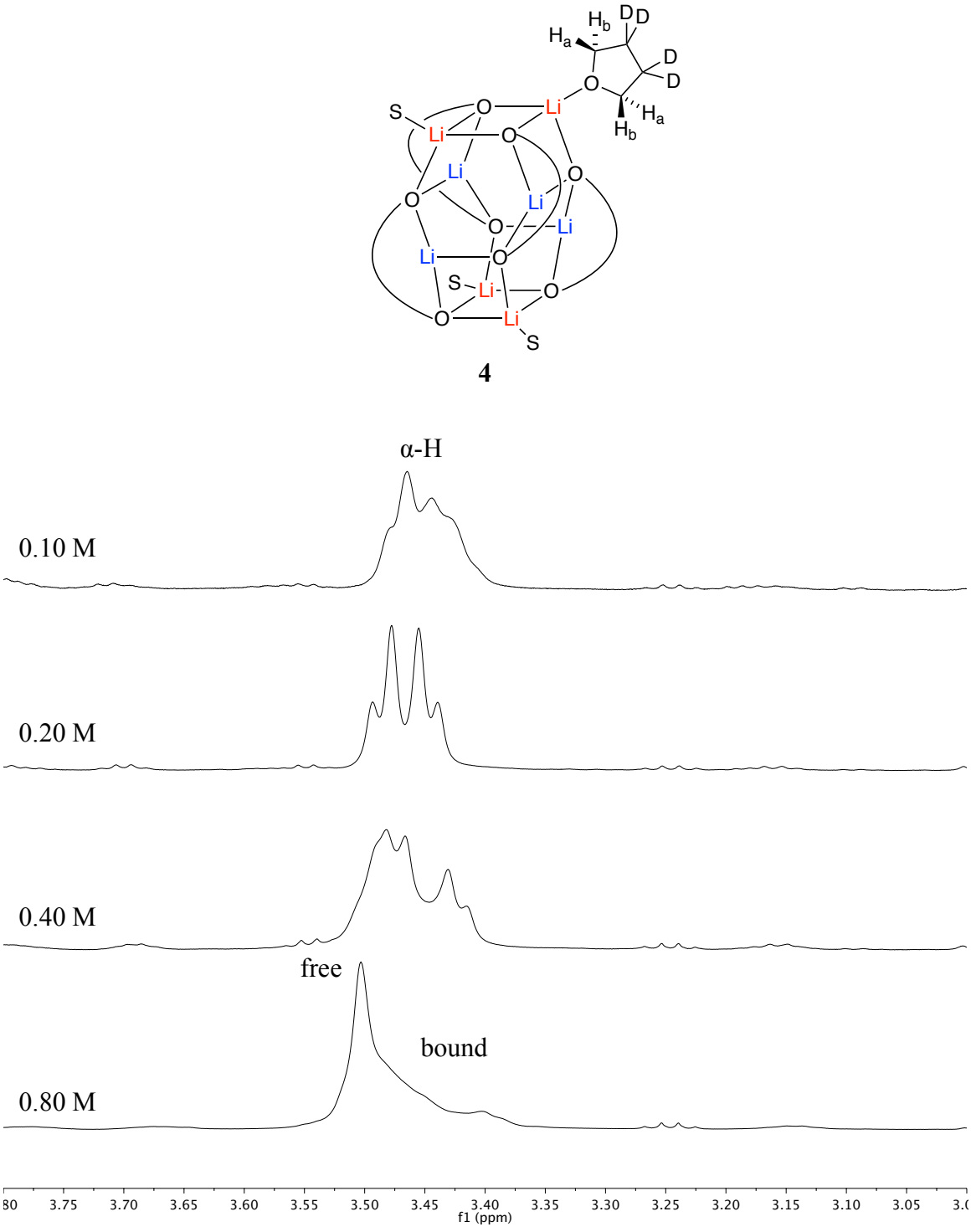


Figure 68. ^{1}H NMR spectra of an aged solution of 0.10 M [^{6}Li]-(*S,S*)-**2** in toluene at 20 °C with varying 3,3,4,4-tetradeuterio-tetrahydrofuran concentrations showing free and bound THF.

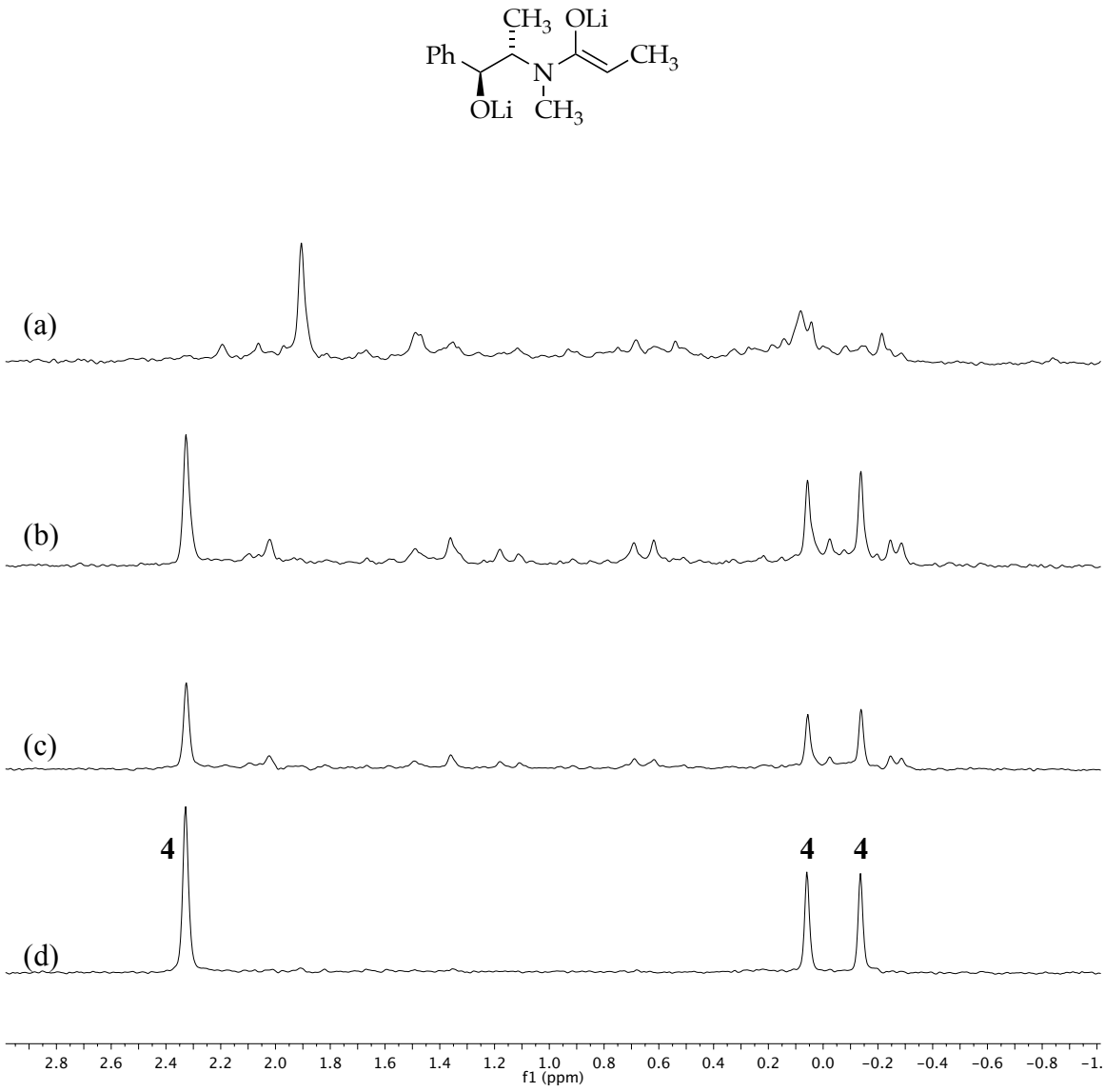


Figure 69. ^{6}Li NMR spectra of a solution of 0.050 M (*S,S*)-**1** in 12.3 M THF at –80 °C with 0.11 M [^{6}Li]LDA at varying aging times, (a) unaged; (b) aged at 0 °C for 3 min; (c) aged at 0 °C for 6 min; (d) aged at 20 °C for 5 min.

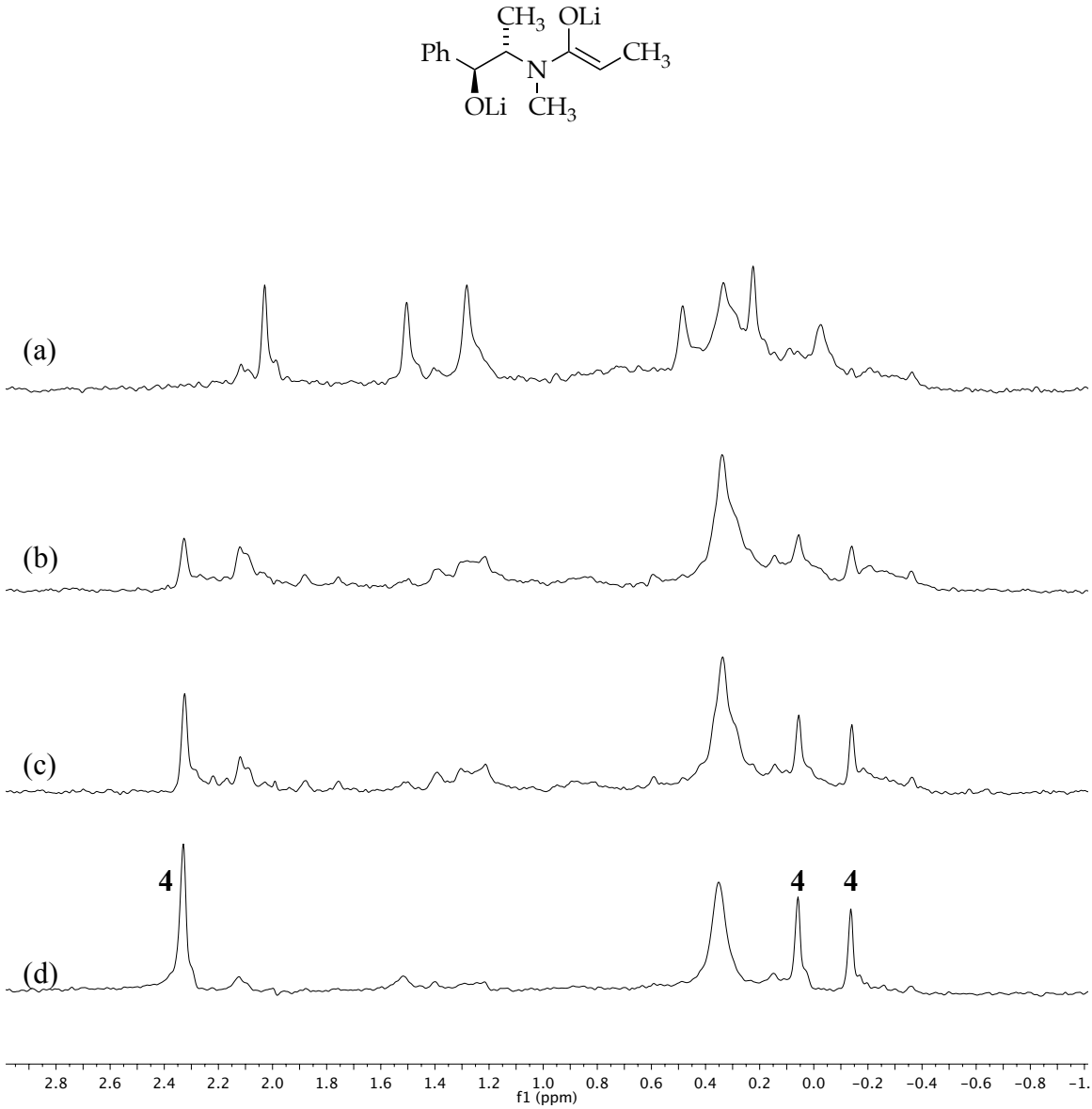


Figure 70. ^{6}Li NMR spectra of a solution of 0.050 M (*S,S*)-**1** in 12.3 M THF at –80 °C with 0.11 M [^{6}Li]LDA, 0.050 M [^{6}Li]LiCl at varying aging times, (a) unaged; (b) aged at 0 °C for 3 min; (c) aged at 0 °C for 6 min; (d) aged at 20 °C for 5 min.

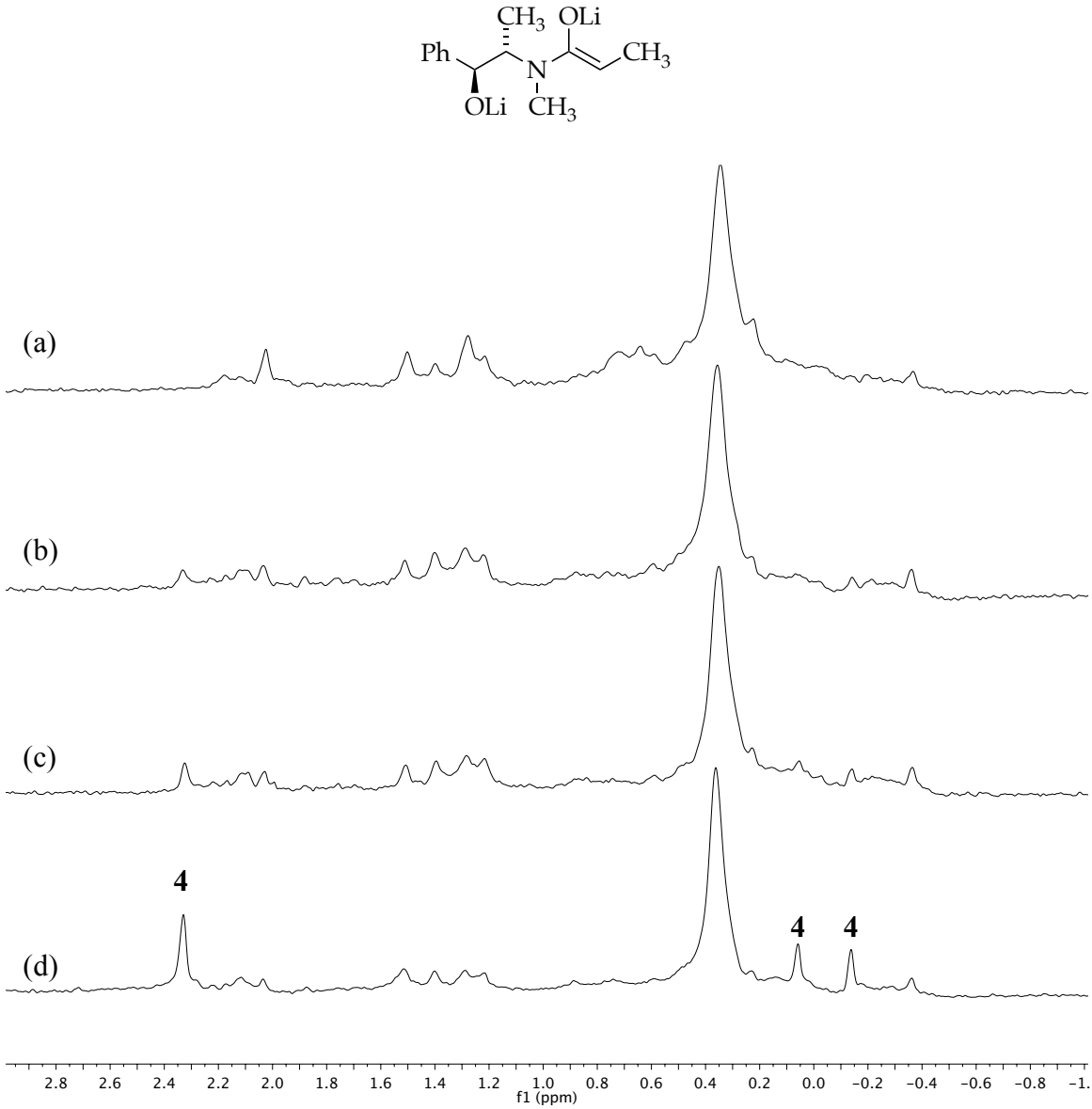
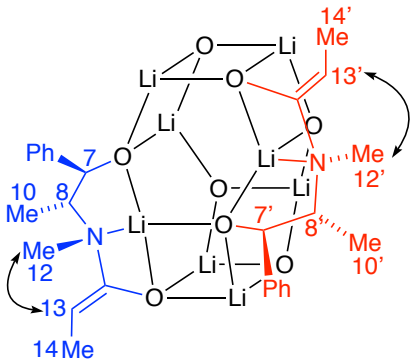


Figure 71. ^{6}Li NMR spectra of a solution of 0.050 M (*S,S*)-**1** in 12.3 M THF at –80 °C with 0.11 M [^{6}Li]LDA, 0.10 M [^{6}Li]LiCl at varying aging times: (a) unaged; (b) aged at 0 °C for 3 min; (c) aged at 0 °C for 6 min; (d) aged at 20 °C for 5 min.

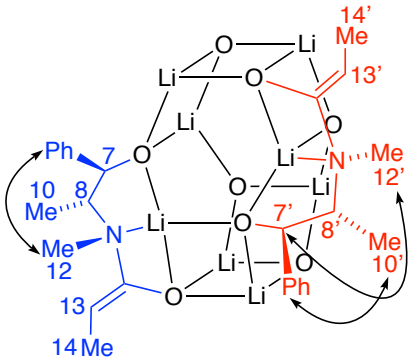
2D NMR analysis of (*R,R*)-1 homoaggregates: A sample prepared from 0.21 M [^{6}Li]LDA, 0.10 M (*R,R*)-**1** in 0.25 M THF and 9.2 M toluene-d_8, after aging at 25 °C for 10 min, was studied by standard 2D NMR techniques. All chemical shifts were assigned using high-field indirect-resolution 2D HSQC, HSQC-TOCSY, and HMBC experiments.

Experimental: 2D NMR spectra were acquired on a 500 MHz Varian INOVA spectrometer operating at 499.92 MHz for ^{1}H observation using a 5 mm Varian inverse-detect probe head with Z-axis pulsed field-gradient. Sample temperature was maintained at –60 °C as calibrated with a neat methanol sample. ^{1}H and ^{13}C chemical shifts were referenced to the residual downfield toluene-d_7 resonance at 2.09 ppm and 20.40 ppm, respectively. 2D experiments were acquired using standard pulse sequences supplied in VnmrJ 3.2A (Agilent Inc.) and processed and analyzed in MestReNova 11.0.3 (Mestrelab Research S.L.).

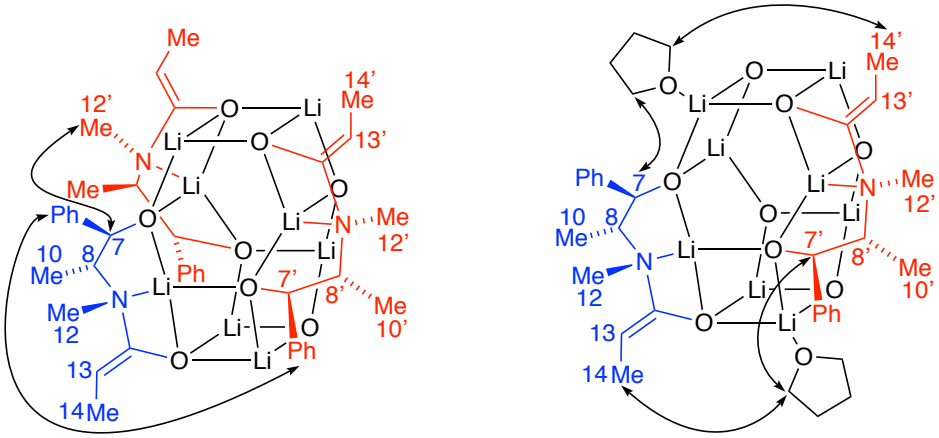
Determination of the 3D aggregate structure: The 3D structure of the aggregate was derived from 2D ROESY (reported as H–H correlations). The enolate is in the Z configuration based on the strong nOe correlation between H-13 and H-12, also between H-13' and H-12' (Figure 72A). The starting point for solving the structure is H-12 gives nOe correlations to H-1, H-2, H-3, H-5, H-6 which indicate phenyl group is on the convex face (blue, Figure 72B). H-7' gives nOe correlation to H-12', and H-10' gives nOe correlation to H-3' and H-5', which suggests the phenyl group is on the concave face (red) (Figure 72B). In addition, intermolecular nOe correlations are also observed (Figure 72C). Phenyl groups of the two subunits correlate to each other. Correlations between H-7 to H-12' further confirm that the two subunits are within one aggregates and rule out all the possible structures with stacked cube or octagonal prisms as the core. The 2D NMR spectroscopy confirmed the octalithio-homoaggregate assignment are fully consistent with the polygonal form observed crystallographically. THF molecules also display informative correlations(Figure 72D). The α-H of THF gives nOe correlations to H-7, H-7', H-14, H-14' which proves that the alkoxides and enolates are alternating.



(A) Z-enolate



(B) convex and concave subunit



(C) intermolecular nOe correlations (D) THF correlations

Figure 72. nOe correlations for homoaggregate **4**.

Table 1. ^{1}H and ^{13}C chemical shifts and assignments for homoaggregate **4** at –60 °C.

Atom	δC, ppm	δH, ppm	HMBC	COSY	HSQC-TOCSY[1]	ROESY[2]
1 C	125.26	7.09	3	5	2,3,5,6	
1' C	125.59	7.02	3',5'		2',3',5'	3',5',12
2 C	127.01	7.21	3,4,6		1,3,5,6	7,8,5',8'
2' C	126.47	7.03	4',6'	3'	1',3',5',6'	3',5',12
3 C	125.87	7.14	1,2,5,6,7	5,7	1,2	7,8,3',5',8'
3' C	127.54	6.74	1',5',7'	2',5',7'	1',2',6'	1',2',6',7',8',10',3,5,12
4 C	151.71	–	2,6,7			
4' C	150.16	–	2',6',7'			
5 C	126.47	8.34	3,7	1,3,6,7	1,2,6	7,8,3',5',8'
5' C	125.85	7.75	1',3',7'	3',6'	1',2',6'	1',2',6',7',8',2,5,6,12
6 C	127.67	7.24	2,3,4	5	1,2,5	7,8,5',8'
6' C	128.82	7.09	2',4'	5'	2',3',5'	3',5',7,12
7 C	80.53	5.02	3,4,5,10	3,5,8		2,3,5,6,8,10,6',12'
7' C	80.08	4.62	3',4',5',8'	3',8'	8',10'	3',5',8',10',12',10
8 C	70.50	3.26	10,12	7,10	10	2,3,5,6,7,10,12
8' C	67.90	3.84	7',11',12'	7',10'	7',10'	3',5',7',10',2,3,5,6
10 C	15.75	2.02	7,8	8	8	7,8,13,7',12'
10' C	12.57	0.98		8'	7',8'	3', 5',7',8'
11 C	163.23	–	12,13,14			
11' C	163.64	–	8',12',13',14'			
12 C	44.39	2.18	8,11			2,3,6,8,13,1',2',3',5',6'
12' C	32.86	2.75	8',11'			7',13',7,10
13 C	75.16	3.68	14	14	14	10,12,14

13' C	73.32	3.82	14'	14'	14'	12',14'
14 C	11.46	1.66	11,13	13	13	13
14' C	11.40	1.83	11',13'	13'	13'	13'
THF α-H	67.24	3.53			β-H	7,7',10,10',14,14', β-H
THF β-H	25.29	1.33			α-H	14,14',α-H

[1]HSQC correlations were omitted from the table. [2]Important correlations that allowed determination of subunit arrangement are marked in red.

	Parameter	Value
1	Experiment	1D
2	Pulse Sequence	s2pul
3	Solvent	toluene
4	Temperature	-60.0
5	Number of Scans	1
6	Receiver Gain	10
7	Relaxation Delay	6.0000
8	Nucleus	1H
9	Spectrometer Frequency	499.92
10	Spectral Width	4669.4
11	Lowest Frequency	-275.5
12	Acquired Size	8192
13	Spectral Size	65536

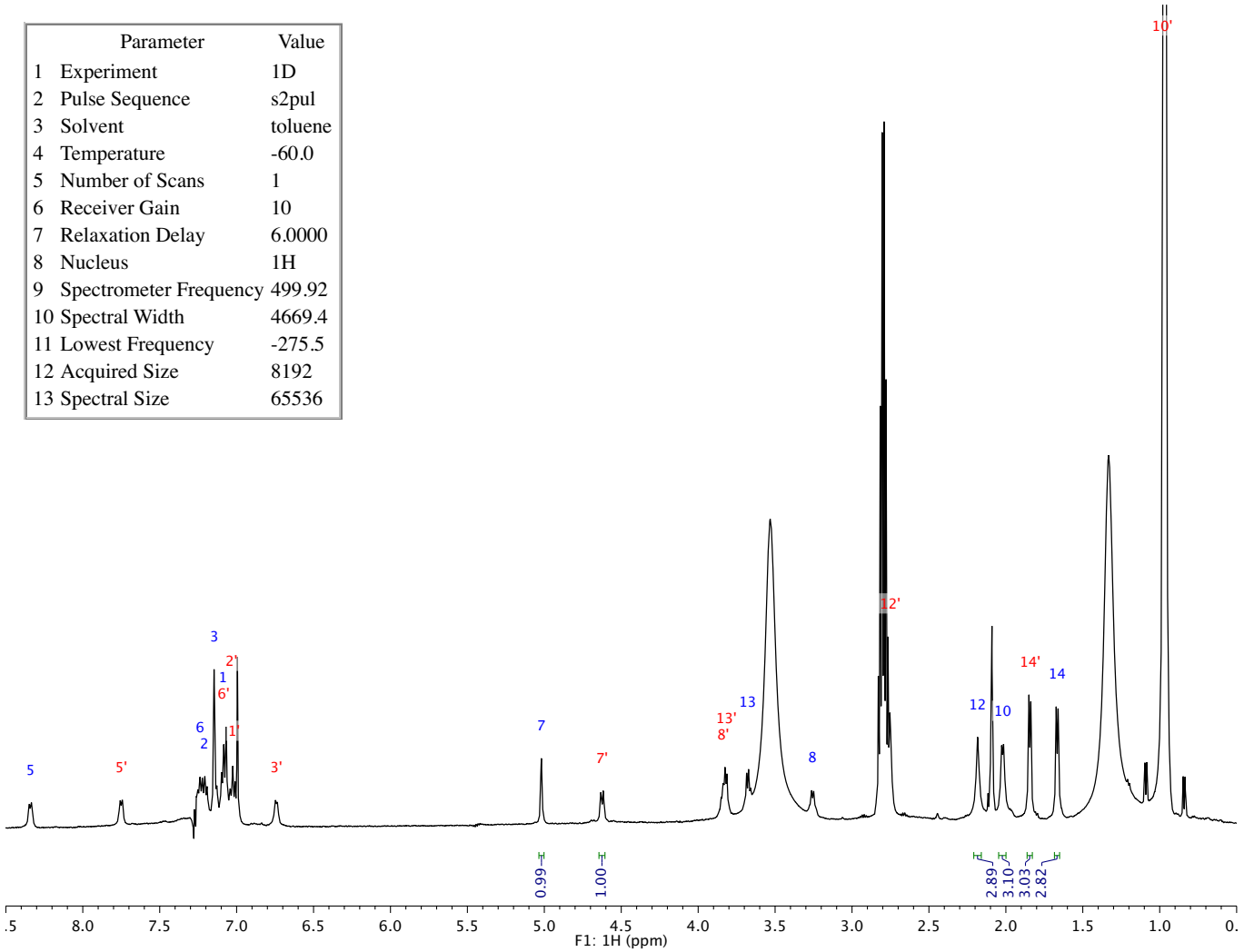


Figure 73. ^{1}H NMR spectrum of an aged solution of 0.10 M *(R,R)*-**1** in 0.25 M THF and 9.2 M toluene-d_8 at –60 °C with 0.21 M [^{6}Li]LDA. Labels indicate assignments by 2D NMR.

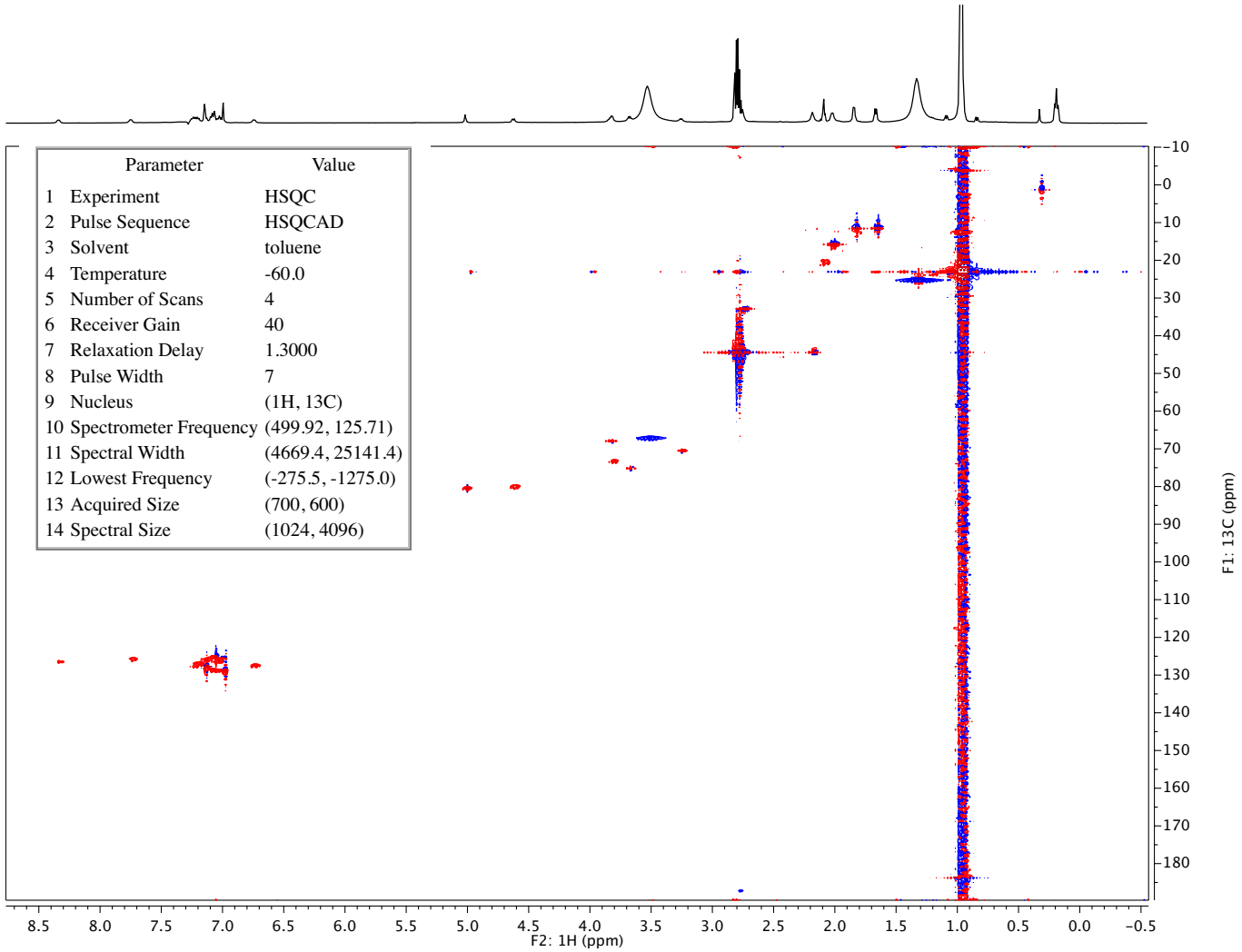


Figure 74. Full-display HSQC spectrum of an aged solution of 0.10 M *(R,R)*-**1** in 0.25 M THF and 9.2 M toluene-d_8 at –60 °C with 0.21 M [^{6}Li]LDA.

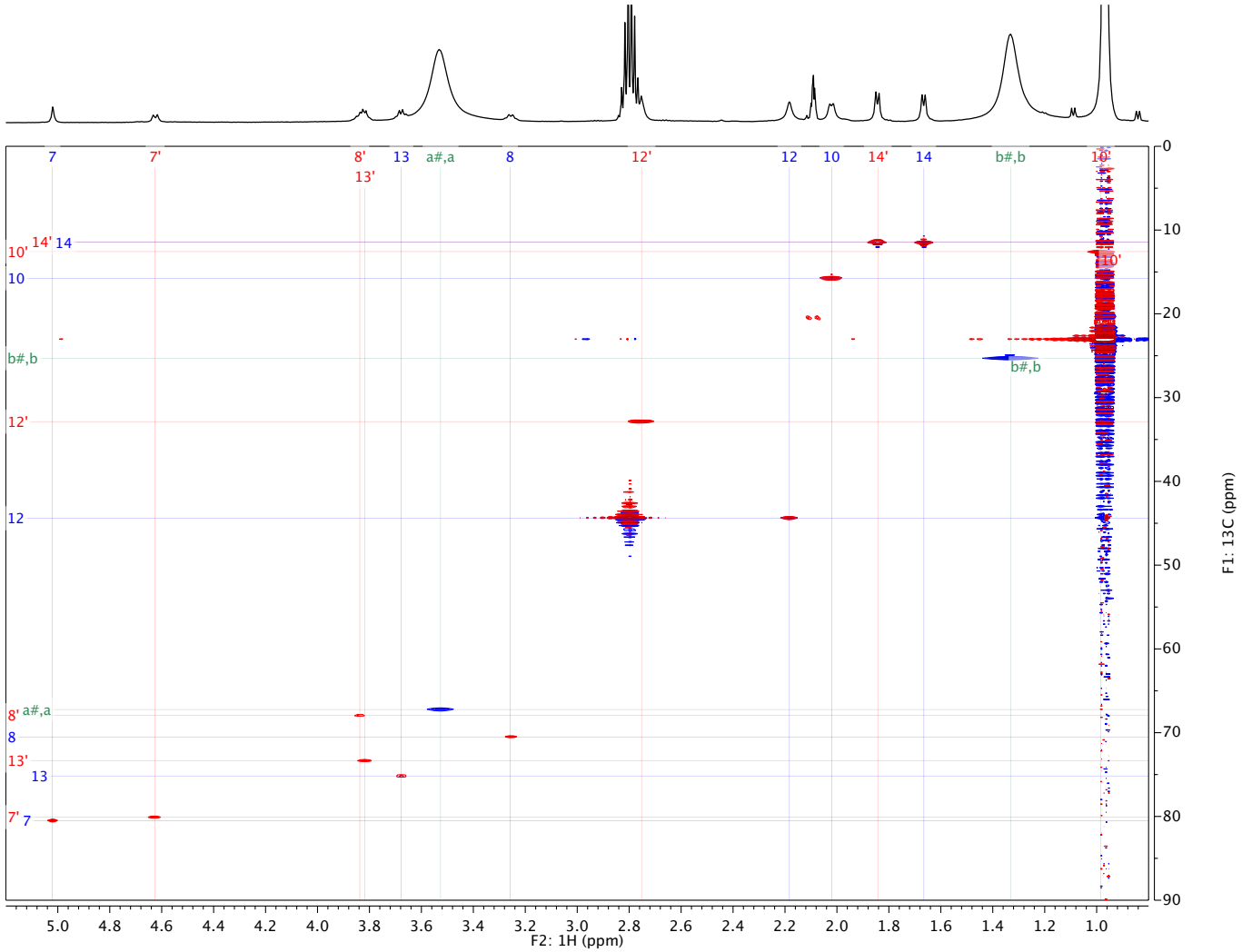


Figure 75. Expansion of the HSQC spectrum of an aged solution of 0.10 M *(R,R)*-**1** in 0.25 M THF and 9.2 M toluene-d_8 at –60 °C with 0.21 M [^{6}Li]LDA.

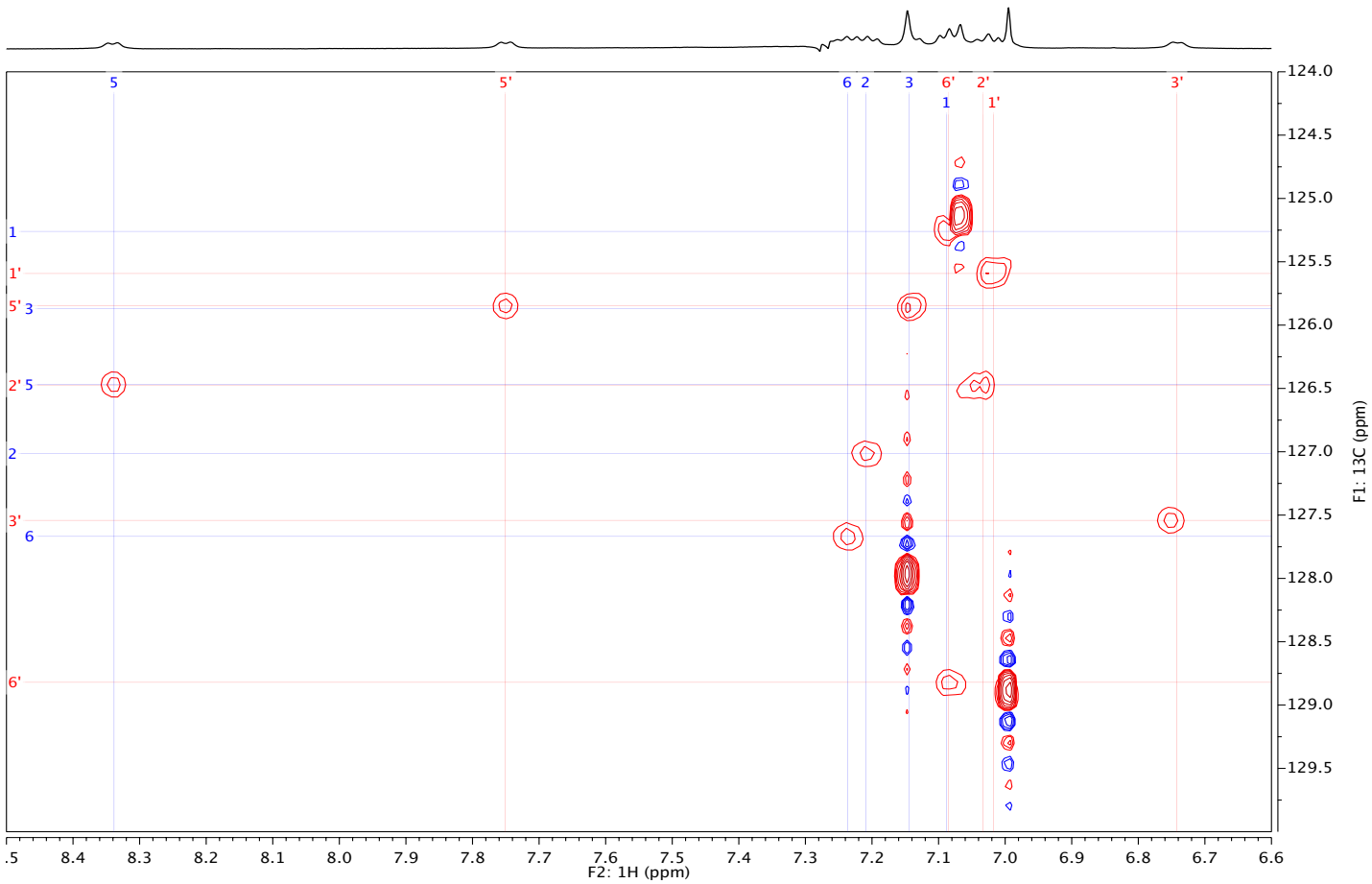


Figure 76. Expansion of the HSQC spectrum of an aged solution of 0.10 M *(R,R)*-**1** in 0.25 M THF and 9.2 M toluene-d_8 at –60 °C with 0.21 M [^{6}Li]LDA.

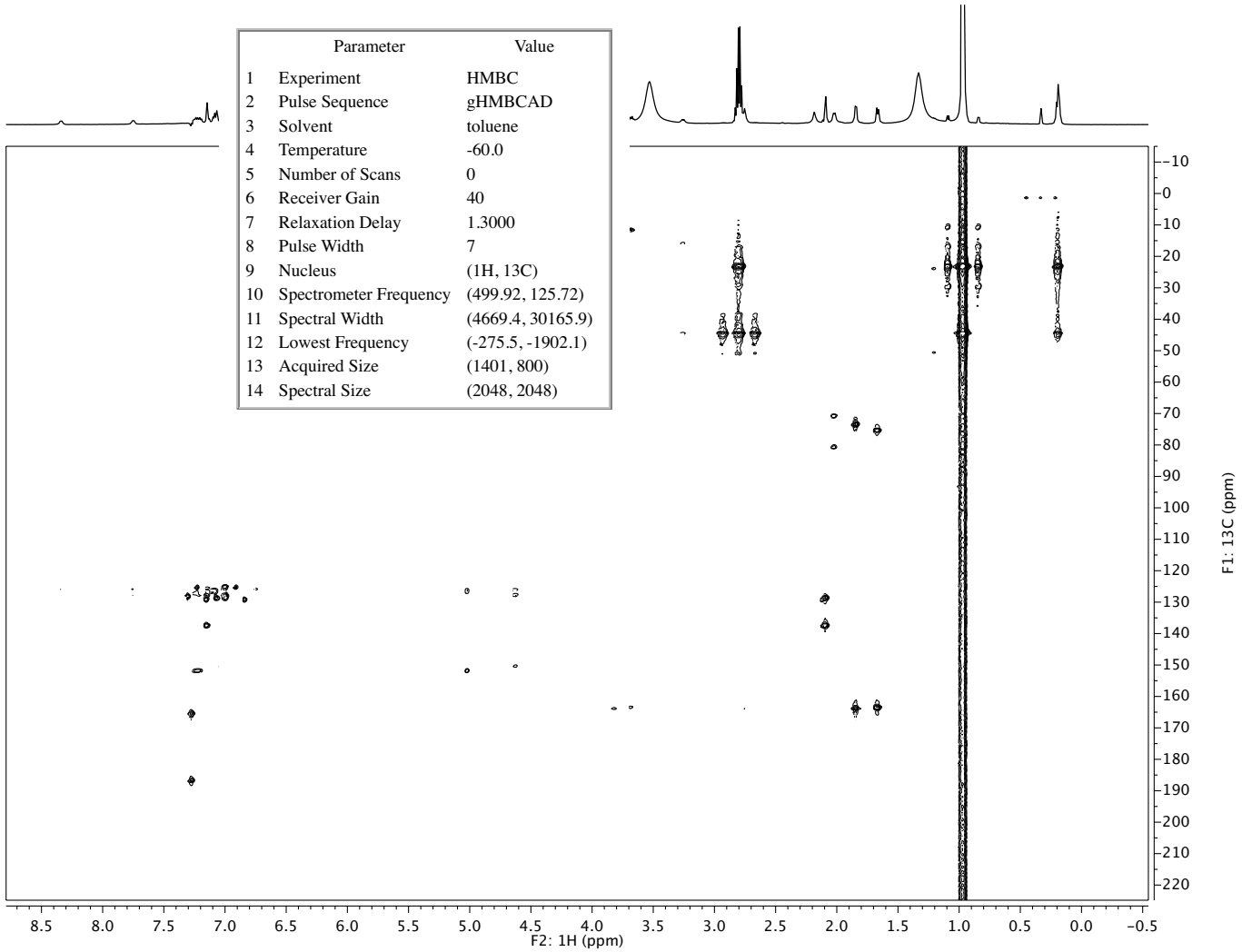


Figure 77. Full-display HMBC spectrum of an aged solution of 0.10 M (*R,R*)-**1** in 0.25 M THF and 9.2 M toluene-d_8 at –60 °C with 0.21 M [^{6}Li]LDA.

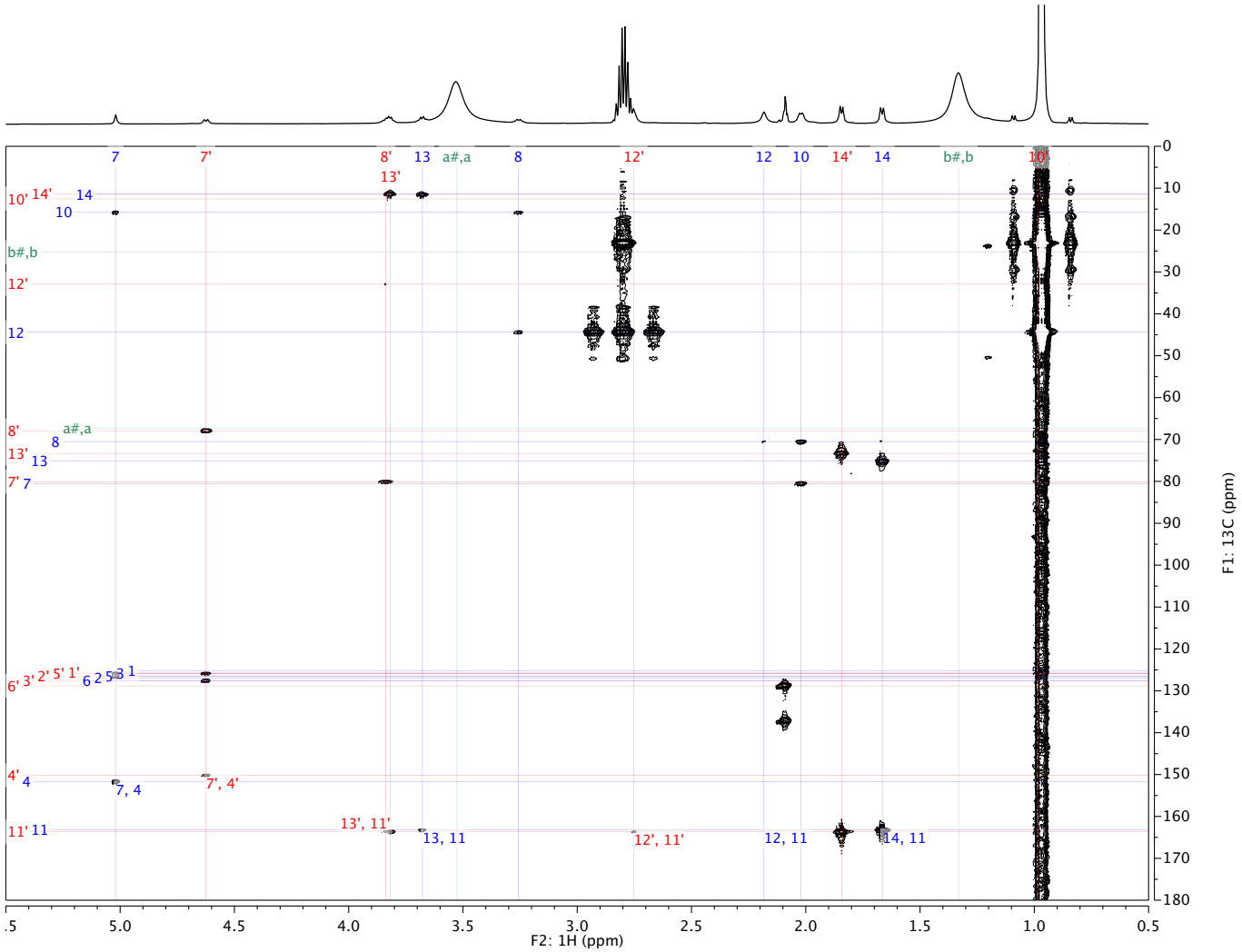


Figure 78. Expansion of the HMBC spectrum of an aged solution of 0.10 M (*R,R*)-**1** in 0.25 M THF and 9.2 M toluene-d_8 at –60 °C with 0.21 M [^{6}Li]LDA.

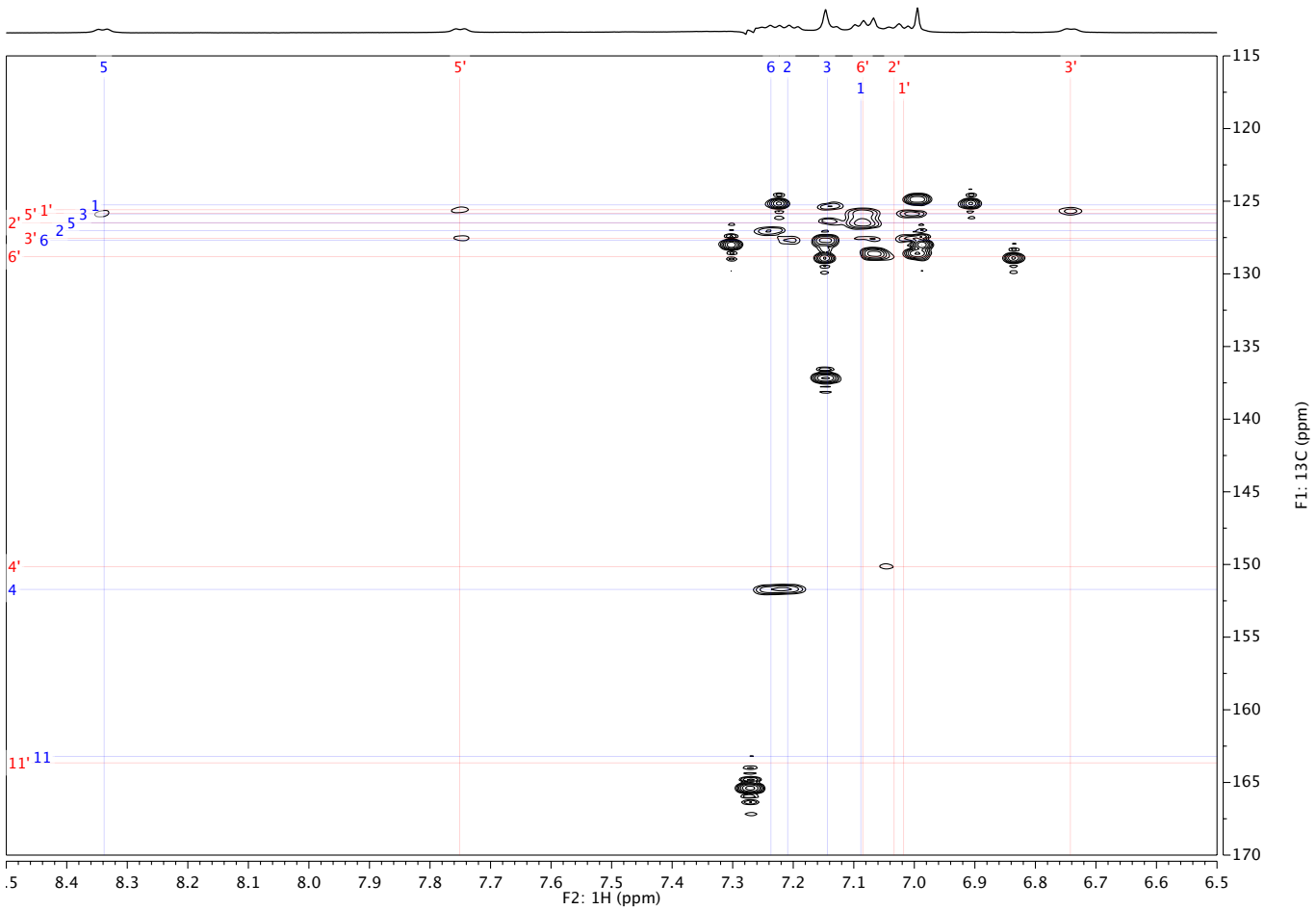


Figure 79. Expansion of the HMBC spectrum of an aged solution of 0.10 M (*R,R*)-**1** in 0.25 M THF and 9.2 M toluene-d_8 at –60 °C with 0.21 M [^{6}Li]LDA.

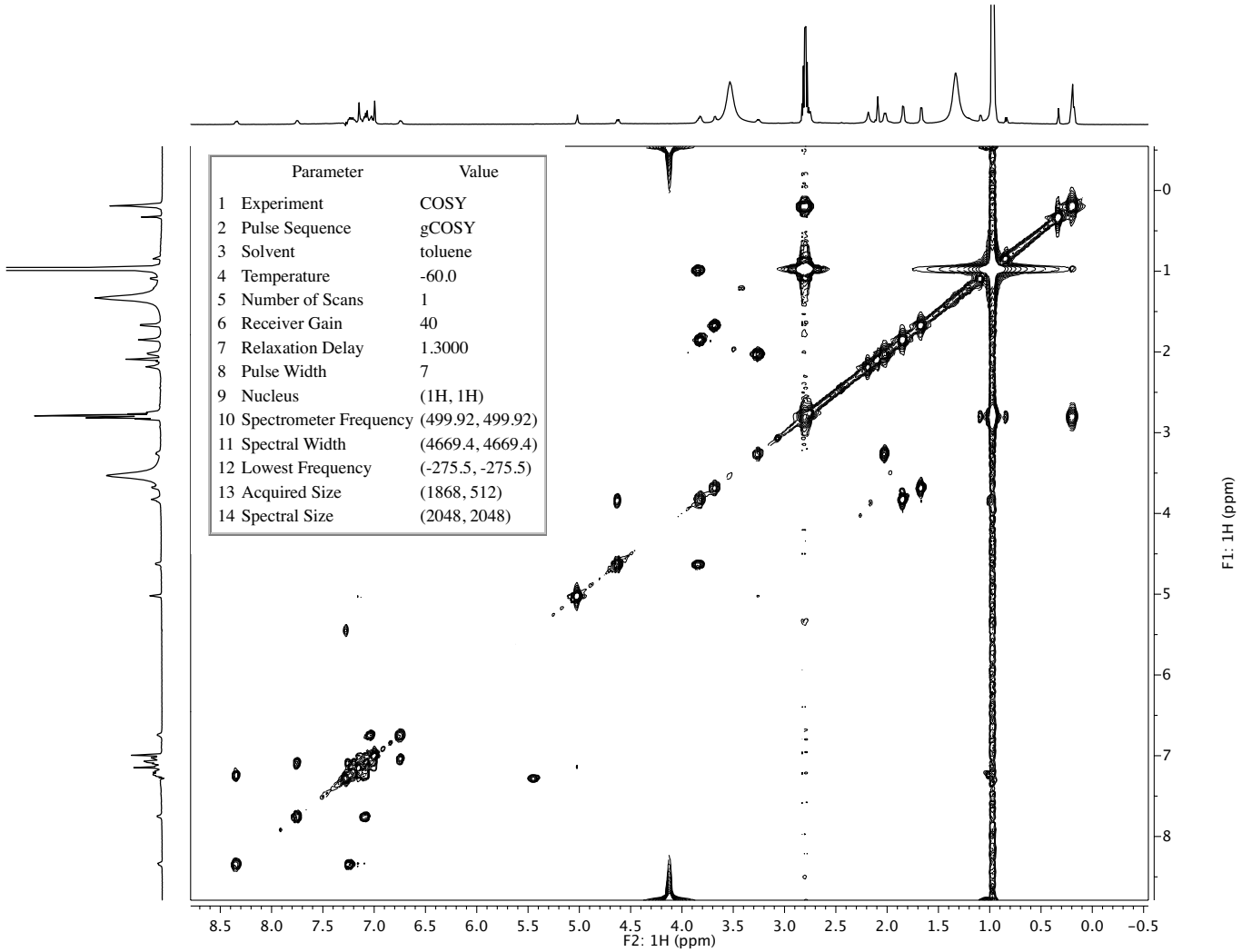


Figure 80. Full-display COSY spectrum of an aged solution of 0.10 M (*R,R*)-**1** in 0.25 M THF and 9.2 M toluene-d_8 at –60 °C with 0.21 M [^{6}Li]LDA.

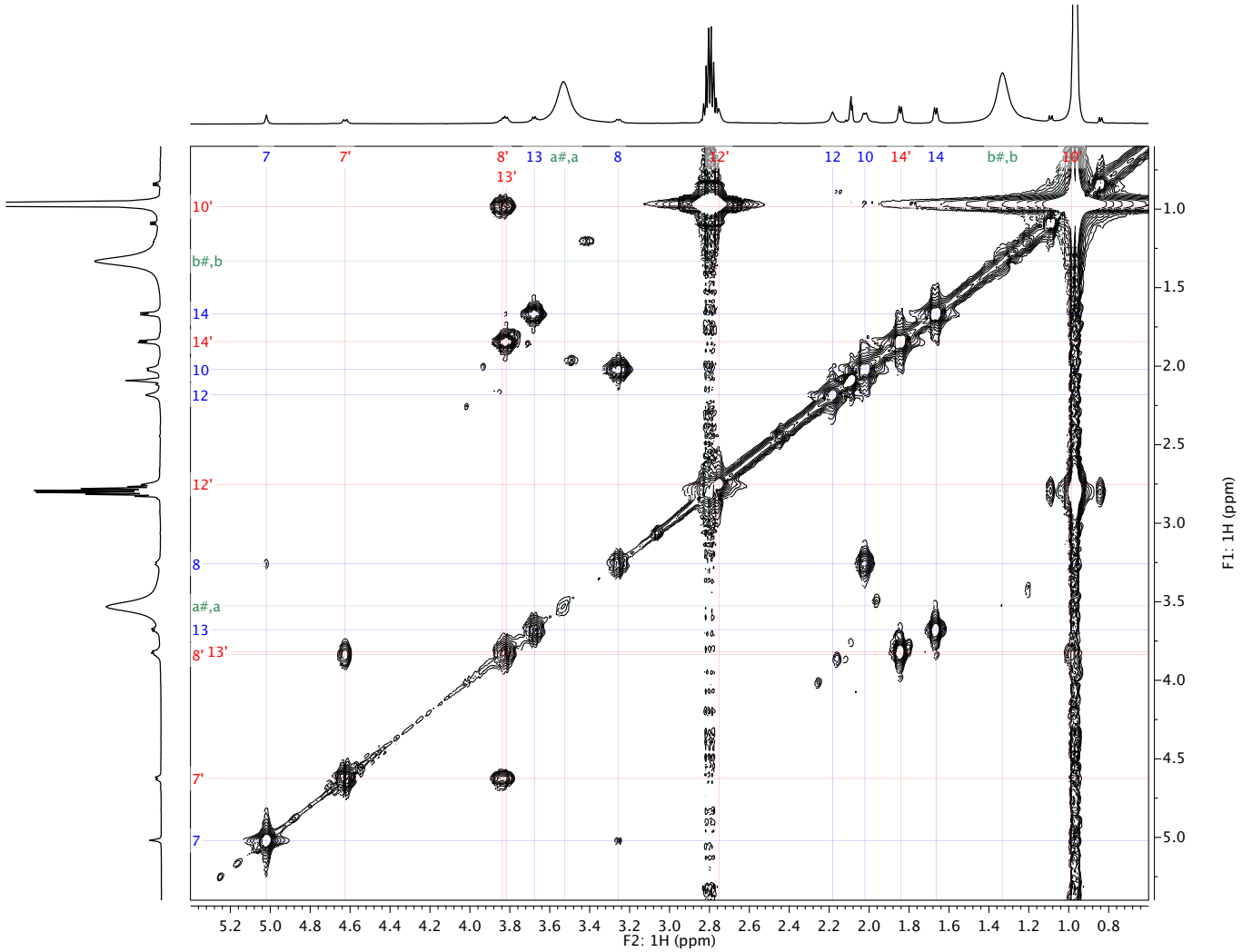


Figure 81. Expansion of the COSY spectrum of an aged solution of 0.10 M (*R,R*)-**1** in 0.25 M THF and 9.2 M toluene-d_8 at –60 °C with 0.21 M [^{6}Li]LDA.

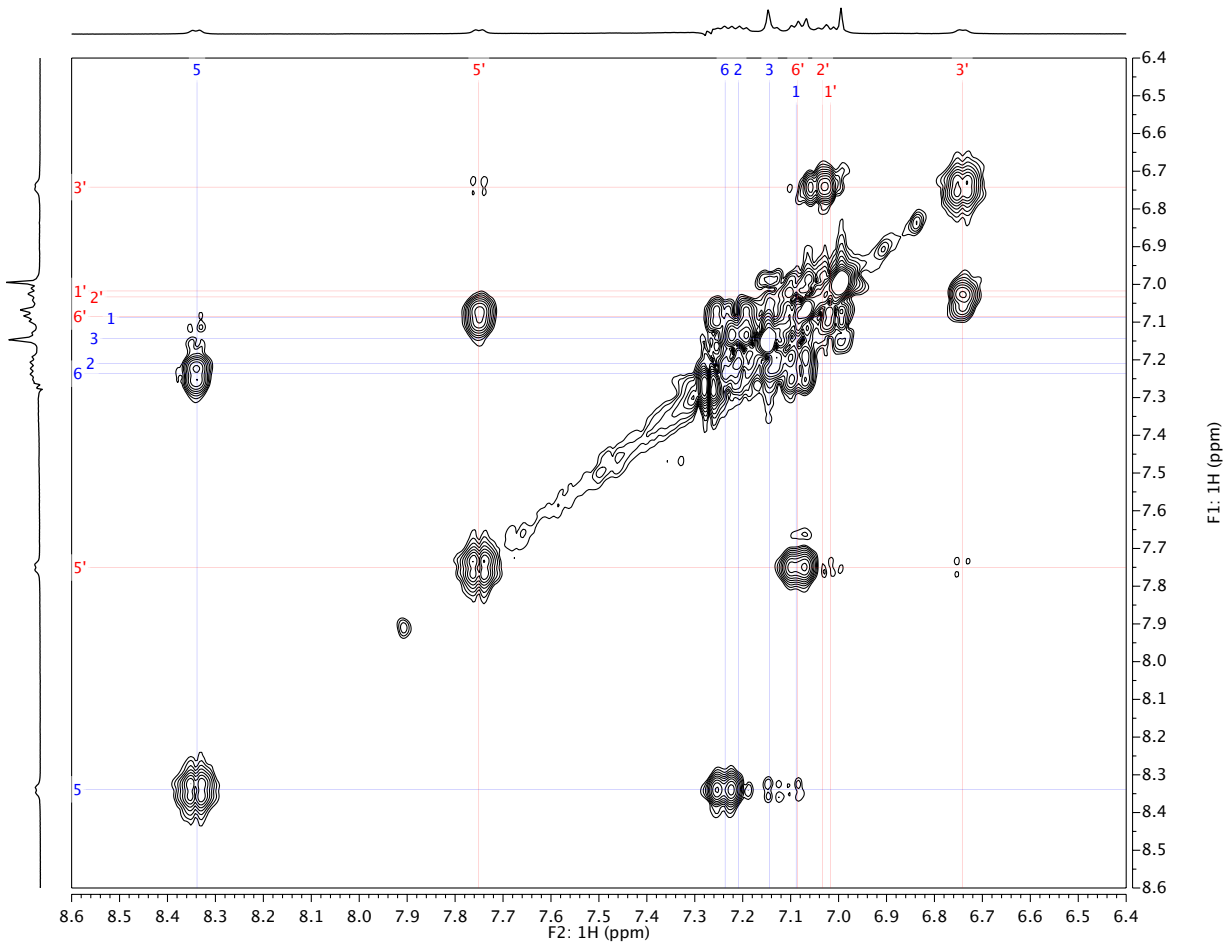


Figure 82. Expansion of the COSY spectrum of an aged solution of 0.10 M (*R,R*)-**1** in 0.25 M THF and 9.2 M toluene-d_8 at –60 °C with 0.21 M [^{6}Li]LDA.

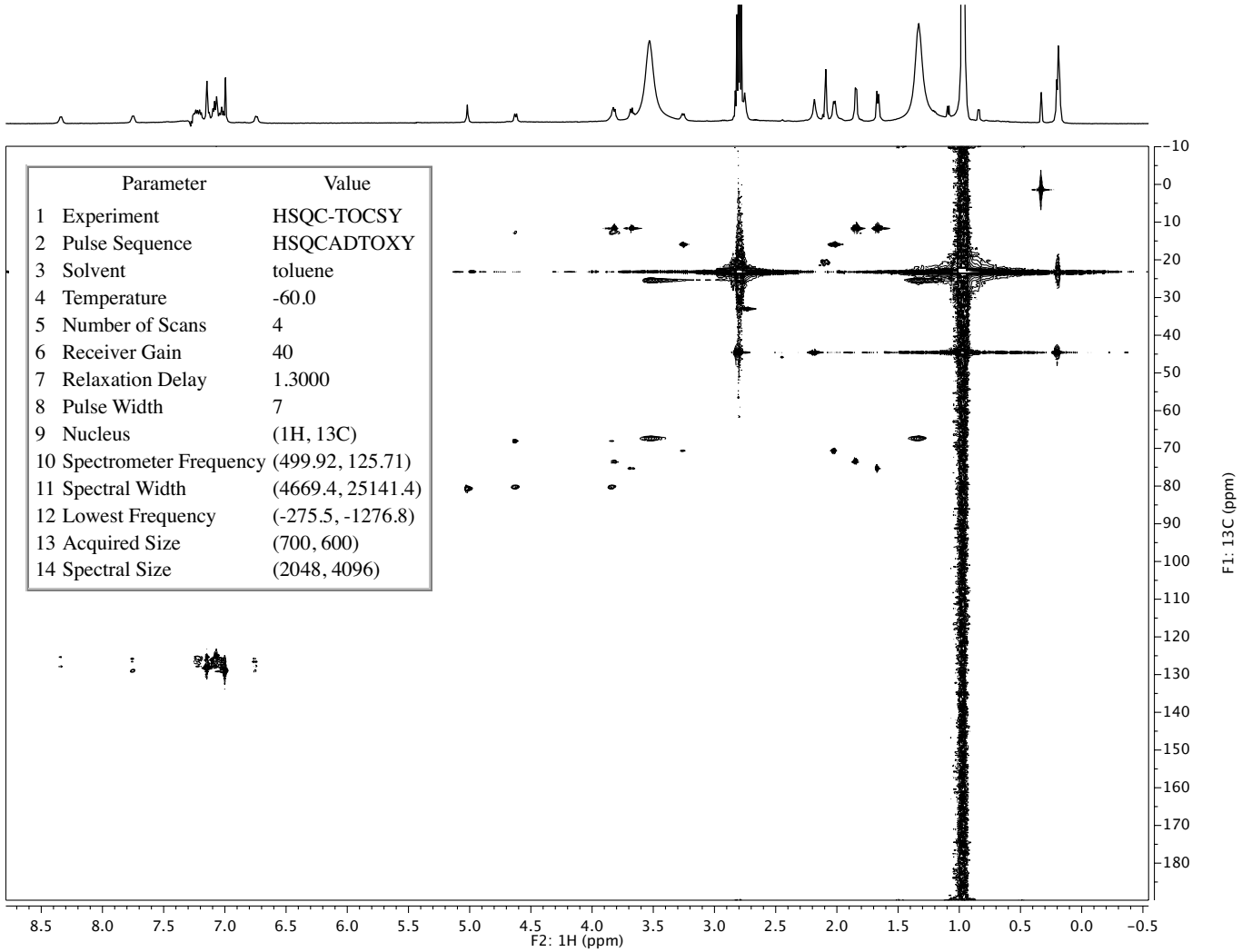


Figure 83. Full-display HSQC-TOCSY spectrum of an aged solution of 0.10 M (*R,R*)-**1** in 0.25 M THF and 9.2 M toluene-d_8 at –60 °C with 0.21 M [^{6}Li]LDA.

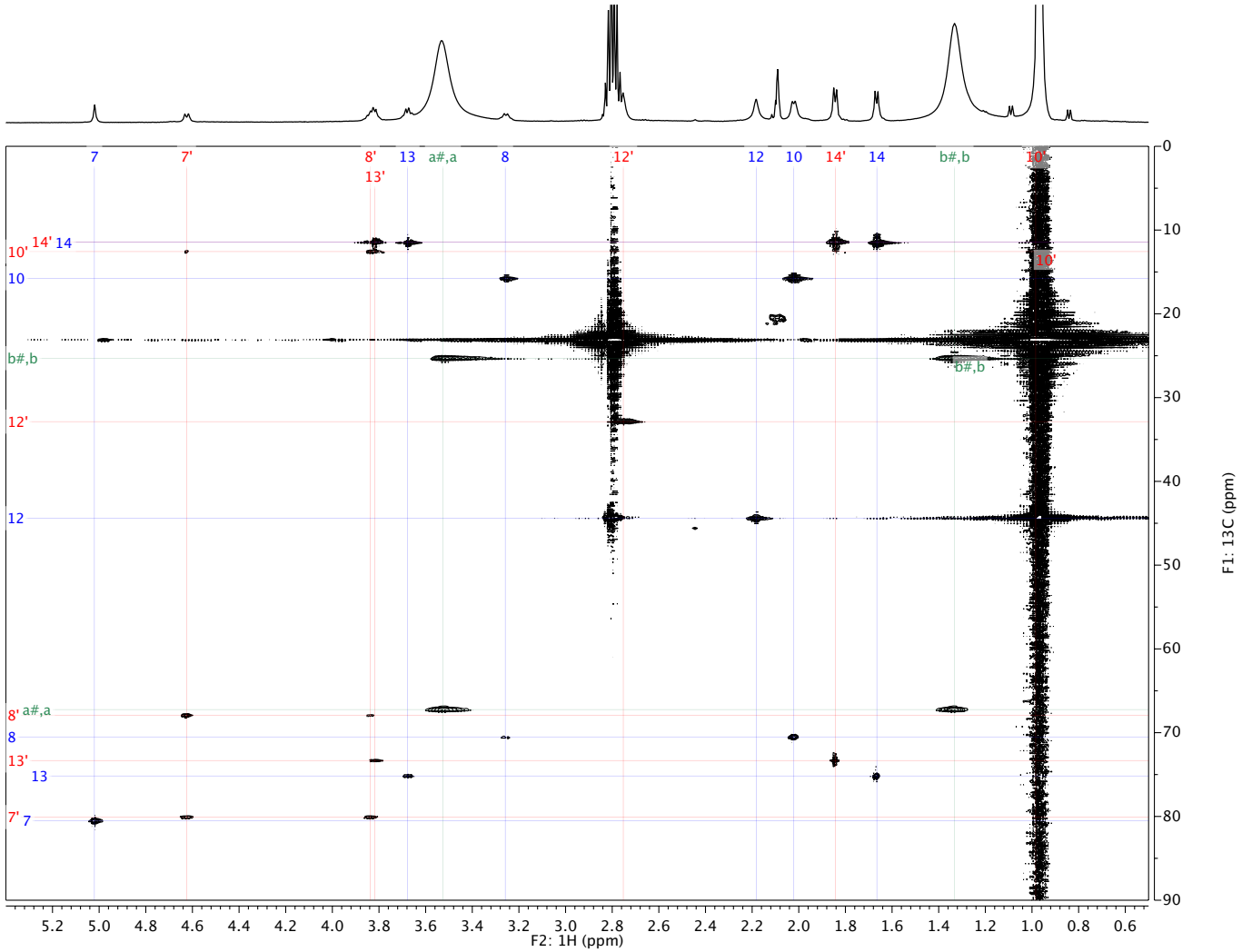


Figure 84. Expansion of the HSQC-TOCSY spectrum of an aged solution of 0.10 M (*R,R*)-**1** in 0.25 M THF and 9.2 M toluene-d_8 at –60 °C with 0.21 M [^{6}Li]LDA.

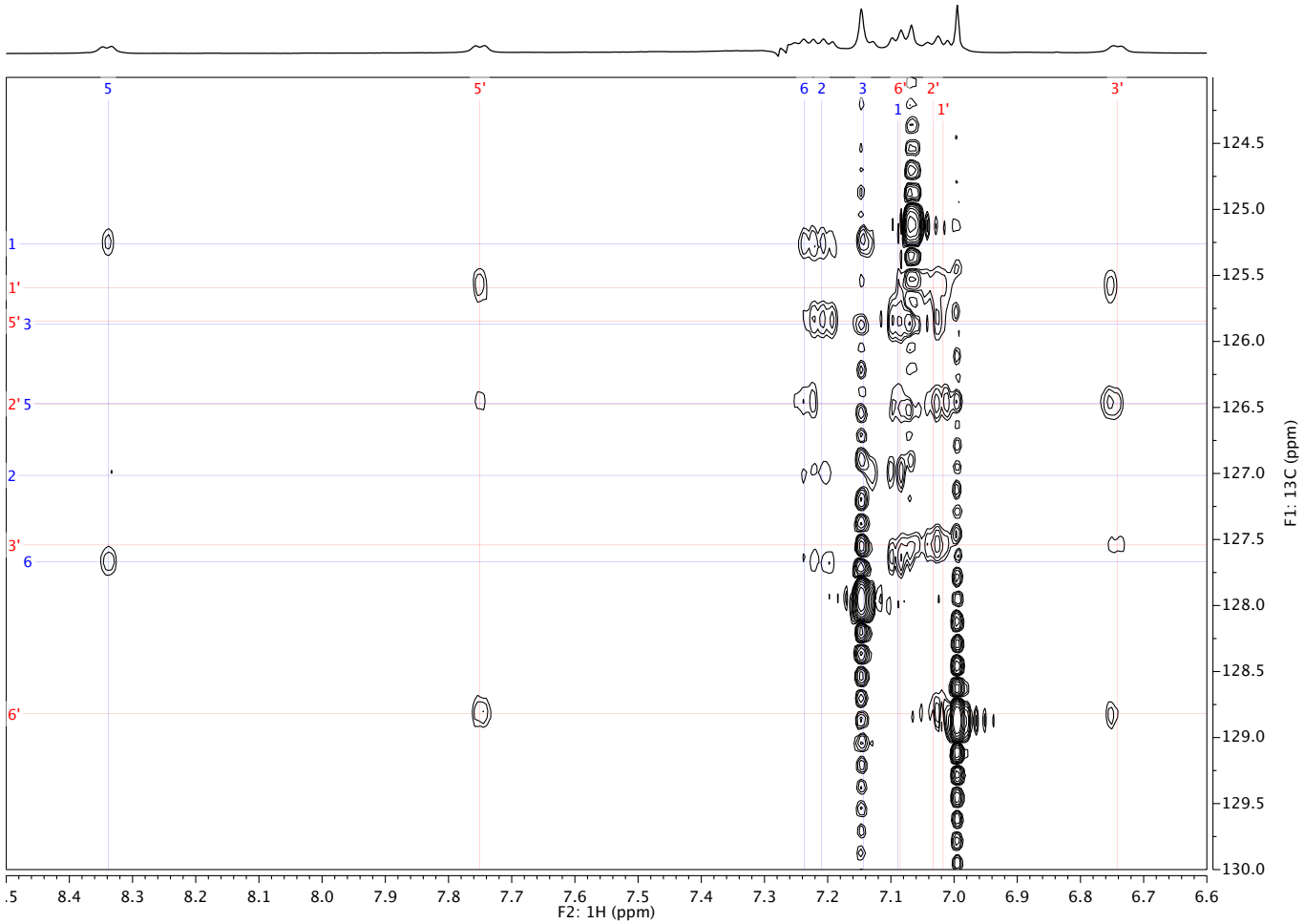


Figure 85. Expansion of the HSQC-TOCSY spectrum of an aged solution of 0.10 M (*R,R*)-**1** in 0.25 M THF and 9.2 M toluene-d_8 at –60 °C with 0.21 M [^{6}Li]LDA.

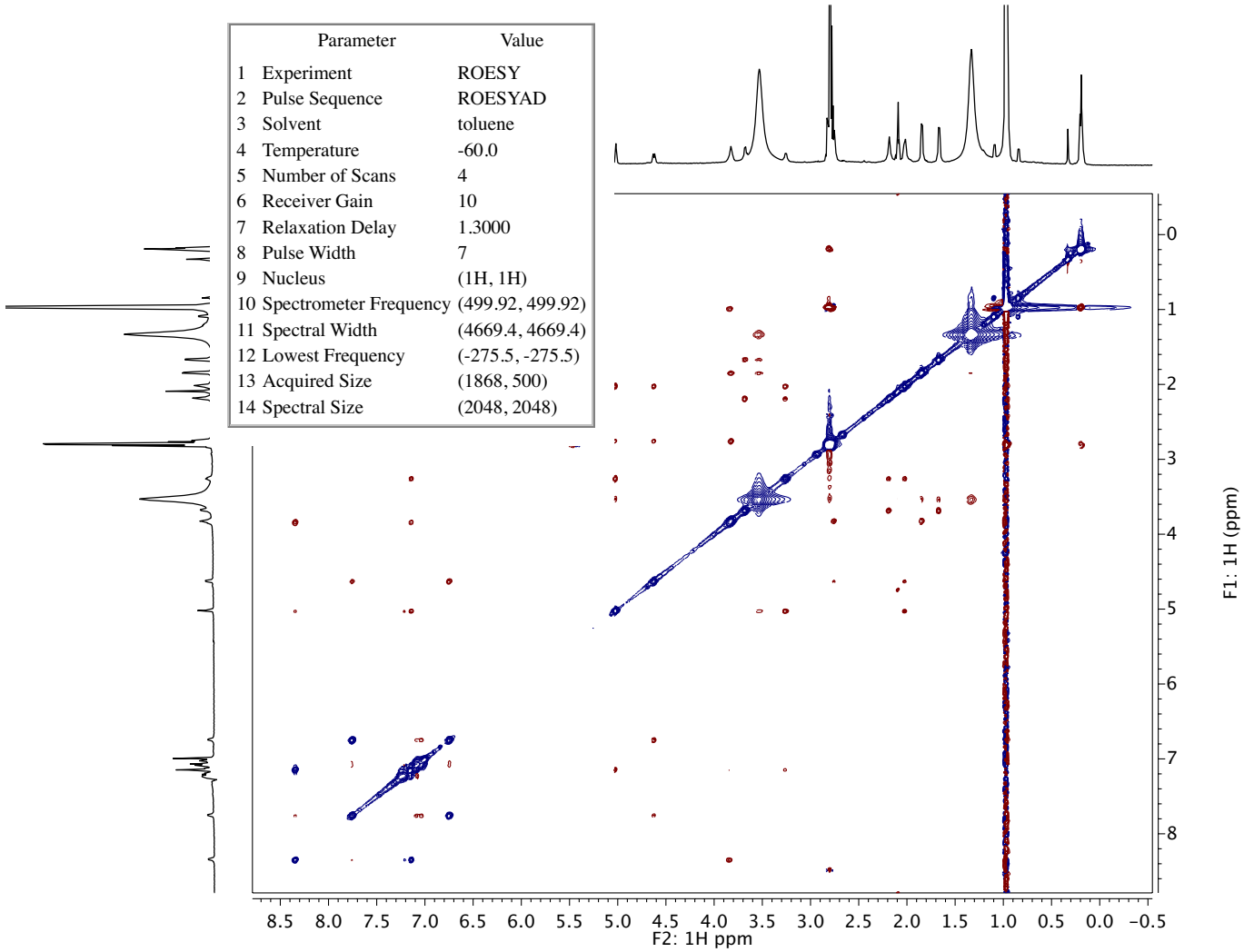


Figure 86. Full-display ROESY spectrum of an aged solution of 0.10 M (*R,R*)-**1** in 0.25 M THF and 9.2 M toluene-d_8 at –60 °C with 0.21 M [^{6}Li]LDA.

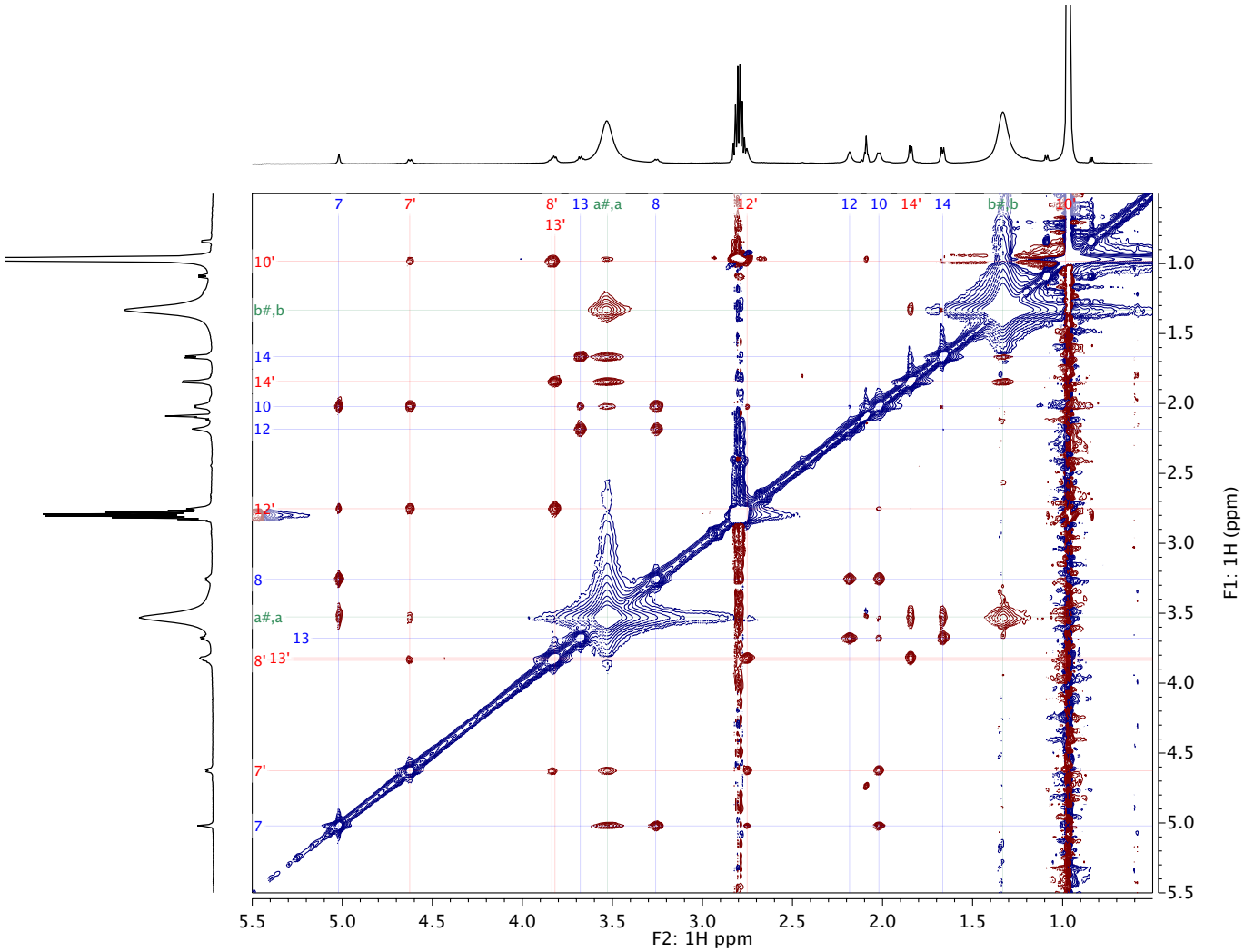


Figure 87. Expansion of the ROESY spectrum of an aged solution of 0.10 M (*R,R*)-**1** in 0.25 M THF and 9.2 M toluene-d_8 at –60 °C with 0.21 M [^{6}Li]LDA.

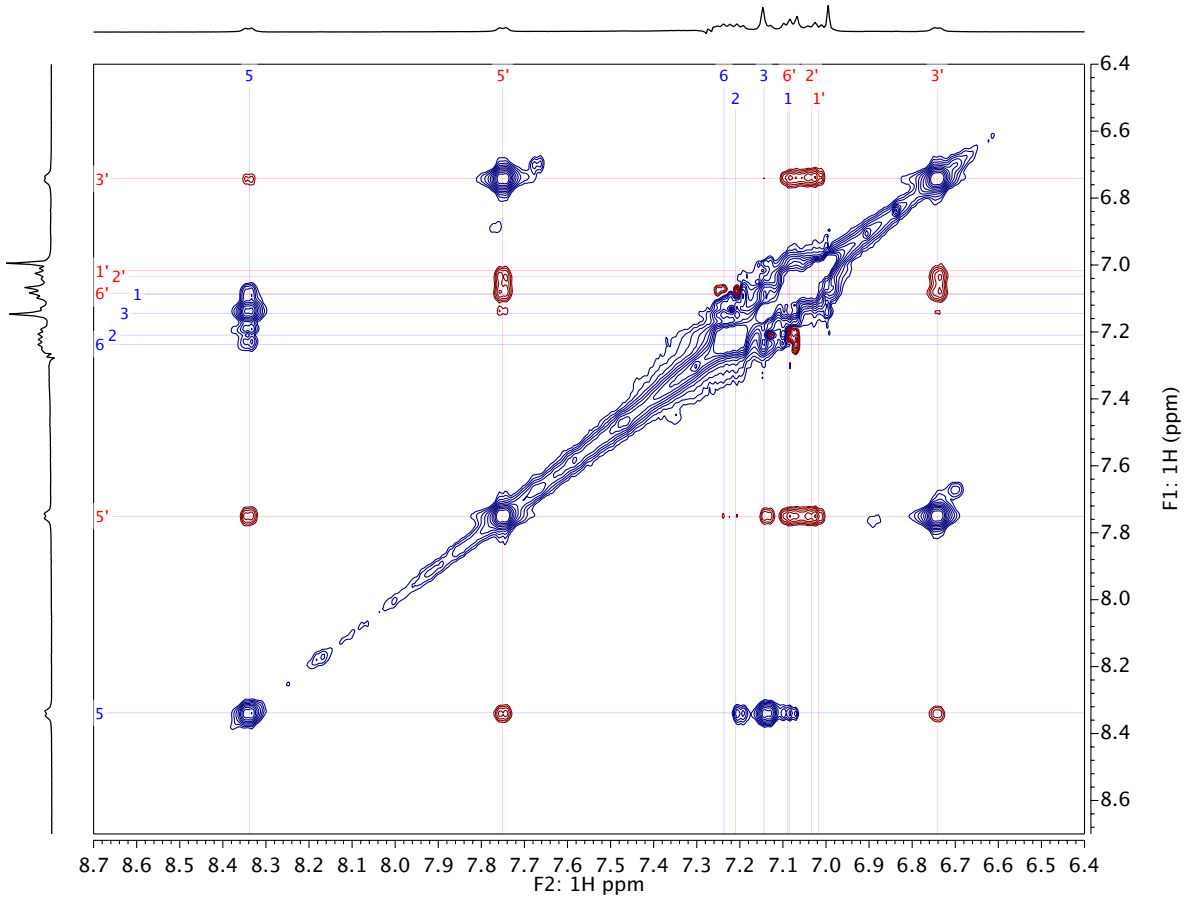


Figure 88. Expansion of the ROESY spectrum of an aged solution of 0.10 M (*R,R*)-**1** in 0.25 M THF and 9.2 M toluene-d_8 at –60 °C with 0.21 M [^{6}Li]LDA.

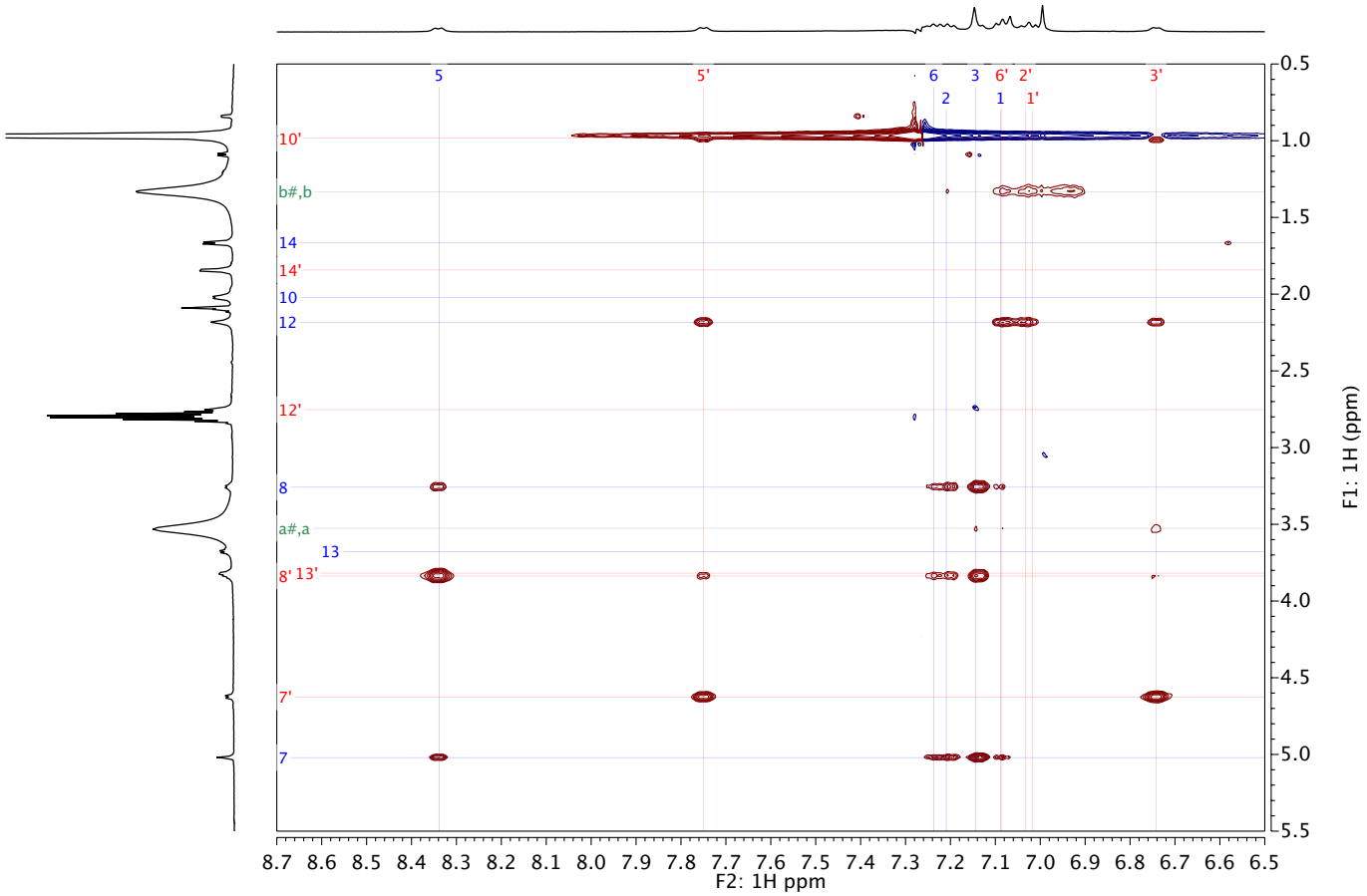
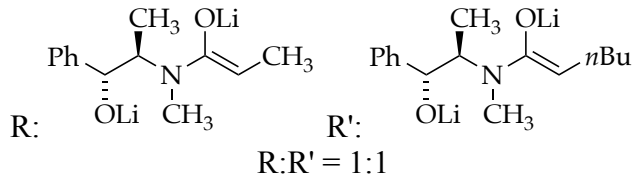


Figure 89. Expansion of the ROESY spectrum of an aged solution of 0.10 M (*R,R*)-**1** in 0.25 M THF and 9.2 M toluene-d_8 at –60 °C with 0.21 M [^{6}Li]LDA.

Part 3 Heteroaggregates Characterization



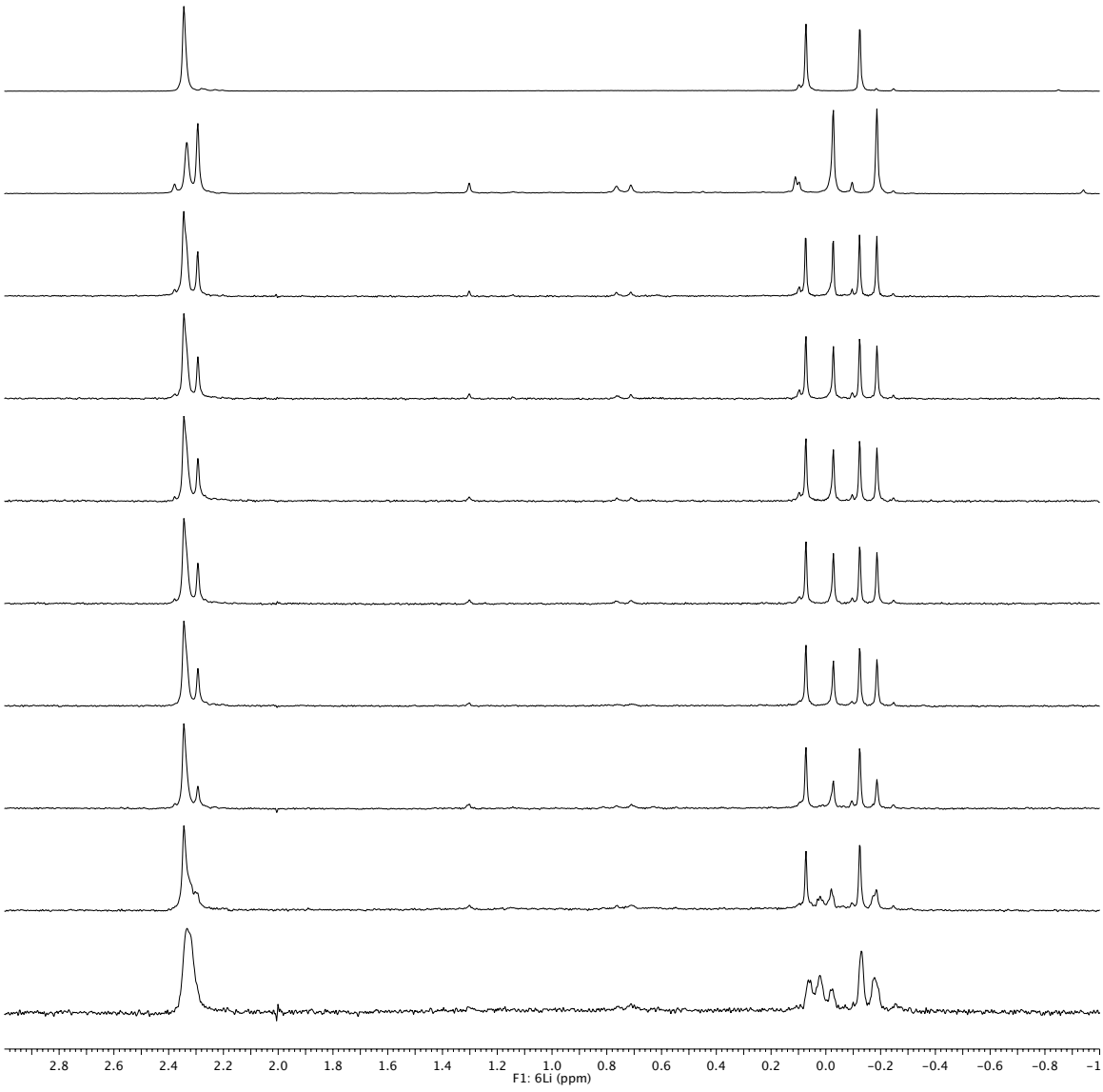


Figure 90. ^{6}Li NMR spectra for 0.10 M pre-aged solutions of [^{6}Li]-(*R,R*)-**2** (R_4) and [^{6}Li]-(*R,R*)-**8** (R'_4) in 12.3 M THF subsequently mixed and recorded at −80 °C: (a) R_4, (b) R'_4, (c) aged at –80 °C for 2 h, (d) aged at –60 °C for 15 min, (e) aged at –40 °C for 15 min, (f) aged at –20 °C for 15 min, (g) aged at –0 °C for 15 min, (h) aged at 20 °C for 15 min, (i) aged at 40 °C for 15 min, (j) aged at 40 °C for 60 min. Subunit exchange does not occur until 40 °C.

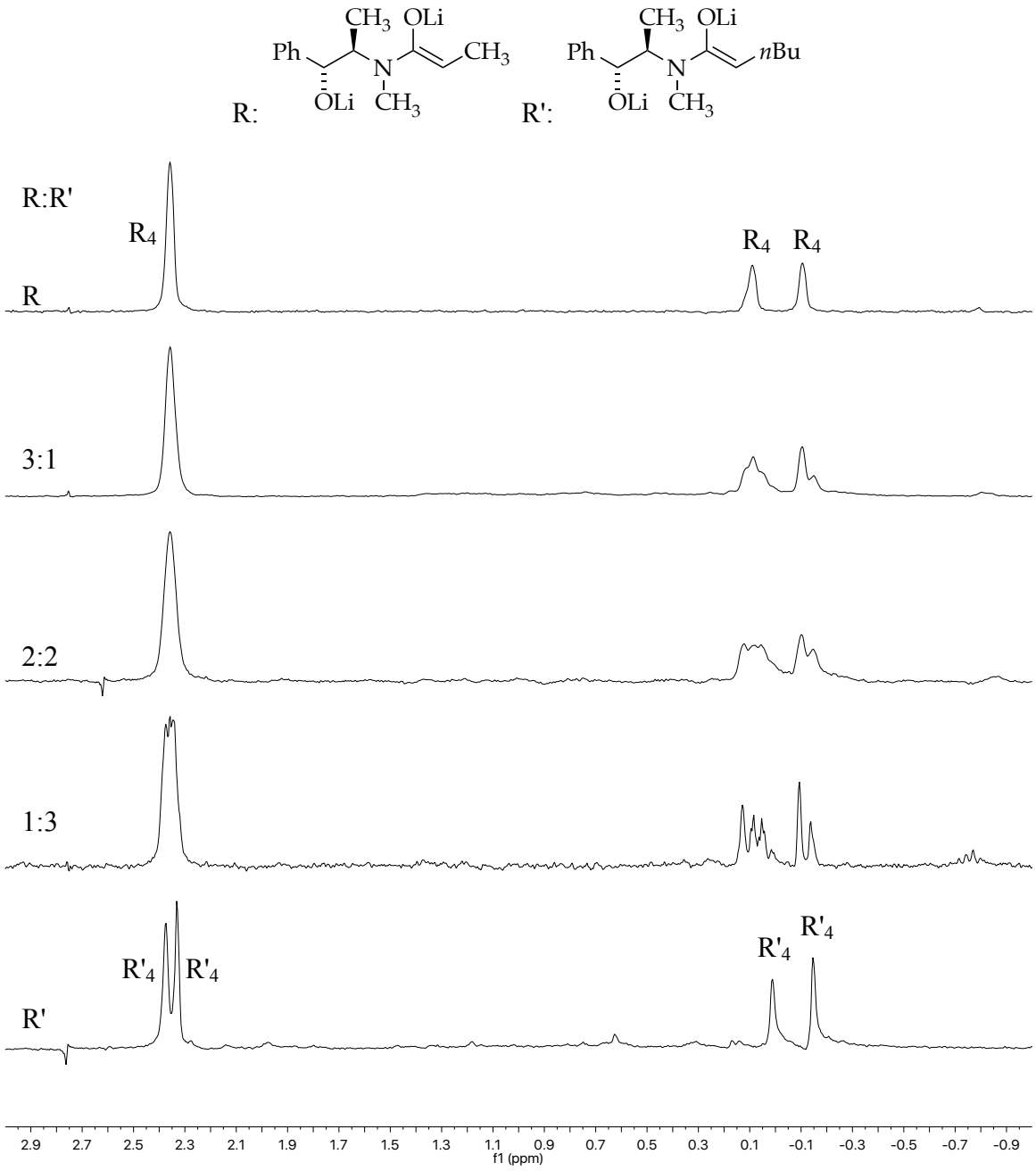


Figure 91. ^{6}Li NMR spectra for 0.10 M pre-aged solutions of [^{6}Li]-(*R,R*)-**2** (R) and [^{6}Li]-(*R,R*)-**8** (R') in 12.3 M THF at −80 °C. T1 relaxation was not optimized for integration. Homochiral heteroaggregates do not resolve owing to the large number (48) of possible species.

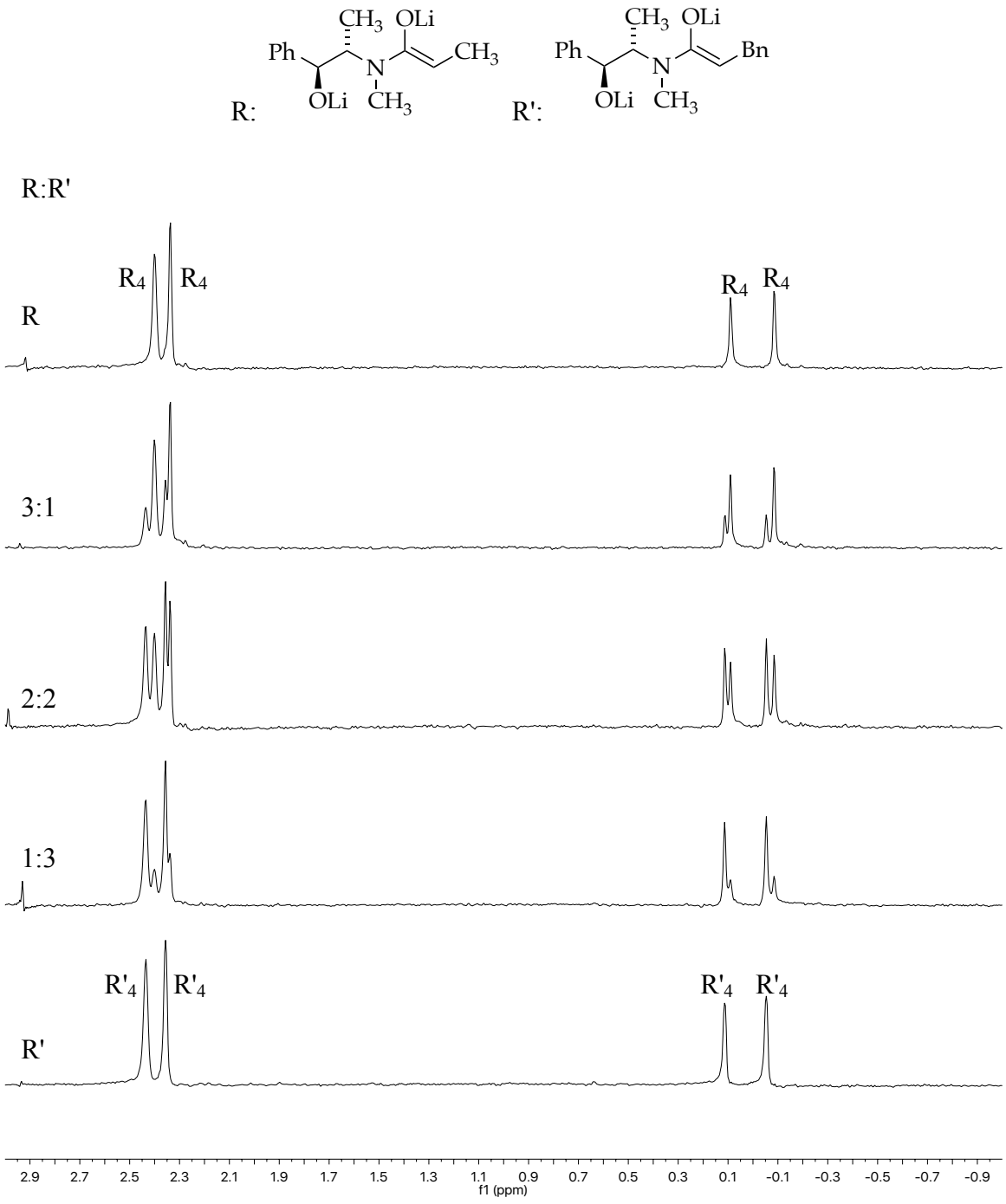


Figure 92. ^{6}Li NMR spectra for 0.10 M pre-aged solutions of [^{6}Li]-(*R,R*)-**2** (R) and [^{6}Li]-(*R,R*)-**11** (R') in 12.3 M THF at −20 °C. T1 relaxation was not optimized for integration. Each enolate was separately formed, aged at 20 °C for 10 min, and then mixed together. At –20 °C, the enolate subunits do not mix.

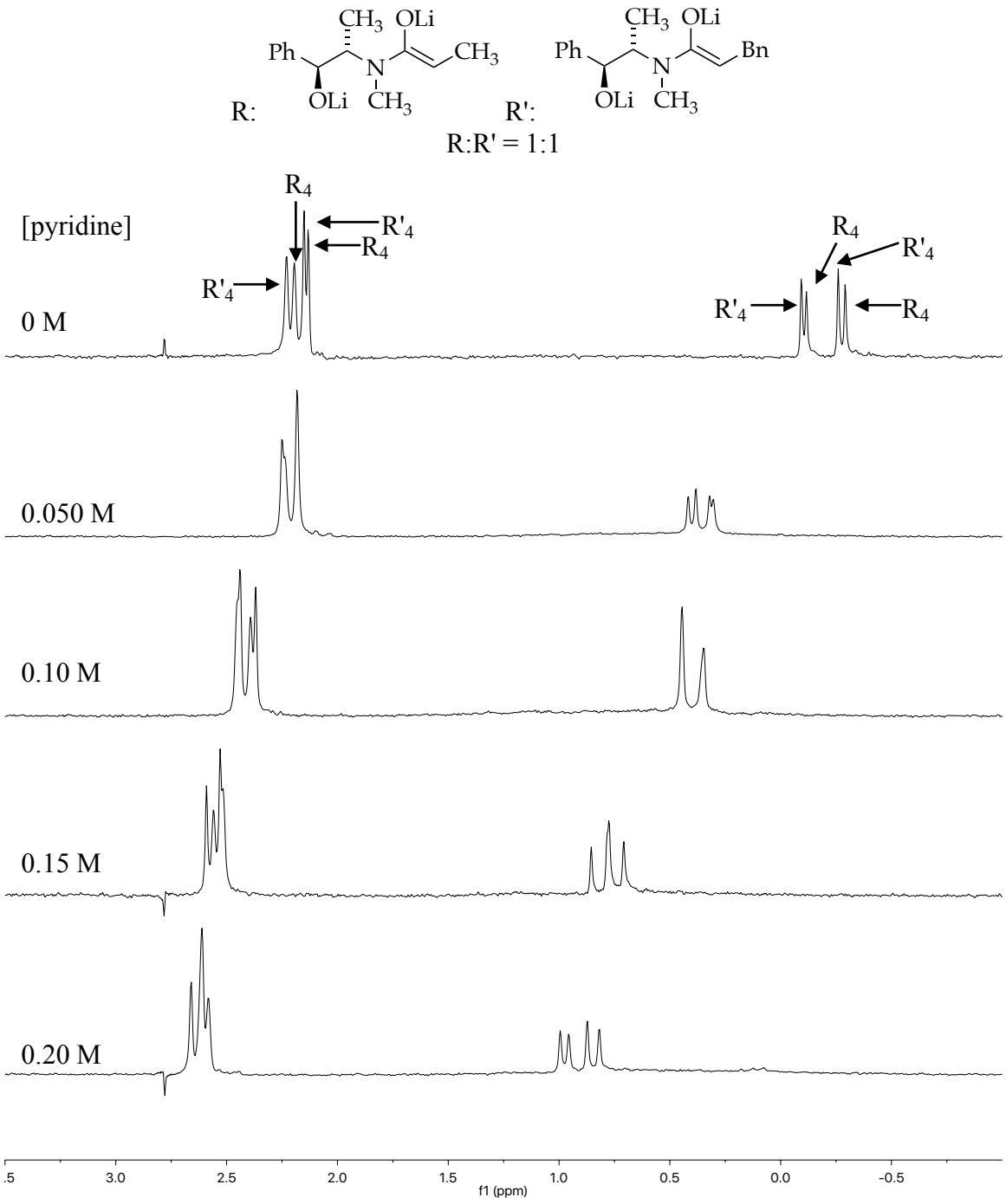


Figure 93. ^{6}Li NMR spectra for 0.10 M pre-aged solutions of 1:1 mixture of [^{6}Li]-(*R,R*)-**2** and [^{6}Li]-(*R,R*)-**11** in 12.3 M THF at −20 °C with varying pyridine concentrations. T1 relaxation was not optimized for integration. All homotetramer resonances are shifted by pyridine. The upfield peaks show a greater downfield shift than downfield peaks owing to direct coordination by pyridine. Each enolate was separately formed, aged at 20 °C for 10 min, and then mixed together. At –20 °C, the enolate subunits do not mix.

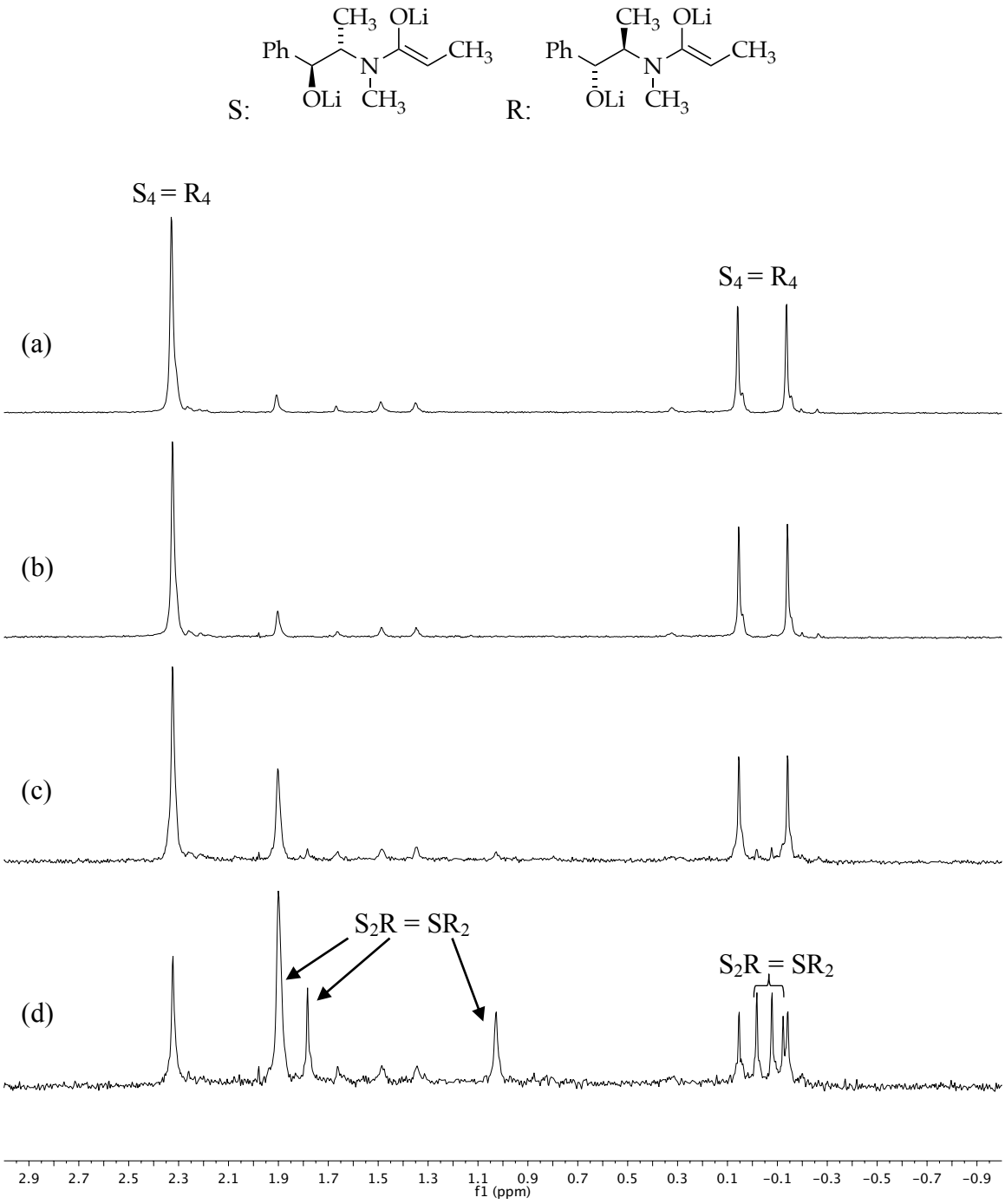


Figure 94. ^{6}Li NMR spectra for 0.10 M pre-aged solutions of [^{6}Li]-(*R,R*)-**2** (R_4) and [^{6}Li]-(*S,S*)-**2** (S_4) in 12.3 M THF subsequently mixed and recorded at −80 °C: (a) aged at –80 °C for 30 min, (b) aged at 0 °C for 15 min, (c) aged at 20 °C for 15 min, (d) aged at 40 °C for 15 min. Subunit exchange does not occur until 20 °C.

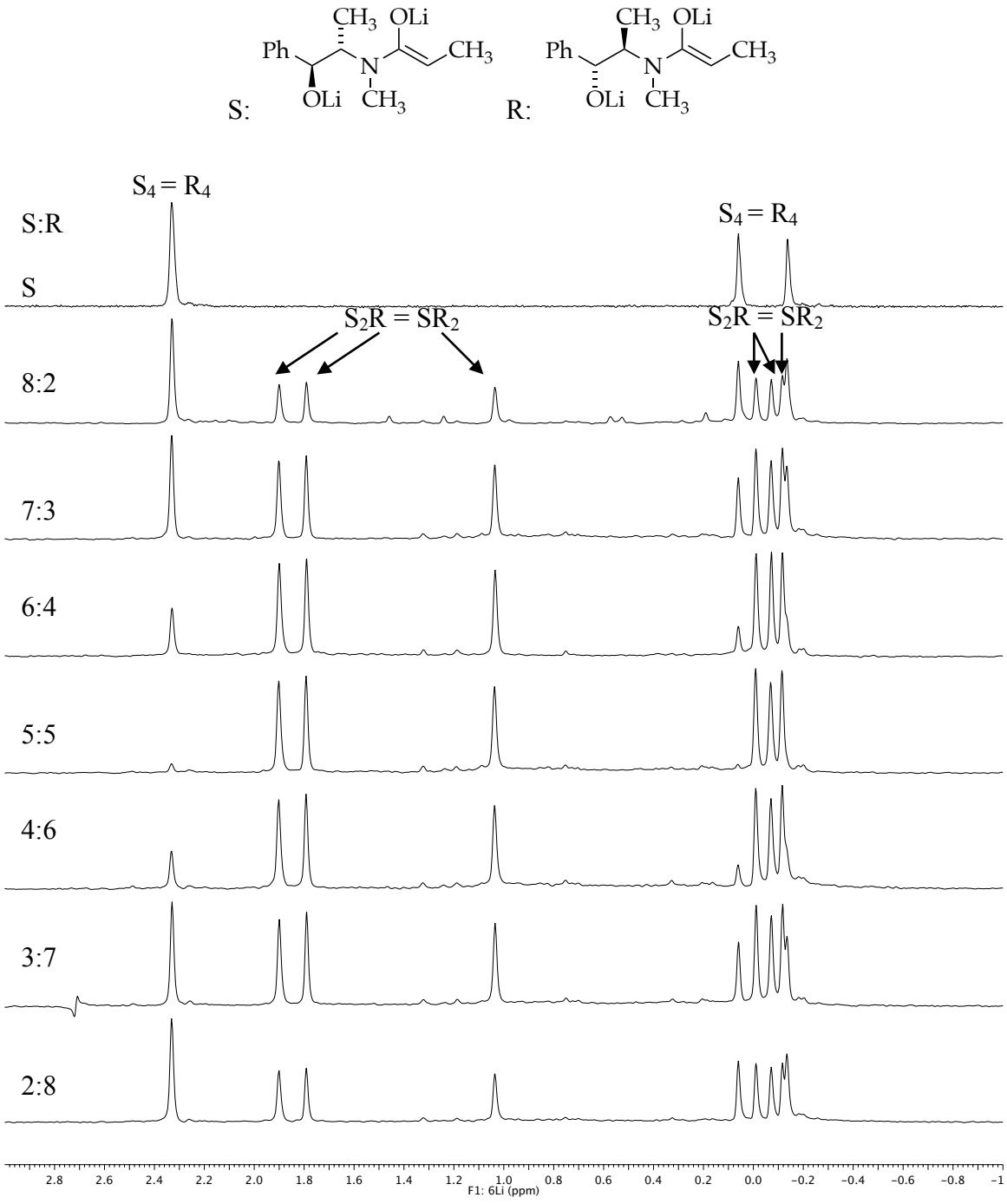


Figure 95. ^{6}Li NMR spectra for 0.10 M pre-aged solutions of [^{6}Li]-(*S,S*)-**2** (S) and [^{6}Li]-(*R,R*)-**2** (R) in 12.3 M THF at –80 °C. The heteroaggregate has 6 resonances (ratio 1:1:1:1:1:1) consistent with a hexalithiated trimer.

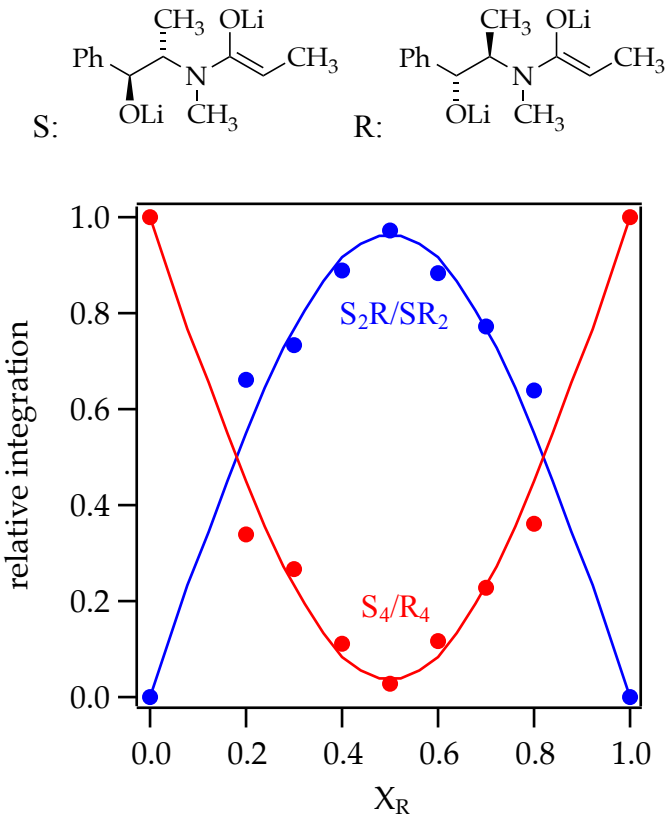


Figure 96. Job plot showing the relative integrations of octalithio-homoaggrgates and hexlithio-heteroaggregates versus intended mole fractions of [^{6}Li]-(*R,R*)-**2** ($\boldsymbol{X_R}$) for 0.10 M mixtures of lithium enolates [^{6}Li]-(*S,S*)-**2** (S) and [^{6}Li]-(*R,R*)-**2** (R) in neat THF at –80 °C monitored by ^{6}Li NMR spectroscopy (Figure 95). The curves result from a parametric fit to tetramer-trimer model.

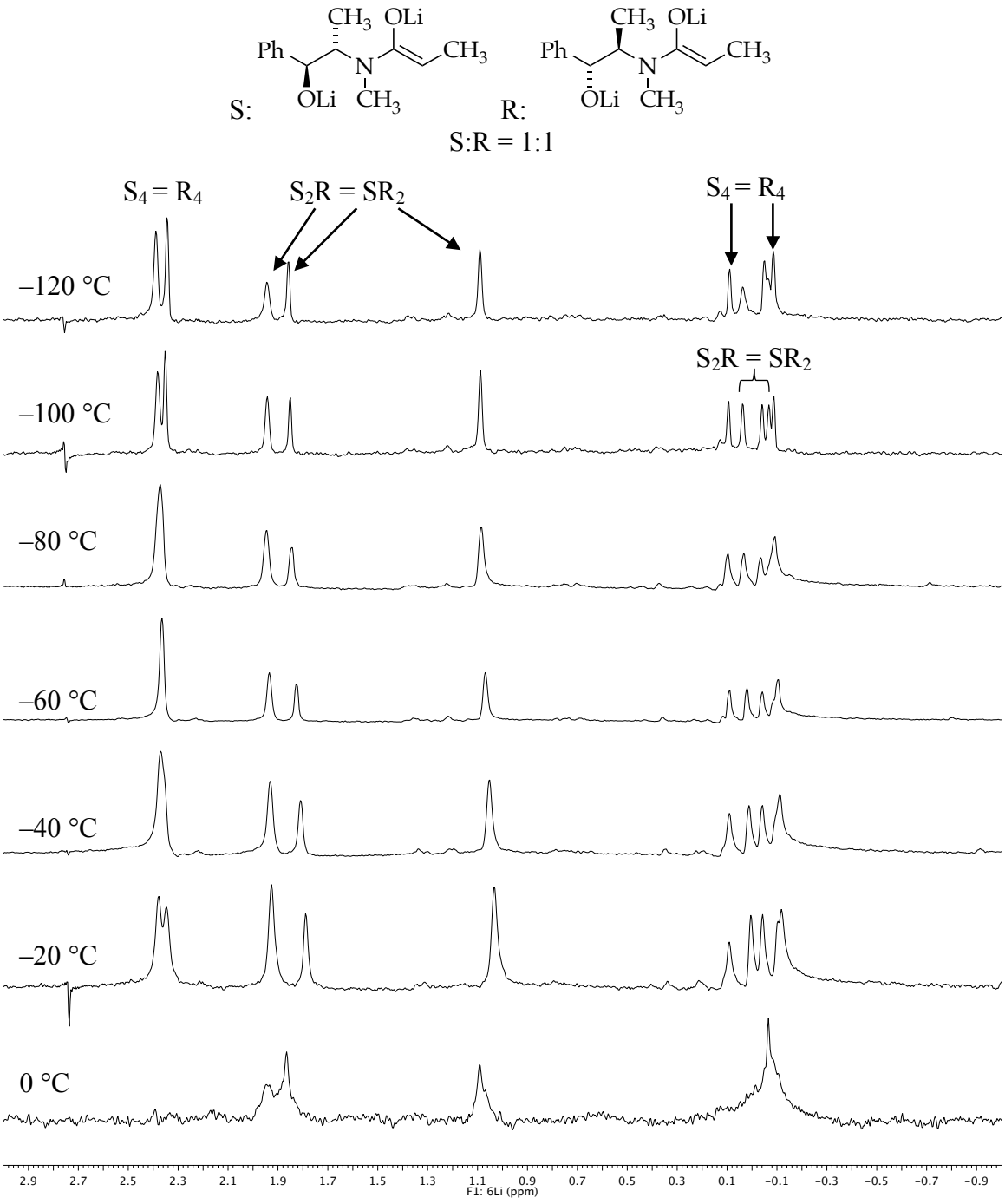


Figure 97. ^{6}Li NMR spectra for 0.10 M aged solutions of a 1:1 mixture of [^{6}Li]-(*S,S*)-**2** and [^{6}Li]-(*R,R*)-**2** in 12.3 M THF at varying temperature. T1 relaxation was not optimized for integration.

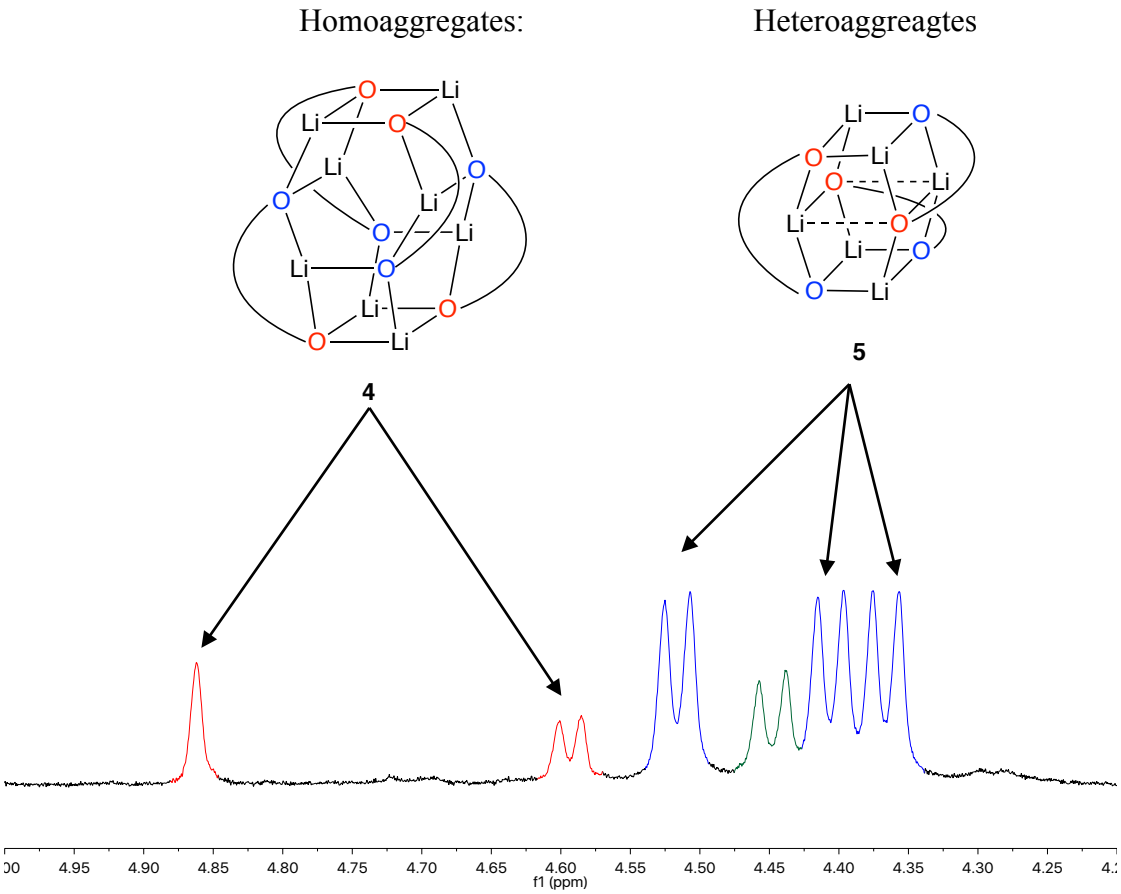


Figure 98. ^{1}H NMR spectrum of a pre-aged solution of 0.060 M [^{6}Li]-(*S,S*)-**2** and 0.040 M [^{6}Li]-(*R,R*)-**2** in 12.3 M THF at 20 °C. Corresponding heteroaggregates and homoaggregates peaks are labeled above. The doublet at 4.45 ppm (green) is LDA-mixed aggregate(s). ^{1}H NMR also shows the different aggregation state of homo- and hetero-aggregates.

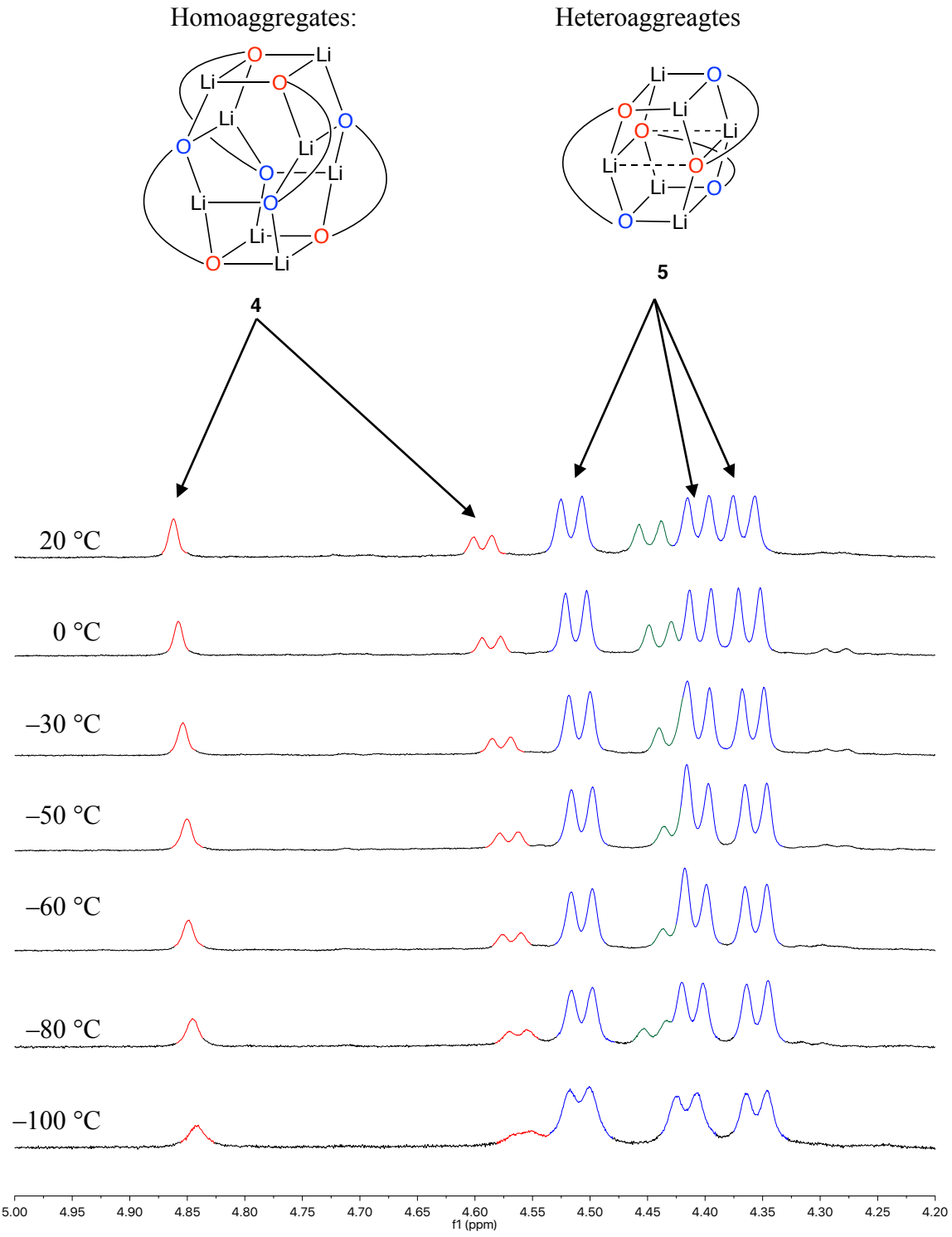


Figure 99. ^{1}H NMR spectra for 0.10 M pre-aged solutions of 0.060 M [^{6}Li]-(*S,S*)-**2** and 0.040 M [^{6}Li]-(*R,R*)-**2** in 12.3 M THF at varying temperature. Corresponding homoaggregate **4** and heteroaggregate **5** resonances are labeled. Varying the temperature shows no structural changes as found by ^{6}Li NMR spectroscopy.

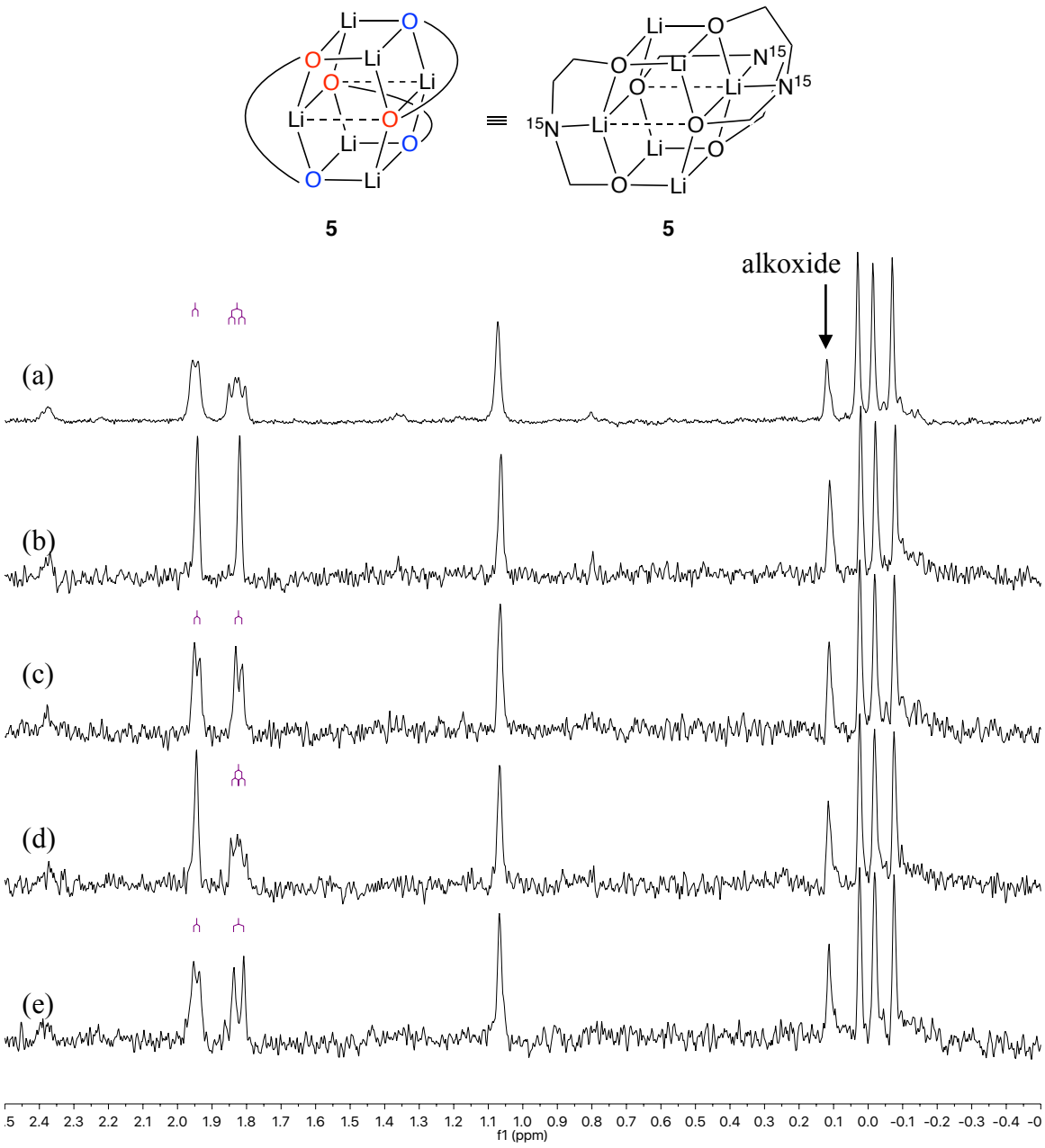


Figure 100. ^{6}Li NMR spectra of 0.050 M pre-aged solutions of 0.025 M [^{6}Li,^{15}N]-(*S,S*)-**2** and 0.025 M [^{6}Li,^{15}N]-(*R,R*)-**2** in 12.3 M THF at –80 °C: (a) direct detect, δ 1.95 ppm (d, J = 1.3 Hz), 1.83 ppm (dd, J = 2.2 Hz, 1.3 Hz); (b) broadband decoupling; (c) selective ^{15}N decoupling at 67.7 ppm; (d) selective ^{15}N decoupling at 57.7 ppm; (e) selective ^{15}N decoupling at 55.6 ppm. A ^{6}Li nucleus (1.87 ppm) is coupled to two ^{15}N nuclei (67.7 ppm and 55.6 ppm). Poor signal to noise of spectra (b) to (e) is caused by detecting through the lock channel. T1 relaxation was not optimized for integration. The peak at 0.10 ppm corresponds to alkoxides owing to a slight deficiency of LDA.

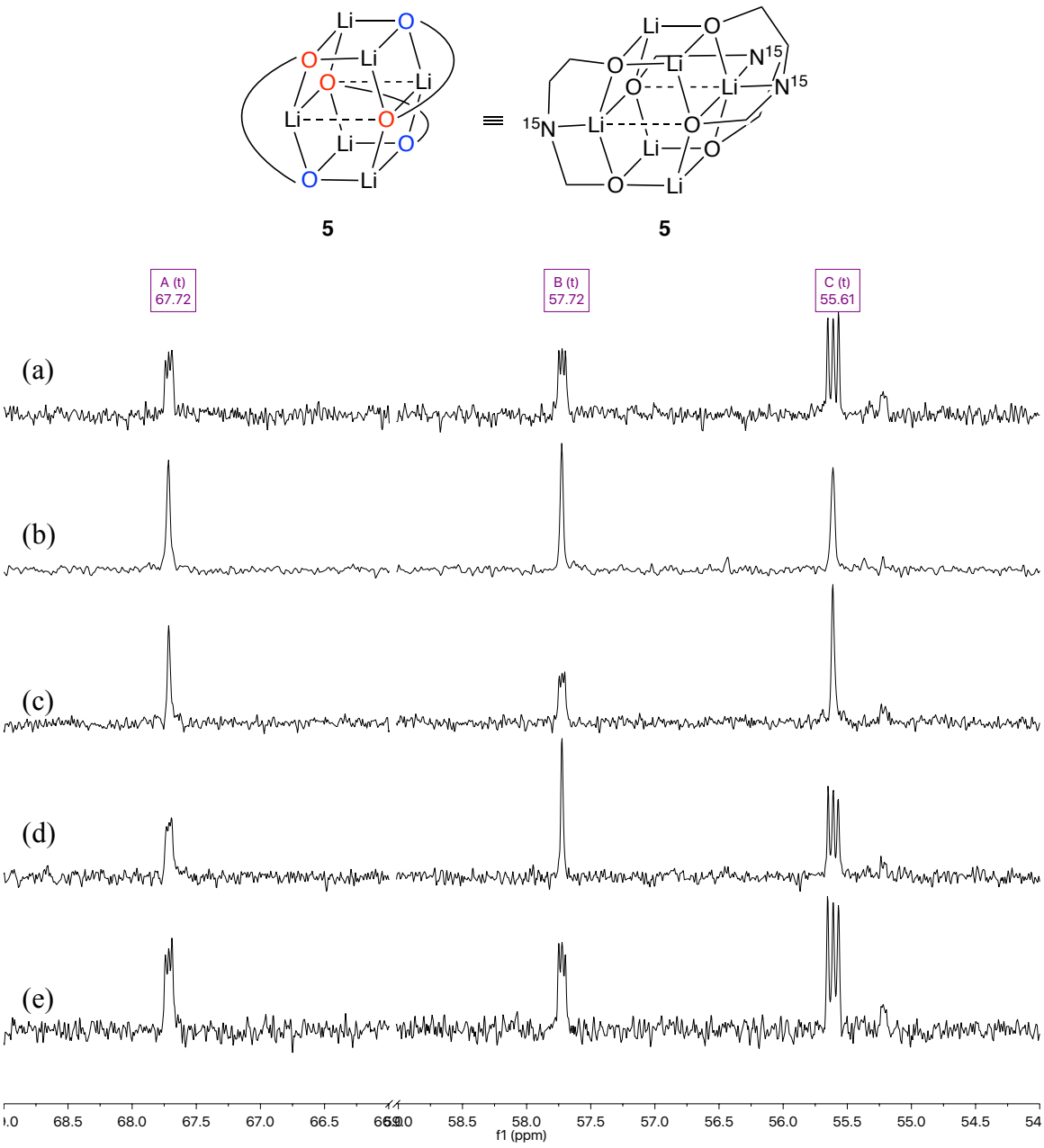


Figure 101. ^{15}N NMR spectra of 0.050 M pre-aged solutions of 0.025 M [^{6}Li,^{15}N]-(*S,S*)-**2** and 0.025 M [^{6}Li,^{15}N]-(*R,R*)-**2** in 12.3 M THF at –80 °C: (a) δ 67.7 ppm (t, J = 1.3 Hz), 57.7 ppm (t, J = 1.3 Hz), 55.6 ppm (t, J = 2.2 Hz); (b) broadband decoupling through direct detect ^{15}N NMR; (c) selective ^{6}Li decoupling at 1.87 ppm; (d) selective ^{6}Li decoupling at 1.97 ppm; (e) selective ^{6}Li decoupling at 1.06 ppm. Two ^{15}N nuclei (67.7 ppm and 55.6 ppm) are coupled to the same ^{6}Li nucleus (1.87 ppm). An ^{15}N nucleus (57.7 ppm) is coupled to a ^{6}Li nucleus (1.97 ppm). Insensitive nuclei enhanced by polarization transfer (INEPT) was applied on spectra (a), (c), (d), and (e), which makes the integrations invalid.

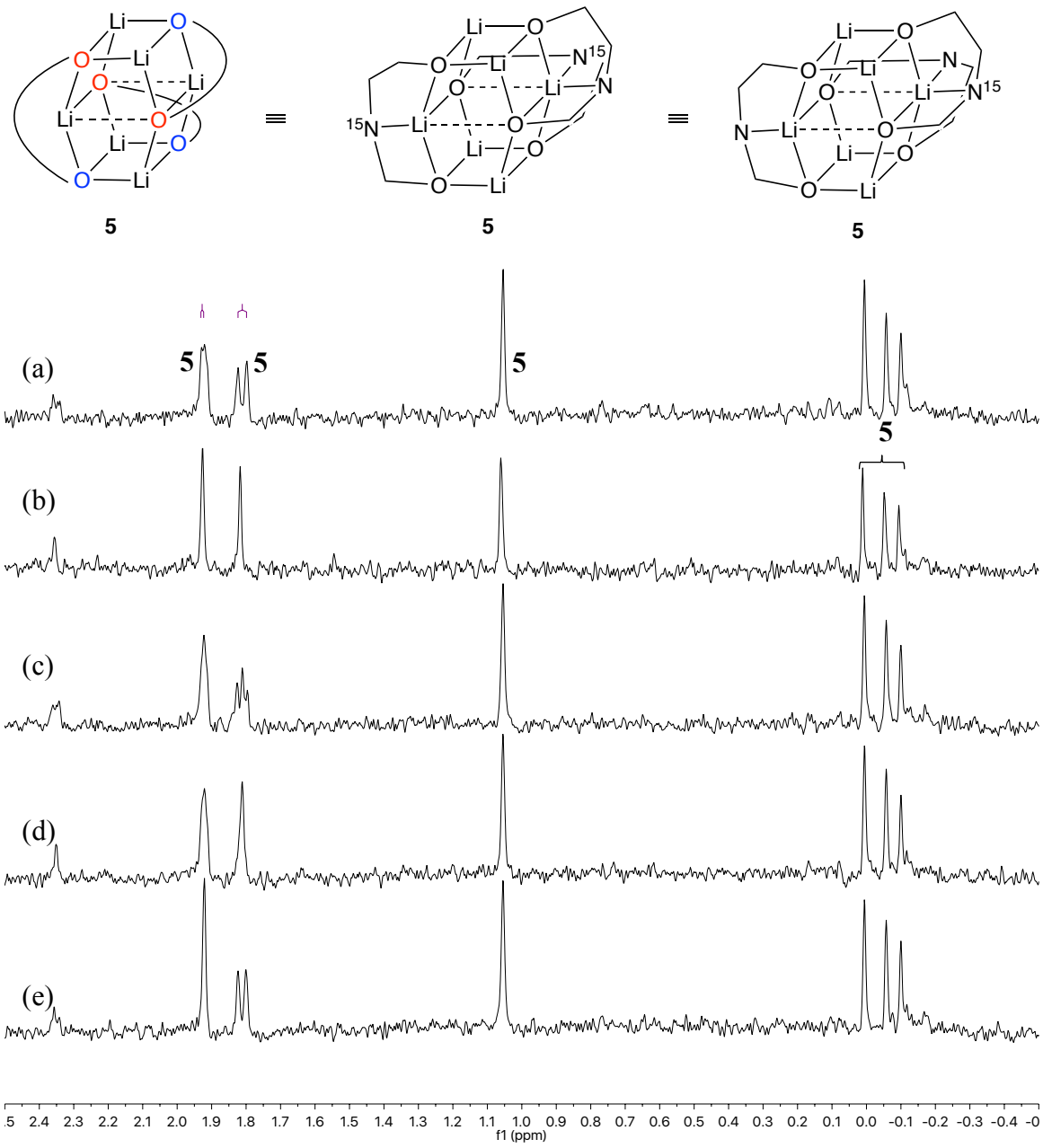


Figure 102. ^{6}Li NMR spectra for 0.050 M pre-aged solutions of 0.033 M [^{6}Li,^{15}N]-(*S,S*)-**2** and 0.017 M [^{6}Li]-(*R,R*)-**2** in 12.3 M THF at –80 °C: (a) no decoupling, δ 1.95 ppm (d, J = 1.3 Hz), 1.83 ppm (dd, J = 2.2 Hz, 1.3 Hz); (b) broadband decoupling; (c) selective ^{15}N decoupling at 67.7 ppm; (d) selective ^{15}N decoupling at 57.7 ppm; (e) selective ^{15}N decoupling at 55.6 ppm. Poor signal to noise is caused by detecting through the lock channel. T1 relaxation was not optimized for integration. Labeling one of the enantiomer shows the core is made of a *R*/*S* pair.

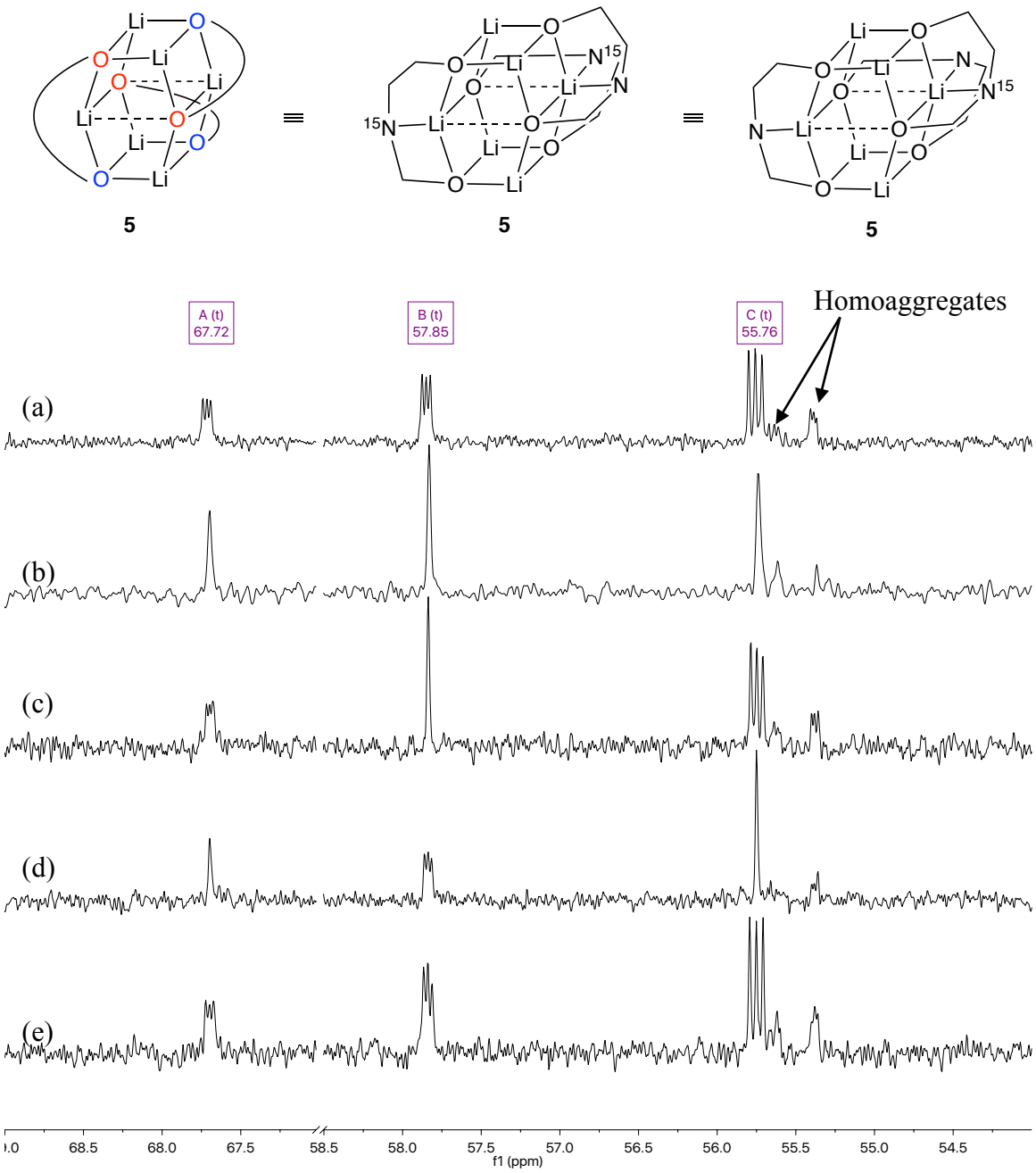


Figure 103. ^{15}N NMR spectra for 0.050 M pre-aged solutions of 0.033 M [^{6}Li,^{15}N]-(*S,S*)-**2** and 0.017 M [^{6}Li]-(*R,R*)-**2** in 12.3 M THF at –80 °C: (a) no decoupling; (b) broadband decoupling with direct detect ^{15}N NMR; (c) selective ^{6}Li decoupling at 1.97 ppm; (d) selective ^{6}Li decoupling at 1.87 ppm; (e) selective ^{6}Li decoupling at 1.06 ppm. Two ^{15}N nuclei (67.7 ppm and 55.6 ppm) are coupled to the same ^{6}Li nucleus (1.87 ppm). And ^{15}N nucleus (57.7 ppm) is coupled to ^{6}Li nucleus (1.97 ppm). Insensitive nuclei enhanced by polarization transfer (INEPT) was used on spectra (a), (c), (d), and (e), which makes the integrations invalid.

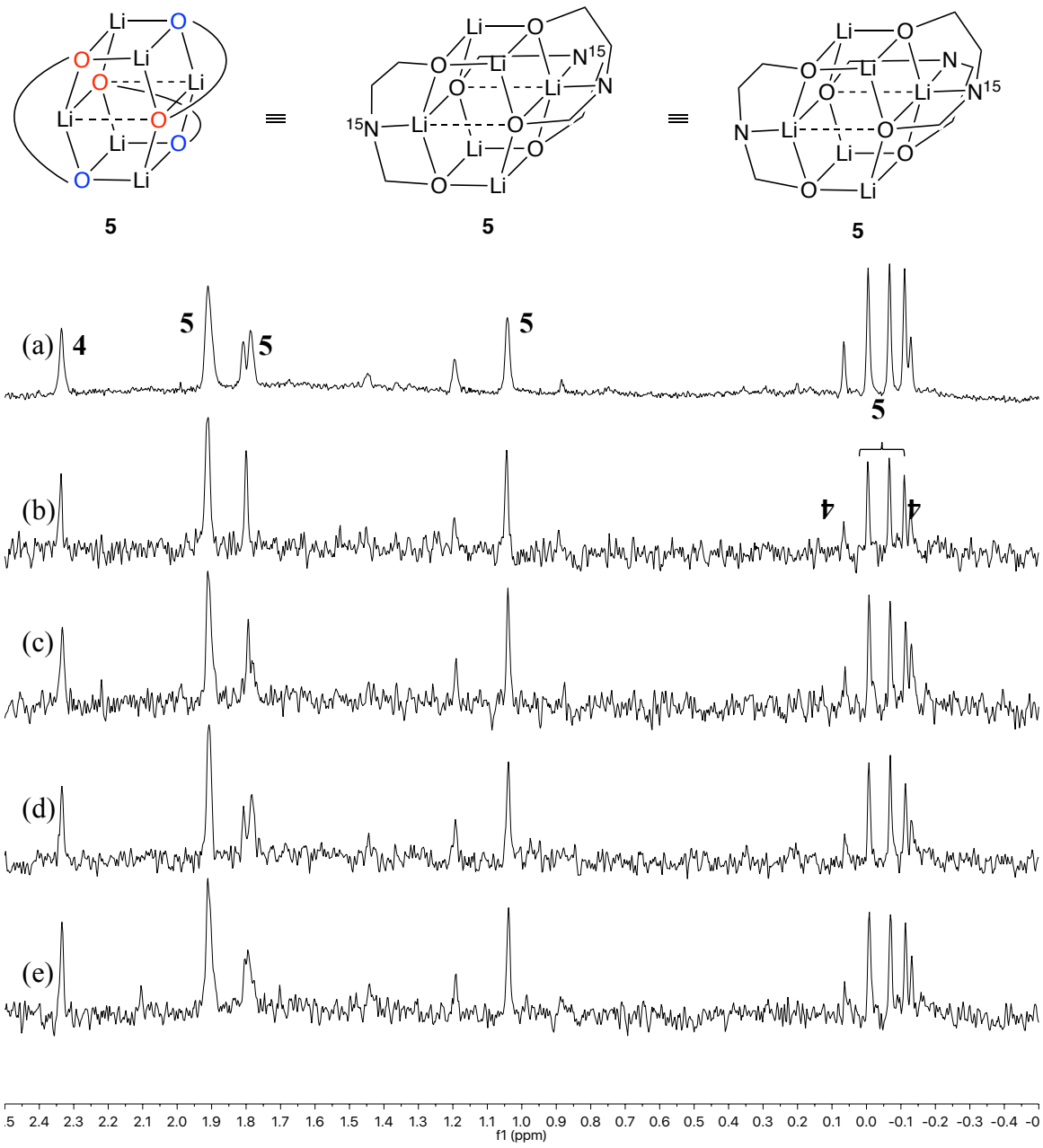


Figure 104. ^{6}Li NMR spectra for 0.050 M pre-aged solutions of 0.017 M [^{6}Li,^{15}N]-(*S,S*)-**2** and 0.033 M [^{6}Li]-(*R,R*)-**2** in 12.3 M THF at –80 °C: (a) direct detect; (b) broadband decoupling; (c) selective ^{15}N decoupling at 67.7 ppm; (d) selective ^{15}N decoupling at 57.7 ppm; (e) selective ^{15}N decoupling at 55.6 ppm. Poor signal to noise is caused by detecting through the lock channel. T1 relaxation was not optimized for integration. Labeling one of the enantiomers shows the core is made of an *R*/*S* pair.

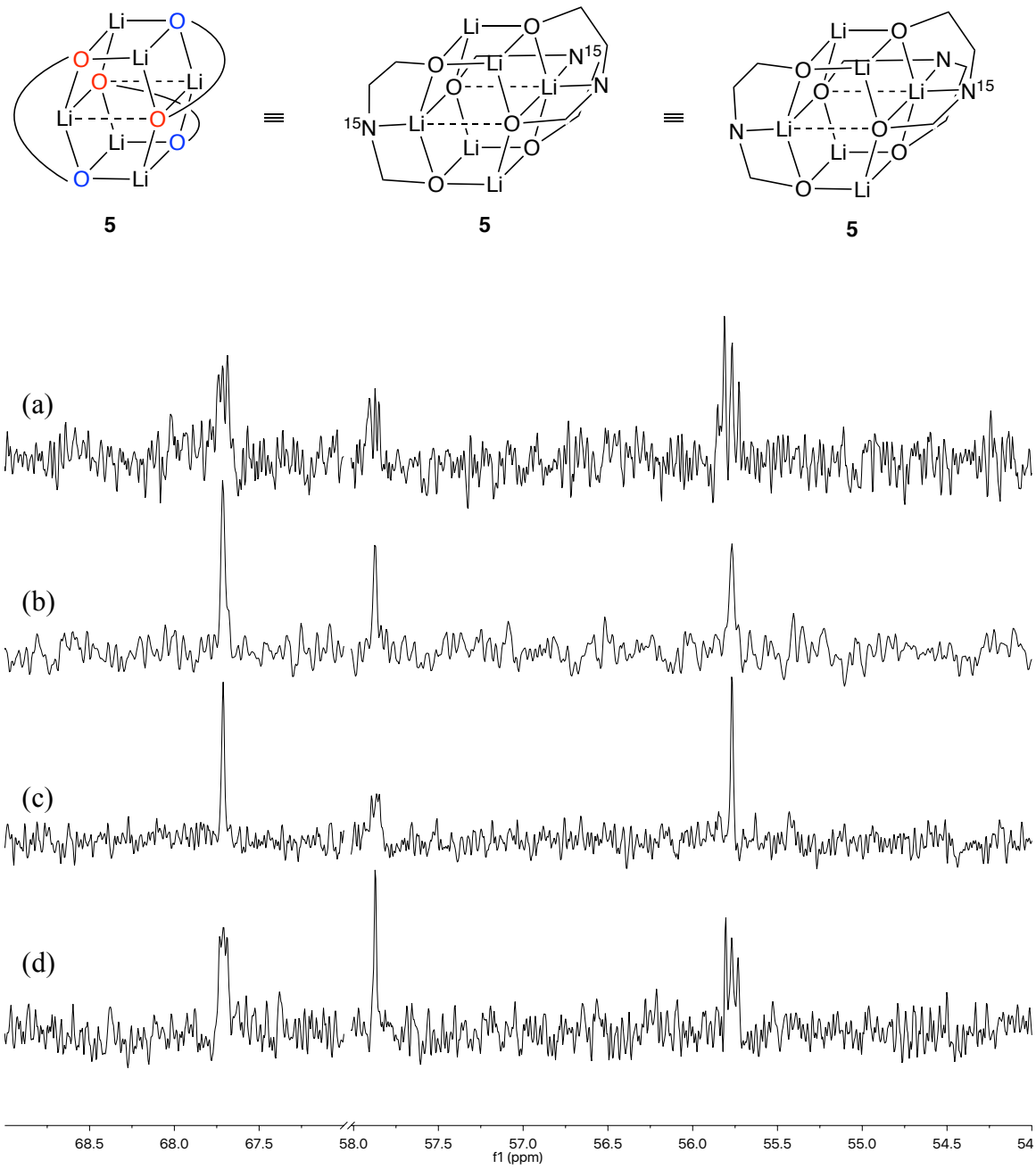


Figure 105. ^{15}N NMR spectra for 0.050 M pre-aged solutions of 0.017 M [^{6}Li,^{15}N]-(*S,S*)-**2** and 0.033 M [^{6}Li]-(*R,R*)-**2** in 12.3 M THF at –80 °C: (a) no decoupling; (b) broadband decoupling; (c) selective ^{6}Li decoupling at 1.87 ppm; (d) selective ^{6}Li decoupling at 1.97 ppm. Poor signal to noise was caused by low concentration of [^{15}N]-labelled substrate. Insensitive nuclei enhanced by polarization transfer (INEPT) was used on spectra (a), (c), (d), and (e), which makes the integrations invalid.

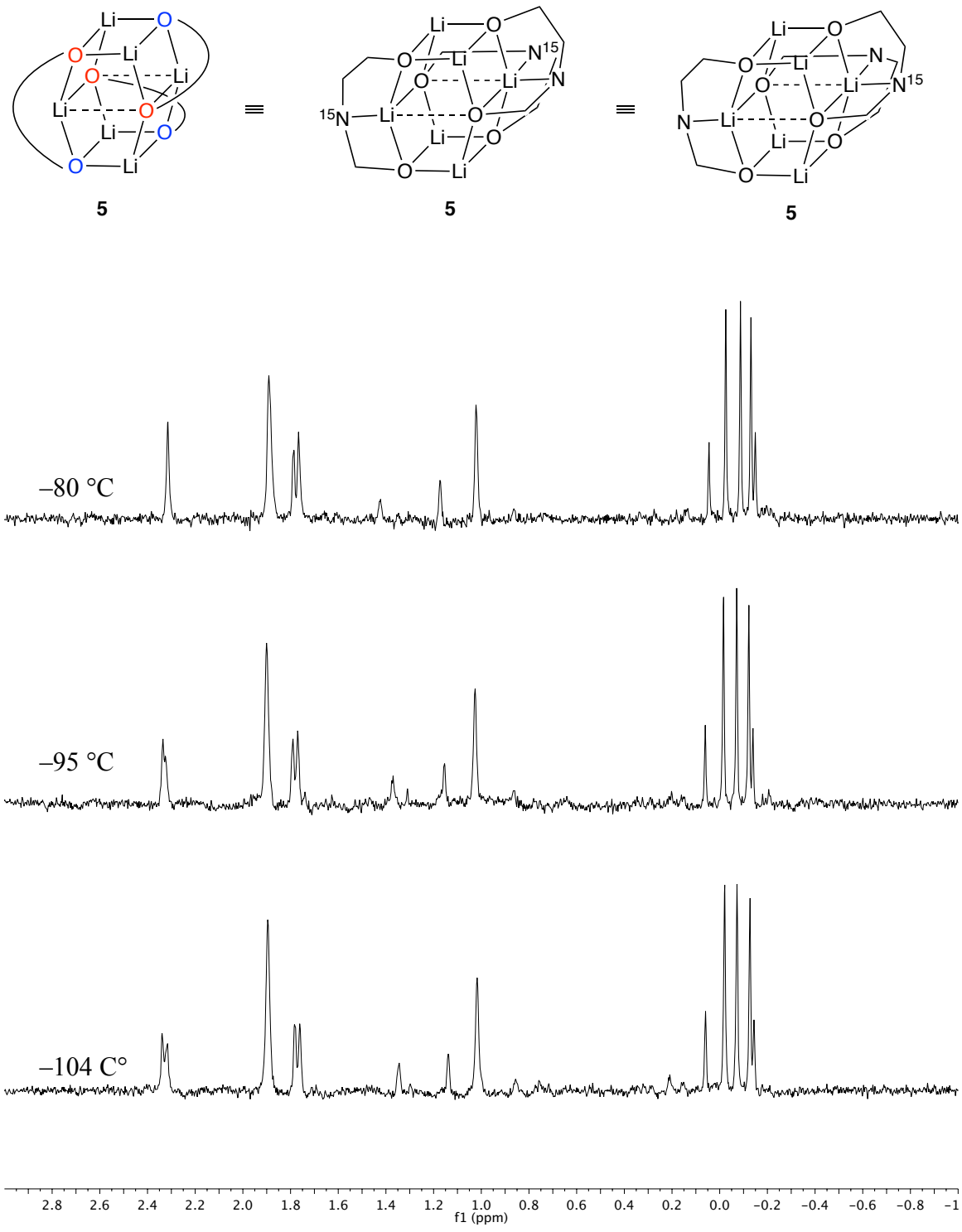


Figure 106. ^{6}Li NMR spectra of for 0.050 M pre-aged solutions of 0.017 M [^{6}Li,^{15}N]-(*S,S*)-**2** and 0.033 M [^{6}Li]-(*R,R*)-**2** in 12.3 M THF at –80 °C at varying temperature. Lowering the temperature (–104 °C) does not resolve more resonances.

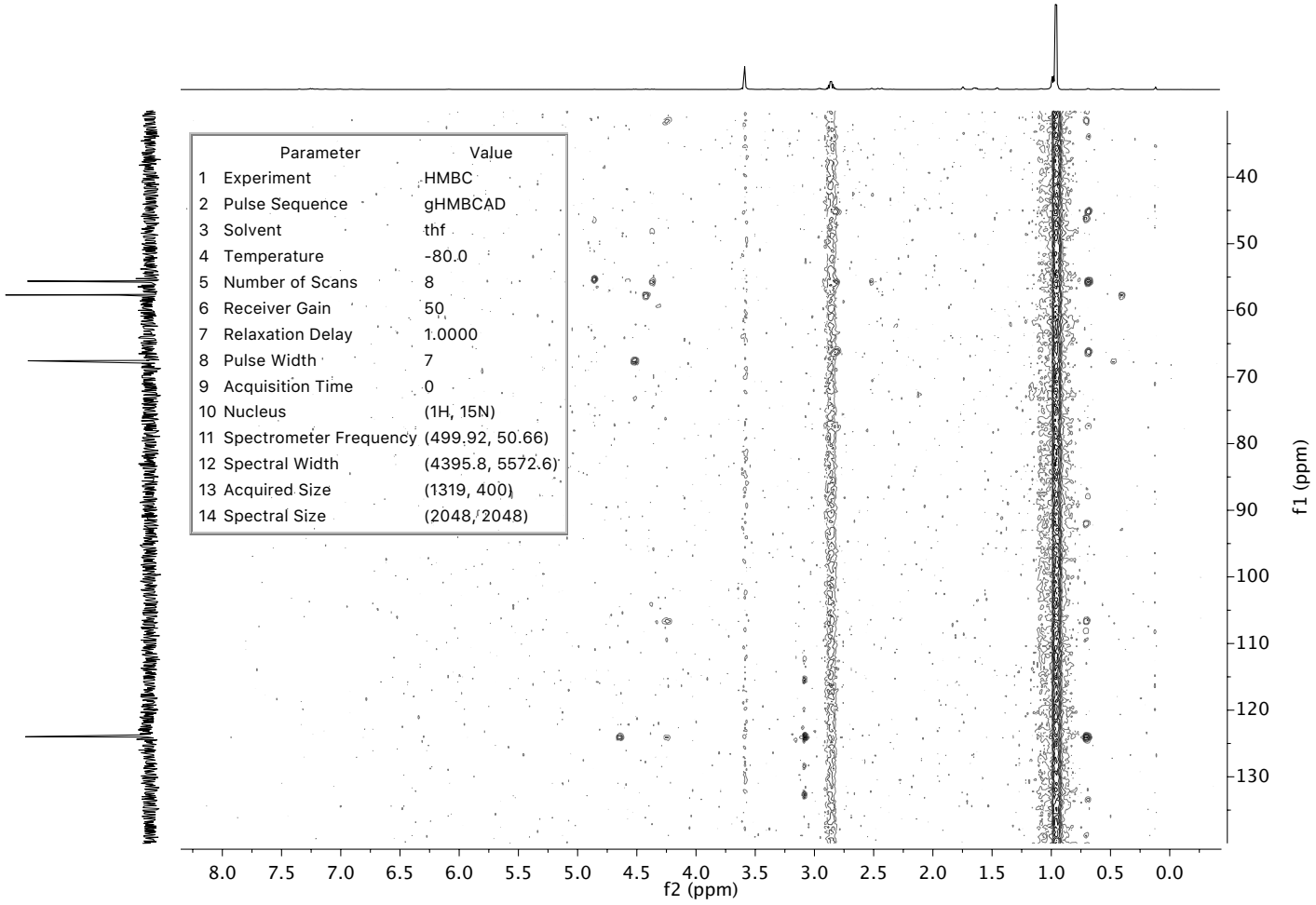


Figure 107. Full-display of ^{1}H-^{15}N HMBC spectrum of a pre-aged solution of 0.025 M [^{6}Li,^{15}N]-(*S,S*)-**2** and 0.025 M [^{6}Li,^{15}N]-(*R,R*)-**2** in 12.3 M THF at –80 °C. Proton resonances are correlated with ^{15}N resonances. A ^{15}N resonance at 123 ppm stems from the alkoxide.

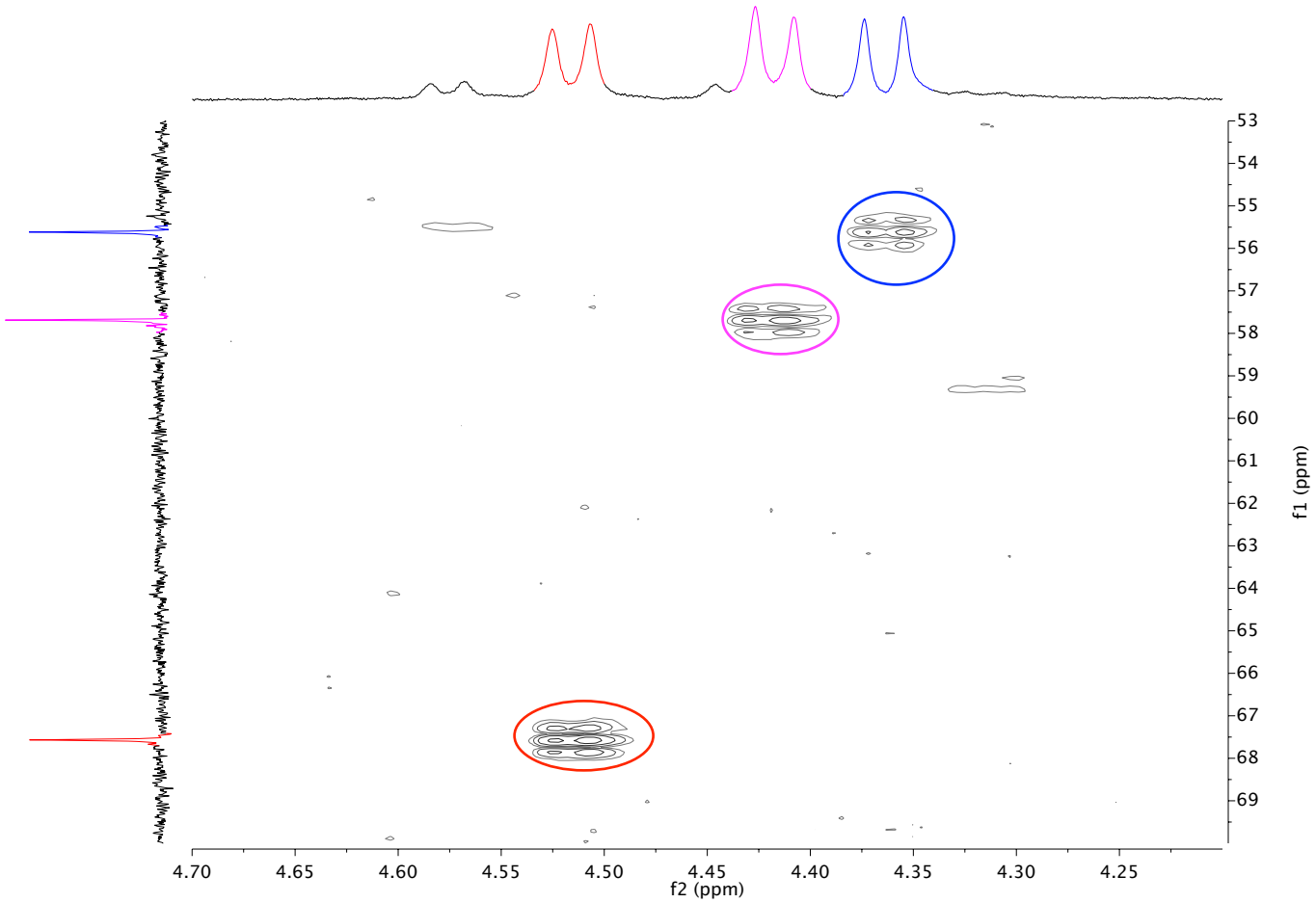


Figure 108. Expansion of ^{1}H-^{15}N HMBC spectrum of a pre-aged solution of 0.025 M [^{6}Li,^{15}N]-(*S,S*)-**2** and 0.025 M [^{6}Li,^{15}N]-(*R,R*)-**2** in 12.3 M THF at –80 °C. Proton resonances are correlated with ^{15}N resonances.

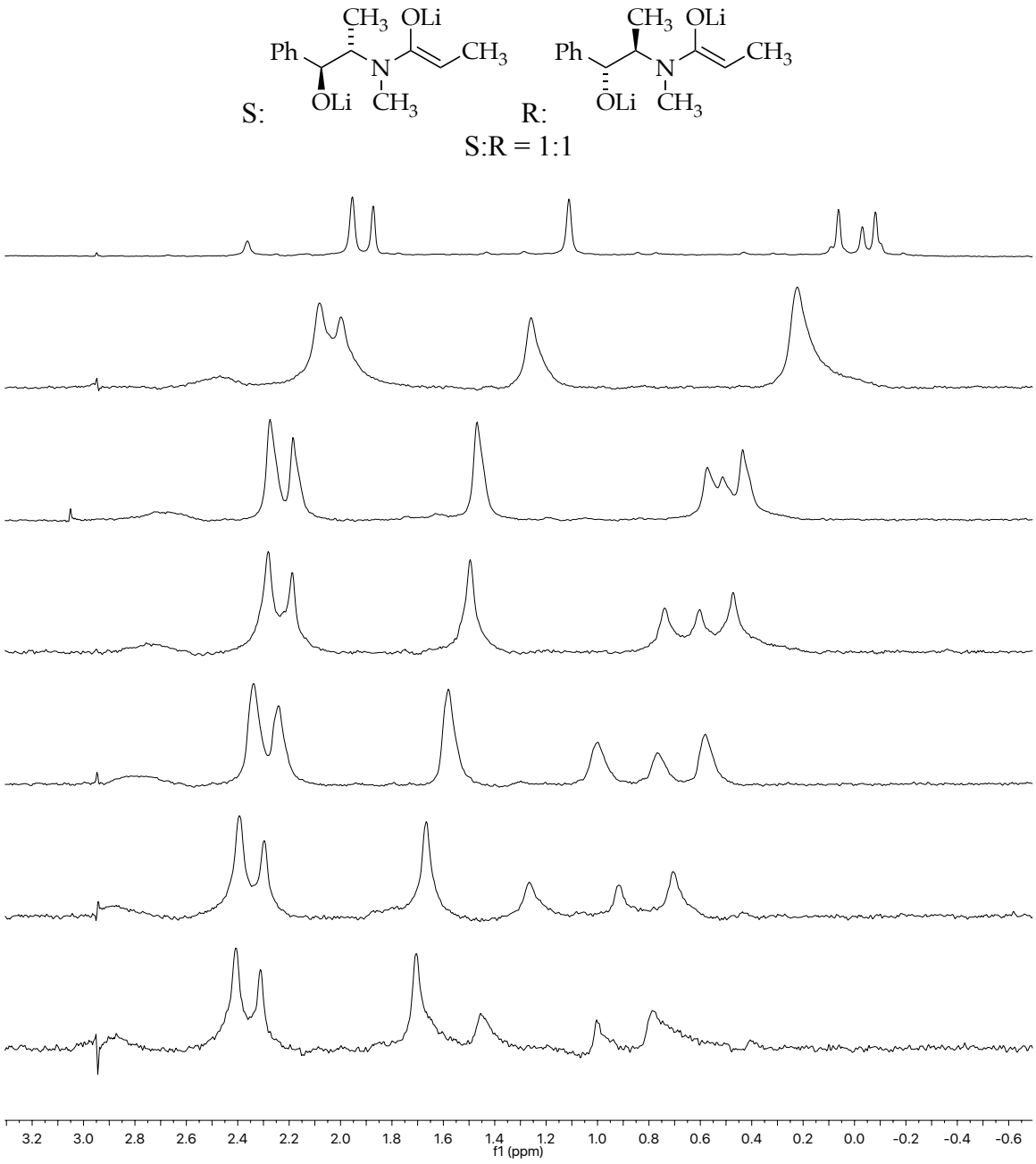


Figure 109. ^{6}Li NMR spectra for 0.10 M pre-aged solutions of 0.05 M [^{6}Li]-(*S,S*)-**2** and 0.05 M [^{6}Li]-(*R,R*)-**2** in 12.3 M THF at −80 °C with varying pyridine concentrations subsequent to aging. T1 relaxation was not optimized for integration. The upfield peaks show a greater shift than do the downfield peaks.

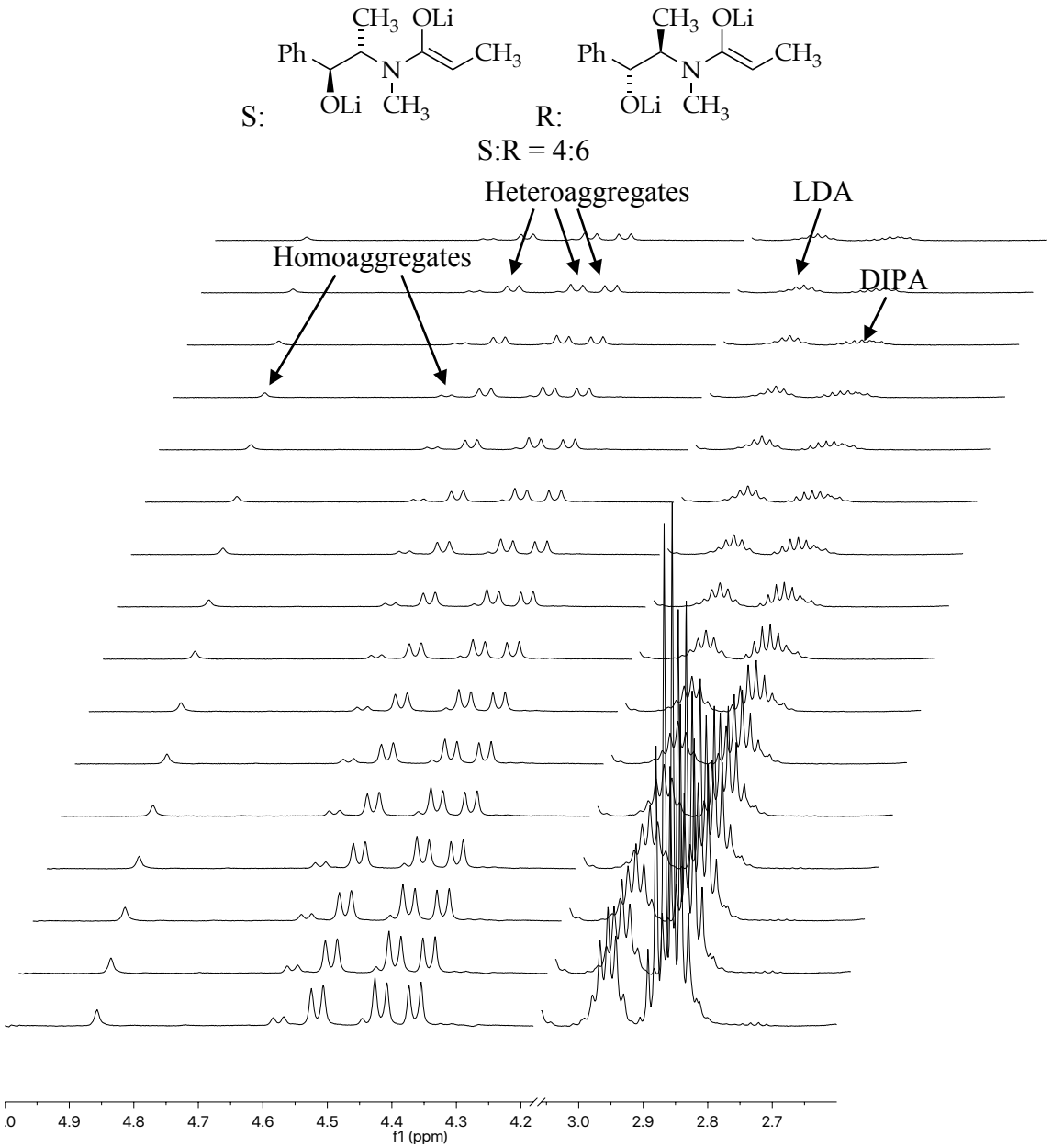


Figure 110. Diffusion NMR spectra for a pre-aged solution of 0.040 M (*S,S*)-**2** and 0.060 M (*R,R*)-**2** in 12.3 M THF at –60 °C.

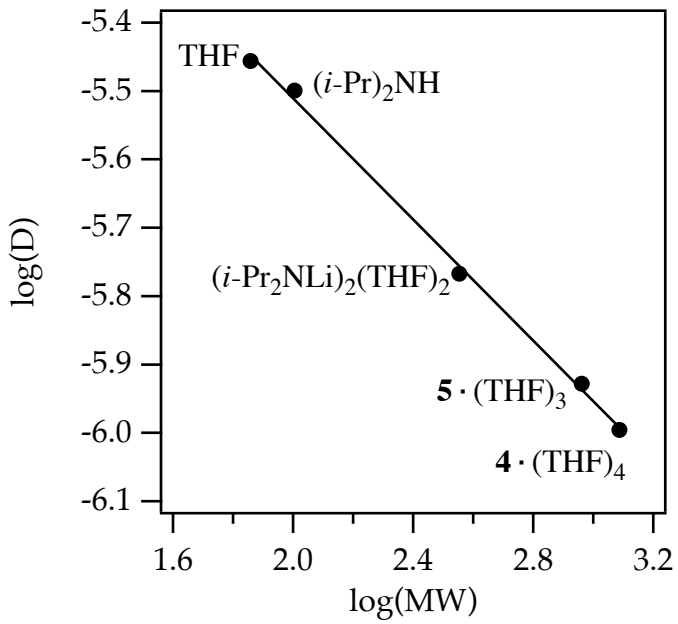


Figure 111. Plot of diffusion coefficient (D) from diffusion NMR vs molecular weight of components in an aged solution of prepared from 0.040 M (*S,S*)-**1** and 0.060 M (*R,R*)-**1** in 12.3 M THF with 0.21 M [^{6}Li]LDA at –60 °C. y = *a* + *b*x such that *a* = –4.622, *b* = 0.443. This experiment assumes four THF solvent molecules per homotetramer **4** and three THF solvent molecules per heterotrimer **5**. LDA is a disolvated dimer.

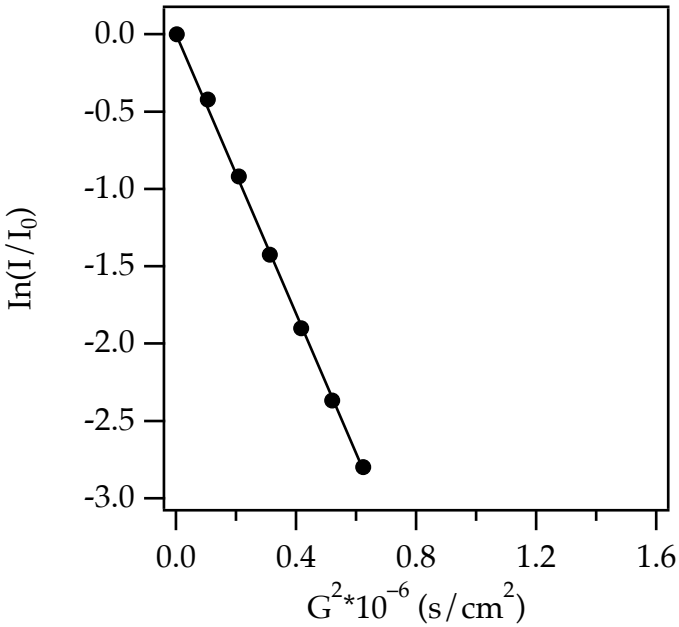


Figure 112. Diffusion coefficient plot of THF signal in an aged solution prepared from 0.040 M (*S,S*)-**1** and 0.060 M (*R,R*)-**1** in 12.3 M THF with 0.21 M [^{6}Li]LDA at –60 °C. *y* = *a* + *bx* such that *a* = 0, *b* = -4.515×10^{-6}.

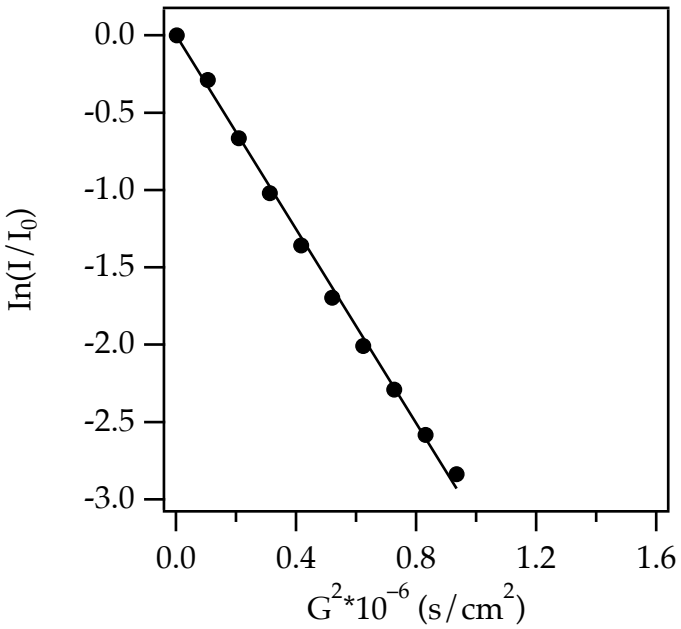


Figure 113. Diffusion coefficient plot of diisopropylamine signal in an aged solution prepared from 0.040 M (*S,S*)-**1** and 0.060 M (*R,R*)-**1** in 12.3 M THF with 0.21 M [^{6}Li]LDA at –60 °C. $y = a + bx$ such that $a = 0$, $b = -3.136 \times 10^{-6}$

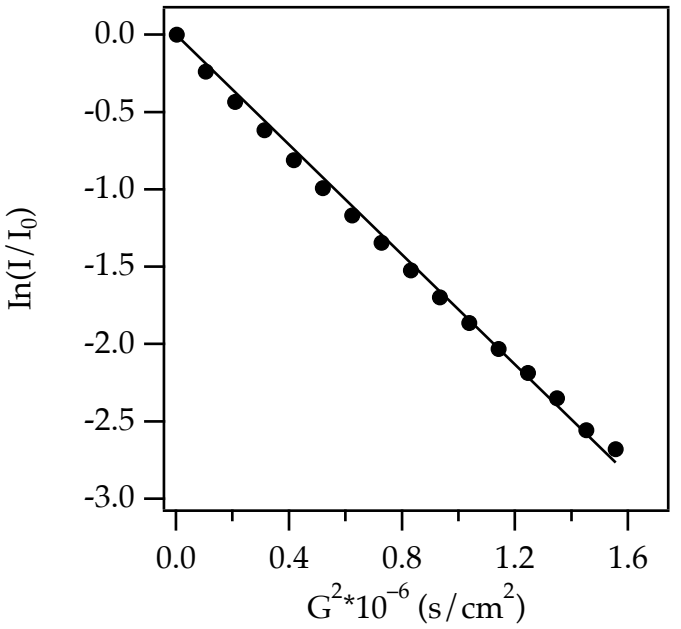


Figure 114. Diffusion coefficient plot of [^{6}Li]LDA signal in an aged solution prepared from 0.040 M (*S,S*)-**1** and 0.060 M (*R,R*)-**1** in 12.3 M THF with 0.21 M [^{6}Li]LDA at –60 °C. $y = a + bx$, such that $a = 0$, $b = -1.707 \times 10^{-6}$.

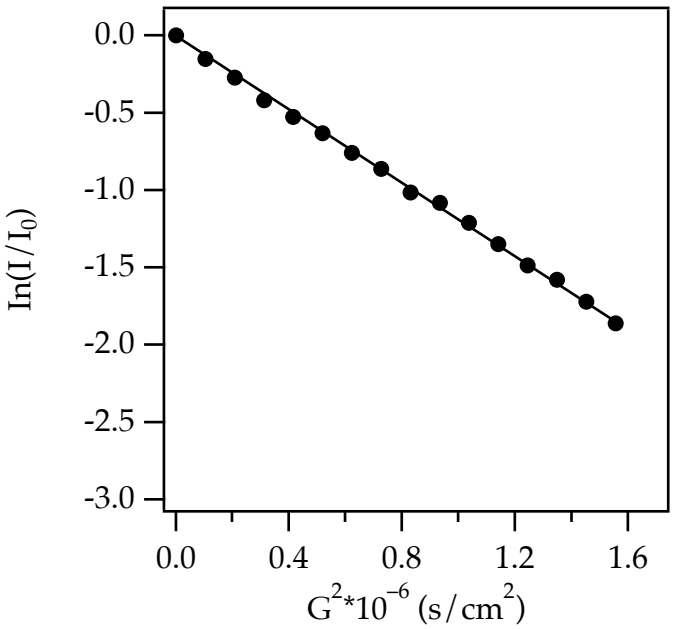


Figure 115. Diffusion coefficient plot of heterotrimer **5** signal in an aged solution prepared from 0.040 M (*S,S*)-**1** and 0.060 M (*R,R*)-**1** in 12.3 M THF with 0.21 M [^{6}Li]LDA at –60 °C. $y = a + bx$ such that $a = 0$, $b = -1.189 \times 10^{-6}$.

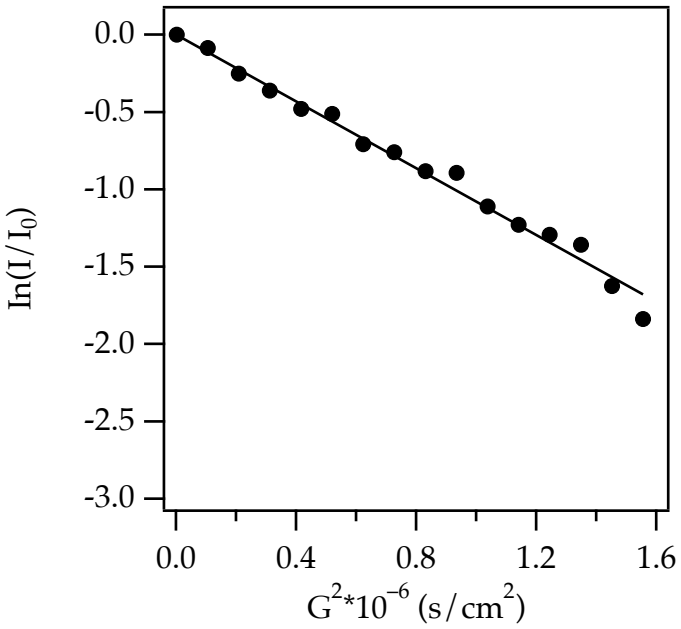


Figure 116. Diffusion coefficient plot of homotetramer **4** signal in an aged solution prepared from 0.040 M (*S,S*)-**1** and 0.060 M (*R,R*)-**1** in 12.3 M THF with 0.21 M [^{6}Li]LDA at –60 °C. $y = a + bx$ such that $a = 0$, $b = -1.079 \times 10^{-6}$.

2D NMR analysis of heteroaggregate 5: Heteroaggregate **5** was prepared as a mixture of two antipodes from 0.21 M [^{6}Li]LDA, 0.050 M (*S,S*)-**1**, and 0.050 M (*R,R*)-**1** in neat THF-d_8, with aging at 25 °C for 10 min. All chemical shifts with the exception of C-1, C-2, C-3, C-4, C-5, C-6 were assigned using high field indirect-resolution 2D HSQC, HSQC-TOCSY, and HMBC experiments.

Experimental: 2D NMR spectra were acquired on a 500 MHz Varian INOVA spectrometer operating at 499.92 MHz for ^{1}H observation using a 5 mm Varian inverse-detect probehead with Z-axis pulsed field-gradient. The sample was maintained at –60 °C as calibrated with a neat methanol sample. ^{1}H and ^{13}C chemical shifts were referenced to the residual downfield toluene-d_7 resonance at 2.09 ppm and 20.40 ppm, respectively. 2D experiments were acquired using standard pulse sequences supplied in VnmrJ 3.2A (Agilent Inc.) and processed and analyzed in MestReNova 11.0.3 (Mestrelab Research S.L.).

Determination of the 3D aggregate structure: The 3D structure of the aggregate was derived from 2D ROESY (reported as H–H correlations) and HSQC-NOESY (reported as C–H correlations) experiments. The enolate is in the Z configuration based on the strong nOe correlation between H-12 and H-13, between H-12' and H-13', between H-12" and H-13". Reciprocal H-12 and H-13 (H-12' and H-13', H-12" and H-13") correlation is also observed. The starting point for solving the structure are N-9 and N-9', which couple to the same lithium resonance. Reciprocal couple from the center lithium to N-9 and N-9' are also observed. This indicates the six-coordinated lithium. C-12' gives nOe correlation to H-8 and H-12. Reciprocal correlations from C-8 and C-12 to H-12' are also observed. This indicates that methyl group 12' projects over the Li/N-9/C-8/C-7 face. The third subunit (blue) does not show any correlations to the first two subunits.

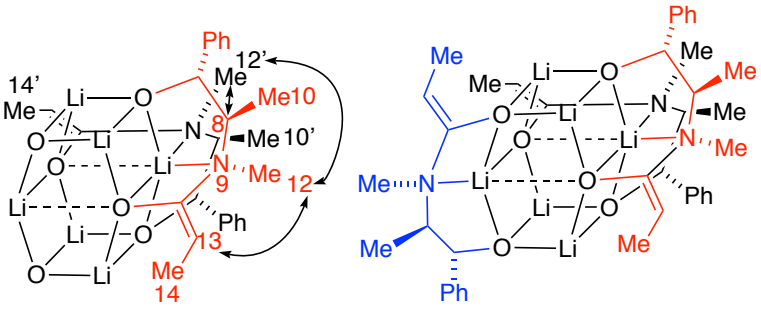


Table 2. ^{1}H and ^{13}C chemical shifts and assignments for heteroaggregate **5** at –60 °C.

Atom	δC, ppm	δH, ppm	HMBC	HSQC-TOCSY[1]	ROESY[2]	HSQC-NOESY[1,2]
1 C[3]	–	–				
1' C	126.55	7.12	3',5',6'	2',3'		2',3'
1" C	126.22	6.80	3",4",5",6"	2",3",5",6"		2",3",5",6"
2 C[3]	–	–				
2' C	128.44	7.24		1',3',5'	8',10'	1'
2" C	129.77	6.08	4",6"	1",3",5",6"	7",10"	1",3",6"
3 C[3]	129.18	–	7			
3' C	128.46	7.23	1',4',7'	1',2',5'		1',7'
3" C	125.38	6.90	1",5",7"	1",2",5",6"	7",8",10"	1",2",5",6",8"
4 C[3]	153.69	–	7,8			
4' C	153.10	–	3',7',8'			
4" C	153.38	–	1",2",6",7",8"			
5 C[3]	127.22	–	7			
5' C	126.91	7.26	1',7'	2',3'		
5" C	128.26	6.98	1",3",7"	1",2",3",6"	7",8",10"	1",3",7"
6 C[3]	–	–				
6' C	129.15	7.21	1'			
6" C	127.83	7.01	1",2",4"	1",2",3",5"		1",2",3"
7 C	81.88	4.35	3,4,5,8,10	8,10	8,10	10
7' C	78.63	4.50	3',4',5',8',10'	8',10'	8',10',12'	3',12'
7" C	80.22	4.40	3",4",5",8",10"	8",10"	2",3",5",8",10",12"	5",8",12"
8 C	68.27	2.81	4,7,10,11,12	7,10	7,10,12'	12,12'

8' C	63.17	3.52	4',7',10',11',12',14'	7',10'	2',7',10'	10',13'
8" C	64.95	3.06	4',7',10',11',12',13',14'	7",10"	3",5",7",10",12"	3",7",10"
9 N	55.61	–	7,10,12			
9' N	67.72	–	7',10'			
9" N	57.73	–	7",10"			
10 C	9.61	0.68	7,8	7,8	7,8,12,13	7,12
10' C	11.91	0.47	7',8'	7',8'	2',7',8',12',13'	8',12'
10" C	11.18	0.39	7",8"	7",8"	2",3",5",7",8",12",13"	8"
11 C	161.26	–	8,11,12,14			
11' C	164.74	–	8',12',13',14'			
11" C	162.73	–	8",12",13",14"			
12 C	42.67	2.50	8,11		8,10,13,12'	8,10,13,12'
12' C	32.52	2.45	8',11',13'		7',10',13',8,12	7',10',13',8,12
12" C	31.71	2.42	8",11"		7",8",10",13"	7",13"
13 C	78.20	3.38	11,14	14	10,12,14	12,14
13' C	68.86	3.25	11',12',14'	14'	10',12',14'	8',12',14'
13" C	71.13	3.11	8",11",14"	14"	10",12",14"	12",14"
14 C	12.14	1.62	8,11,13	13	7,13	13
14' C	13.05	1.64	8',11',13'	13'	13'	13'
14" C	11.52	1.44	8",11",13"	13"	13"	13"

[1]HSQC correlations were omitted from the assignment table. [2]Important correlations that allowed determination of subunit arrangement are marked in red. [3]Not determined.

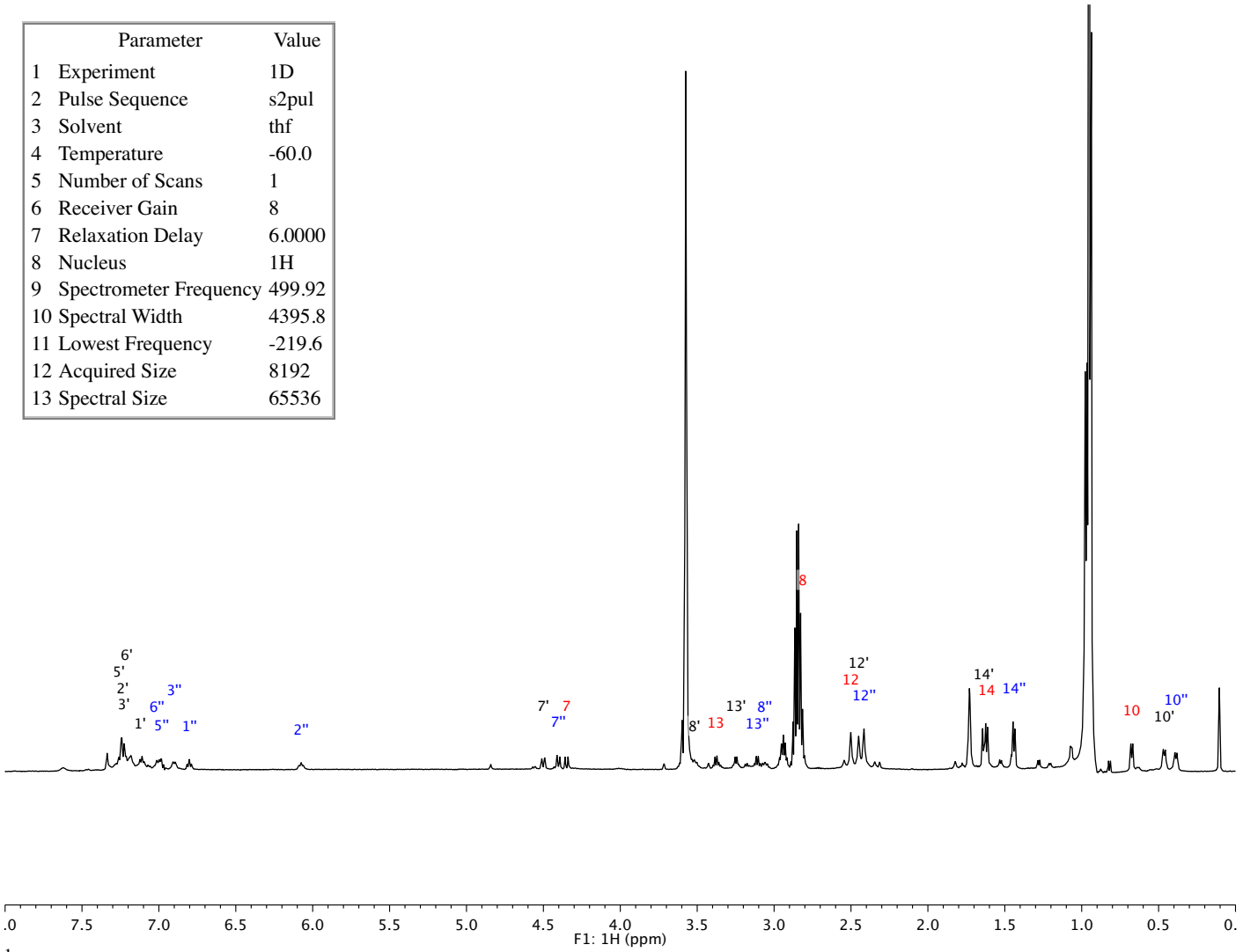


Figure 117. ^{1}H NMR spectrum of a pre-aged solution of **5** prepared from 0.050 M (*S,S*)-**1** and 0.050 M (*R,R*)-**1** in 12.3 M THF-d_8 with 0.21 M [^{6}Li]LDA at –60 °C.

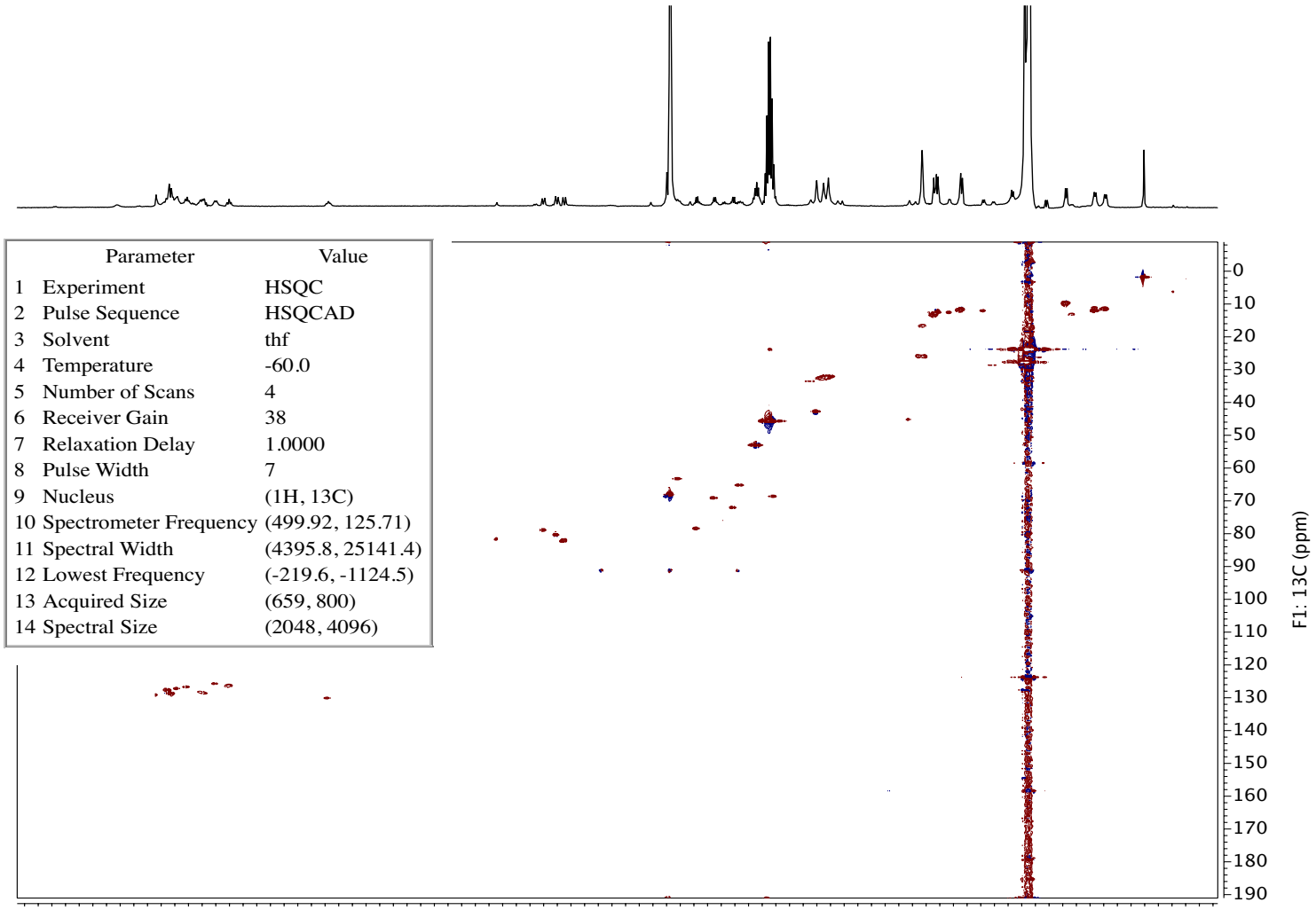


Figure 118. Full-display HSQC spectrum of an aged solution of **5** prepared from 0.050 M (*S,S*)-**1** and 0.050 M (*R,R*)-**1** in 12.3 M THF-d_8 with 0.21 M [^{6}Li]LDA at –60 °C.

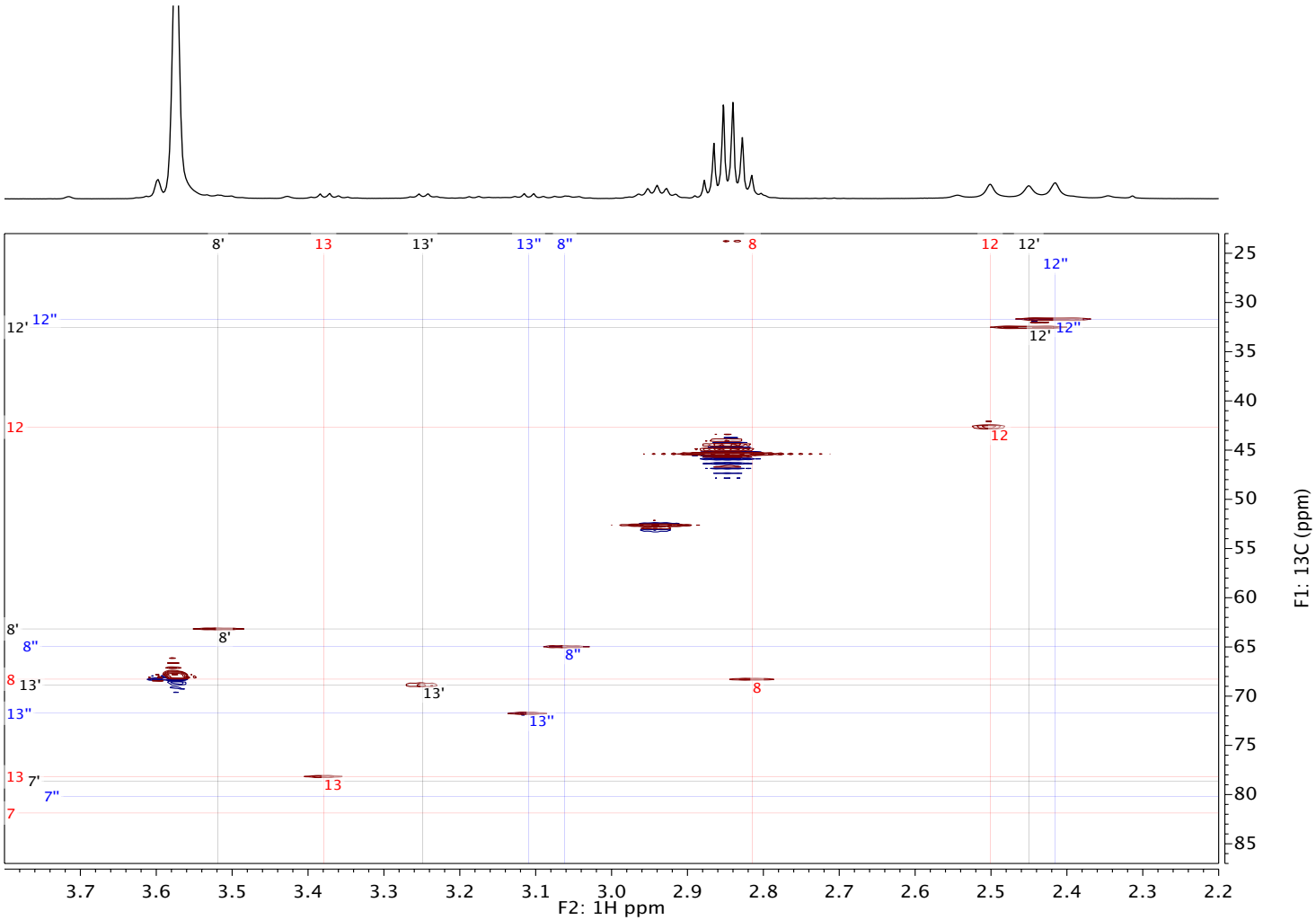


Figure 119. Expansion of the HSQC spectrum of an aged solution of **5** prepared from 0.050 M (*S,S*)-**1** and 0.050 M (*R,R*)-**1** in 12.3 M THF-d_8 with 0.21 M [^{6}Li]LDA at –60 °C.

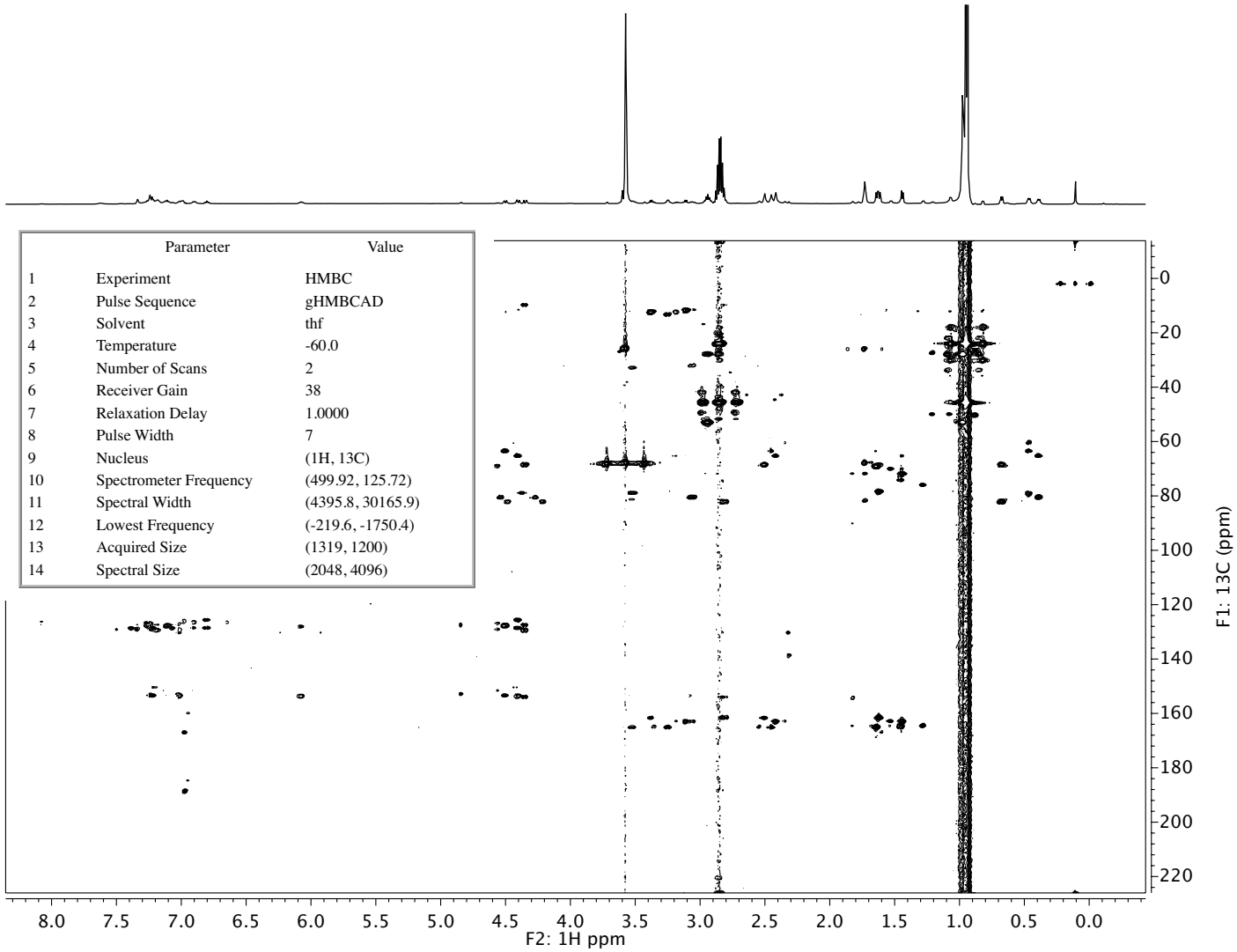


Figure 120. Full-display HMBC spectrum of an aged solution of **5** prepared from 0.050 M (*S,S*)-**1** and 0.050 M (*R,R*)-**1** in 12.3 M THF-d_8 with 0.21 M [^{6}Li]LDA at –60 °C.

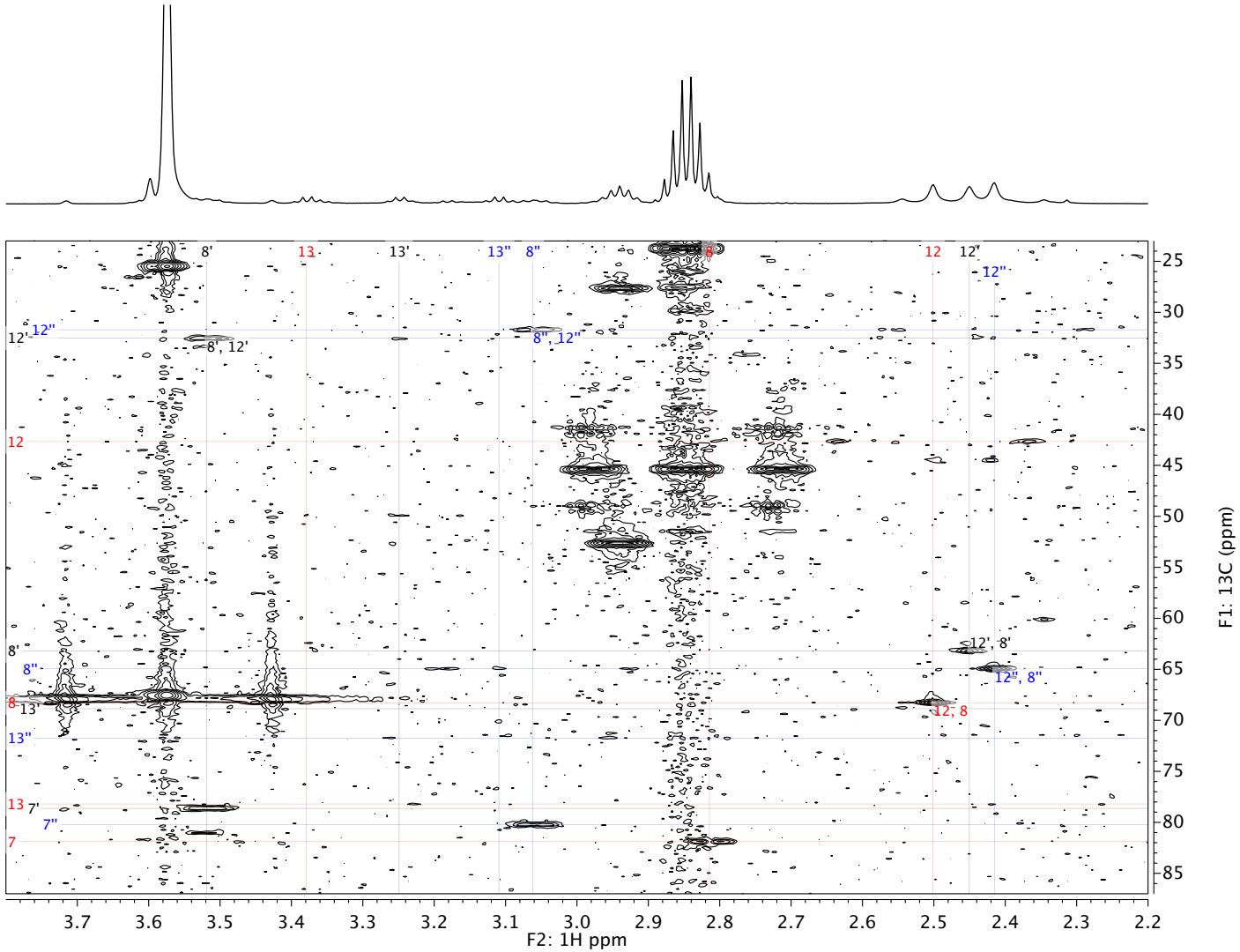


Figure 121. Expansion of the HMBC spectrum of an aged solution of **5** prepared from 0.050 M (*S,S*)-**1** and 0.050 M (*R,R*)-**1** in 12.3 M THF-d_8 with 0.21 M [^{6}Li]LDA at –60 °C.

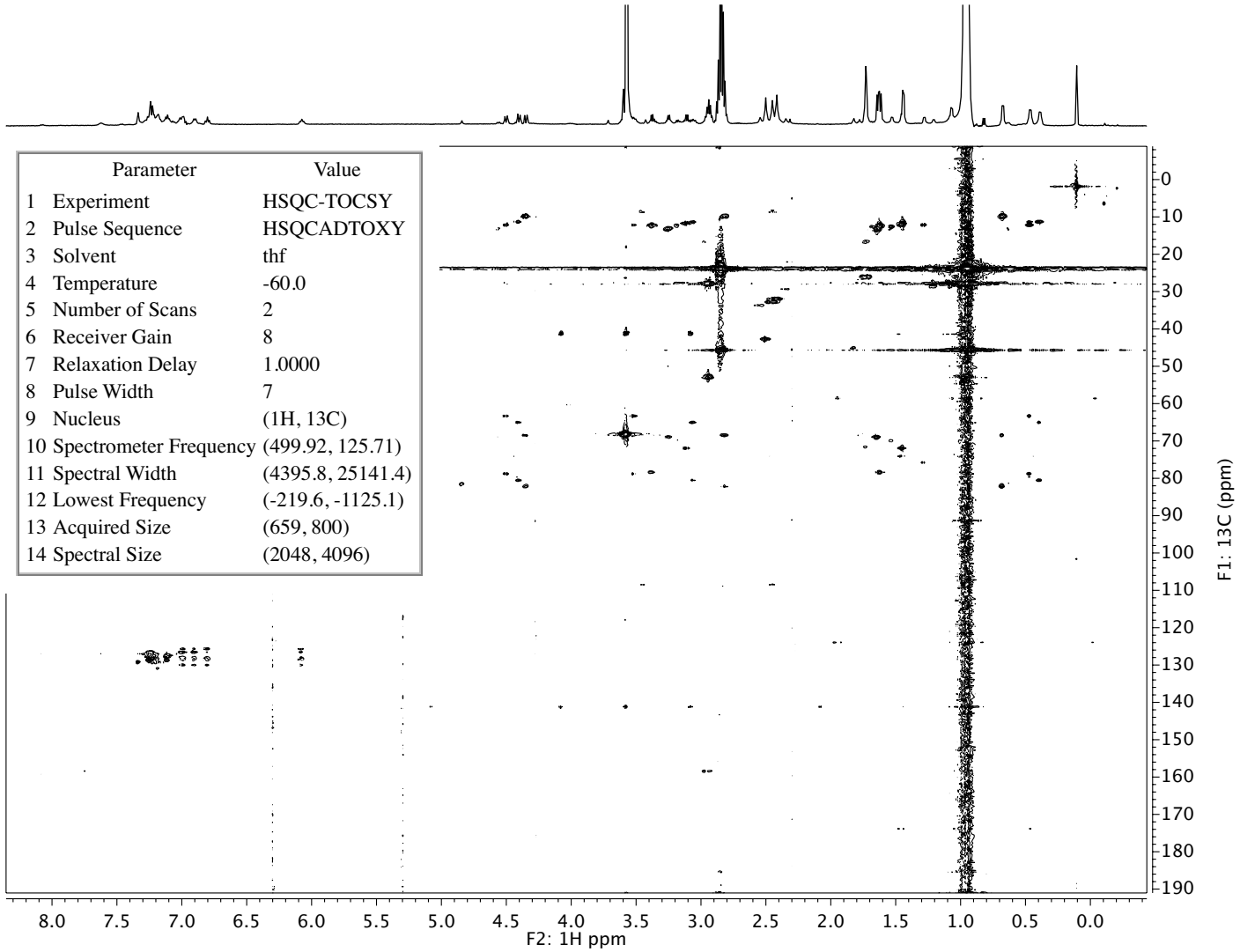


Figure 122. Full-display HSQC-TOCSY spectrum of an aged solution of **5** prepared from 0.050 M (*S,S*)-**1** and 0.050 M (*R,R*)-**1** in 12.3 M THF-d_8 with 0.21 M [^{6}Li]LDA at –60 °C.

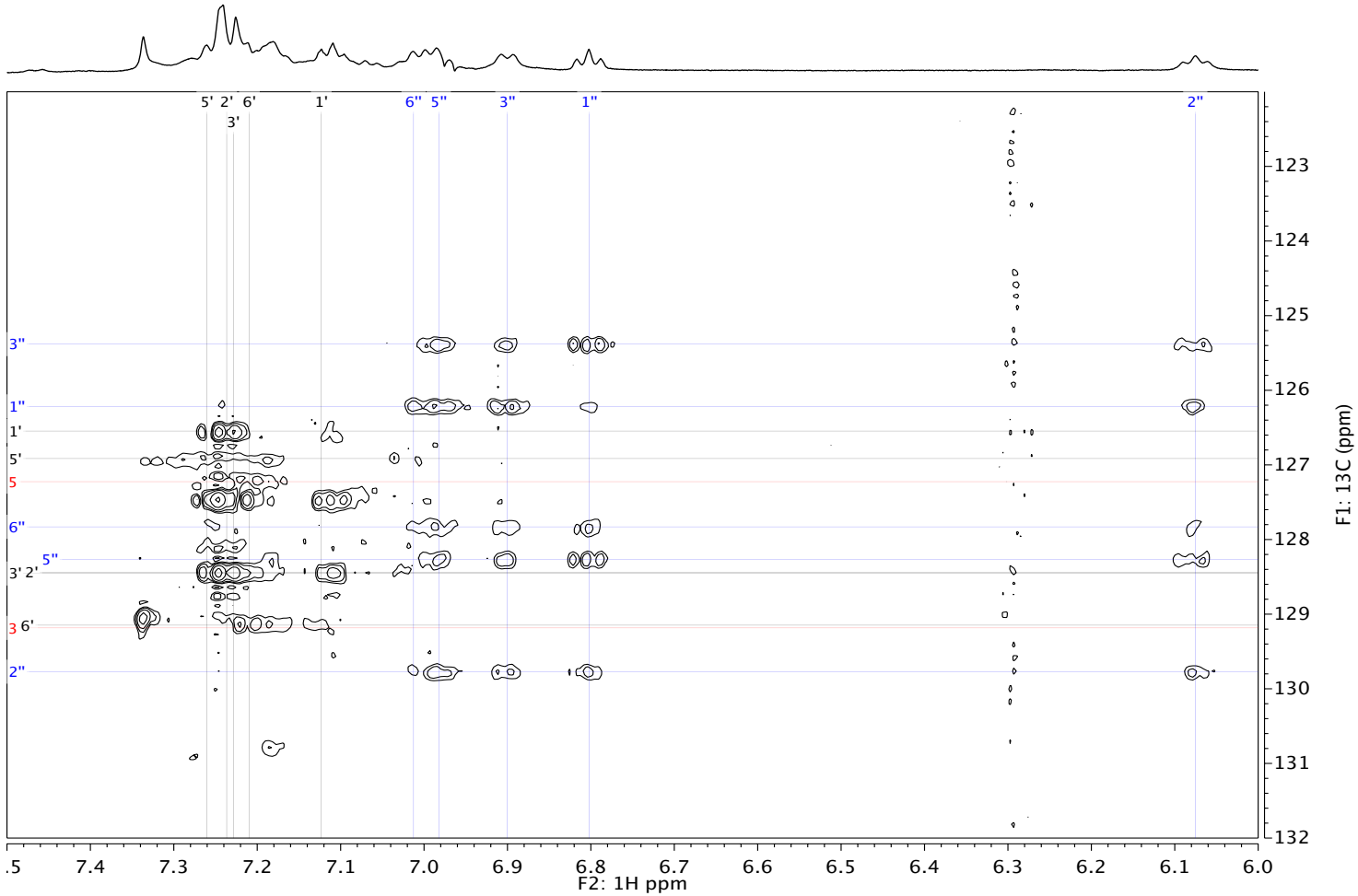


Figure 123. Expansion of the HSQC-TOCSY spectrum of an aged solution of **5** prepared from 0.050 M (*S,S*)-**1** and 0.050 M (*R,R*)-**1** in 12.3 M THF-d_8 with 0.21 M [^{6}Li]LDA at –60 °C.

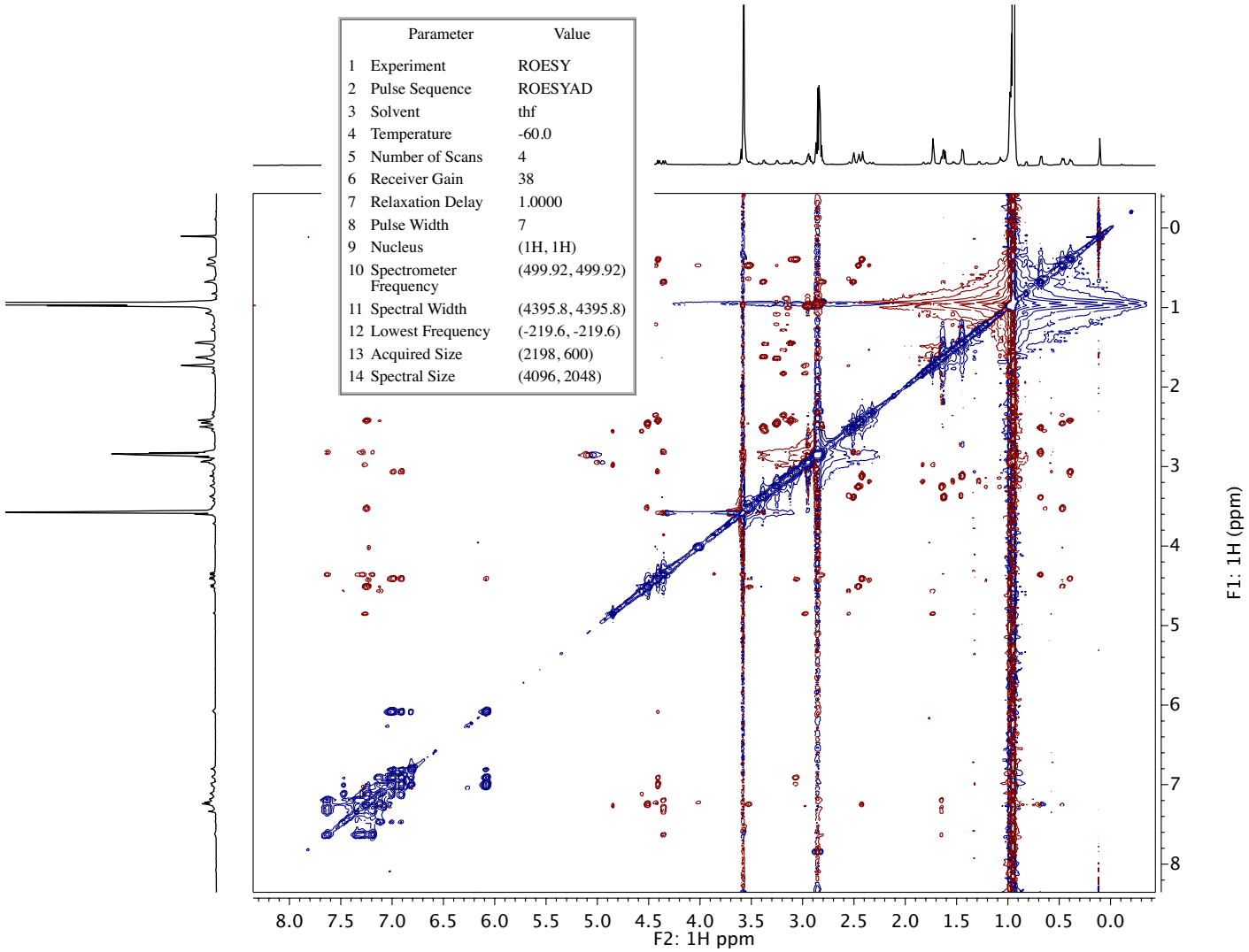


Figure 124. Full-display ROESY spectrum of an aged solution of **5** prepared from 0.050 M (*S,S*)-**1** and 0.050 M (*R,R*)-**1** in 12.3 M THF-d_8 with 0.21 M [^{6}Li]LDA at –60 °C.

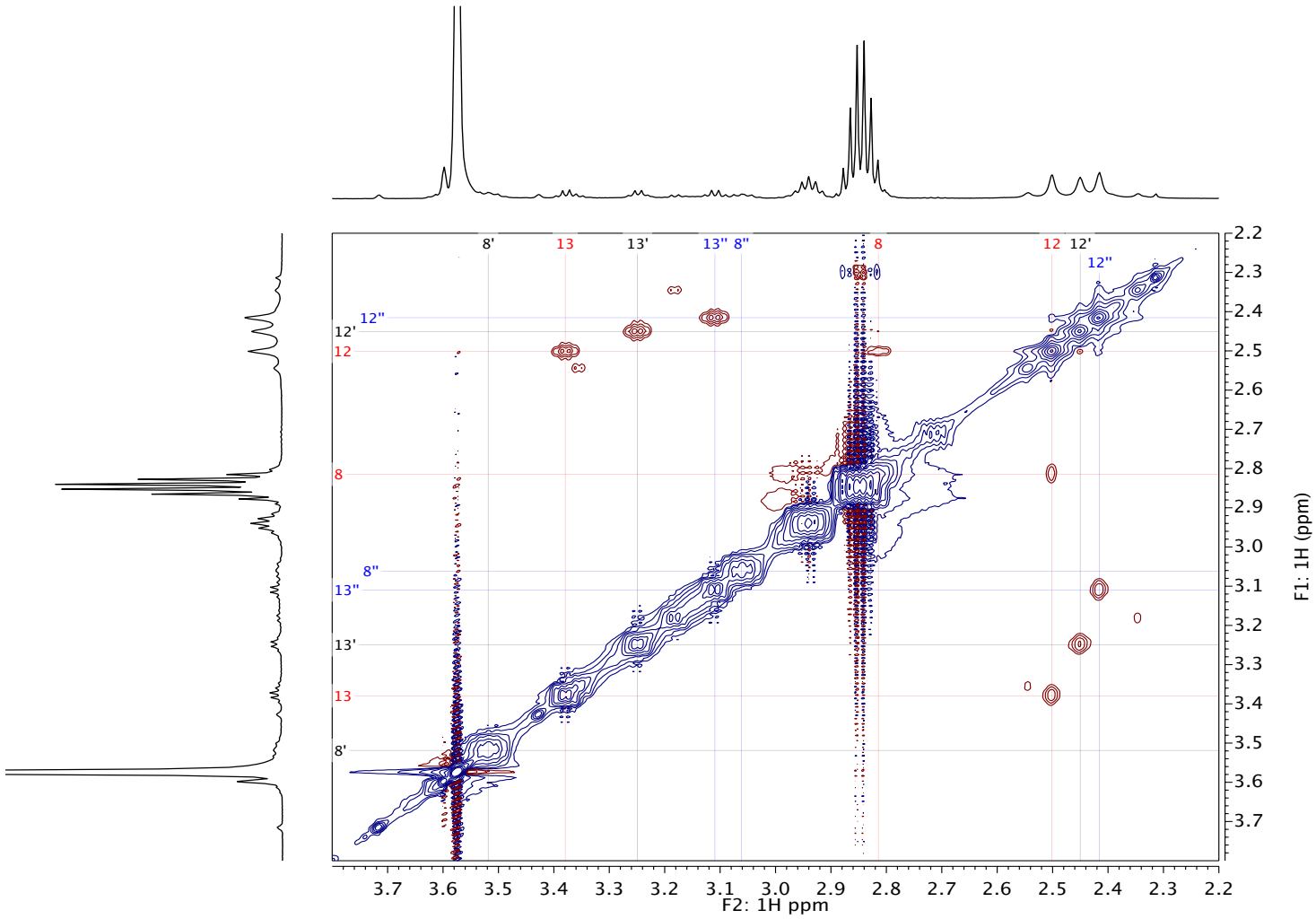


Figure 125. Expansion of the ROESY spectrum of an aged solution of **5** prepared from 0.050 M (*S,S*)-**1** and 0.050 M (*R,R*)-**1** in 12.3 M THF-d_8 with 0.21 M [^{6}Li]LDA at –60 °C.

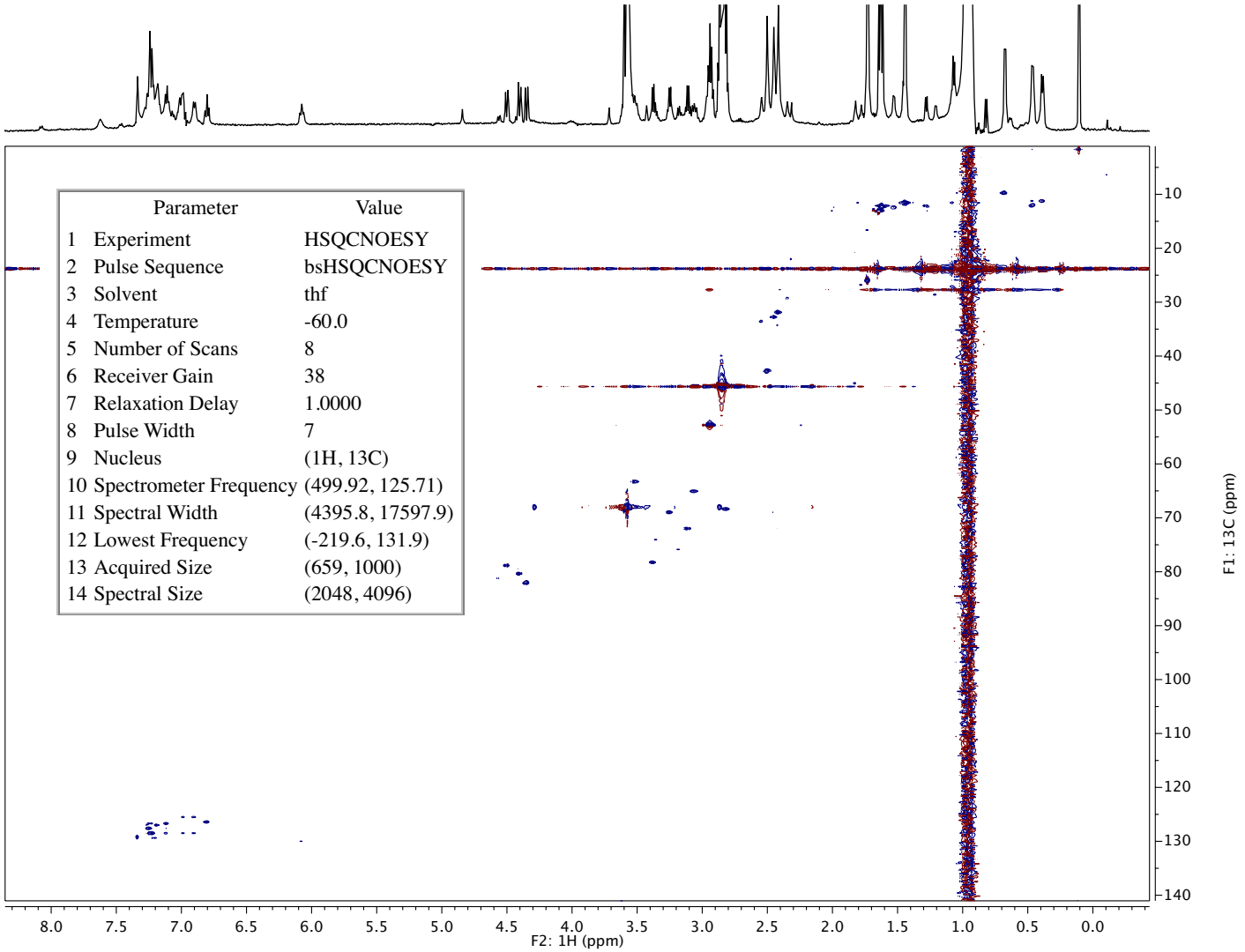


Figure 126. Full-display HSQC-NOESY spectrum of an aged solution of **5** prepared from 0.050 M (*S,S*)-**1** and 0.050 M (*R,R*)-**1** in 12.3 M THF-d_8 with 0.21 M [^{6}Li]LDA at –60 °C.

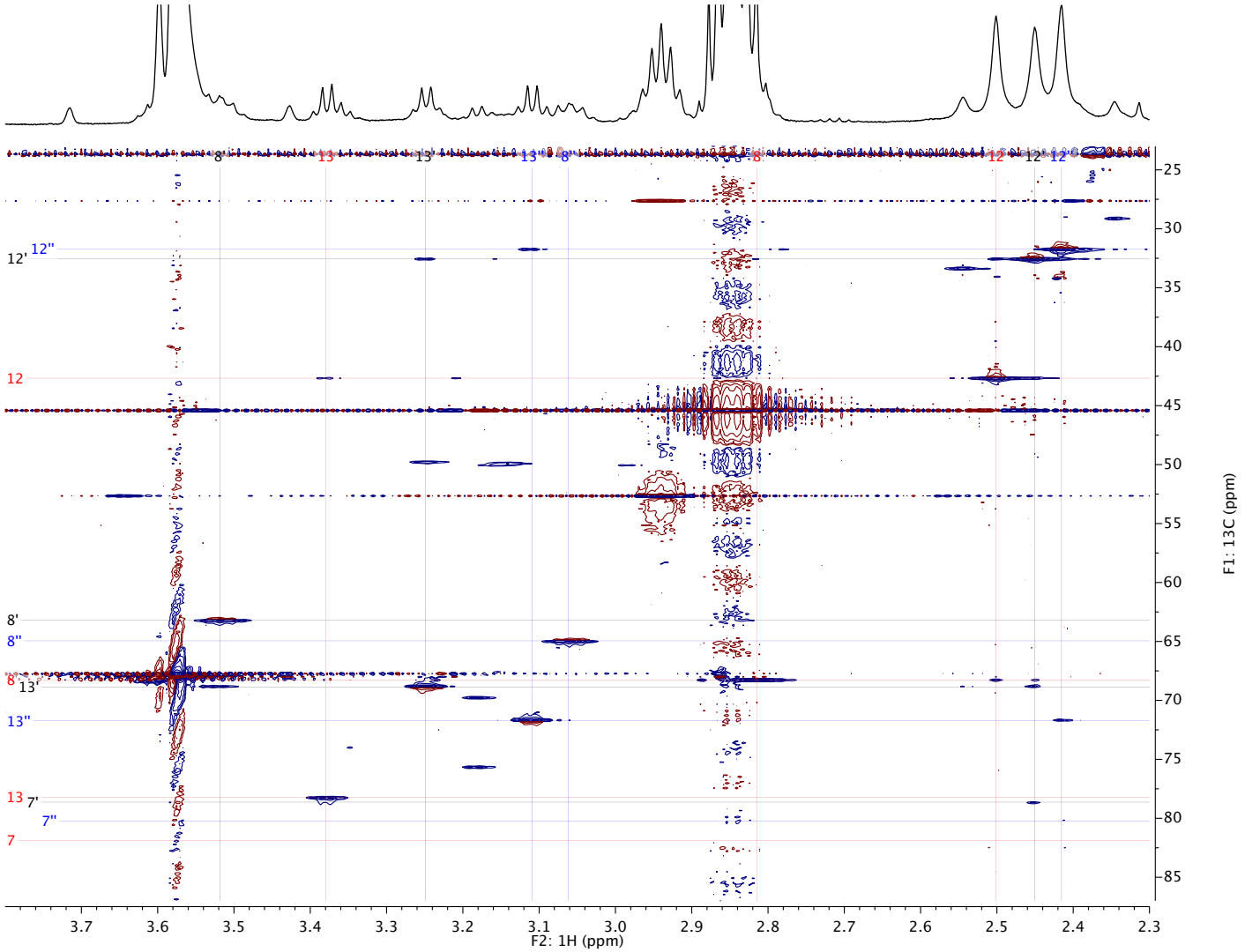


Figure 127. Expansion of the HSQC-NOESY spectrum of an aged solution of **5** prepared from 0.050 M (*S,S*)-**1** and 0.050 M (*R,R*)-**1** in 12.3 M THF-d_8 with 0.21 M [^{6}Li]LDA at –60 °C.

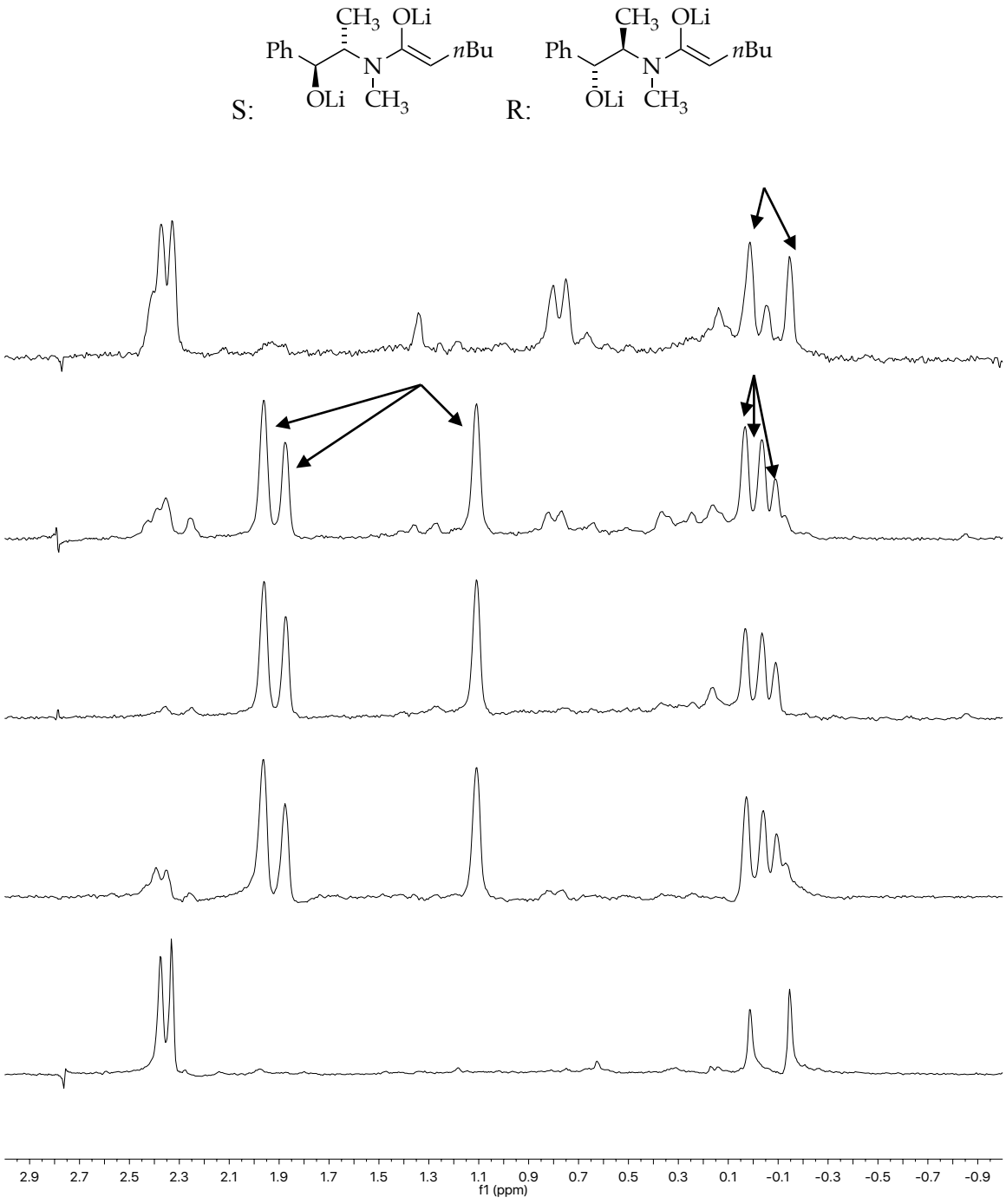


Figure 128. ^{6}Li NMR spectra for 0.10 M pre-aged solutions of [^{6}Li]-(*S,S*)-**8** (S) and [^{6}Li]-(*R,R*)-**8** (R) in 12.3 M THF at −80 °C. T1 relaxation was not optimized for integration. Minor peaks in the first spectrum are from reproducible, uncharacterized isomers. Heteroaggregates consistently showed six new resonances corresponding to hexalithio heterochiral trimers.

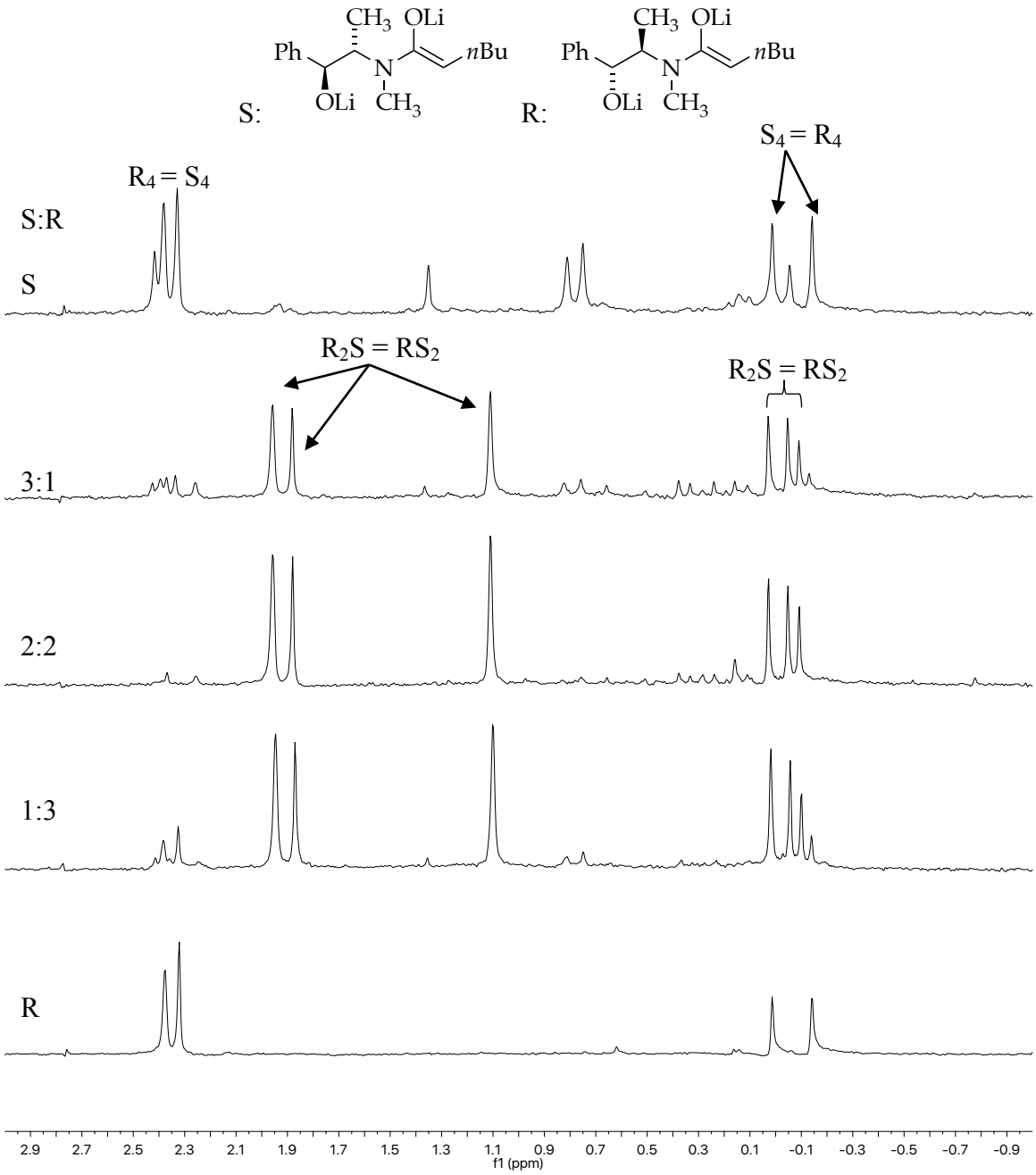


Figure 129. ^{6}Li NMR spectra for 0.10 M pre-aged solutions of [^{6}Li]-(*S,S*)-**8** (S) and [^{6}Li]-(*R,R*)-**8** (R) in 12.3 M THF at −60 °C. T1 relaxation was not optimized for integration. Minor peaks in the first spectrum are from reproducible, uncharacterized isomers. Heteroaggregates consistently showed six new resonances corresponding to hexalithio heterochiral trimers.

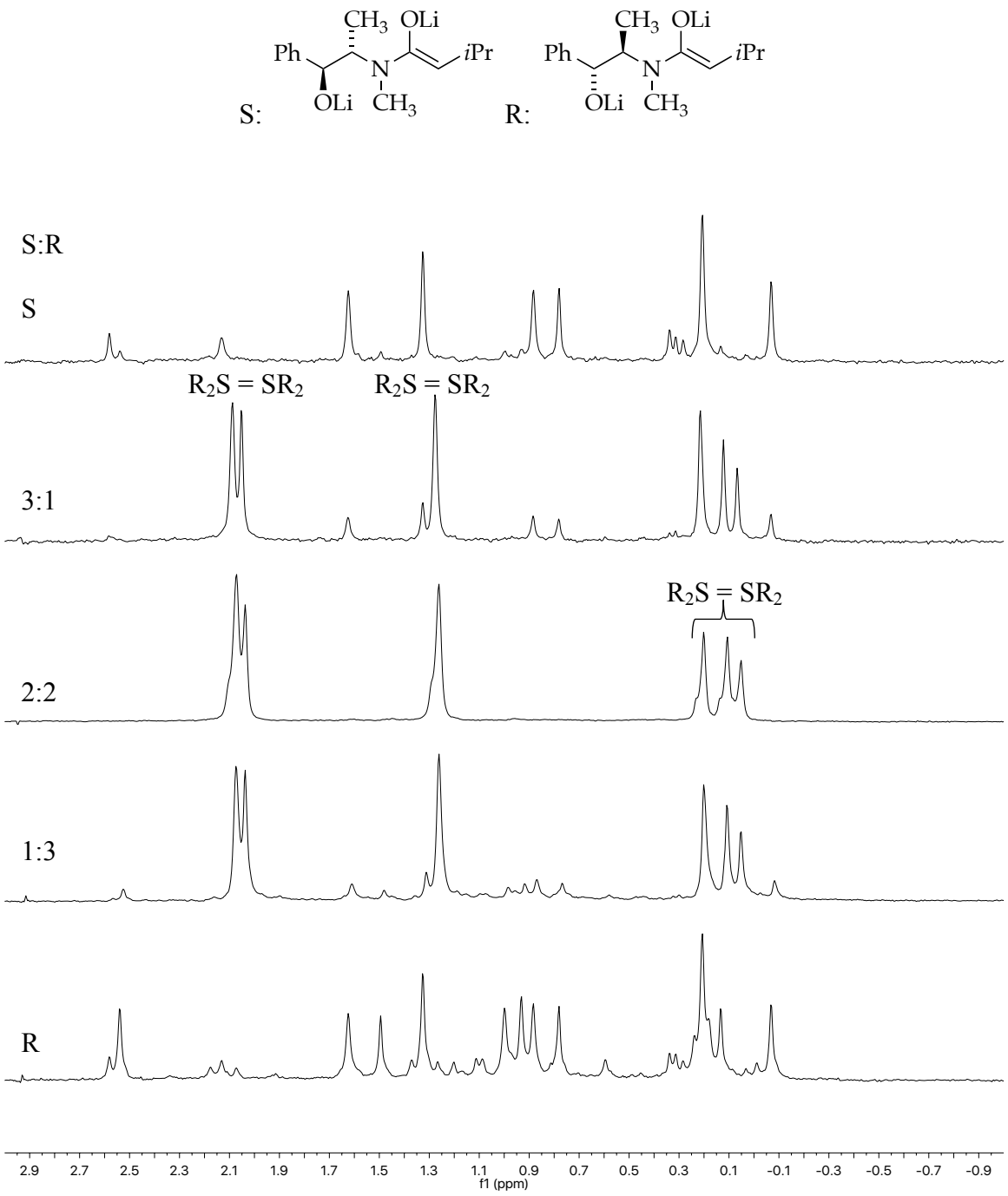


Figure 130. ^{6}Li NMR spectra for 0.10 M aged solutions of [^{6}Li]-(*S,S*)-**9** (S) and [^{6}Li]-(*R,R*)-**9** (R) in 12.3 M THF at −80 °C. T1 relaxation was not optimized for integration. Minor peaks in the first and last spectra were reproducible, uncharacterized isomers. Heteroaggregates consistently showed six new resonances corresponding to hexalithio heterochiral trimers.

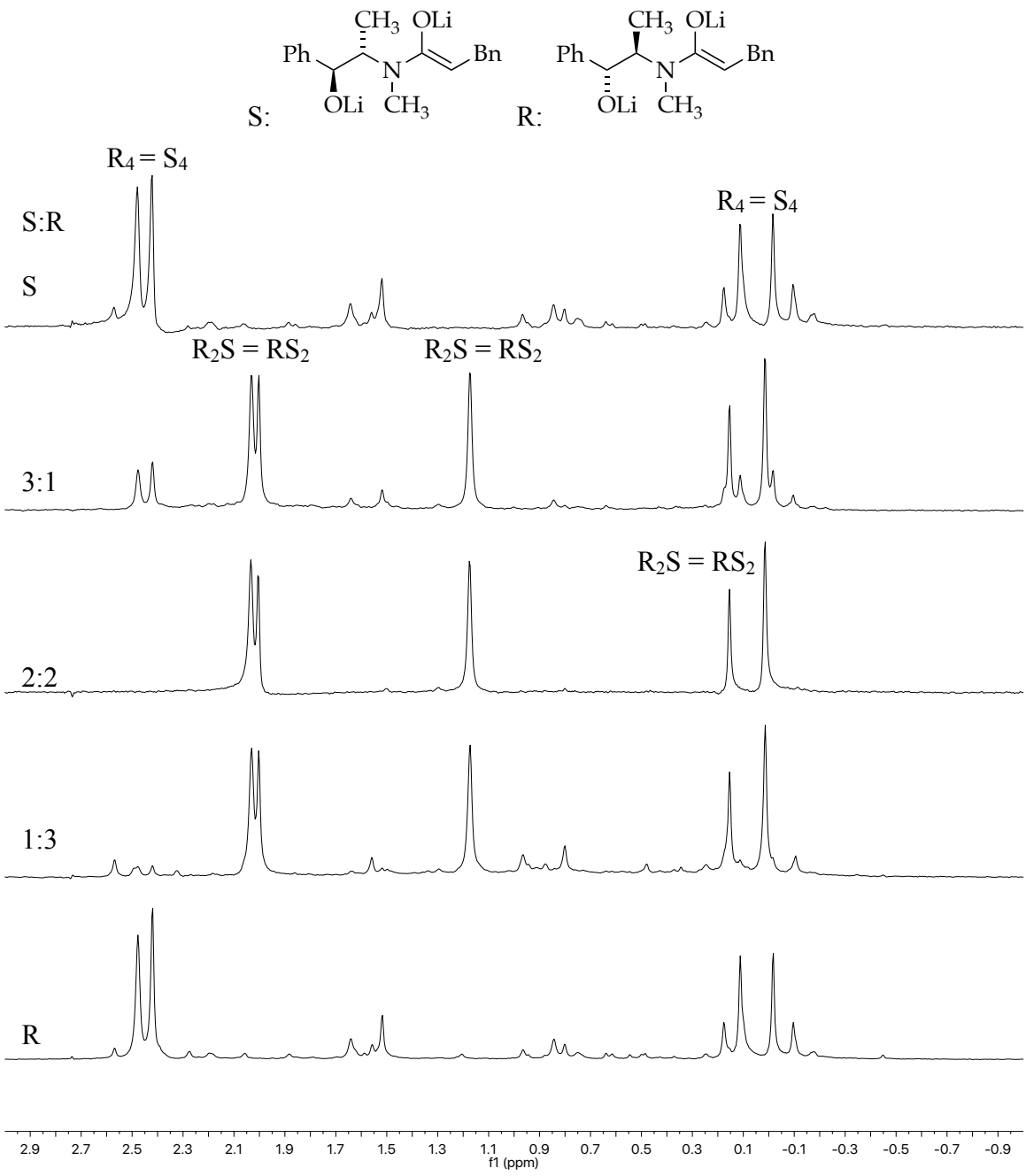


Figure 131. ^{6}Li NMR spectra for 0.10 M aged solutions of [^{6}Li]-(*S,S*)-**11** (S) and [^{6}Li]-(*R,R*)-**11** (R) in 12.3 M THF at –80 °C. Heteroaggregates consistently showed six (5 was shown in the spectra owing to overlaps) new resonances corresponding to heterochiral hexalithio heterochiral trimers. Minor peaks in the first spectrum were reproducible, uncharacterized isomers.

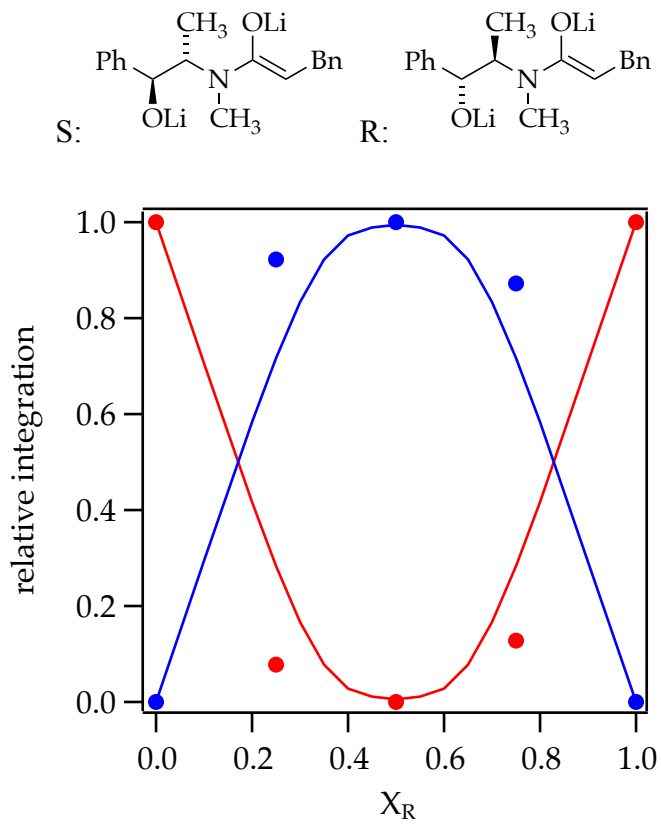


Figure 132. Job plot showing the relative integrations of octalithio homoaggregates and hexalithio heteroaggregates versus intended mole fractions of [^{6}Li]-(*R,R*)-**11** ($\boldsymbol{X_R}$) for 0.10 M mixtures of lithium enolates [^{6}Li]-(*S,S*)-**11** (S) and [^{6}Li]-(*R,R*)-**11** (R) in neat THF at –80 °C monitored by ^{6}Li NMR spectroscopy (Figure 131). The curves result from a parametric fit to tetramer-trimer model.

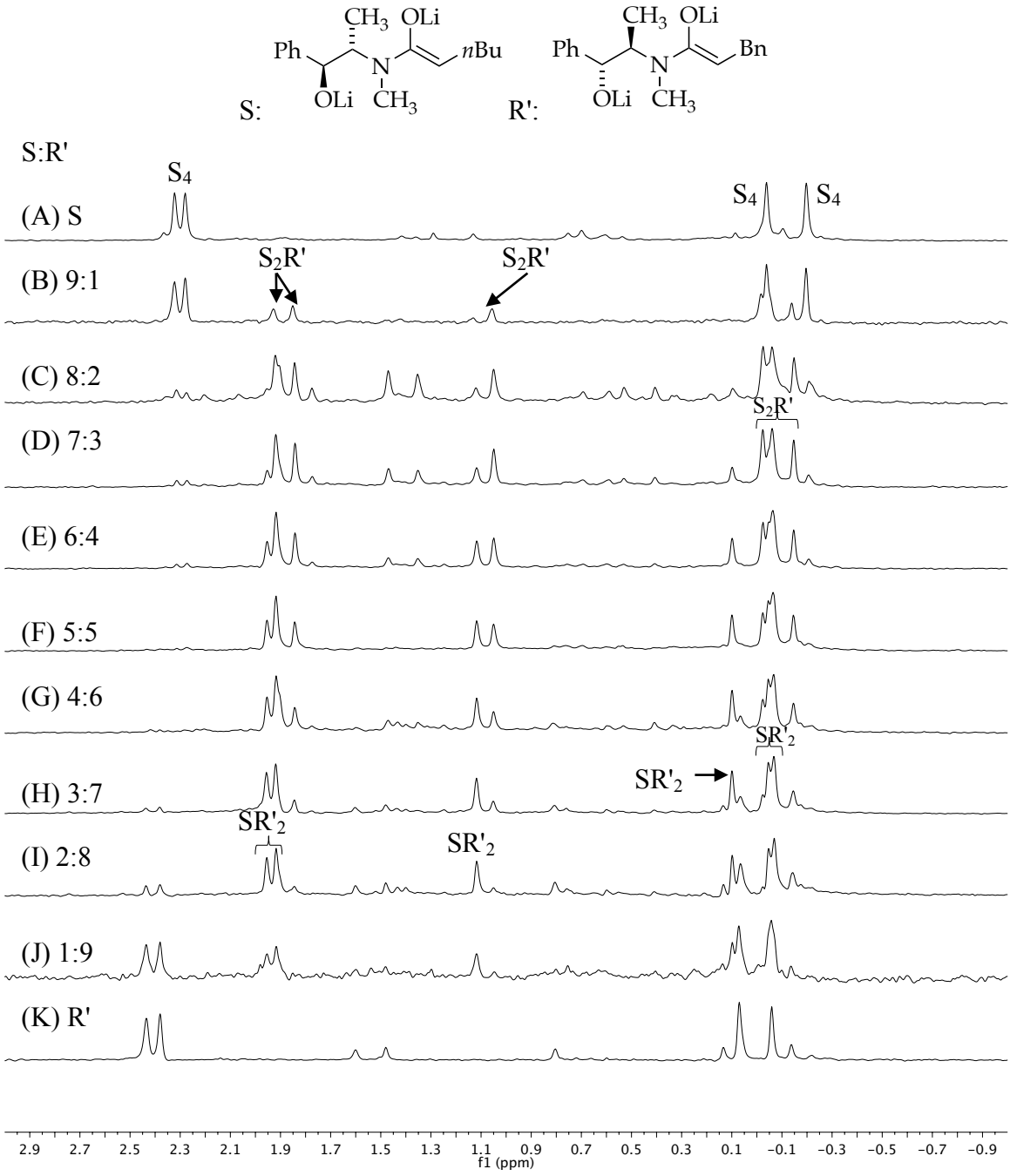


Figure 133. ^{6}Li NMR spectra for 0.10 M pre-aged solutions of [^{6}Li]-(*S,S*)-**8** (S) and [^{6}Li]-(*R,R*)-**11** (R') in 12.3 M THF at −80 °C. The measured mole fractions of (*R,R)*-**11** ($\chi_{R'}$) are 0.00, 0.18, 0.34, 0.40, 0,46, 0.50, 0.54, 0.57, 0.62, 0.88 and 1.00 for A−K, respectively. Six new resonances are found for S_2R' and SR'_2 each, which are consistent with the hexalithio trimer assignment.

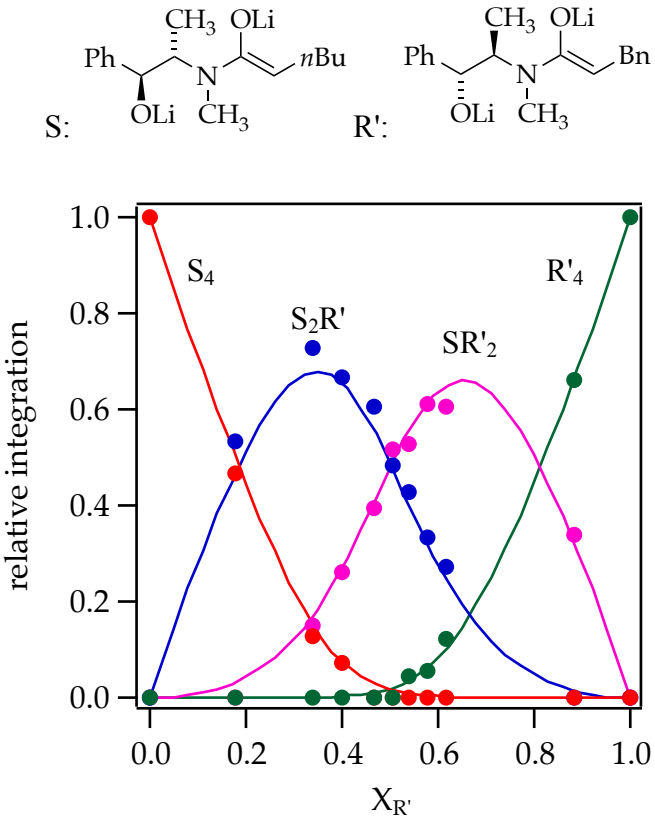


Figure 134. Job plot showing the relative integrations of octalithio-homoaggregates and hexalithio-heteroaggregates versus measured mole fractions of [^{6}Li]-(*R,R*)-**11** ($\boldsymbol{X_{R'}}$) for 0.10 M mixtures of lithium enolates [^{6}Li]-(*S,S*)-**8** (S) and [^{6}Li]-(*R,R*)-**11** (R') in neat THF at –80 °C monitored by ^{6}Li NMR spectroscopy (Figure 133). The curves result from a parametric fit to tetramer-trimer model.

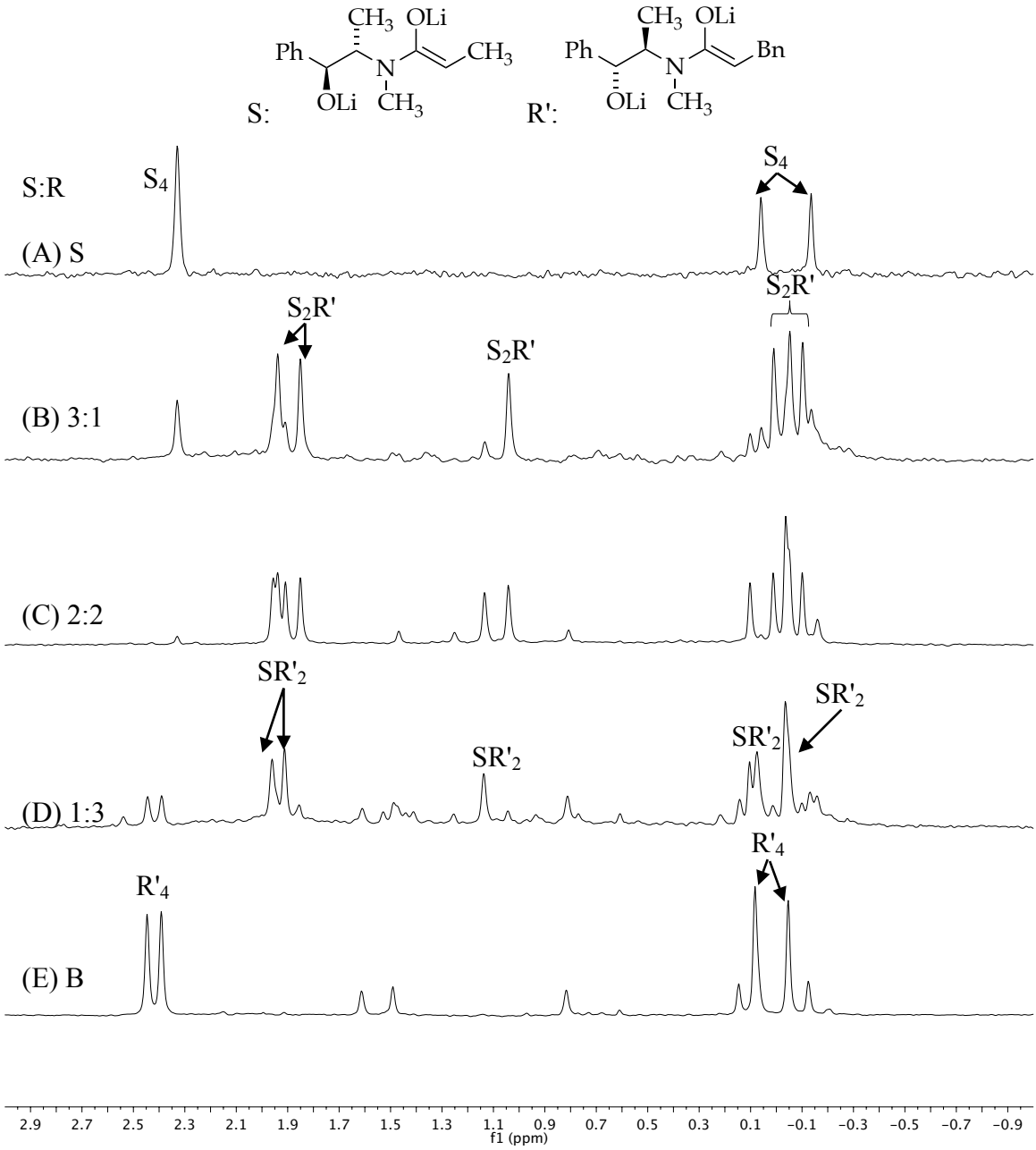


Figure 135. ^{6}Li NMR spectra for 0.10 M aged solutions of [^{6}Li]-(*S,S*)-**2** (S) and [^{6}Li]-(*R,R*)-**11** (R') in 12.3 M THF at –80 °C. The measured mole fractions of (*R,R)*-**11** ($\chi_{R'}$) are 0.00, 0.27, 0.47, 0.76 and 1.00 for A−E, respectively. Six new resonances are found for S_2R' and SR'_2 each, which are consistent with the hexalithio trimer assignment.

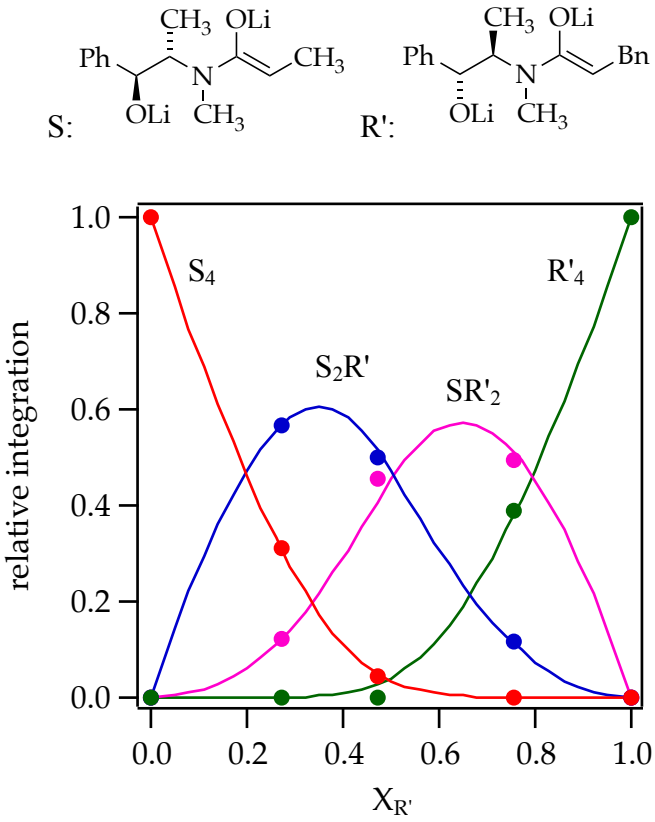


Figure 136. Job plot showing the relative integrations of octalithio homoaggregates and hexalithio heteroaggregates versus measured mole fractions of [^{6}Li]-(*R,R*)-**11** ($\boldsymbol{X_{R'}}$) for 0.10 M mixtures of lithium enolates [^{6}Li]-(*S,S*)-**2** (S) and [^{6}Li]-(*R,R*)-**11** (R') in neat THF at –80 °C monitored by ^{6}Li NMR spectroscopy (Figure 135). The curves result from a parametric fit to tetramer-trimer model.

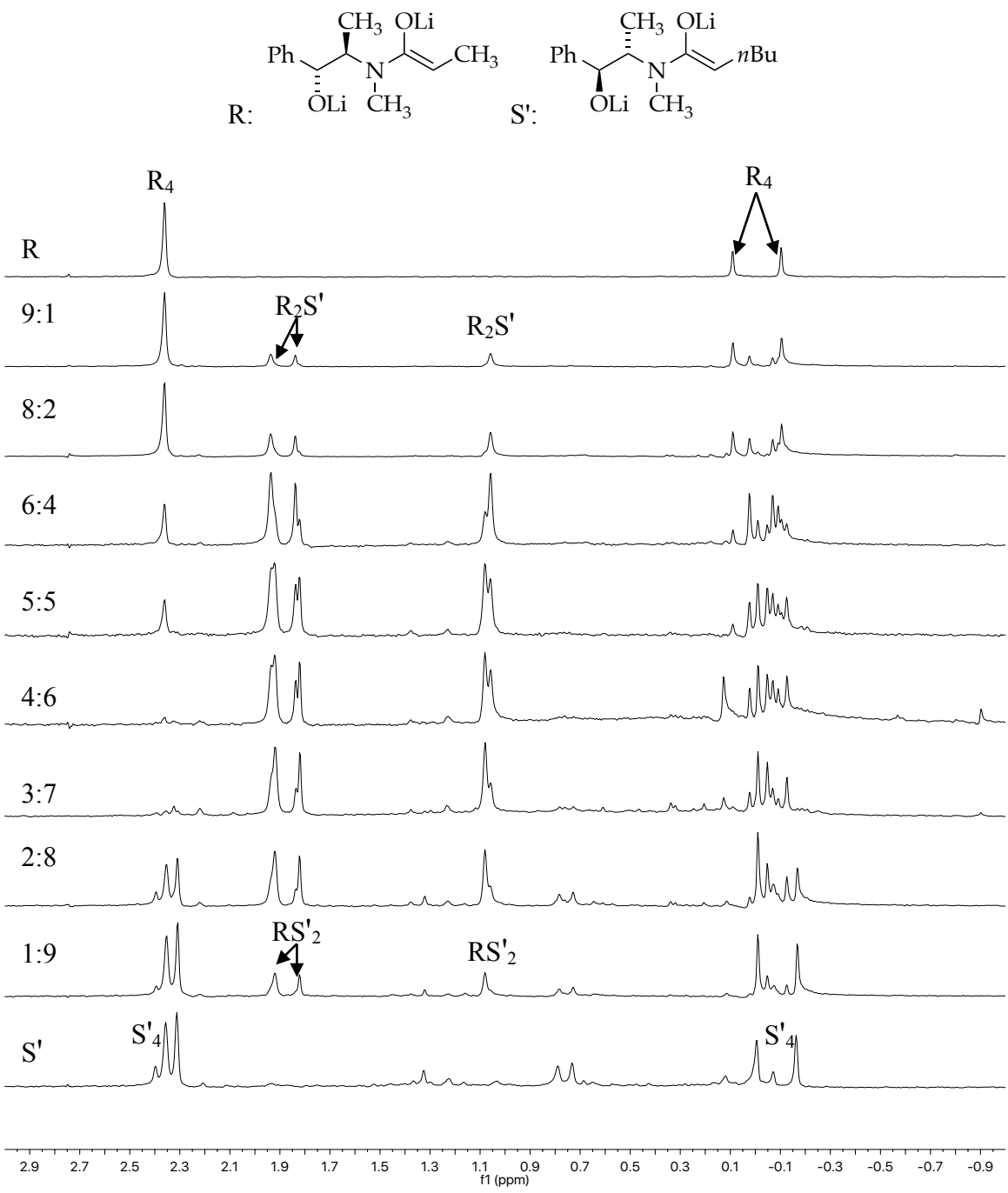


Figure 137. ^{6}Li NMR spectra for 0.10 M aged solutions of [^{6}Li]-(*S,S*)-**8** (S') and [^{6}Li]-((*R,R*)-**2** (R) in 12.3 M THF at −80 °C. T1 relaxation was not optimized for integration When enolate S' and R are not enantiomeric, heteroaggregates S'_2R and $S'R_2$ are not the same. Six new resonances were found for S'_2R and six new resonance were found for $S'R_2$. Assignments are not made for resonances from 0.1 ppm to –0.2 ppm owing to overlapping.

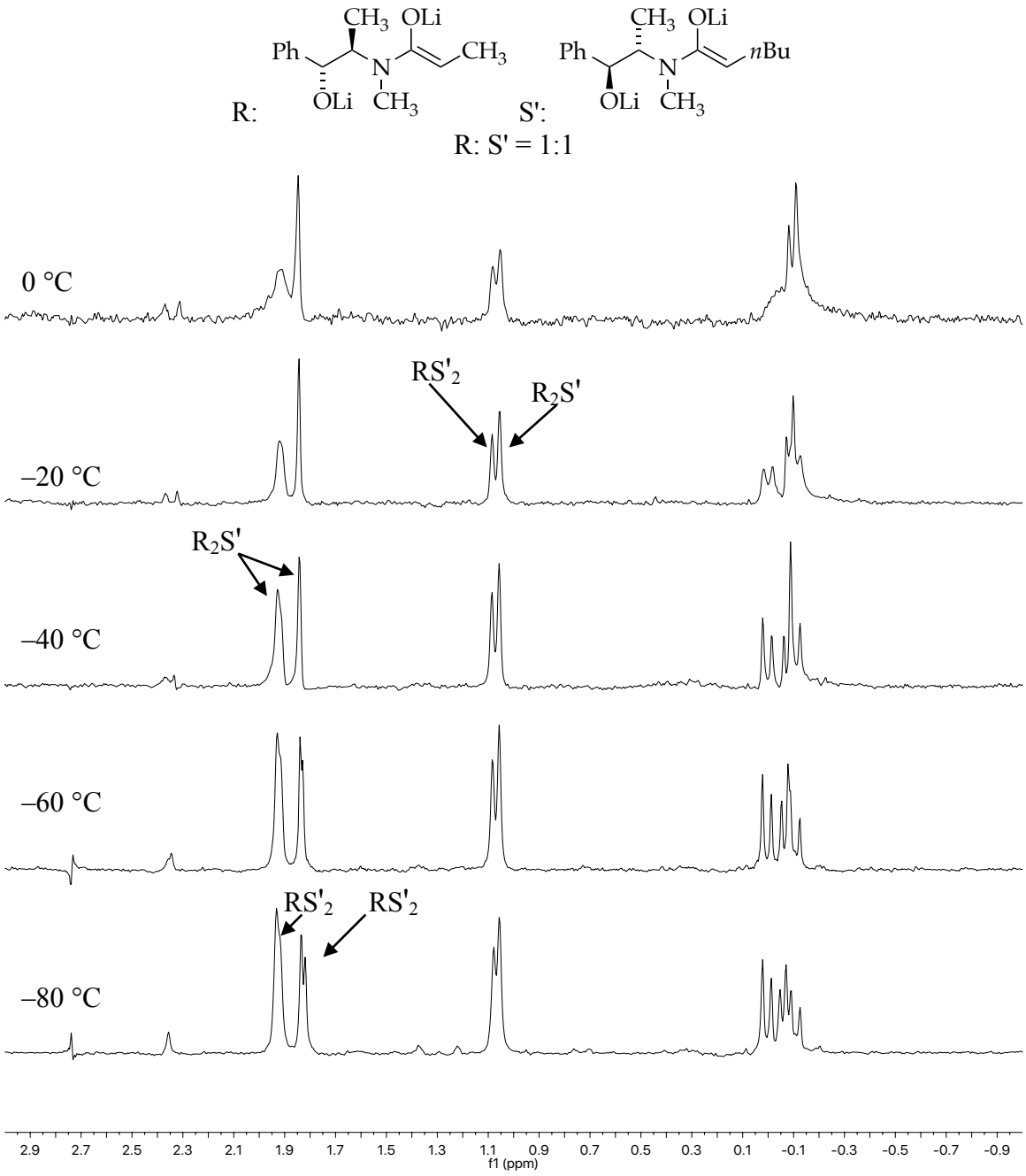


Figure 138. ^{6}Li NMR spectra for 0.10 M aged solutions of 1:1 mixture of [^{6}Li]-(*S,S*)-**8** (S') and [^{6}Li]-(*R,R*)-**2** (R) in 12.3 M THF at varying temperature. T1 relaxation was not optimized for integration. Changing temperature does not change the spectra. At temperature over 0 °C, signal-to-noise ratio becomes problematic.

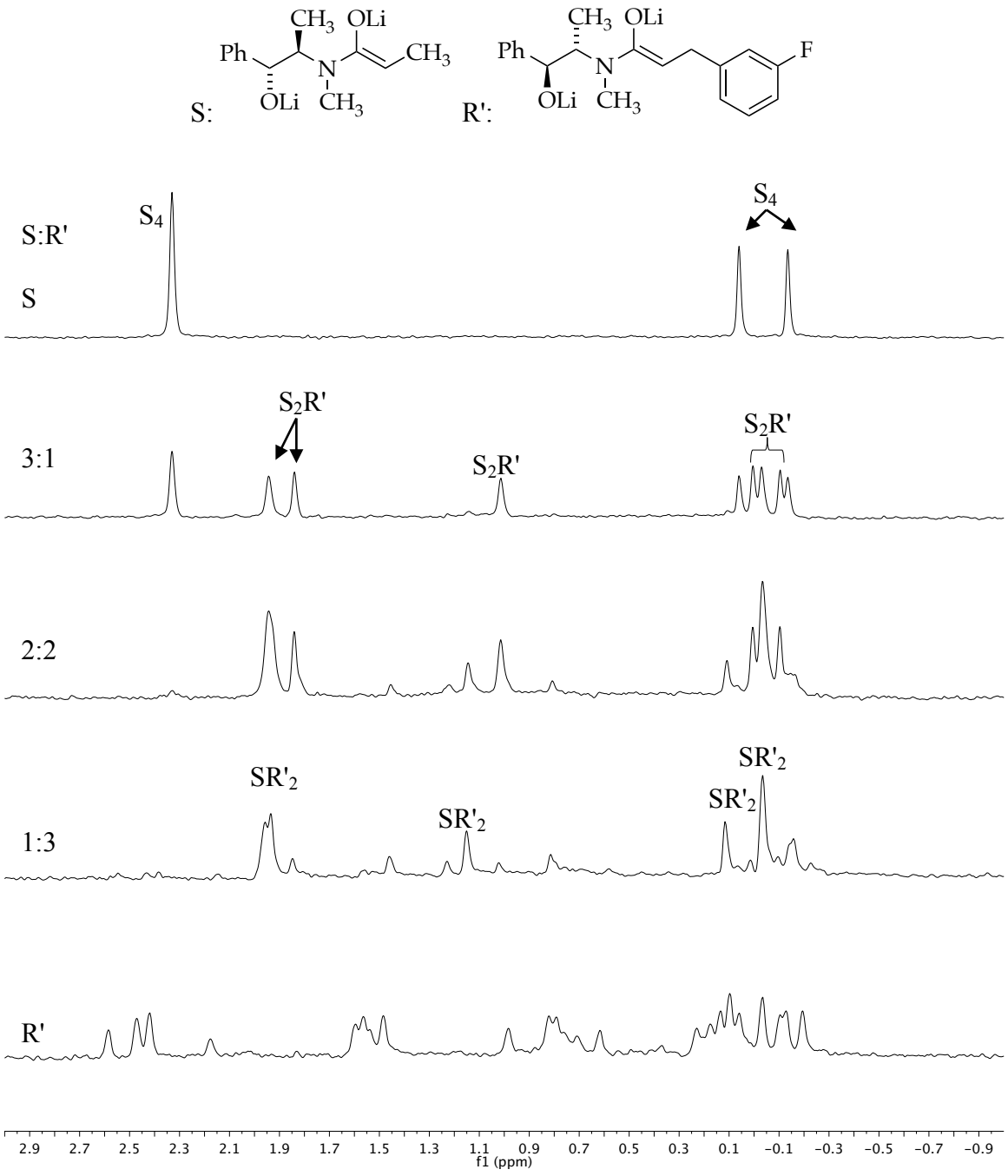


Figure 139. ^{6}Li NMR spectra for 0.10 M aged solutions of [^{6}Li]-(*R,R*)-**12** (R') and [^{6}Li]-(*S,S*)-**2** (S) in 12.3 M THF at –80 °C. T1 relaxation was not optimized for integration. Lithium enolate of **12** does not give a clean spectrum. However, the heteroaggregates still gives approximately 12 new resonances.

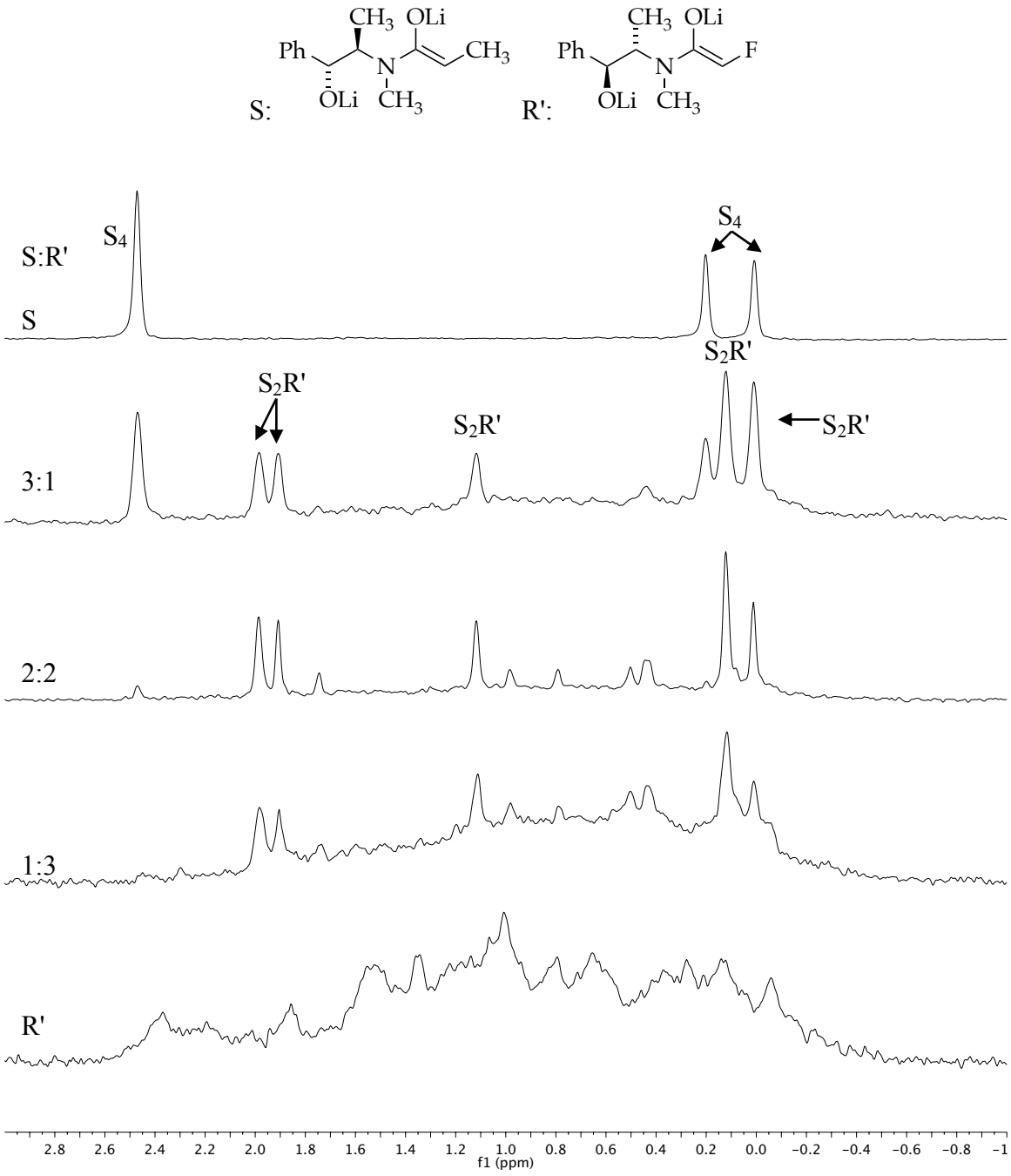


Figure 140. ^{6}Li NMR spectra for 0.10 M aged solutions of [^{6}Li]-(*R,R*)-**19** (R') and [^{6}Li]-(*S,S*)-**2** (S) in 12.3 M THF at –80 °C. T1 relaxation was not optimized for integration. Lithium enolate of **19** does not give a clean spectrum. However, the heteroaggregates (S_2R') still give 6 new resonances (5 were shown in the spectra owing to overlaps).

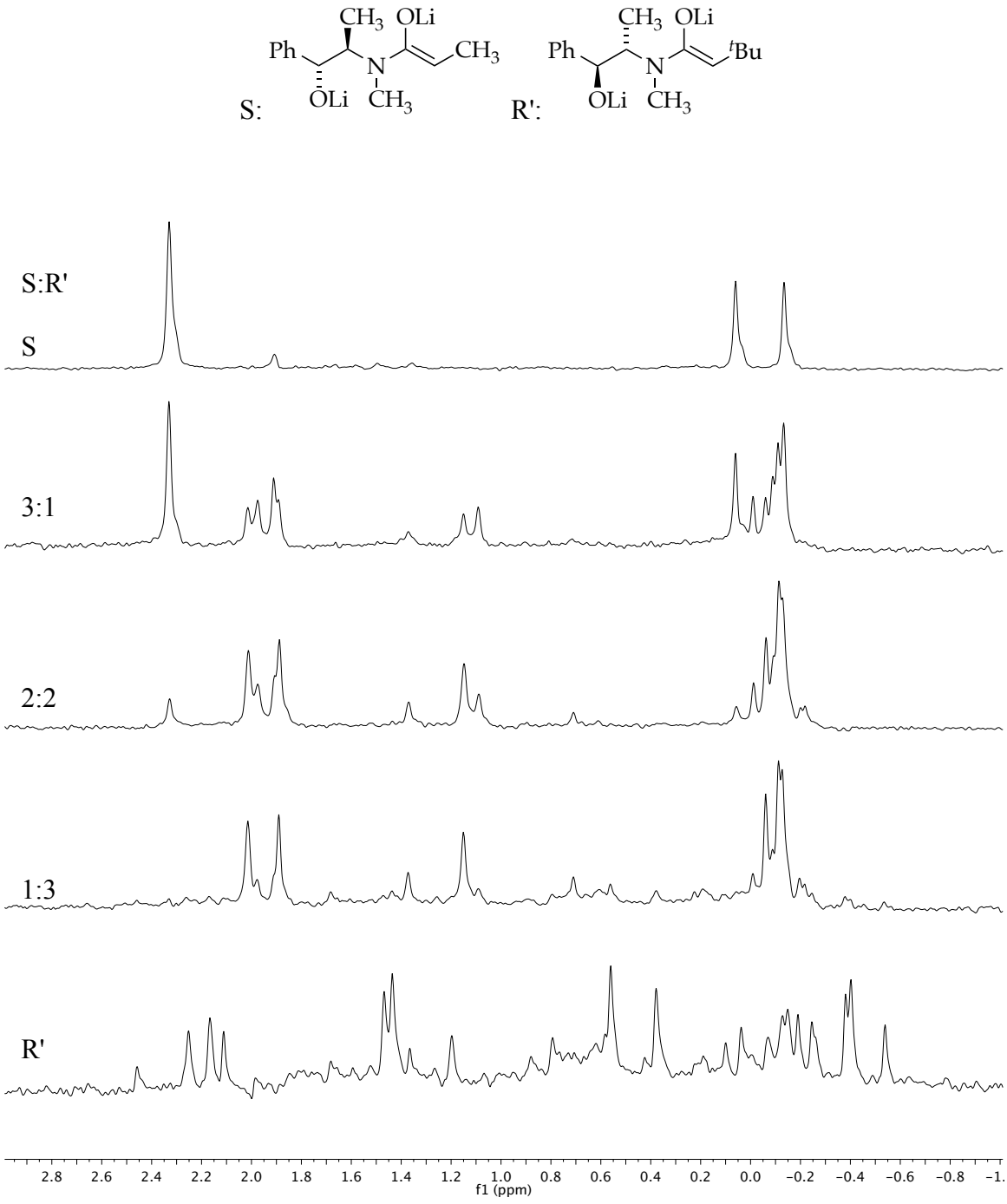


Figure 141. ^{6}Li NMR spectra for 0.10 M aged solutions of [^{6}Li]-(*R,R*)-**10** (R') and [^{6}Li]-(*S,S*)-**2** (S) in 12.3 M THF at –80 °C. T1 relaxation was not optimized for integration. The bulky *tert*-butyl group may cause deaggregation to homotetramers.

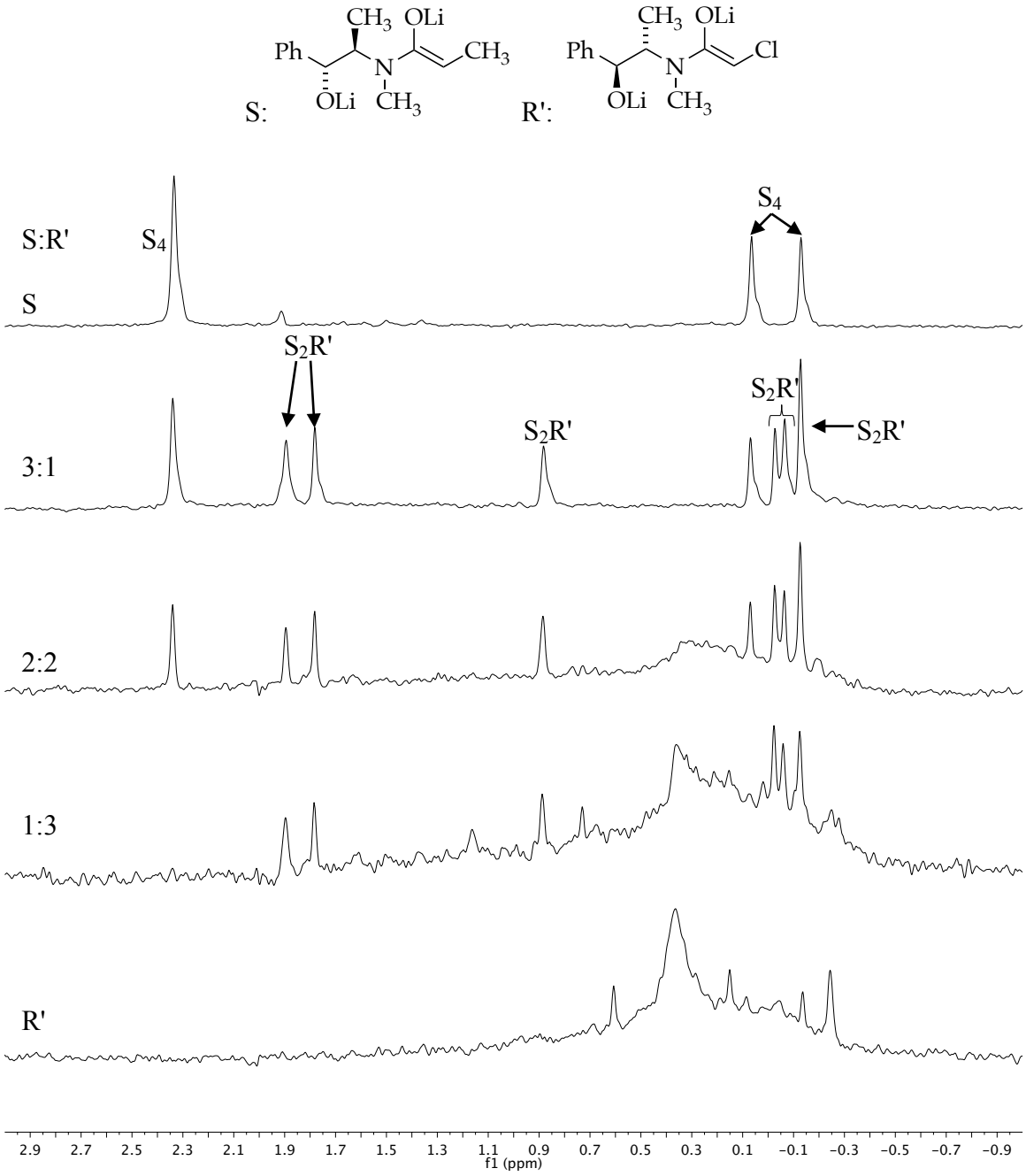


Figure 142. ^{6}Li NMR spectra for 0.10 M pre-aged solutions of [^{6}Li]-(*R,R*)-**20** (R') and [^{6}Li]-(*S,S*)-**2** (S) in 12.3 M THF at −80 °C. T1 relaxation was not optimized for integration. Lithium enolate of **20** does not give a clean spectrum. However, the heteroaggregates (S_2R') still gives 6 new resonances.

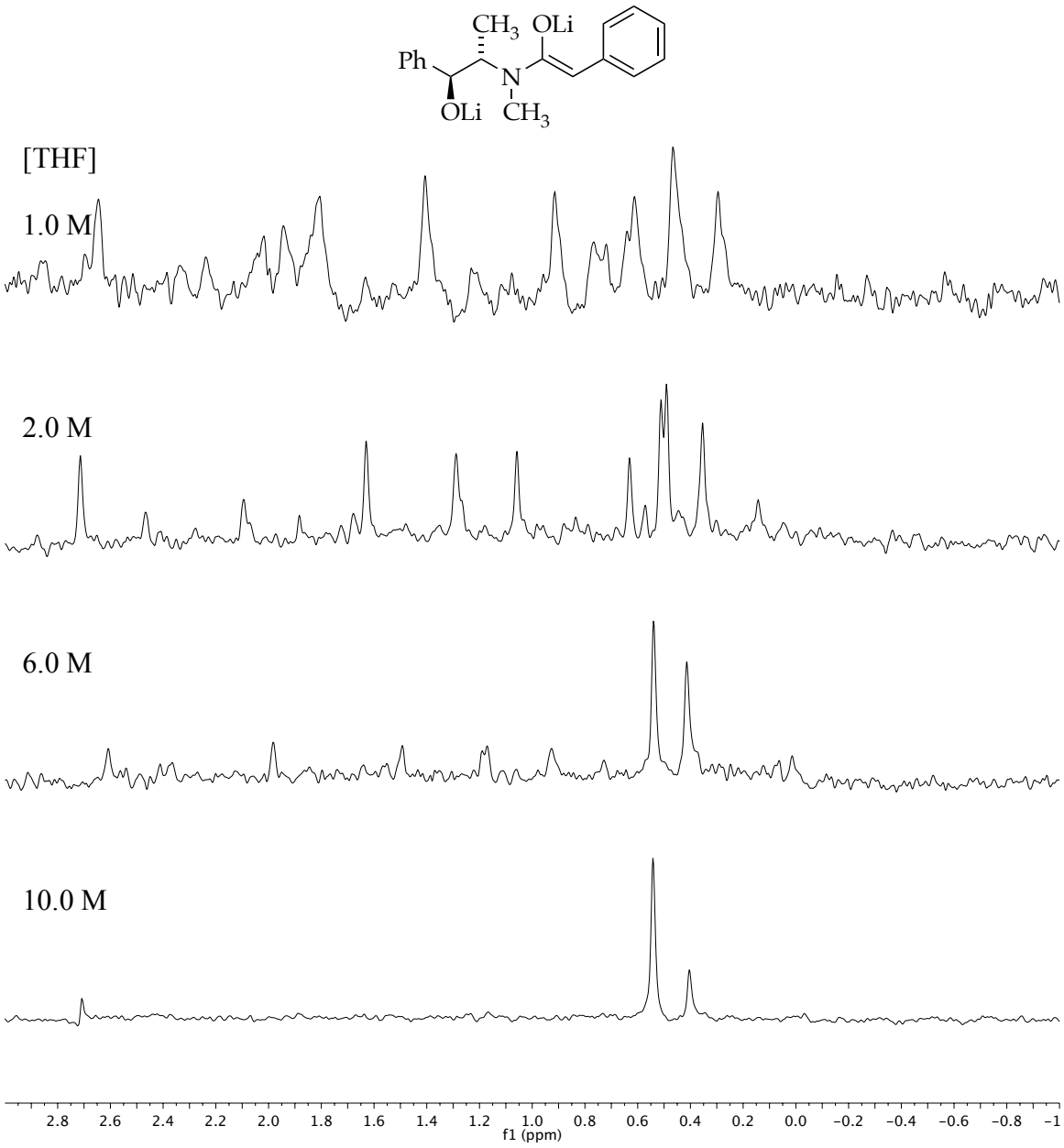


Figure 143. ^{6}Li NMR spectra for a pre-aged solution of 0.10 M [^{6}Li]-(*S,S*)-**13** in toluene at −80 °C with varying THF concentrations showing the deaggregation of **13** at low THF concentrations.

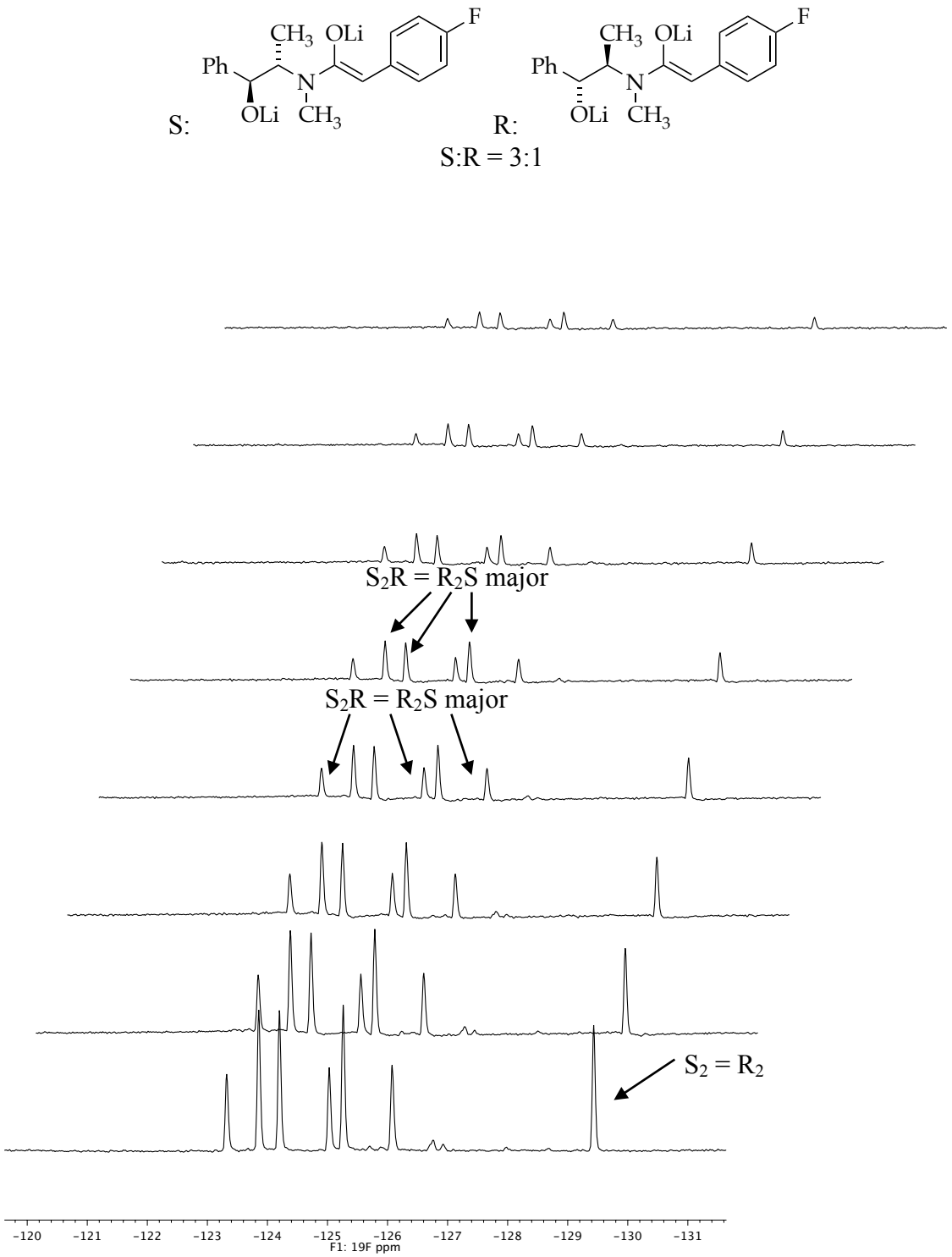


Figure 144. Diffusion ^{19}F NMR spectra for 0.10 M pre-aged solutions prepared from 0.075 M (*S,S*)-**16** and 0.025 M (*R,R*)-**16** in 12.3 M THF at –80 °C showing homoaggregates **16** is "smaller" than heteroaggregates **16**.

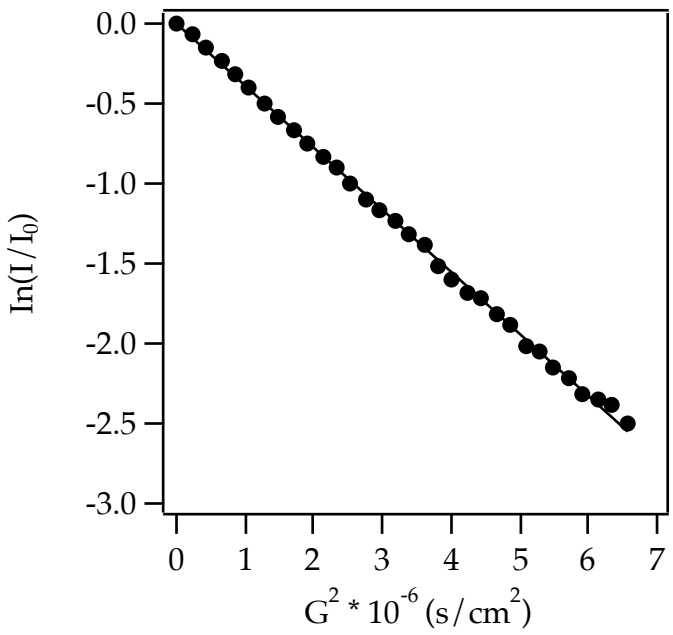


Figure 145. Diffusion coefficient plot of heteroaggregate (SR_2/S_2R major) signal in a pre-aged solution prepared from 0.075 M (*S,S*)-**16** and 0.025 M (*R,R*)-**16** in 12.3 M THF at –80 °C. $y = a + bx$ such that $a = 0$, $b = -3.876 \times 10^{-7}$. Three ^{19}F resonances corresponding to heteroaggregate (SR_2/S_2R major) are averaged.

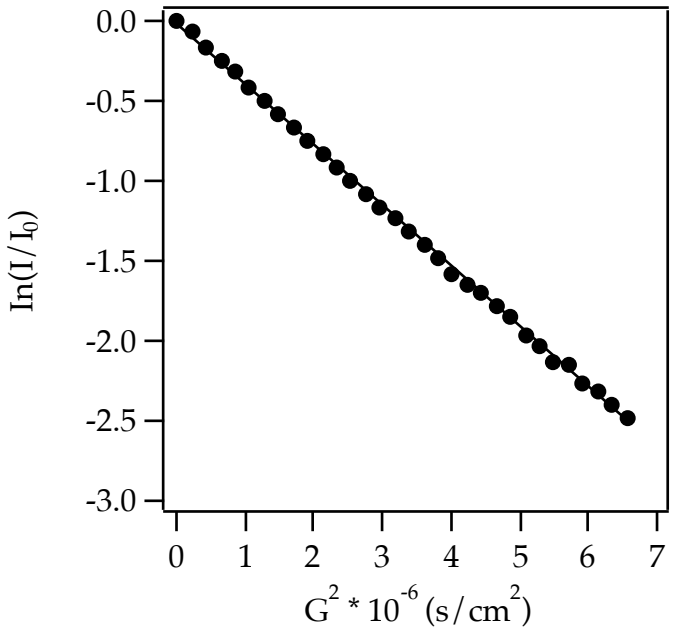


Figure 146. Diffusion coefficient plot of heteroaggregate (SR_2/S_2R minor) signal in a pre-aged solution prepared from 0.075 M (*S,S*)-**16** and 0.025 M (*R,R*)-**16** in 12.3 M THF at –80 °C. $y = a + bx$ such that $a = 0$, $b = -3.799 \times 10^{-7}$. Three ^{19}F resonances corresponding to heteroaggregate (SR_2/S_2R minor) are averaged.

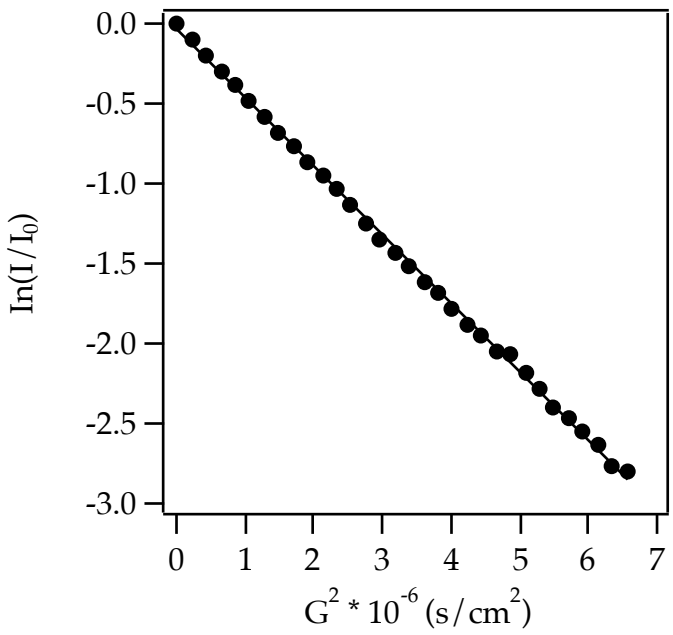


Figure 147. Diffusion coefficient plot of homoaggregate (S_2/R_2) signal in a pre-aged solution prepared from 0.075 M (*S,S*)-**16** and 0.025 M (*R,R*)-**16** in 12.3 M THF at –80 °C. $y = a + bx$ such that $a = 0$, $b = -4.279 \times 10^{-7}$.

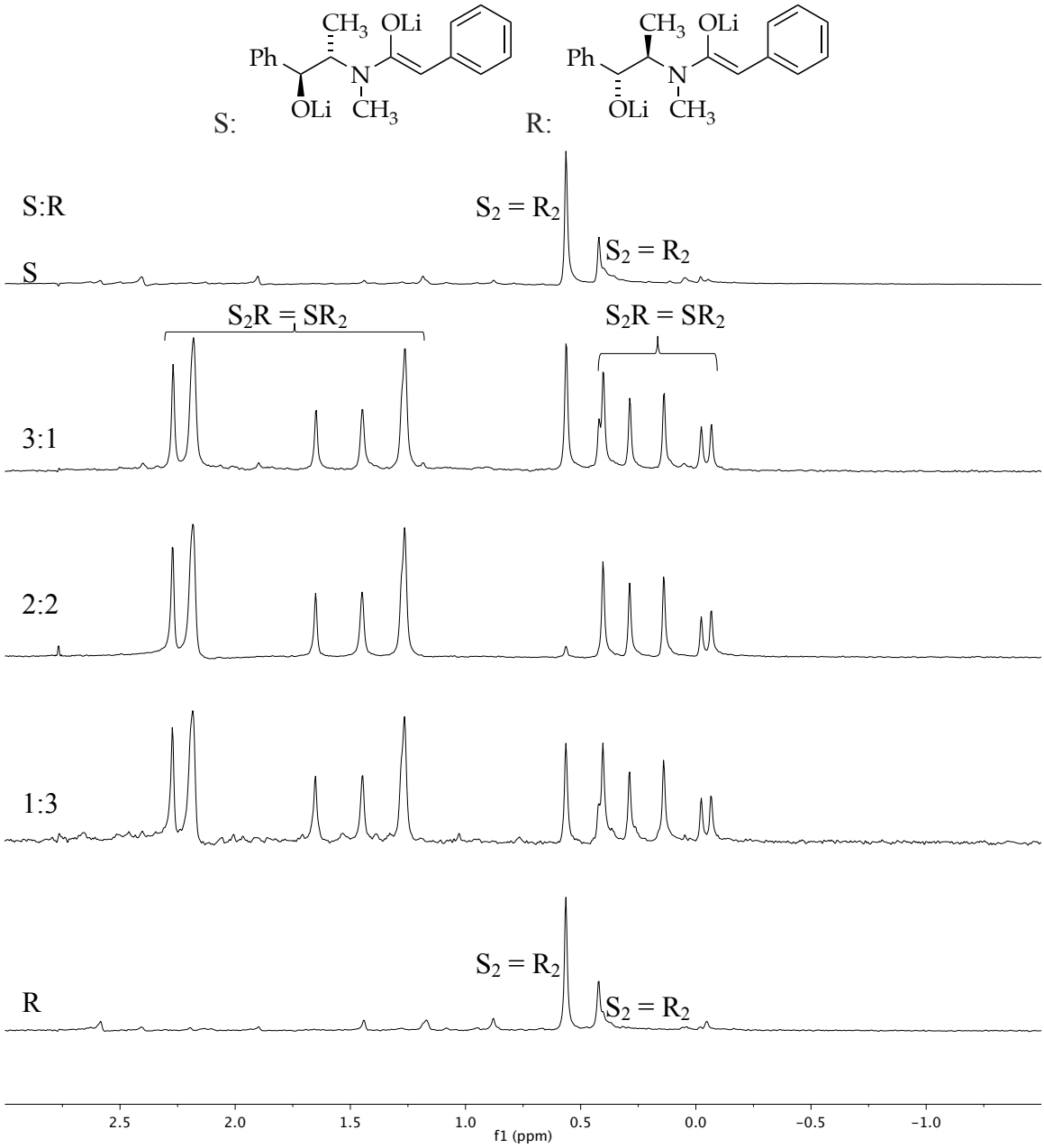


Figure 148. ^{6}Li NMR spectra for 0.10 M pre-aged solutions of [^{6}Li]-(*S,S*)-**13** (S) and [^{6}Li]-(*R,R*)-**13** (R) in 12.3 M THF at −80 °C. T1 relaxation was not optimized for integration. Hexalithio hetero-trimers show 10 new resonances. In principle, 12 resonances should be detected, 6 resonances each for major and minor isomers.

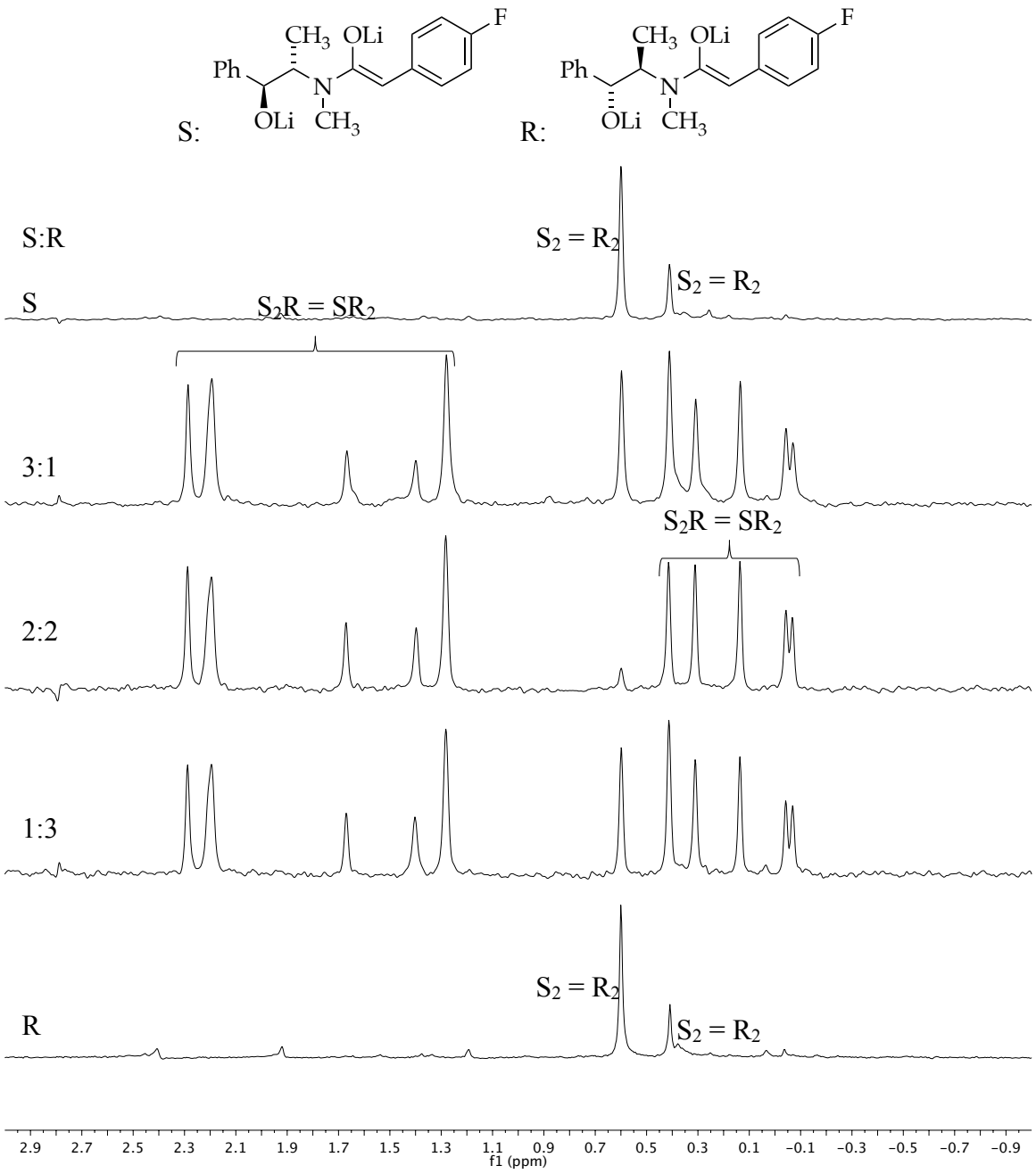


Figure 149. ^{6}Li NMR spectra for 0.10 M pre-aged solutions of [^{6}Li]-(*S,S*)-**16** (S) and [^{6}Li]-(*R,R*)-**16** (R) in 12.3 M THF at –80 °C. T1 relaxation was not optimized for integration. Hexalithio hetero-trimers show 10 new resonances. In principle, 12 resonances should be detected, 6 resonances each for major and minor isomers. Enolates **16** and **13** give similar results.

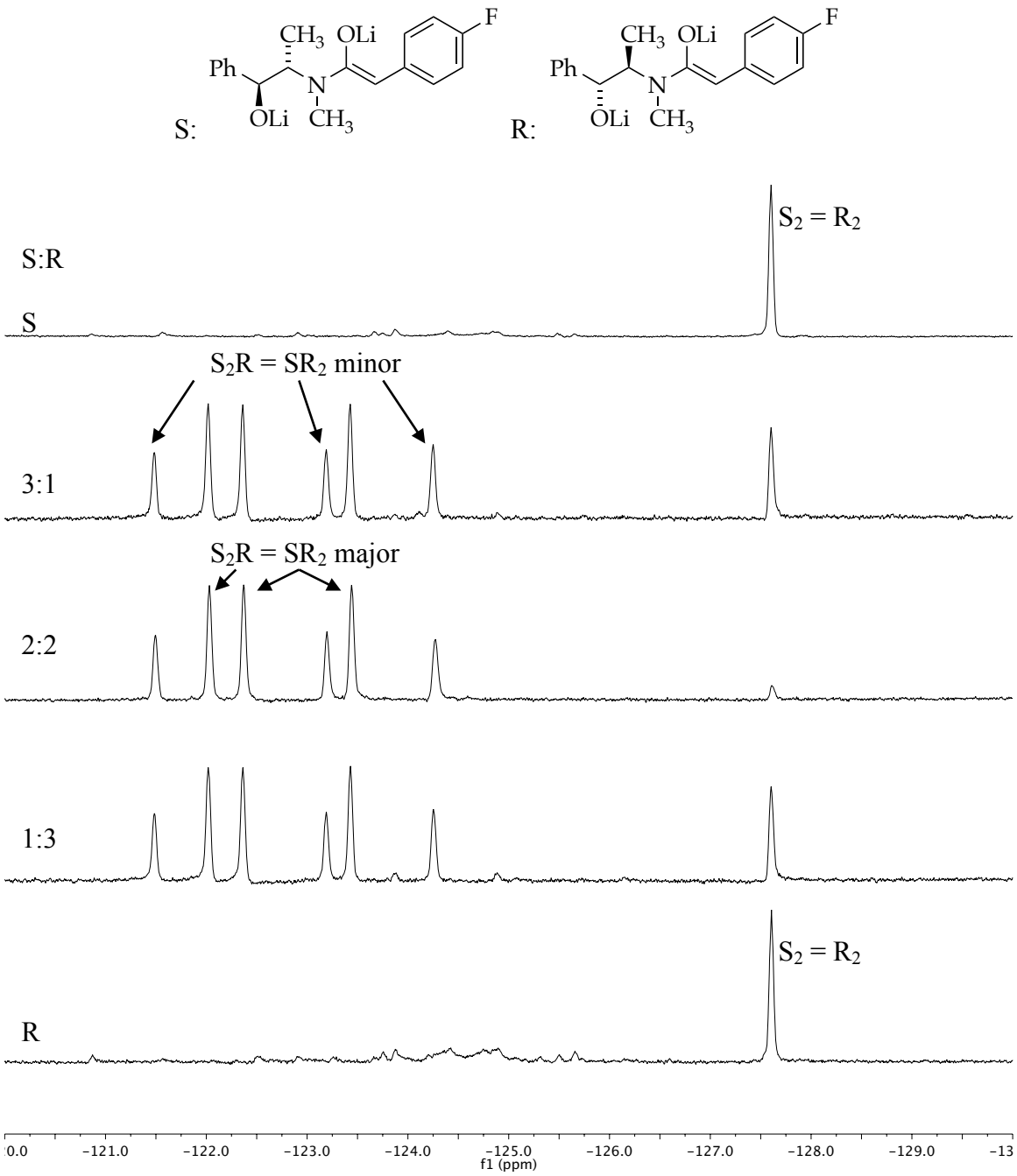


Figure 150. ^{19}F NMR spectra for 0.10 M pre-aged solutions of [^{6}Li]-(*S,S*)-**16** (S) and [^{6}Li]-(*R,R*)-**16** (R) in 12.3 M THF at –80 °C. ^{19}F rather than ^{6}Li NMR spectroscopy reduces the number of resonances to one half. This experiment shows 6 new resonances for hetero-trimers, 3 resonances for major and minor isomers each.

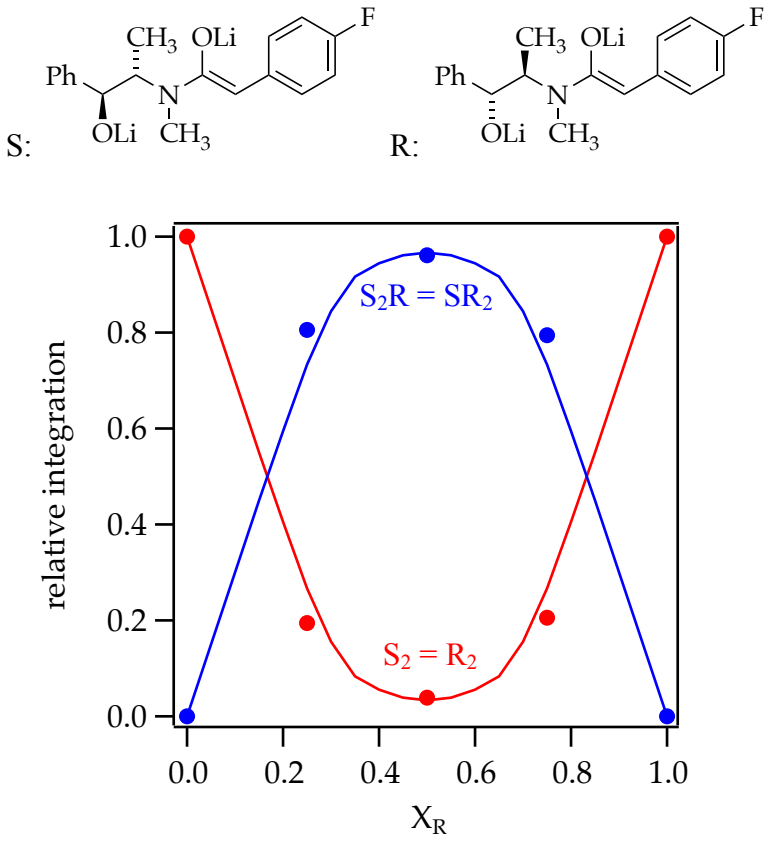


Figure 151. Job plot showing the relative integrations of tetralithio homoaggregates and hexalithio heteroaggregates versus intended mole fractions of [^{6}Li]-(*R,R*)-**16** (R) ($\boldsymbol{X_R}$) for 0.10 M pre-aged solutions of lithium enolates [^{6}Li]-(*S,S*)-**16** (S) and [^{6}Li]-(*R,R*)-**16** (R) in neat THF at –80 °C monitored by ^{19}F NMR spectroscopy (See Figure 150). The curves result from a parametric fit to a dimer-trimer model. The Job plot shows heteroaggregates are non-statistically favored when mixing two enantiomers.

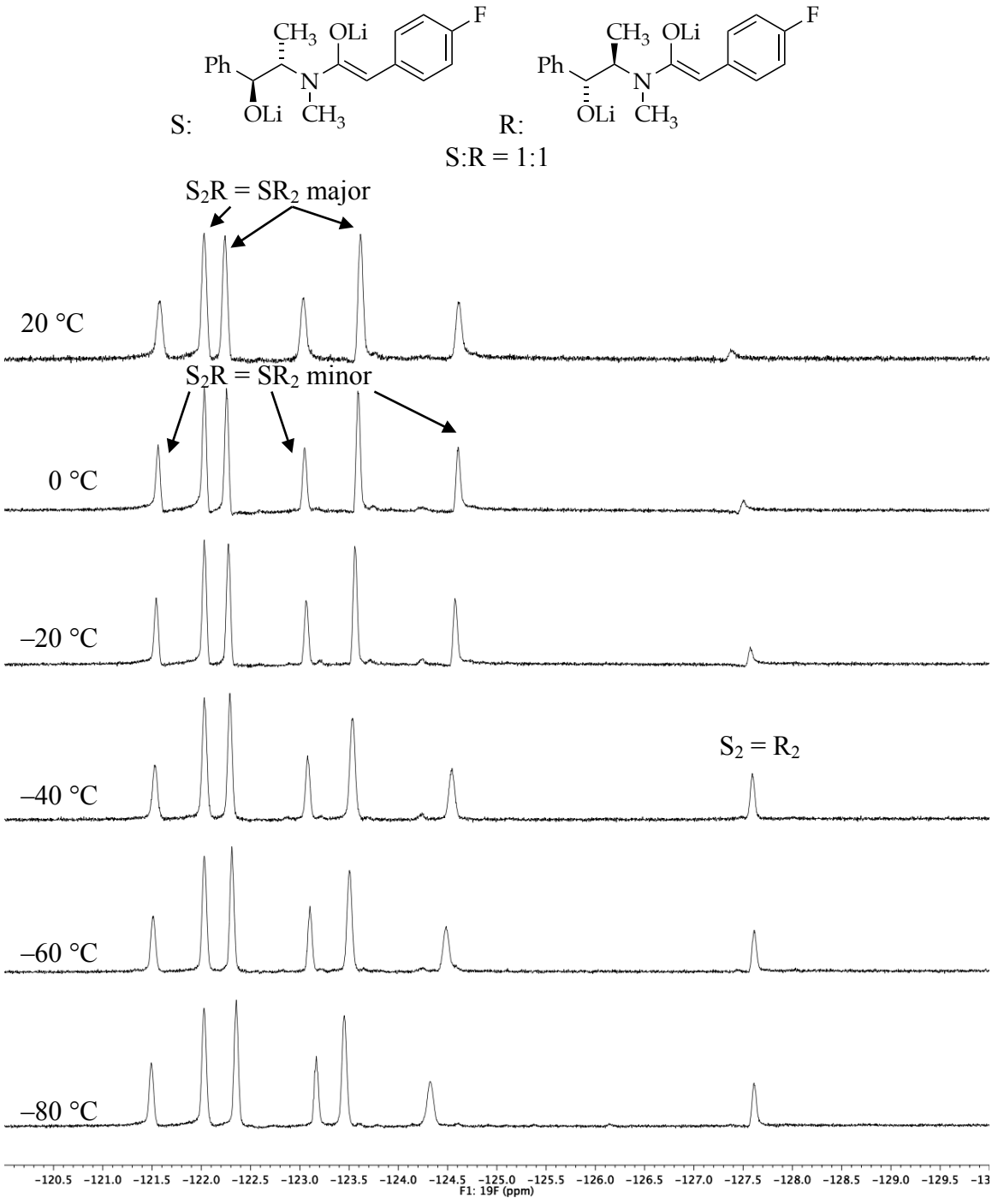


Figure 152. ^{19}F NMR spectra for 0.10 M pre-aged solutions of 1:1 mixture of [^{6}Li]-(*S,S*)-**16** (S) and [^{6}Li]-(*R,R*)-**16** (R) in 12.3 M THF at varying temperature. Varying temperature does not resolve or coalesce peaks.

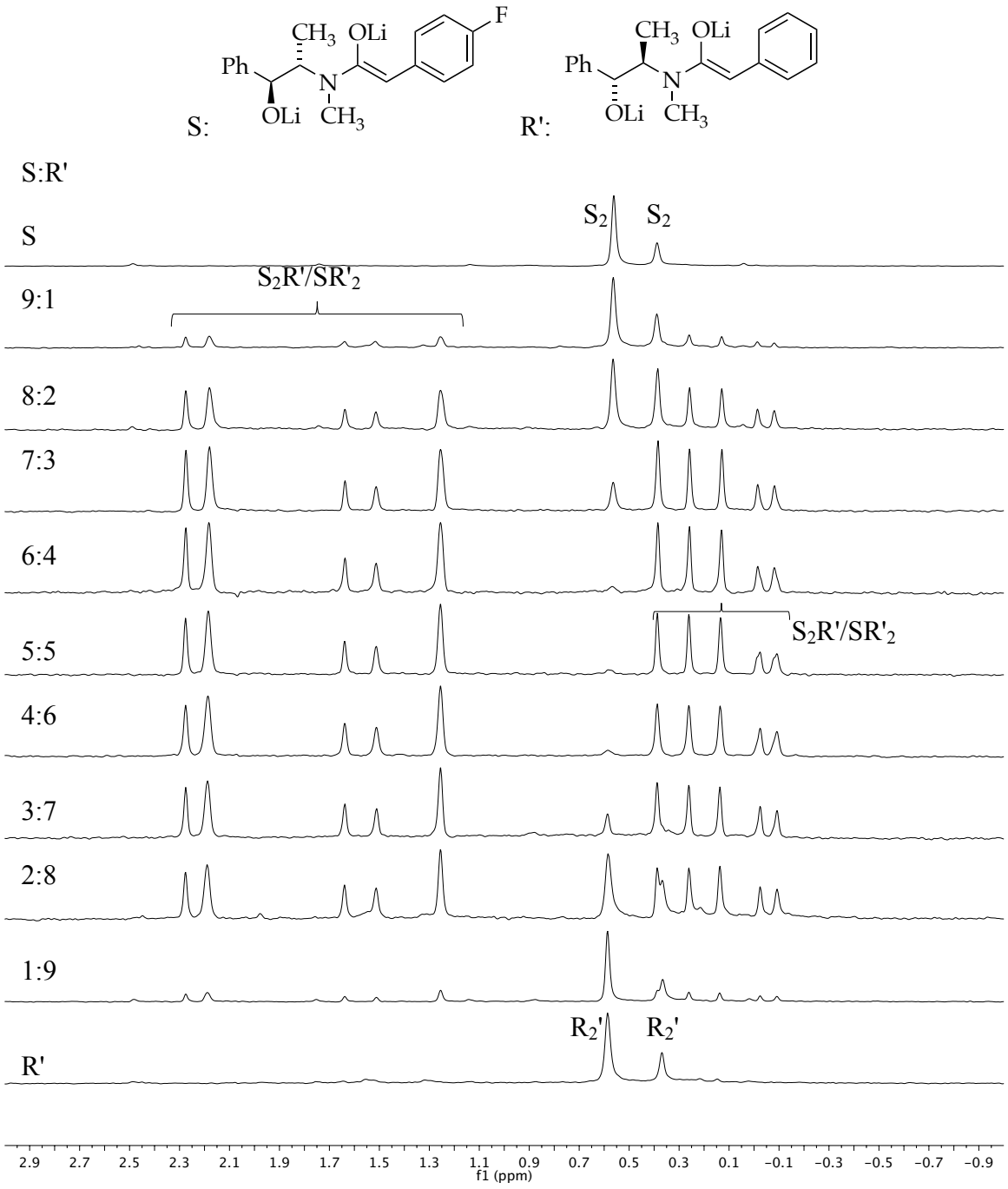


Figure 153. ^{6}Li NMR spectra for 0.10 M pre-aged solutions of [^{6}Li]-(*S,S*)-**16** (S) and [^{6}Li]-(*R,R*)-**13** (R') in 12.3 M THF at –80 °C. T1 relaxation was not optimized for integration.

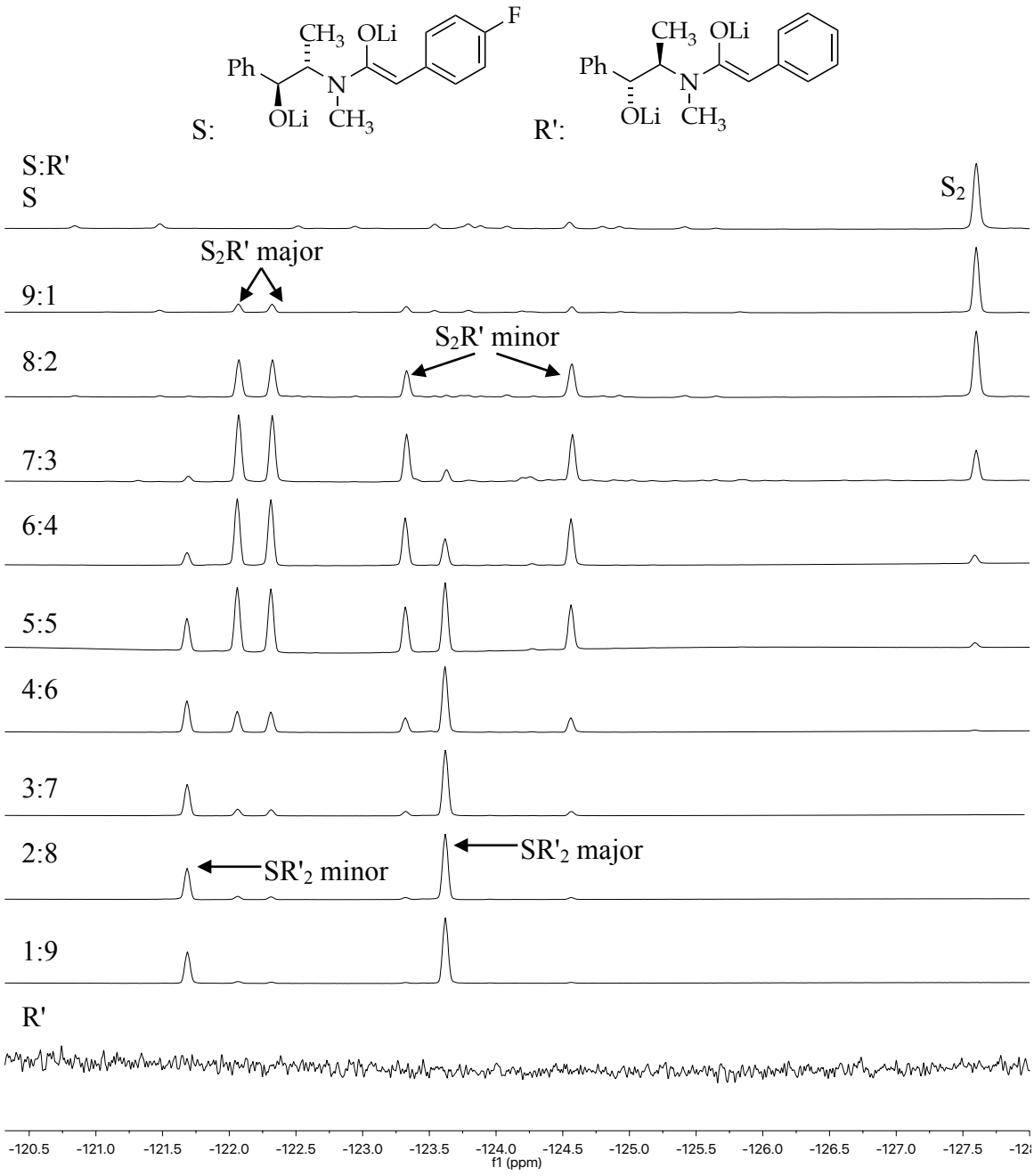


Figure 154. ^{19}F NMR spectra for 0.10 M pre-aged solutions of [^{6}Li]-(*S,S*)-**16** (S) and [^{6}Li]-(*R,R*)-**13** (R') in 12.3 M THF at –80 °C. Six new resonances are shown for hetero-trimers, one resonance for R'$_2$S major isomer and R'$_2$S minor isomer each, two resonances each for R'S$_2$ major isomers and R'S$_2$ minor isomers.

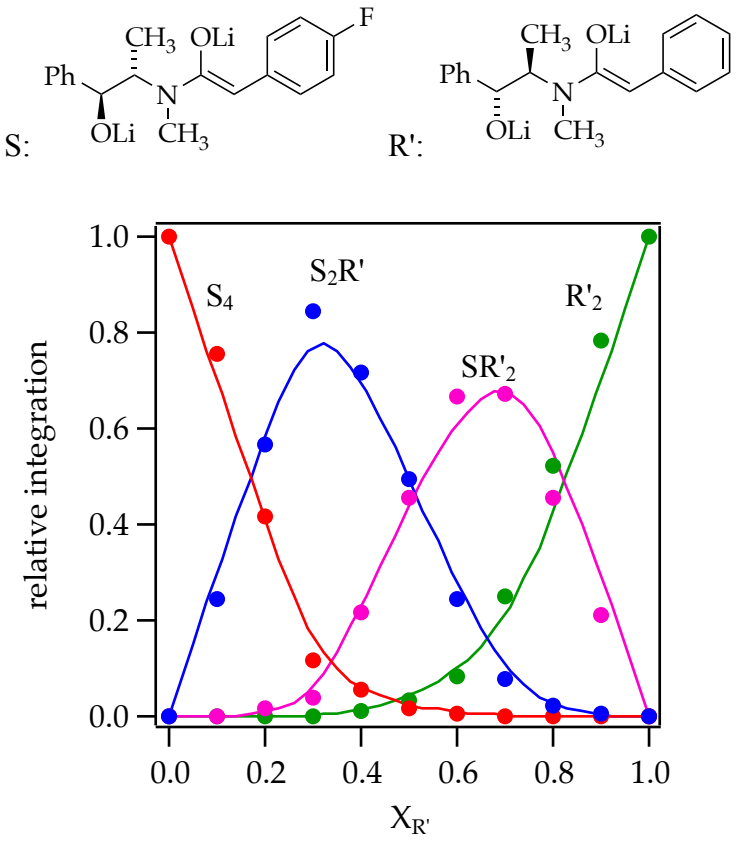


Figure 155. Job plot showing the relative integrations of tetralithio homoaggregates and hexalithio heteroaggregates versus intended mole fractions of [^{6}Li]-(*R,R*)-**13** (R') ($\boldsymbol{X_{R'}}$) for 0.10 M pre-aged solutions of lithium enolates [^{6}Li]-(*S,S*)-**16** (S) and [^{6}Li]-(*R,R*)-**13** (R') in neat THF at –80 °C monitored by ^{19}F NMR spectroscopy (See Figure 154). The curves result from a parametric fit to a dimer-trimer model. Integration of R_2 is derived from the intended mole fraction.

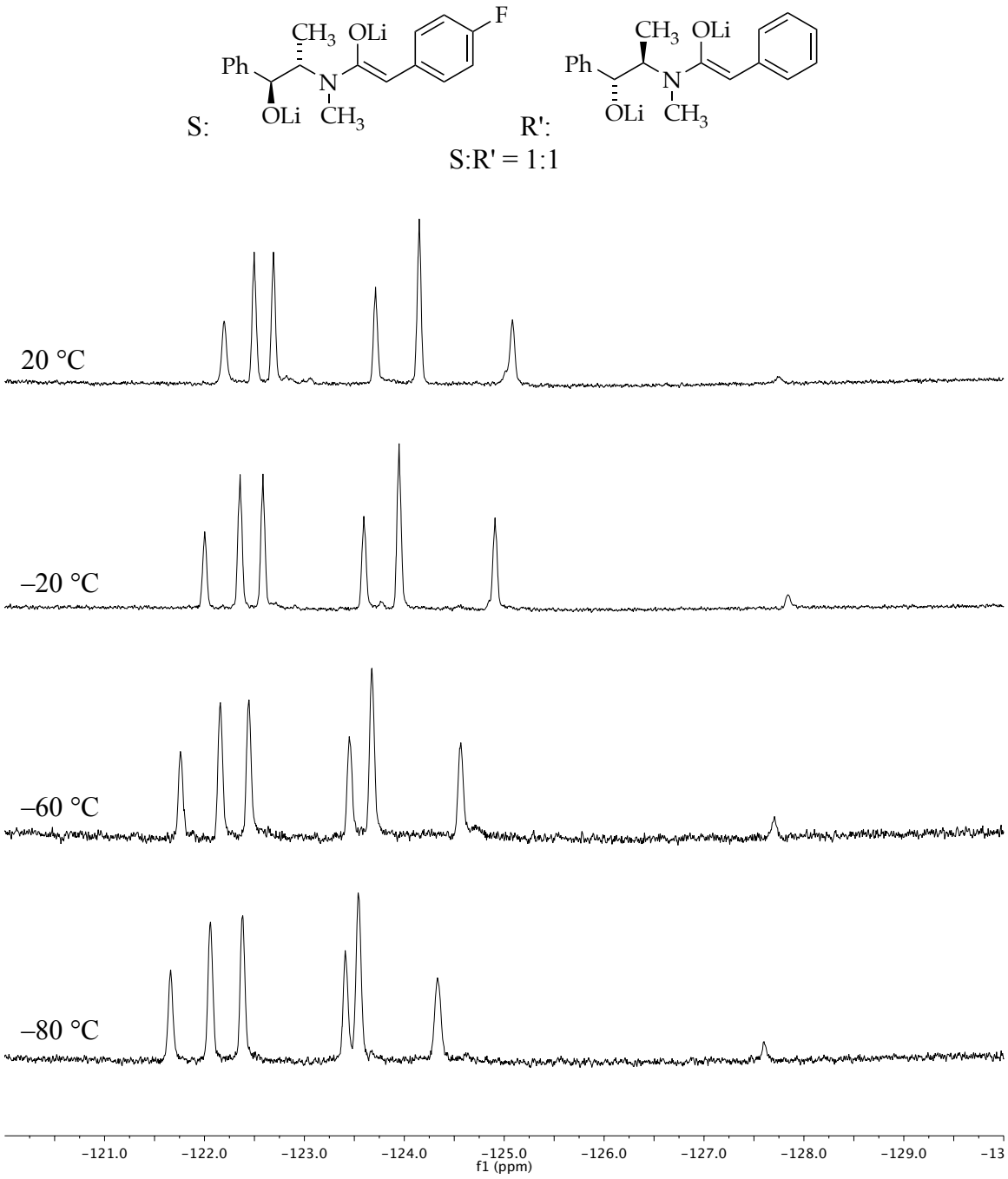


Figure 156. ^{19}F NMR spectra for 0.10 M pre-aged solutions of 1:1 mixture of [^{6}Li]-(*S,S*)-**16** (S) and [^{6}Li]-(*R,R*)-**13** (R') in 12.3 M THF at varying temperature. Varying the temperature does not resolve or coalesce peaks.

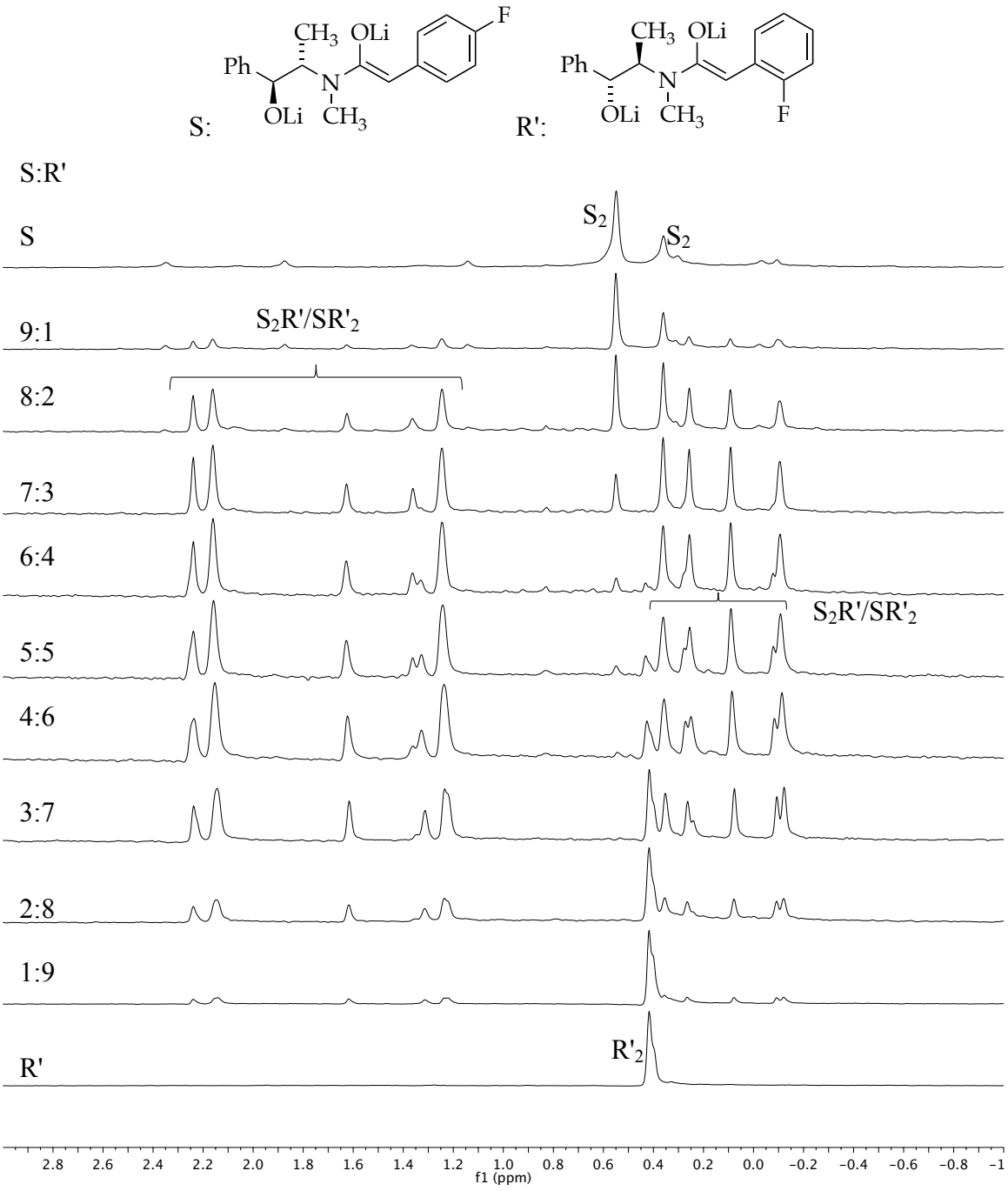


Figure 157. ^{6}Li NMR spectra of 0.10 M pre-aged solutions of [^{6}Li]-(*S,S*)-**16** (S) and [^{6}Li]-(*R,R*)-**14** (R') in 12.3 M THF at –80 °C. T1 relaxation was not optimized for integration. Mixing heterochiral hetero-substrates, in theory, should produce 24 new resonances (corresponding to $S_2R'_{\text{major/minor}}$ and $SR'_{2\ \text{major/minor}}$).

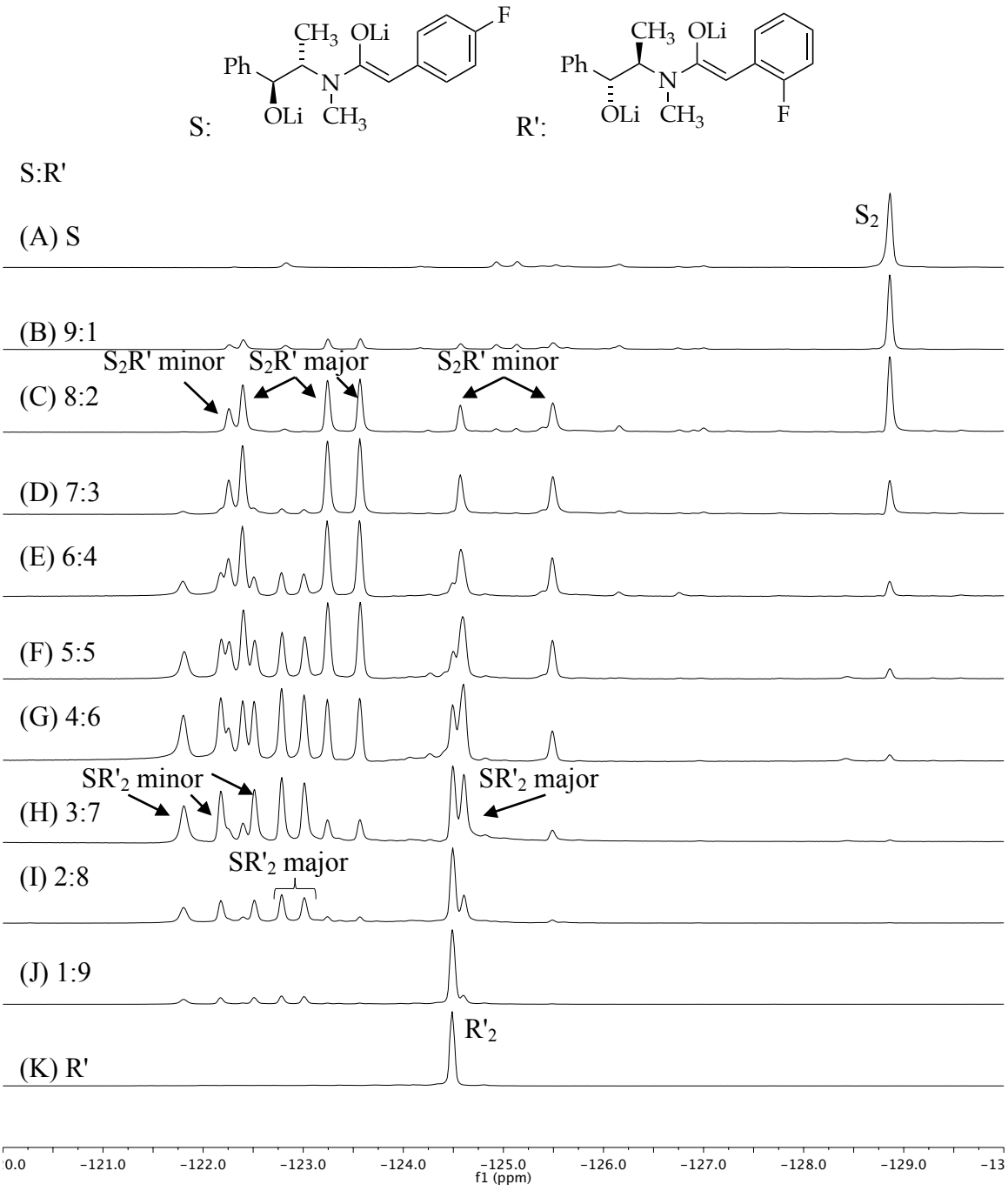


Figure 158. ^{19}F NMR spectra for 0.10 M pre-aged solutions of [^{6}Li]-(*S,S*)-**16** (S) and [^{6}Li]-(*R,R*)-**14** (R') in 12.3 M THF at –80 °C. The measured mole fractions of [^{6}Li]-(*R,R*)-**14** ($\chi_{R'}$) are 0.00, 0.15, 0.26, 0.34, 0.42, 0.50, 0.56, 0.68, 0.75, 0.88 and 1.00 for A−K, respectively. ^{19}F NMR spectra give improved resolution. SR'$_2$ and S$_2$R' each form two isomers.

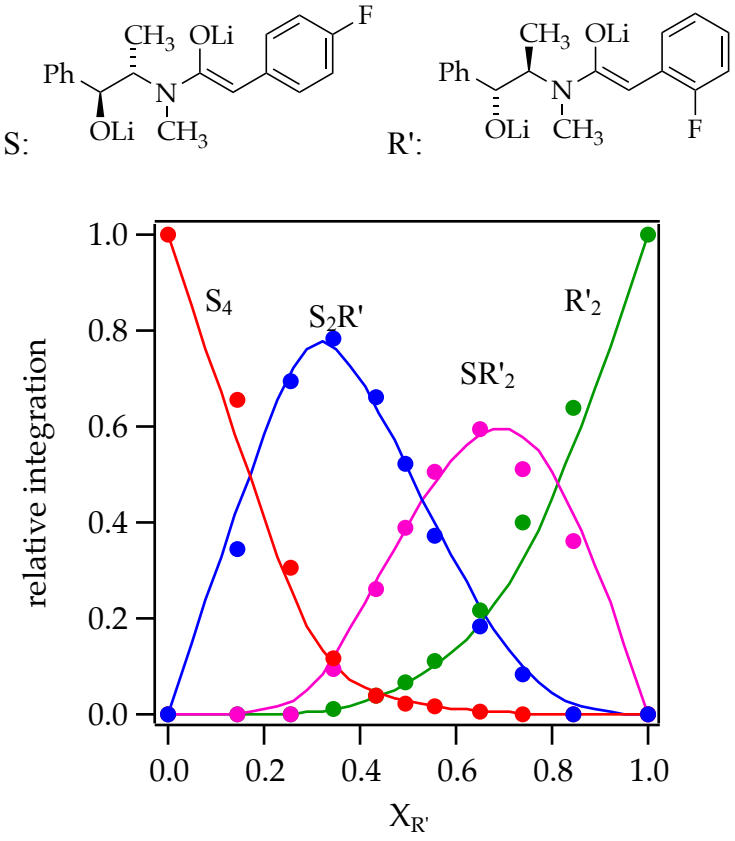


Figure 159. Job plot showing the relative integrations of tetralithio homoaggregates and hexalithio heteroaggregates versus measured mole fractions of [^{6}Li]-(*R,R*)-**14** (R') ($\boldsymbol{X_{R'}}$) for 0.10 M pre-aged solutions of lithium enolates [^{6}Li]-(*S,S*)-**16** (S) and [^{6}Li]-(*R,R*)-**14** (R') in neat THF at –80 °C monitored by ^{19}F NMR spectroscopy (See Figure 158). The curves result from a parametric fit to dimer-trimer model.

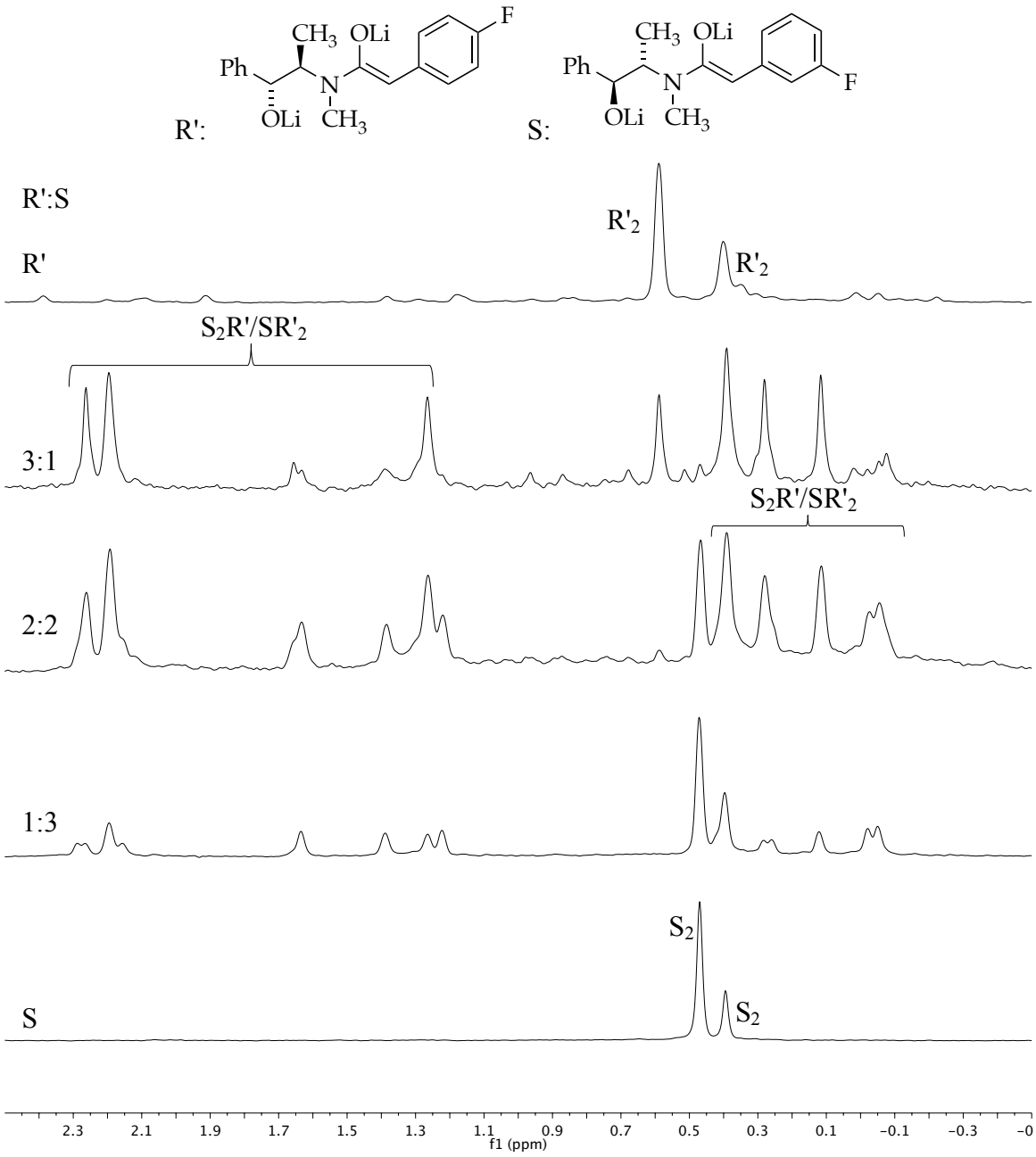


Figure 160. ^{6}Li NMR spectra for 0.10 M pre-aged solutions of [^{6}Li]-(*R,R*)-**16** (R') and [^{6}Li]-(*S,S*)-**15** (S) in 12.3 M THF at –80 °C. T1 relaxation was not optimized for integration. Overlap is significant.

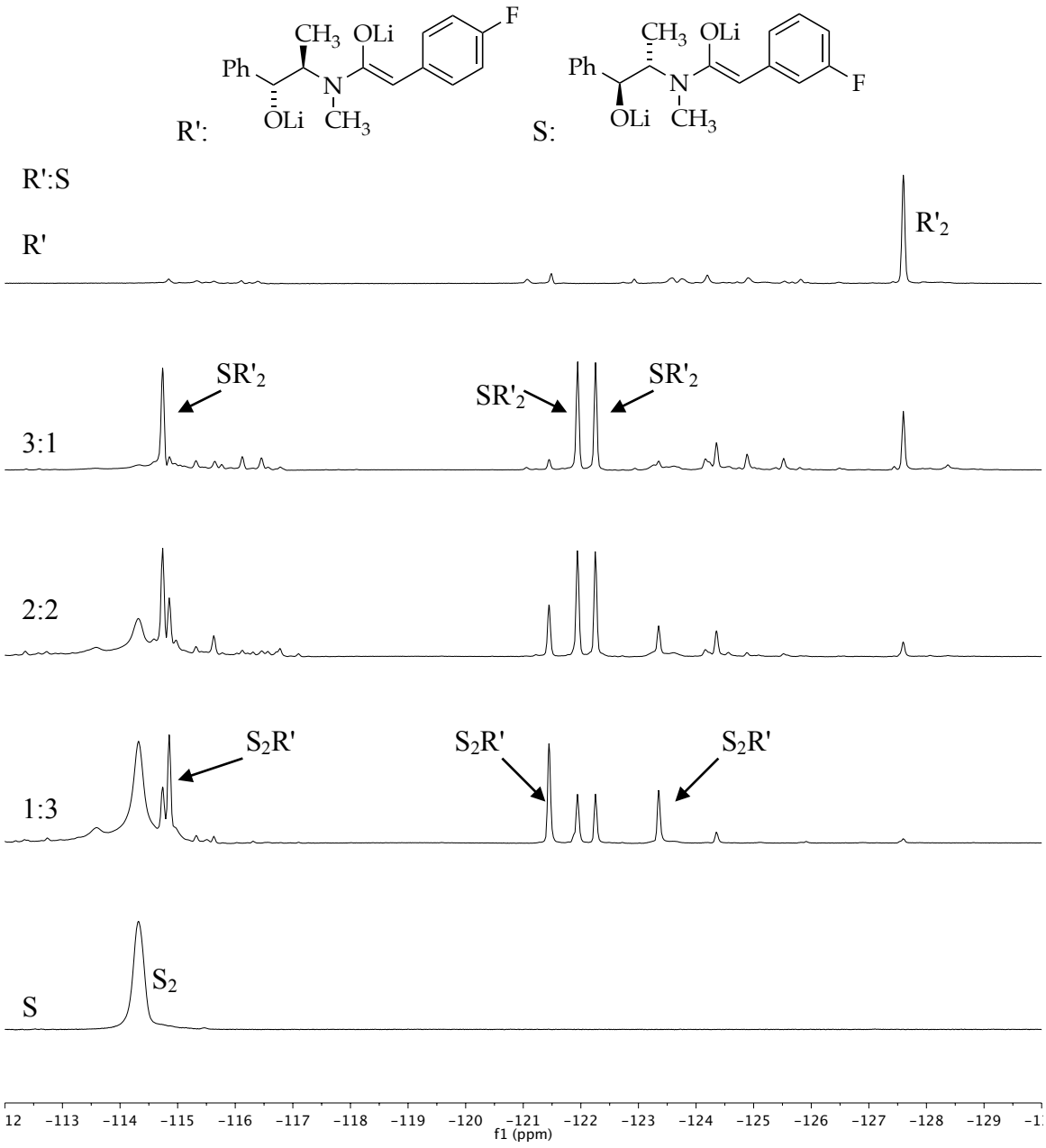


Figure 161. ^{19}F NMR spectra for 0.10 M pre-aged solutions of [^{6}Li]-(*R,R*)-**16** (R') and [^{6}Li]-(*S,S*)-**15** (S) in 12.3 M THF at –80 °C. Six new peaks are found for heteroaggregates. Minor peaks in the spectra come from minor isomers or deaggregated homo/hetero-aggregates.

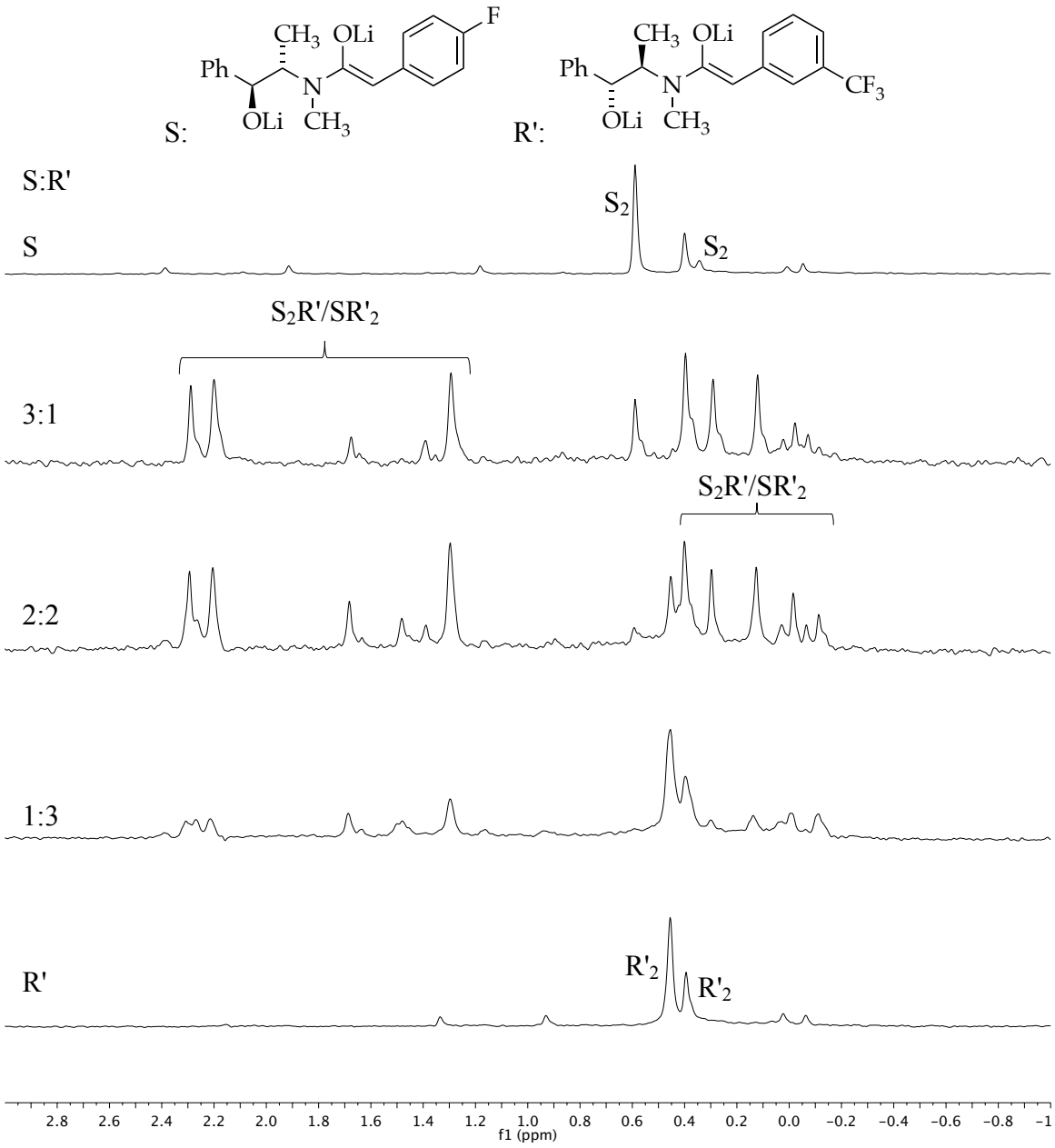


Figure 162. ^{6}Li NMR spectra for 0.10 M pre-aged solutions of [^{6}Li]-(*S,S*)-**16** (S) and [^{6}Li]-(*R,R*)-**17** (R') in 12.3 M THF at –80 °C. T1 relaxation was not optimized for integration. The CF_3 group on the phenyl ring does not provide adequate resolution.

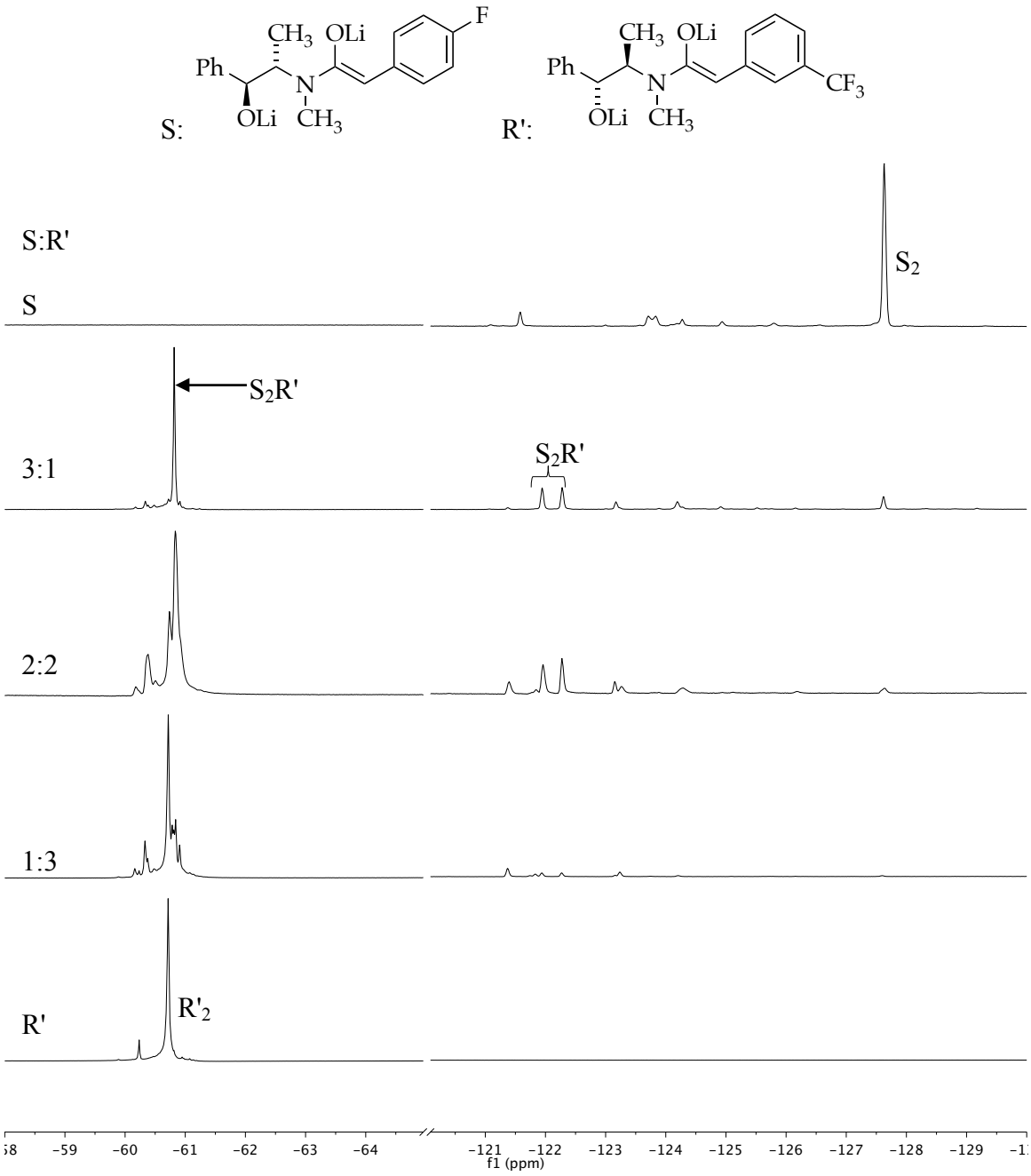


Figure 163. ^{19}F NMR spectra for 0.10 M aged solutions of [^{6}Li]-(*S,S*)-**16** (S) and [^{6}Li]-(*R,R*)-**17** (R') in 12.3 M THF at –80 °C. CF_3 group on phenyl ring does not give adequate resolution.

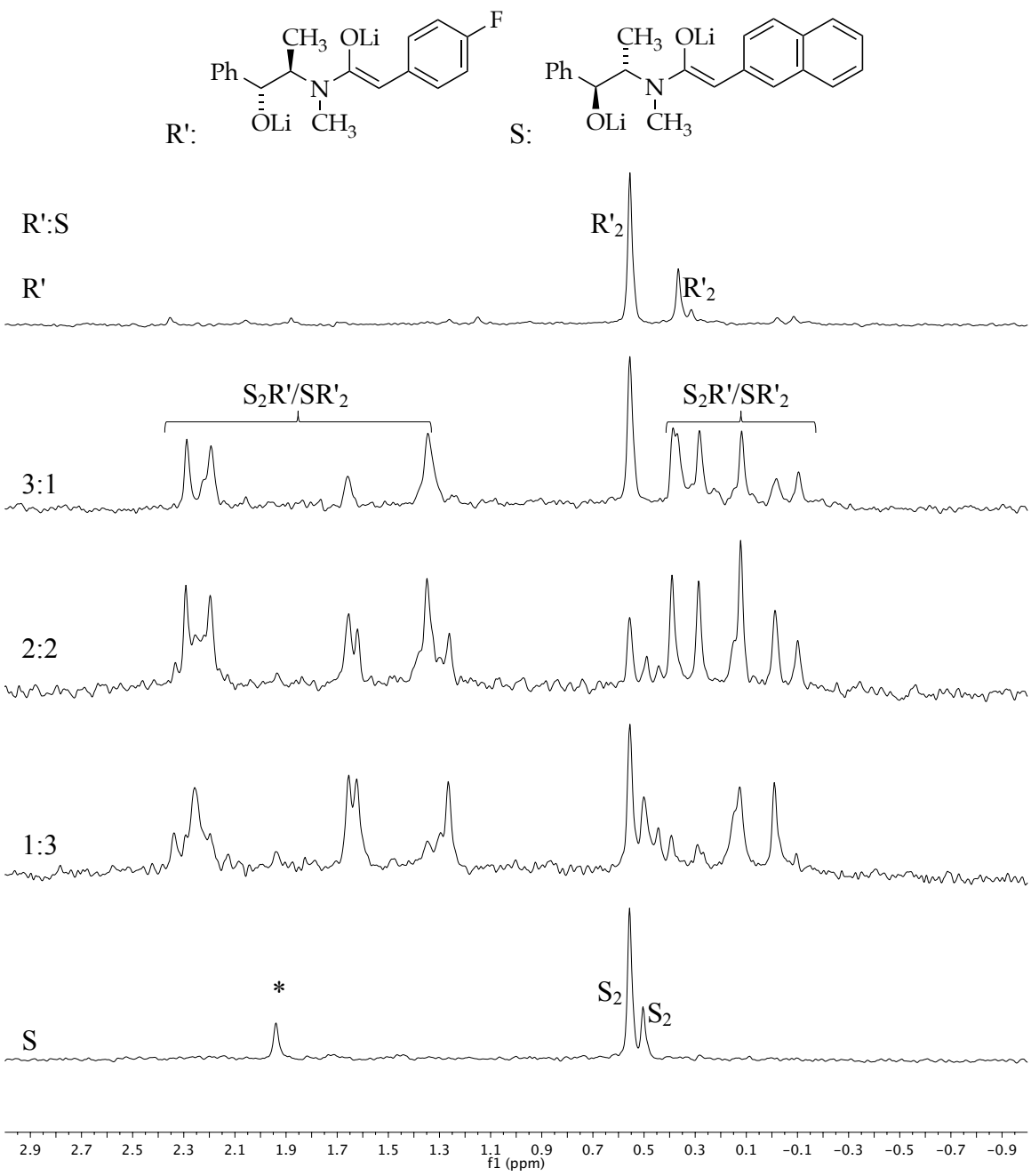


Figure 164. ^{6}Li NMR spectra for 0.10 M aged solutions of [^{6}Li]-(*R,R*)-**16** (R') and [^{6}Li]-(*S,S*)-**18** (S) in 12.3 M THF at –80 °C showing inadequate resolution. T1 relaxation was not optimized for integration. Peak at 1.94 ppm (*) is [^{6}Li]LDA caused by trace amount of extra LDA.

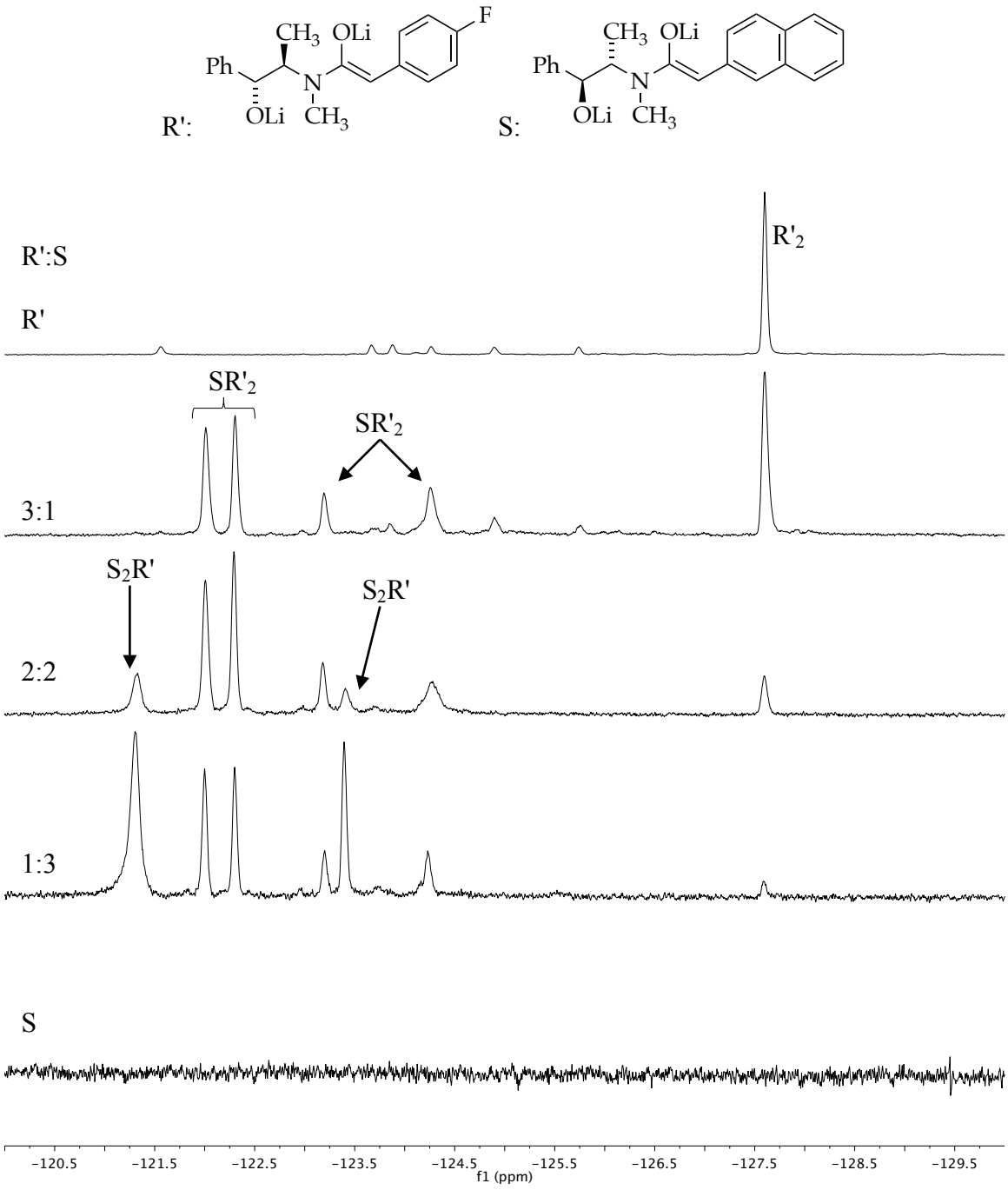


Figure 165. ^{19}F NMR spectra for 0.10 M aged solutions of [^{6}Li]-(*R,R*)-**16** (R') and [^{6}Li]-(*S,S*)-**18** (S) in 12.3 M THF at –80 °C with 0.22 M [^{6}Li]LDA. ^{19}F NMR follows a similar pattern as mixtures of enolates **13** and **16**.

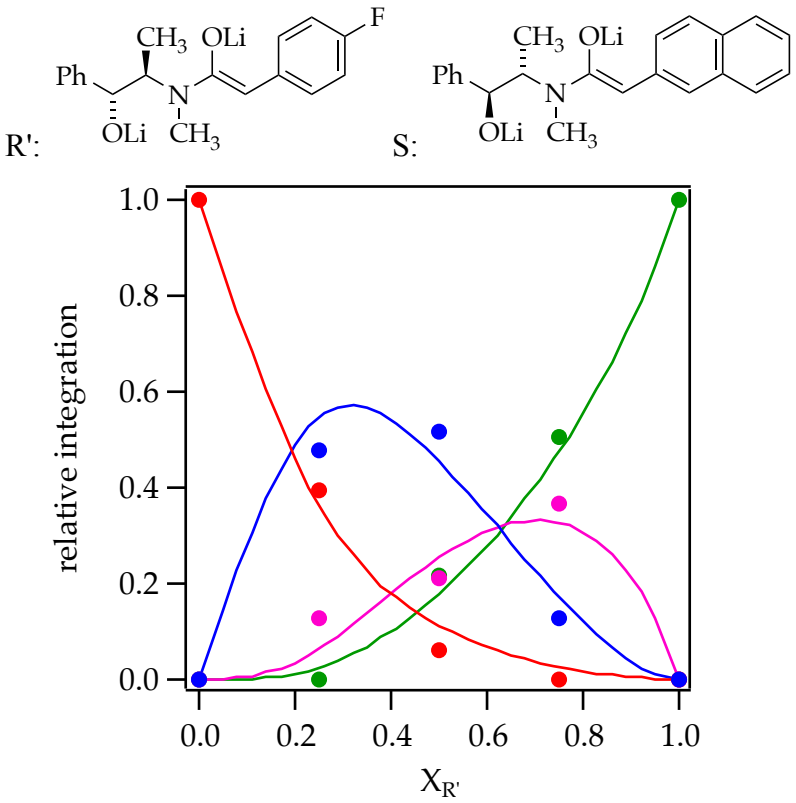


Figure 166. Job plot showing the relative integrations of tetralithio homoaggregates and hexalithio heteroaggregates versus measured mole fractions of [^{6}Li]-(*R,R*)-**16** (R') ($\boldsymbol{X_{R'}}$) for 0.10 M mixtures of lithium enolates [^{6}Li]-(*S,S*)-**18** (S) and [^{6}Li]-(*R,R*)-**16** (R') in neat THF at –80 °C monitored by ^{19}F NMR spectroscopy (See Figure 165). The curves result from a parametric fit to dimer-trimer model. Integration of R'$_2$ is derived from the intended mole fraction.

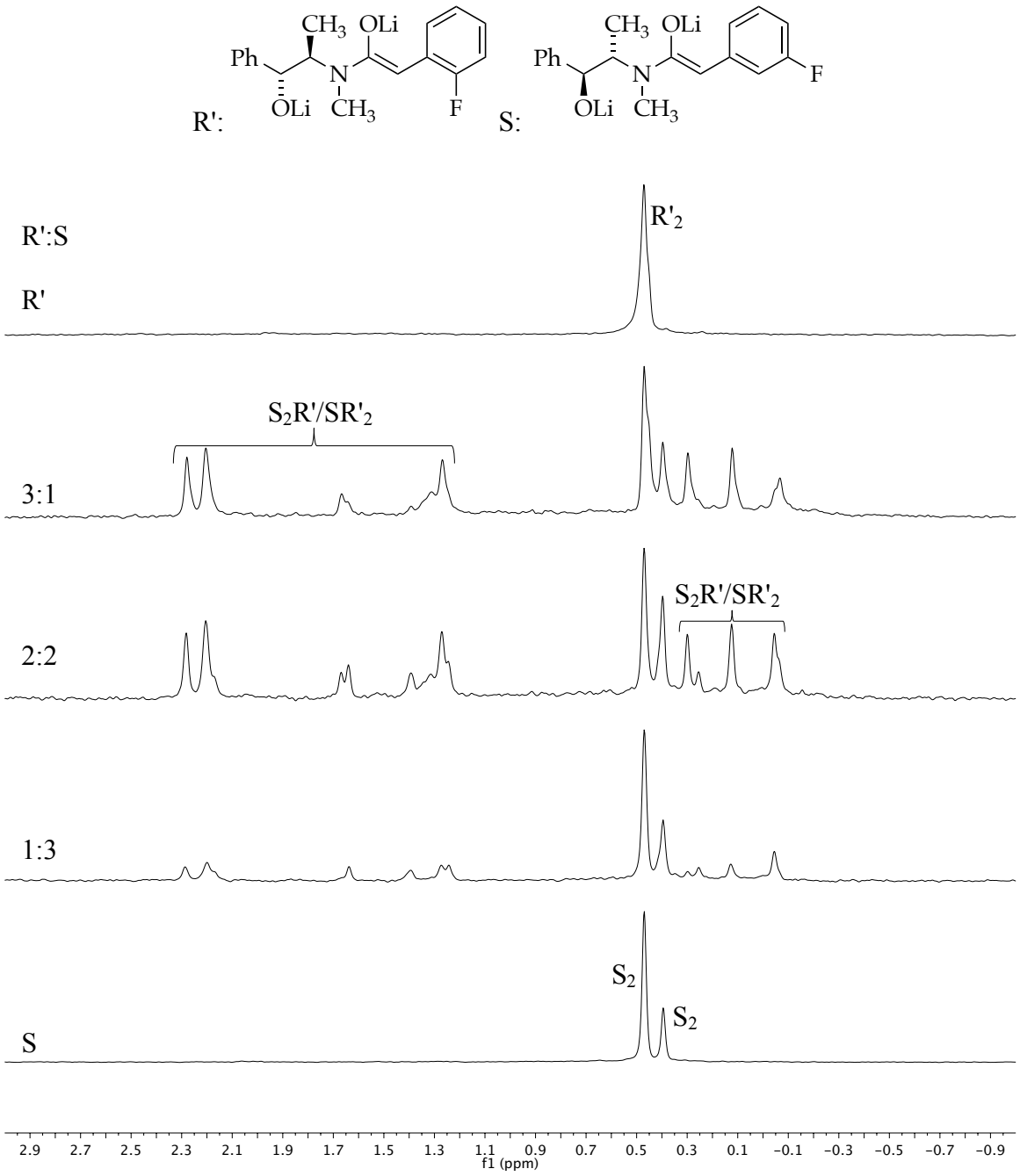


Figure 167. ^{6}Li NMR spectra for 0.10 M aged solutions of [^{6}Li]-(*R,R*)-**14** (R') and [^{6}Li]-(*S,S*)-**15** (S) in 12.3 M THF at –80 °C with 0.22 M [^{6}Li]LDA. T1 relaxation was not optimized for integration. ^{6}Li NMR spectra show overlapping issues.

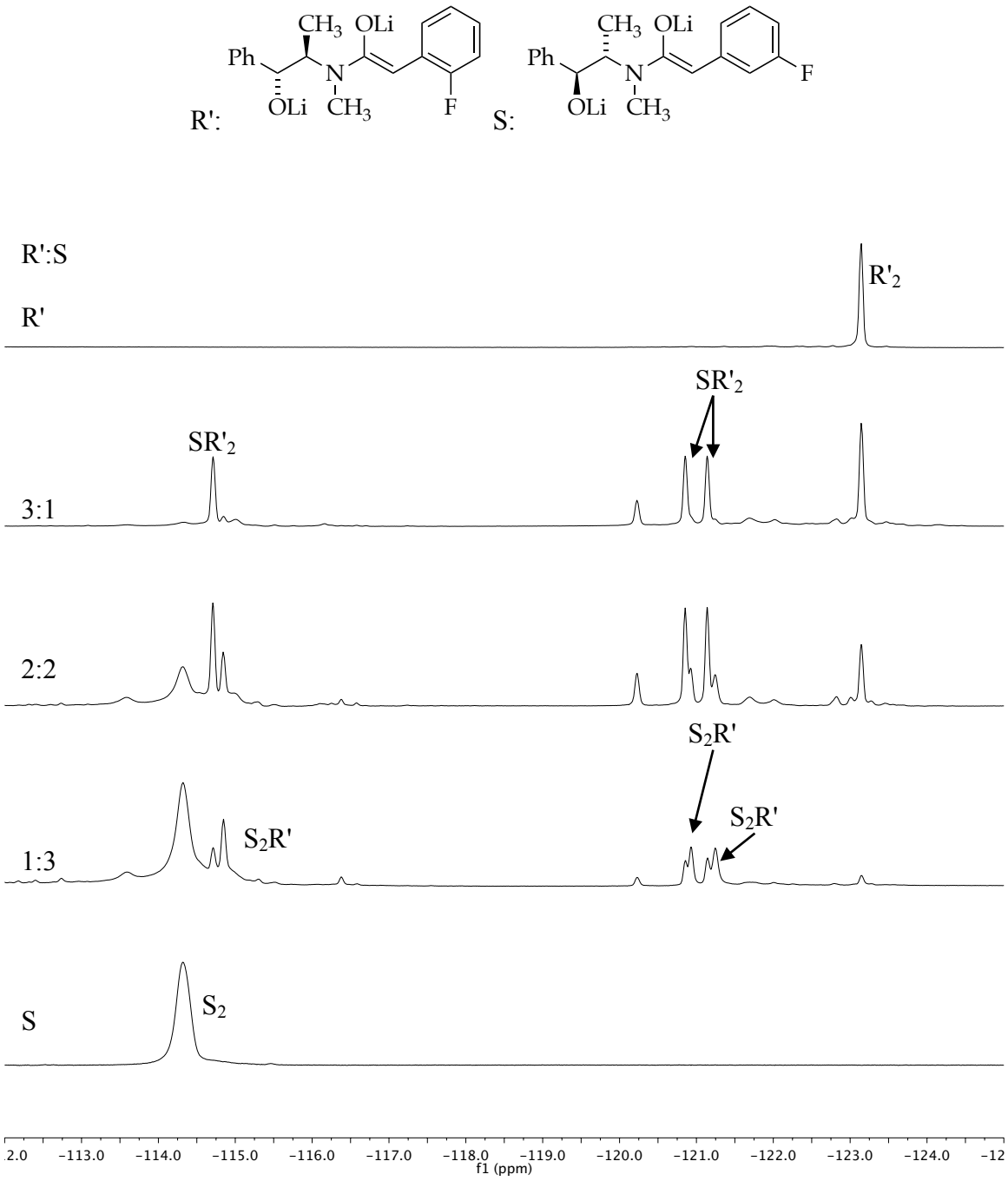


Figure 168. ^{19}F NMR spectra of 0.10 M aged solutions of [^{6}Li]-(*R,R*)-**14** (R') and [^{6}Li]-(*S,S*)-**15** (S) in 12.3 M THF at –80 °C. ^{19}F NMR shows similar patterns as mixtures of enolates **16** and **14**.

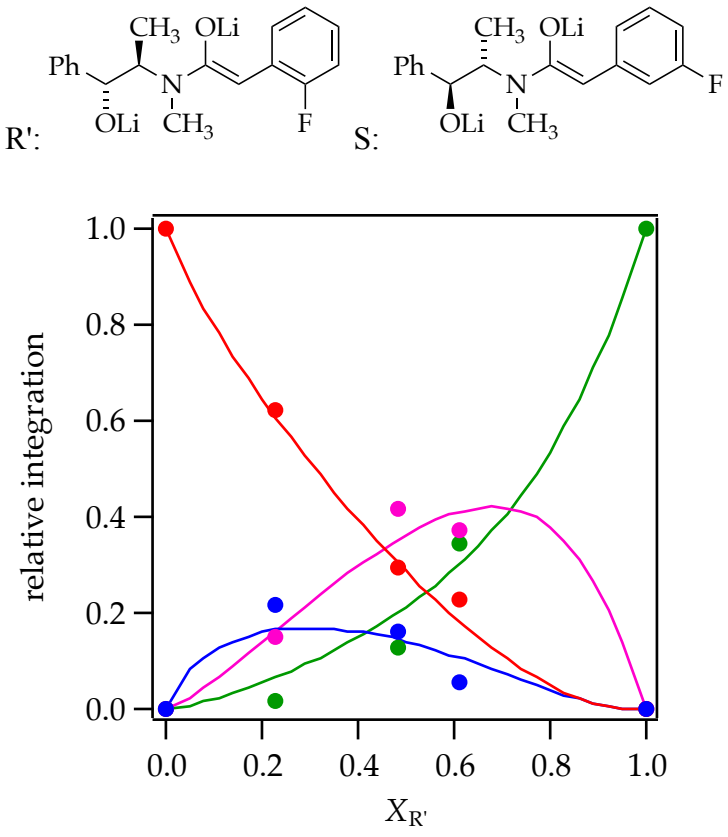


Figure 169. Job plot showing the relative integrations of tetralithio homoaggregates and hexalithio heteroaggregates versus measured mole fractions of [^{6}Li]-(*R,R*)-**14** (R') ($\boldsymbol{X}_{\mathbf{R'}}$) for 0.10 M mixtures of lithium enolates [^{6}Li]-(*S,S*)-**15** (S) and [^{6}Li]-(*R,R*)-**14** (R') in neat THF at –80 °C monitored by ^{19}F NMR spectroscopy (See Figure 168). The curves result from a parametric fit to a dimer-trimer model.

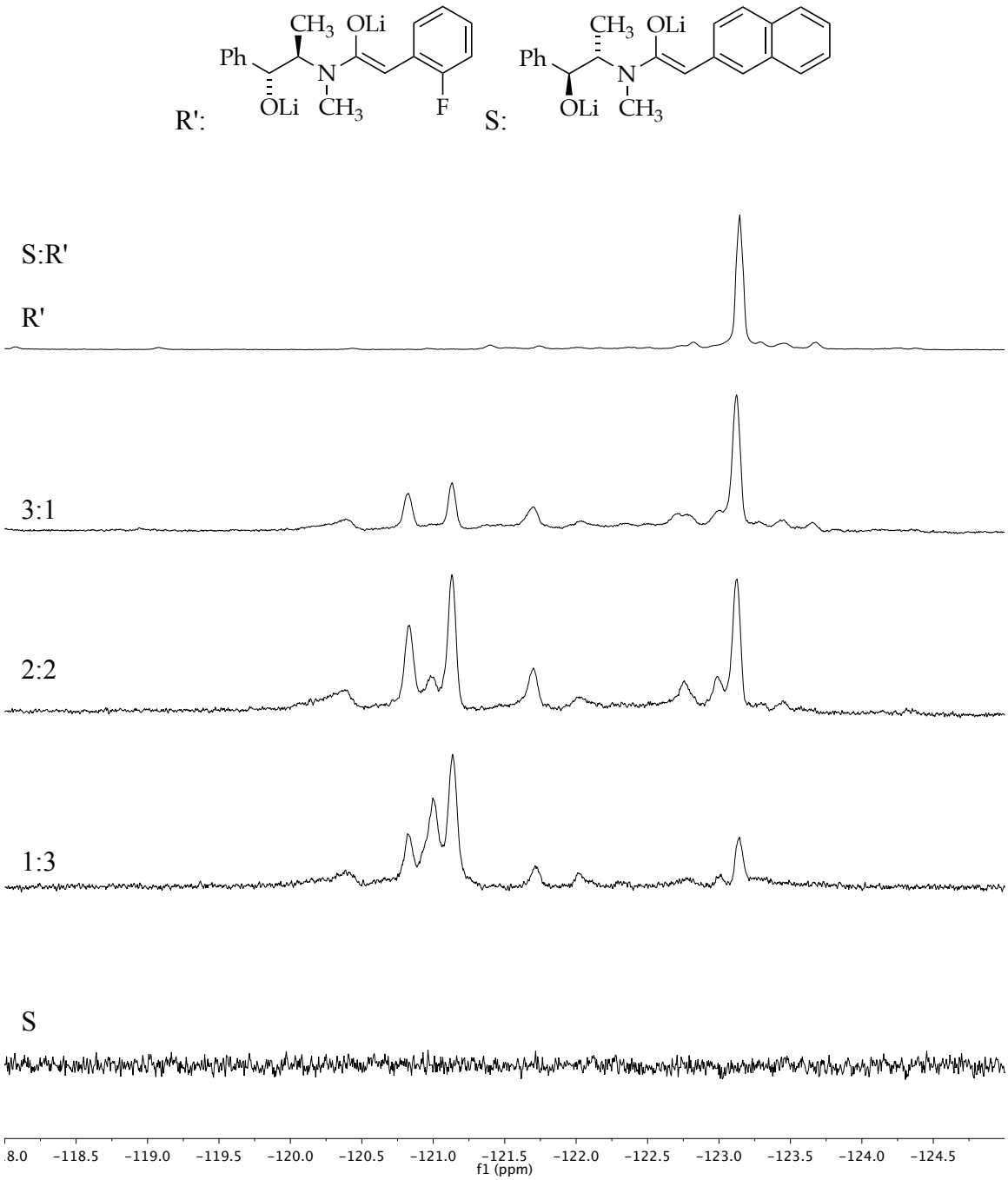


Figure 170. ^{19}F NMR spectra for 0.10 M aged solutions of [^{6}Li]-(*R,R*)-**14** (R') and [^{6}Li]-(*S,S*)-**18** (S) in 12.3 M THF at –80 °C.

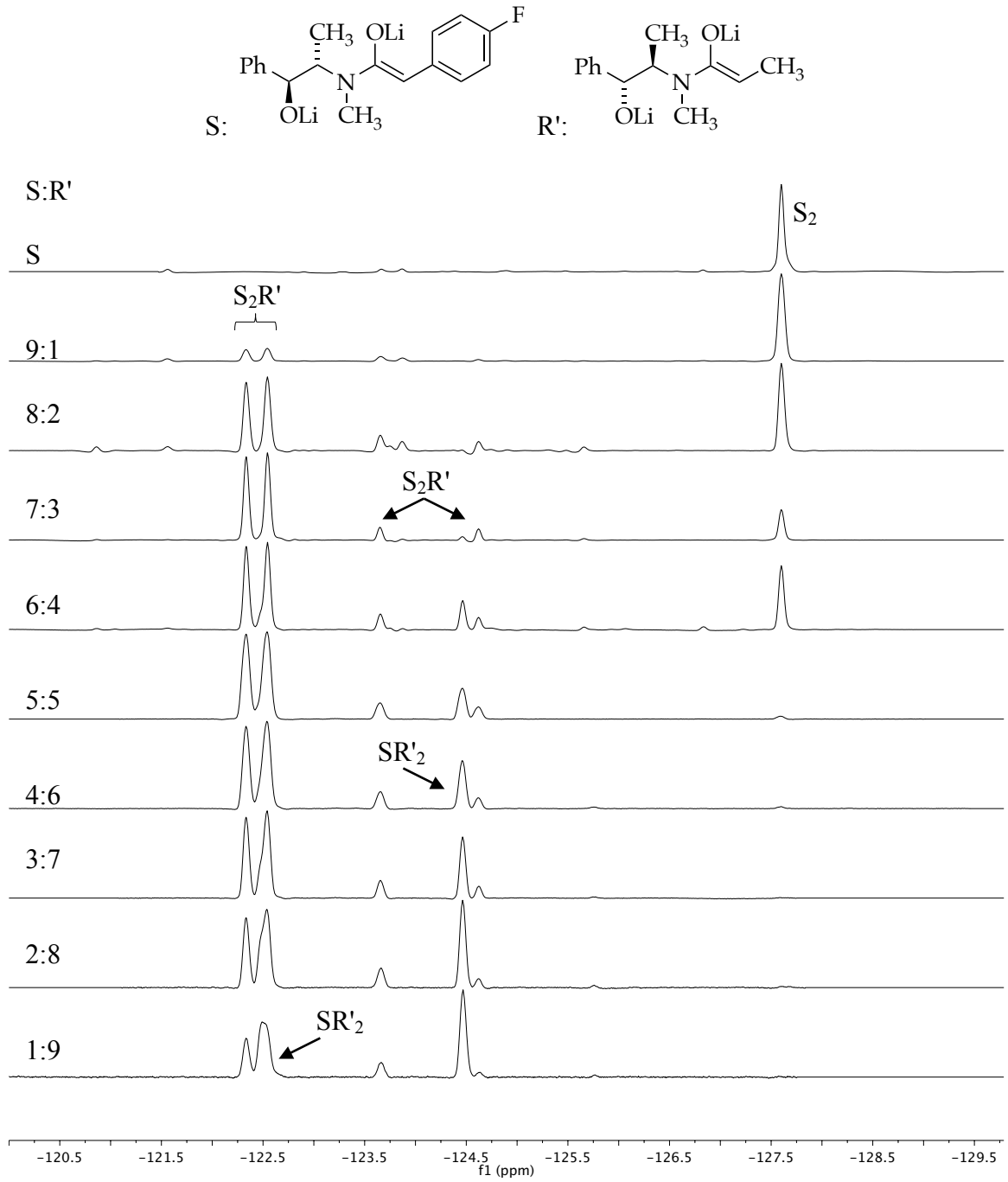


Figure 171. ^{19}F NMR spectra of 0.10 M aged solutions of [^{6}Li]-(*S,S*)-**16** (S) and [^{6}Li]-(*R,R*)-**2** (R') in 12.3 M THF at −80 °C. This experiment shows two new resonances for SR'_2 and four new resonance for S_2R', which proves that the heteroaggregates formed when mixing α-aryl enolates and α-alkyl enolates.

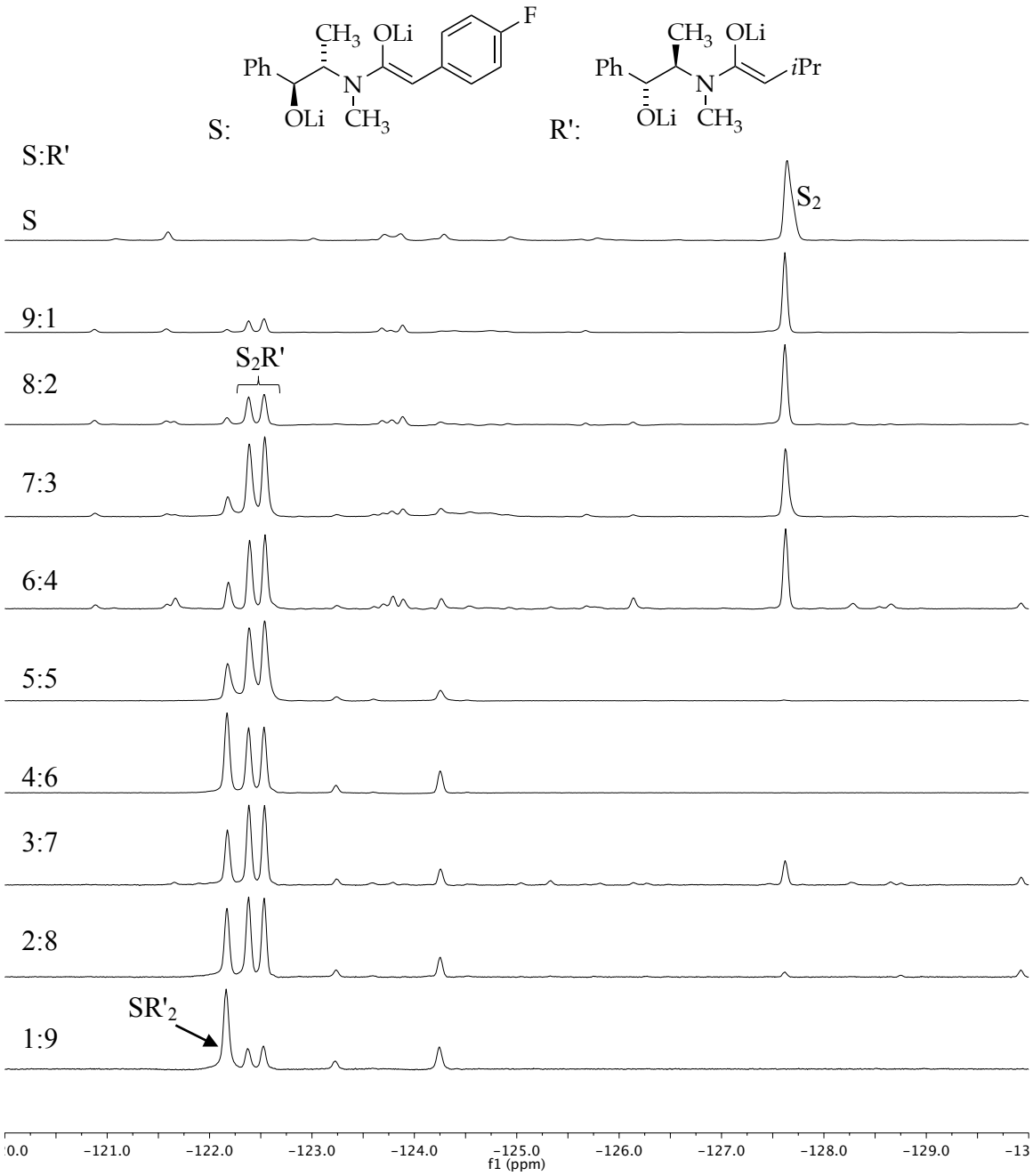


Figure 172. ^{19}F NMR spectra of 0.10 M aged solutions of [^{6}Li]-(*S,S*)-**16** (S) and [^{6}Li]-(*R,R*)-**9** (R') in 12.3 M THF at −80 °C. This experiment shows one new resonance for SR'_2 and two new resonance for S_2R', which proves that the heteroaggregates formed when mixing α-aryl enolates and α-alkyl enolates similar to mixing enolates **16** and **2**.

Part 4. LDA-mixed Aggregate Characterization

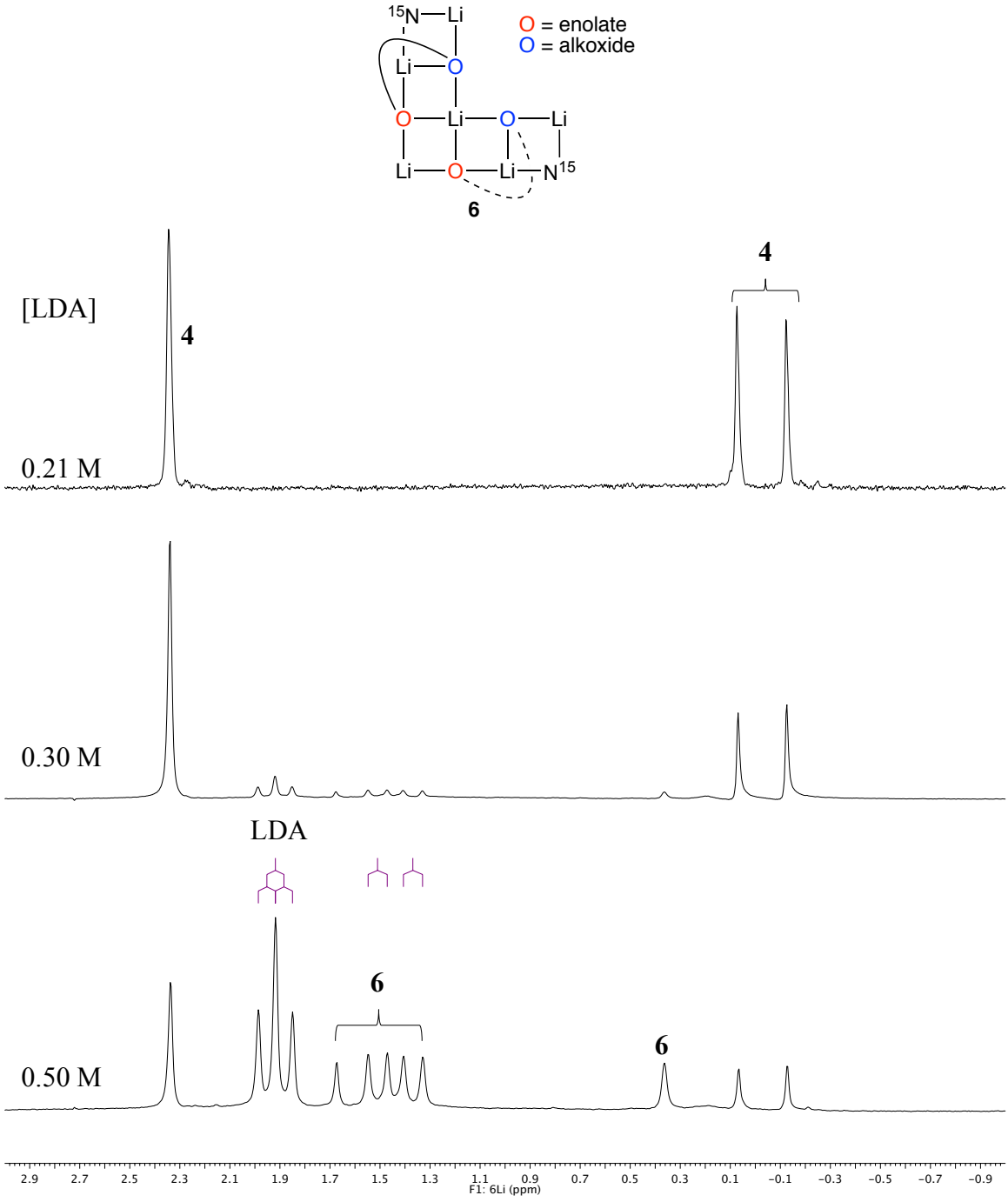


Figure 173. ^{6}Li NMR spectra of a pre-aged solution of 0.10 M (*S,S*)-**1** in neat THF at –80 °C with varying [^{6}Li,^{15}N]LDA concentrations. As a control experiment, extra LDA was added to enolate, and LDA-mixed aggregates were formed.

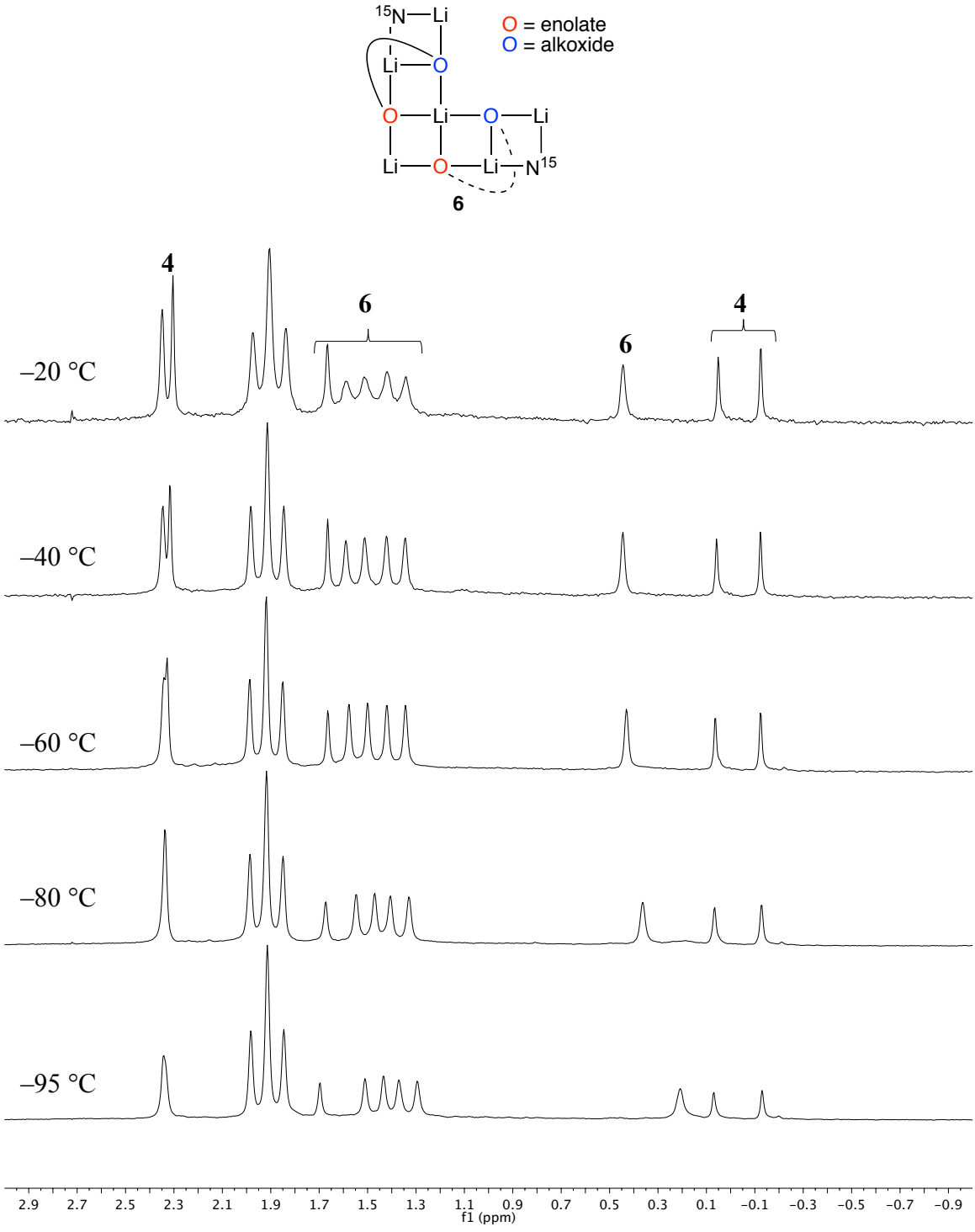


Figure 174. ^{6}Li NMR spectra of a pre-aged solution of 0.10 M (*S,S*)-**1** in neat THF with 0.50 M [^{6}Li,^{15}N]LDA at varying temperature. T1 relaxation was not optimized for integration. No obvious change was detected.

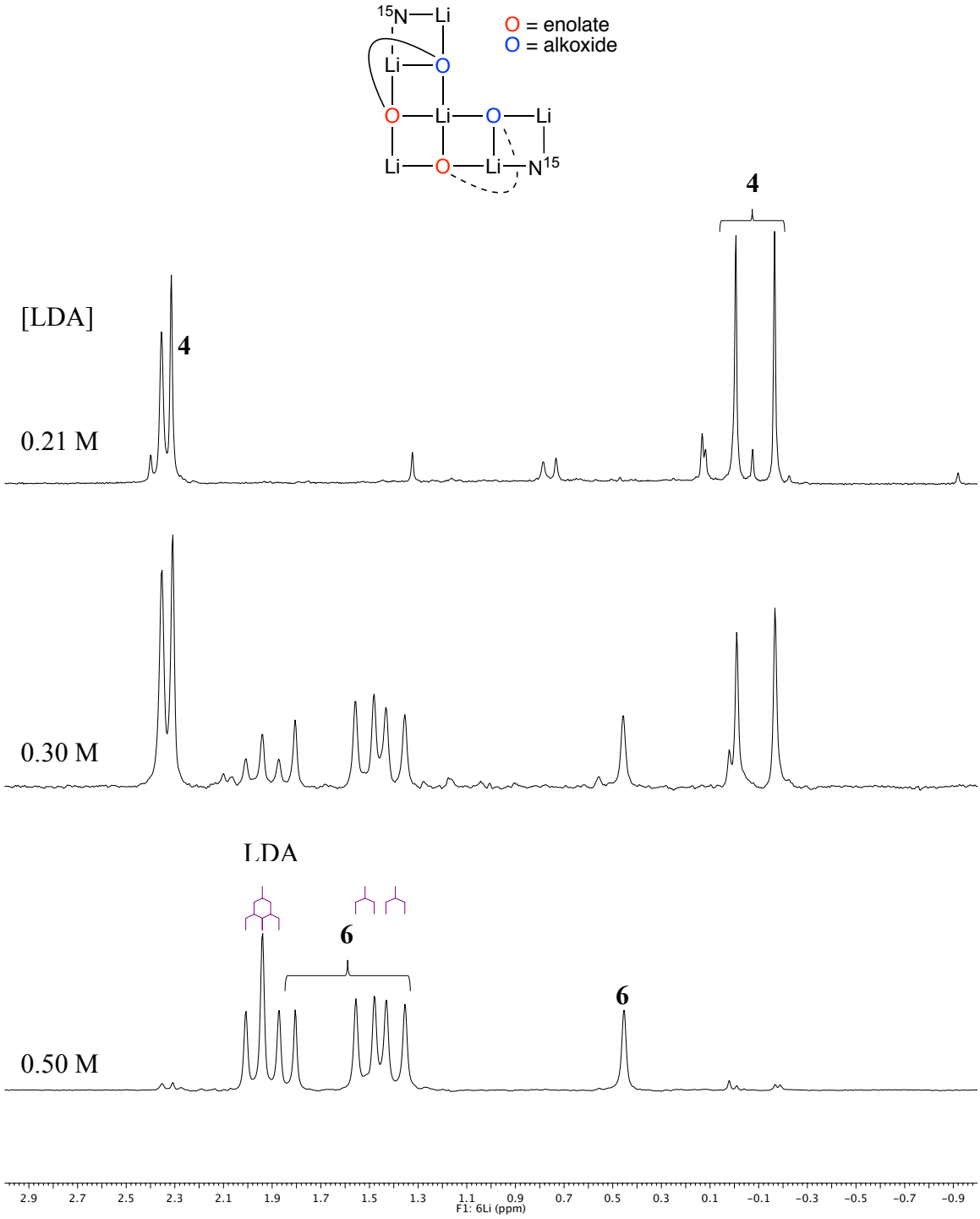


Figure 175. ^{6}Li NMR spectra of a pre-aged solution of 0.10 M (*S,S*)-**4** in neat THF at –80 °C with varying [^{6}Li,^{15}N]LDA concentrations. As a control experiment, extra LDA was added to enolate, and LDA-mixed aggregates were formed.

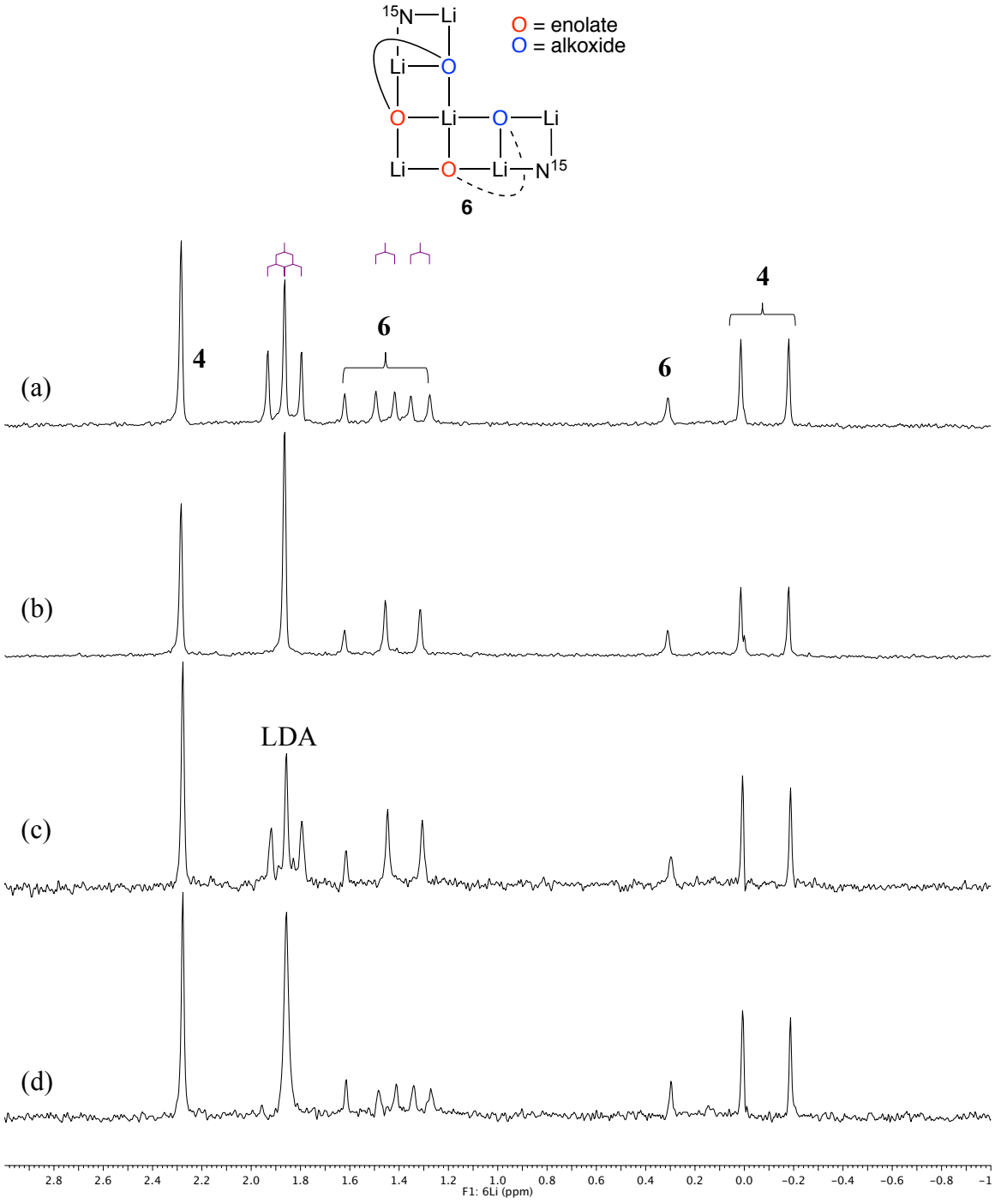


Figure 176. ^{6}Li NMR spectra of a pre-aged solution of 0.10 M (*S,S*)-**1** in neat THF at –80 °C with 0.40 M [^{6}Li,^{15}N]LDA, (a) direct detect, δ 1.86 ppm (t, *J* = 5.02 Hz), 1.46 ppm (d, *J* = 5.45 Hz), 1.32 ppm (d, *J* = 5.45 Hz); (b) broadband decoupling; (c) selective ^{15}N decoupling at 81.2 ppm; (d) selective ^{15}N decoupling at 78.2 ppm. T1 relaxation was not optimized for integration. Two different kinds of lithium atoms (1.46 ppm and 1.32 ppm) are coupled to the same nitrogen atom (81.2 ppm).

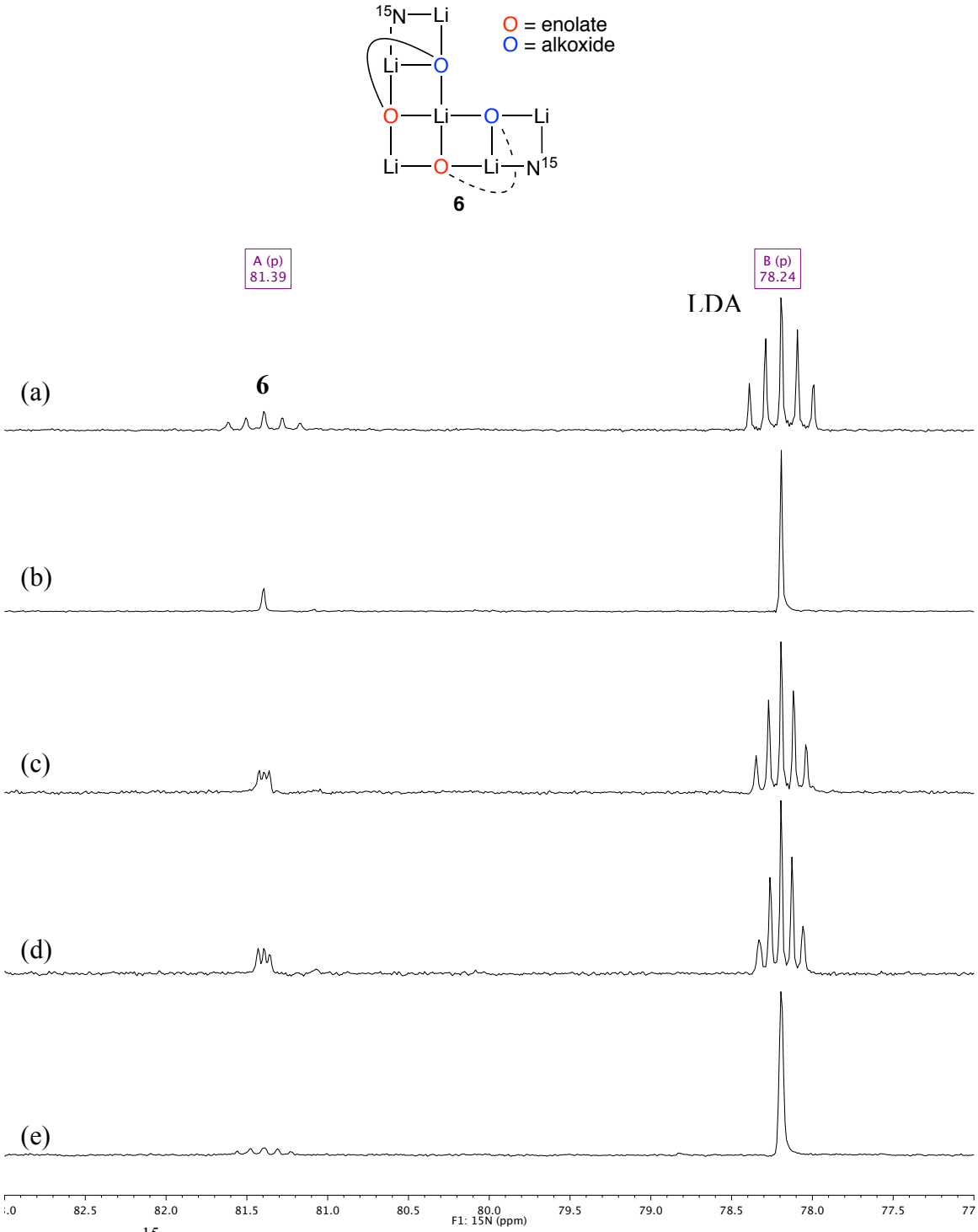


Figure 177. ^{15}N NMR spectra of a pre-aged solution of 0.10 M (*S,S*)-**1** in neat THF at –80 °C with 0.40 M [^{6}Li,^{15}N]LDA: (a) direct detect, δ 81.4 ppm (quintet, J = 5.45 Hz), 78.2 ppm (quintet, J = 5.02 Hz); (b) broadband decoupling; (c) selective ^{6}Li decoupling at 1.46 ppm ; (d) selective ^{6}Li decoupling at 1.32 ppm; (e) selective ^{6}Li decoupling at 1.86 ppm. T1 relaxation was not optimized for integration. Two different kinds of lithium atoms (1.46 ppm and 1.32 ppm) are coupled to the same nitrogen atom (81.4 ppm).

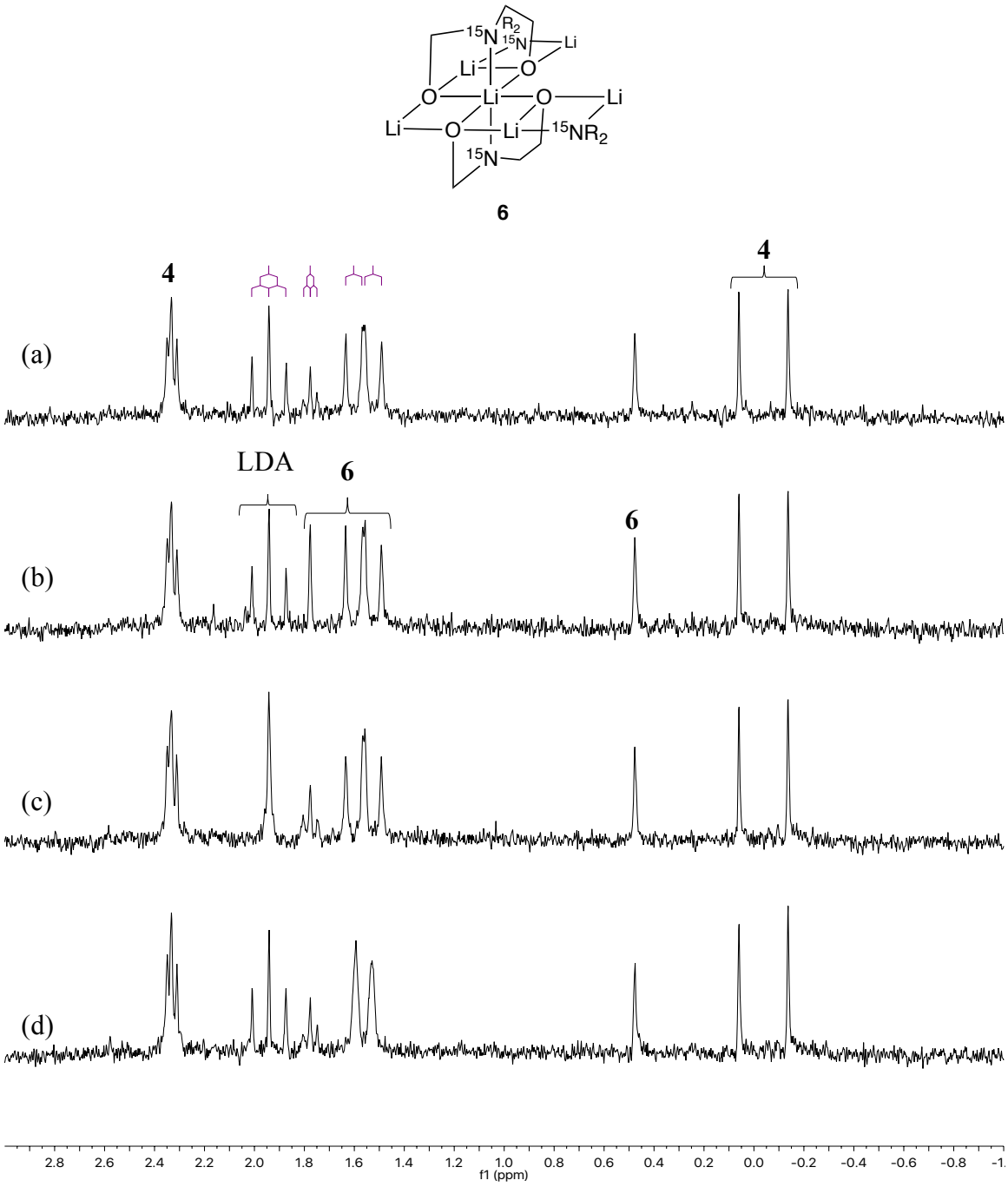


Figure 178. ^{6}Li NMR spectra of a pre-aged solution of 0.050 M [^{15}N]-(*S,S*)-**1** in 2.0 M THF and 7.9 M toluene at –80 °C with 0.40 M [^{6}Li,^{15}N]LDA, (a) no decoupling; (b) selective ^{15}N decoupling at 63.4 ppm; (c) selective ^{15}N decoupling at 78.2 ppm; (d) selective decoupling ^{15}N signal at 81.4 ppm. The middle lithium atom is coupled to two nitrogen atoms.

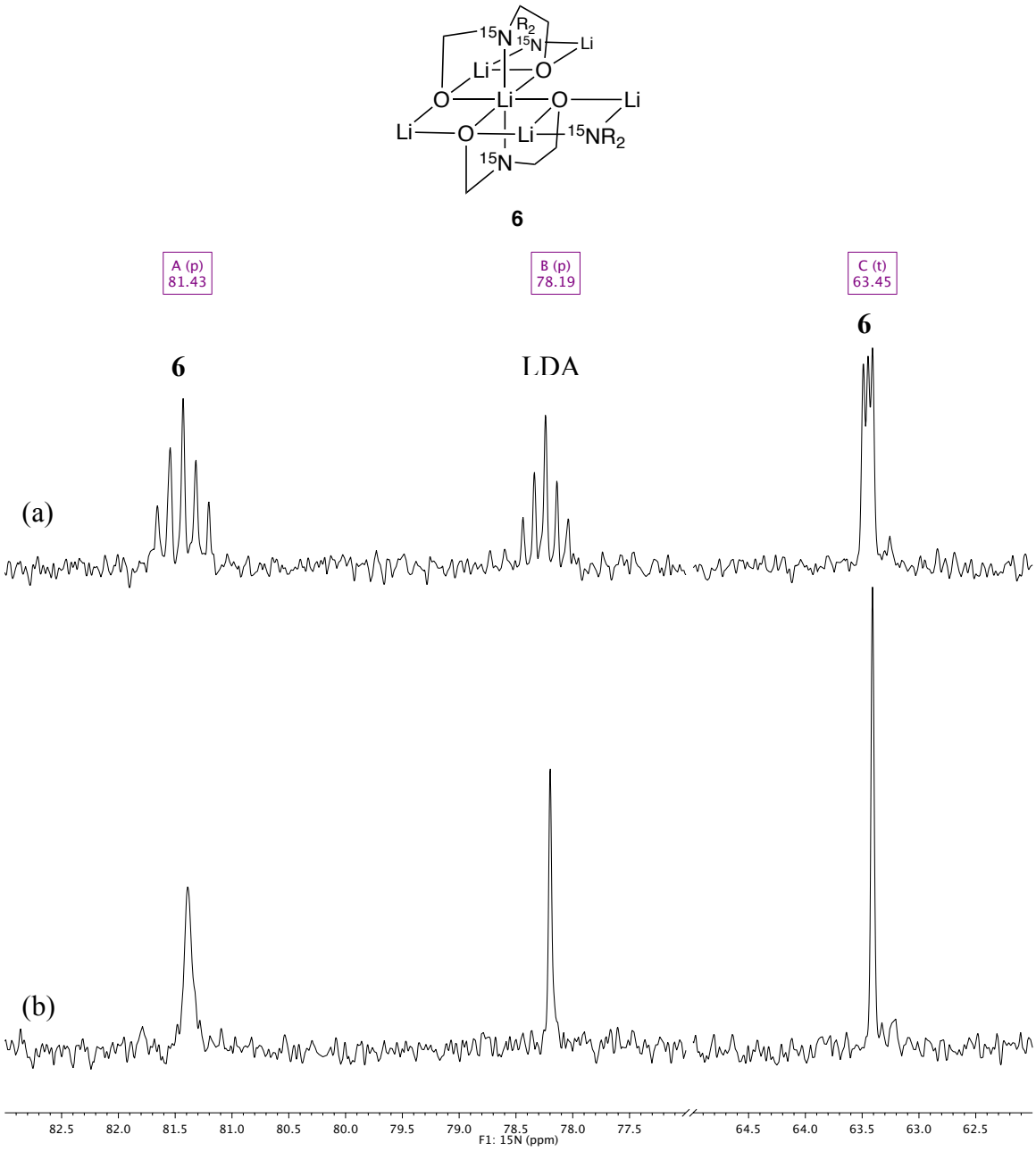


Figure 179. ^{15}N NMR spectra of a pre-aged solution of 0.050 M [^{15}N]-(*S,S*)-**1** in 2.0 M THF and 7.9 M toluene at –80 °C with 0.40 M [^{6}Li,^{15}N]LDA, (a) no decoupling, (b) broadband decoupling.

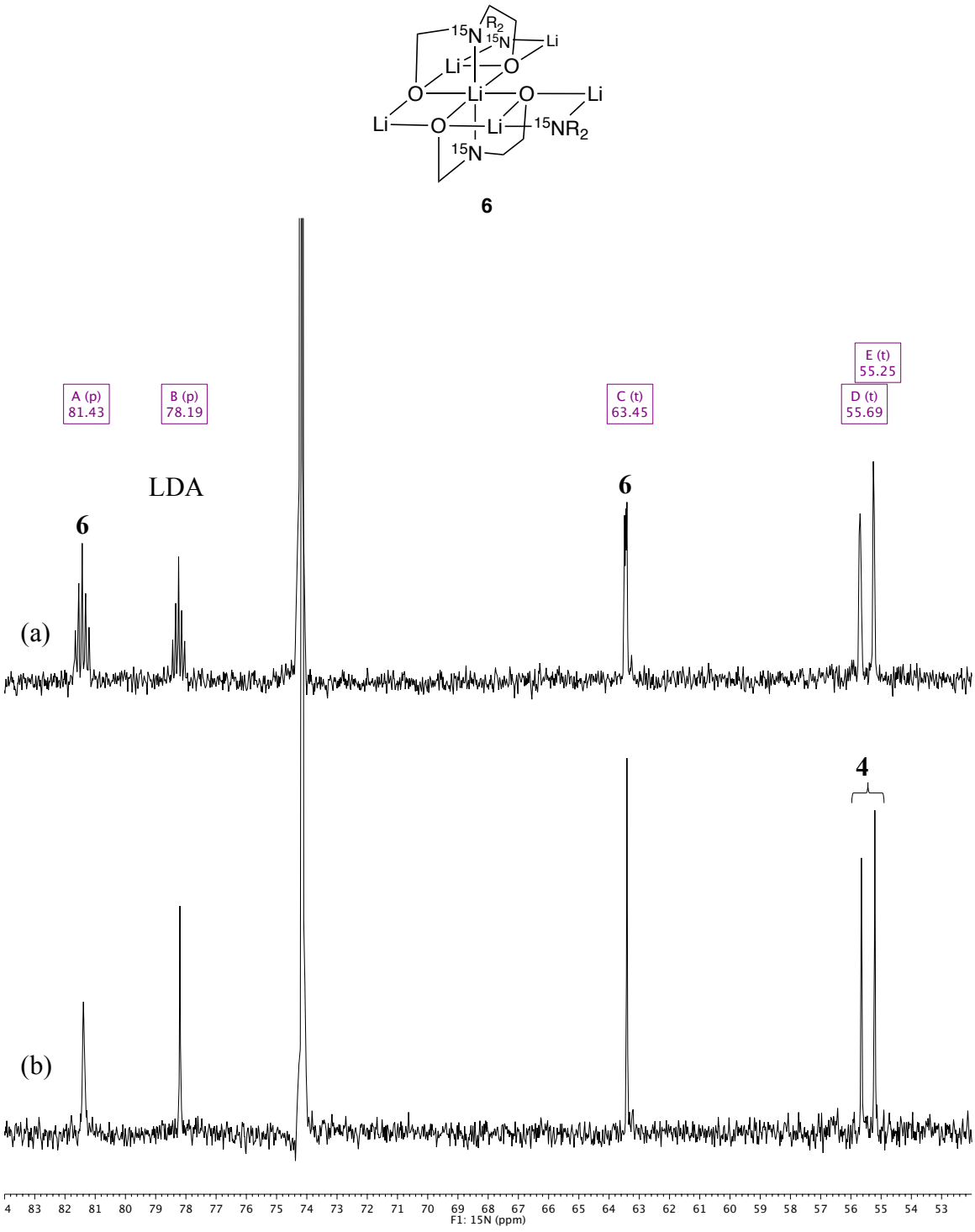


Figure 180. Full spectra of ^{15}N NMR spectra of 0.050 M [^{15}N]-(*S,S*)-**1** in 2.0 M THF and 7.9 M toluene at –80 °C with 0.40 M [^{6}Li,^{15}N]LDA: (a) no decoupling; (b) broadband decoupling.

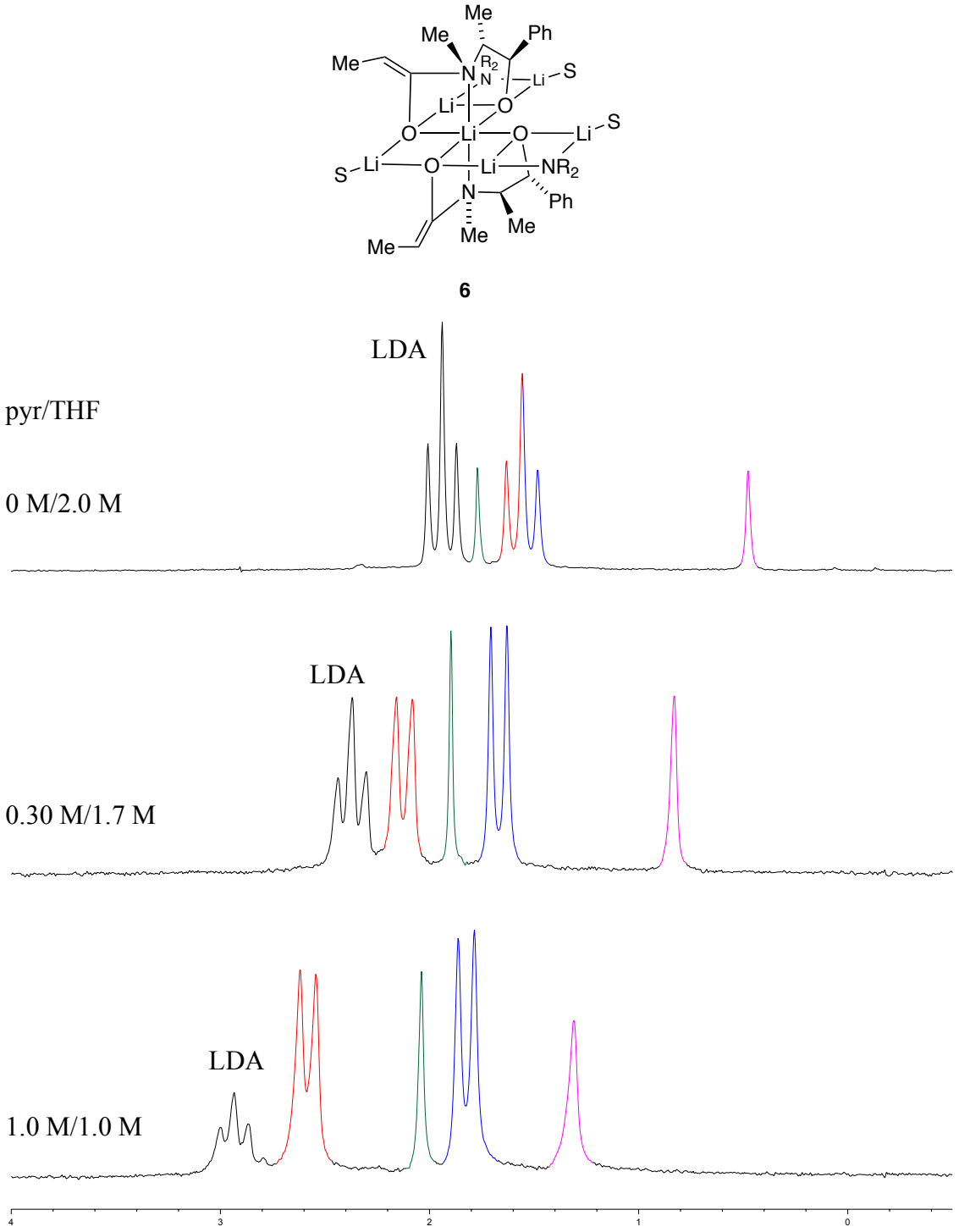


Figure 181. ^{6}Li NMR spectra of a pre-aged solution of 0.10 M (*S,S*)-**1** in toluene at –80 °C with 0.40 M [^{6}Li, ^{15}N]LDA and varying pyridine and THF concentrations. All six peaks from the LDA-mixed aggregates are shifted by pyridine. Lithium atom at 0.76 ppm (magenta) and 1.60 ppm (red) show greater shifts than lithium atom at 1 52ppm (blue) and 1.77ppm (green) owing to direct coordination by pyridine.

2D NMR analysis of 1:1 LDA mixed aggregates: A sample prepared from 0.40 M [^{6}Li]LDA, 0.010 M **(*S*,*S*)-1** in 2.0 M THF-d_8 and 7.9 M toluene-d_8, after aging at 25 °C for 10 min, was studied by standard 2D NMR techniques. All chemical shifts with the exception of C-1, C-2, C-3, C-4, C-5, C-6 were assigned using high field indirect-resolution 2D HSQC, and HMBC experiments.

Experimental: 2D NMR spectra were acquired on a 500 MHz Varian INOVA spectrometer operating at 499.92 MHz for ^{1}H observation using a 5 mm Varian inverse-detect probehead with Z-axis pulsed field-gradient. Sample temperature was maintained at –80 °C as calibrated with a neat methanol sample. ^{1}H and ^{13}C chemical shifts were referenced to the residual downfield toluene-d_7 resonance at 2.09 ppm and 20.40 ppm, respectively. 2D experiments were acquired using standard pulse sequences supplied in VnmrJ 3.2A (Agilent Inc.) and processed and analyzed in MestReNova 11.0.3 (Mestrelab Research S.L.).

Determination of the 3D aggregate structure: The 2D experiment shows that in the LDA-mixed aggregates, the ratio between enolate and LDA is 1:1. The 3D structure of the aggregate was derived from 2D ROESY (reported as H–H correlations). Only one enolate subunit was detected in the 2D NMR. The enolate is in the Z configuration based on the strong nOe correlation between H-13 and H-12. The starting point for solving the structure is H-12 gives nOe correlations to H-1, H-3, H-6 which indicate phenyl group is on the convex face. With the study of labeled base and labeled substrate, a molecule with C2 axis was confirmed.

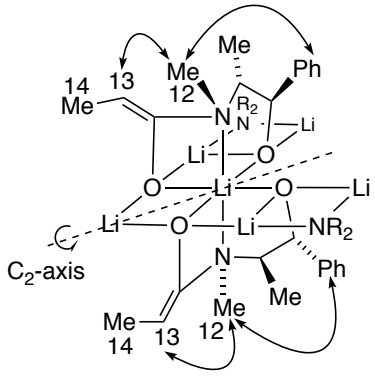


Table 3. [1]H and [13]C chemical shift assignments for LDA-mixed aggregates at –80 °C.

Atom	δC, ppm	δH, ppm	HMBC[1]	COSY[1]	ROESY
1 C	128.8	6.98	2,3,6	6	5
2 C	125.06	7.04	1,6		
3 C	126.20	6.99	1,5		5
4 C	148.46	–	6,7		
5 C[2]	–	6.96	3,7	6	1,3,6,7,8,10,20,21,24,25
6 C	127.92	7.12	1,2,4	1,5	5,24,25
7 C	78.31	4.72	4,5,8,10	8	5,8,10,12,21,22
8 C	59.29	4.23	7,10	7,10	5,7,10,24,25
10 C	10.40	0.68	7,8	8	5,7,8,12
11 C	160.65	–	13,14		
12 C	21.06	2.11			7,10,13
13 C	69.34	3.59	11,14	14	12,14
14 C	11.84	1.86	11,13	13	13,21,22
20 C	48.91	3.75	21,23	21,22	5,21,22,24,25
21 C	27.38	1.69	20	20	5,7,14,20,22,23
22 C	25.62	1.49	23	20	7,14,20,21,23
23 C	49.02	3.59	20,25	24,25	21,22,24,25
24 C[2]	–	1.33		23	5,6,8,20,23
25 C[2]	–	1.30	23	23	5,6,8,20,23

[1]HSQC correlations were omitted from the assignment table.[2]Not determined

	Parameter	Value
1	Experiment	1D
2	Pulse Sequence	s2pul
3	Solvent	toluene
4	Temperature	-80.0
5	Number of Scans	1
6	Receiver Gain	12
7	Relaxation Delay	6.0000
8	Nucleus	1H
9	Spectrometer Frequency	499.92
10	Spectral Width	4101.1
11	Lowest Frequency	-118.1
12	Acquired Size	8192
13	Spectral Size	65536

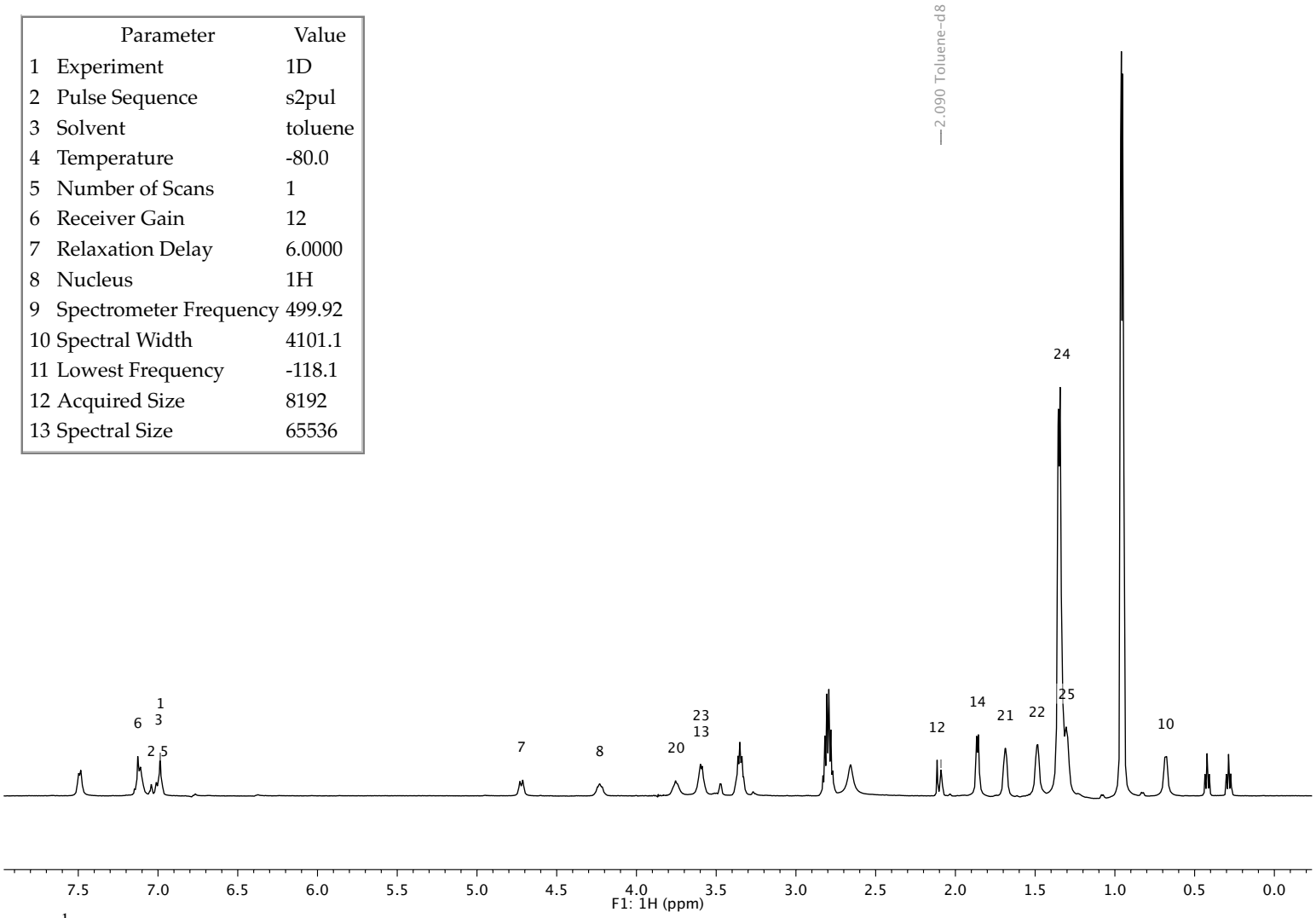


Figure 182. ^{1}H NMR spectrum of a pre-aged solution prepared from 0.10 M (*S,S*)-**1** in 2.0 M THF-d_8 and 7.9 M toluene-d_8 at –80 °C with 0.40 M [^{6}Li]LDA. Labels indicate assignments by 2D NMR.

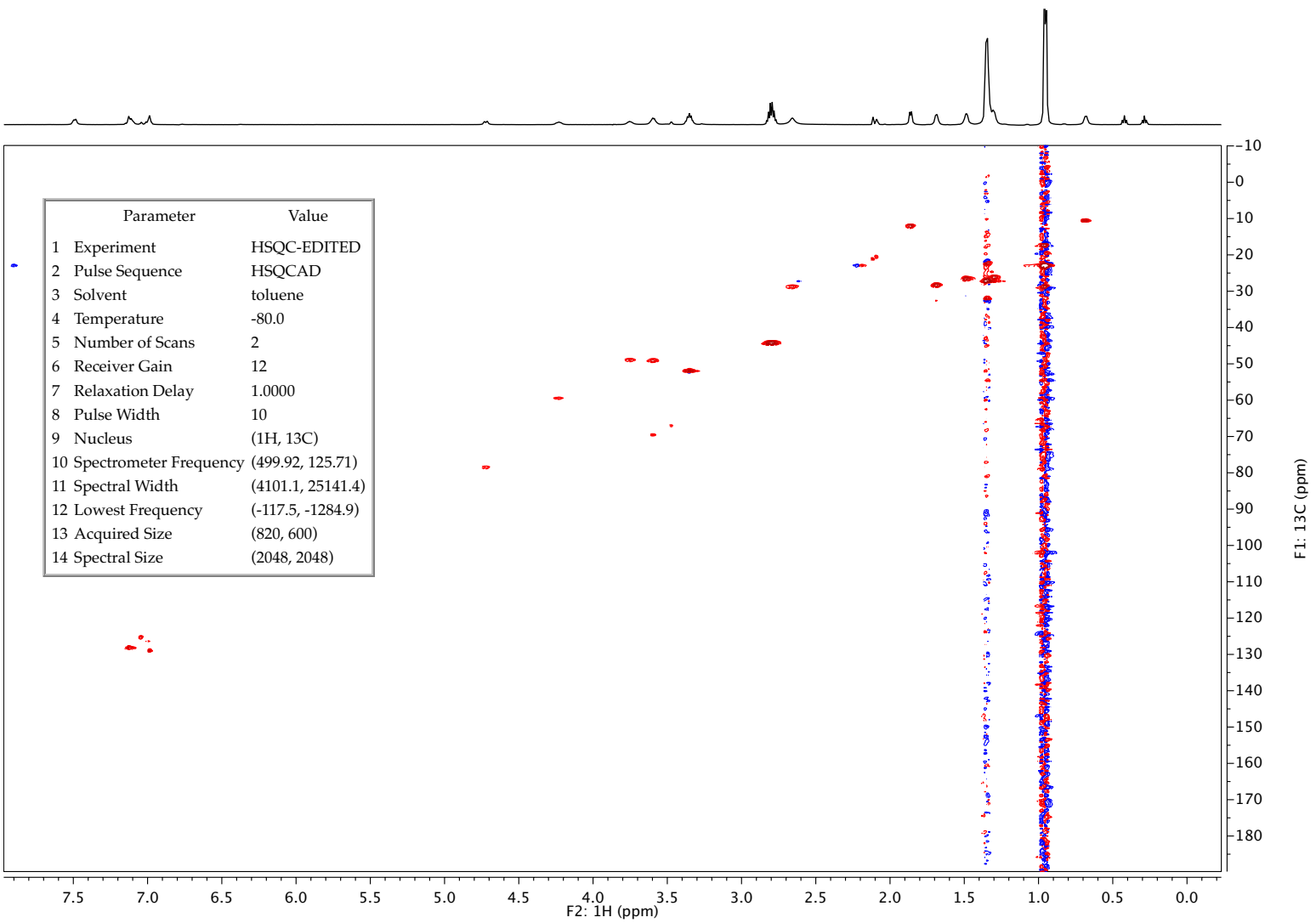


Figure 183. Full-display HSQC spectrum of a pre-aged solution prepared from 0.10 M (*S,S*)-**1** in 2.0 M THF-d_8 and 7.9 M toluene-d_8 at –80 °C with 0.40 M [^{6}Li]LDA.

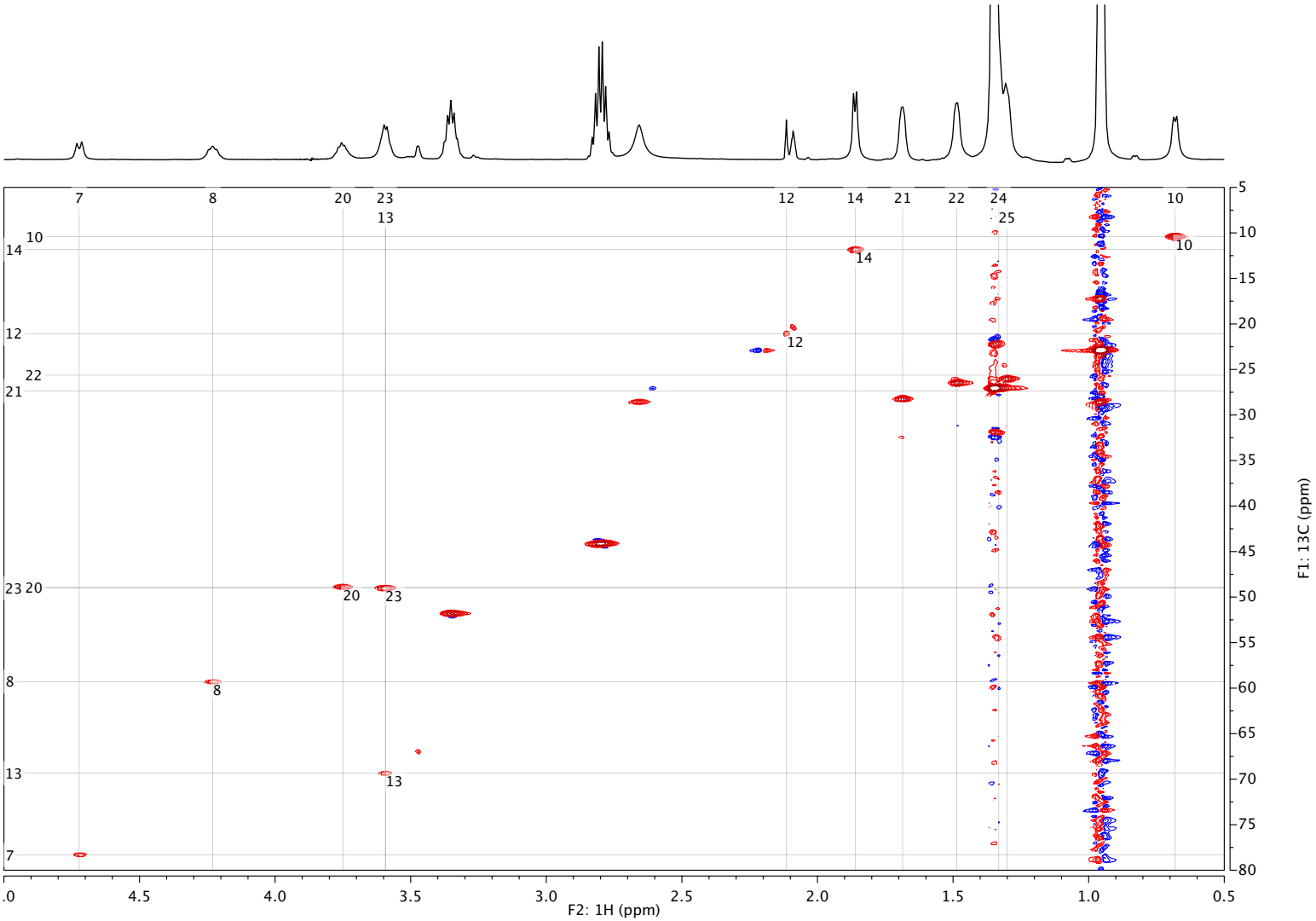


Figure 184. Expansion of the HSQC spectrum of a pre-aged solution prepared from 0.10 M (*S,S*)-**1** in 2.0 M THF-d_8 and 7.9 M toluene-d_8 at –80 °C with 0.40 M [^{6}Li]LDA.

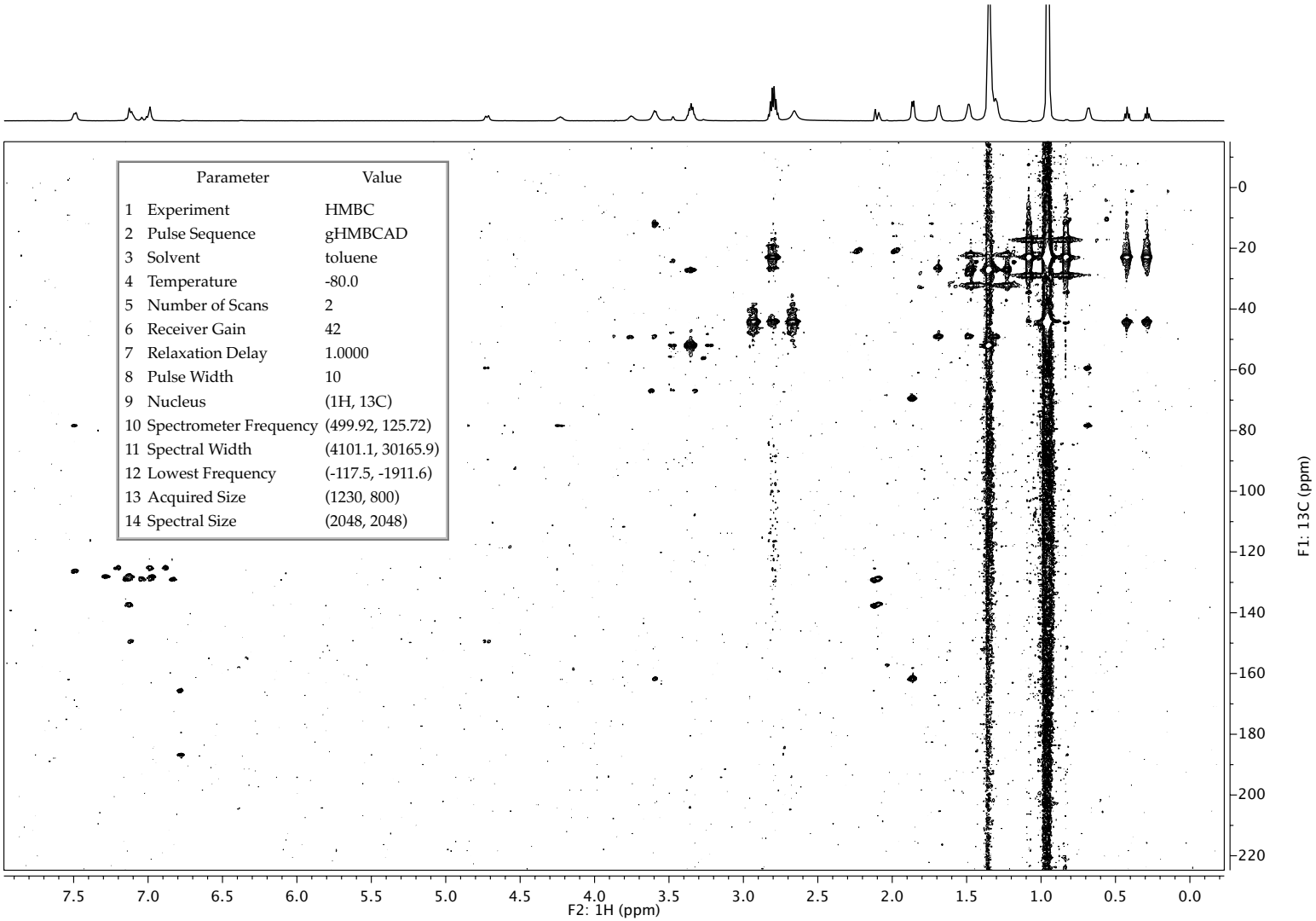


Figure 185. Full-display HMBC spectrum of a pre-aged solution prepared from 0.10 M (*S,S*)-**1** in 2.0 M THF-d_8 and 7.9 M toluene-d_8 at –80 °C with 0.40 M [^{6}Li]LDA.

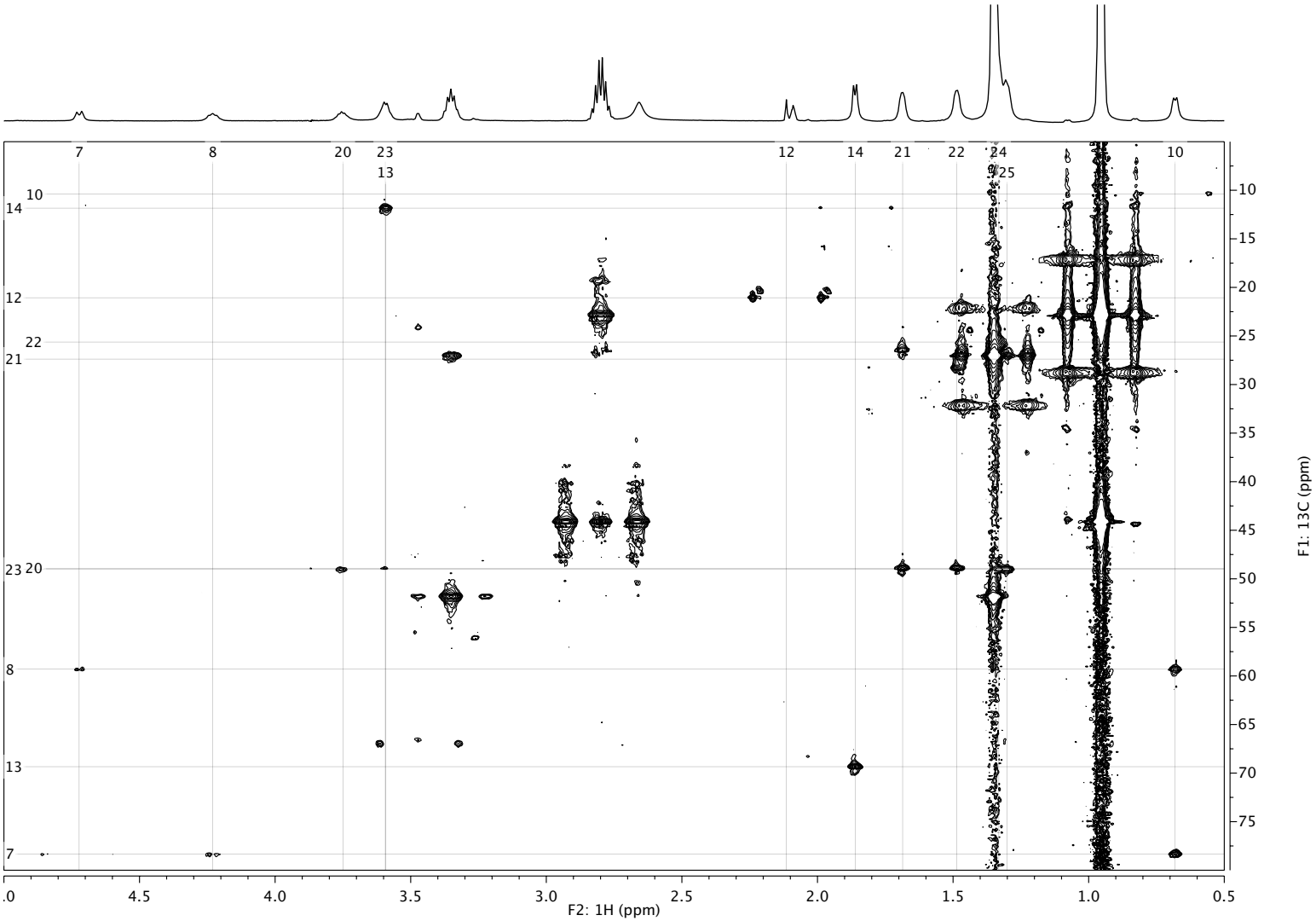


Figure 186. Expansion of the HMBC spectrum of a pre-aged solution prepared from 0.10 M (*S,S*)-**1** in 2.0 M THF-d_8 and 7.9 M toluene-d_8 at –80 °C with 0.40 M [^{6}Li]LDA.

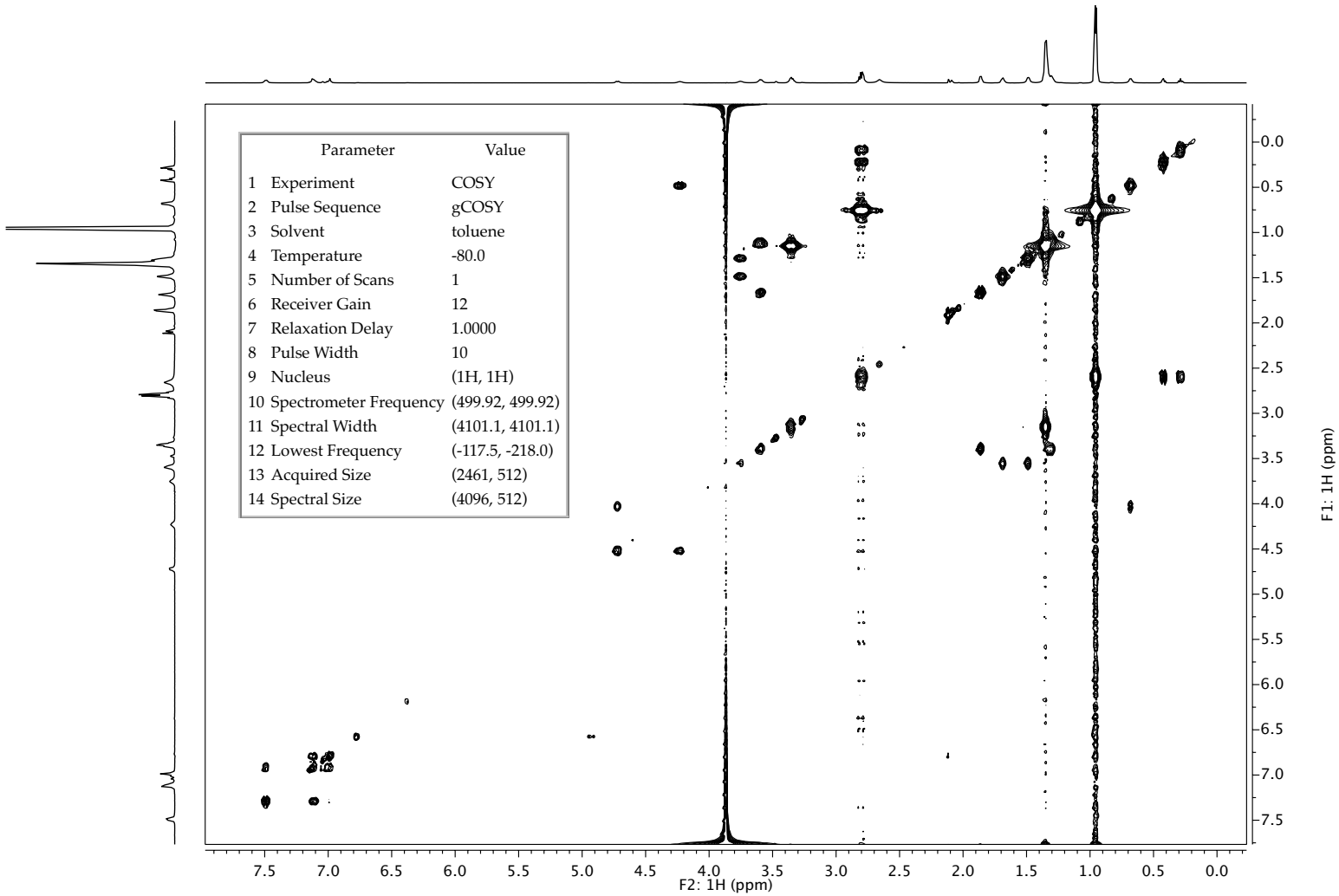


Figure 187. Full-display COSY spectrum of a pre-aged solution prepared from 0.10 M (*S,S*)-**1** in 2.0 M THF-d_8 and 7.9 M toluene-d_8 at –80 °C with 0.40 M [^{6}Li]LDA.

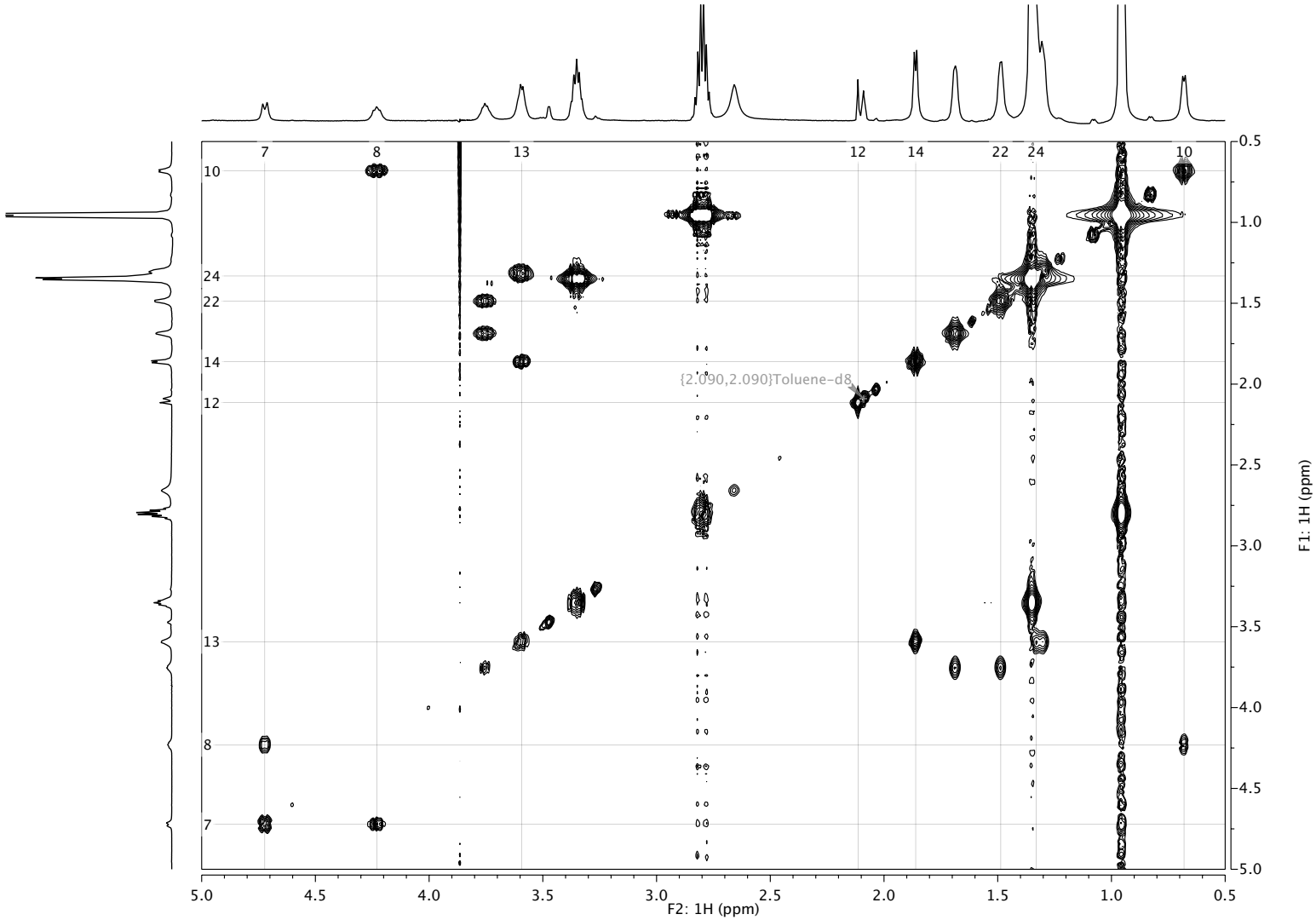


Figure 188. Expansion of the COSY spectrum of a pre-aged solution prepared from 0.10 M (*S,S*)-**1** in 2.0 M THF-d_8 and 7.9 M toluene-d_8 at –80 °C with 0.40 M [^{6}Li]LDA.

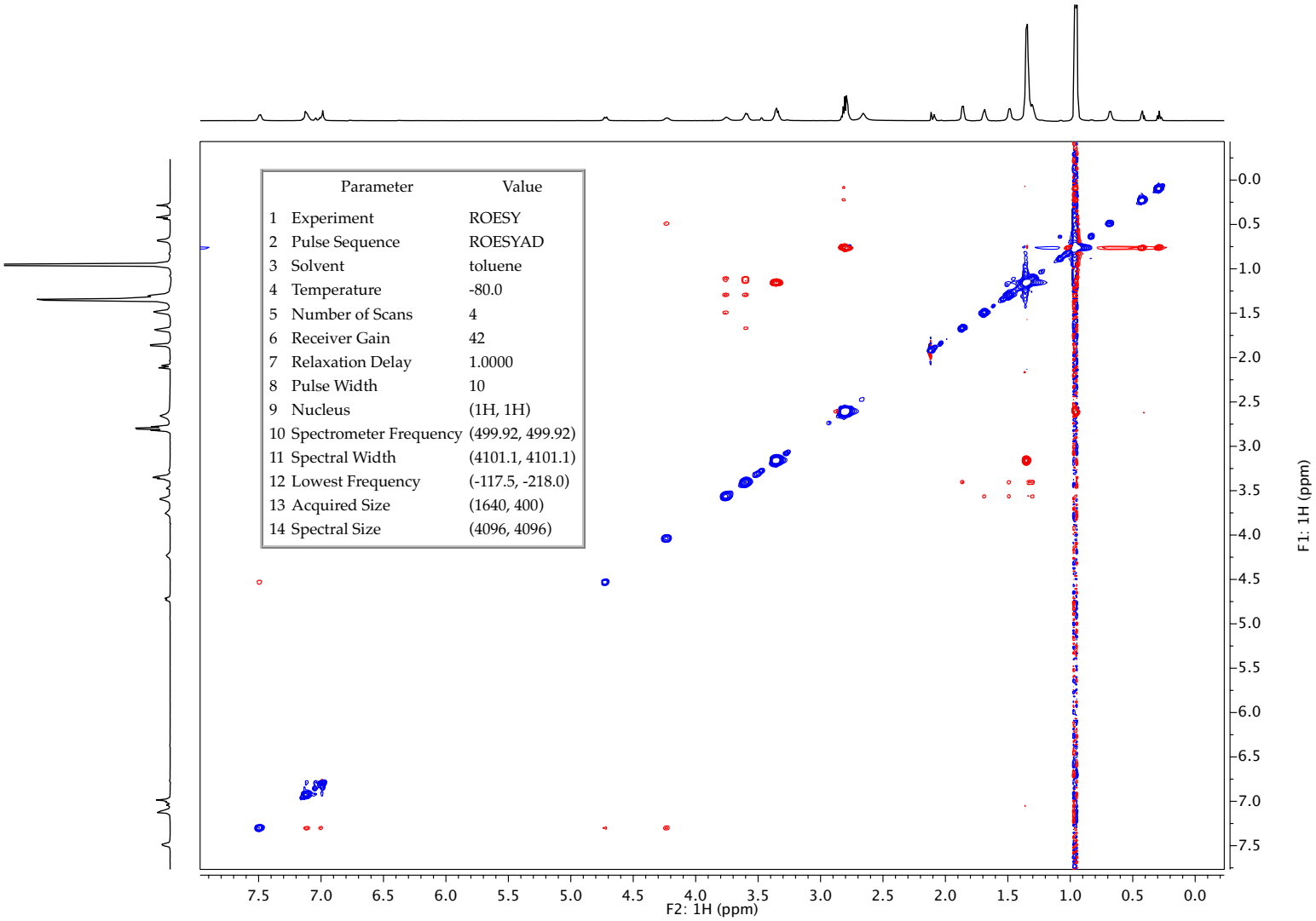


Figure 189. Full-display ROESY spectrum of a pre-aged solution prepared from 0.10 M (*S,S*)-**1** in 2.0 M THF-d_8 and 7.9 M toluene-d_8 at –80 °C with 0.40 M [^{6}Li]LDA.

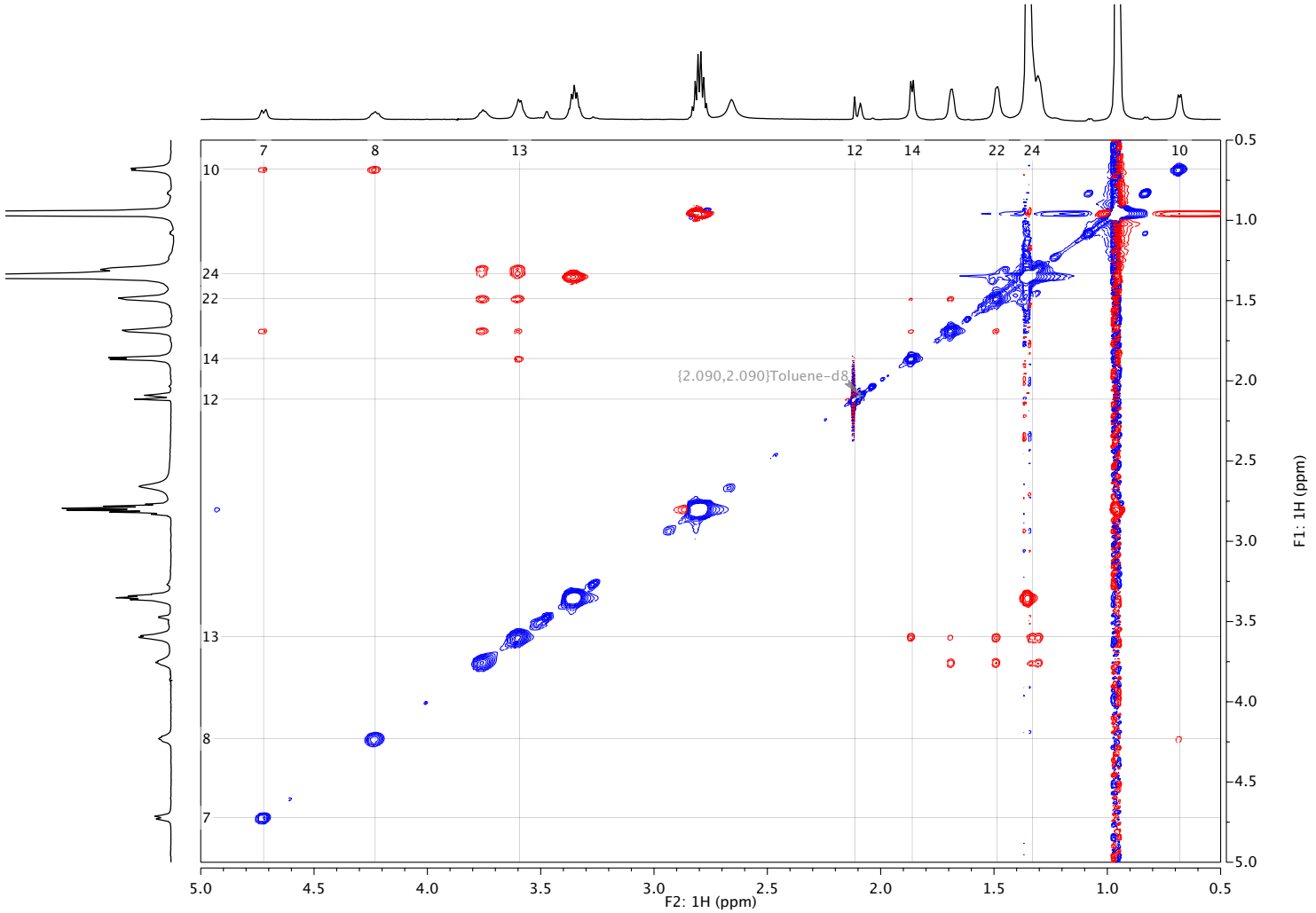


Figure 190. Expansion of the ROESY spectrum of a pre-aged solution prepared from 0.10 M (*S,S*)-**1** in 2.0 M THF-d_8 and 7.9 M toluene-d_8 at –80 °C with 0.40 M [^{6}Li]LDA.

Part 5. LiCl- adduct Characterization

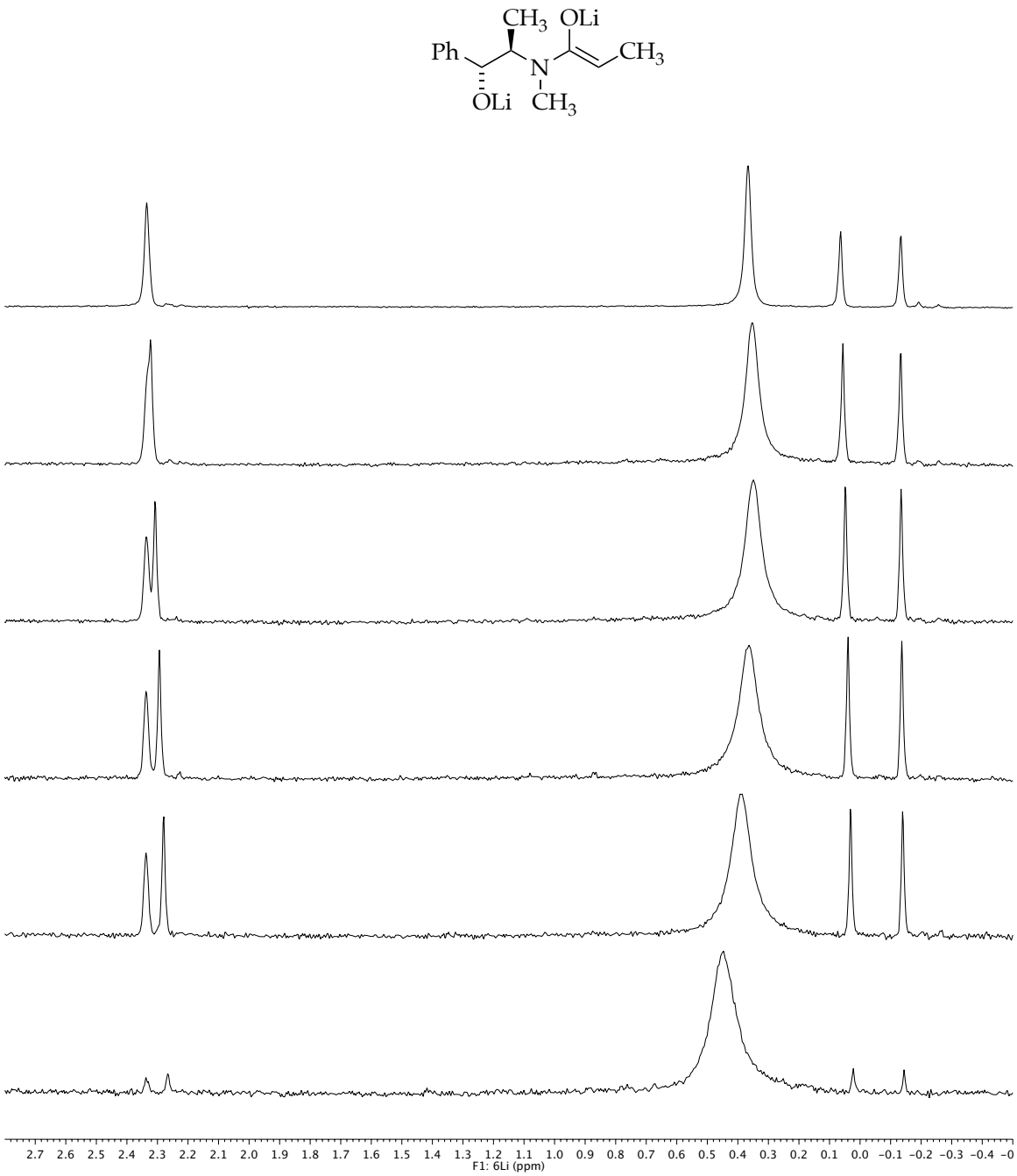


Figure 191. ^{6}Li NMR spectra of 0.10 M [^{6}Li]-(*R,R*)-**2** and 0.20 M [^{6}Li]LiCl in 12.3 M THF at varying temperature. The sample was kept at each temperature for 20 min before the spectra were taken. With increasing temperature, LiCl-adduct (**2$_{LiCl}$**) was formed.

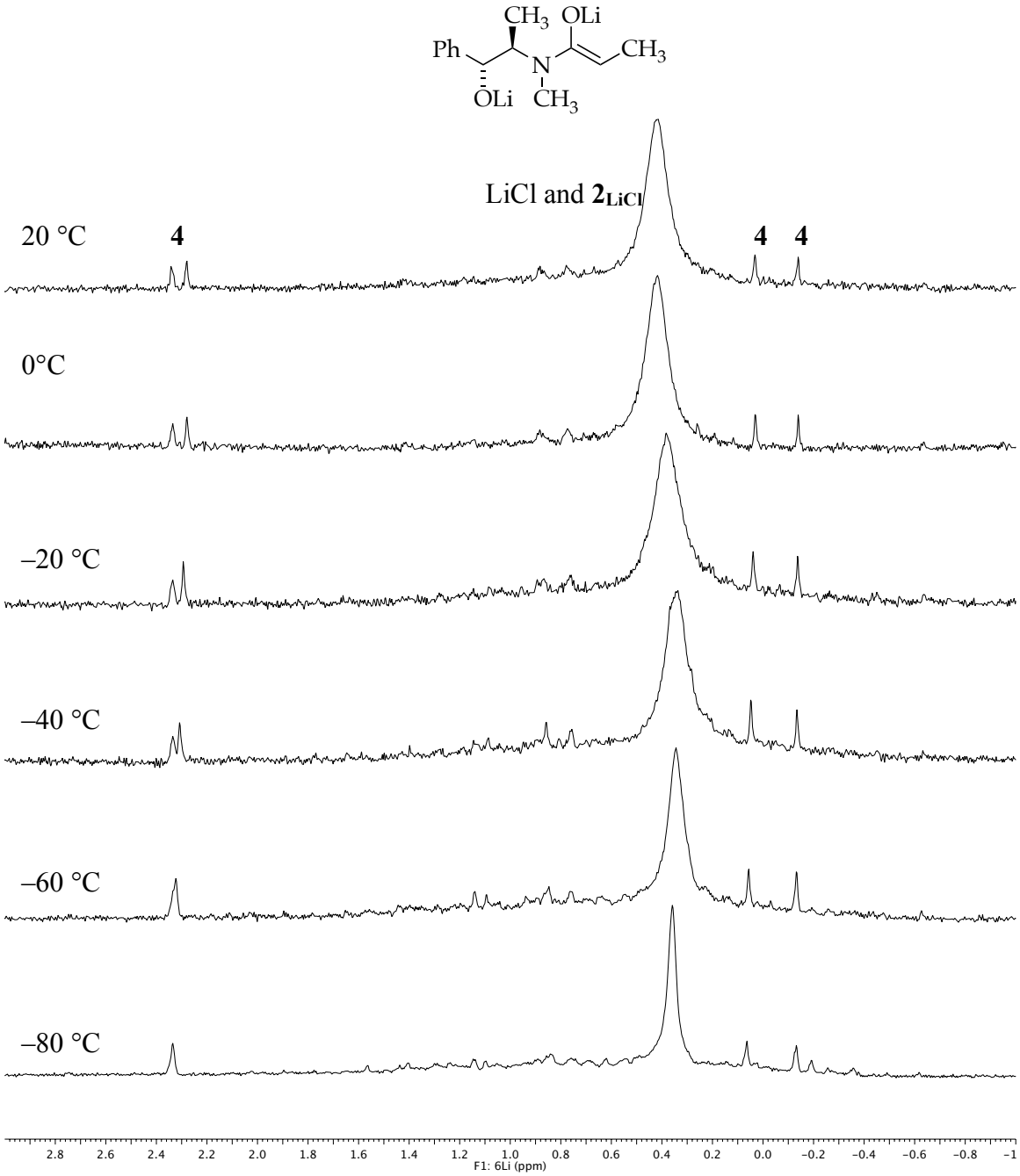


Figure 192. ^{6}Li NMR spectra of 0.10 M [^{6}Li]-(*R,R*)-**2** and 0.20 M [^{6}Li]LiCl in 12.3 M THF at varying temperature. The sample was kept at each temperature for 20 min before spectra were taken. Formation of LiCl-adduct (**2$_{LiCl}$**) was not reversible.

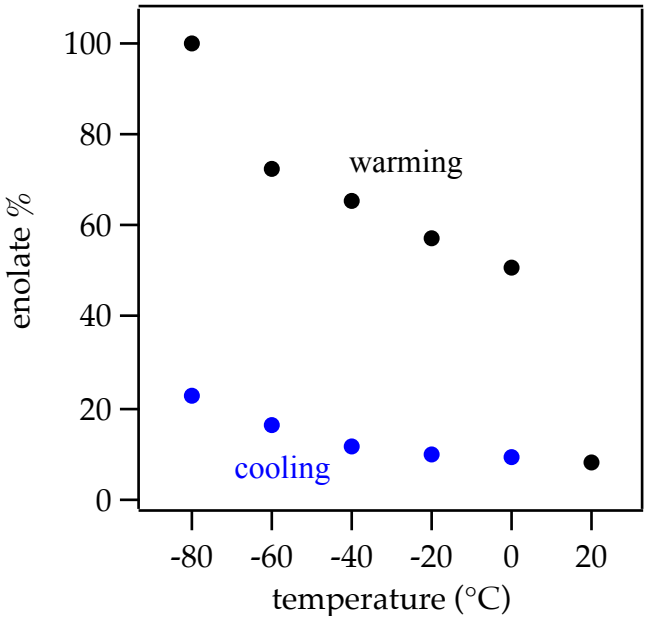


Figure 193. Plot of percent enolate **4** (Figure 192 and 193) vs temperature. Percent enolate on incremental temperature increases (black) versus temperature decreases (blue).

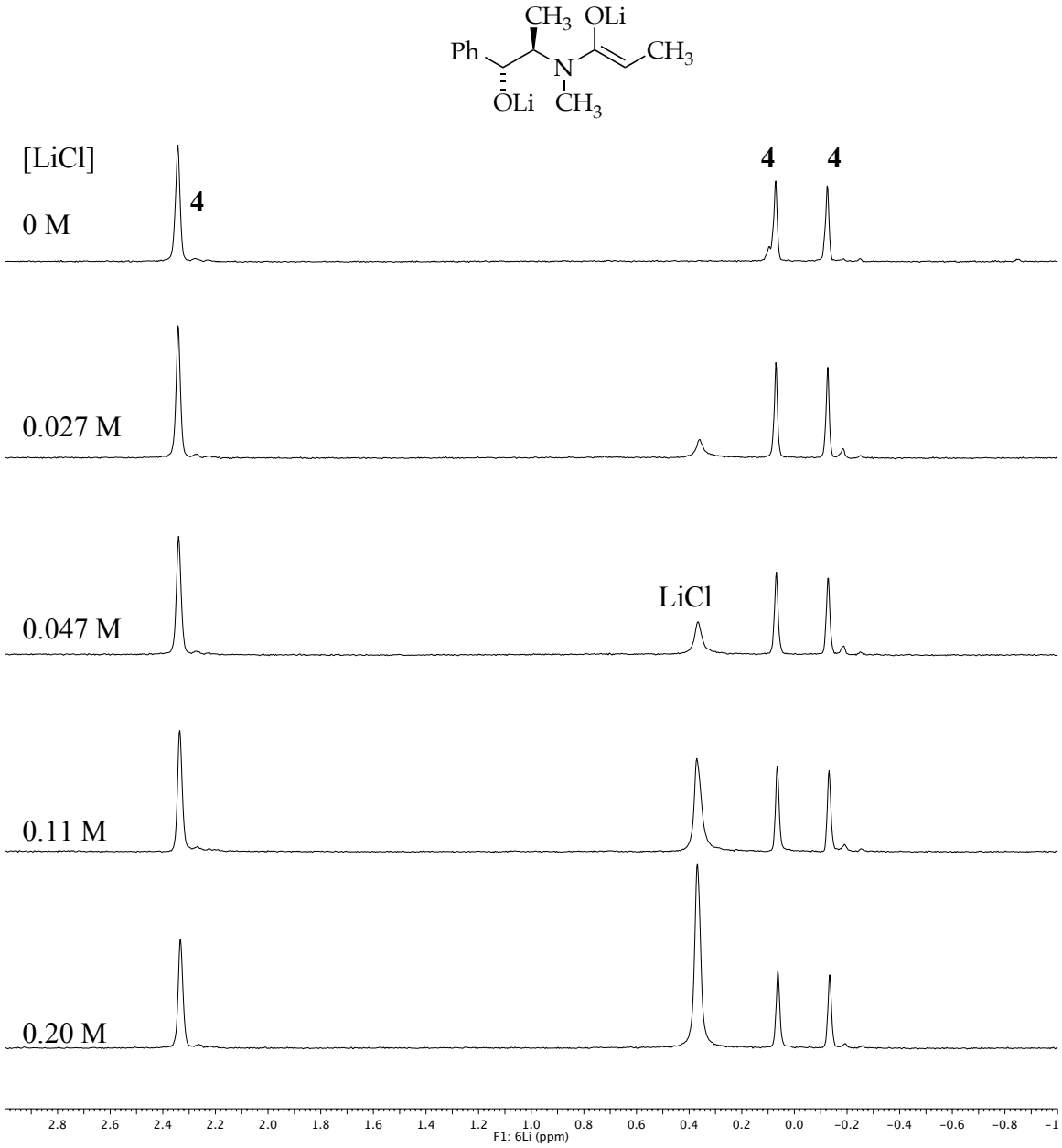


Figure 194. ^{6}Li NMR spectra of 0.10 M [^{6}Li]-(*R,R*)-**2** in 12.3 M THF at –80 °C with varying LiCl concentrations. Samples were kept at –80 °C (unaged).

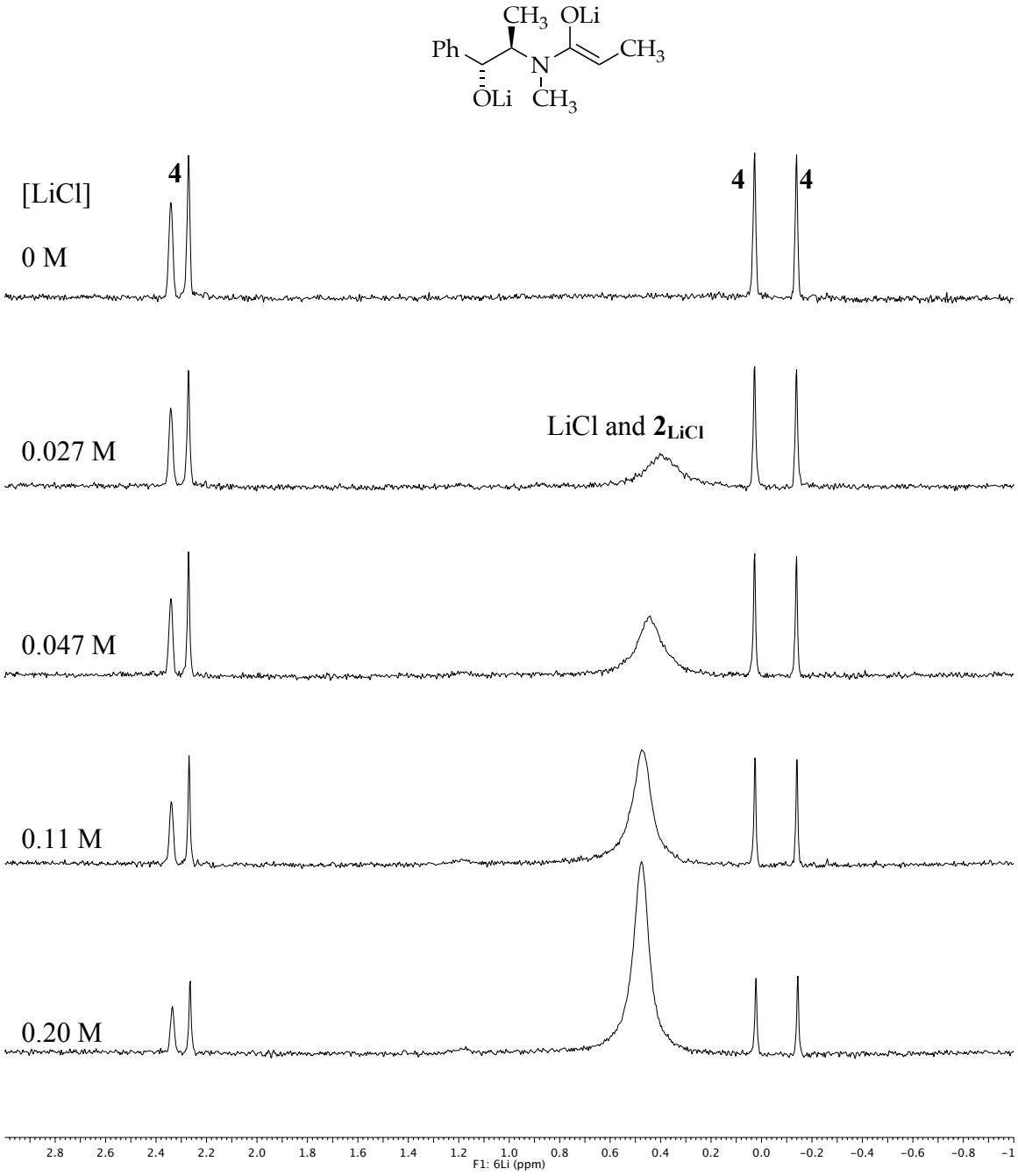


Figure 195. ^{6}Li NMR spectra of 0.10 M [^{6}Li]-(*R,R*)-**2** in 12.3 M THF at 20 °C with varying LiCl concentrations. Samples were aged at 20 °C for 20 m. The integration of LiCl resonance at 0.50 ppm was increased.

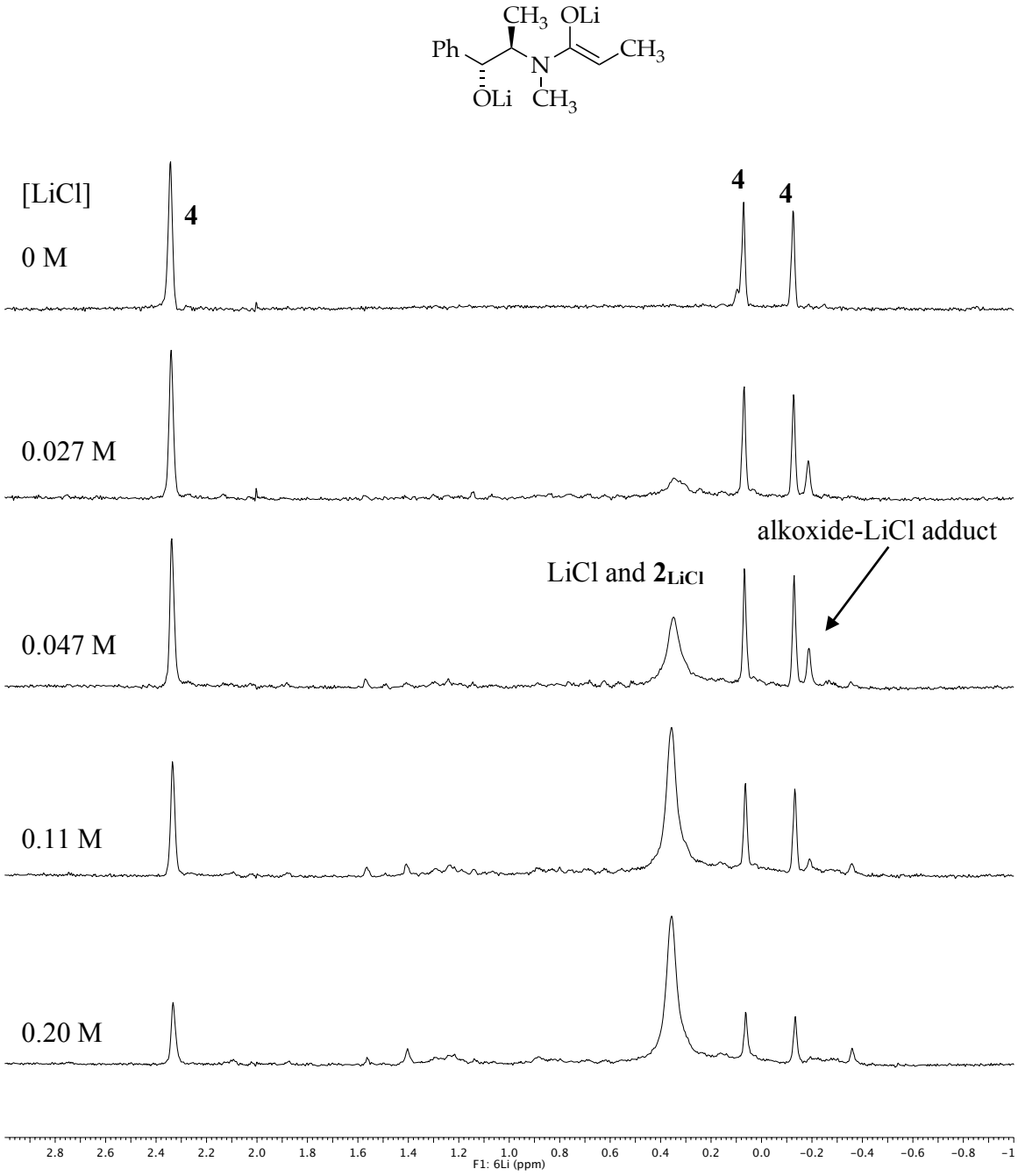


Figure 196. ^{6}Li NMR spectra of 0.10 M [^{6}Li]-(*R,R*)-**2** in 12.3 M THF at –80 °C with varying LiCl concentrations. Samples were aged at 20 °C for 20 m. The integration of LiCl resonance at 0.50 ppm was increased.

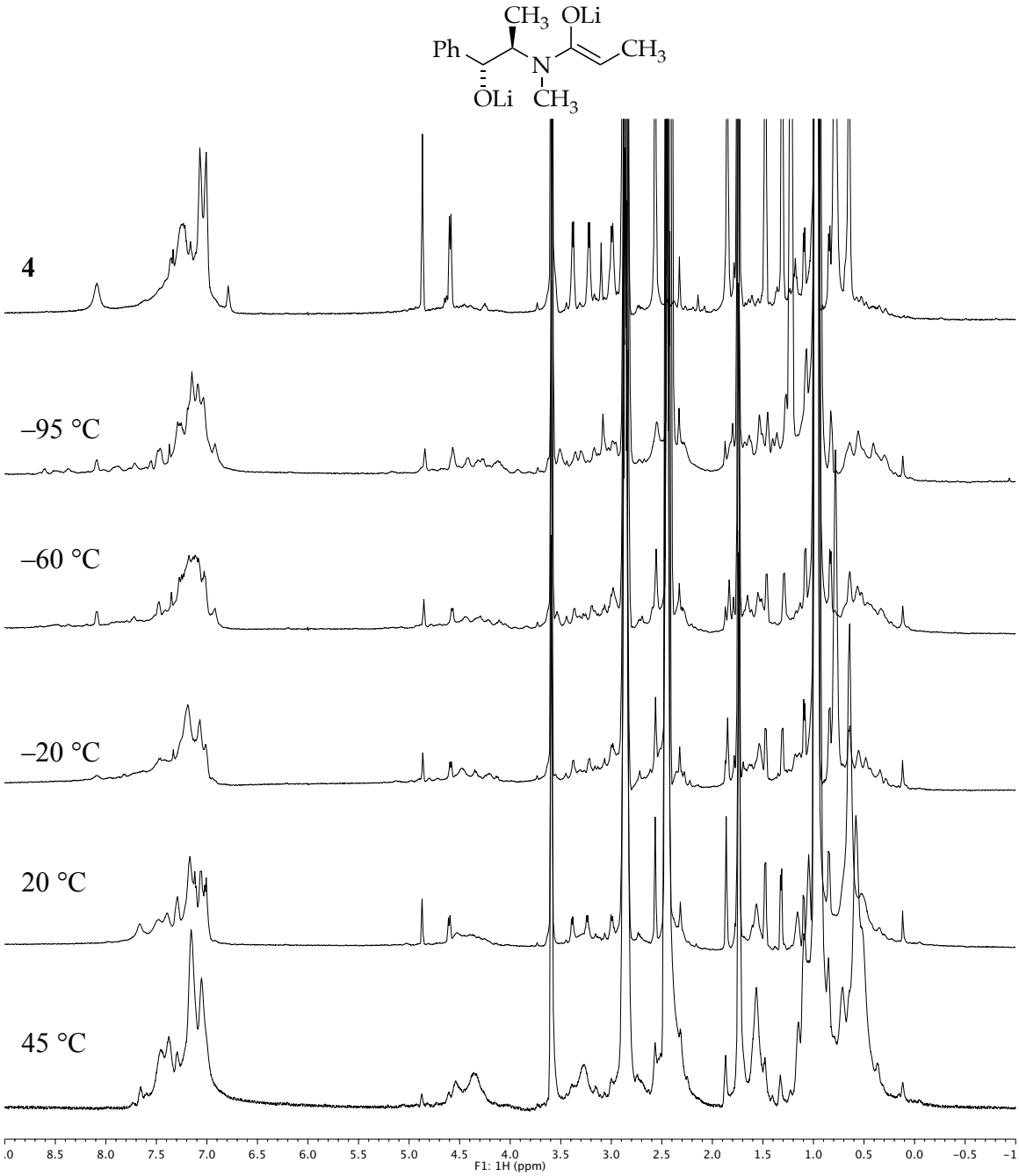


Figure 197. ^{1}H NMR spectra of 0.10 M [^{6}Li]-(*R,R*)-**2** in 12.3 M THF with 0.15 M [^{6}Li]LiCl at varying temperature. First spectrum was taken at –20 °C. Samples were aged at 20 °C for 20 min. LiCl adduct does not give a sharp resonance.

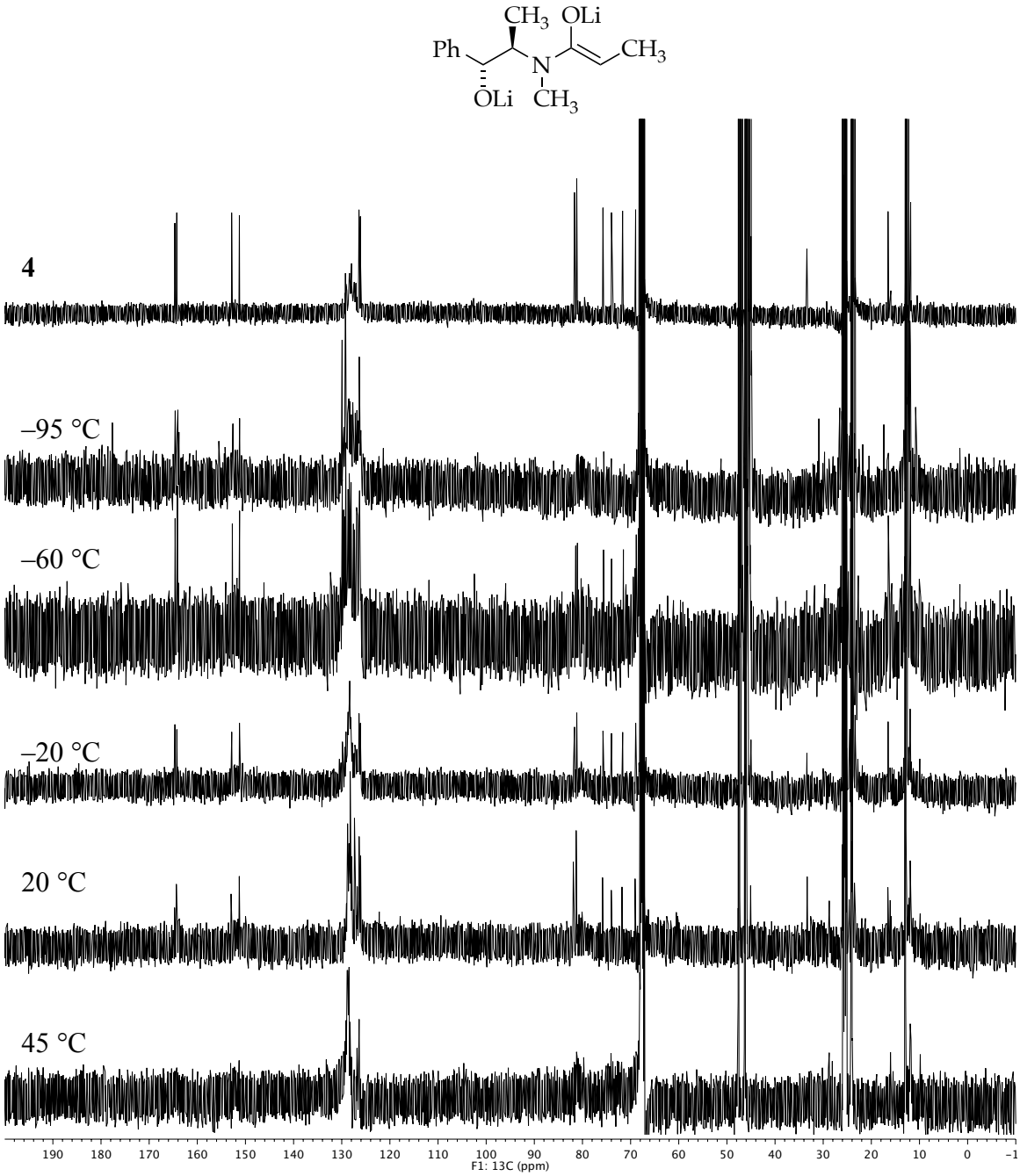


Figure 198. ^{13}C NMR spectra of 0.10 M [^{6}Li]-(*R,R*)-**2** in 12.3 M THF with 0.15 M [^{6}Li]LiCl at varying temperature. First spectrum was taken at –20 °C. Samples were aged at 20 °C for 20 min. LiCl adduct does not give a sharp resonance.

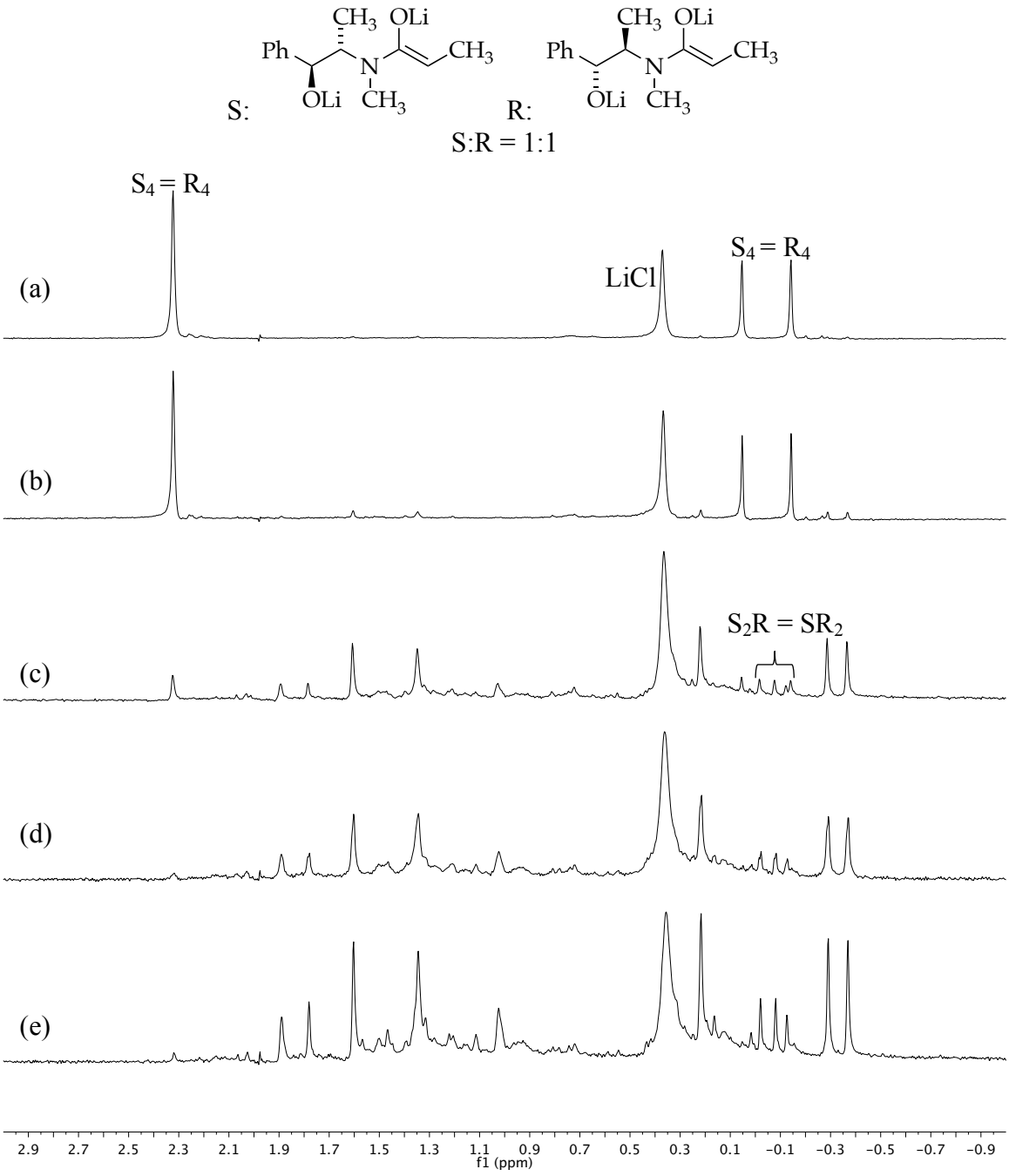


Figure 199. ^{6}Li NMR spectra of 0.10 M solutions of 0.050 M [^{6}Li]-(*S,S*)-**2** and 0.050 M [^{6}Li]-(*R,R*)-**2** and 0.10 M [^{6}Li]LiCl in neat THF at –80 °C: (a) aged at –80 °C for 30 min; (b) aged at 0 °C for 15 min; (c) aged at 20 °C for 15 min; (d) aged at 40 °C for 15 min; (e) aged at 60 °C for 15 min. Each enolate was separately formed, aged at 20 °C for 10 min, and then mixed together. With LiCl, heteroaggregates begin to appear at 20 °C. Without LiCl (Figure 94), heteroaggregates begin to appear at 40 °C.

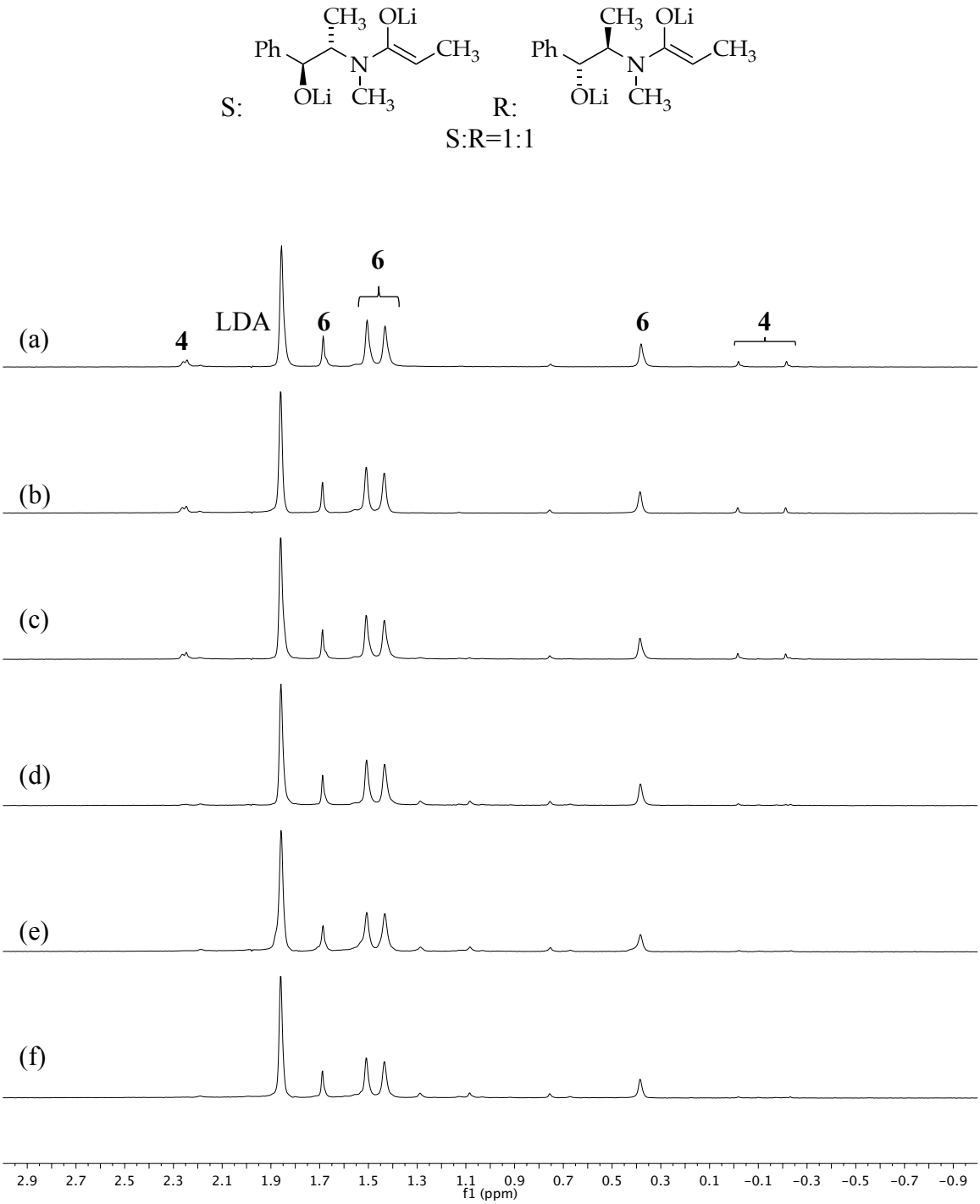


Figure 200. ^{6}Li NMR spectra of 0.10 M solutions of 0.050 M [^{6}Li]-(*S,S*)-**6** and 0.050 M [^{6}Li]-(*R,R*)-**6** in 0.40 M THF and toluene at –80 °C. (*S,S*)-**6** or (*R,R*)-**6** was prepared by mixing [^{6}Li]-(*S,S*)-**2** or (*R,R*)-**6** with 0.15 M [^{6}Li]LDA: (a) aged at –80 °C for 30 min; (b) aged at 0 °C for 15 min; (c) aged at 20 °C for 15 min; (d) aged at 40 °C for 15 min; (e) aged at 60 °C for 15 min; (f) aged at 80 °C for 15 min. Each LDA-mixed aggregates was separately formed, aged at 20 °C for 10 min, and then mixed together. LDA-mixed aggregates did not form heteroaggregates.

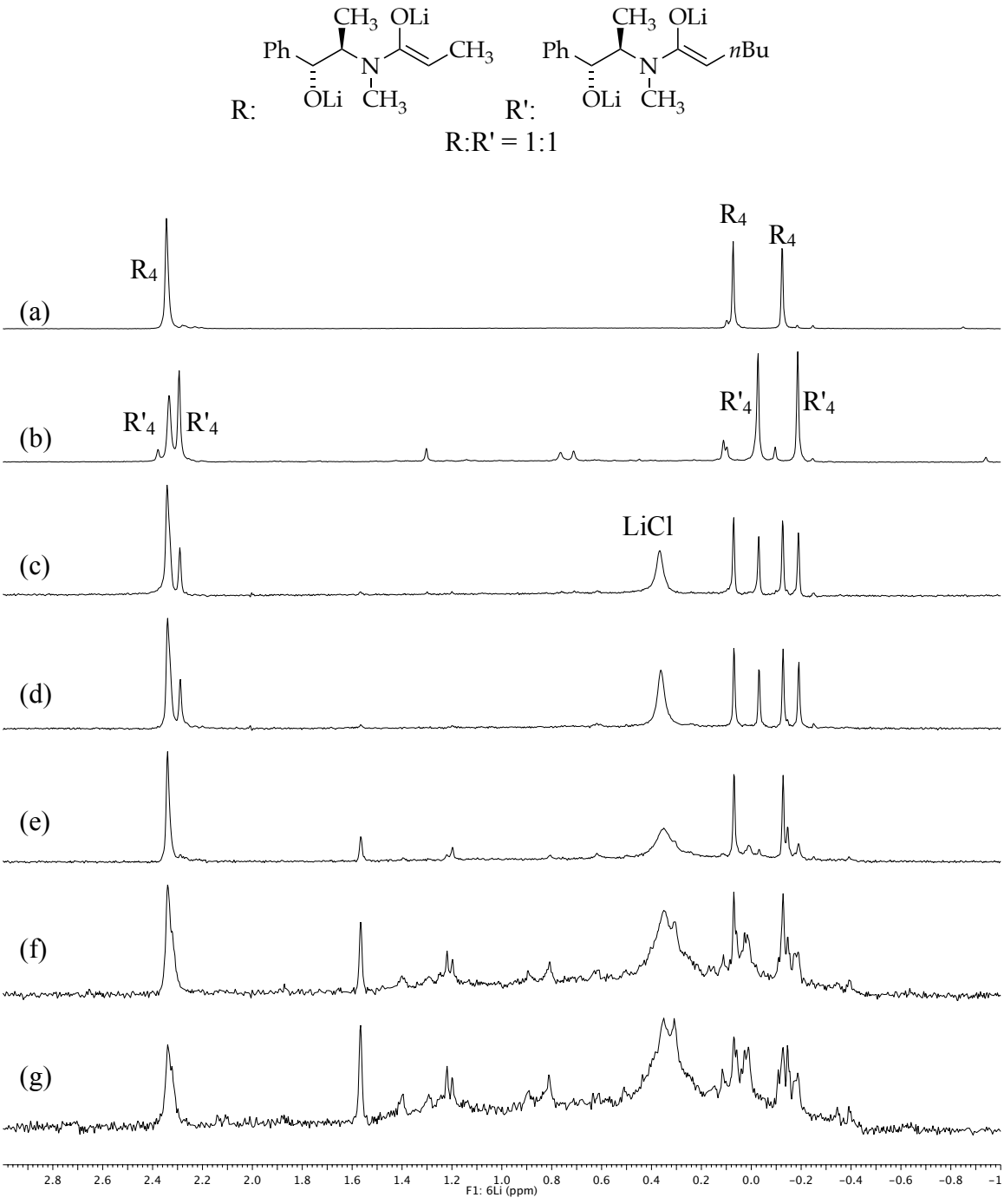


Figure 201. ^{6}Li NMR spectra of 0.10 M solutions of [^{6}Li]-(*R,R*)-**2** (R) and [^{6}Li]-(*R,R*)-**8** (R') and 0.10 M [^{6}Li]LiCl in 12.3 M THF at −80 °C: (a) R_4; (b) R'_4; (c) aged at –80 °C for 2 h; (d) aged at –40 °C for 15 min; (e) aged at 0 °C for 15 min; (f) aged at 20 °C for 15 min; (g) aged at 40 °C for 15 min. Each enolate was separately formed, aged at 20 °C for 10 min, and then mixed together. With LiCl, heteroaggregates begin to appear at 0 °C. Without LiCl (Figure 90), heteroaggregates begin to appear at 40 °C.

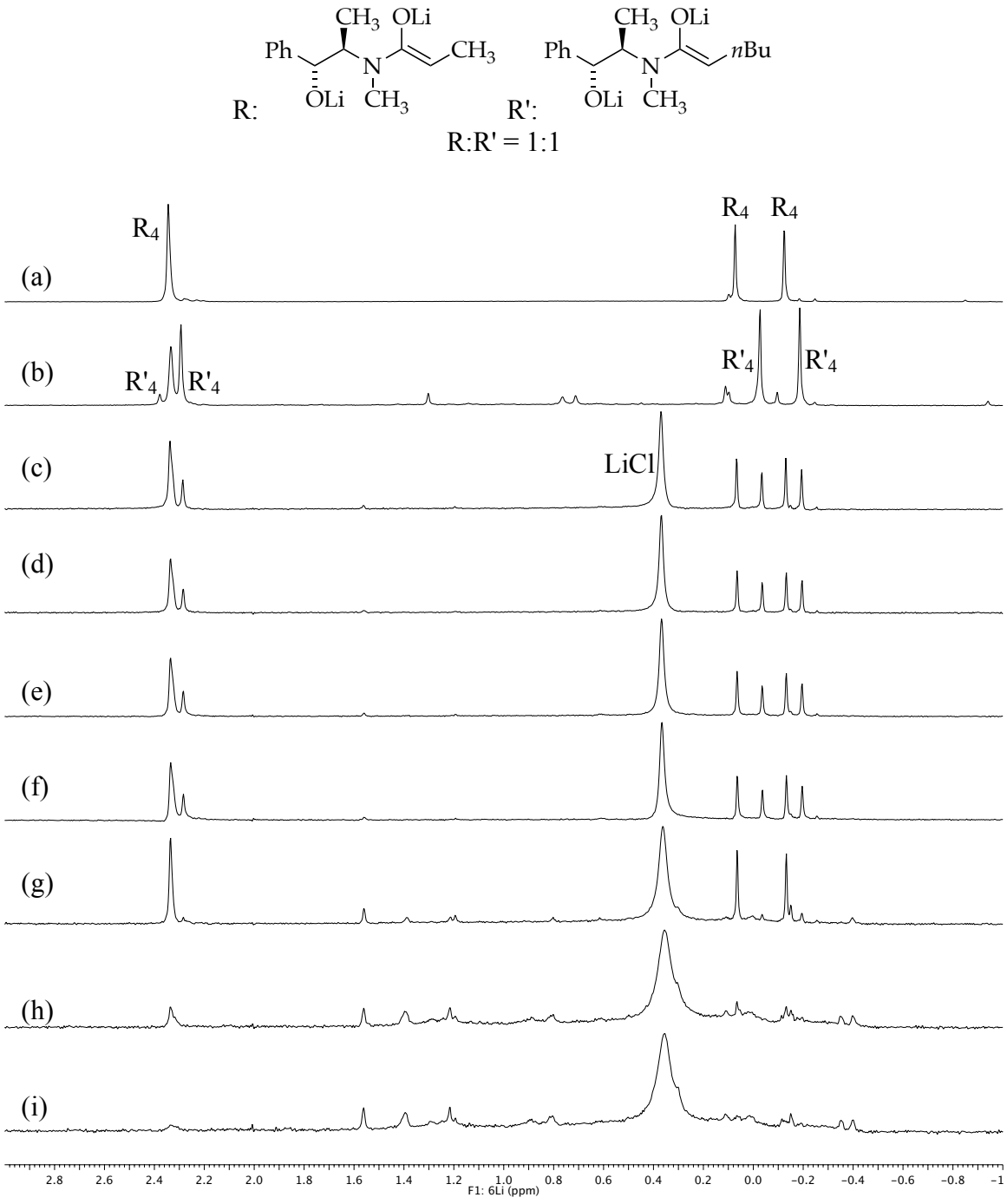
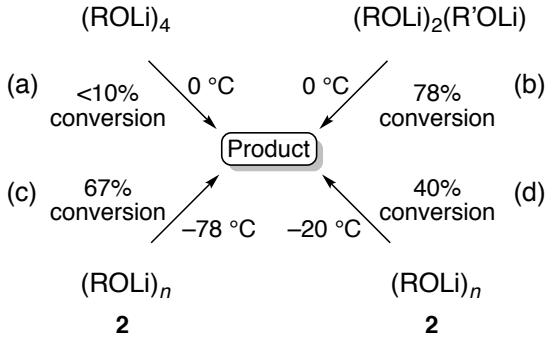


Figure 202. ^{6}Li NMR spectra of 0.10 M solutions of [^{6}Li]-(*R,R*)-**2** (R) and [^{6}Li]-(*R,R*)-**8** (R'$_4$) and 0.20 M [^{6}Li]LiCl in 12.3 M THF at −80 °C: (a) R$_4$; (b) R'$_4$; (c) aged at –80 °C for 2 h; (d) aged at –60 °C for 15 min; (e) aged at –40 °C for 15 min; (f) aged at –20 °C for 15 min; (g) aged at –0 °C for 15 min; (h) aged at 20 °C for 15 min; (i) aged at 40 °C for 15 min. Each enolate was separately formed, aged at 20 °C for 10 min, and then mixed together. With LiCl, heteroaggregates begin to appear at 0 °C. Without LiCl (Figure 90), heteroaggregates begin to appear at 40 °C.



Reaction (a):
0.50 mL (*R,R*)-**1** (0.16 M in THF, 0.50 equiv) was mixed with 1.0 mL anhydrous THF in a 5 mL Kimble® vial which was flame dried and flushed with argon. 0.50 mL LDA (0.34 M in THF, 2.1 equiv) was added to the vial. The solution was warmed to 20 °C for 10 min and then cooled back to 0 °C. Allyl bromide (15.0 μL, 0.17 mmol) was then added in one portion, and the reaction mixture was stirred for 1 h at 0 °C. Reaction was quenched at 0 °C by the addition of saturated aqueous ammonium chloride (0.50 mL) and the mixture was partitioned between saturated aqueous ammonium chloride (1 mL) and EtOAc (3 mL). The organic layer was collected and the aqueous layer was extracted with EtOAc (30 mL × 3). The combined organic layers were dried over anhydrous sodium sulfate and solvent was removed under reduced pressure to afford a yellow oil that was purified by flash chromatography (30% EtOAc in hexanes) to provide product (10% yield).

Reaction (b):
0.25 mL (*R,R*)-**1** (0.16 M in THF, 0.50 equiv) and 0.25 mL (*S,S*)-**1** (0.16 M in THF, 0.50 equiv) were mixed with 1.0 mL anhydrous THF in a 5 mL Kimble® vial which was flame dried and flushed with argon. 0.50 mL LDA (0.34 M in THF, 2.1 equiv) was added to the vial. The solution was warmed to 20 °C for 10 min and then cooled back to 0 °C. Allyl bromide (15.0 μL, 0.17 mmol) was then added in one portion, and the reaction mixture was stirred for 1 h at 0 °C. Reaction workup was the same as reaction (a). Yield was 78%.

Reaction (c):
0.50 mL (*R,R*)-**1** (0.16 M in THF, 0.50 equiv) was mixed with 1.0 mL anhydrous THF in a 5 mL Kimble® vial which was flame dried and flushed with argon. The solution was then cooled to –78 °C with dry ice acetone bath. 0.50 mL LDA (0.34 M in THF, 2.1 equiv) was slowly added to the vial to avoid temperature rise. The solution was kept at –78 °C for 10 min. Allyl bromide (15.0 μL, 0.17 mmol) was then added in one portion, and the reaction mixture was stirred for 1 h at –78 °C. The reaction was quenched at –78 °C. Reaction workup was the same as reaction (a). Yield was 67%.

Reaction (d):
0.50 mL (*R,R*)-**1** (0.16 M in THF, 0.50 equiv) was mixed with 1.0 mL anhydrous THF in a 5 mL Kimble® vial which was flame dried and flushed with argon. The solution was then cooled to 0 °C with ice water bath. 0.50 mL LDA (0.34 M in THF, 2.1 equiv) was

slowly added to the vial to avoid temperature rise. The solution was kept at 0 °C for 3 min. Allyl bromide (15.0 µL, 0.17 mmol) was then added in one portion, and the reaction mixture was stirred for 1 h at 0°C. Reaction workup was the same as reaction (a). Yield was 40%.

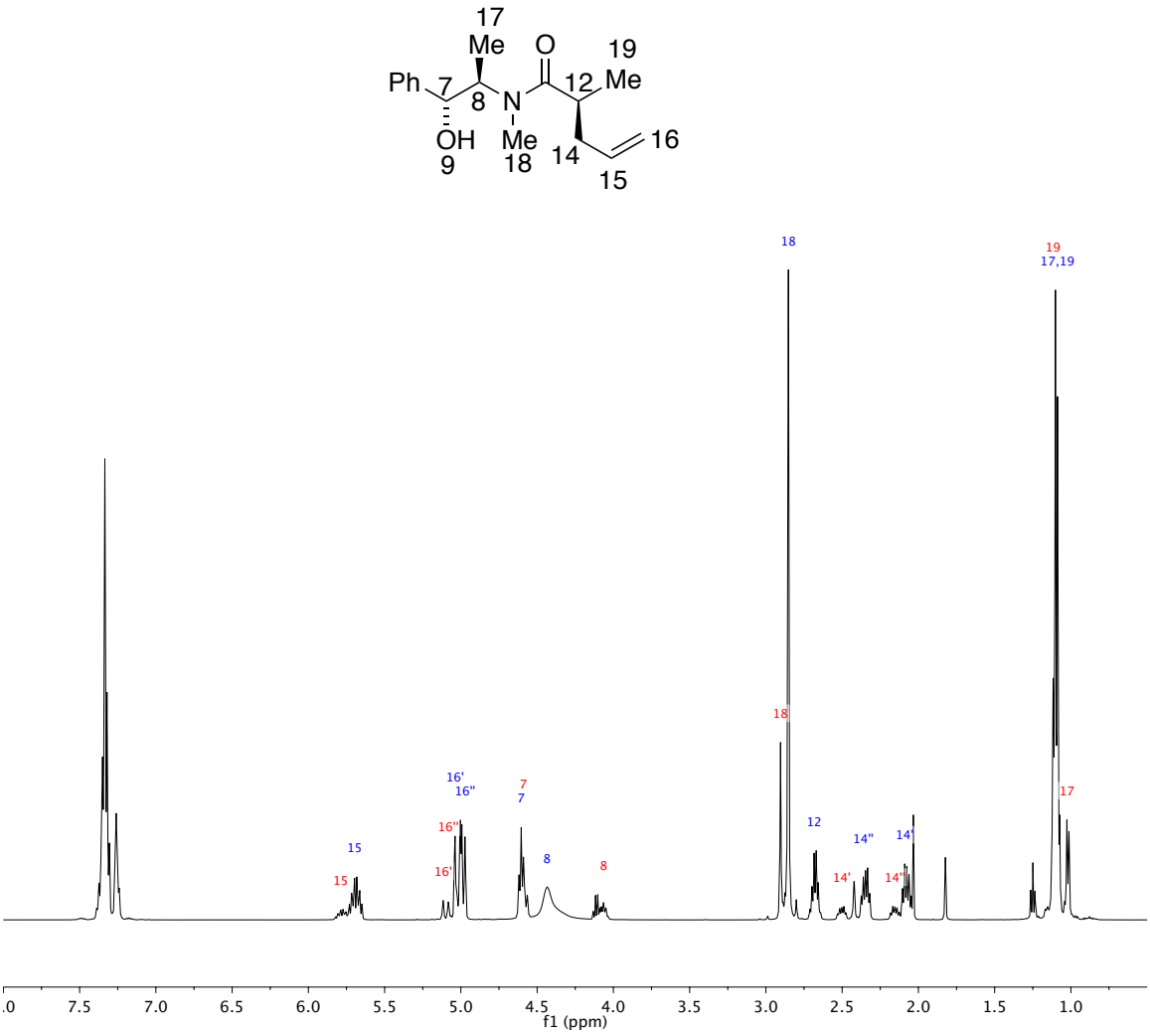


Figure 203. ^{1}H NMR of product **53** in $CDCl_3$ at 25 °C. Red and blue denotes the two rotamers.

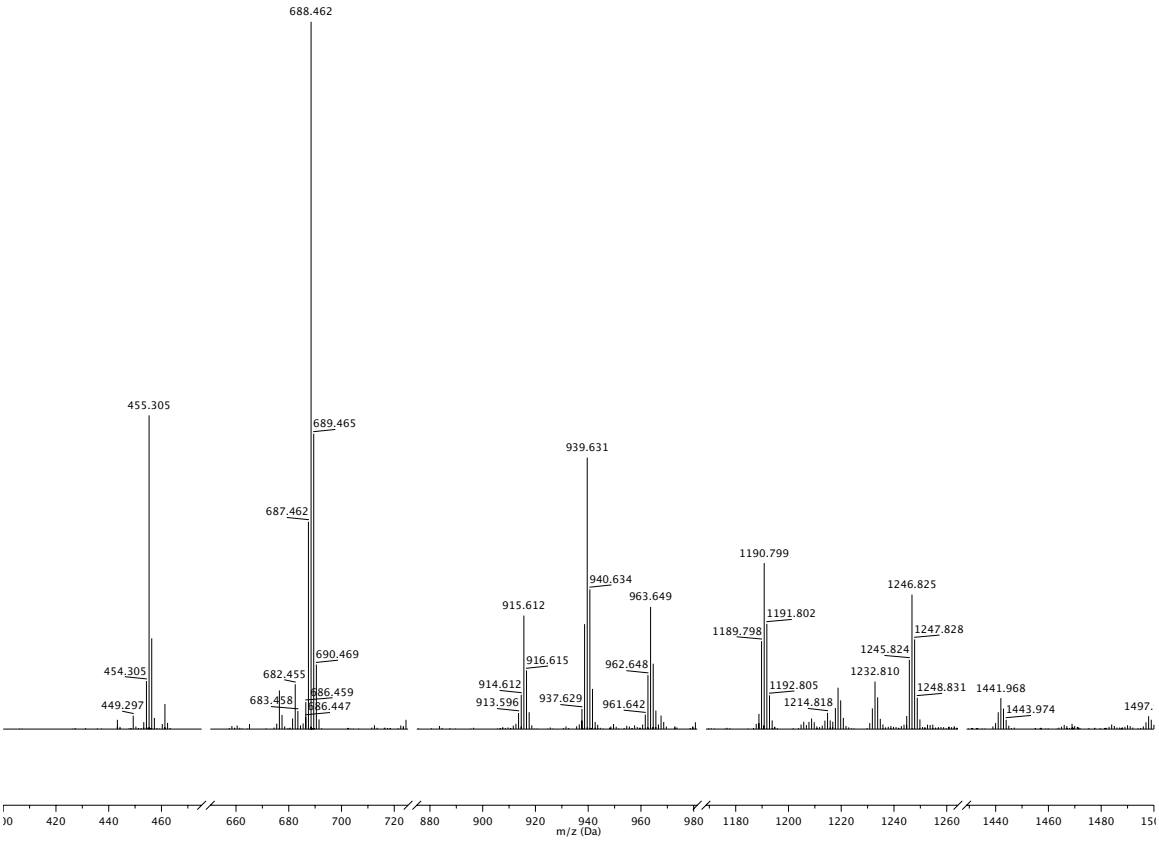
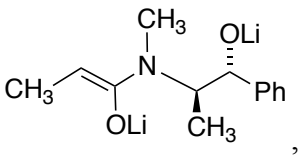
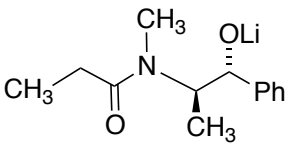


Figure 204. Mass spectrum of homoaggregate **4**. DART-MS spectrum was acquired in positive ion mode with helium DART gas at 400 °C on a Thermo Scientific Exactive mass spectrometer equipped with an IonSense DART SVP ion source. Resolution was 100,000 at 1 Hz repetition rate, scan range was m/z 200-2000. DART is an open atmosphere ionization method where heat is used to desorb the analyte from the surface where it ionizes by interacting with metastable DART gas

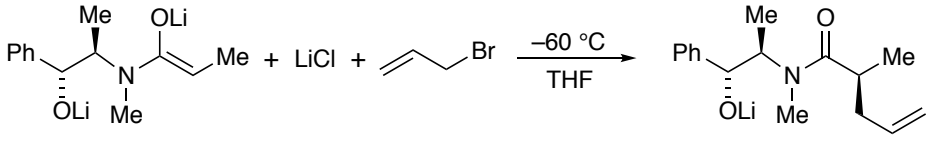
observed m/z	calculated m/z	formula	possible composition	error (ppm)
455.3054	455.3068	$C_{26}H_{37}Li_2N_2O_4$	$[A_2+H]^+$	–3.14
688.4623	688.4647	$C_{39}H_{54}Li_4N_3O_6$	$[E_1A_2+H]^+$	–3.48
915.6122	915.6145	$C_{52}H_{72}Li_5N_4O_8$	$[E_1A_3+H]^+$	–2.54
939.6306	939.6332	$C_{52}H_{74}Li_6N_4O_9$	$[E_2A_2+H_2O+H]^+$	–2.80
963.6491	963.6520	$C_{52}H_{74}Li_7N_4O_{10}$	$[E_3A_1+2H_2O+H]^+$	–2.97
1190.7991	1190.8017	$C_{65}H_{92}Li_8N_5O_{12}$	$[E_3A_2+2H_2O+H]^+$	–2.20
1441.9675	1441.9702	$C_{78}H_{111}Li_{10}N_6O_{15}$	$[E_4A_2+3H_2O+H]^+$	–1.87

E = 

, A = 

Ref: Gross, Jürgen H. *Analytical and bioanalytical chemistry* **2014**, *406*, 63.

Part 6. Kinetic Data



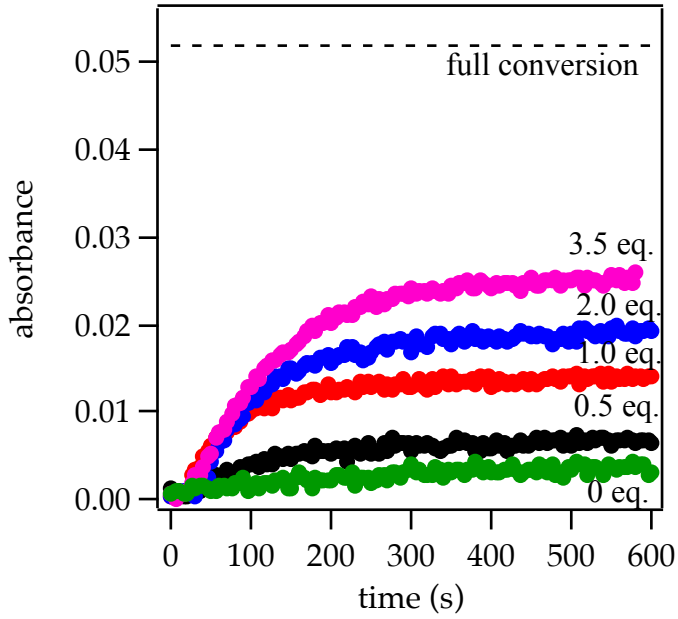


Figure 205. Plot following the formation of alkoxide product (1610 cm^{-1}) versus time (IR spectroscopy) for the alkylation of (*R,R*)-**2** (0.040 M) in neat THF at –60 °C with allyl bromide (0.092 M) and varying LiCl equivalencies. Plot shows LiCl-concentration-dependent intial rates and percent conversions.

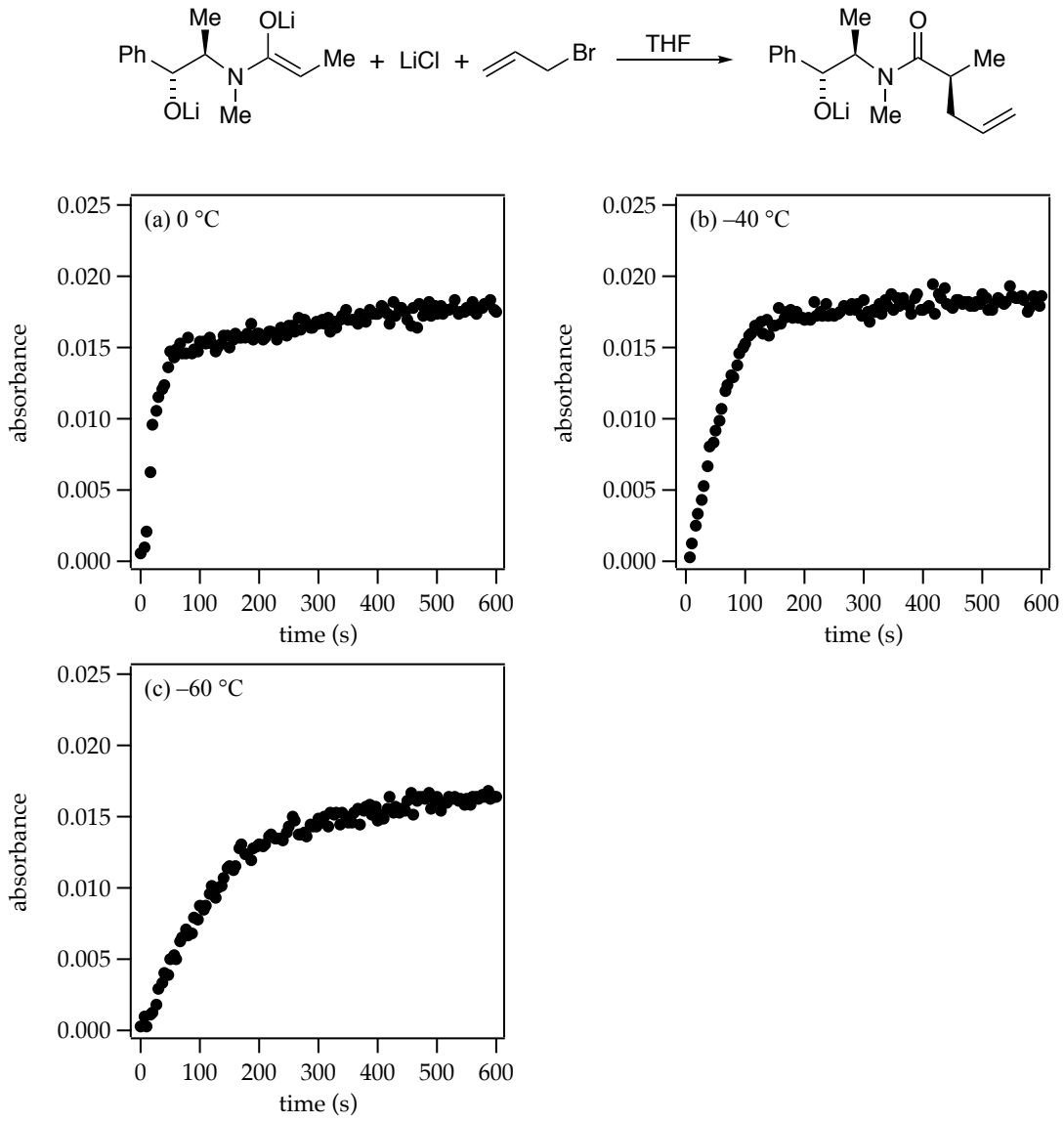


Figure 206. Plots following the formation of alkoxide product (1610 cm^{-1}) versus time (IR spectroscopy) for the alkylation of (*R,R*)-**2** (0.040 M) with allyl bromide (0.092 M) in neat THF with 0.040 M LiCl (1.0 eq) at varying temperature. Plot shows temperature-independent percent conversion and temperature-dependent initial rates.

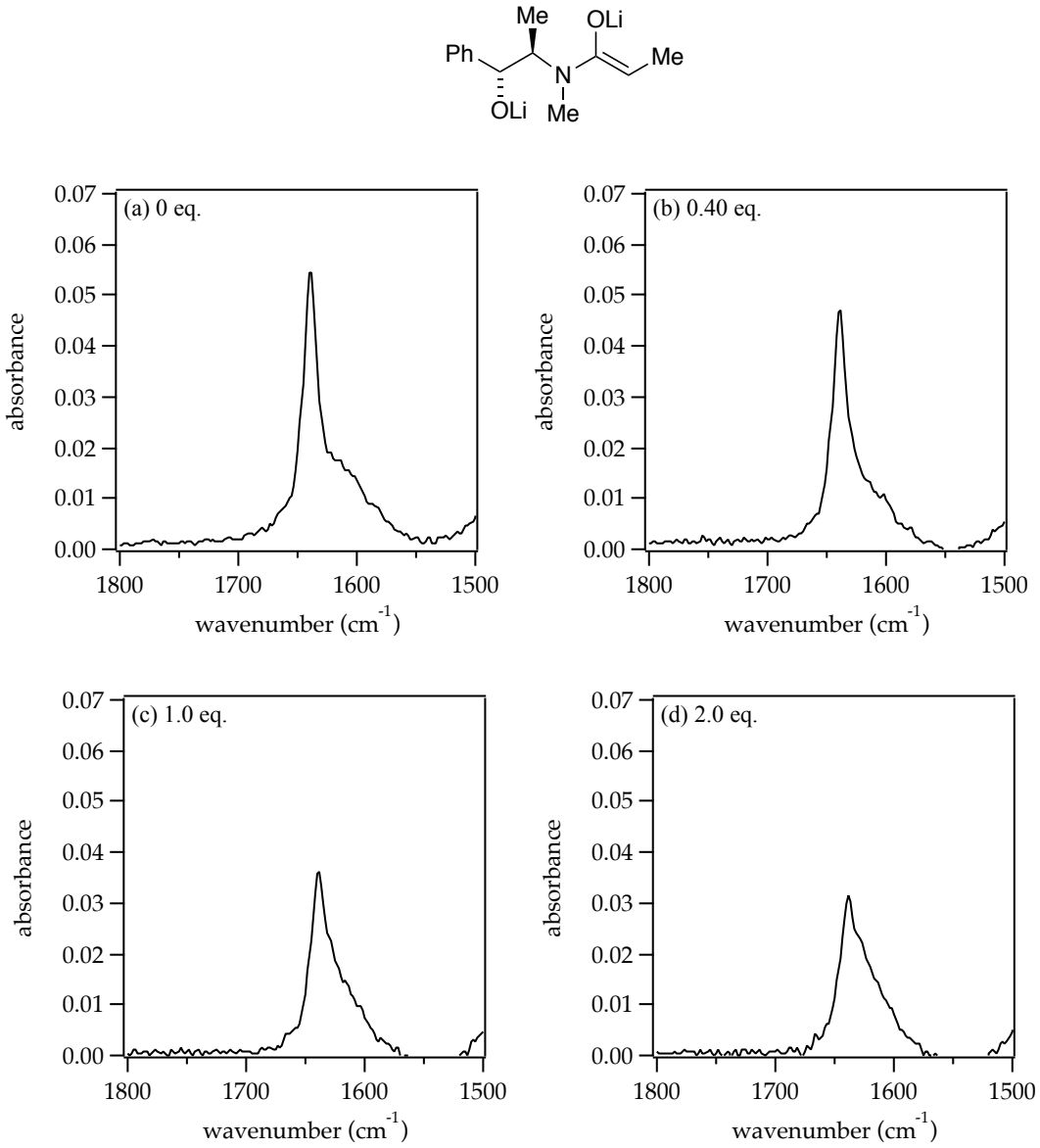


Figure 207. IR spectra of enolate **2** in neat THF at 20 °C with varying LiCl equivalencies. No change in frequency (1640 cm^{-1}) was observed. The attenuated absorbance with increasing LiCl can be accounted for by the dilution.

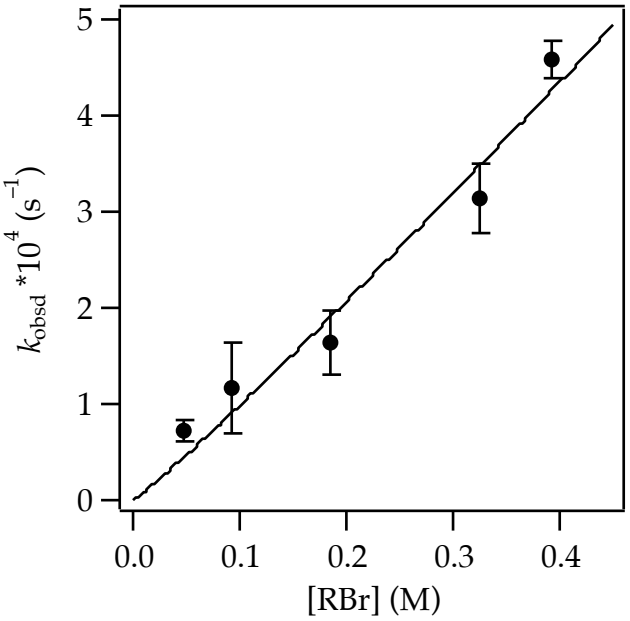


Figure 208. Plot of initial rate constants (k_{obsd}) vs allyl bromide concentrations for alkylation of 0.040 M (*R,R*)-**2** and 0.040 M LiCl in neat tetrahydrofuran (THF) at −60 °C. The curve depicts an unweighted least-squares fit to the function $f(x) = ax^n$ such that $a = (1.2 \pm 0.26) \times 10^{-2}$, $n = 1.1 \pm 0.19$.

[RBr] (M)	Initial Rate × 10^4 (s^{-1})	Standard Deviation × 10^4 (s^{-1})
0.046	0.73	0.098
0.092	1.2	0.48
0.18	1.6	0.33
0.32	3.1	0.35
0.39	4.6	0.18

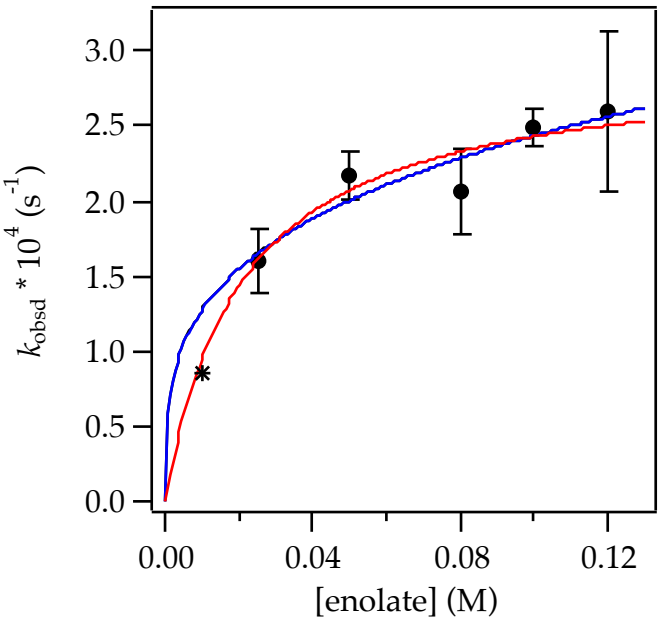


Figure 209. Plot of initial rate constants (k_{obsd}) vs enolate ((*R*,*R*)-**2**) concentration for alkylation with 0.080 M LiCl and 0.18 M allyl bromide in neat tetrahydrofuran (THF) at −60 °C. The black curve (overlapped with blue curve) depicts an unweighted least-squares fit to the function $f(x) = ax^n$ such that $a = (4.6 \pm 0.86) \times 10^{-4}$, $n = 0.28 \pm 0.071$. The blue curve (overlapped with black curve) depicts an unweighted least-squares fit to the function $f(x) = ax^n/(bx^n+1)$ such that $a = (0.47 \pm 4.0) \times 10^{-3}$, $b = 0.027 \pm 10.7$, $n = 0.28 \pm 1.33$. The red curve depicts an unweighted least-squares fit to the function $f(x) = ax/(bx+1)$ such that $a = (1.4 \pm 0.4) \times 10^{-2}$, $b = 47.7 \pm 18.0$. Asterisk (*) denotes a point at 0.010 M enolate where the absorbance at 0.010 M enolate is too low.

[enolate] (M)	Initial Rate × 10^4 (s^{-1})	Standard Deviation × 10^4 (s^{-1})
0.010	0.85	n/a
0.025	1.6	0.21
0.050	2.2	0.17
0.080	2.1	0.28
0.10	2.4	0.13
0.12	2.6	0.53

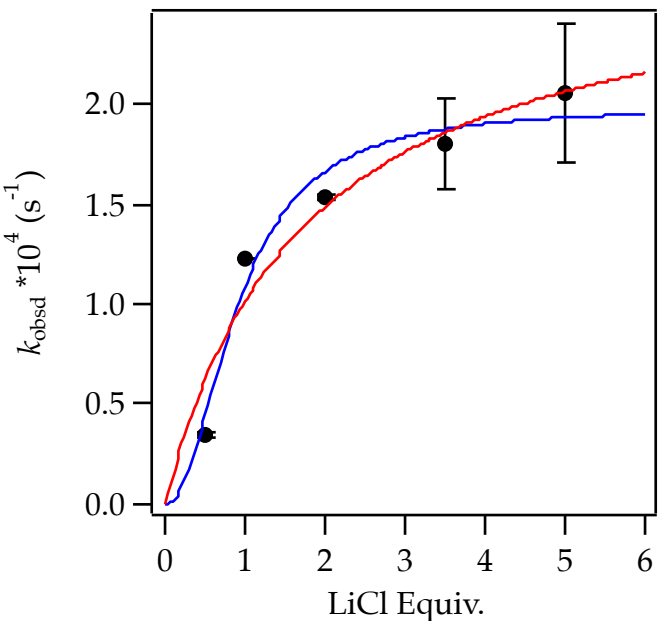


Figure 210. Plot of initial rate constants (k_{obsd}) vs LiCl equivalence (per enolate) for alkylation of 0.040 M (*R,R*)-**2** with 0.092 M allyl bromide in neat THF at −60 °C. The red curve depicts an unweighted least-squares fit to the function $f(x) = ax/(bx+1)$ such that $a = (1.6 \pm 0.45) \times 10^{-4}$, $b = 0.57 \pm 0.25$. The blue curve depicts an unweighted least-squares fit to the function $f(x) = ax^n/(bx^n+1)$ such that $a = (2.3 \pm 0.86) \times 10^{-4}$, $b = 1.2 \pm 0.52$, $n = 2.1 \pm 0.77$.

LiCl Equiv.	Initial Rate × 10^4 (s^{-1})	Standard Deviation × 10^4 (s^{-1})
0.5	0.34	0.019
1.0	1.2	0.000071
2.0	1.5	0.0070
3.5	1.8	0.23
5.0	2.0	0.35

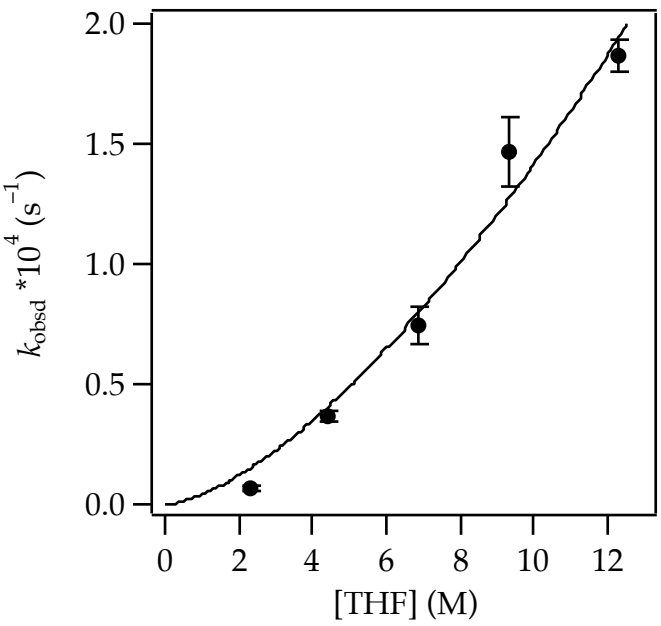


Figure 211. Plot of initial rate constants (k_{obsd}) vs THF concentration for alkylation of 0.040 M (*R,R*)-**2** with 0.092 M allyl bromide and 0.040 M LiCl, in hexanes cosolvent at −60 °C. The curve depicts an unweighted least-squares fit to the function $f(x) = ax^n$ such that $a = (0.042 \pm 0.020) \times 10^{-4}$, $n = 1.5 \pm 0.21$.

[THF] (M)	Initial Rate × 10^4 (s^{-1})	Standard Deviation × 10^4 (s^{-1})
2.3	0.068	0.010
4.4	0.36	0.020
6.9	0.75	0.079
9.3	1.5	0.14
12.3	1.9	0.070

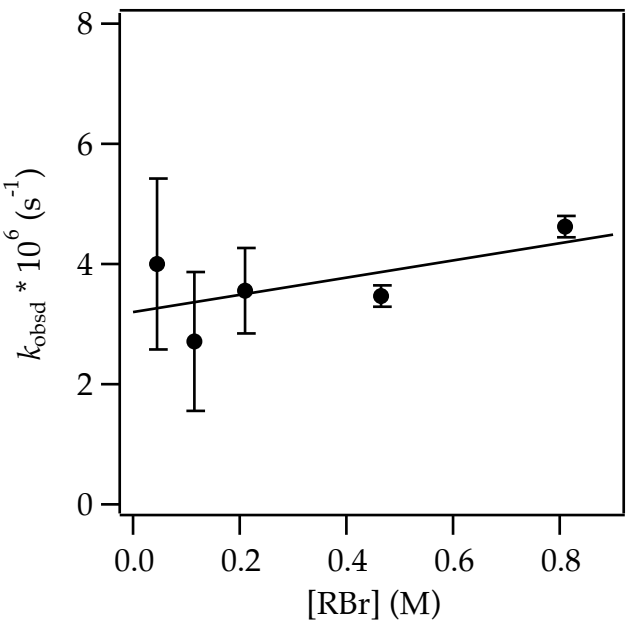


Figure 212. Plot of initial rate constants (k_{obsd}) vs allyl bromide concentration for alkylation of 0.040 M (*R*,*R*)-**2** with 0.092 M allyl bromide in neat THF at 0 °C. The curve depicts an unweighted least-squares fit to the function $f(x) = a + bx$ such that $a = (3.2 \pm 0.43) \times 10^{-6}$, $b = (1.5 \pm 1.1) \times 10^{-6}$.

[allyl bromide] (M)	Initial Rate × 10^6 (s^{-1})	Standard Deviation × 10^6 (s^{-1})
0.046	4.0	1.4
0.12	2.7	1.1
0.21	3.6	0.71
0.46	3.5	0.16
0.81	4.6	0.20

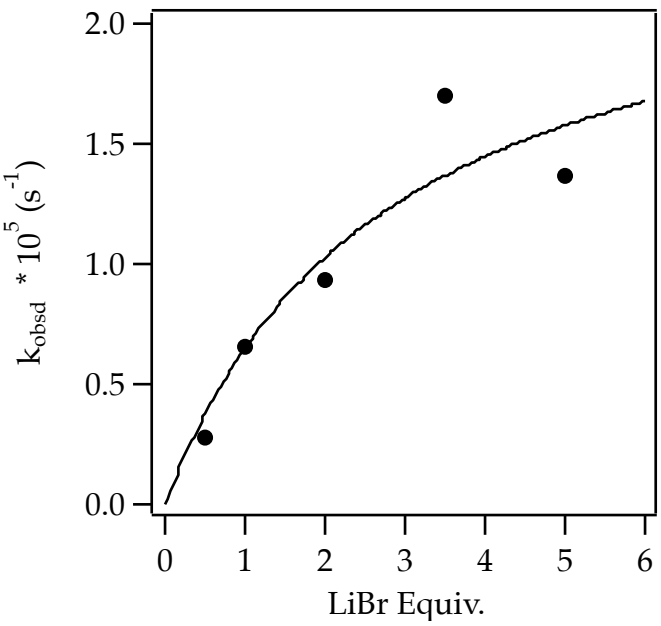


Figure 213. Plot of initial rate constants (k_{obsd}) vs LiBr equivalence (per enolate) for alkylation of 0.040 M (*R,R*)-**2** with 0.092 M allyl bromide in neat THF at −60 °C. The curve depicts an unweighted least-squares fit to the function $f(x) = ax/(bx+1)$ such that $a = (8.8 \pm 3.8) \times 10^{-6}$, $b = 0.36 \pm 0.28$. Initial rates with LiCl are approximately 15 times faster than initial rates with LiBr. The catalytic effect of LiBr byproduct can be ignored.

LiBr Equiv.	Initial Rate × 10^5 (s^{-1})
0.5	0.28
1.0	0.65
2.0	0.92
3.5	1.7
5.0	1.3

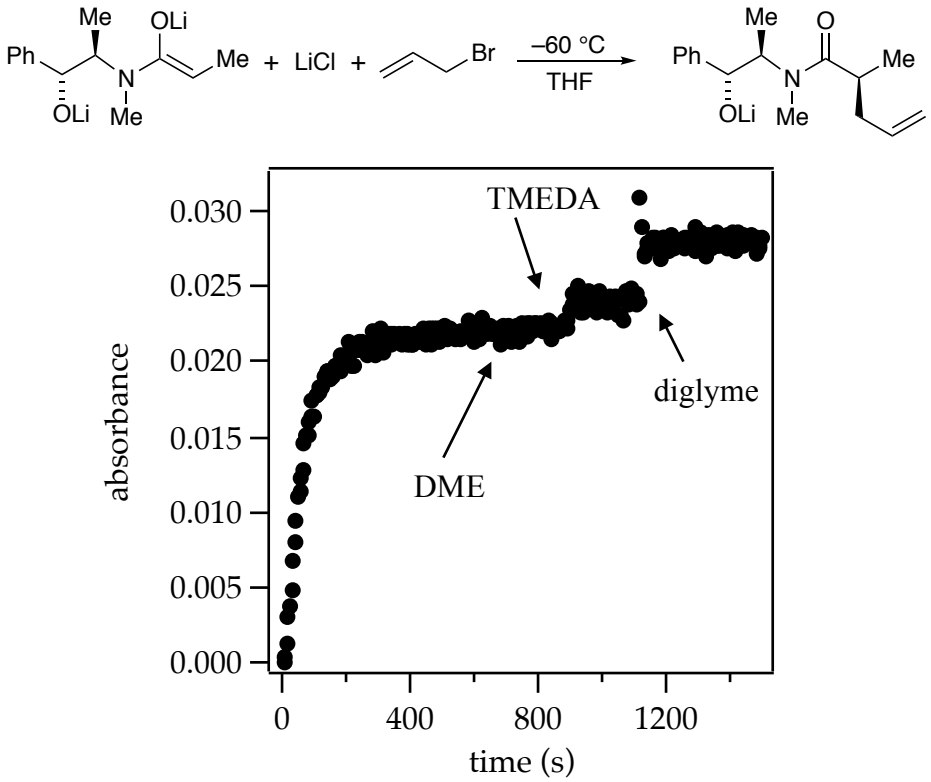


Figure 214. Plot following growth of product in 0.040 M (*R,R*)-**2** and 0.40 M allyl bromide with 0.040 M LiCl in neat THF at –60 °C with 2.0 equiv of different ligands. No visible acceleration was found.

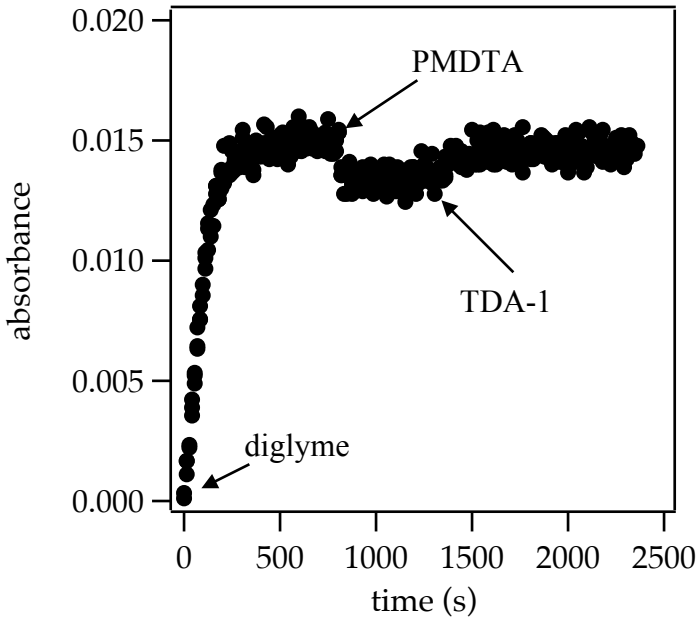
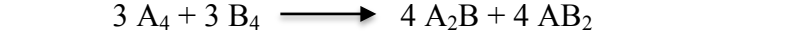


Figure 215. Plot following growth of product in 0.040 M (*R,R*)-**2** and 0.20 M allyl bromide with 0.040 M LiCl in neat THF at –60 °C with 2.0 equiv of different ligands. No visible acceleration was found.

Part 7. Coding for Mathematica

i. Simulation of the tetramer (homoaggregates 4) and trimer (heteroaggregates 5) model using *Mathematica*

To construct a generic model for tetramer and trimer (assuming same amount of solvent per lithium atom) consider the following equilibrium:



$$3\ A_4 + 3\ B_4 \longrightarrow 4\ A_2B + 4\ AB_2$$

for which $K_{eq} = \{[A_2B]^4[AB_2]^4\}/\{[A_4]^3[B_4]^3\}$. Code for fitting the data from integration of NMR spectra is listed below.

For (*S,S*)-**8** and (*R,R*)-**11**: k1 = 25, k2 = 35

```
Manipulate[
 Show[Plot[{Evaluate[
    Interpolation[
     Join[Flatten[
      Table[{x, 4 b4} /.
       NSolve[{k1 (a4*b4^0.5) == a2b^2, k2 (a4^0.5*b4) == ab2^2,
         x == 4 a4 + 2 a2b + ab2, 1 - x == 4 b4 + 2 ab2 + a2b,
         a2b > 0, ab2 > 0}, {a4, a2b, ab2, b4},
        WorkingPrecision -> 1], {x, 0.1, 0.9, 0.1}], 1], {{0, 1}, {1, 0}}], f]],
   Evaluate[
    Interpolation[
     Join[Flatten[
      Table[{x, 3 ab2} /.
       NSolve[{k1 (a4*b4^0.5) == a2b^2, k2 (a4^0.5*b4) == ab2^2,
         x == 4 a4 + 2 a2b + ab2, 1 - x == 4 b4 + 2 ab2 + a2b,
         a2b > 0, ab2 > 0}, {a4, a2b, ab2, b4},
        WorkingPrecision -> 1], {x, 0.1, 0.9, 0.1}], 1], {{0, 0}, {1, 0}}], f]],
   Evaluate[
    Interpolation[
     Join[Flatten[
      Table[{x, 3 a2b} /.
       NSolve[{k1 (a4*b4^0.5) == a2b^2, k2 (a4^0.5*b4) == ab2^2,
         x == 4 a4 + 2 a2b + ab2, 1 - x == 4 b4 + 2 ab2 + a2b,
         a2b > 0, ab2 > 0}, {a4, a2b, ab2, b4},
        WorkingPrecision -> 1], {x, 0.1, 0.9, 0.1}], 1], {{0, 0}, {1, 0}}], f]],
   Evaluate[
    Interpolation[
     Join[Flatten[
      Table[{x, 4 a4} /.
       NSolve[{k1 (a4*b4^0.5) == a2b^2, k2 (a4^0.5*b4) == ab2^2,
         x == 4 a4 + 2 a2b + ab2, 1 - x == 4 b4 + 2 ab2 + a2b,
```

```
          a2b > 0, ab2 > 0}, {a4, a2b, ab2, b4},
         WorkingPrecision -> 1], {x, 0.1, 0.9, 0.1}], 1], {{0, 0}, {1, 1}}], f]]},
        {f, 0, 1}, AspectRatio -> 1],
 ListPlot[{{{0.`, 1.`}, {0.122`, 0.635`}, {0.302`, 0.224`}, {0.372`, 0.130`}, {0.465`, 0.`},
{0.505`, 0.`}, {0.559`, 0.`}, {0.597`, 0.`}, {0.657`, 0.`}, {0.932`, 0.`}, {1.`, 0.`}},
{{0.`, 0.`}, {0.122`, 0.365`}, {0.302`, 0.645`}, {0.372`, 0.624`}, {0.465`, 0.606`},
{0.505`, 0.486`}, {0.559`, 0.408`}, {0.597`, 0.314`}, {0.657`, 0.245`}, {0.932`, 0.`}, {1.`,
0.`}},
{{0.`, 0.`}, {0.122`, 0.`}, {0.302`, 0.131`}, {0.372`, 0.246`}, {0.465`, 0.394`}, {0.505`,
0.514`}, {0.559`, 0.508`}, {0.597`, 0.581`}, {0.657`, 0.538`}, {0.932`, 0.205`}, {1.`,
0.`}},
{{0.`, 0.`}, {0.122`, 0.`}, {0.302`, 0.`}, {0.372`, 0.`}, {0.465`, 0.`}, {0.505`, 0.`},
{0.559`, 0.085`}, {0.597`, 0.105`}, {0.657`, 0.217`}, {0.932`, 0.795`}, {1.`, 1.`}}}]],
{{k1, 25, "k1"}, 0, 1000}, {{k2, 35, "k2"}, 0, 1000}]
```

Code for plotting the data is listed below.

```
Manipulate[
 ListPlot[Flatten[
  Table[{{x, 4 a4}, {x, 3 a2b}, {x, 3 ab2}, {x, 4 b4}} /.
    NSolve[{k1 == a2b^2/(a4*b4^0.5), k2 == ab2^2/(a4^0.5*b4),
      x == 4 a4 + 2 a2b + ab2, 1 - x == 4 b4 + 2 ab2 + a2b,
      a2b > 0, ab2 > 0}, {a4, a2b, ab2, b4}], {x, 0.05, 0.95, 0.05}], 2], PlotRange -> {0,
1}],
      {{k1, 25, "k1"}, 0, 1000}, {{k2, 35, "k2"}, 0, 1000}]

Manipulate[
 Flatten[Table[{x, 4 a4, 3 a2b, 3 ab2, 4 b4} /.
   NSolve[{k1 == a2b^2/(a4*b4^0.5), k2 == ab2^2/(a4^0.5*b4),
     x == 4 a4 + 2 a2b + ab2, 1 - x == 4 b4 + 2 ab2 + a2b,
     a2b > 0, ab2 > 0}, {a4, a2b, ab2, b4}, WorkingPrecision -> 5], {x, 0.05, 0.95, 0.03}],
1],
     {{k1, 25, "k1"}, 0, 1000}, {{k2, 35, "k2"}, 0, 1000}]
```

For (*S,S*)-**2** and (*R,R*)-**11**: k1 = 25, k2 = 30

```
ListPlot[{{{0.`, 1.`}, {0.269`, 0.311`}, {0.471`, 0.0426`}, {0.756`, 0.`}, {1.`, 0.`}},
{{0.`, 0.`}, {0.269`, 0.569`}, {0.471`, 0.502`}, {0.756`, 0.118`}, {1.`, 0.`}},
{{0.`, 0.`}, {0.269`, 0.120`}, {0.471`, 0.456`}, {0.756`, 0.493`}, {1.`, 0.`}},
{{0.`,0.`}, {0.269`, 0.`}, {0.471`, 0.`}, {0.756`, 0.388`}, {1.`, 1.`}}}]],
{{k1, 25, "k1"}, 0, 1000}, {{k2, 30, "k2"}, 0, 1000}]
```

ii. Simulation of the tetramer (homoaggregates 4) and trimer (heteroaggregates 5) model with enantiomer pairs using *Mathematica*

To construct a generic model for tetramer and trimer (assuming same amount of solvent per lithium atom) consider the following equilibrium:

$$3\ A_4 + 3\ B_4 \longrightarrow 4\ A_2B + 4\ AB_2$$

where A_4=B_4, A_2B = AB_2, for which K_{eq} = {$[A_2B]^4[AB_2]^4$}/{$[A_4]^3[B_4]^3$}. Code for fitting the data from integration of NMR spectra is listed below.

For (*S,S*)-**2** and (*R,R*)-**2**: k1 = 25, k2 = 35

```
Manipulate[
 Show[
  Plot[{
    Evaluate[
    Interpolation[
     Join[Flatten[
      Table[{x, 4 b4 + 4 a4} /.
       NSolve[{k1 (a4*b4^0.5) == a2b^2, k2 (a4^0.5*b4) == ab2^2,
         x == 4 a4 + 2 a2b + ab2, 1 - x == 4 b4 + 2 ab2 + a2b,
         a2b > 0, ab2 > 0}, {a4, a2b, ab2, b4},
         WorkingPrecision -> 1], {x, 0.05, 1, 0.1}], 1], {{0, 1}, {1, 1}}], f]],
   Evaluate[
    Interpolation[
     Join[Flatten[
      Table[{x, 3 ab2 + 3 a2b} /.
       NSolve[{k1 (a4*b4^0.5) == a2b^2, k2 (a4^0.5*b4) == ab2^2, x == 4 a4 + 2 a2b +
ab2,
         1 - x == 4 b4 + 2 ab2 + a2b, a2b > 0, ab2 > 0}, {a4, a2b, ab2, b4},
         WorkingPrecision -> 1], {x, 0.05, 0.95, 0.1}], 1],
         {{0, 0}, {1, 0}}], f]]}, {f, 0, 1}, AspectRatio -> 1],
ListPlot[{{{0.`, 1.`}, {0.2`, 0.341`}, {0.3`, 0.264`}, {0.4`, 0.112`}, {0.5`, 0.026`}, {0.6`,
0.117`}, {0.7`, 0.226`}, {0.8`, 0.362`}, {1.`, 1.`}}, {{0.`, 0.`}, {0.2`, 0.658`}, {0.3`,
0.735`}, {0.4`, 0.887`}, {0.5`, 0.974`}, {0.6`, 0.883`}, {0.7`, 0.773`}, {0.8`, 0.637`}, {1`,
0.`}}}]], {{k1, 1000, "k1"}, 0, 100}, {{k2, 1000, "k2"}, 0, 100}]
```

Code for plotting the data from integration of NMR spectra is listed below.

```
Manipulate[
 ListPlot[Flatten[
  Table[{{x, 4 a4 + 4 b4}, {x, 3 a2b}, {x, 3 ab2}, {x, 4 b4}} /.
    NSolve[{k1 == a2b^2/(a4*b4^0.5), k2 == ab2^2/(a4^0.5*b4), x == 4 a4 + 2 a2b +
ab2,
1 - x == 4 b4 + 2 ab2 + a2b, a2b > 0, ab2 > 0}, {a4, a2b, ab2, b4}], {x, 0.05, 0.95, 0.05}],
```

```
2], PlotRange -> {0, 1}], {{k1, 1, "k1"}, 0, 1000}, {{k2, 1, "k2"}, 0, 1000}]

Manipulate[
 Flatten[Table[{x, 4 a4, 3 a2b, 3 ab2, 4 b4} /.
   NSolve[{k1 == a2b^2/(a4*b4^0.5), k2 == ab2^2/(a4^0.5*b4),
     x == 4 a4 + 2 a2b + ab2, 1 - x == 4 b4 + 2 ab2 + a2b, a2b > 0, ab2 > 0}, {a4, a2b,
ab2, b4},
     WorkingPrecision -> 5], {x, 0.05, 0.95, 0.03}], 1], {{k1, 4, "k1"}, 0, 1000}, {{k2,
6.5, "k2"},
      0, 1000}]
```

For (*S,S*)-**11** and (*R,R*)-**11**: k1 = k2 = 80

```
ListPlot[{{{0.`, 1.`}, {0.2`, 0.341`}, {0.3`, 0.264`}, {0.4`, 0.112`}, {0.5`, 0.026`}, {0.6`,
0.117`}, {0.7`, 0.226`}, {0.8`, 0.362`}, {1.`, 1.`}}, {{0.`, 0.`}, {0.2`, 0.658`}, {0.3`,
0.735`}, {0.4`, 0.887`}, {0.5`, 0.974`}, {0.6`, 0.883`}, {0.7`, 0.773`}, {0.8`, 0.637`}, {1`,
0.`}}}]], {{k1, 80, "k1"}, 0, 100}, {{k2, 80, "k2"}, 0, 100}]
```

iii. Simulation of the dimer and trimer model using *Mathematica*

To construct a generic model for tetramer and trimer (assuming same amount of solvent per lithium atom) consider the following equilibrium:

$$3\ A_2 + 3\ B_2 \longrightarrow 2\ A_2B + 2\ AB_2$$

for which $K_{eq} = \{[A_2B]^2[AB_2]^2\}/\{[A_2]^3[B_2]^3\}$. Code for fitting the data from integration of NMR spectra is listed below.

For (*S,S*)-**16** and (*R,R*)-**14**: k1 = 35, k2 = 70

```
Manipulate[
 Show[
  Plot[{
    Evaluate[
     Interpolation[
      Join[Flatten[
        Table[{x, 2 b2} /.
          NSolve[{k1 (a2*b2^0.5) == a2b, k2 (a2^0.5*b2) == ab2,
            x == 2 a2 + 2 a2b + ab2, 1 - x == 2 b2 + 2 ab2 + a2b,
            a2b > 0, ab2 > 0}, {a2, a2b, ab2, b2},
           WorkingPrecision -> 1], {x, 0.1, 0.9, 0.1}], 1], {{0, 1}, {1, 0}}], f]],
    Evaluate[
     Interpolation[
      Join[Flatten[
        Table[{x, 3 ab2} /.
          NSolve[{k1 (a2*b2^0.5) == a2b, k2 (a2^0.5*b2) == ab2,
            x == 2 a2 + 2 a2b + ab2, 1 - x == 2 b2 + 2 ab2 + a2b,
            a2b > 0, ab2 > 0}, {a2, a2b, ab2, b2},
           WorkingPrecision -> 1], {x, 0.1, 0.9, 0.1}], 1], {{0, 0}, {1, 0}}], f]],
    Evaluate[
     Interpolation[
      Join[Flatten[
        Table[{x, 3 a2b} /.
          NSolve[{k1 (a2*b2^0.5) == a2b, k2 (a2^0.5*b2) == ab2,
            x == 2 a2 + 2 a2b + ab2, 1 - x == 2 b2 + 2 ab2 + a2b,
            a2b > 0, ab2 > 0}, {a2, a2b, ab2, b2},
           WorkingPrecision -> 1], {x, 0.1, 0.9, 0.1}], 1], {{0, 0}, {1, 0}}], f]],
    Evaluate[
     Interpolation[
      Join[
       Flatten[
        Table[{x, 2 a2} /.
          NSolve[{k1 (a2*b2^0.5) == a2b, k2 (a2^0.5*b2) == ab2,
            x == 2 a2 + 2 a2b + ab2, 1 - x == 2 b2 + 2 ab2 + a2b,
```

```
          a2b > 0, ab2 > 0}, {a2, a2b, ab2, b2},
         WorkingPrecision -> 1],
          {x, 0.1, 0.9, 0.1}], 1], {{0, 0}, {1, 1}}], f]]}, {f, 0, 1}, AspectRatio -> 1],
  ListPlot[{{{0.`, 1.`}, {0.147`, 0.656`}, {0.258`, 0.305`}, {0.343`, 0.114`}, {0.433`,
0.038`}, {0.493`, 0.021`}, {0.557`,0.014`}, {0.651`, 0.003`}, {0.737`, 0.`}, {0.846`, 0.`},
{1.`, 0.`}},
{{0.`, 0.`}, {0.147`, 0.344`}, {0.258`, 0.695`}, {0.343`, 0.784`}, {0.433`, 0.660`},
{0.493`, 0.523`}, {0.557`, 0.370`}, {0.651`, 0.183`}, {0.737`, 0.085`}, {0.846`, 0.`}, {1.`,
0.`}},
{{0.`, 0.`}, {0.147`, 0.`}, {0.258`, 0.`}, {0.343`, 0.093`}, {0.433`, 0.261`}, {0.493`,
0.387`}, {0.557`, 0.504`}, {0.651`, 0.597`}, {0.737`,0.512`}, {0.846`, 0.363`}, {1.`,
0.`}},
{{0.`, 0.`}, {0.147`, 0.`}, {0.258`, 0.`}, {0.343`, 0.009`}, {0.433`, 0.041`}, {0.493`,
0.068`}, {0.557`, 0.112`}, {0.651`, 0.216`}, {0.737`, 0.402`}, {0.846`, 0.637`}, {1.`,
1.`}}}]],
{{k1, 35, "k1"}, 0, 1000}, {{k2, 70, "k2"}, 0, 1000}]
```

Code for plotting the data is listed below.

```
Manipulate[
 ListPlot[Flatten[
   Table[{{x, 2 a2}, {x, 3 a2b}, {x, 3 ab2}, {x, 2 b2}} /.
     NSolve[{k1 == a2b/(a2*b2^0.5), k2 == ab2/(a2^0.5*b2),
       x == 2 a2 + 2 a2b + ab2, 1 - x == 2 b2 + 2 ab2 + a2b,
      a2b > 0, ab2 > 0}, {a2, a2b, ab2, b2}], {x, 0.05, 0.95, 0.05}], 2],
     PlotRange -> {0, 1}], {{k1, 35, "k1"}, 0, 1000}, {{k2, 70, "k2"}, 0, 1000}]

Manipulate[
 Flatten[Table[{x, 2 a2, 3 a2b, 3 ab2, 2 b2} /.
    NSolve[{k1 == a2b/(a2*b2^0.5), k2 == ab2/(a2^0.5*b2),
      x == 2 a2 + 2 a2b + ab2, 1 - x == 2 b2 + 2 ab2 + a2b,
      a2b > 0, ab2 > 0}, {a2, a2b, ab2, b2}, WorkingPrecision -> 5],
     {x, 0.05, 0.95, 0.03}], 1], {{k1, 35, "k1"}, 0, 1000}, {{k2, 70, "k2"}, 0, 1000}]
```

For (*S,S*)-**15** and (*R,R*)-**14**: k1 = 3, k2 = 1

```
ListPlot[{{{0.`, 1.`}, {0.23`, 0.620`}, {0.483`, 0.296`}, {0.75`, 0.229`}, {1.`, 0.`}},
{{0.`, 0.`}, {0.23`, 0.216`}, {0.483`, 0.162`}, {0.613`, 0.054`}, {1.`, 0.`}},
{{0.`, 0.`}, {0.23`, 0.148`}, {0.483`, 0.414`}, {0.613`, 0.374`}, {1.`, 0.`}},
{{0.`, 0.`}, {0.23`, 0.015`}, {0.483`, 0.126`}, {0.613`, 0.343`}, {1.`, 1.`}}}]],
{{k1, 3, "k1"}, 0, 100}, {{k2, 1, "k2"}, 0, 100}]
```

For (*S,S*)-**16** and (*R,R*)-**13**: k1 = 60, k2 = 90

```
ListPlot[{{{0.`, 1.`}, {0.1`, 0.756`}, {0.2`, 0.417`}, {0.3`, 0.119`}, {0.4`, 0.053`}, {0.5`,
```

```
0.016`}, {0.6`, 0.005`}, {0.7`, 0.`}, {0.8`, 0.`}, {0.9`, 0.`}, {1.`, 0.`}},
{{0.`, 0.`}, {0.1`, 0.244`}, {0.2`, 0.565`}, {0.3`, 0.842`}, {0.4`, 0.718`}, {0.5`, 0.493`},
{0.6`, 0.2243`}, {0.7`, 0.075`}, {0.8`, 0.019`}, {0.9`, 0.004`}, {1.`, 0.`}},
{{0.`, 0.`}, {0.1`, 0.`}, {0.2`, 0.018`}, {0.3`, 0.038`}, {0.4`, 0.219`}, {0.5`, 0.455`},
{0.6`, 0.668`}, {0.7`, 0.674`}, {0.8`, 0.455`}, {0.9`, 0.212`}, {1.`, 0.`}},
{{0.`, 0.`}, {0.1`, 0.`}, {0.2`, 0.`}, {0.3`, 0.`}, {0.4`, 0.009`}, {0.5`, 0.034`}, {0.6`,
0.083`}, {0.7`, 0.250`}, {0.8`, 0.524`}, {0.9`, 0.783`}, {1.`, 1.`}}}]],
{{k1, 60, "k1"}, 0, 1000}, {{k2, 90, "k2"}, 0, 1000}]
```

For (*S,S*)-**18** and (*R,R*)-**16**: k1 = 4, k2 = 9

```
ListPlot[{{{0.`, 1.`}, {0.25`, 0.393`}, {0.5`, 0.0614`}, {0.75`, 0.0013`}, {1.`, 0.`}},
{{0.`, 0.`}, {0.25`, 0.480`}, {0.5`, 0.515`}, {0.75`, 0.126`}, {1.`, 0.`}},
{{0.`, 0.`}, {0.25`, 0.127`}, {0.5`, 0.209`}, {0.75`, 0.368`}, {1.`, 0.`}},
{{0.`, 0.`}, {0.25`, 0.`}, {0.5`, 0.214`}, {0.75`, 0.504`}, {1.`, 1.`}}}]],
{{k1, 4, "k1"}, 0, 100}, {{k2, 9, "k2"}, 0, 100}]
```

iv. Simulation of the dimer and trimer model with enantiomer pairs using *Mathematica*

To construct a generic model for tetramer and trimer (assuming same amount of solvent per lithium atom) consider the following equilibrium:

$$3\ A_2 + 3\ B_2 \longrightarrow 2\ A_2B + 2\ AB_2$$

where A_2=B_2, A_2B = AB_2, for which K_{eq} = {$[A_2B]^2[AB_2]^2$}/{$[A_2]^3[B_2]^3$}. Code for fitting the data from integration of NMR spectra is listed below.

For (*S,S*)-**16** and (*R,R*)-**16**: k1 = k2 = 190

```
Manipulate[
 Show[
  Plot[{
    Evaluate[
     Interpolation[
      Join[Flatten[
        Table[{x, 2 b2 + 2 a2} /.
          NSolve[{k1 (a2*b2^0.5) == a2b, k2 (a2^0.5*b2) == ab2,
            x == 2 a2 + 2 a2b + ab2, 1 - x == 2 b2 + 2 ab2 + a2b,
            a2b > 0, ab2 > 0}, {a2, a2b, ab2, b2},
          WorkingPrecision -> 1], {x, 0.05, 1, 0.1}], 1], {{0, 1}, {1, 1}}], f]],
    Evaluate[
     Interpolation[
      Join[Flatten[
        Table[{x, 3 ab2 + 3 a2b} /.
          NSolve[{k1 (a2*b2^0.5) == a2b, k2 (a2^0.5*b2) == ab2,
            x == 2 a2 + 2 a2b + ab2, 1 - x == 2 b2 + 2 ab2 + a2b,
            a2b > 0, ab2 > 0}, {a2, a2b, ab2, b2},
          WorkingPrecision -> 1],
          {x, 0.05, 0.95, 0.1}], 1], {{0, 0}, {1, 0}}], f]]}, {f, 0, 1}, AspectRatio -> 1],
  ListPlot[{{{0.`, 1.`}, {0.25`, 0.197`}, {0.5`, 0.0388`}, {0.75`, 0.204`}, {1.`, 1.`}}, {{0.`,
0.`}, {0.25`, 0.803`}, {0.5`, 0.962`}, {0.75`, 0.796`}, {1`, 0.`}}}]], {{k1, 190, "k1"}, 0,
1000}, {{k2, 190, "k2"}, 0, 1000}]

K1=190, K2=190

Manipulate[
 ListPlot[
  Flatten[
   Table[{{x, 2 a2 + 2 b2}, {x, 3 a2b + 3 ab2}} /.
     NSolve[{k1 == a2b/(a2*b2^0.5), k2 == ab2/(a2^0.5*b2),
       x == 2 a2 + 2 a2b + ab2, 1 - x == 2 b2 + 2 ab2 + a2b,
       a2b > 0, ab2 > 0}, {a2, a2b, ab2, b2}], {x, 0.05, 0.95, 0.05}], 2], PlotRange -> {0,
```

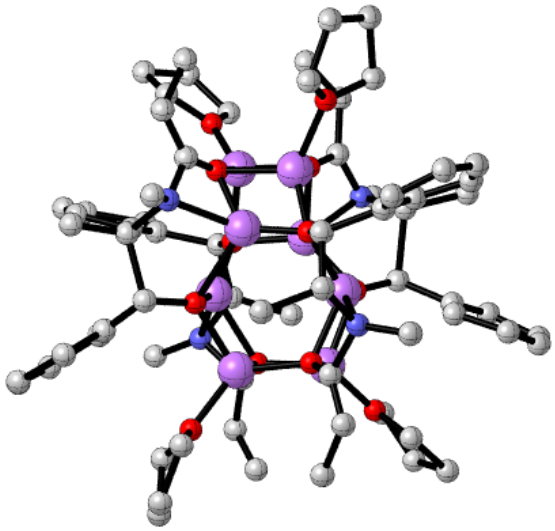
```
1}],
     {{k1, 190, "k1"}, 0, 1000}, {{k2, 190, "k2"}, 0, 1000}]


Manipulate[
 Flatten[
  Table[{x, 2 a2 + 2 b2, 3 a2b + 3 ab2} /.
    NSolve[{k1 == a2b/(a2*b2^0.5), k2 == ab2/(a2^0.5*b2),
      x == 2 a2 + 2 a2b + ab2, 1 - x == 2 b2 + 2 ab2 + a2b,
      a2b > 0, ab2 > 0}, {a2, a2b, ab2, b2}, WorkingPrecision -> 5],
     {x, 0.05, 0.95, 0.05}], 1], {{k1, 190, "k1"}, 0, 1000}, {{k2, 190, "k2"}, 0, 1000}]
```

Part 8. Crystal Structure Data

Owing to the low resolution of the crystal, only coordinates (xyz) are presented.

Table 4. Crystal structure for (*R,R*)-**4**

Samples for X-ray spectroscopy were prepared from 0.11 M (*R,R*)-**1** and 0.23 M LDA in neat THF, aged at 25 °C for 10 min. The sample was kept at –20 °C for 3-5 days until crystals have grown out.



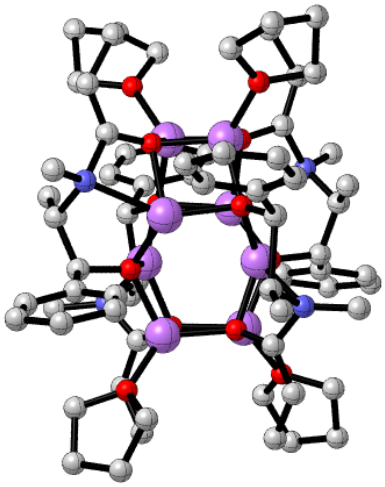
Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	Li	5.19180000	-1.69246000	-0.34364100
O	0.24932400	0.11012000	1.84358900	O	6.53668100	-2.56767000	-1.49298200
C	-0.07333000	1.26355000	2.36137200	C	6.92240100	-3.90078000	-1.40707100
N	1.05156000	2.12137000	2.61213800	C	8.25701100	-3.94715000	-2.14775700
C	1.59860500	1.35049000	3.89614800	C	8.52100100	-2.78793000	-2.55873400
C	1.42261200	2.00545000	5.44485900	C	7.14239100	-1.84316000	-2.56105600
C	0.98262900	3.55301000	2.60052800	Li	3.62252700	-1.21139000	2.57730900
Li	1.96525800	0.82884000	1.30026400	C	6.99426100	-3.10092000	2.56337800
O	3.54186300	0.56802000	2.47282400	C	8.13969100	-2.46334000	1.69034300
C	3.39373600	1.57074000	3.38765200	C	5.04513900	-3.57620000	4.68791600
C	4.21503700	1.36788000	4.76453900	C	4.00384600	-4.72382000	1.33509300
C	4.56115700	2.52710000	5.42627900	C	1.89486000	-3.51824000	4.46037000
C	5.38245900	2.28366000	6.68939900	C	1.66900200	-2.34742000	5.01762900
C	5.58485100	1.11285000	6.90532900	C	1.46954400	-2.41698000	6.50131900
C	5.21233200	-0.08694000	6.40611900	C	1.21728700	-3.47766000	6.91461900
C	4.54355800	0.13910000	5.04780900	C	1.30528300	-4.72382000	6.35968900
Li	5.35312700	0.16229000	1.54406300	C	1.72620000	-4.72382000	4.99208900
O	5.01287300	0.26082000	-0.30416900	Li	0.43998300	-1.87794000	1.96432700
C	5.30912900	1.27514000	-1.04253300	O	-1.08382400	-2.64302000	3.19957800
N	4.08744200	1.53017000	-2.08274400	C	-1.52527400	-1.76781000	4.27694000

C	4.34116600	1.90112000	-3.48285000	C	-2.96255200	-2.41118000	4.55092400
C	3.07988100	2.60824000	-1.36992100	C	-2.90388700	-3.68632000	3.84738800
C	1.70126800	1.88373000	-1.33973600	C	-1.48127600	-3.93555000	3.15778400
O	1.78779800	0.70712000	-0.62226900	C	-1.43727700	-3.59938000	-0.75693900
Li	3.12388000	-0.55643000	-0.95197900	C	-2.63989800	-3.06034000	-0.14395800
O	3.37613700	-2.15036000	-1.04021100	C	0.80663600	-5.34401000	-0.81498700
C	3.18547700	-3.24582000	-2.02005300	C	1.05596000	-4.00511000	-3.41551500
C	1.44461100	-3.28060000	-2.21741400	C	3.75158900	-3.01397000	-3.25530400
N	0.83156800	-3.77326000	-0.89393100	C	4.26783500	-4.25434000	-3.99831200
C	-0.20972500	-3.01397000	-0.49224300	C	4.73715100	-3.83122000	-5.42395800
O	0.13492800	-1.91272000	-0.04643800	C	4.70781800	-2.71837000	-5.78849700
Li	1.73060000	-2.45755000	0.55725600	C	4.38516400	-1.69826000	-5.24749400
O	2.08405300	-2.46334000	2.22670200	C	3.78385400	-1.83157000	-3.76380000
C	2.23364700	-3.61677000	2.84432800	C	1.12635700	1.55915000	-2.87451200
C	3.63719300	-4.18479000	2.81414300	C	1.03249400	0.44050000	-3.20886600
N	4.60808900	-3.12410000	3.29477600	C	0.45464900	0.23184000	-4.57646500
C	5.70658100	-2.71837000	2.32190000	C	0.14959500	1.15342000	-5.18248100
O	5.30032900	-1.71565000	1.62300800	C	0.24932400	2.29525000	-4.95029100
C	0.73623900	2.78213000	-3.50839100	H	3.97602511	-3.90943331	0.64162323
C	3.75452200	3.07773000	0.04876000	H	1.63136659	-1.43265557	4.46383336
C	6.57041100	1.79099000	-1.56728200	H	1.07952526	-5.61945549	6.89984686
C	7.69970100	1.17081000	-0.98448600	H	1.89228995	-5.62538391	4.44027686
O	6.63788100	1.27514000	2.35672900	H	-0.90355849	-1.92963830	5.13261600
C	6.70241100	2.71257000	2.21277100	H	-1.65560231	-0.77890929	3.88965469
C	8.03702100	2.92703000	2.80949900	H	-3.04036845	-2.61415534	5.59860984
C	8.44767100	1.94169000	3.87757300	H	-3.69647109	-1.80007989	4.06841035
C	7.49438100	0.57961000	3.36211100	H	-3.00926731	-4.44427276	4.59525337
C	-1.52527400	1.61711000	2.55176800	H	-3.61393533	-3.61937906	3.04973502
O	-1.38008000	0.96795000	-0.79873400	H	-0.86523948	-4.52182967	3.80714919
C	-1.72473300	2.28366000	-0.65013200	H	-1.62295651	-4.23493589	2.14033881
C	-2.91855400	2.30685000	-1.60211100	H	-2.38235100	-2.22365100	0.47128266
C	-3.02121600	0.93897000	-2.41477600	H	-3.10334942	-3.81519223	0.45630101
C	-2.25857900	0.24343000	-1.68802100	H	-3.31931953	-2.74535507	-0.90820330
H	1.02561513	0.44731030	3.92528642	H	0.37511746	-5.64753676	0.11590679
H	1.85221091	1.34016198	6.16439818	H	1.80578262	-5.72052756	-0.88456121
H	0.38295260	2.13968308	5.65931135	H	0.22204771	-5.73248260	-1.62260421
H	1.92129082	2.95101313	5.49100883	H	0.37930887	-4.79136393	-3.15312594
H	1.33828477	3.93480138	3.53468233	H	1.92592722	-4.42268895	-3.87777560
H	-0.03164450	3.86006688	2.45265867	H	0.57645207	-3.33478624	-4.09789187
H	1.58978937	3.93288856	1.80557608	H	3.42743347	-0.97903750	-3.22430697
H	3.81254835	2.44207695	2.92910196	H	3.11229993	3.78353982	0.53278821
H	5.36001542	-1.03465427	6.88038397	H	3.88690550	2.22429259	0.68043966
H	4.35636576	-0.66663033	4.36909131	H	4.70463589	3.53174997	-0.14110698
H	5.39628064	1.96048562	-3.65050687	H	7.37753970	0.44237397	-0.26999804
H	3.89359683	2.85137962	-3.68678257	H	8.29942040	1.90952974	-0.49506820
H	3.91824519	1.16142002	-4.13006088	H	8.27666031	0.69124505	-1.74739845

H	2.92246999	3.54047448	-1.87098053	H	5.96179369	3.16082726	2.84162028
H	1.01171252	2.54777055	-0.86175756	H	6.74072495	2.95866331	1.17216054
H	3.64568808	-4.14526320	-1.66776378	H	7.97802638	3.87393389	3.30426425
H	1.04423365	-2.30488541	-2.39791056	H	8.73234196	2.78413774	2.00886764
H	3.70486865	-5.02679996	3.47090721	H	8.08431767	2.28279327	4.82442194
H	7.10912725	-4.12401841	-0.37741187	H	9.48452351	1.70742497	3.75527511
H	6.21738804	-4.48412782	-1.96165377	H	6.88186240	0.25404369	4.17680575
H	7.37866704	-0.84952008	-2.24206801	H	8.12832157	-0.11884693	2.85696026
H	6.59358448	-1.99812306	-3.46642766	H	-1.60099260	2.59253461	2.98502720
H	7.21995880	-3.81603314	3.32664316	H	-2.07099000	2.44405979	0.34950693
H	9.08481293	-2.86039219	1.99692756	H	-0.94521816	2.89716227	-1.05121999
H	8.13932568	-1.40145872	1.82190290	H	-3.79429403	2.36295945	-0.98987646
H	7.97308647	-2.69502677	0.65909901	H	-2.71866590	3.07332910	-2.32145413
H	4.18236698	-3.83115421	5.26715929	C	-2.51557244	0.69912114	2.01312166
H	5.57663244	-2.78250620	5.17006212	H	-2.11891169	-0.29463804	2.01483956
H	5.68237120	-4.43142885	4.60178395	H	-3.39814107	0.73191654	2.61718877
H	3.29346533	-5.46770763	1.04032106	H	-2.75852638	0.98444310	1.01089177
H	4.98476696	-5.15114974	1.34422330	H	6.25310113	0.98922464	7.73180256
H	5.74224744	3.07014818	7.31938997	H	0.84672593	-3.47511614	7.91840086
H	4.28112417	3.50253142	5.08714016	H	1.33688777	-0.37297620	-2.58396529
H	-2.63304915	1.04120717	-3.40662985	H	0.33069018	-0.75319136	-4.97552319
H	-4.02040215	0.55618154	-2.41497242	H	-0.30587820	0.93196308	-6.12503126
H	-1.65332448	-0.36282708	-2.32912888	H	0.01388847	3.01585370	-5.70540716
H	-2.86847988	-0.40500915	-1.09434803	H	0.76389404	3.77643140	-3.11405621
H	9.25290018	-2.34357814	-1.91703702	H	4.30032684	-5.24780549	-3.60224306
H	8.91140822	-2.84590524	-3.55327966	H	5.09875774	-4.58403206	-6.09284855
H	9.02724412	-4.27835817	-1.48296975	H	5.03157325	-2.58684202	-6.79982431
H	8.18518017	-4.61699736	-2.97904807	H	4.49217569	-0.74823791	-5.72802135
H	1.56918678	-4.32774874	2.39946639	H	-1.49969862	-4.44476265	-1.40987983
H	1.55239687	-1.55789386	7.13377960	H	6.63334409	2.55604798	-2.31268505

Table 5. Crystal structure for (*S,S*)-**4**

Samples for X-ray spectroscopy were prepared from 0.040 M (*S,S*)-**1**, 0.040 M (*R,R*)-**1** and 0.17 M LDA in neat THF, aged at 25 °C for 10 min. The sample was kept at –20 °C for at least 7 days until crystals have grown out. (Protons are omitted)



Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	C	1.43721900	3.67941900	-4.65528700
O	1.53969600	0.05647300	1.20247900	C	1.07214900	3.93427100	-6.00148100
C	1.86248100	-0.25774700	2.43952300	C	1.89872900	4.21663400	-6.99839300
N	1.60105300	0.91949300	3.47645600	C	3.21239200	4.31510000	-6.66366300
C	2.80086200	1.83898600	3.49646700	C	3.79211200	4.07328000	-5.40297000
C	2.27062200	3.20591600	3.24905900	C	2.73064200	3.80394900	-4.42970800
O	1.69919700	3.27542100	1.97017400	C	-0.15100400	1.83898600	-3.86030400
Li	1.39521900	5.03042200	1.19520200	N	1.04880300	0.91949300	-3.84029300
O	-0.05956800	4.94933300	-0.05275600	C	0.78737500	-0.25774700	-2.80335900
C	-1.29294700	5.33450600	-0.17828000	O	1.11016000	0.05647300	-1.56631600
N	-2.14728400	4.33682000	-0.50391400	Li	2.64985200	0.00000000	-0.36383700
C	-2.25618500	3.81987700	0.74586400	O	4.05171200	-1.43788400	-0.43296500
C	-3.45215900	4.27889900	1.53357000	C	5.11028200	-1.62323000	0.53665800
C	-3.27120100	4.42370100	-1.37712100	C	5.70842200	-3.03215400	0.08914000
Li	-0.30718300	3.20302000	-0.71675800	C	5.62440200	-2.90038400	-1.38439800
O	-0.80908000	1.71735200	0.28743100	C	4.25846200	-2.32117600	-1.57177300
C	-2.16583600	1.96785900	0.39840100	O	3.45893200	1.71735200	-0.65126700
C	-2.79843000	1.27281000	1.59542200	C	4.81569200	1.96785900	-0.76223700
C	-4.16731800	0.96583000	1.58086900	C	5.44828200	1.27281000	-1.95925900
C	-4.75838700	0.43440600	2.71240000	C	6.81717200	0.96583000	-1.94470600
C	-4.05335000	0.25630000	3.86030400	C	7.40824200	0.43440600	-3.07623700
C	-2.71920000	0.50680700	3.91124100	C	6.70320200	0.25630000	-4.22414000
C	-2.08742600	1.02664600	2.76151800	C	5.36905200	0.50680700	-4.27507800
Li	0.66960300	1.89111400	1.62089100	C	4.73728200	1.02664600	-3.12535500
O	0.95065800	3.27542100	-2.33401100	Li	2.95704200	3.20302000	0.35292100

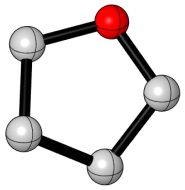
C	0.37923400	3.20591600	-3.61289500	O	2.70942200	4.94933300	-0.31108000
C	3.94280200	5.33450600	-0.18555700	H	-4.13660649	4.03198949	-0.88464215
N	4.79714200	4.33682000	0.14007700	H	-3.44194371	5.44728426	-1.63793557
C	4.90604200	3.81987700	-1.10970100	H	-3.07843602	3.85702444	-2.26403663
C	6.10201200	4.27889900	-1.89740700	H	-2.61872288	1.53459800	-0.46882352
C	5.92106200	4.42370100	1.01328400	H	-5.79163743	0.15789520	2.68349785
C	4.39411200	6.57835500	0.04729900	H	-4.55775823	-0.08718361	4.73921887
C	3.60855200	7.76862700	0.08550100	H	-2.16003317	0.31430828	4.80296780
Li	1.25463700	5.03042200	-1.55903900	H	-0.46324213	3.85957111	-3.70160218
O	1.25817500	6.36260000	-2.88340300	H	0.02871274	3.89484142	-6.23511763
C	2.47454200	7.01565700	-3.32910300	H	1.55424042	4.35788936	-8.00152536
C	1.98760600	8.30005100	-3.84211200	H	3.88107177	4.60928265	-7.44547112
C	0.54061500	8.15235300	-4.16592700	H	3.04278035	3.69502874	-3.41206070
C	0.14697300	6.78542200	-3.70203500	H	-0.63902059	1.84210836	-4.81252774
Li	1.98025300	1.89111400	-1.98472800	H	4.66725688	-1.73549978	1.50414146
C	0.53206100	-1.55806900	-3.18174900	H	5.85456849	-0.87213990	0.37294701
C	0.63508000	-2.81350300	-2.32855300	H	5.03769033	-3.80450827	0.40296783
C	1.42635500	0.57631200	-5.21013700	H	6.73974737	-3.07190523	0.37143031
C	-1.34375700	1.36113900	-3.03985300	H	6.34376716	-2.17315793	-1.69833431
C	-1.74425500	6.57835500	-0.41113500	H	5.63467746	-3.88174438	-1.81069159
C	-0.95869700	7.76862700	-0.44933800	H	3.55333543	-3.12208394	-1.49276041
O	1.39168100	6.36260000	2.51956700	H	4.28204237	-1.71407744	-2.45255408
C	0.17531500	7.01565700	2.96526600	H	5.26857914	1.53459660	0.10498669
C	0.66225000	8.30005100	3.47827500	H	8.44149265	0.15789593	-3.04733593
C	2.10924200	8.15235300	3.80209000	H	7.20760938	-0.08718441	-5.10305504
C	2.50288200	6.78542200	3.33819800	H	4.80988432	0.31430830	-5.16680428
C	1.21263700	3.67941900	4.29145000	H	4.05437286	4.18472919	-1.64490429
C	1.57770600	3.93427100	5.63764700	H	6.67809492	4.96013450	-1.30668992
C	0.75112700	4.21663400	6.63455700	H	6.70461839	3.43341194	-2.15609054
C	-0.56254000	4.31510000	6.29982700	H	5.77427114	4.76975077	-2.78990376
C	-1.14225900	4.07328000	5.03913300	H	5.61791322	4.85887593	1.94259751
C	-0.08078600	3.80394900	4.06587100	H	6.31257493	3.44358116	1.18930309
C	3.99361200	1.36113900	2.67601600	H	6.67608192	5.03384099	0.56320167
C	1.22350100	0.57631200	4.84630000	H	5.44435789	6.68674136	0.22089616
C	2.11779200	-1.55806900	2.81791200	H	4.24079152	8.60675743	0.29216634
C	2.01477600	-2.81350300	1.96471600	H	2.86795489	7.68270815	0.85298642
O	-1.40185300	-1.43788400	0.06912900	H	3.12772997	7.90913399	-0.85999779
C	-2.46042200	-1.62323000	-0.90049500	H	3.08312476	7.20873742	-2.47047213
C	-3.05856800	-3.03215400	-0.45297600	H	2.87090477	6.45700372	-4.15111460
C	-2.97454200	-2.90038400	1.02056100	H	2.05950430	9.00561884	-3.04092247
C	-1.60860400	-2.32117600	1.20793700	H	2.49841916	8.48371431	-4.76419535
H	3.28888114	1.84210860	4.44868944	H	0.00406719	8.86079138	-3.56999789
H	3.11309803	3.85957108	3.33776733	H	0.44648201	8.16947934	-5.23164069
H	-1.40451689	4.18473009	1.28106831	H	-0.70947634	6.88625031	-3.06860925
H	-3.44337589	3.81539717	2.49792933	H	0.10646012	6.14559223	-4.55870096
H	-3.41685273	5.34211959	1.64852845	H	0.94843928	-2.54846197	-1.34039349

H	-4.34719788	4.00577977	1.01471426	H	-0.32025993	-3.29325538	-2.28312980
H	1.34951367	-3.48173541	-2.76208498	H	7.39956298	1.14163201	-1.06447058
H	1.47192684	-0.48789417	-5.31156896	H	4.84064348	4.08449084	-5.19000039
H	2.38479492	0.99710928	-5.43199859	H	0.22475129	-1.70186204	-4.19653189
H	0.69870598	0.96851722	-5.88954996	H	-4.74970926	1.14163173	0.70063371
H	-1.10777732	0.42445335	-2.57959917	H	-1.03835072	1.23536707	2.78938489
H	-1.56869518	2.08362480	-2.28333658	H	-2.19079023	4.08449064	4.82616218
H	-2.19194874	1.23995531	-3.68077834	H	2.42509736	-1.70186285	3.83269609
H	-2.79450105	6.68674160	-0.58473102	H	4.32677326	0.41506357	3.04863492
H	0.06632944	7.52564346	-0.26177523	H	3.70351950	1.25873466	1.65119422
H	-1.30650755	8.44969120	0.29904651	H	1.08483083	1.47304906	5.41333900
H	-1.04673433	8.22326558	-1.41393801	H	1.99769917	-0.01195423	5.29290948
H	-0.22104820	6.45700389	3.78727750	H	0.31161025	0.01663751	4.83535804
H	-0.43326729	7.20873720	2.10663475	H	2.27983031	-3.66717319	2.55284304
H	0.15143680	8.48371398	4.40035839	H	1.01113551	-2.92237936	1.61010112
H	0.59035139	9.00561893	2.67708558	H	2.68091126	-2.73390033	1.13115303
H	2.20337544	8.16947952	4.86780365	H	-3.20470695	-0.87213783	-0.73678651
H	2.64578997	8.86079094	3.20616051	H	-2.01739548	-1.73550241	-1.86797751
H	2.54339468	6.14559248	4.19486416	H	-4.08989451	-3.07190042	-0.73526283
H	3.35933125	6.88624955	2.70477201	H	-2.38784091	-3.80451120	-0.76680641
H	2.62114201	3.89484059	5.87128463	H	-2.98481604	-3.88174475	1.44685376
H	1.09561581	4.35789003	7.63768919	H	-3.69390696	-2.17315863	1.33449939
H	-1.23121998	4.60928187	7.08163523	H	-1.63218555	-1.71407730	2.08871795
H	-0.39292361	3.69502891	3.04822345	H	-0.90347702	-3.12208367	1.12892529
H	4.78769266	2.07423471	2.75237307	H	3.68820695	1.23536820	-3.15322224

Part 9. Computations

Geometries are optimized at the B3LYP level of theory using the 6-31G(d) basis set. Energies are defined as follows: G is the sum of electronic and thermal free energies calculated at the B3LYP level of theory (T = 195 K). G_{MP2} is derived from an MP2 SP calculation corresponding to the DFT-optimized geometry and includes a thermal correction from the DFT calculation

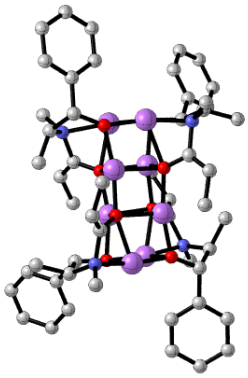
Table 6. Geometric coordinates and thermally corrected MP2 energies for THF



G = –232.349381
G_{MP2} = –231.5698764

Atom	X	Y	Z	Atom	X	Y	Z
C	0.00000000	0.00000000	0.00000000	H	-1.96355800	1.58402400	-1.17939400
O	-1.16524900	-0.82153300	0.13025400	H	-2.51080100	2.19080000	0.39446500
C	-2.33080700	-0.00114700	0.26375800	H	-3.11492500	-0.39466800	-0.39376200
C	-1.90010100	1.42632300	-0.09596600	H	-2.69929400	-0.05338700	1.30020700
C	-0.43282000	1.42743400	0.35786600	H	0.78283500	-0.39219300	0.65989000
H	0.17708000	2.19204100	-0.13334200	H	0.37125700	-0.05275000	-1.03537400
H	-0.36976200	1.58669800	1.44108900				

Table 7. Geometric coordinates and thermally corrected MP2 energies for **S_4** with stacked cube as the core (Chart 5)



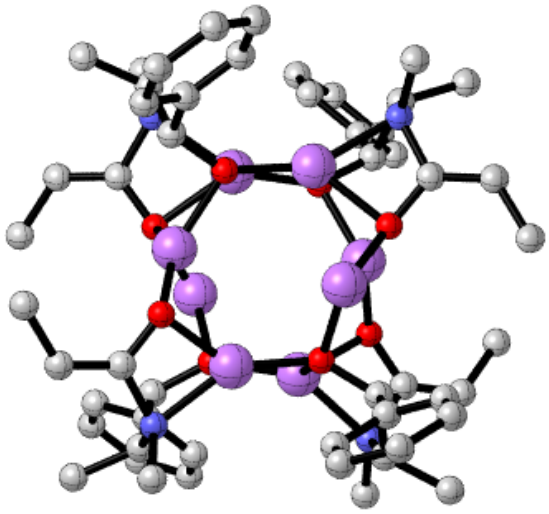
G = –2903.175789

G_{MP2} = –2893.662496

Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	O	-4.08369900	1.87412300	0.09445000
O	-0.06825700	-0.19043800	2.03792600	Li	-2.12711600	1.73473000	-0.00028400
C	0.48103500	-1.07697800	2.88419700	H	-3.08139600	3.67738400	-0.08164800
N	1.91518700	-1.26421300	2.67988000	Li	-4.10864600	1.19459600	1.87749000
C	2.37927700	-2.11110400	1.52838300	O	-3.88594800	-0.58310000	1.69446000
C	1.96856400	-1.53431800	0.12322500	C	-4.39639400	-1.86871700	1.57723100
O	1.95668600	-0.13888100	0.09443200	C	-3.66660200	-2.66087700	0.42721700
Li	1.98193600	0.54054700	1.87752400	N	-3.57764500	-1.83003700	-0.82893100
O	1.75874700	2.31816600	1.69460900	C	-2.28079300	-1.26006600	-1.16784600
C	2.26892800	3.60391400	1.57762300	C	-1.62253400	-1.60834000	-2.29660800
C	1.53892000	4.39610700	0.42777700	C	-0.41188300	-0.91390500	-2.85967700
N	1.45015100	3.56549400	-0.82851100	H	-0.20999700	0.03904600	-2.35978000
C	0.15353200	2.99519800	-1.16761800	H	0.49864700	-1.52477900	-2.79483100
C	-0.50464100	3.34323600	-2.29650800	H	-0.55535500	-0.68263000	-3.92440300
C	-1.71480300	2.64825300	-2.85996000	H	-2.01105200	-2.43795700	-2.87835500
H	-2.62558300	3.25879900	-2.79557100	O	-1.89909400	-0.29681200	-0.30885400
H	-1.57079700	2.41687000	-3.92459100	Li	-2.00555500	-0.19942800	1.76645000
H	-1.91654000	1.69530300	-2.35999800	H	-1.60568600	-2.49260900	1.20081300
H	-0.11628300	4.17299000	-2.87817100	C	-2.32281100	-3.24876100	0.87100600
O	-0.22802300	2.03182800	-0.30867200	H	-2.48440200	-3.94001700	1.70571000
Li	-0.12164600	1.93436700	1.76621300	H	-1.85711800	-3.80735000	0.05250800
H	-0.52167800	4.22733400	1.20228300	C	-0.16244900	-1.65873000	3.92062500
C	0.19502300	4.98359400	0.87179400	H	0.37073000	-2.39887400	4.50772700
H	0.35666700	5.67528200	1.70613200	C	-1.56497000	-1.32687400	4.35691000
H	-0.27120700	5.54164100	0.05323300	H	-1.67466800	-1.46335500	5.43978200
O	-2.05890000	1.92503200	2.03797200	H	-1.82356700	-0.28170500	4.14288500
C	-2.60786600	2.81165600	2.88438500	H	-2.33390500	-1.95848600	3.88668000
N	-4.04196300	2.99930400	2.68014000	Li	-3.94910500	0.07111200	-0.16299100
C	-4.50590500	3.84627000	1.52863100	C	-4.32665400	-2.43740800	-1.93622900
C	-4.09504800	3.26957300	0.12351500	H	-5.36057800	-2.59309200	-1.61569000

H	-4.32274600	-1.76212400	-2.79525500	C	2.19918300	4.17310500	-1.93565600
H	-3.91577700	-3.40827300	-2.25648200	H	3.23302800	4.32899000	-1.61496100
H	-4.30138300	-3.51667900	0.17214700	H	2.19554500	3.49788800	-2.79473500
C	-5.91706700	-1.90262200	1.36622100	H	1.78814200	5.14390700	-2.25589600
C	-6.62367600	-3.09282400	1.59989100	H	2.17346400	5.25212400	0.17283300
C	-7.99982200	-3.17103900	1.39297500	C	3.78958600	3.63818000	1.36661000
C	-8.70680200	-2.05110000	0.94672900	C	4.49595300	4.82848400	1.60049000
C	-8.02192000	-0.85835800	0.71938200	C	5.87208600	4.90700900	1.39359800
C	-6.64069200	-0.78557000	0.93192300	C	6.57929400	3.78728800	0.94716700
H	-6.13334400	0.16154400	0.76670500	C	5.89465200	2.59444800	0.71960400
H	-8.56045300	0.02371800	0.38140700	C	4.51343700	2.52135200	0.93211800
H	-9.78027100	-2.10731100	0.78747800	H	4.00626200	1.57417800	0.76671700
H	-8.52324100	-4.10389800	1.58731700	H	6.43336400	1.71253800	0.38147900
H	-6.08680700	-3.96945100	1.95884100	H	7.65275300	3.84374000	0.78793800
H	-4.20811900	-2.45160300	2.49899200	H	6.39531700	5.83993800	1.58810600
C	-5.01245000	3.85898600	-0.95172400	H	3.95890800	5.70494200	1.95958900
C	-4.62899400	4.96817100	-1.71503000	H	2.08052500	4.18657800	2.49949800
C	-5.48288900	5.50526600	-2.68242500	C	2.88652500	-2.12323300	-0.95182500
C	-6.73675300	4.93545100	-2.90192800	C	2.50404800	-3.23292300	-1.71489300
C	-7.12755300	3.82325100	-2.15129500	C	3.35847600	-3.76958000	-2.68205700
C	-6.27130900	3.29023400	-1.18811000	H	-0.30305300	2.01575100	4.14161200
H	-6.56857400	2.41327200	-0.61982300	Li	1.82168000	1.66412400	-0.16287900
H	-8.10036700	3.36802200	-2.32046000	C	4.61190600	-3.19881400	-2.90157600
H	-7.40205700	5.34858000	-3.65554400	C	5.00172600	-2.08610800	-2.15119000
H	-5.16318900	6.36414400	-3.26720100	C	4.14494800	-1.55352900	-1.18823400
H	-3.64863500	5.41311800	-1.55695300	H	4.44143900	-0.67617800	-0.62014800
H	-5.60029800	3.77706100	1.57765000	H	5.97418700	-1.63013100	-2.32037200
C	-4.09982400	5.31846100	1.67688200	H	5.27761900	-3.61160300	-3.65501700
H	-4.46439000	5.74212700	2.61820800	H	3.03952700	-4.62886400	-3.26664600
H	-3.00967900	5.42536100	1.66070000	H	1.52403700	-3.67863500	-1.55681800
H	-4.51782800	5.91745500	0.86275400	H	0.95512700	-1.94248600	-0.08232100
C	-4.82099400	3.27010300	3.89626400	H	3.47366000	-2.04185500	1.57752800
H	-4.69040400	4.28562500	4.29723600	C	1.97325700	-3.58331600	1.67652300
H	-5.88494100	3.13420500	3.67044800	H	2.33759600	-4.00694500	2.61795600
H	-4.53018000	2.55988200	4.67377200	H	0.88312500	-3.69030000	1.66004600
C	-1.96415800	3.39303700	3.92088500	H	2.39153400	-4.18228700	0.86251800
H	-2.49706100	4.13333600	4.50804900	C	2.69433200	-1.53479700	3.89598500
C	-0.56182600	3.06055300	4.35728700	H	2.56408000	-2.55037600	4.29693200
H	0.20726600	3.69307900	3.88852200	H	3.75823300	-1.39855700	3.67015500
H	-0.45277600	3.19518400	5.44046600	H	2.40330500	-0.82469600	4.67352300

Table 8. Geometric coordinates and thermally corrected MP2 energies for **S_4** with octagonal prism as the core (Chart 5). Four dimethylether molecules were omitted.



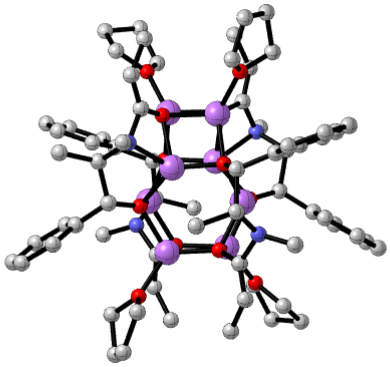
G = –3523.019427

G_{MP2} = –3511.436748

Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	H	-0.01343400	-2.76062900	4.07414400
N	1.10191100	-1.30188000	1.11934600	C	-1.89515300	-0.96979800	3.52450000
C	1.93201200	-0.10700200	1.39159400	C	-1.86283200	-0.66295400	4.89079900
O	1.46881000	0.96713400	0.77040900	C	-2.89480800	-1.06515700	5.74476000
Li	0.46483200	2.42413900	1.23430400	C	-3.97884100	-1.78392600	5.24128400
O	0.20003600	4.05283600	0.21223100	C	-4.02388600	-2.09637700	3.87896800
C	1.25101700	4.72983700	0.84169600	C	-2.99408300	-1.68940700	3.03158100
C	0.74250300	5.81171000	1.85295000	H	-3.04175600	-1.92378300	1.97217600
N	-0.45548200	5.33184200	2.62051600	H	-4.86347500	-2.65901400	3.47774000
C	-0.31590400	4.06968200	3.36074300	H	-4.78186700	-2.09980100	5.90219400
C	0.15295500	4.03369200	4.62543200	H	-2.84756600	-0.81669800	6.80215900
C	0.28935400	2.79112600	5.45925400	H	-1.01915200	-0.10763800	5.29348800
H	1.28450400	2.72844000	5.91957300	H	-0.12632400	0.16916100	3.15290300
H	-0.43861700	2.75625700	6.28475400	Li	-2.40460600	-0.00460400	-0.03482300
H	0.14982800	1.89445600	4.84932000	O	-1.08278400	0.19263300	-1.50459700
H	0.45782900	4.97020800	5.08349400	C	-1.62114600	-0.49931900	-2.61302500
O	-0.73800900	3.01567700	2.65135100	C	-2.52195400	-1.70692200	-2.21139000
Li	-2.00973300	1.68290400	2.45011500	N	-3.50167100	-1.30639300	-1.15968200
O	-1.32279300	0.18641500	1.47109300	C	-4.33717800	-0.11388200	-1.42572600
C	-0.78200800	-0.50921700	2.57610700	C	-5.46031500	-0.19588900	-2.17350600
C	0.12330800	-1.71159800	2.16846100	C	-6.39637400	0.95389100	-2.41772700
H	-0.52469500	-2.45188700	1.67484500	H	-6.43093100	1.24894700	-3.47741600
C	0.75850900	-2.37619600	3.40175700	H	-7.43003800	0.70517000	-2.13180500
H	1.39345400	-3.22002400	3.11348800	H	-6.08948400	1.83032500	-1.83862600
H	1.37678200	-1.66289500	3.95619100	H	-5.71924800	-1.15452300	-2.61380900

O	-3.87780800	0.95955400	-0.80041600	H	-1.87110800	-2.44745300	-1.72189800
Li	-2.88370500	2.42506100	-1.25863500	C	-0.50651800	-0.95099400	-3.56397600
O	-1.68201500	3.02486300	-2.67342400	C	-0.54024900	-0.63725000	-4.92866500
Li	-0.40435600	1.69735900	-2.47617500	C	0.49323400	-1.03088500	-5.78479700
C	-2.10768900	4.07982200	-3.37924100	C	1.58017600	-1.74795000	-5.28517100
N	-1.97187100	5.34004200	-2.63497500	C	1.62655800	-2.06737900	-3.92451700
C	-3.17130900	5.81401400	-1.86611200	C	0.59523900	-1.66891400	-3.07493400
C	-3.67682000	4.72731800	-0.85841100	H	0.64393700	-1.90855700	-2.01674800
O	-2.62390100	4.05131500	-0.23123300	H	2.46838900	-2.62881300	-3.52630900
Li	-0.96156100	4.23206900	-1.21314100	H	2.38439300	-2.05716000	-5.94778500
Li	-1.46276900	4.22538000	1.19520200	H	0.44489400	-0.77710500	-6.84088500
C	-4.64018300	5.34499000	0.15747400	H	-1.38611800	-0.08313800	-5.32841200
C	-6.00928800	5.05417700	0.14032800	H	-2.27936800	0.17961000	-3.18626900
C	-6.87788600	5.60707300	1.08725900	C	-1.09018000	6.40968800	3.38616900
C	-6.38265200	6.46151500	2.07264400	H	-1.29408800	7.25136500	2.71281300
C	-5.01681300	6.76058400	2.10282200	H	-2.04069400	6.05200700	3.79131700
C	-4.15761600	6.20721500	1.15315800	H	-0.48606100	6.79011300	4.22243800
H	-3.09640100	6.44134400	1.18863400	C	1.88774700	6.32680100	2.73679300
H	-4.62257200	7.43152400	2.86277400	H	2.27586100	5.52644400	3.37549400
H	-7.05294300	6.89537000	2.81056500	H	2.70804000	6.69940700	2.11614000
H	-7.93430800	5.35984400	1.03736500	H	1.56405700	7.14979800	3.38263100
H	-6.41424900	4.38471600	-0.61492200	H	0.35923900	6.65132200	1.25593300
H	-4.28981000	4.02216700	-1.46258700	C	2.21254900	5.35369100	-0.17215000
H	-2.79055700	6.65274200	-1.26623700	C	1.72770100	6.21851500	-1.16448400
C	-4.31795000	6.32875900	-2.74833800	C	2.58531200	6.77732600	-2.11239000
H	-3.99652500	7.15474800	-3.39147400	C	3.95184100	6.48130100	-2.08375500
H	-4.70384200	5.52940300	-3.38963500	C	4.44936000	5.62438400	-1.10166900
H	-5.13926800	6.69707300	-2.12648000	C	3.58233200	5.06601600	-0.15652100
C	-1.34008400	6.42204200	-3.39719000	H	3.98906400	4.39458400	0.59600800
H	-1.94515700	6.80330400	-4.23238600	H	5.50635400	5.37935600	-1.05303400
H	-1.13860100	7.26222700	-2.72124200	H	4.62089200	6.91942800	-2.82027700
H	-0.38851600	6.06825300	-3.80327900	H	2.18927300	7.45016000	-2.86973000
C	-2.57703700	4.04647900	-4.64381600	H	0.66595200	6.45041000	-1.19884100
C	-2.71019000	2.80615700	-5.48150700	H	1.86603000	4.02445000	1.44346600
H	-3.70480100	2.74293700	-5.94289300	C	3.05449800	-0.18745300	2.14052700
H	-1.98139500	2.77518200	-6.30643800	C	3.98492900	0.96546700	2.39138200
H	-2.56945000	1.90793500	-4.87413800	H	5.02072200	0.72159000	2.10908500
H	-2.88475800	4.98356300	-5.09879200	H	3.67677600	1.84208800	1.81322900
C	-4.24096700	-2.44138200	-0.60334600	H	4.01399100	1.25808000	3.45193300
H	-3.52873300	-3.20769500	-0.26994200	H	3.31697600	-1.14685700	2.57702300
H	-4.81791400	-2.10165800	0.26178900	C	1.84645200	-2.43075200	0.55763600
H	-4.94200700	-2.91554800	-1.30599300	H	2.54976900	-2.90492600	1.25797900
C	-3.15533300	-2.36733000	-3.44789800	H	1.13782600	-3.19881300	0.22059500
H	-3.77595100	-1.65322600	-3.99866700	H	2.42170100	-2.08420300	-0.30593000
H	-2.38239600	-2.74605100	-4.12239000	H	-3.78763300	-3.21452500	-3.16372800

Table 9. Geometric coordinates and thermally corrected MP2 energies for $\mathbf{R_4 \cdot (THF)_4}$



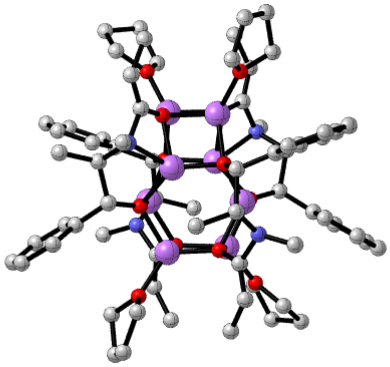
G = –3832.614098

G_{MP2} = –3820.055651

Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	C	0.58531600	-3.78850900	-3.08501100
O	1.98157400	0.20213400	-0.28976800	C	-0.34503300	-6.77935700	-1.38663800
C	2.49655700	0.58110200	-1.45152000	C	0.52036500	-7.89754600	-0.87505700
N	2.96084600	-0.56646200	-2.21822600	O	3.56441100	-6.20975900	-1.36604300
C	4.26900800	-1.10872000	-1.73233600	C	3.24643300	-6.47856100	-2.74634300
C	5.47000900	-0.56663800	-2.52003500	C	3.99013900	-7.76883400	-3.08645300
C	2.82116000	-0.48994400	-3.67015900	C	5.27477700	-7.61601600	-2.25734200
Li	1.75586400	-1.72192900	-0.90855900	C	4.77398500	-6.91785400	-0.98695800
O	3.23354600	-2.98901800	-0.60574100	C	2.56824400	1.84295600	-1.94289700
C	4.14998900	-2.66582200	-1.62086400	O	-1.15570000	1.40852800	-0.90236000
C	5.52555400	-3.31651300	-1.46531000	C	-1.11530900	1.68926100	-2.32054400
C	6.18890400	-3.82282700	-2.59240900	C	-1.93626900	2.96400900	-2.50067900
C	7.47447400	-4.36108300	-2.50125900	C	-3.03133400	2.77576800	-1.43881100
C	8.12522800	-4.41057600	-1.26737700	C	-2.26034100	2.11806900	-0.28943000
C	7.47527500	-3.91776600	-0.13355000	H	4.35990500	-0.75776100	-0.69935000
C	6.19008100	-3.37870900	-0.23302800	H	6.40612400	-0.81695200	-2.01382100
Li	2.57790700	-4.82459900	-0.23997700	H	5.40331700	0.52494100	-2.59137900
O	0.63828500	-4.96285700	-0.16925400	H	5.52893100	-0.97405000	-3.53536800
C	-0.25677000	-5.48064300	-1.00407400	H	3.48521600	0.24078800	-4.15616000
N	-1.23525500	-4.49398500	-1.44680100	H	1.78909600	-0.22099700	-3.91095400
C	-2.57160100	-5.02273100	-1.73580400	H	3.03109600	-1.47284900	-4.10610200
C	-0.80094600	-3.51142600	-2.49780400	H	3.76665700	-3.01617500	-2.59917100
C	-0.91275600	-2.03521900	-1.97865800	H	7.97011700	-3.94855800	0.83373300
O	-0.16679300	-1.82960700	-0.81524200	H	5.70625700	-3.00663800	0.66425300
Li	-0.42687400	-3.35718800	0.30665400	H	-2.87963500	-5.69195100	-0.93006100
O	-0.29382600	-3.37947400	2.21274900	H	-2.62055600	-5.58048300	-2.68670600
C	-1.23090500	-3.27084600	3.25611200	H	-3.28068900	-4.19365000	-1.79950500
C	-1.68511200	-1.77887700	3.39625100	H	-1.50908100	-3.61301900	-3.33268500
N	-0.51218600	-0.96567000	3.85047600	H	-0.51449200	-1.41835600	-2.81065400
C	-0.33319300	0.25788800	3.07977700	H	-0.75258600	-3.53689400	4.21870000
O	0.21795400	0.00344800	1.89879900	H	-1.88851500	-1.44419200	2.37459500

H	4.37930500	-2.97818700	4.98813600	H	3.41306200	-8.63843000	-2.75046200
H	1.43246700	-6.81433800	4.30442400	H	5.99412000	-6.97891200	-2.78203800
H	-0.21268100	-6.39112400	4.84895800	H	5.76263300	-8.57070600	-2.03756000
H	-1.05131200	-7.39379300	1.26506100	H	5.48730500	-6.19597700	-0.58309000
H	-1.96451700	-7.11615800	2.77200400	H	4.50714500	-7.63509100	-0.20572400
H	4.83903400	-6.39217700	3.72691600	H	3.05118600	1.99005600	-2.90510500
H	4.31208500	-8.21861000	2.01287700	H	-0.06582200	1.77867300	-2.60852100
H	2.78829000	-7.39362100	1.62433300	H	-1.57235100	0.85124200	-2.86116000
H	3.00569400	-8.19534600	3.18460400	H	-1.32760900	3.84794800	-2.27558000
H	6.28438800	-3.11003900	3.51464700	H	-2.33071600	3.06735900	-3.51635000
H	6.27123400	-4.65019200	2.62570500	C	2.01769000	3.06708600	-1.26375500
H	5.93585200	-4.62347500	4.37233500	H	1.51827600	2.80427900	-0.32662200
H	2.02714500	-3.01194700	5.49538500	H	2.80365200	3.80206300	-1.03266200
H	2.56294200	-4.64291500	5.04990600	H	1.28785600	3.59830200	-1.89401800
H	1.61159300	-3.68365900	3.90681900	H	9.12523400	-4.82901000	-1.18914400
H	4.95655500	-0.80172800	1.41953400	H	7.96602300	-4.74161000	-3.39368400
H	7.24135600	0.39382200	5.65189100	H	5.69052800	-3.78969800	-3.55961400
H	5.01073900	-0.66614300	5.70197000	H	-3.80945600	2.10060600	-1.81195400
H	5.06935400	2.30132300	1.96996000	H	-3.50751800	3.71280900	-1.13391300
H	3.94155200	2.52242900	0.60200700	H	-2.86237900	1.40217600	0.27630400
H	4.72167500	4.71489100	2.10949800	H	-1.84522100	2.85857100	0.40085600
H	3.03902300	4.55882300	1.57650300	H	0.11112200	-9.30887100	2.24339000
H	4.12664000	4.12786000	4.35743600	H	-1.49333200	-9.51984100	2.97085600
H	2.47134200	4.48570100	3.85991300	H	0.85064800	-9.13431900	4.49595100
H	3.76577800	1.81611300	4.29097700	H	3.59952800	-5.64263800	-3.36670700
H	2.02053000	2.13225600	4.07842200	H	2.16007100	-6.55163600	-2.82752900
H	0.08995900	2.64538600	1.94760400	H	4.17656200	-7.87519300	-4.15980300
H	0.12198000	3.49368800	3.50400000	H	-0.74332100	-8.65117900	5.08045600
H	-1.40326300	3.28726700	2.65871500	H	2.91780400	-1.06228100	4.43786400
H	0.59671900	-0.36881300	5.51575400	H	7.21313500	0.22605700	1.35294000
H	-0.33291800	-1.86463700	5.73455400	H	8.37019200	0.83162400	3.47391200
H	-1.15260300	-0.29389900	5.80418800	H	-2.37218800	-1.52576100	0.29681200
H	-3.12245500	-0.44752600	4.32202600	H	-4.78085100	-0.96868300	0.50243200
H	-2.88641000	-1.95189900	5.23627800	H	-6.17677900	-0.70224300	-1.54419300
H	-3.82335200	-1.96847700	3.74300200	H	-5.13312100	-1.01265700	-3.78572700
H	-2.75411800	-3.88799000	1.01569800	H	-2.74314800	-1.60207800	-3.97149700
H	0.77953800	-3.07780800	-3.89661300	H	-2.41736600	-4.74752300	5.20990300
H	1.37968500	-3.68773800	-2.34189700	H	-4.43195500	-6.17542100	5.08275000
H	0.63285200	-4.79956700	-3.49860300	H	-5.62521200	-6.45940300	2.91308700
H	1.21903400	-7.54103900	-0.11336900	H	-4.76382200	-5.30185400	0.88400100
H	1.11674400	-8.36206500	-1.67500100	H	-1.13843600	1.50527200	4.56279900
H	-0.07500500	-8.71253900	-0.43538000	H	-1.10917600	-7.05093800	-2.10902900

Table 10. Geometric coordinates and thermally corrected MP2 energies for $S_4 \cdot (THF)_4$



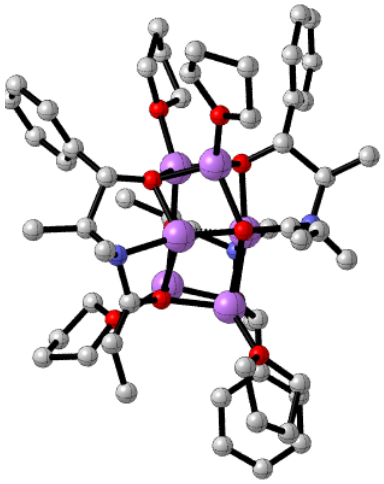
G = –3832.613034
G_{MP2} = –3820.053988

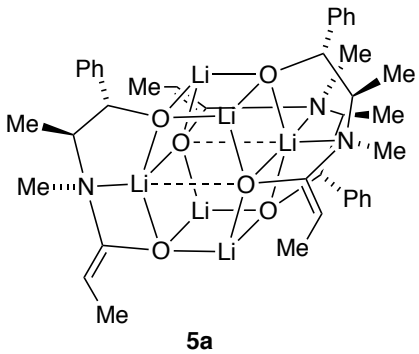
Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	C	-6.47207900	4.38977300	0.53736000
O	0.08210500	0.07054800	-1.99779000	C	-5.14812200	3.94008200	0.56926400
C	0.99307400	-0.34048500	-2.87650400	C	-3.09387400	1.70388600	2.36865500
N	1.83200900	0.75007700	-3.35987200	N	-3.68807300	0.77881900	1.34509300
C	1.24770200	1.68113000	-4.38372400	C	-2.86032300	-0.31988800	0.86137300
C	1.22323400	3.16044700	-3.85849500	O	-1.94461600	0.08264400	-0.01638100
O	0.51840600	3.27805700	-2.65704900	Li	-1.86361900	0.00831900	-2.01348100
Li	0.18404200	5.06440300	-1.82998800	O	-2.72256400	-1.48260900	-3.10207500
O	0.00295800	5.06365000	0.06930500	C	-2.37428100	-1.74135500	-4.47693300
C	0.56743000	5.37530300	1.22866700	C	-2.94509100	-3.12450200	-4.78034900
N	0.91366400	4.17882900	1.98333400	C	-4.24382500	-3.11318900	-3.95842500
C	2.14348200	3.49156900	1.47361700	C	-3.85079800	-2.30876400	-2.71171500
C	3.41138700	3.88288200	2.24605100	O	-2.72555400	1.76637800	-2.36956500
C	0.81130700	4.26562100	3.43779700	C	-3.68486400	1.98554500	-3.37322100
Li	-0.42590900	3.17720200	0.68423800	C	-4.97783100	1.18759800	-3.19853400
O	0.88130700	1.74933500	0.35420400	C	-5.58597100	0.59287900	-4.31343400
C	1.84217800	1.95942500	1.35833300	C	-6.79733600	-0.09356200	-4.20359500
C	3.12685300	1.14796000	1.18493200	C	-7.42774400	-0.20368300	-2.96308200
C	3.72897400	0.54863500	2.30064400	C	-6.83244200	0.37833400	-1.84144500
C	4.93307900	-0.15060800	2.19159900	C	-5.62126100	1.06451100	-1.95969700
C	5.56199800	-0.26922400	0.95110400	Li	-1.40404500	3.18136600	-2.70004500
C	4.97235600	0.31689400	-0.17137600	O	-1.81514100	5.07380900	-2.08701200
C	3.76834700	1.01569200	-0.05394000	C	-2.37598800	5.38897000	-3.24719500
Li	0.95877800	1.78491600	-1.55511600	N	-2.73428400	4.19475200	-3.99984300
O	-2.34793700	3.29309700	0.64154400	C	-3.97056800	3.52051500	-3.48881300
C	-3.05330200	3.18281500	1.84333500	C	-5.23500700	3.92502700	-4.26008300
C	-4.47957700	3.74625100	1.78112200	C	-2.63125100	4.27779300	-5.45448700
C	-5.16666100	4.04990800	2.96778800	C	-2.57399300	6.63278400	-3.74909400
C	-6.48529400	4.50506800	2.94469300	C	-2.14522500	7.91111800	-3.08292400
C	-7.14856900	4.67027900	1.72554700	Li	-1.99562400	5.07632000	-0.18714600

O	-3.02491600	6.62778600	0.57241000	H	-4.66203200	3.92387200	3.92459400
C	-4.11107000	7.29295100	-0.09276800	H	-6.99545800	4.73190200	3.87784000
C	-4.01191800	8.74030900	0.39498600	H	-8.17714900	5.02076900	1.70330200
C	-3.49828500	8.58579800	1.85062100	H	-4.61597200	3.74928000	-0.35625500
C	-3.01869800	7.11585000	1.92684500	H	-3.77244800	1.69067600	3.23356000
Li	-2.80266400	1.80488800	-0.46059700	H	-1.28759300	-1.67450800	-4.55892700
C	-3.09503200	-1.59740700	1.24973700	H	-2.83394200	-0.97467300	-5.11699500
C	-2.42034700	-2.81705100	0.68782000	H	-2.26344300	-3.90312300	-4.41851100
C	-5.06483800	0.41702700	1.69627000	H	-3.11123000	-3.28469400	-5.85037600
C	-1.72838000	1.26223800	2.90101400	H	-5.03811600	-2.59706800	-4.50784400
C	0.77819000	6.61806500	1.72796400	H	-4.60273300	-4.11565900	-3.70559700
C	0.36183300	7.89909400	1.05909600	H	-3.51907800	-2.95464900	-1.89416900
O	1.23050000	6.60472500	-2.58880000	H	-4.65212000	-1.65918500	-2.35267200
C	2.32557900	7.25664400	-1.92496900	H	-3.27899900	1.67532300	-4.35564400
C	2.24337500	8.70579800	-2.41135600	H	-7.24701800	-0.54183100	-5.08658400
C	1.71806500	8.56024500	-3.86402400	H	-8.37012400	-0.73715000	-2.87032000
C	1.22912900	7.09373800	-3.94270500	H	-7.31272300	0.30218400	-0.86927700
C	2.65553200	3.70836300	-3.79518600	H	-4.08177300	3.86846300	-2.45707500
C	3.34647700	4.00522800	-4.98135300	H	-5.28589300	5.01665100	-4.34274600
C	4.66986600	4.44635400	-4.95734500	H	-5.26761700	3.50238300	-5.27037300
C	5.33429500	4.60379100	-3.73779400	H	-6.13087800	3.58277400	-3.73504400
C	4.65411000	4.33017900	-2.55010500	H	-1.63951500	4.65583000	-5.71682900
C	3.32537800	3.89484400	-2.58289500	H	-2.74277000	3.27599700	-5.88355800
C	-0.12277600	1.25445100	-4.91556000	H	-3.37956700	4.93026000	-5.92930100
C	3.20498500	0.37391800	-3.71083500	H	-3.07952300	6.72324700	-4.70641700
C	1.21464500	-1.61996000	-3.26608500	H	-1.51326800	8.52781300	-3.73975500
C	0.52808700	-2.83325700	-2.70485600	H	2.79072400	3.70998700	-1.65760900
O	0.84621200	-1.49653000	1.09064100	H	-0.43200300	1.94775100	-5.70619600
C	0.49429400	-1.75380500	2.46507400	H	-0.07352200	0.25007700	-5.34520800
C	1.05195100	-3.14254800	2.76798000	H	-0.89086800	1.25400200	-4.13889100
C	2.34939600	-3.14448200	1.94422700	H	3.81332700	1.27692400	-3.80361200
C	1.96088500	-2.33914600	0.69702800	H	3.27277300	-0.17637100	-4.66492000
H	1.92584700	1.66043200	-5.24885500	H	3.62202000	-0.25604100	-2.92249700
H	0.72060000	3.73522100	-4.66319400	H	-0.02093500	-3.39539300	-3.47554100
H	2.25961400	3.83818400	0.44200200	H	1.24631100	-3.54621800	-2.27135700
H	4.30399500	3.53099700	1.72183600	H	-0.19030200	-2.56001700	-1.92698800
H	3.47399900	4.97389200	2.32866700	H	0.96046900	-0.99191500	3.10607900
H	3.43865200	3.46003900	3.25640900	H	-0.59178900	-1.67712600	2.54655500
H	0.91090600	3.26336700	3.86874700	H	-1.57834700	7.70621200	-2.16986600
H	1.56717700	4.91007300	3.91157800	H	-3.00187900	8.54701300	-2.81182000
H	-0.17589000	4.65598600	3.69920700	H	-3.96847000	7.15789200	-1.16561200
H	1.43268200	1.65420600	2.34081700	H	-5.06081100	6.83132400	0.21028200
H	5.37831400	-0.60210500	3.07519900	H	-3.28691500	9.28948100	-0.21383200
H	6.49883500	-0.81248100	0.85897500	H	-4.97068500	9.26476400	0.33614700
H	5.45148000	0.23401000	-1.14357300	H	-2.68554400	9.28673400	2.06076700
H	-2.54397600	3.75193500	2.64786000	H	-4.29166000	8.77120900	2.58146400

H	-0.20403700	7.69758800	0.14468000	H	-2.00206400	6.99542400	2.30463000
H	1.22459500	8.52742400	0.78978000	H	-3.70512900	6.50489700	2.52664600
H	-0.26703400	8.52186100	1.71319500	H	-1.70415700	-2.55082200	-0.09449300
H	3.26913100	6.78394800	-2.23006400	H	-1.87134800	-3.38171900	1.45669900
H	2.18343100	7.12237300	-0.85194000	H	-3.14621200	-3.52546900	0.25972100
H	3.20996900	9.21634600	-2.35844900	H	-5.48843600	-0.20896600	0.90828100
H	1.53065700	9.26522900	-1.79744200	H	-5.66371700	1.32639800	1.78855500
H	2.50645500	8.74455800	-4.60050000	H	-5.13826600	-0.13210900	2.65062500
H	0.90741200	9.26639800	-4.06446300	H	-1.78859900	0.25781200	3.32910500
H	1.91265800	6.47900200	-4.54207300	H	-0.95959200	1.25485600	2.12507300
H	0.21229700	6.98027600	-4.32211200	H	-1.41266100	1.95111600	3.69297300
H	2.84109400	3.88498200	-5.93850600	H	1.28450000	6.70559400	2.68516400
H	5.18287700	4.66822100	-5.89012800	H	-5.17840100	1.50527000	-1.07266900
H	6.36652100	4.94334100	-3.71484200	H	-5.10275500	0.67199300	-5.28555900
H	1.21786100	-3.30405100	3.83784100	H	-3.85519400	-1.77266400	2.00517400
H	0.36227800	-3.91463100	2.40731000	H	1.97293300	-1.80244900	-4.02168900
H	2.69889500	-4.15056400	1.69255500	H	3.24686300	0.63434800	3.27274100
H	3.14917700	-2.63427800	2.49119900	H	3.32954100	1.45941900	-0.94146200
H	2.76863900	-1.70137500	0.33136300	H	-6.97188100	4.52250700	-0.41925500
H	1.61650200	-2.98370000	-0.11643900	H	5.15473700	4.45720600	-1.59314800

Table 11. Geometric coordinates and thermally corrected MP2 energies for heteroaggregate **5a**. THFs are omitted in the chemdraw representation.





5a

G = –3106.790811
G_{MP2} = –3096.583583

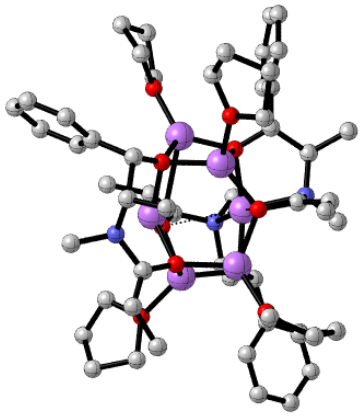
Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000
Li	1.93880000	-1.11749200	-0.59223700
Li	2.07774800	0.51018500	-2.46873900
Li	0.04056400	-1.24730100	-2.89498200
Li	-1.29765800	1.06614800	-2.34318900
O	-1.71321200	0.79479500	-0.41215400
C	-1.74780900	1.40258100	0.77114500
N	-0.42015500	1.47967800	1.35985400
C	0.47264100	2.48725800	0.70075700
C	1.85651400	1.83024300	0.37704000
O	1.68376100	0.74550400	-0.49203500
C	-0.32522200	1.40926100	2.81450000
H	0.72300100	1.26799200	3.10029100
H	-0.69841000	2.30191300	3.33913100
H	-0.89857500	0.54706400	3.16599100
C	-2.84804200	1.85577000	1.41869000
C	-4.25902400	1.71320300	0.91753800
H	-4.91226400	1.22422100	1.65622900
H	-4.72333100	2.68809200	0.70336500
H	-4.29130100	1.12229200	-0.00271600
H	-2.70983900	2.36287800	2.36963500
Li	-2.11660400	-1.04331800	-0.93628200
O	-1.91518000	-0.77741300	-2.73639500
C	-2.49066300	-1.12705800	-3.95315400
C	-1.85501100	-0.24345500	-5.06808900

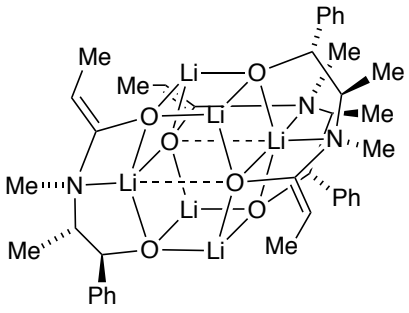
Atom	X	Y	Z
C	1.55173900	2.89684900	-5.43931800
H	1.84406000	3.01032400	-4.39158600
H	2.46418800	2.96755900	-6.04988700
H	0.94168600	3.77382700	-5.71011000
H	0.64623000	1.30734900	-6.69212400
C	0.21434400	-1.23356200	-6.10009000
H	-0.24565700	-2.22943700	-6.11408400
H	0.10964900	-0.80488100	-7.10972100
H	1.28130700	-1.35349100	-5.89713300
H	-2.03908000	0.79308200	-4.76008700
H	-2.25231200	-2.17567300	-4.22415000
O	-0.02680200	-1.77619900	-0.45129800
C	-0.08484000	-3.07199800	-0.74725500
N	0.02412000	-3.36473400	-2.18492000
C	1.35087800	-3.79704800	-2.71004800
C	2.44566600	-2.75022700	-2.34835000
O	1.99950300	-1.43852100	-2.48452800
H	2.70967700	-2.97517000	-1.29013700
H	1.22485500	-3.78098600	-3.80199800
C	-1.06644900	-4.20150300	-2.69065800
H	-1.07377300	-5.23122300	-2.30045900
H	-2.02120400	-3.73485300	-2.43728400
H	-0.99228200	-4.25938300	-3.78373800
C	-0.29311500	-4.06542000	0.15049100
H	-0.32829800	-5.08767600	-0.21476100

N	-0.36890100	-0.43877500	-5.02307300	C	-0.54018800	-3.85980000	1.61901900
C	0.33816400	0.79435300	-4.67945900	C	1.55173900	2.89684900	-5.43931800
O	0.40962900	1.00131200	-3.37223000	H	1.84406000	3.01032400	-4.39158600
C	0.81896800	1.60108100	-5.65949400	H	2.46418800	2.96755900	-6.04988700
H	0.94168600	3.77382700	-5.71011000	H	-3.94087900	5.56883500	-2.34343200
H	0.64623000	1.30734900	-6.69212400	H	-2.25135500	5.57381700	-1.80769800
C	0.21434400	-1.23356200	-6.10009000	H	-3.29690800	4.69482700	-4.55690100
H	-0.24565700	-2.22943700	-6.11408400	H	-1.98655500	5.84764200	-4.23446100
H	0.10964900	-0.80488100	-7.10972100	H	-0.51881000	4.08461100	-3.40846900
H	1.28130700	-1.35349100	-5.89713300	H	-1.35959700	3.19784600	-4.69343900
H	-2.03908000	0.79308200	-4.76008700	O	3.90604100	1.04726900	-3.24096200
H	-2.25231200	-2.17567300	-4.22415000	C	5.09098300	1.06290300	-2.41122300
O	-0.02680200	-1.77619900	-0.45129800	C	6.29100500	0.85574700	-3.35521200
C	-0.08484000	-3.07199800	-0.74725500	C	5.70609900	1.19036600	-4.73765300
N	0.02412000	-3.36473400	-2.18492000	C	4.27525300	0.68336900	-4.58747400
C	1.35087800	-3.79704800	-2.71004800	H	4.22850000	-0.40586800	-4.69926900
C	2.44566600	-2.75022700	-2.34835000	H	3.54940400	1.14262900	-5.25819700
O	1.99950300	-1.43852100	-2.48452800	H	6.24259100	0.70444500	-5.55872300
H	2.70967700	-2.97517000	-1.29013700	H	5.71050500	2.27293000	-4.91228900
H	1.22485500	-3.78098600	-3.80199800	H	6.61988300	-0.18905700	-3.33293400
C	-1.06644900	-4.20150300	-2.69065800	H	7.14326900	1.48606700	-3.08247700
H	-1.07377300	-5.23122300	-2.30045900	H	5.11791700	2.02783300	-1.89946700
H	-2.02120400	-3.73485300	-2.43728400	H	5.01206400	0.26692700	-1.66249700
H	-0.99228200	-4.25938300	-3.78373800	O	3.18180500	-1.73789900	0.86502300
C	-0.29311500	-4.06542000	0.15049100	C	4.43242300	-1.07634600	1.16342400
H	-0.32829800	-5.08767600	-0.21476100	C	4.87464600	-1.62122400	2.52414000
C	-0.54018800	-3.85980000	1.61901900	C	4.27699700	-3.03742500	2.51214500
H	0.22085200	-4.34967900	2.24552200	C	2.93948900	-2.80682800	1.80927000
H	-0.54162100	-2.79392200	1.86684300	H	2.16349800	-2.48459900	2.51425600
H	-1.50691500	-4.28152400	1.93327400	H	2.56486200	-3.66903600	1.25230500
O	-3.57150100	-1.97808400	0.00257000	H	4.15571900	-3.46632900	3.51132500
C	-4.48235100	-2.93727900	-0.55692300	H	4.90878700	-3.71456100	1.92468700
C	-5.82248900	-2.62200300	0.11601700	H	4.43468300	-1.02967500	3.33584900
C	-5.40975900	-2.08699500	1.51352900	H	5.96195300	-1.60801000	2.64518200
C	-3.88075100	-1.88440300	1.40502800	H	5.15432600	-1.32711800	0.37525900
H	-3.33499800	-2.67042200	1.94327300	H	4.25959800	0.00259400	1.14939500
H	-3.53120300	-0.90815700	1.74618700	C	3.73614900	-3.01420500	-3.13468300
H	-5.65162500	-2.79590600	2.31158100	C	4.94371200	-3.24292700	-2.46385300
H	-5.92045700	-1.14730700	1.74085500	C	3.75587000	-3.00600800	-4.53737600
H	-6.47189500	-3.50087800	0.17264500	C	6.13613500	-3.45371200	-3.16265100
H	-6.34615700	-1.85040900	-0.45552300	H	4.94714400	-3.26128500	-1.37559700
H	-4.48391200	-2.79843700	-1.63887800	C	4.93936700	-3.22561900	-5.24291200
H	-4.13299000	-3.95240300	-0.31606000	H	2.83460400	-2.82001300	-5.08221500
O	-2.08980600	2.87057300	-2.79039600	C	6.13752800	-3.44778300	-4.55788800
C	-1.50257200	3.76064800	-3.76891700	H	7.06004500	-3.63104900	-2.61690400
C	-2.47242400	4.93545500	-3.87459900	H	4.92781000	-3.22227200	-6.33034500

C	-2.98381400	5.04527800	-2.42967400
C	-3.08461100	3.57564700	-2.00896200
H	-4.07004700	3.15776800	-2.25111100
H	-2.87925200	3.40083000	-0.95070800
C	-6.21046400	-1.91998600	-4.52023400
H	-4.33758400	-2.84437900	-5.04468700
C	-6.05282100	0.12509100	-3.25292400
H	-4.05611100	0.78078200	-2.77223100
C	-6.83558400	-0.85167600	-3.87520300
H	-6.80712200	-2.69102700	-5.00210800
H	-6.52967300	0.95995700	-2.74413600
H	-7.92023500	-0.78208300	-3.85368100
C	1.78284100	-5.21650800	-2.30422900
H	2.72965500	-5.47687400	-2.78776000
H	1.92118200	-5.29027900	-1.22015700
H	1.04345300	-5.96754800	-2.60203500
C	-2.47303100	-0.40611000	-6.46231700
H	-1.97030500	0.24057200	-7.18941700
H	-2.41917500	-1.43761900	-6.82908000
H	-3.52879700	-0.12195600	-6.43603600
H	2.28163400	1.49276000	1.34533400
H	7.05980900	-3.61882900	-5.10716300
C	-4.01736900	-1.03034500	-3.92803200
H	0.01536700	2.68522800	-0.27431800
C	2.81507100	2.88525100	-0.17110100
C	3.91972200	3.31442100	0.57456000
C	2.58584700	3.47762900	-1.42201900
C	4.77456400	4.31018900	0.09318600
H	4.10983200	2.86722700	1.54890700
C	3.43239800	4.47540300	-1.90524800
H	1.74595700	3.13981900	-2.02401600
C	4.53080400	4.89686400	-1.14933300
H	5.62739400	4.62712600	0.68894300
H	3.23754600	4.92164100	-2.87738400
H	5.19020300	5.67407100	-1.52738000
C	0.53867100	3.81307600	1.47284100
H	1.11134000	3.72755200	2.40357500
H	1.01456000	4.58721100	0.86569100
H	-0.47292000	4.15250400	1.72362000
C	-4.81573000	-2.00488200	-4.54307200
C	-4.65994300	0.03273000	-3.27610900

Table 12. Geometric coordinates and thermally corrected MP2 energies for heteroaggregate **5b**. THFs are omitted in the chemdraw representation.





5b

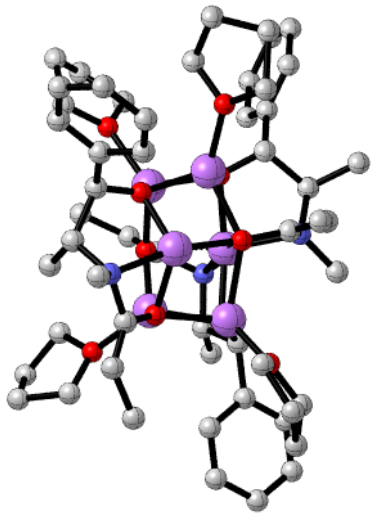
G = – 3106.788851
G_{MP2} = – 3096.578490

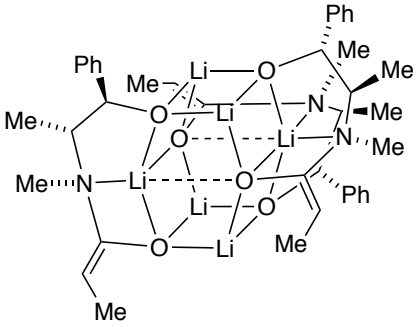
Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	C	-3.01488300	-2.63901800	-2.34539500
Li	-2.26061600	-0.40975100	-0.85721000	O	-2.51448100	-2.30511800	-1.09118900
Li	-2.13999600	-2.40806400	0.78327500	H	-2.63891400	-3.62773500	-2.67834600
Li	-0.57380500	-2.85459500	-1.33135100	H	-2.72807300	-0.62147000	-3.00192200
Li	1.21292600	-2.61876000	0.72322100	C	-0.34609300	-2.41588700	-4.45801500
O	1.64810900	-0.74046600	0.53834100	H	-0.48539700	-1.96056200	-5.45156900
Li	2.25816300	-1.35081200	-1.15835100	H	0.72578500	-2.48444300	-4.26515800
O	1.44156000	-3.02258500	-1.23080800	H	-0.75614000	-3.43184400	-4.49602700
C	1.88501100	-4.34762500	-1.17449000	C	0.41063300	0.28900300	-3.87845100
C	0.77138500	-5.37031200	-1.55860800	H	0.51098600	-0.07857300	-4.89502800
N	-0.53249100	-4.98874000	-0.94288400	C	1.05278100	1.61323500	-3.56307800
C	-0.55949900	-4.76754200	0.51694700	H	0.80765900	2.36760300	-4.32525200
O	-0.49004200	-3.48916500	0.85846200	H	0.70219200	1.99250500	-2.59786400
C	-0.69662400	-5.81328200	1.37120900	H	2.15347500	1.57320000	-3.51858700
C	-0.83022600	-5.68781800	2.86412900	O	3.94604200	-0.78724900	-1.99507300
H	-0.72336200	-4.64375000	3.17244000	C	5.17258200	-0.69205400	-1.23277200
H	-1.80437500	-6.04916500	3.22830100	C	6.22287800	-0.18545100	-2.21960700
H	-0.07213700	-6.27747600	3.40179800	C	5.75651200	-0.83118900	-3.53358700
H	-0.75041200	-6.81544700	0.95547000	C	4.23351400	-0.74068800	-3.41618600
C	-1.63798400	-5.81953400	-1.42594200	H	3.71112500	-1.57033200	-3.89614400
H	-1.63031100	-5.82277800	-2.52342400	H	3.84725800	0.20499100	-3.81159600
H	-1.60517500	-6.86677000	-1.08873500	H	6.07023900	-1.88026800	-3.57722500
H	-2.58195600	-5.38463000	-1.08896600	H	6.13405000	-0.32131800	-4.42520700
H	0.60103100	-5.27395300	-2.64123300	H	7.23857800	-0.47295400	-1.93130900
H	2.18351000	-4.61411700	-0.14143100	H	6.18160500	0.90782300	-2.28887200
O	-0.57885100	-0.06507400	-1.74472900	H	4.99232300	-0.01971200	-0.39123800
C	-0.33497100	-0.42240100	-2.98980100	H	5.42907100	-1.69116900	-0.85623800

N	-0.95856200	-1.68442100	-3.35484000	C	2.07027900	0.01611600	1.63278400
C	-2.45824100	-1.60998200	-3.38658800	C	0.87079600	0.40040300	2.57638600
N	-0.21633900	1.11085500	1.82169400	H	-1.88577900	2.71071600	-1.26260100
C	-1.54911400	0.50527400	1.83872200	H	-2.05284700	1.94061900	-2.85373400
O	-1.64955900	-0.49481400	0.96947500	H	-3.23890100	4.39522900	-2.38469500
C	-2.53625200	0.99542300	2.62367100	H	-4.10642500	3.16776300	-3.32688500
C	-3.95708600	0.50665200	2.61838700	H	-4.35333500	3.68417900	-0.31092100
H	-4.26411000	0.12767100	3.60560000	H	-5.68344100	3.57328900	-1.47941200
H	-4.67269600	1.30642500	2.36884200	H	-5.39146300	1.17927000	-1.72894800
H	-4.08967700	-0.30771300	1.89977500	H	-4.88909800	1.34974600	-0.02750500
H	-2.29693800	1.79915000	3.31425800	C	3.12922100	-4.58568900	-2.03984900
C	-0.18122000	2.55644400	2.05691500	C	4.30280100	-5.12354100	-1.49596400
H	0.80232600	2.94356000	1.77981700	C	3.12246600	-4.28003400	-3.40869700
H	-0.93840200	3.04409600	1.43773400	C	5.43582800	-5.34657800	-2.28450600
H	-0.36778100	2.82984700	3.10947600	H	4.32477100	-5.38764700	-0.44065700
H	1.26243700	1.11126800	3.31945800	C	4.24515200	-4.50759800	-4.20513800
H	2.73344400	-0.58415800	2.28413700	H	2.22350700	-3.86038700	-3.84854000
O	2.70595200	-3.34834500	1.97190300	C	5.41107700	-5.03971900	-3.64507400
C	2.47900100	-4.43396700	2.90498500	H	6.33275500	-5.76760200	-1.83622000
C	3.86759100	-4.94259300	3.30659700	H	4.21018000	-4.27489600	-5.26709300
C	4.74332900	-3.69422000	3.11864400	H	6.28513100	-5.22069300	-4.26553500
C	4.11558300	-3.06140700	1.87659200	C	1.21897000	-6.81406900	-1.27229100
H	4.51346300	-3.50813800	0.95579500	H	2.13589600	-7.04852200	-1.82134900
H	4.23674800	-1.97712800	1.81887900	H	1.41134800	-6.95784600	-0.20363500
H	5.80472000	-3.92344600	2.98257800	H	0.45911000	-7.54050500	-1.57829500
H	4.64605200	-3.02251800	3.98005700	C	-4.54253200	-2.74287400	-2.37870900
H	4.19583900	-5.74109800	2.63030000	C	-5.18469900	-3.67861600	-3.20192900
H	3.88659500	-5.33757300	4.32675300	H	-0.02483400	-1.59990000	2.71080100
H	1.92626000	-4.03363500	3.76285100	H	1.21426800	-1.24403400	3.93141800
H	1.86030100	-5.18518200	2.40917700	H	-0.40730000	-0.53311500	4.06691600
O	-3.68601700	-3.08547400	1.89712100	C	-5.34256900	-1.91271800	-1.58216000
C	-3.70642600	-3.24826700	3.33230200	C	-6.57737500	-3.76907500	-3.24846700
C	-4.55120500	-4.50981000	3.62208100	H	-4.58457600	-4.34949100	-3.81380300
C	-4.71817700	-5.15787100	2.23451300	C	-6.73581900	-1.99495900	-1.62556900
C	-4.68674500	-3.94116100	1.31552800	H	-4.86056200	-1.21915800	-0.90138400
H	-5.65577900	-3.42147700	1.29780500	C	-7.36083500	-2.92242500	-2.46232700
H	-4.38215700	-4.14253000	0.28827500	H	-7.04967300	-4.50640200	-3.89336400
H	-5.64191100	-5.73754800	2.14134300	H	-7.33508300	-1.34067400	-0.99601000
H	-3.86979400	-5.81097300	2.00557500	H	-8.44525000	-2.99204200	-2.49269300
H	-5.52777700	-4.23112800	4.03371500	C	-3.05505800	-1.69161000	-4.79824300
H	-4.06472800	-5.17327300	4.34306300	H	-2.58428900	-0.95326900	-5.45693100
H	-2.66885800	-3.34870000	3.66051900	H	-2.93823500	-2.68023000	-5.25645000
H	-4.13413400	-2.34884600	3.78893500	H	-4.12583800	-1.47291900	-4.76156800
O	-3.34490300	1.23723400	-1.40027100	C	2.89286000	1.24852200	1.23952900
C	-4.68038900	1.66899000	-1.05192700	C	3.80795700	1.79740600	2.15132000
C	-4.68956200	3.18938500	-1.22965400	C	2.76358500	1.86230700	-0.01248300

C	-3.65685200	3.38445300	-2.35019100
C	-2.60590700	2.33273300	-1.99869200
H	5.26279200	3.33332400	2.55638800
H	3.38924900	3.45707700	-1.31538000
H	4.99622400	4.41806000	0.32954400
C	0.37826700	-0.82085800	3.36240200
C	4.55886900	2.92948200	1.83254500
H	3.93519600	1.32796200	3.12578700
C	3.51190600	2.99749100	-0.33750400
H	2.07934600	1.44614100	-0.74378800
C	4.41193000	3.53724500	0.58320800

Table 13. Geometric coordinates and thermally corrected MP2 energies for heteroaggregate **5c**. THFs are omitted in the chemdraw representation.





5c

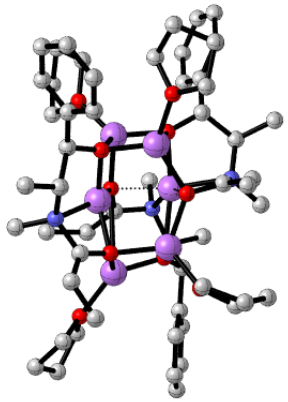
G = –3106.785041
G_{MP2} = –3096.579279

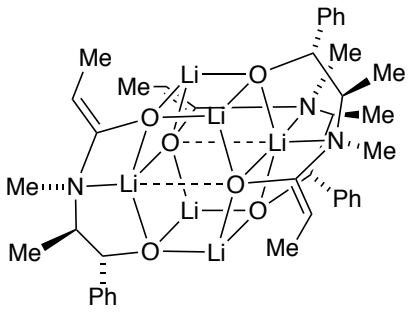
Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	C	3.03554300	-3.79771100	-0.78996600
Li	-1.93126700	-1.19499000	-0.77338800	C	2.70737900	-4.78188900	0.37318200
Li	-1.48066200	-2.60218200	1.19032300	N	1.23266900	-5.06177600	0.33221400
Li	0.35579800	-3.17062100	-0.70383700	C	0.53188500	-4.59733200	1.52425600
Li	1.85715300	-2.05167900	1.23803200	O	0.33625500	-3.28437300	1.53046000
O	1.75825500	-0.16816000	0.67594700	C	0.15223000	-5.47367300	2.48963000
C	1.77475100	1.04947500	1.21165800	C	-0.57414800	-5.10343000	3.75376700
N	0.43498100	1.58433300	1.41433900	H	-0.94649500	-4.07607700	3.70499300
C	-0.41692500	1.00036200	2.51214600	H	-1.43145700	-5.76536600	3.94783800
C	-1.73882600	0.34872700	1.95195600	H	0.07230100	-5.17903900	4.64331900
O	-1.48072100	-0.59395400	0.96106600	H	0.42283500	-6.51925300	2.36846500
H	-2.18581800	-0.13478000	2.84105000	C	0.86191300	-6.37767300	-0.17950000
H	-0.71710700	1.84650900	3.14631900	H	1.27773200	-6.50791100	-1.18549800
C	0.33252000	3.04635700	1.38192600	H	1.19997200	-7.22877300	0.43296100
H	-0.71813100	3.33183100	1.30119900	H	-0.22477700	-6.43427500	-0.25501400
H	0.74689400	3.52766800	2.28398200	H	2.89310000	-4.21976400	1.29469700
H	0.86914600	3.43126200	0.51123100	H	2.72008400	-4.31385700	-1.71908000
C	2.88420800	1.79100100	1.45547100	O	-0.07394500	-0.84436000	-1.64669000
C	4.28101400	1.38873800	1.06934000	C	-0.22490900	-1.40052100	-2.84881700
H	4.75139900	2.12812800	0.40199000	N	0.00991000	-2.85212300	-2.86855500
H	4.94939600	1.30212000	1.93962700	C	-1.15963500	-3.77128400	-2.98887000
H	4.28241000	0.42483200	0.55259300	C	-2.23561200	-3.41741100	-1.91047600
H	2.76897200	2.75855100	1.93364800	O	-1.65827500	-3.09927500	-0.68328200
Li	2.04255300	-0.91688200	-1.14878500	H	-2.78072200	-2.54849900	-2.33001000

O	2.30336900	-2.63387400	-0.58610400	H	-0.75246000	-4.76076700	-2.72981000
C	1.11556300	-3.23003100	-3.75212800	H	-5.32838200	-3.10977400	4.78163600
H	0.92922500	-3.03640300	-4.81981000	H	-3.12939500	-2.26550100	4.23417100
H	2.01205600	-2.67858700	-3.45676800	H	-4.06300600	-1.40435900	2.98667900
H	1.31852000	-4.30146700	-3.63405900	O	-3.72999200	-0.55592400	-1.44665800
C	-0.50886900	-0.72054900	-3.98543800	C	-4.89678100	-0.80968300	-0.62581600
H	-0.57976500	-1.28013600	-4.91365200	C	-6.06343100	-0.11988800	-1.33938800
C	-0.65620300	0.77335300	-4.07718600	C	-5.62186400	-0.16744500	-2.81093200
H	-1.63511500	1.07482500	-4.47940000	C	-4.11427900	0.05746200	-2.69389400
H	-0.54366500	1.23568300	-3.09156300	H	-3.87156300	1.12726400	-2.65100300
H	0.09703600	1.21820600	-4.74541800	H	-3.52614100	-0.40642100	-3.49021900
O	3.11540700	0.15571300	-2.39694800	H	-6.10976700	0.58682800	-3.43588900
C	4.30272700	-0.25308100	-3.10767500	H	-5.82946800	-1.15426900	-3.24147700
C	5.17824800	0.99644700	-3.14986000	H	-6.15403600	0.91832300	-1.00132200
C	4.12990600	2.10778200	-3.32635000	H	-7.01756300	-0.62415100	-1.15821800
C	2.94028800	1.59165600	-2.50108100	H	-5.03696300	-1.89530800	-0.56182800
H	1.97493300	1.79106000	-2.97582700	H	-4.69976200	-0.41048200	0.37177900
H	2.92816400	1.99557700	-1.48344000	C	-3.28000000	-4.53668000	-1.81452100
H	3.85326700	2.20214200	-4.38296100	C	-4.49784700	-4.45869600	-2.50354200
H	4.47708900	3.08642300	-2.98184500	C	-3.04008900	-5.67339100	-1.03184800
H	5.91612800	0.96715700	-3.95737400	C	-5.44204100	-5.48637300	-2.42770300
H	5.71042700	1.11402300	-2.19911300	H	-4.70596400	-3.58379000	-3.11675400
H	4.74129100	-1.09223400	-2.56511300	C	-3.97452200	-6.70691000	-0.95594900
H	4.02409400	-0.58147300	-4.11918200	H	-2.12147600	-5.72255800	-0.45727400
O	2.96465300	-2.26149400	2.96109000	C	-5.18125300	-6.61881200	-1.65560900
C	2.51418300	-3.09516300	4.05391900	H	-6.38004100	-5.40050200	-2.97140400
C	3.64137900	-3.03631700	5.08053800	H	-3.76243100	-7.58239700	-0.34629700
C	4.10399500	-1.57700900	4.94487500	H	-5.91114400	-7.42218300	-1.59518800
C	3.95574300	-1.31865600	3.43912900	C	4.53408200	-3.53211600	-0.94179300
H	4.89126000	-1.51329900	2.90148300	C	5.28932700	-4.19695400	-1.91735200
H	3.61653100	-0.30751300	3.20145100	C	5.19150400	-2.60752500	-0.11701400
H	5.12704600	-1.40900900	5.29503700	C	6.65796200	-3.95619000	-2.06359500
H	3.44036300	-0.91649700	5.51547400	H	4.79633600	-4.90977200	-2.57577100
H	4.44834700	-3.72551500	4.80349900	C	6.55936400	-2.36482700	-0.25507900
H	3.30411900	-3.29166400	6.08996200	H	4.61463000	-2.06714100	0.62609200
H	1.58203400	-2.68208700	4.46005900	C	7.29986900	-3.03873800	-1.23053500
H	2.30440600	-4.08848200	3.65312500	H	7.22021400	-4.48124900	-2.83226400
O	-3.09844200	-3.12132400	2.34859300	H	7.04787000	-1.64317200	0.39592100
C	-3.80138000	-2.39287800	3.37506900	H	8.36384800	-2.84603500	-1.34262700
C	-5.02580900	-3.24140600	3.73828100	C	-2.74471100	1.42947600	1.53377900
C	-4.54358000	-4.66342600	3.41367600	C	-3.66780200	1.92154000	2.46799500
C	-3.69440500	-4.42797800	2.16589400	C	-2.76073700	1.98102300	0.24478100
H	-4.30206000	-4.41527200	1.25453900	C	-4.57103500	2.93419000	2.13679900
H	-2.88235000	-5.14556800	2.03540500	H	-3.67756500	1.50418500	3.47384200
H	-5.36206200	-5.36747600	3.23523900	C	-3.65438300	3.00017000	-0.09119500
H	-3.92524800	-5.05484900	4.22991600	H	-2.06741100	1.61008600	-0.50335900

H	-5.87861900	-2.97495200	3.10247500	C	-4.56603300	3.48106900	0.85291600
H	-5.27825100	3.29332600	2.88063700	H	3.28593000	-6.68210700	1.27357100
H	-3.63637200	3.42332600	-1.09309900	H	3.55879100	-6.62780100	-0.47893500
H	-5.26314100	4.27249900	0.58979400	H	4.62962100	-5.74326800	0.60894300
C	-1.77006400	-3.87122100	-4.39738700	C	0.31226900	0.01061700	3.42613200
H	-2.51963000	-4.66721500	-4.43250500	H	0.46225800	-0.95815500	2.94693200
H	-2.25592100	-2.93298300	-4.68714500	H	1.28344600	0.40564300	3.73902100
H	-1.00934200	-4.10315400	-5.15029800	H	-0.29384200	-0.15067400	4.32574600
C	3.58896400	-6.03574400	0.44253300				

Table 14. Geometric coordinates and thermally corrected MP2 energies for heteroaggregate **5d**. THFs are omitted in the chemdraw representation.





5d

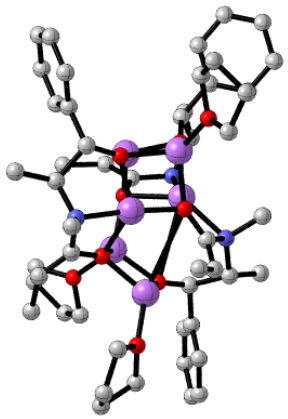
G = –3106.777111
G_{MP2} = –3096.568241

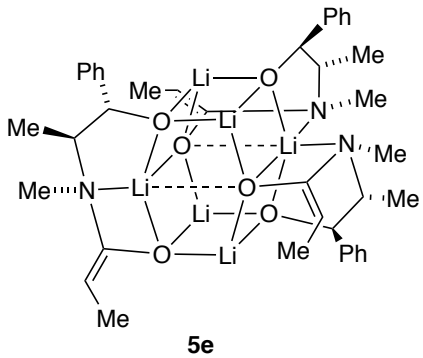
Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	C	-2.23291900	-4.29837800	-0.00931200
Li	-2.68554500	-0.85207200	0.10064000	C	-2.78306000	-3.43666900	1.20030500
Li	-1.44144400	-0.84784100	2.43308200	O	-2.19512600	-2.19099400	1.29925100
Li	0.19743100	-2.68702900	1.16102600	H	-2.53968400	-4.03596100	2.10110000
Li	2.10493400	-0.76280500	1.88313700	H	-2.94378600	-4.24873000	-0.84947700
O	1.84057000	0.31486200	0.33295400	C	-0.15025100	-4.72792300	-1.27650200
Li	2.01101600	-1.50340400	-0.51090800	H	-0.71366200	-5.06993000	-2.16153100
O	2.19263500	-2.57871200	1.02085800	H	0.75316500	-4.22017300	-1.62298200
C	2.87966200	-3.41262800	1.89105100	H	0.15990900	-5.60106900	-0.69662700
C	1.91912600	-4.31719200	2.73935100	C	-1.78241500	-2.20620600	-2.14603100
N	0.66424900	-3.58843200	3.09588000	H	-2.52495800	-2.95539000	-2.40705000
C	0.76299800	-2.24302100	3.69429500	C	-1.70414000	-0.98041900	-3.01945100
O	0.44043900	-1.26765300	2.85460300	H	-2.55237600	-0.29297600	-2.88163800
C	1.11183700	-2.08833000	4.99725300	H	-0.78869200	-0.41626000	-2.81367200
C	1.18643200	-0.76768800	5.71492600	H	-1.69366100	-1.25358000	-4.08489100
H	1.11657200	0.06277700	5.00544900	O	3.01872600	-1.65652700	-2.21009400
H	0.38189200	-0.64176500	6.45629400	C	4.42799200	-1.97670000	-2.31939900
H	2.12668300	-0.65471600	6.27348300	C	4.66469100	-2.36387500	-3.78844600
H	1.32177400	-2.97901200	5.58266800	C	3.26012800	-2.77044500	-4.26624800
C	-0.28827900	-4.44694600	3.80139100	C	2.37683200	-1.79439200	-3.49247500
H	-0.42640300	-5.37751300	3.23741600	H	1.35633400	-2.14073200	-3.31503100
H	0.01479900	-4.71583700	4.82511500	H	2.33680300	-0.81406600	-3.98929200
H	-1.25390800	-3.93790500	3.86084800	H	3.03493700	-3.80155100	-3.96951300
H	1.57384600	-5.13129000	2.08385500	H	3.13208500	-2.68890900	-5.35002500
H	3.45414400	-2.82131400	2.62868800	H	5.40270100	-3.16503100	-3.88847500
O	0.06778700	-1.70089900	-0.74080100	H	5.02357100	-1.50194200	-4.36302900
C	-0.91013500	-2.48399700	-1.14196700	H	5.01009400	-1.10228300	-2.00996500

N	-0.91260000	-3.78249400	-0.44328000	H	4.63241500	-2.80347900	-1.63308100
C	2.05574300	1.62371000	-0.11988000	H	-4.70156900	-1.29016800	-2.61908400
C	0.86801700	2.55135500	0.30607700	H	-5.35896100	-2.02214700	-1.13198300
N	-0.38961100	2.00479800	-0.28793600	H	-6.96470500	-0.47298200	-2.82236000
C	-1.49577800	1.79964000	0.65015900	H	-7.21020200	-0.51843700	-1.06772500
O	-1.65238300	0.51333200	0.95727500	H	-5.54847600	1.53271900	-2.63557700
C	-2.23119300	2.84157300	1.09695700	H	-6.79969400	1.87304600	-1.42293700
C	-3.37106200	2.74374600	2.07103200	H	-5.40279100	1.00219700	0.38189300
H	-3.17057300	3.31547600	2.98987600	H	-4.16453500	1.79283700	-0.62312700
H	-4.30765200	3.14968200	1.65928500	C	3.90244300	-4.30023700	1.16489600
H	-3.55012400	1.70254300	2.35580200	C	5.20299600	-4.48307000	1.65200400
H	-1.96865000	3.83364300	0.73722800	C	3.55005400	-4.95420900	-0.02460900
C	-0.78501900	2.55522000	-1.58358900	C	6.12316900	-5.29514500	0.98196600
H	0.05513200	2.49335900	-2.28493500	H	5.50042900	-3.98586000	2.57320600
H	-1.60250800	1.95365300	-1.99121900	C	4.46010100	-5.77157200	-0.69593500
H	-1.11958100	3.60363200	-1.54267600	H	2.55248600	-4.80248300	-0.42228200
O	3.97755800	-0.46673600	2.73914000	C	5.75436000	-5.94520600	-0.19549900
C	4.39086900	-0.46471900	4.12088300	H	7.12736500	-5.41750600	1.38121200
C	5.85469400	-0.91152600	4.12325000	H	4.15972600	-6.27723000	-1.61127800
C	6.35302400	-0.39033800	2.76678700	H	6.46522100	-6.57983500	-0.71868600
C	5.13023200	-0.59383700	1.86908800	C	2.66435300	-4.95768600	3.92335100
H	5.11417200	-1.59462600	1.42302400	H	3.51332400	-5.54507000	3.56055700
H	5.04130000	0.15271200	1.07892400	H	3.04616700	-4.19437700	4.60952800
H	7.23328600	-0.92473100	2.39585000	H	2.01969700	-5.63442200	4.49384200
H	6.60058000	0.67457600	2.83188800	C	-4.33127000	-3.35232700	1.19203600
H	5.91985200	-2.00549600	4.16168600	C	-4.94227700	-2.26541800	1.83809900
H	6.41178500	-0.51025200	4.97578100	C	-5.17735700	-4.31404000	0.61362100
H	4.28234000	0.55311600	4.51991200	C	-6.33136100	-2.14468900	1.91286800
H	3.72602400	-1.13433000	4.67072900	H	-4.30705500	-1.50270700	2.27524900
O	-2.55519100	-0.44209800	4.11943800	C	-6.56894300	-4.19428600	0.67854600
C	-2.18274000	0.65310600	4.99406400	H	-4.76326300	-5.17162100	0.09403900
C	-2.57318400	0.22671500	6.42005400	C	-7.15590200	-3.11019500	1.33140500
C	-2.68402500	-1.30325700	6.30743400	H	-6.77000200	-1.29260500	2.42810800
C	-3.21493100	-1.46810000	4.88696400	H	-7.19332800	-4.95479000	0.21522700
H	-4.30318800	-1.31681000	4.84464900	H	-8.23786200	-3.02060700	1.38787400
H	-2.97983400	-2.42876200	4.42460700	C	-2.12521800	-5.76941200	0.42568000
H	-3.34697700	-1.74298300	7.05921400	H	-1.98500000	-6.45384600	-0.41721000
H	-1.69834900	-1.77245600	6.39207500	H	-1.28966500	-5.90264300	1.12227700
H	-3.54117300	0.65843300	6.70013900	H	-3.03401400	-6.07549000	0.95164400
H	-1.83634200	0.54950500	7.16143400	H	2.07788900	1.64215600	-1.22886100
H	-1.10553900	0.80336800	4.88534000	C	3.39579500	2.20492000	0.33353600
H	-2.70246000	1.55750100	4.66540400	C	4.41124900	2.45435800	-0.59816500
O	-4.31350500	-0.24497100	-0.88021800	C	3.64087200	2.52864200	1.67715600
C	-4.94467400	1.02885200	-0.61546300	C	5.63579800	3.00640200	-0.20976100
C	-6.00403400	1.17616000	-1.70379700	H	4.23517300	2.21753500	-1.64591900
C	-6.49031500	-0.27383300	-1.85662200	C	4.85366400	3.09426600	2.07000200

C	-5.20124400	-1.08327300	-1.66640400	H	2.87060400	2.34218100	2.42044900
C	5.85937800	3.33350900	1.12761100	H	1.92077600	4.43080600	0.61355600
H	6.40812100	3.18936600	-0.95315100	H	1.32634600	4.23132400	-1.03510900
H	5.01476900	3.35561500	3.11348500	H	0.19684900	4.62514400	0.27508100
H	6.80390200	3.77581000	1.43438500				
H	0.75509800	2.42460500	1.38893300				
C	1.08947100	4.04463700	0.01878800				

Table 15. Geometric coordinates and thermally corrected MP2 energies for heteroaggregate **5e**. THFs are omitted in the chemdraw representation.





5e

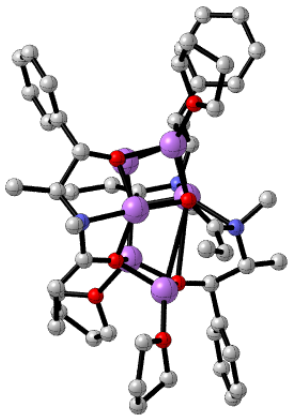
G = -3106.786758
G_{MP2} = –3096.554593

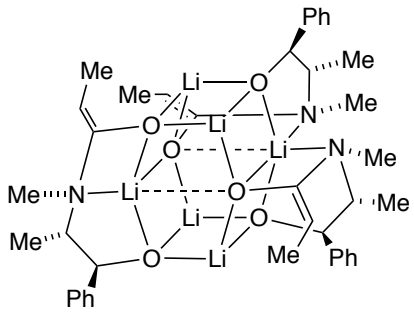
Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	H	7.74908500	-0.02436700	-4.17528000
Li	1.92655700	-0.83984200	-1.55284100	H	7.02278000	-1.90313500	-5.63800000
Li	2.07429300	1.54506500	-1.03673700	C	3.70844800	3.33010600	-4.92756800
O	1.87463600	0.16156600	0.15684200	H	4.10607300	3.94675400	-4.11462500
C	2.23763700	0.15141600	1.50638400	H	4.54767000	2.80186600	-5.39111800
C	1.13498900	0.86896400	2.34708900	H	3.28123400	3.99652300	-5.68397700
N	-0.17744300	0.19497300	2.09122600	C	-3.88505300	2.41709000	-3.93537200
C	-1.27240100	1.11085900	1.76185100	C	-3.96848400	3.67924100	-4.53779400
O	-1.42500400	1.24578000	0.44665200	C	-5.08446100	1.73999000	-3.66660600
Li	-2.76876100	0.63043600	-0.82281500	C	-5.20244700	4.25452400	-4.85541700
Li	-1.14023900	2.66289300	-1.01215000	H	-3.05038200	4.21881600	-4.76310700
O	0.72361500	2.73275100	-1.65044600	C	-6.31981500	2.30341200	-3.98765400
Li	0.49938000	1.09675800	-2.93545800	H	-5.04729700	0.75702000	-3.20418300
O	2.34917200	0.61165700	-2.68662900	C	-6.38484200	3.56733500	-4.58129900
C	3.31760700	1.35448400	-3.35029000	H	-5.23770300	5.23677900	-5.32095300
C	2.67770500	2.31504400	-4.40547600	H	-7.23552700	1.75411200	-3.77953300
N	1.39902300	2.88911600	-3.88583500	H	-7.34699200	4.00734200	-4.83096900
C	1.39032100	3.47737800	-2.53797100	C	-2.26546000	0.66997500	-5.78849100
C	2.01045100	4.65095700	-2.27562200	H	-3.17483400	1.19128900	-6.09948100
C	2.05933100	5.32205500	-0.93076000	H	-1.40970100	1.29115900	-6.08086300
H	1.61126000	4.68207100	-0.16408800	H	-2.21759200	-0.26782400	-6.34942100
H	3.08980400	5.54508000	-0.62157200	C	3.61807700	0.77723100	1.70483800
H	1.51304100	6.27882600	-0.92563000	H	3.87198600	2.01081700	-2.64300800
H	2.49281300	5.16693100	-3.10100800	O	-2.37084400	1.76843600	-2.17337500
C	0.70975000	3.71812200	-4.87494500	C	-2.52369900	1.82077200	-3.54580600
H	0.59286300	3.15032400	-5.80719700	C	-2.30189700	0.44776700	-4.27042500
H	-0.28611800	3.96937600	-4.50003500	N	-1.04587900	-0.17559200	-3.76491700

H	1.22701000	4.66096800	-5.11354700	C	-1.11913600	-0.85784100	-2.46260700
H	2.36205000	1.69384200	-5.25725000	O	-0.03292300	-0.66915700	-1.74524500
C	-2.16289600	-1.64800900	-2.09852800	H	-0.73286500	-0.57940600	4.03381300
H	-2.98611900	-1.78829800	-2.79200400	H	-1.40400600	-1.41470900	2.61847700
C	-2.15853500	-2.50582200	-0.85582000	H	1.03010800	1.87138900	1.91519200
H	-3.17570300	-2.81260000	-0.58401800	H	2.30332900	-0.88845300	1.88369500
H	-1.57164500	-3.42964500	-0.98539900	O	5.62357800	5.82519800	-0.05138000
H	-1.72828300	-1.99227500	0.01425500	C	5.77179000	7.17501800	0.39233200
C	-0.38343900	-1.10682500	-4.70217900	C	5.79484600	8.01169700	-0.88713200
H	-1.03308200	-1.94504200	-5.00255800	C	6.60411300	7.10183400	-1.82796100
H	-0.04489400	-0.58191700	-5.59905300	C	6.21458300	5.68449800	-1.35583100
H	0.49843600	-1.51628200	-4.20274800	H	7.08298800	5.01580700	-1.29480200
H	-3.15525300	-0.21238200	-4.05852400	H	5.46803000	5.21680100	-2.00774100
H	-1.76068900	2.49061800	-3.98985700	H	7.67774200	7.27308500	-1.68844900
O	-1.97145700	4.45284300	-0.46541100	H	6.37693500	7.26610100	-2.88542000
C	-1.50550800	5.52849300	0.35800800	H	6.24550100	8.99940600	-0.74773300
C	-1.95756200	6.81487900	-0.36211600	H	4.77427100	8.14758400	-1.26291500
C	-3.13736300	6.34012800	-1.25704300	H	4.93491200	7.39956400	1.06012100
C	-3.27723000	4.84812600	-0.91135400	H	6.71080500	7.29500200	0.95805900
H	-3.54647900	4.20103700	-1.74478000	O	2.83105500	-2.57970300	-1.60378400
H	-3.99619700	4.70079500	-0.09009700	C	4.26601000	-2.62736300	-1.38601100
H	-2.89422300	6.46461300	-2.31647000	C	4.56358500	-4.05079600	-0.90094500
H	-4.06394300	6.88890600	-1.06238500	C	3.42037200	-4.86258400	-1.53126400
H	-1.14596900	7.22206200	-0.97236000	C	2.24987400	-3.88543200	-1.42339900
H	-2.25589500	7.58854200	0.35232700	H	1.77268600	-3.93761000	-0.43488700
H	-1.96782000	5.44648500	1.35288000	H	1.48203400	-4.02149300	-2.18980100
H	-0.42508200	5.42680000	0.45748600	H	3.22571300	-5.80970700	-1.01888700
O	-4.52724000	0.13048600	0.01933000	H	3.63879800	-5.07995400	-2.58348400
C	-5.77451800	0.79206700	-0.27794100	H	4.50798700	-4.10561300	0.19283600
C	-6.46431000	0.96588300	1.07232600	H	5.55693200	-4.39274100	-1.20619800
C	-6.05761000	-0.32614700	1.79921200	H	4.75870400	-2.40022800	-2.33678400
C	-4.62994200	-0.57163400	1.28687300	H	4.52705100	-1.85547300	-0.65620700
H	-4.41822300	-1.63150500	1.11494200	C	4.37086300	0.45516900	-4.00338200
H	-3.86781600	-0.15797600	1.95465500	C	3.97557400	-0.61492200	-4.81996300
H	-6.72045700	-1.14933700	1.50770700	C	5.73898200	0.64963000	-3.78231100
H	-6.09337700	-0.23656700	2.88889900	C	4.92067200	-1.45556800	-5.40758500
H	-7.54804500	1.08536700	0.97810100	H	2.91546700	-0.79382700	-4.97677600
H	-6.06279300	1.84267800	1.59153000	C	6.69147100	-0.19235800	-4.36447200
H	-5.54135600	1.72594500	-0.79287400	H	6.06264500	1.46721600	-3.14122200
H	-6.37047700	0.15868500	-0.95081200	C	6.28543100	-1.24722300	-5.18183600
C	-1.99807400	1.70550900	2.73576900	H	4.59396300	-2.27568200	-6.04303100
C	-3.12593400	2.67105600	2.50737100	C	4.67778600	0.03306900	2.23589100
H	-4.06805500	2.33036400	2.96473400	C	3.87360600	2.10241300	1.31514400
H	-2.91241200	3.65555600	2.95061500	C	5.95441400	0.58685400	2.36960800
H	-3.29709800	2.81960200	1.43785700	H	4.49969100	-0.99480400	2.54706200
H	-1.73205300	1.48881900	3.76759600	C	5.14475900	2.66517800	1.44317700

C	-0.51929000	-0.89631700	3.00104300	H	3.06505200	2.71640900	0.91940700
H	0.30488200	-1.61833300	3.03453200	C	6.19126500	1.90238500	1.97168600
H	6.76266700	-0.01271300	2.78210700	H	1.69117100	0.06588300	4.31429900
H	5.31615300	3.69289500	1.13227600	H	2.36831700	1.65510500	3.94991700
H	7.18359100	2.33473900	2.07253500	H	0.65597200	1.50734000	4.37449400
C	1.47953700	1.02832300	3.83414900				

Table 16. Geometric coordinates and thermally corrected MP2 energies for heteroaggregate **5f**. THFs are omitted in the chemdraw representation.





5f

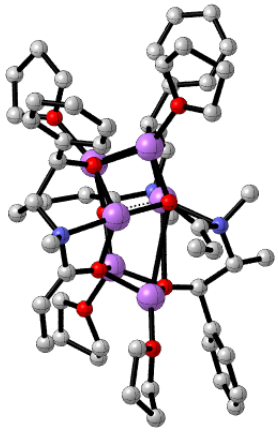
G = –3106.787289
G_{MP2} = –3096.555365

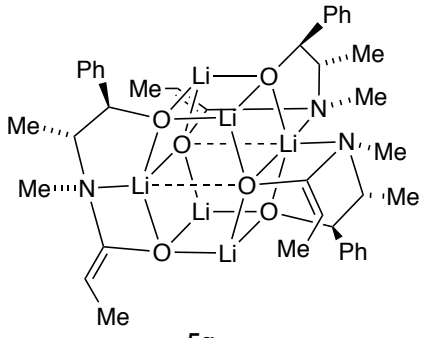
Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	H	3.89091700	1.81306700	-2.80414500
Li	1.91751500	-0.93473400	-1.51101300	O	-2.35710000	1.67810900	-2.28190100
Li	2.08673900	1.47328800	-1.14397900	C	-2.51761700	1.64071900	-3.65414500
O	1.87702600	0.16698000	0.13401800	C	-2.31831600	0.21877300	-4.28447500
C	2.24100900	0.25599500	1.48091300	N	-1.06605600	-0.38211900	-3.74456200
C	1.14462900	1.04756300	2.26081500	C	-1.13803900	-0.97444200	-2.40053800
N	-0.16928400	0.35270400	2.07510000	O	-0.04051300	-0.76399800	-1.70793000
C	-1.26863900	1.23765000	1.68294800	C	-2.19031900	-1.71574000	-1.96469700
O	-1.41302900	1.28891700	0.36091200	H	-3.03261400	-1.88688600	-2.62693000
Li	-2.76757000	0.62097600	-0.86891700	C	-2.16299400	-2.47721000	-0.65935600
Li	-1.11762400	2.62407000	-1.17365900	H	-3.14160000	-2.92356500	-0.44810700
O	0.74507600	2.63680000	-1.81760600	H	-1.42787000	-3.29726300	-0.66844400
Li	0.49429300	0.93088000	-3.00120200	H	-1.90293500	-1.84921000	0.20532800
O	2.34238600	0.44299800	-2.73609100	C	-0.41554000	-1.37893200	-4.62079800
C	3.31085700	1.12702200	-3.46040300	H	-1.07394200	-2.22898700	-4.86308600
C	2.66973100	2.03600700	-4.56077000	H	-0.07628500	-0.91681600	-5.55122600
N	1.40148000	2.65236900	-4.06380900	H	0.46454400	-1.76223300	-4.09821100
C	1.41190800	3.32013100	-2.75309000	H	-3.17751200	-0.41571400	-4.02288400
C	2.04587100	4.50066800	-2.56622200	H	-1.74746100	2.26730200	-4.14602700
C	2.11352100	5.24848900	-1.26347100	O	-1.91630500	4.44958500	-0.71994300
H	1.67451800	4.65420300	-0.45567600	C	-1.43409200	5.53997900	0.07431100
H	3.14834900	5.48675100	-0.98161000	C	-1.87657400	6.81374200	-0.67396700
H	1.56857100	6.20515800	-1.30597500	C	-3.06194900	6.32963400	-1.55629900
H	2.52544400	4.96208800	-3.42476900	C	-3.21823900	4.84848200	-1.17316900
C	0.71247800	3.43044800	-5.09377900	H	-3.49727700	4.18436100	-1.98999400
H	0.57221800	2.80816500	-5.98720800	H	-3.93753900	4.72954300	-0.34772300
H	-0.27318400	3.72244900	-4.72178600	H	-2.81754700	6.42484900	-2.61849000

H	1.24243100	4.34733400	-5.39657700	H	-3.98227300	6.89347200	-1.37548200
H	2.34017000	1.37359700	-5.37548200	H	-1.06277800	7.20084300	-1.29426000
H	-2.16729500	7.60544600	0.02365300	H	1.76093000	-4.00630600	-0.26075000
H	-1.89047100	5.48717600	1.07372600	H	1.49325100	-4.14493000	-2.01576400
H	-0.35408800	5.42909900	0.16924000	H	3.23687100	-5.88135500	-0.76609000
O	-4.54105800	0.20135400	-0.01322500	H	3.65742100	-5.20300100	-2.35160900
C	-5.77551300	0.86824000	-0.34958600	H	4.49736400	-4.12472100	0.39527700
C	-6.48873000	1.08490200	0.98239500	H	5.55973100	-4.45620600	-0.98408600
C	-6.10266400	-0.18741900	1.75421000	H	4.74921000	-2.51805300	-2.19926500
C	-4.66642000	-0.45169200	1.27786300	H	4.51737800	-1.90611700	-0.54166400
H	-4.45096200	-1.51674800	1.14977800	C	4.33401700	0.17083000	-4.08000500
H	-3.91703700	-0.01237500	1.94404100	C	3.90101900	-0.94929300	-4.80501200
H	-6.76256400	-1.01640900	1.47254700	C	5.71061000	0.36313900	-3.91730100
H	-6.16014400	-0.06674700	2.83998700	C	4.81740200	-1.84155200	-5.36114800
H	-7.56983600	1.20706000	0.86445100	H	2.83436700	-1.12427000	-4.91371700
H	-6.09227700	1.97430400	1.48357800	C	6.63462500	-0.52999600	-4.46841300
H	-5.52344500	1.78575300	-0.88484500	H	6.06361500	1.21971000	-3.34643100
H	-6.36585400	0.22370000	-1.01645200	C	6.19091100	-1.63518500	-5.19467800
C	-2.00815800	1.88273300	2.61366600	H	4.46148200	-2.70045800	-5.92574000
C	-3.14915600	2.81447200	2.31941100	H	7.69959600	-0.36259800	-4.32561200
H	-4.08048900	2.50375400	2.81802200	H	6.90600600	-2.33123700	-5.62613600
H	-2.94240300	3.83599800	2.67338900	C	3.70673600	3.00990500	-5.14527600
H	-3.33744200	2.86891600	1.24375700	H	4.11666600	3.66574300	-4.36985900
H	-1.74494300	1.73667600	3.65849400	H	4.53682800	2.44809700	-5.58533500
C	-0.49565100	-0.65782200	3.07874300	H	3.28033400	3.63825400	-5.93402600
H	0.32947800	-1.37510900	3.15783800	C	-3.87159500	2.23255800	-4.07554600
H	-0.69072900	-0.25583000	4.08519400	C	-3.93675900	3.46358200	-4.74154700
H	-1.38695300	-1.20510700	2.75677500	C	-5.08070500	1.58811800	-3.77253100
H	1.03819900	2.00607000	1.73884700	C	-5.16217600	4.04055900	-5.08757400
H	2.29535400	-0.75220100	1.93715400	H	-3.01080000	3.97696800	-4.99405400
O	5.66657700	5.79076600	-0.41662200	C	-6.30775600	2.15271700	-4.12210900
C	5.85762900	7.13098700	0.04643100	H	-5.05851300	0.63008600	-3.25969100
C	6.09077900	7.96685200	-1.21297500	C	-6.35446900	3.38582800	-4.77887100
C	6.90316700	6.98826300	-2.07679500	H	-5.18316400	4.99814800	-5.60273000
C	6.28896200	5.62666300	-1.70402700	H	-7.23140500	1.62842800	-3.88634300
H	7.03928500	4.82882700	-1.64359300	H	-7.31018100	3.82683300	-5.05057400
H	5.51564900	5.31469000	-2.41695500	C	-2.28893800	0.33601000	-5.81432600
H	7.96164700	7.02410700	-1.79323100	H	-3.19232100	0.84935000	-6.15464100
H	6.83711500	7.19747200	-3.14869000	H	-1.42575400	0.92222400	-6.15334100
H	6.61426700	8.90687100	-1.01228500	H	-2.25951300	-0.63833200	-6.31070900
H	5.13332500	8.20146000	-1.69265200	C	3.62850800	0.87900900	1.63206900
H	4.96810300	7.42025800	0.61444300	C	4.67994800	0.16205600	2.21442500
H	6.72946200	7.18039300	0.71891900	C	3.89947000	2.16932200	1.14718400
O	2.82330400	-2.67463700	-1.45457800	C	5.96363600	0.70789400	2.30640200
C	4.25867500	-2.70802500	-1.23911600	H	4.48951900	-0.83849200	2.59878700
C	4.56183600	-4.10986400	-0.69931100	C	5.17769800	2.72395400	1.23329000

C	3.42897100	-4.95105600	-1.30930200	H	3.09799900	2.76412500	0.70964800
C	2.25025600	-3.97949800	-1.24422100	C	6.21573300	1.98825800	1.81428100
H	6.76521900	0.12967000	2.76031300	H	1.71527400	0.43227500	4.29234300
H	5.36049800	3.72487800	0.84980200	H	2.37834300	1.98587900	3.77993300
H	7.21349700	2.41447200	1.88272500	H	0.66828900	1.86502700	4.22181700
C	1.49429600	1.34422900	3.72549300				

Table 17. Geometric coordinates and thermally corrected MP2 energies for heteroaggregate **5g**. THFs are omitted in the chemdraw representation.





5g

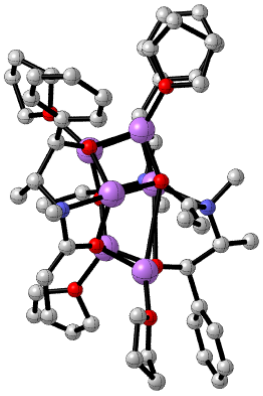
G = –3106.784881
G_{MP2} = –3096.573261

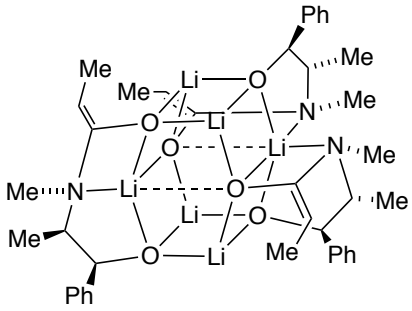
Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	H	-1.34223200	-5.59453300	-1.35116500
Li	-2.07840500	-1.24302800	-1.04814200	H	-2.88256100	-4.30126600	0.91783100
Li	-1.61393900	-2.11322800	1.26129300	O	2.78754800	-2.23365900	-0.64533300
O	-1.72654200	-0.30758400	0.66007800	C	3.04923700	-3.27388700	-1.51934500
C	-2.08409000	0.72690600	1.51208000	C	2.32054800	-3.15408000	-2.90654500
C	-0.83721600	1.23877000	2.32925500	N	0.92423200	-2.69207300	-2.69519200
N	0.27107100	1.65395800	1.40350600	C	0.74430600	-1.25591100	-2.44416900
C	1.58381200	1.02567900	1.58648000	O	-0.19547800	-1.02783700	-1.55200200
O	1.72938800	-0.07227800	0.84493600	C	1.42068100	-0.29012100	-3.11929600
Li	2.82911800	-0.42580700	-0.71963400	H	2.13378100	-0.57976100	-3.88474700
Li	1.96242300	-2.09857100	1.09147300	C	1.10012200	1.18062600	-2.99779500
O	0.19126100	-2.97003600	1.38279200	H	1.91377500	1.79622100	-3.39981100
Li	-0.07559700	-2.99209800	-0.72087400	H	0.18908400	1.46065900	-3.55154200
O	-2.00606800	-3.02602600	-0.44305800	H	0.93315100	1.49871900	-1.95986900
C	-2.54800700	-4.26849200	-0.13788000	C	-0.02435200	-3.07136200	-3.75989900
C	-1.49509000	-5.41822300	-0.27502700	H	0.27927300	-2.70451900	-4.75455800
N	-0.15530600	-4.96616000	0.21211100	H	-0.14746100	-4.15632900	-3.80472700
C	-0.07280000	-4.26911100	1.50824200	H	-0.99657000	-2.63593600	-3.51510700
C	-0.24207600	-4.94898500	2.66831300	H	2.85790600	-2.43028100	-3.53592800
C	-0.19016700	-4.35092600	4.04686700	H	2.68070000	-4.22614500	-1.09522600
H	-0.03194800	-3.26907000	3.99967900	O	3.39726500	-2.67084800	2.44124000
H	-1.12051000	-4.53726500	4.60449400	C	3.18664500	-3.54290900	3.57671000
H	0.61549900	-4.77946800	4.66210100	C	4.56675300	-4.10123300	3.95197600
H	-0.43250700	-6.01654600	2.60669100	C	5.33612800	-4.00104500	2.62578800
C	0.87277500	-5.99614400	0.06090100	C	4.78680200	-2.69795200	2.05065300
H	0.88407900	-6.35135000	-0.97750700	H	4.81697400	-2.63100600	0.96251500
H	1.85020400	-5.56083400	0.28447800	H	5.30132600	-1.82900600	2.48601000

H	0.73604800	-6.86939400	0.71780700	H	5.08583000	-4.84019300	1.96643400
H	6.42280400	-3.97988700	2.75407400	H	-2.57971300	0.88353500	-3.53628300
H	4.50707100	-5.12073400	4.34544300	H	-2.46226900	-0.73957700	-4.25195600
H	5.04420600	-3.47377200	4.71411900	H	-4.46392500	0.99572700	-5.06490200
H	2.72377600	-2.96471900	4.38258600	H	-4.79582300	-0.73793400	-4.89246200
H	2.49315700	-4.33098000	3.26842900	H	-5.27890900	1.44339200	-2.78719000
O	4.32523000	0.90103400	-0.99721100	H	-6.44331100	0.22344600	-3.34492200
C	5.71061200	0.66679400	-0.67005000	H	-5.24932300	-1.56129200	-2.19470900
C	6.43389300	1.91484900	-1.16543200	H	-4.91025500	-0.20812400	-1.07811100
C	5.43063700	3.02048700	-0.79417100	C	-3.78509900	-4.58027900	-0.98957300
C	4.06431800	2.33057600	-0.96721900	C	-3.77142100	-4.34085500	-2.37133700
H	3.58310900	2.58974700	-1.91448700	C	-4.95919300	-5.09034500	-0.42101200
H	3.37842200	2.54301200	-0.14137400	C	-4.89072300	-4.61170900	-3.15880200
H	5.52410300	3.91230600	-1.42092400	H	-2.87460400	-3.92422700	-2.81927700
H	5.57508300	3.32767300	0.24730900	C	-6.08668400	-5.35911100	-1.20301200
H	6.57499600	1.86413700	-2.25157700	H	-4.98918300	-5.28456300	0.64964700
H	7.41383600	2.04929500	-0.69724900	C	-6.05619100	-5.12093800	-2.57691600
H	5.81790100	0.55223200	0.41700500	H	-4.85525700	-4.42730100	-4.23035700
H	6.01236100	-0.26102100	-1.15709400	H	-6.98714900	-5.75276400	-0.73721900
C	2.51089400	1.58030800	2.39921300	H	-6.92955900	-5.32931900	-3.18979800
C	3.89041600	1.03814500	2.63733600	C	-2.02111500	-6.72667500	0.34019700
H	4.67773300	1.76768500	2.38916800	H	-2.24606600	-6.60387400	1.40497900
H	4.04435200	0.76984500	3.69343300	H	-2.94098300	-7.03399600	-0.16655100
H	4.05978400	0.13662300	2.04418100	H	-1.30257700	-7.54598500	0.23604100
C	-3.46309100	-2.37343600	3.93668800	C	4.55584600	-3.47312500	-1.74950900
C	-4.78355100	-3.13338600	4.06588800	C	5.20862800	-4.61973300	-1.27894600
C	-5.60470000	-2.58592600	2.87423400	C	5.32558400	-2.51325300	-2.42538600
C	-4.53722500	-1.98561300	1.92548900	C	6.58175400	-4.80517000	-1.46538400
H	-4.64923500	-0.89836800	1.82680200	H	4.62876900	-5.38271500	-0.76285300
H	-4.53091100	-2.43134500	0.93003800	C	6.69526700	-2.69458400	-2.62333000
H	-6.30890200	-1.81349100	3.19988300	H	4.84201400	-1.61591900	-2.80423200
H	-6.18474500	-3.37328200	2.38458500	C	7.33138900	-3.84189400	-2.14018600
H	-5.27187100	-2.97283100	5.03201900	H	7.06241400	-5.70512200	-1.08883200
H	-4.60172800	-4.20702100	3.95030400	H	7.26793500	-1.94365700	-3.16356500
H	-2.59897400	-2.88459200	4.36195600	H	8.39791500	-3.98403800	-2.29492000
H	-3.53761100	-1.36581600	4.37599500	C	2.38502300	-4.50649500	-3.62913500
O	-3.39720700	-0.65584800	-2.41079600	H	3.42509800	-4.84226700	-3.67193500
C	-4.80974200	-0.56063300	-2.10832600	H	1.81000100	-5.27363800	-3.09640200
C	-5.38503100	0.41147600	-3.13998000	H	2.01664000	-4.45260100	-4.65781600
C	-4.47731500	0.16309400	-4.35498100	H	-2.79014500	0.37217300	2.29015600
C	-3.11466900	-0.06135700	-3.69503500	H	-1.14793100	2.13141200	2.89463400
C	-2.60641800	2.15515500	-0.55392800	C	-0.41343200	0.18493300	3.35907200
C	-4.32546700	3.78508100	0.91489800	H	-1.27071300	-0.05187200	4.00011500
H	-3.85969600	2.50297800	2.57837700	H	-0.07373500	-0.74078500	2.88494000
C	-3.24503000	3.23626100	-1.16850400	H	0.39660300	0.55403500	3.99293900
H	-1.94587500	1.51483700	-1.12925800	C	-2.80502000	1.88005400	0.80512100

C	-4.10753800	4.05660200	-0.43770600	C	-3.68036900	2.70769800	1.52384100
H	-5.00130000	4.40954700	1.49446600	H	2.22907800	2.46828800	2.95941800
H	-3.06401600	3.44106900	-2.22159000	C	0.31926300	3.10970000	1.23763800
H	-4.60620300	4.89534900	-0.91676500	H	-0.64912200	3.46859000	0.88283500
H	1.07663900	3.36905300	0.49264900	H	0.55746400	3.64628400	2.17206900
O	-3.25598400	-2.27372100	2.52339500				

Table 18. Geometric coordinates and thermally corrected MP2 energies for heteroaggregate **5h**. THFs are omitted in the chemdraw representation.





5h

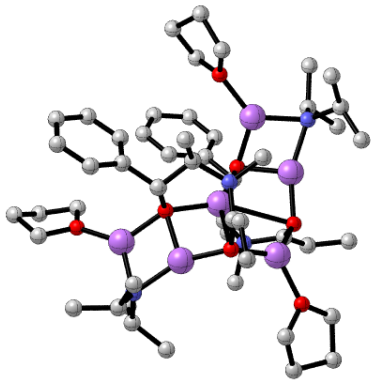
G = –3106.787421
G_{MP2} = –3096.574402

Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	H	-1.52685000	-5.72723600	-0.96944100
Li	-2.11288200	-1.26890500	-0.91630500	H	-2.97196100	-4.17020500	1.18650100
Li	-1.58300000	-2.05746000	1.40372900	O	2.78881400	-2.34215300	-0.51480300
O	-1.70378800	-0.26917000	0.74837400	C	2.98229600	-3.43654000	-1.33898600
C	-2.01676000	0.81907700	1.55125000	C	2.26884600	-3.33250000	-2.73271000
C	-0.73342200	1.37468900	2.27662200	N	0.87883100	-2.83981800	-2.53758600
N	0.33428800	1.72530100	1.27904100	C	0.71524700	-1.39460100	-2.34184900
C	1.65203300	1.10645600	1.44976600	O	-0.24075200	-1.12070300	-1.48134000
O	1.75320900	-0.05214200	0.80161200	C	1.41740200	-0.45540900	-3.02909500
Li	2.84516500	-0.54242900	-0.73499900	H	2.14820200	-0.76845200	-3.76755200
Li	1.95634600	-2.05324600	1.18975700	C	1.08472500	1.01771700	-2.95587800
O	0.19683200	-2.94606000	1.49988700	H	1.80414800	1.60906100	-3.53416100
Li	-0.12993600	-3.05788900	-0.56138800	H	0.08532400	1.24085800	-3.36112900
O	-2.04295500	-3.02785000	-0.25377000	H	1.09004200	1.41759900	-1.93147900
C	-2.62599700	-4.22456100	0.13471700	C	-0.08208600	-3.24609400	-3.58182800
C	-1.62048600	-5.42443900	0.08420600	H	0.21760200	-2.91706800	-4.59068200
N	-0.23689700	-4.99904700	0.45641600	H	-0.21678100	-4.33052500	-3.58782000
C	-0.02697200	-4.24279700	1.70492700	H	-1.04725800	-2.79138100	-3.34453300
C	-0.02714500	-4.87393400	2.90383200	H	2.82227800	-2.63050100	-3.37259800
C	0.26273500	-4.21676900	4.22453200	H	2.54481700	-4.34022300	-0.87616300
H	0.20347400	-3.12735100	4.13985300	O	3.36651600	-2.35601200	2.65335700
H	-0.44531800	-4.53403400	5.00330100	C	3.34290300	-2.13579100	4.07105000
H	1.26577300	-4.46803000	4.60373900	C	4.22894200	-3.24444000	4.68674900
H	-0.18851100	-5.94802500	2.91525900	C	5.00026300	-3.82313800	3.46979200
C	0.72833900	-6.08782000	0.28797700	C	4.68737800	-2.82605800	2.34826600
H	0.66155300	-6.47691900	-0.73621100	H	4.66291800	-3.24382100	1.34289300
H	1.73741700	-5.69978800	0.44424000	H	5.38934800	-1.97709000	2.36616700

H	0.58473800	-6.93165900	0.98046600	H	4.61571800	-4.81373400	3.20722200
H	6.07523700	-3.91714300	3.65196200	H	-3.19786300	0.68716400	-3.63007800
H	3.62376600	-4.01496200	5.17305100	H	-2.71843800	-0.97750700	-4.04201900
H	4.90373100	-2.82985800	5.44240100	H	-5.11208600	0.01719200	-4.98497400
H	3.75007600	-1.13848800	4.28626900	H	-5.03244800	-1.65157500	-4.38036700
H	2.30124900	-2.17002600	4.39031200	H	-5.88480600	0.83829800	-2.80440200
O	4.38880100	0.69225300	-1.13706700	H	-6.76314400	-0.69823600	-2.92505800
C	5.77148900	0.40844700	-0.84012100	H	-5.17784300	-1.82700400	-1.48095800
C	6.54150300	1.56013800	-1.47862900	H	-5.00848900	-0.17544900	-0.81853000
C	5.61464700	2.75186800	-1.18289400	C	-3.86631400	-4.55249100	-0.70783400
C	4.20823900	2.12880200	-1.25382700	C	-3.80131400	-4.49347900	-2.10816900
H	3.71840900	2.31590900	-2.21376300	C	-5.09042800	-4.89378900	-0.12041300
H	3.55442000	2.46547000	-0.44331400	C	-4.91972100	-4.77311900	-2.89281100
H	5.73599300	3.57702300	-1.89098500	H	-2.86277600	-4.21212800	-2.57662400
H	5.81074300	3.14221500	-0.17827400	C	-6.21868100	-5.16911700	-0.90041200
H	6.63675000	1.39884700	-2.55901200	H	-5.16163700	-4.94977400	0.96439500
H	7.54502800	1.68169300	-1.05940500	C	-6.13697800	-5.11047200	-2.29119100
H	5.91752300	0.38903000	0.24822700	H	-4.84328700	-4.73260100	-3.97729100
H	6.00052500	-0.57735400	-1.24578200	H	-7.15867400	-5.42930000	-0.41934500
C	2.62127900	1.72200100	2.16472600	H	-7.00980800	-5.32643200	-2.90217200
C	4.01128200	1.19556200	2.37948400	C	-2.17511400	-6.62625200	0.86843900
H	4.78332200	1.83048300	1.91586900	H	-2.28833700	-6.38415700	1.93065300
H	4.26094600	1.15366200	3.45018500	H	-3.15821800	-6.90641200	0.47663700
H	4.11398500	0.18508800	1.97430000	H	-1.52860400	-7.50593500	0.78677200
H	2.37217000	2.66042700	2.65335400	C	4.47504900	-3.74774300	-1.53323700
C	0.37273800	3.16556800	1.00981400	C	5.05187500	-4.87049700	-0.92492500
H	-0.61005100	3.49839100	0.66961400	C	5.31076100	-2.91880600	-2.29815600
H	0.64633400	3.76667800	1.89397900	C	6.41385400	-5.15508200	-1.05998800
H	1.09984500	3.37037500	0.21906800	H	4.42031300	-5.53590100	-0.33905900
O	-3.05627400	-2.20084400	2.82403200	C	6.66958800	-3.20139400	-2.44680500
C	-3.07213100	-2.93856100	4.06949500	H	4.88982500	-2.04473600	-2.78928500
C	-4.54679600	-3.05986200	4.47587200	C	7.22953400	-4.32020700	-1.82340600
C	-5.18749100	-1.85335300	3.77192600	H	6.83373100	-6.03318200	-0.57478200
C	-4.39772300	-1.80480600	2.46565200	H	7.29327200	-2.55164600	-3.05714500
H	-4.34108400	-0.81416300	2.01030700	H	8.28769900	-4.54054300	-1.93895100
H	-4.79877500	-2.51101200	1.72685700	C	2.31037700	-4.70019000	-3.42830900
H	-5.02332100	-0.93657500	4.35096400	H	3.34544300	-5.04992800	-3.47331400
H	-6.26365600	-1.96748700	3.60932200	H	1.73068500	-5.44942000	-2.87547100
H	-4.68003500	-3.05136300	5.56185800	H	1.93343000	-4.66180600	-4.45449600
H	-4.97596900	-3.99297800	4.09196700	H	-2.68077500	0.51779100	2.38662400
H	-2.58413600	-3.90257300	3.90526900	H	-1.01613100	2.30269400	2.79825700
H	-2.49027700	-2.37081100	4.80499500	C	-0.26985400	0.38326800	3.35073700
O	-3.55403600	-0.75248100	-2.17313700	H	-1.09849000	0.19410700	4.04313400
C	-4.93100300	-0.78776400	-1.72165300	H	0.03613700	-0.57375500	2.91815800
C	-5.76668500	-0.24824500	-2.88793400	H	0.57240900	0.78380300	3.92034600
C	-4.89765200	-0.59898500	-4.10634600	C	-2.77606400	1.92778200	0.81324700

C	-3.48881800	-0.37022100	-3.55921700	C	-3.60583100	2.80362800	1.52913000
C	-2.66359100	2.11180300	-0.57089300	C	-4.15880200	4.01949500	-0.48695700
C	-4.28973800	3.83980000	0.89189300	H	-4.92861900	4.50314700	1.47023600
H	-3.71855300	2.66934200	2.60409600	H	-3.23194500	3.28142400	-2.28868700
C	-3.34317100	3.15013000	-1.21444600	H	-4.68936100	4.82482500	-0.98862700
H	-2.04217200	1.43300400	-1.14531100				

Table 19. Geometric coordinates and thermally corrected MP2 energies for LDA-mixed aggregate **6** with three THF attached

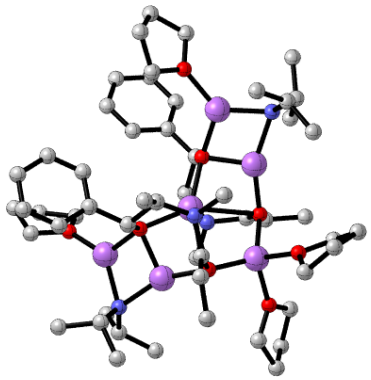


G = –2747.060282
G_{MP2} = –2737.755837

Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	H	3.26192000	-9.62655400	0.96690100
O	1.34174600	-1.08335600	0.70680400	C	0.73313600	-4.58443400	3.29436600
O	-1.52332500	-0.64496500	-0.85852900	H	1.03632200	-5.63365000	3.36275900
Li	0.12207200	-2.84981600	-0.56541000	H	1.49545500	-3.97785500	3.79411200
Li	2.73663500	-2.04393600	-0.10352100	H	-0.20367700	-4.47616800	3.85095700
Li	-2.69132200	-2.13369900	-0.68305700	H	-1.96652800	-3.41430500	1.87823900
O	1.88599100	-3.81499000	-0.25743600	H	-1.29900700	-2.62008000	3.31768700
O	-1.52024000	-3.62716000	-1.26734000	H	-1.71254200	-1.66091200	1.88945900
N	-4.34626000	-3.14995200	-0.17554700	H	0.75051100	-1.73297900	3.92992800
N	4.61212400	-2.34159300	-0.81260900	H	2.41239700	0.46136200	2.48960700
Li	-2.89642700	-4.50277700	-0.26923000	H	1.42702800	0.78339600	3.92927500
Li	3.63668900	-4.08941200	-1.04048900	H	2.86148300	-0.23042500	4.05779000
C	0.91377600	-1.64960600	1.84156700	C	-1.35904600	-0.71946200	-2.17837300
N	0.02488600	-2.79630900	1.61243400	N	-0.20708500	-1.54481000	-2.57754900
C	0.57037900	-4.16664300	1.82179100	C	-0.45757800	-2.79742500	-3.34565800
C	1.90703400	-4.35488700	1.04469500	C	-1.58057700	-3.64788000	-2.67099700
C	1.18249200	-1.19974600	3.08760200	C	-2.12647300	-0.08126300	-3.09507400
C	2.01220600	0.01363700	3.40368700	C	-3.29146500	0.81094600	-2.76125300
C	-1.29535000	-2.61656700	2.21722400	C	0.85941700	-0.72729100	-3.15898800
H	-0.17519500	-4.82928200	1.35830700	H	0.48501100	-3.35827800	-3.25254900
H	2.67268600	-3.84443900	1.66150000	H	-2.53523600	-3.20923900	-3.02020400
C	2.29069500	-5.83955900	1.03153400	C	-1.53701500	-5.08057000	-3.21171600
C	3.42505200	-6.30403600	1.70861000	C	-2.57252000	-5.59575100	-4.00066600
C	1.51417800	-6.77066200	0.32316500	C	-0.45538300	-5.92124500	-2.90295900
C	3.77891400	-7.65765000	1.68474600	C	-2.53530200	-6.91180500	-4.47365200
H	4.03459800	-5.60020700	2.27162600	H	-3.41699200	-4.95811000	-4.25262300
C	1.85928100	-8.12210400	0.29986800	C	-0.41122500	-7.23291400	-3.37687200
H	0.63452800	-6.42679700	-0.21279400	H	0.34849700	-5.53741100	-2.28029200
C	2.99612900	-8.57248800	0.98028500	C	-1.45304600	-7.73526900	-4.16440300
H	4.66098400	-7.99484200	2.22392400	H	-3.35137300	-7.28909500	-5.08497600
H	1.23933000	-8.82838100	-0.24855400	H	0.43753000	-7.86824200	-3.13248100

H	-1.41804100	-8.75721800	-4.53338900
C	-0.73950300	-2.63378400	-4.85099800
H	-0.73579800	-3.61391900	-5.33846900
H	-1.71691400	-2.17498700	-5.03031200
H	0.02207000	-2.02070600	-5.34359100
H	1.74054300	-1.34789300	-3.34550300
H	0.58272200	-0.23470100	-4.10433800
H	1.14346300	0.05777900	-2.44943900
H	-1.87762800	-0.19585800	-4.14593100
H	-3.42274100	0.88958800	-1.67826500
H	-3.15554500	1.82693800	-3.16233800
H	-4.23349400	0.43627700	-3.18717100
C	-5.21823500	-2.55398900	0.84540400
C	-5.09383700	-3.71525800	-1.31113500
H	-6.26029300	-2.51220300	0.48708900
H	-4.34597000	-4.20482200	-1.96407500
C	5.64518100	-2.08338900	0.19964500
C	5.03084000	-1.77589100	-2.10222600
H	6.07487700	-1.07130900	0.06085800
H	6.12740700	-1.86104600	-2.22667900
C	1.76655500	2.41258200	-0.03277800
C	0.60373500	3.92881000	-1.44724600
C	2.00697900	3.33944400	-1.22057700
H	2.46599800	1.57788100	0.04778000
H	1.76084800	2.96688900	0.91590700
H	0.44748800	4.28343200	-2.47010900
H	0.43605600	4.77444100	-0.77061200
H	2.33296600	2.76020800	-2.09208400
H	2.76489200	4.10075100	-1.01332800
O	0.45526900	1.85434600	-0.26822000
C	-0.33001400	2.75951200	-1.09220800
H	-1.21061700	3.07461900	-0.52418600
H	-0.66182700	2.19450300	-1.96812600
C	5.57069700	-6.30074700	-1.77513200
C	4.51309400	-7.35818200	-3.63869700
C	5.53322500	-7.63603100	-2.52321400
H	5.74757500	-6.41070200	-0.70220200
H	6.31744400	-5.61384900	-2.19031600
H	4.06185600	-8.26603100	-4.04999000
H	4.98335400	-6.80716900	-4.46170900
H	5.16808400	-8.43070100	-1.86276800
H	6.51806200	-7.92852200	-2.89918900
C	3.49392100	-6.47705800	-2.91718500
H	4.65099300	-3.08911200	1.86307300
H	5.84714700	-1.89203400	2.36886200
H	2.97131800	-5.77509100	-3.57328900
H	2.75451100	-7.07388700	-2.37141500
O	4.26076000	-5.71048000	-1.96107300
C	-2.84917300	-7.51983000	-0.30108500
C	-3.28371200	-8.12675000	1.95496900
C	-2.59329300	-8.65462000	0.68745100
H	-2.10520500	-7.43414100	-1.09499500
H	-3.84685100	-7.59943600	-0.75335500
H	-2.91569800	-8.59000900	2.87506200
H	-4.36500500	-8.29784800	1.89792100
H	-1.51699300	-8.77662800	0.85808100
H	-2.99807200	-9.61020900	0.34079500
O	-2.79192100	-6.31002200	0.49464600
C	-2.97275600	-6.62732400	1.89923200
H	-3.77437500	-5.99839900	2.29483400
H	-2.03925600	-6.38680600	2.42122200
C	-5.78107900	-2.66044000	-2.21167800
H	-6.54945600	-2.10658000	-1.65819600
H	-5.04399700	-1.93474600	-2.57447100
H	-6.27016000	-3.11997200	-3.08214200
C	-6.10820600	-4.83010900	-0.94948600
H	-6.93345300	-4.44428400	-0.33922600
H	-6.54966500	-5.27676600	-1.85076400
H	-5.61758000	-5.62765300	-0.37739800
C	-4.83386300	-1.09242800	1.15338900
H	-3.80694600	-1.02621100	1.53680400
H	-4.88883400	-0.48136700	0.24510000
H	-5.49294000	-0.64473400	1.91024800
C	-5.25545300	-3.36464900	2.15945200
H	-5.60694000	-4.38571800	1.97195000
H	-4.25119300	-3.42820400	2.59904200
H	-5.91871000	-2.90994100	2.90942600
C	4.42065100	-2.55569300	-3.27800700
H	3.32774900	-2.62394000	-3.17891800
H	4.62760500	-2.07489500	-4.24252500
H	4.81449900	-3.57772500	-3.31462900
C	4.70641300	-0.26947500	-2.23638700
H	5.11566600	0.16337000	-3.16085500
H	3.62039200	-0.10983400	-2.23804100
H	5.12477500	0.29077700	-1.39198200
C	6.83383100	-3.07008500	0.12540100
H	6.50117200	-4.08198600	0.39563400
H	7.25101600	-3.11308900	-0.88740600
H	7.64804800	-2.78813400	0.80817200
C	5.07098600	-2.10321900	1.62244700
H	4.27684700	-1.35699400	1.75020400

Table 20. Geometric coordinates and thermally corrected MP2 energies for LDA-mixed aggregate **6** with four THF attached



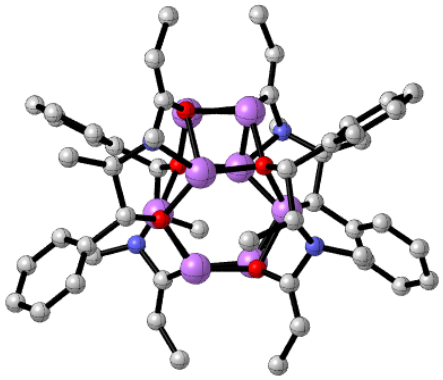
G = –2979.407402
G_{MP2} = –2969.338951

Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	H	-5.43868700	-7.14529800	-3.55487300
O	-1.53420100	-0.68433900	-0.96487000	H	-2.39030800	-8.49248300	-0.83260100
O	1.08797800	-1.30822400	0.92633100	H	-4.33134300	-8.99633500	-2.31126000
Li	-0.67994500	-2.95722500	0.16434900	C	-1.15123800	-4.02898200	-3.93392200
Li	-3.12023200	-1.56562900	-0.38645100	H	-1.47596400	-5.05579900	-4.13047300
Li	2.09097700	-2.81404000	0.34256200	H	-1.85252000	-3.35407100	-4.43455900
O	-2.57266000	-3.45816500	-0.44781400	H	-0.16747600	-3.90091400	-4.39797100
O	0.78002700	-4.26264200	0.68937800	H	1.48553600	-3.26822000	-2.16874300
N	3.73504300	-3.90297300	-0.15921700	H	1.02278700	-2.24744100	-3.54393000
N	-5.12834900	-1.69921400	0.11723800	H	1.38094300	-1.50546100	-1.97453000
Li	2.18943400	-5.19330600	-0.20406000	H	-1.12483500	-1.26076000	-4.22682200
Li	-4.38559400	-3.55683500	0.20621100	H	-2.47893900	1.04729600	-2.64953300
C	-1.21110700	-1.23892200	-2.12837500	H	-1.56695400	1.30307200	-4.14805500
N	-0.45965000	-2.49881800	-1.98794900	H	-3.10138200	0.44411000	-4.19558400
C	-1.10360900	-3.76834200	-2.41653200	C	0.74317100	-1.56253900	2.18422700
C	-2.52322700	-3.89000000	-1.78757800	N	-0.48488300	-2.36829900	2.29620300
C	-1.47046900	-0.71702500	-3.35250700	C	-0.36310400	-3.75967900	2.81661600
C	-2.18985800	0.58179200	-3.59636900	C	0.79407700	-4.48987200	2.07879400
C	0.91961400	-2.37348200	-2.45397000	C	1.39513300	-1.12143800	3.28761200
H	-0.47477300	-4.55060000	-1.96577100	C	2.64757300	-0.28796900	3.26580800
H	-3.17539700	-3.26019000	-2.42000000	C	-1.58124000	-1.62177400	2.91197900
C	-3.03562300	-5.32565200	-1.94288400	H	-1.30688000	-4.24263700	2.52016700
C	-4.12493800	-5.62501800	-2.76995900	H	1.71955600	-4.08076000	2.52826300
C	-2.42468600	-6.37888800	-1.24448300	C	0.79171400	-5.98474800	2.41449900
C	-4.59473600	-6.93674800	-2.90154600	C	1.84347800	-6.56267200	3.13732500
H	-4.60721000	-4.82373700	-3.32605400	C	-0.25588200	-6.81827300	1.99326600
C	-2.88473500	-7.68938600	-1.37529800	C	1.85267000	-7.92943600	3.43614600
H	-1.58089000	-6.15811200	-0.59788000	H	2.66406700	-5.93406000	3.47528800

C	-3.97541400	-7.97459300	-2.20463100	C	-0.25455700	-8.18106400	2.28958700
H	-1.07734500	-6.38719900	1.42977400	C	-4.59383700	-6.04058000	1.91189400
C	0.80227100	-8.74432500	3.01318400	H	-4.17681600	-5.39449700	2.68999900
H	2.67920500	-8.35279500	4.00160400	H	-3.78118500	-6.61081300	1.44658600
H	-1.08231600	-8.80686200	1.96273800	O	-5.20069600	-5.19572400	0.90998900
H	0.80200600	-9.80582200	3.24773800	C	2.63629800	-8.15025200	-0.55911900
C	-0.22748900	-3.90396700	4.34367000	C	1.84498700	-8.63767100	-2.74869200
H	-0.32683200	-4.95519600	4.63158800	C	2.05317000	-9.29982500	-1.37785600
H	0.74605300	-3.55013300	4.69734300	H	2.42535200	-8.21658300	0.51045100
H	-1.00530300	-3.34419000	4.87303700	H	3.72027400	-8.05649000	-0.70919900
H	-2.49579600	-2.22052200	2.86269600	H	1.10245400	-9.14758000	-3.36940200
H	-1.40861400	-1.35515400	3.96683500	H	2.78973900	-8.60882200	-3.30388600
H	-1.74187700	-0.69550000	2.35322400	H	1.09441000	-9.61859000	-0.95280900
H	0.99077200	-1.37883200	4.26232600	H	2.71867600	-10.1675690	-1.41337600
H	2.96667600	-0.09744900	2.23728400	O	1.99026700	-6.95923000	-1.06723200
H	2.50960100	0.68573300	3.76176900	C	1.40226700	-7.22137600	-2.36550000
H	3.47941700	-0.78234100	3.78783300	H	1.75285100	-6.45672200	-3.06530500
C	4.63644600	-3.70064300	-1.30224700	H	0.31357800	-7.14486900	-2.26881700
C	4.46469600	-4.07762200	1.11130700	C	5.38030100	-2.89993000	1.52407500
H	5.67140100	-3.97360300	-1.03405500	H	6.22714000	-2.78467100	0.83633800
H	3.69622000	-4.13949200	1.89992000	H	4.81938900	-1.95823000	1.52970300
C	-5.99814900	-1.24091500	-0.97506200	H	5.79577200	-3.05366100	2.52927500
C	-5.63431400	-1.16322400	1.39022800	C	5.26277700	-5.40300200	1.21212800
H	-6.26374900	-0.17282400	-0.83164800	H	6.05378900	-5.45480100	0.45417100
H	-6.72027200	-0.97243700	1.32068000	H	5.74289200	-5.51463000	2.19421400
C	-1.77451000	2.36660700	0.57914600	H	4.60055900	-6.26440500	1.06067400
C	-1.51729600	2.73804000	2.98010700	C	4.70252900	-2.23264300	-1.78358600
C	-2.38267800	3.15591500	1.76355500	H	3.71870200	-1.90025100	-2.13820200
H	-2.49123600	1.76247300	0.02174100	H	5.00360500	-1.57191700	-0.96423500
H	-1.25408900	3.03618300	-0.12050900	H	5.41742300	-2.10087600	-2.60937500
H	-2.04709500	2.00097200	3.59181200	C	4.27156400	-4.60851100	-2.49295600
H	-1.24973000	3.58142400	3.62399200	H	4.32037100	-5.66347000	-2.20007000
H	-3.43453600	2.90150400	1.91757000	H	3.25069500	-4.40266500	-2.84324000
H	-2.32567300	4.23345200	1.57961300	H	4.94453400	-4.45528900	-3.34792900
O	-0.81831000	1.45539100	1.15436400	C	-5.47522100	-2.16224600	2.54742800
C	-0.29363500	2.08690200	2.33094500	H	-4.43085900	-2.48373400	2.65370200
H	0.45659100	2.84138600	2.04472300	H	-5.77659800	-1.72644600	3.50915100
H	0.18403800	1.30854100	2.92869600	H	-6.08163800	-3.05755200	2.36941500
C	-6.45755000	-5.76192500	0.46433300	C	-4.99642900	0.19592700	1.75751100
C	-5.71791400	-6.95183500	2.40306900	H	-5.44933100	0.64290300	2.65512000
C	-6.54898700	-7.14140700	1.12434200	H	-3.92070700	0.07990500	1.94243000
H	-6.44407600	-5.80791900	-0.62783000	H	-5.11940100	0.90427300	0.92896100
H	-7.26487000	-5.09301700	0.78481900	C	-7.33716200	-2.01309800	-1.06065500
H	-5.34174700	-7.89124200	2.81902200	H	-7.14770000	-3.06077700	-1.33386800
H	-6.30968100	-6.44757400	3.17606200	H	-7.86615800	-2.00877000	-0.10096700
H	-6.08911300	-7.89973200	0.48093700	H	-8.01283400	-1.58279300	-1.81375500

H	-7.58319200	-7.43961800	1.32026600	C	-5.30393900	-1.32353400	-2.33907500
H	-4.37525800	-0.74224800	-2.36164600	H	3.01089600	0.93561800	-3.36705500
H	-5.05860200	-2.36350100	-2.59114900	H	2.68701100	2.65620900	-3.66064000
H	-5.95255400	-0.94147000	-3.13755000	H	4.46686300	1.98861900	-1.69063300
C	2.71040800	1.25978000	-0.59548000	H	3.25146300	3.23124700	-1.34762500
O	1.37592000	1.01285100	-1.10455200	H	3.21768200	0.29519300	-0.50064500
C	1.20986000	1.64372700	-2.39164400	H	0.59432100	0.97964300	-3.00176100
C	2.62877800	1.85797900	-2.91431000	H	0.68472200	2.60139100	-2.26242400
C	3.39182400	2.17795500	-1.61882200	H	2.62860200	1.70824000	0.39934800

Table 21. Geometric coordinates and thermally corrected MP2 energies for homoaggregate **4** (R_4)

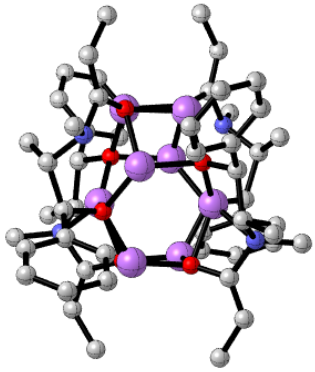


G = –2903.209366
G_{MP2} = –2893.686916

Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	C	-1.89276800	3.38164800	1.57398300
O	1.90683500	-0.37759300	-0.12966100	N	-0.62125500	3.79296600	0.88842300
C	2.40920400	-1.55295300	-0.52925000	C	-0.33395000	3.04181200	-0.32283600
N	2.69999100	-2.41327100	0.60588500	O	0.17199000	1.83533600	-0.03608100
C	3.97312700	-2.07033100	1.32523100	Li	2.07646800	1.44864200	0.05482000
C	5.14520800	-2.98725300	0.95093200	C	-0.51001000	3.55422000	-1.55823800
H	6.08249100	-2.58754500	1.34646500	C	-0.13611900	2.85552300	-2.83545500
H	5.23938900	-3.05579100	-0.13847600	H	0.33951200	1.89050800	-2.63265600
H	5.02654100	-4.00020900	1.35118800	H	0.55993400	3.45217700	-3.44299900
C	3.66259700	-1.97817500	2.84911500	H	-1.01419000	2.66261100	-3.46898500
O	2.75547100	-0.91659200	3.07971700	H	-0.95038200	4.54358400	-1.64515900
Li	1.44888700	-1.14974200	1.69571700	C	-0.38085600	5.23475600	0.83202700
O	-0.44710900	-0.94189100	1.57531800	H	0.62678400	5.40782800	0.44499300
C	-1.22794600	-2.10439000	1.61247100	H	-0.43920600	5.65248100	1.84303200
C	-1.41203600	-2.62500600	3.08080900	H	-1.08855100	5.78894800	0.19855400
N	-1.92130800	-1.53612600	3.98419700	C	-3.06853800	4.32495900	1.28701500
C	-1.07822300	-1.15828900	5.10924600	H	-3.16197300	4.49753500	0.20914800
O	-0.05364100	-0.38209700	4.73060700	H	-2.95521600	5.29531500	1.78306600
Li	1.81006800	-0.48542000	4.64369200	H	-4.00414900	3.88450900	1.64115200
O	2.13811100	1.40054500	4.80192500	H	-2.13812000	2.39827400	1.15929500
C	3.16785000	2.13283200	5.24778200	C	-2.82738300	2.94207100	3.93952300
N	4.00919100	2.60921300	4.15965300	C	-3.07298400	3.78019900	5.03444700
C	3.49905600	3.77579400	3.35833700	C	-4.19573300	3.60084600	5.84711800
C	3.31632100	3.39044300	1.84908100	C	-5.10149400	2.57803000	5.56833200
O	2.53081200	2.23956100	1.70694400	C	-4.87233000	1.73558300	4.47699300
Li	0.63413000	2.43805600	1.85453900	C	-3.74390000	1.91248600	3.67593200
O	-0.66955800	2.07640500	3.21506700	H	-3.58378300	1.24597400	2.83160800
Li	-0.98790500	0.16910400	3.03952900	H	-5.57685600	0.94064900	4.24625000

Li	0.27587000	1.50948700	4.73472900	H	-5.97944500	2.43715500	6.19304700
C	-1.58225900	3.14999100	3.08268600	H	-4.36229100	4.26307600	6.69289200
H	-2.37704000	4.58862100	5.25134300	C	-2.56876400	-1.93889600	0.88492000
H	-1.11239300	4.08291100	3.44761300	C	-3.04595300	-0.68338100	0.49078300
Li	3.07220400	0.99743100	3.06719900	C	-4.26404600	-0.55249600	-0.18616900
C	4.65833100	3.28367600	1.11261500	C	-5.02552700	-1.68153100	-0.48445400
C	5.12328100	2.06797400	0.59742800	C	-4.55604800	-2.94321600	-0.10717200
C	6.34269300	1.99082500	-0.08558500	C	-3.34091400	-3.06703400	0.56446800
C	7.11737700	3.13527600	-0.26862900	H	-2.98102300	-4.05738900	0.83783100
C	6.65996000	4.35874800	0.22987200	H	-5.13396900	-3.83268200	-0.34526300
C	5.44378800	4.42934200	0.90732700	H	-5.96958800	-1.58342000	-1.01343600
H	5.09410500	5.39189000	1.27656200	H	-4.61089500	0.43429600	-0.48275100
H	7.24851000	5.26078400	0.08227800	H	-2.45561200	0.20180800	0.70976200
H	8.06242900	3.07956000	-0.80201100	H	-0.71072500	-2.93091300	1.08549100
H	6.67987400	1.03425100	-0.47708000	C	4.90721900	-1.85977700	3.72305000
H	4.52271800	1.17221100	0.72718800	C	5.14525500	-2.80052500	4.73300200
H	2.80372400	4.26309200	1.39715700	C	6.26750200	-2.70763800	5.56062500
C	2.22655500	4.41721900	3.92379900	C	7.18040500	-1.66891500	5.38237900
H	2.00837700	5.33658100	3.36837300	C	6.95910800	-0.72435400	4.37625700
H	2.35700900	4.67746900	4.97808700	C	5.83119100	-0.81599600	3.56022600
H	1.35839300	3.75729600	3.84505000	H	5.67804400	-0.07064400	2.78302700
H	4.27578600	4.55102600	3.40636900	H	7.66953200	0.08412000	4.22366700
C	5.42879800	2.77687200	4.49175600	H	8.05804100	-1.59428100	6.01886300
H	5.99796800	2.90302700	3.56652700	H	6.42809900	-3.44911200	6.33912600
H	5.78776500	1.88704400	5.01125300	H	4.44364900	-3.62133400	4.87063600
H	5.62050900	3.65701100	5.12787500	H	3.18618400	-2.93794200	3.12523000
C	3.46284100	2.36159500	6.54476200	H	4.22328600	-1.05359400	1.00416800
C	2.71578200	1.77719300	7.71005700	C	2.45628600	-3.84320000	0.41716000
H	3.38368600	1.22927600	8.39051200	H	3.15880600	-4.33702700	-0.26976000
H	1.94025300	1.08116900	7.37545800	H	1.44577700	-3.97843000	0.02251500
H	2.22237700	2.55120500	8.31707500	H	2.52083600	-4.35301700	1.38465200
H	4.30881700	3.00116900	6.77726600	C	2.57760900	-1.94891100	-1.80780600
C	-1.36627100	-1.51029400	6.37981000	H	3.01304500	-2.92758700	-1.98938900
C	-0.61616600	-1.03396100	7.59149600	C	2.19883600	-1.13400400	-3.01265800
H	0.14118300	-0.29146800	7.32140300	H	1.74565300	-0.18170300	-2.71865800
H	-0.09968700	-1.85561300	8.11050400	H	3.07143100	-0.90299500	-3.64083800
H	-1.28579100	-0.57264100	8.33167000	H	1.48220900	-1.66160500	-3.65914000
H	-2.20790200	-2.17384100	6.55377300	H	0.07445000	-4.18397700	2.94893600
C	-3.34054400	-1.73250700	4.30171900	H	0.72953300	-2.65677000	3.56593800
H	-3.69777800	-0.89354600	4.90072300	H	-0.27124800	-3.67272800	4.61216100
H	-3.53265200	-2.66696100	4.85494400	H	-2.18957900	-3.40051600	3.05740200
H	-3.91095700	-1.77181500	3.36940200	C	-0.14079700	-3.31824900	3.58570000

Table 22. Geometric coordinates and thermally corrected MP2 energies for homoaggregate **4** (S_4)

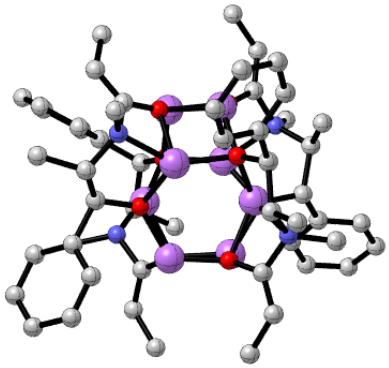


G = –2903.209644
G_{MP2} = –2893.687127

Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	H	-3.86927900	0.37974800	-1.86403300
O	-0.32806200	1.88843800	0.12197000	H	-5.85709200	0.56894100	-0.42169900
C	-1.35620400	2.63174400	0.55292900	H	-6.24285400	-1.06937900	1.41078500
N	-2.19702600	3.08734900	-0.54444000	H	-4.61442000	-2.91883900	1.76718400
C	-1.68556900	4.23658100	-1.36944600	H	-2.63403600	-3.12568600	0.29772800
C	-1.50219400	3.81971700	-2.87032100	H	-1.37985000	-2.48140000	-1.46595000
O	-0.71908500	2.66441700	-2.98862500	Li	-1.26346400	1.45209800	-1.60376200
Li	-0.26745800	1.83904100	-4.62515800	O	2.25305400	-0.52164700	-3.05927200
O	-0.10066400	0.00956900	-4.77688200	C	3.03367300	-1.68323400	-2.99822100
C	-0.61083700	-1.17108800	-5.15014600	C	4.37433500	-1.53265600	-3.72932400
N	-0.89792900	-2.00807900	-3.99655100	C	5.14761100	-2.66681500	-4.02484800
C	-2.16958400	-1.65055200	-3.28175500	C	6.36248300	-2.55667800	-4.69936600
C	-3.34251300	-2.57490500	-3.63437200	C	6.83060600	-1.30319000	-5.10461200
H	-4.27887300	-2.16665300	-3.24543900	C	6.06796400	-0.16861600	-4.83143600
H	-3.43884200	-2.66636100	-4.72189200	C	4.85000800	-0.28569800	-4.15164700
H	-3.22322800	-3.57918700	-3.21299800	H	4.25887500	0.60359500	-3.95226100
H	-2.42043600	-0.64069300	-3.62345900	H	6.41366400	0.81170600	-5.14999800
C	-0.65434700	-3.44144800	-4.15728600	H	7.77450200	-1.21588400	-5.63578100
H	-0.71600000	-3.93218500	-3.17974300	H	6.94131100	-3.45060000	-4.91774600
H	-1.35838000	-3.94914800	-4.83245600	H	4.78890900	-3.65125000	-3.72941200
H	0.35522600	-3.58415600	-4.55170000	C	3.21850300	-2.17313900	-1.51955000
Li	0.35653400	-0.72387900	-2.93510600	N	3.72954200	-1.06564000	-0.63982000
O	-0.94742400	-0.46161400	-1.55406800	C	2.88820400	-0.66348600	0.47797900
C	-1.85585400	-1.52704700	-1.76082800	O	1.86308400	0.10426100	0.08407300
C	-3.09848300	-1.38894900	-0.88688800	Li	1.53427000	1.99572100	0.05004400
C	-3.33497000	-2.30718700	0.14394600	O	2.48037300	2.53067400	-1.48081400
C	-4.45494200	-2.19479400	0.97222500	C	3.39224500	3.60211400	-1.63452000
C	-5.36703000	-1.15901600	0.77374500	C	4.63491200	3.41459300	-0.76955100

C	-5.14726200	-0.23690000	-0.25331300	C	4.87444000	4.27529800	0.30908800
C	-4.02164200	-0.34786600	-1.07009300	C	5.99417800	4.11476400	1.12978200
C	6.90298700	3.08829400	0.87551900	H	3.99554600	-2.94943500	-1.52719100
C	6.68001400	2.22343000	-0.19948400	H	2.51609400	-2.52043700	-3.50776200
C	5.55455800	2.38178400	-1.00858000	C	-0.79101600	-1.59048600	-6.41952400
H	5.39908000	1.69833100	-1.84015500	C	-0.41853800	-0.80007700	-7.64252800
H	7.38711100	1.42547800	-0.41120400	H	0.04145200	0.15535400	-7.36998500
H	7.77862400	2.96181500	1.50653500	H	-1.29526200	-0.57676300	-8.26773400
H	6.15605400	4.79438100	1.96257500	H	0.29030200	-1.34304800	-8.28483700
H	4.17618000	5.08662300	0.50680700	H	-1.23250200	-2.57038000	-6.57869300
H	2.92024900	4.54232400	-1.29166700	C	-2.84391000	3.70105200	-3.60549600
Li	1.17806000	2.86292200	-2.84907700	C	-3.62498900	4.84465900	-3.83727800
O	1.63842500	2.21930900	-4.72501300	C	-4.84071200	4.76343700	-4.51435400
C	2.15027600	3.41655900	-5.03842400	C	-5.30201600	3.53081300	-4.98600800
N	2.43560500	4.19551400	-3.84423400	C	-4.53168500	2.38795400	-4.77653700
C	3.70622500	3.80092800	-3.14721300	C	-3.31271500	2.47585200	-4.09405000
C	4.88125600	4.73946800	-3.45211800	H	-2.71565700	1.58094600	-3.94374000
H	4.97767100	4.88733100	-4.53338600	H	-4.87194500	1.42413000	-5.14703700
H	4.76474000	5.72073500	-2.97883700	H	-6.24667800	3.46657000	-5.51911600
H	5.81652100	4.30893300	-3.08513900	H	-5.42577400	5.66410900	-4.68266200
H	3.95459300	2.80909300	-3.53957100	H	-3.27210300	5.81391700	-3.48924100
C	2.19445100	5.63542800	-3.93497700	H	-0.98735100	4.68185800	-3.33955700
H	1.18659000	5.79862400	-4.32575800	C	-0.41359100	4.88995800	-0.81639100
H	2.25268600	6.07755800	-2.93432400	H	-0.19620500	5.79856000	-1.38959300
H	2.90161500	6.17481200	-4.58172900	H	-0.54449600	5.17074300	0.23257900
C	2.33428200	3.89813600	-6.28497700	H	0.45544300	4.22980500	-0.88220200
C	1.96432300	3.16986500	-7.54672000	H	-2.46203000	5.01288600	-1.33826200
H	1.26501500	3.74910300	-8.16734700	C	-3.61646600	3.26327900	-0.21587000
H	1.49404700	2.20682400	-7.32296400	H	-4.18539100	3.37118800	-1.14359500
H	2.84366800	2.96839900	-8.17573000	H	-3.80737700	4.15622900	0.40240700
H	2.77822900	4.88376900	-6.39371500	H	-3.97631500	2.38446700	0.32139900
Li	1.80638200	0.38471900	-4.65520800	C	-1.65009000	2.88792900	1.84501900
Li	2.79702400	0.62017900	-1.61903500	C	-0.90362400	2.32563200	3.02152000
C	3.17831300	-0.98744900	1.75555000	H	-1.57266600	1.79508300	3.71448500
C	2.43043000	-0.48431200	2.95770500	H	-0.13157200	1.61943400	2.70049800
H	1.66963900	0.24885700	2.67224900	H	-0.40602900	3.11032700	3.61117400
H	1.91856100	-1.29490700	3.49817500	H	-2.49474400	3.53376700	2.06470300
H	3.10085600	-0.00289100	3.68427200	C	1.94748900	-2.85482300	-0.99877800
H	4.02032300	-1.64684500	1.94289500	H	2.07868400	-3.18642600	0.03521500
C	5.14901200	-1.25656200	-0.31987800	H	1.07708700	-2.19404700	-1.03266000
H	5.50794800	-0.40500900	0.26006200	H	1.73175200	-3.73460900	-1.61586200
H	5.71815200	-1.31735100	-1.25181200	H	5.34075700	-2.17878500	0.25360700

Table 23. Geometric coordinates and thermally corrected MP2 energies for RS_3 (using the same core as **4**) with the R-unit being concave

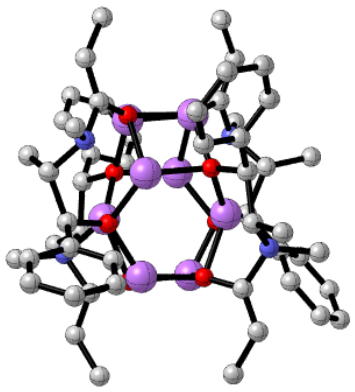


G = –2903.201961
G_{MP2} = –2893.677609

Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	H	-4.51752100	-0.69370700	-0.21718000
O	1.84675800	0.41450400	-0.25581300	H	-5.36660000	-2.79388200	-1.25738300
C	2.75115400	-0.26914800	-0.96658200	H	-3.92315200	-4.82466000	-1.26416700
N	3.62232200	-1.05464600	-0.10824300	H	-1.68187500	-4.75744000	-0.23164900
C	4.66188100	-0.29963700	0.67086900	H	0.20522600	-3.30769800	0.37685700
C	4.50211300	-0.51308000	2.22891300	Li	1.98798100	-0.99658600	1.22746100
O	3.15881700	-0.47279500	2.63150800	O	-0.87671700	1.10218500	3.49943000
Li	2.31828800	-0.79961500	4.30013700	C	-2.27710500	1.21659900	3.45567000
O	0.54557500	-1.34178100	4.41631800	C	-2.87630800	0.98463600	4.84765400
C	-0.27404000	-2.37598800	4.65510900	C	-3.94932700	0.11031800	5.05607500
N	-1.10011300	-2.69593700	3.49827100	C	-4.46291800	-0.10714000	6.33779400
C	-0.45910300	-3.50129100	2.40139200	C	-3.90615500	0.54680400	7.43708500
H	-1.08983300	-4.38785900	2.25114300	C	-2.83706400	1.42582800	7.24480000
C	0.93988700	-4.01295700	2.74579900	C	-2.32988400	1.64126600	5.96232300
H	1.29116800	-4.68186500	1.95200200	H	-1.50534600	2.33781200	5.81955700
H	1.64602800	-3.18564700	2.83262200	H	-2.40166600	1.94818500	8.09313000
H	0.94303400	-4.56358800	3.69034100	H	-4.30092800	0.37528500	8.43480800
C	-2.44586900	-3.19299000	3.80750400	H	-5.29453100	-0.79344400	6.47598700
H	-2.44750800	-4.23027200	4.18229400	H	-4.38717800	-0.40779400	4.20581000
H	-2.90475700	-2.55139200	4.56208400	C	-2.77312500	2.58999400	2.89418400
H	-3.05293400	-3.16333400	2.89839700	N	-1.90259900	3.11403600	1.79864000
Li	-0.50499000	-0.71682200	2.86426500	C	-1.71067000	2.31803200	0.57654200
O	0.10804300	-1.42491900	1.21325400	O	-0.51106700	1.73261500	0.53033100
C	-0.43682400	-2.70521700	1.04773800	Li	1.37535100	2.09761600	0.37897300
C	-1.82035700	-2.69540100	0.38838600	O	1.83266500	2.75697900	2.08490800
C	-2.30691100	-3.86616700	-0.21581800	C	2.61690500	3.86532300	2.48822900
C	-3.57148500	-3.90634100	-0.80056600	C	2.07392300	5.17598600	1.92722200
C	-4.38124300	-2.76676700	-0.79996200	C	2.72593500	5.79243400	0.85101700

C	-3.90618700	-1.59252300	-0.21760400	C	2.24626800	6.98241600	0.29753000
C	-2.63509100	-1.55791100	0.36716100	C	1.10484200	7.58578700	0.82562900
H	-2.28323800	-0.62977000	0.80769000	H	-2.70405800	0.44160200	2.78955900
C	0.92278700	5.79072900	2.44070700	C	0.44670700	6.98658700	1.90245600
H	0.39564100	5.33662400	3.27695400	C	-0.39774000	-3.01787700	5.83522300
H	-0.44018100	7.45302100	2.32406100	C	0.33521100	-2.64869400	7.09424700
H	0.73186200	8.51612300	0.40576400	H	0.96811000	-1.76842300	6.94234100
H	2.76983500	7.44017800	-0.53787500	H	0.98514400	-3.46395200	7.44535500
H	3.62779300	5.33627500	0.44644200	H	-0.35483400	-2.42410100	7.92072600
H	3.63822300	3.76131400	2.07513600	H	-1.08248100	-3.85870000	5.89511400
Li	2.64149500	1.32292900	3.06476500	C	5.26111500	-1.75326800	2.71626500
O	1.99569000	1.00219500	4.95532100	C	6.66552200	-1.75558800	2.69286800
C	2.93016400	1.81941700	5.45767400	C	7.39369400	-2.85882200	3.13441400
N	3.55182200	2.61690900	4.40999400	C	6.73048900	-3.98999400	3.61862300
C	2.77698900	3.84938700	4.03781500	C	5.33705300	-3.99955900	3.65604900
C	3.35464200	5.13206600	4.65162100	C	4.61261300	-2.88848100	3.21069300
H	3.51137300	4.99906600	5.72755500	H	3.52988200	-2.90798400	3.23876200
H	4.30970400	5.41602200	4.19626000	H	4.80638600	-4.87070400	4.03223500
H	2.66577800	5.96871600	4.51292100	H	7.29592600	-4.84986300	3.96755500
H	1.77326800	3.69523300	4.45083400	H	8.48028400	-2.83343800	3.10927600
C	5.00175600	2.79126200	4.51102100	H	7.19666200	-0.87643400	2.33150300
H	5.46360700	1.81010600	4.64928100	H	5.05021900	0.33941300	2.67487000
H	5.38270000	3.22402200	3.57912900	C	4.73776500	1.19605200	0.33487900
H	5.32540700	3.43868600	5.33875200	H	5.65676000	1.61076600	0.76480500
C	3.31293000	1.89462000	6.74834100	H	4.76606600	1.35641700	-0.74698600
C	2.76845500	1.04116400	7.85905600	H	3.89143200	1.75476900	0.74322700
H	3.56496900	0.49687500	8.38668900	H	5.63178900	-0.72367000	0.37964500
H	2.05643700	0.30208400	7.47827400	C	4.16974300	-2.28249400	-0.69339900
H	2.24693400	1.64123300	8.61939200	H	4.60593300	-2.89159600	0.10325900
H	4.07868300	2.61923100	7.01202300	H	4.95462000	-2.09275900	-1.44436600
Li	0.20478500	0.51874700	4.92044200	H	3.36608300	-2.84837900	-1.17137500
Li	-0.03974300	2.37987200	2.38198900	C	2.82366200	-0.30920300	-2.31441000
C	-2.62910500	2.28632700	-0.41249700	C	1.86517900	0.38626700	-3.24093800
C	-2.41271500	1.64106400	-1.75464100	H	2.36783400	1.14759100	-3.85590400
H	-1.34372600	1.50127600	-1.95714600	H	1.38845700	-0.31288100	-3.94360500
H	-2.89646800	0.65742000	-1.84446900	H	1.07046000	0.89298000	-2.68325600
H	-2.81865700	2.26606100	-2.56077600	H	3.62621000	-0.87832000	-2.77396100
H	-3.56694100	2.81094500	-0.25778900	H	-4.65267900	3.49829800	2.22616900
C	-2.19512000	4.52341100	1.50293000	H	-4.45874000	1.80093500	1.75472900
H	-1.43701600	4.91317000	0.82131100	H	-4.84931700	2.22584700	3.43212600
H	-2.15124400	5.10201700	2.43315400	H	-2.64030100	3.32336400	3.70241100
H	-3.18239000	4.68632800	1.04728900	C	-4.27068800	2.52602400	2.55332500

Table 24. Geometric coordinates and thermally corrected MP2 energies for RS_3 (using the same core as **4**) with the R-unit being convex

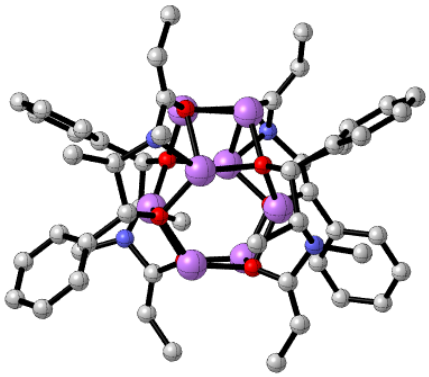


G = –2903.203492
G_{MP2} = –2893.679377

Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	H	-3.81601400	0.93808800	1.48396900
O	-0.53179800	-1.66236500	0.81004500	H	-5.69843100	0.21864700	0.06775800
C	-1.63143500	-2.42575800	0.75057500	H	-5.71792300	0.74468700	-2.36334700
N	-2.52607300	-2.17918900	1.87184500	H	-3.83135000	2.03101000	-3.35670100
C	-2.16615200	-2.81595100	3.18590800	H	-1.95831600	2.78652000	-1.92497100
C	-1.94844000	-1.73407300	4.29967600	H	-0.95868700	3.03815000	0.07911000
O	-1.02799000	-0.76005900	3.89139400	Li	-1.35772100	-0.33833400	2.05941600
Li	-0.47283300	0.71430100	4.93302800	O	2.49628300	1.68002500	2.73442000
O	-0.01610200	2.34889600	4.18544300	C	3.65231300	2.28928000	2.20515200
C	-0.47713400	3.58365700	3.94472800	C	3.53958900	2.21686000	0.64151100
N	-0.66768000	3.80849000	2.52085000	N	3.85270700	0.79712100	0.26041900
C	-1.93232400	3.20159900	1.98083200	C	2.86895100	0.15928300	-0.59505800
C	-3.06602000	4.21762200	1.78475300	O	1.82749800	-0.29562300	0.11243700
H	-4.00621300	3.69884500	1.58075100	Li	1.30455200	-1.90064800	1.03945700
H	-3.20207300	4.81752800	2.69126400	O	2.16443000	-1.73564600	2.70391900
H	-2.87959900	4.89670800	0.94583400	C	2.97593900	-2.63984600	3.43101100
H	-2.25413900	2.48043900	2.73871300	C	4.26266900	-2.96395500	2.67859700
C	-0.38797000	5.15751000	2.02274200	C	4.43341300	-4.22652900	2.09666500
H	-0.39766500	5.14417200	0.92738800	C	5.59052300	-4.54441000	1.38076300
H	-1.10681400	5.92044800	2.35418000	C	6.60810700	-3.60032600	1.24589800
H	0.60763200	5.46356500	2.34823500	C	6.45572500	-2.33796200	1.82554500
Li	0.60099000	2.07001700	2.27332200	C	5.29180100	-2.02212700	2.52709600
O	-0.75604500	1.27173000	1.13496200	H	5.19183000	-1.03478700	2.97385600
C	-1.55352600	2.36642100	0.72681500	H	7.24788000	-1.59922100	1.73389400
C	-2.74052800	1.91485500	-0.11877900	H	7.51407300	-3.84453300	0.69775700
C	-2.77242500	2.21100000	-1.48773100	H	5.69808500	-5.53083100	0.93698100
C	-3.83134900	1.78962300	-2.29681700	H	3.65049900	-4.97396500	2.21203700
C	-4.88798600	1.06906800	-1.74138000	H	2.44045100	-3.60017900	3.54996800

C	-4.87365200	0.77005600	-0.37621000	Li	0.82440200	-1.21542100	3.98585900
C	-3.80745100	1.18190600	0.42393500	O	1.33334600	0.19172700	5.38779400
C	1.64088500	-0.77613200	6.25978400	H	6.06389000	3.55416400	2.35270400
N	1.89009500	-2.03433000	5.57746700	H	4.54248800	1.67851800	2.45469000
C	3.21304500	-2.08872500	4.86876000	C	-0.68916700	4.54389300	4.86899400
C	4.29615300	-2.81554700	5.67781900	C	-0.41499600	4.39333600	6.33935300
H	4.32263000	-2.42957000	6.70279900	H	0.04328300	3.42375700	6.55929600
H	4.12856000	-3.89759100	5.72051500	H	-1.33508200	4.46555800	6.93769000
H	5.28095200	-2.65506900	5.23187900	H	0.26098200	5.17545900	6.71439500
H	3.51611700	-1.04264000	4.75030900	H	-1.08549500	5.49880700	4.53514000
C	1.52104800	-3.25222700	6.29816700	C	-3.27310200	-1.13163600	4.78470700
H	0.48910000	-3.15618300	6.64579600	C	-4.18440200	-1.91892400	5.50663200
H	1.57975700	-4.10840000	5.61779700	C	-5.39193800	-1.39105000	5.96092500
H	2.15451700	-3.47180600	7.16984800	C	-5.71378500	-0.05384000	5.71037800
C	1.65910200	-0.65611600	7.60384300	C	-4.81304700	0.74518600	5.00761300
C	1.30538500	0.59607700	8.35652700	C	-3.60358900	0.20821300	4.55227200
H	0.45924000	0.44170600	9.04251500	H	-2.90384200	0.83935200	4.01268700
H	1.03665900	1.40732200	7.67237500	H	-5.04411900	1.78987200	4.81470600
H	2.14368700	0.95103700	8.97323700	H	-6.65236000	0.36038500	6.06847000
H	1.94435100	-1.52188100	8.19446100	H	-6.07992400	-2.02082600	6.51941800
Li	1.82989000	1.71596500	4.47993200	H	-3.94145700	-2.95796500	5.72224600
Li	2.71976400	-0.06576600	1.91918100	H	-1.54998000	-2.29894200	5.16583600
C	3.04279200	0.02148400	-1.92602000	C	-0.97477000	-3.77834500	3.11156500
C	2.11617100	-0.72671100	-2.84310200	H	-0.86219900	-4.28644800	4.07608300
H	1.33082700	-1.24273500	-2.28077600	H	-1.13383300	-4.53821300	2.34124800
H	1.62191200	-0.06279100	-3.56835900	H	-0.03673300	-3.26312200	2.88636200
H	2.65101500	-1.48522300	-3.43241200	H	-3.02987900	-3.42518600	3.48587000
H	3.92820500	0.46276600	-2.37493500	C	-3.95459400	-2.34350700	1.57969200
C	5.25228700	0.55406800	-0.08879600	H	-4.53728700	-1.90323600	2.39375100
H	5.40420600	-0.52013700	-0.20636100	H	-4.25584300	-3.39995300	1.48270100
H	5.89539500	0.90387200	0.72742700	H	-4.19606400	-1.82677800	0.64960400
H	5.58071000	1.05609400	-1.01058200	C	-1.93591500	-3.28178200	-0.24713500
C	4.29682000	3.26523000	-0.18135000	C	-1.11334900	-3.48037200	-1.48914300
H	5.37544000	3.26396900	0.00223900	H	-1.69340000	-3.28297400	-2.40258700
H	4.13206200	3.08794500	-1.25012600	H	-0.24269400	-2.81671200	-1.50057800
H	3.92641700	4.26657300	0.05771900	H	-0.74134100	-4.51223300	-1.57615700
H	2.47332900	2.35162600	0.42712000	H	-2.84655000	-3.86754400	-0.16467100
C	3.95558200	3.66423000	2.80236000	C	2.97236900	4.44178700	3.42375800
C	5.27120700	4.15539200	2.79342000	H	1.95410100	4.07676600	3.47921200
C	5.58563200	5.39284000	3.35362900	H	2.49453100	6.25812500	4.47193500
C	4.58865200	6.16551400	3.95485000	H	4.83284700	7.12649800	4.39962600
C	3.28181500	5.68117000	3.99341200	H	6.61280100	5.74843000	3.33339300

Table 25. Geometric coordinates and thermally corrected MP2 energies for R_3S (using the same core as **4**) with the S-unit being concave

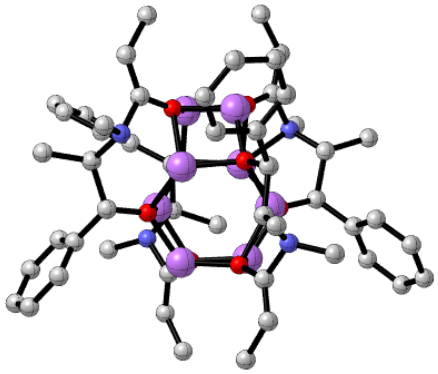


G = –2903.208982
G_{MP2} = –2893.686881

Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	C	0.60862900	3.79192500	-0.53671200
O	-1.90744400	-0.27497600	0.20395500	C	0.21644600	3.85568500	0.91321700
C	-2.77380100	-0.98758500	0.93138800	H	-0.31488500	2.94800500	1.21847400
N	-2.60423200	-2.43461800	0.73284500	H	-0.43694800	4.71444600	1.12500500
C	-3.64575700	-3.19775600	-0.01381200	H	1.09167200	3.96175700	1.57096400
C	-3.84945800	-2.62104900	-1.45023300	H	1.08305200	4.67231500	-0.96140400
O	-2.63524300	-2.29916400	-2.08649300	C	0.49093900	4.00488300	-3.45936600
Li	-1.31882000	-1.92256900	-0.79008200	H	-0.51361800	4.36467700	-3.22169200
O	0.56598800	-1.61546100	-0.77113400	H	0.55169300	3.83916800	-4.54075200
C	1.36332400	-2.60829200	-0.19039700	H	1.20693700	4.79837700	-3.20053400
C	1.52202300	-3.84318200	-1.14458100	C	3.16156600	2.95149000	-3.38507100
N	1.99042200	-3.41961600	-2.50925400	H	3.27006300	3.66255200	-2.55861500
C	1.11030100	-3.71091200	-3.63165800	H	3.04841900	3.51910100	-4.31537800
O	0.09403300	-2.84104900	-3.71173800	H	4.08980000	2.37960700	-3.46240600
Li	-1.78164000	-2.89144400	-3.64771800	H	2.21859200	1.39584800	-2.25404000
O	-2.05282400	-1.41376100	-4.86044900	C	2.89127600	0.37969700	-4.90534400
C	-3.11758000	-1.06447000	-5.59643800	C	3.12567300	0.49897200	-6.28102300
N	-3.95014600	-0.08207300	-4.91540400	C	4.24203700	-0.09170700	-6.87965300
C	-3.48959500	1.34886400	-4.94810900	C	5.15231700	-0.80742100	-6.10287400
C	-3.28707900	1.90776300	-3.49463100	C	4.93386200	-0.93259800	-4.72809700
O	-2.45585400	1.06856300	-2.74206000	C	3.81153400	-0.35074100	-4.13790200
Li	-0.56479100	1.11900300	-2.91668000	H	3.65953300	-0.46055200	-3.06663400
O	0.73776400	0.04000100	-3.82282400	H	5.64166400	-1.48202600	-4.11271500
Li	1.04716400	-1.45963500	-2.61984200	H	6.02543700	-1.26369100	-6.56160600
Li	-0.19655900	-1.27438800	-4.79280300	H	4.40032400	0.01299100	-7.94999600
C	1.65352500	1.01756600	-4.28250600	H	2.42626400	1.06717500	-6.89176500
C	1.97602400	2.01229900	-3.12587000	H	1.18214400	1.61846700	-5.08336200
N	0.71322200	2.73898900	-2.75999700	Li	-2.88518500	-0.72165700	-3.18087700

C	0.40633500	2.72596300	-1.33804100	C	-4.62098700	2.20046300	-2.79820300
O	-0.14343400	1.56160300	-0.97107400	C	-5.09401600	1.41753000	-1.73827700
Li	-2.04506300	1.20872300	-0.91508000	C	-6.31782300	1.70144300	-1.12226900
C	-7.08757900	2.78164300	-1.55233100	H	3.18590300	-3.84592600	1.43700700
C	-6.62116700	3.57999300	-2.60063000	H	5.36642000	-3.01687100	2.23749300
C	-5.40126700	3.29215200	-3.21110000	H	6.16576400	-0.75157400	1.57996100
H	-5.04412200	3.92965400	-4.01819200	H	4.73960200	0.67329700	0.11886900
H	-7.20505700	4.43308300	-2.93708500	H	2.55233900	-0.16745600	-0.68182000
H	-8.03621400	3.00637800	-1.07229500	H	0.87030700	-3.01559300	0.71480700
H	-6.66247700	1.07549100	-0.30294000	C	-4.65978800	-3.59423800	-2.30855700
H	-4.50419300	0.57696200	-1.38489100	C	-5.97001500	-3.30323900	-2.70537400
H	-2.80644600	2.89524000	-3.63823000	C	-6.68717400	-4.18259800	-3.52194600
C	-2.23670700	1.58465400	-5.80014200	C	-6.10027400	-5.37050500	-3.95784100
H	-2.04876100	2.66215600	-5.87175300	C	-4.79319000	-5.67565500	-3.56812900
H	-2.37098800	1.19231100	-6.81198200	C	-4.08239500	-4.79494300	-2.75202400
H	-1.34952500	1.11124300	-5.37012900	H	-3.06863700	-5.04680500	-2.44524600
H	-4.29495800	1.93152700	-5.41729200	H	-4.32991700	-6.60330800	-3.89507500
C	-5.39044500	-0.19155700	-5.17649800	H	-6.65453900	-6.05424900	-4.59507800
H	-5.93188400	0.41910600	-4.44952600	H	-7.70302000	-3.93518700	-3.81956000
H	-5.70119200	-1.23258500	-5.06558400	H	-6.43458100	-2.37767800	-2.37202600
H	-5.67306200	0.15345300	-6.18503700	H	-4.46486200	-1.70985800	-1.32532600
C	-3.45079100	-1.58835200	-6.79401800	C	-4.98969700	-3.35995400	0.71462300
C	-2.70636000	-2.69608200	-7.48373700	H	-5.51616300	-2.40342700	0.79235700
H	-3.35950400	-3.55242500	-7.70628300	H	-5.63347400	-4.05988900	0.17343400
H	-1.87972300	-3.06068800	-6.86665900	H	-4.85071600	-3.75444100	1.72661600
H	-2.28141000	-2.37136000	-8.44529700	H	-3.20360600	-4.19724300	-0.13298100
H	-4.32806300	-1.19694900	-7.30055900	C	-2.15349700	-3.12140300	1.94848800
C	1.35945100	-4.70804000	-4.50662100	H	-2.91149200	-3.16077800	2.74486100
C	0.56802200	-4.97000900	-5.75669200	H	-1.27593400	-2.60414100	2.34846300
H	-0.20013400	-4.20500800	-5.90743500	H	-1.86456300	-4.14969000	1.69877000
H	0.05864800	-5.94517200	-5.72890200	C	-3.65863300	-0.47538100	1.81133000
H	1.20699300	-4.98017500	-6.65166300	H	-4.29599400	-1.16313700	2.35828100
H	2.19994700	-5.36723500	-4.31181000	C	-3.78886500	0.98939500	2.12940500
C	3.40249500	-3.76160900	-2.71462700	H	-2.89958300	1.54313300	1.80632100
H	3.72984700	-3.38463100	-3.68479700	H	-4.66076600	1.45599700	1.64689500
H	3.59298900	-4.84710500	-2.67613000	H	-3.90400800	1.15148500	3.20916200
H	4.00047500	-3.28925300	-1.93006900	C	2.71894300	-2.07550100	0.29198000
C	0.25301500	-4.70406200	-1.15753100	C	3.17494700	-0.79872700	-0.05491300
H	0.05073200	-5.06417900	-0.14215600	C	4.40933700	-0.32315200	0.40180100
H	-0.62459800	-4.15135700	-1.50441900	C	5.20828900	-1.11940500	1.22112900
H	0.38004300	-5.57267900	-1.80981300	C	4.75924400	-2.39145700	1.58779000
H	2.31299300	-4.47961800	-0.72546500	C	3.52788300	-2.85870500	1.13104700

Table 26. Geometric coordinates and thermally corrected MP2 energies for R_3S (using the same core as **4**) with the S-unit being convex

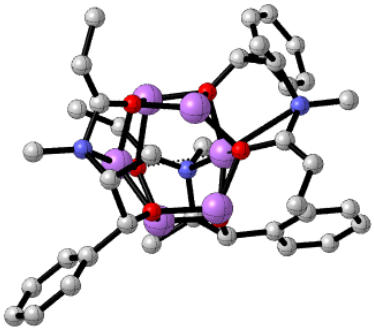


G = –2903.203171
G_{MP2} = –2893.676637

Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	C	-1.81294800	2.37740300	2.80872200
O	1.87358300	-0.28574500	-0.42506700	N	-0.69818800	3.17104400	2.18637400
C	2.30910100	-1.22882300	-1.26905800	C	-0.45317200	2.85494600	0.79013600
N	2.66681700	-2.44391700	-0.55600300	O	0.22911000	1.70900700	0.66264400
C	3.99464800	-2.36997300	0.14217200	Li	2.12867300	1.34178600	0.41773100
C	5.12605100	-3.03847700	-0.65077800	C	-0.83324000	3.66402700	-0.22020800
H	6.09768900	-2.79265900	-0.21543800	C	-0.50258500	3.43969200	-1.66912000
H	5.12009900	-2.68196200	-1.68667900	H	0.15165900	2.57112000	-1.79626400
H	5.03940500	-4.13062000	-0.66078800	H	0.00678800	4.30821900	-2.11113500
C	3.80183600	-2.88440400	1.60033500	H	-1.40282800	3.26449700	-2.27671900
O	2.94574800	-2.00079400	2.30205800	H	-1.40330600	4.55655900	0.02151600
Li	1.53903300	-1.68340000	1.02362300	C	-0.70544300	4.59321300	2.53127000
O	-0.35873100	-1.46802200	1.12656800	H	0.18192400	5.06009300	2.10376000
C	-1.12981100	-2.58778700	0.78871000	H	-0.67059000	4.70217500	3.62164700
C	-1.19314500	-3.61973900	1.96874000	H	-1.58743300	5.14106100	2.16953200
N	-1.62977700	-2.96239400	3.24832500	C	-3.12545500	3.16156700	2.94344000
C	-0.69792700	-3.00164500	4.36436500	H	-3.38690100	3.63401400	1.99021900
O	0.28957100	-2.10656700	4.22657200	H	-3.07389300	3.93996700	3.71232200
Li	2.13972300	-2.17683700	3.99601200	H	-3.93995200	2.48684200	3.21896200
O	2.50325900	-0.49099900	4.84580900	H	-1.99281200	1.54108000	2.12596500
C	3.57295500	0.04602700	5.44507900	C	-2.34036900	1.19962300	5.05872100
N	4.41170100	0.75935800	4.49471500	C	-2.42076700	1.67079100	6.37538700
C	3.94854900	2.15723100	4.18530100	C	-3.38384500	1.18316000	7.26335400
C	3.86352800	2.27670700	2.63429100	C	-4.29448500	0.21596700	6.84028400
O	2.78933400	1.47414000	2.17497500	C	-4.22949000	-0.26234700	5.52862500
Li	0.87650800	1.69796900	2.56843400	C	-3.25798200	0.21892700	4.65070900
O	-0.31054600	0.75666500	3.78447700	H	-3.22514400	-0.16727900	3.63430800
Li	-0.70490500	-0.97365700	2.93594600	H	-4.94230800	-1.00842400	5.18716200

Li	0.65634100	-0.34503900	4.93636200	H	-5.05027000	-0.16251000	7.52323800
C	-1.26652500	1.74378600	4.12157700	H	-3.42346800	1.56379900	8.28079200
H	-1.72135000	2.43550600	6.70858900	C	-3.06646100	-0.93796500	0.45331000
H	-0.77314500	2.56611200	4.67413500	C	-4.34276400	-0.61855600	-0.02345100
Li	3.27493800	-0.22353400	2.97336400	C	-5.10268800	-1.57906500	-0.68975800
C	3.78347800	3.69644200	2.08258700	C	-4.57373000	-2.85892800	-0.88080900
C	2.87188300	4.64577500	2.56670400	C	-3.30094100	-3.16967200	-0.40494400
C	2.81801100	5.93062100	2.02537200	H	-2.89633600	-4.16619000	-0.57391800
C	3.66520900	6.28896400	0.97365700	H	-5.15105900	-3.61308900	-1.40980300
C	4.57174000	5.35410600	0.47476000	H	-6.09245800	-1.33334600	-1.06487700
C	4.63053600	4.07381200	1.03171700	H	-4.73640600	0.38397700	0.12443500
H	5.35408500	3.35521800	0.65021700	H	-2.47773000	-0.18214900	0.96375900
H	5.24014200	5.62102800	-0.33982100	H	-0.65380100	-3.14320300	-0.04367000
H	3.62028400	7.28941300	0.55197800	C	5.10979100	-3.12462300	2.34766100
H	2.11632800	6.65704400	2.42760200	C	5.34473300	-4.35948600	2.96584200
H	2.20322100	4.38295400	3.38283400	C	6.52910100	-4.60635100	3.66518600
H	4.81809500	1.86664500	2.25126900	C	7.50970000	-3.61805300	3.74590300
C	4.76658800	3.24106300	4.90100000	C	7.29229500	-2.38231000	3.13080300
H	5.78290600	3.33081800	4.50293100	C	6.10085100	-2.13724900	2.44750100
H	4.28779600	4.21681000	4.78986200	H	5.94539900	-1.16962600	1.97520200
H	4.83327200	3.02020800	5.97186900	H	8.05425400	-1.60861500	3.18223300
H	2.91781000	2.21466900	4.55416800	H	8.43679100	-3.80727200	4.28027000
C	5.85549900	0.62251600	4.69780500	H	6.68684400	-5.57247500	4.13770000
H	6.38490500	1.01690400	3.82245600	H	4.59198300	-5.14227400	2.89148900
H	6.09541100	-0.43683300	4.79499100	H	3.31586700	-3.87429500	1.51543300
H	6.23894500	1.14785500	5.58404900	H	4.21838100	-1.30007100	0.22227400
C	3.89481700	-0.07107500	6.74958600	C	2.39470500	-3.70584300	-1.24411600
C	3.12470600	-0.87616100	7.75814800	H	3.03727800	-3.89402800	-2.11633400
H	3.76615300	-1.60445700	8.27482000	H	1.35541800	-3.70385100	-1.58321900
H	2.31034800	-1.43228300	7.28293400	H	2.52866500	-4.53778100	-0.54432900
H	2.68013500	-0.24352000	8.54097400	C	2.36490000	-1.12993400	-2.61361000
H	4.78731200	0.43722900	7.10369200	H	2.75672600	-1.97394700	-3.17413700
C	-0.87447300	-3.81040500	5.43064200	C	1.91548600	0.06510300	-3.40656700
C	-0.02561200	-3.79035100	6.67080800	H	1.52864800	0.85249300	-2.75214900
H	0.71322600	-2.98339400	6.63364000	H	2.73890200	0.49877600	-3.99254600
H	0.52458500	-4.73287600	6.81296900	H	1.12392900	-0.19066700	-4.12636900
H	-0.63012400	-3.64542700	7.57792200	H	0.28272500	-4.96789100	1.15605200
H	-1.69536600	-4.52095600	5.41151200	H	0.97810200	-3.76071000	2.25304000
C	-3.01431700	-3.31893300	3.57683500	H	0.06646700	-5.12685500	2.90959400
H	-3.31961500	-2.79003200	4.48089200	H	-1.96930600	-4.35437400	1.71522100
H	-3.15311400	-4.40062300	3.74179700	C	-2.52820100	-2.21758100	0.27891000
H	-3.66498600	-3.02021300	2.75016100	C	0.11517700	-4.41038500	2.08459900

Table 27. Geometric coordinates and thermally corrected MP2 energies for R_3 (using the same core as **5**)

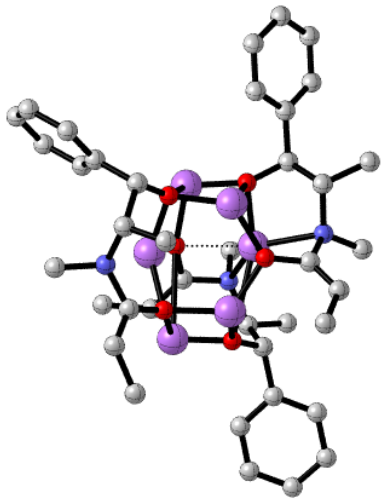


G = – 2177.361786
G_{MP2} = – 2170.213258

Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	H	-2.37069200	-1.56379700	-5.15553700
Li	-3.41237800	-0.57362900	-0.83075300	H	-2.39990900	-0.43449600	-6.49949700
O	-3.43845500	1.24725500	-0.18362300	H	-1.43163700	-0.05741700	-5.07483000
Li	-2.01184800	1.56541800	-1.39602900	H	-4.39379900	0.47190500	-5.48519400
O	-2.60668100	0.36416200	-2.67338900	Li	-1.60289500	-1.20177100	-2.61156500
C	-3.62689700	0.59229700	-3.50685900	O	0.05387800	-1.05206700	-1.60262500
N	-4.79478400	1.14692900	-2.89209900	C	1.33963600	-0.81387000	-2.09499000
C	-4.66079400	2.36860400	-2.04771900	C	1.71675800	0.71077800	-1.97758800
C	-4.50363100	2.09840500	-0.50696300	N	1.59032600	1.19787500	-0.55241300
C	-5.81913400	1.62932500	0.12287800	C	0.63039000	2.26167400	-0.27008100
C	-6.38628000	2.36967000	1.16859600	O	-0.62355200	1.78880500	-0.16810900
C	-7.57484900	1.96625600	1.78290700	Li	-2.04868100	1.11305700	1.00373600
C	-8.22523000	0.80948800	1.35272600	O	-1.37233800	-0.89330600	0.90684700
C	-7.67421700	0.06139200	0.30928000	Li	-0.98820700	-2.08709100	-0.51225300
C	-6.48245600	0.46469200	-0.29491400	O	-2.58647700	-2.28675100	-1.40485100
H	-6.07130400	-0.12279900	-1.10925500	C	-3.27845500	-3.33832400	-0.80991200
H	-8.17135800	-0.84054300	-0.03949100	C	-3.25522800	-3.20881100	0.76562600
H	-9.15238300	0.49381400	1.82429700	N	-3.49697500	-1.79555100	1.21425300
H	-7.99179500	2.55797700	2.59425300	C	-2.37794100	-1.07481300	1.76603800
H	-5.89014500	3.27783000	1.50648600	C	-2.39431600	-0.50543300	3.00199600
H	-4.31951200	3.10406600	-0.08191200	C	-1.25617200	0.29379100	3.58877600
C	-3.63983200	3.38300300	-2.60562100	H	-0.50326500	0.56740500	2.83901100
H	-3.92709200	3.68084600	-3.61963100	H	-1.60678900	1.21844600	4.06941300
H	-3.61381600	4.28330600	-1.98178200	H	-0.71956300	-0.27154800	4.36563400
H	-2.61406600	3.00577400	-2.69486200	H	-3.24181800	-0.68071100	3.65381100
H	-5.62660300	2.87962500	-2.12801800	C	-4.75315400	-1.67499000	1.96468700
C	-5.99873100	1.16926000	-3.71849900	H	-5.55839100	-2.10966000	1.36925400
H	-6.86324500	1.38637900	-3.08503200	H	-4.72364600	-2.19020600	2.93968500
H	-5.96375200	1.91727600	-4.52992500	H	-4.98326100	-0.62095700	2.12593800

H	-6.14703900	0.18701000	-4.17366400	C	-2.01899100	-3.87620900	1.39565600
C	-3.57213500	0.24273100	-4.81859000	H	-1.05298700	-3.50079800	1.03606000
C	-2.38893300	-0.48638200	-5.40487400	H	-2.01592000	-3.73792400	2.48157100
H	-2.04175200	-4.95091500	1.18545300	H	3.45370600	0.42063600	0.01603200
H	-4.10234200	-3.78143300	1.15327200	H	2.77854800	0.80644000	-2.24206700
C	-4.70774700	-3.49955200	-1.35324000	C	0.93240300	1.53906000	-3.00047500
C	-5.55556100	-4.50778500	-0.86544600	H	1.24662700	1.25039600	-4.01012100
C	-6.83988300	-4.68299700	-1.37837200	H	-0.14510000	1.36386700	-2.93568400
C	-7.30404800	-3.85638500	-2.40525700	H	1.12511100	2.60829000	-2.87682200
C	-6.46359600	-2.86887200	-2.91636500	H	1.38331300	-1.02855600	-3.17948400
C	-5.17582400	-2.69446000	-2.39758500	C	2.40430600	-1.70855200	-1.45133000
H	-4.52144600	-1.94267300	-2.82657800	C	3.59469000	-1.97870900	-2.14268100
H	-6.80168700	-2.23432500	-3.73174100	C	4.59625600	-2.76918600	-1.57976300
H	-8.30325500	-3.99333300	-2.81035400	C	4.42658200	-3.31441000	-0.30489800
H	-7.47636700	-5.46998400	-0.98128200	C	3.24634800	-3.06137900	0.39434500
H	-5.20720300	-5.17995900	-0.08346400	C	2.24624000	-2.26882800	-0.17728000
H	-2.77657200	-4.30350600	-1.02670200	H	1.33611500	-2.08682700	0.38983000
C	0.99618100	3.54112300	-0.05955800	H	3.09866600	-3.48090100	1.38642800
C	0.05848100	4.63342900	0.37235100	H	5.20287700	-3.93457700	0.13484700
H	0.39744800	5.11874800	1.29898400	H	5.50632200	-2.96724500	-2.14037600
H	-0.02124600	5.42863900	-0.38337600	H	3.73468200	-1.56902300	-3.14156100
H	-0.94835900	4.24111900	0.54599400	C	2.90614700	1.36412100	0.07808500
H	2.03963200	3.80985200	-0.19677500	H	3.51687500	2.14574500	-0.40185600
H	2.77526400	1.62660900	1.13083100				

Table 28. Geometric coordinates and thermally corrected MP2 energies for S_3 (using the same core as **5**)

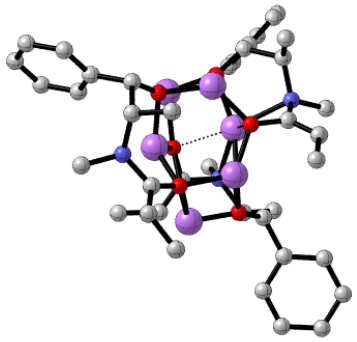


G = –2177.373661
G_{MP2} = –2170.217749

Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	C	-1.94380800	-3.15486500	-3.12117200
Li	-1.36382600	-3.06381700	-0.20351300	H	-2.19908000	-4.21240800	-3.02729200
O	-3.50151000	-1.14288100	0.30306100	H	-2.34825500	-2.77127000	-4.07043100
Li	-2.76198000	0.35783700	-0.27678400	H	-0.85453200	-3.07467100	-3.15226100
O	-0.54326100	-1.17142500	-1.38675900	C	-2.24098600	0.02840300	-2.53039900
C	-1.72428800	-1.09994100	-1.95998500	C	-1.46581700	1.31142100	-2.73287900
N	-2.43152400	-2.39189100	-1.94764800	H	-1.18636500	1.44526300	-3.78849900
C	-3.92124600	-2.35062100	-1.80572800	H	-2.04220800	2.20629900	-2.45466700
C	-4.29853700	-2.09836900	-0.30070000	H	-0.53442100	1.32606700	-2.15711100
C	-5.78413500	-1.74661000	-0.16839100	H	-3.20056100	-0.03835700	-3.03458400
C	-6.66455000	-2.58563000	0.52401900	Li	1.06530100	-2.11751200	-0.93747200
C	-8.01236700	-2.24947600	0.67881200	O	1.41406200	-1.07774900	0.63096900
C	-8.50298400	-1.06168400	0.13749100	C	2.31798800	-0.20222300	1.23516300
C	-7.63562500	-0.21253800	-0.55575300	C	1.55572600	0.88816300	2.07461300
C	-6.29161100	-0.55324200	-0.70291600	N	0.59005600	1.65554800	1.20893800
H	-5.62412000	0.12105700	-1.23629700	C	-0.82249600	1.65017500	1.57814500
H	-8.00838000	0.71618300	-0.98118700	O	-1.46847800	0.58378900	1.07444400
H	-9.55022100	-0.79596700	0.25598200	Li	-2.28075200	-1.07911100	1.66803000
H	-8.67581800	-2.91493600	1.22576900	O	-1.25795300	-2.63163000	1.94052600
H	-6.28705100	-3.51021300	0.95599400	Li	0.51302800	-2.53382000	1.36337500
H	-4.16284200	-3.07659200	0.20254400	O	0.46695800	-3.66552300	-0.21644600
H	-4.32951600	-1.53407800	-2.41679600	C	0.50999000	-5.04347200	-0.00671400
C	-4.58566500	-3.64669200	-2.28480200	C	-0.24373700	-5.34075300	1.32913700
H	-4.17859400	-4.52360400	-1.76640300	N	-1.64128100	-4.79263800	1.21773500
H	-5.65513900	-3.59802400	-2.06178800	C	-1.93238400	-3.76390200	2.19675400

H	-4.48186100	-3.80343900	-3.36216700
C	-3.21595000	-2.86378200	4.17972600
H	-2.53269700	-2.00726400	4.13636300
H	-4.23701400	-2.48944400	4.00897800
H	-3.19030900	-3.23999200	5.21149200
H	-3.29396800	-4.90441700	3.31508300
C	-2.68787100	-5.78407500	0.97427500
H	-2.84967700	-6.49165400	1.80125000
H	-3.62931800	-5.26083000	0.79069500
H	-2.43606500	-6.36482800	0.08029900
C	-0.18100900	-6.79115300	1.82267700
H	-0.57079700	-7.50460900	1.08862300
H	0.85612100	-7.06716100	2.03032800
H	-0.75168000	-6.90678100	2.75010700
H	0.25809800	-4.73474000	2.09636800
C	1.93704000	-5.58908600	-0.01396000
C	3.00060900	-4.83355600	0.50004400
C	4.30207900	-5.33978700	0.51171000
C	4.56599600	-6.61143100	-0.00077300
C	3.51905200	-7.36840800	-0.52942900
C	2.21984300	-6.85804700	-0.53686300
H	1.41260800	-7.45181000	-0.96131300
H	3.71451200	-8.35377500	-0.94519000
H	5.57944600	-7.00388700	0.00150300
H	5.11174600	-4.73498600	0.91253200
H	2.81279200	-3.82800400	0.86825300
H	-0.04208600	-5.58059400	-0.80378800
C	-1.39826400	2.64804700	2.27611100
C	-2.86657500	2.74540600	2.58398400
C	-2.81918400	-3.93466900	3.20015700
C	3.01589200	0.51195500	-1.13094000
H	2.07391500	0.12834000	-1.51478800
H	3.67757400	1.16238900	-3.07531200
H	5.84220800	2.06240700	-2.23758600
H	6.38024900	1.89800900	0.18862500
H	4.77566400	0.85141000	1.74798200
H	2.94411300	-0.73847600	1.97473800
H	-0.76278300	3.44731900	2.64757700
C	1.11973300	2.97687800	0.84762500
H	0.42956000	3.46941200	0.15798600
H	1.26589800	3.63471500	1.72005500
H	2.08496400	2.85530600	0.35057100
C	0.90836700	0.25719100	3.31240300
H	0.15716300	-0.49438800	3.05125800
H	1.68348600	-0.23139600	3.91466100
H	0.42261700	1.01483400	3.93264300
H	2.30347900	1.60752500	2.43891200
C	3.29896500	0.42074400	0.23783900
C	4.52612200	0.92708800	0.69099500
H	-3.05778000	2.72851900	3.66679600
H	-3.30352800	3.68199400	2.20766400
H	-3.42576500	1.91314600	2.14328400
C	5.43412400	1.51714300	-0.18771600
C	5.13469000	1.60805300	-1.54928800
C	3.92220600	1.10157300	-2.01767800

Table 29. Geometric coordinates and thermally corrected MP2 energies for S_2R (using the same core as **5**)

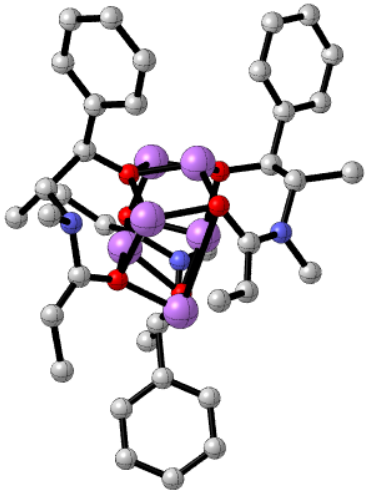


G = –2177.367688
G_{MP2} = -2170.214347

Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000
Li	2.53067900	2.19814300	0.31505100
O	3.61542100	-0.79343300	0.25125400
Li	2.27578600	-1.57608400	-0.58109700
O	1.10774600	1.13843300	-1.05819600
C	2.09546900	0.61435600	-1.75400900
N	3.35153400	1.36302500	-1.58378600
C	4.62717700	0.57763100	-1.53113400
C	4.77143100	-0.15113600	-0.14967600
H	5.03746300	0.64399900	0.57526300
C	5.95432600	-1.12711100	-0.18201900
C	7.08816800	-0.91628400	0.61084300
C	8.15085900	-1.82430200	0.60894200
C	8.09538200	-2.96339200	-0.19355400
C	6.96849400	-3.18884000	-0.98932400
C	5.91085900	-2.28049400	-0.97876800
H	5.03329400	-2.47296900	-1.59273300
H	6.91482400	-4.07486000	-1.61755900
H	8.91920800	-3.67243400	-0.19802900
H	9.01889600	-1.64159500	1.23774400
H	7.13567700	-0.03283100	1.24421900
H	4.62615100	-0.17686100	-2.33288700
C	5.84552800	1.48458300	-1.75269300
H	5.84592400	2.32532100	-1.04783100
H	6.75744500	0.90630700	-1.58305700
H	5.89872700	1.88675300	-2.76799300
C	3.35562500	2.38479600	-2.66010700
H	4.04387800	3.19804400	-2.42315000
H	3.62399200	1.95500800	-3.63754700
C	1.97515900	-0.45473400	-2.59433200
C	0.65793700	-1.09166500	-2.98299600
H	0.20038600	-0.58997800	-3.84975500
H	0.78621500	-2.14513400	-3.26383200
H	-0.08945300	-1.06210200	-2.18097400
H	2.84476900	-0.74433800	-3.17827200
Li	-0.03376900	2.53046400	-0.31815400
O	-0.84643400	1.37645300	0.95416600
C	-2.07094200	0.87076900	1.39277100
C	-1.91072900	-0.61658900	1.87750900
N	-1.35838400	-1.48476300	0.77782400
C	-0.11367300	-2.20394500	1.02998600
O	0.96461700	-1.44378000	0.77410600
Li	2.43769000	-0.49399000	1.61469800
O	2.24328000	1.27652400	2.21312800
Li	0.57959300	2.07164800	1.92867300
O	1.11199000	3.48216300	0.72685900
C	1.56439900	4.63346800	1.35933800
C	2.58327400	4.27511900	2.50534200
N	3.54077700	3.19532300	2.07808600
C	3.33848800	1.89125000	2.68319800
C	4.20277400	1.34450700	3.56563400
C	4.07050100	-0.04948300	4.12062000
H	3.02690800	-0.39134200	4.11368200
H	4.66926900	-0.78987700	3.56697500
H	4.40964700	-0.09102000	5.16333500
H	5.05960600	1.92411800	3.89304400
C	4.92414500	3.68072300	2.06369500
H	5.29360500	3.98281700	3.05811900

H	2.35091900	2.80560400	-2.74177900
C	1.87220900	3.98845600	3.83751700
H	1.14771500	3.16613400	3.78514000
H	2.59092900	3.72095900	4.61706600
H	1.32770600	4.88337600	4.15822900
H	3.19877100	5.16133400	2.69085400
C	2.13984000	5.67967300	0.39329700
C	2.22390800	5.43502400	-0.97951300
C	2.72323800	6.40202600	-1.85813500
C	3.14147100	7.64071400	-1.37418900
C	3.04632000	7.90697600	-0.00547900
C	2.54723100	6.93857400	0.86405000
H	2.46246000	7.17284900	1.92378000
H	3.35529000	8.87387700	0.38407300
H	3.52796900	8.39533700	-2.05406000
H	2.77746300	6.18663400	-2.92277300
H	1.88237100	4.47752800	-1.35488000
H	0.72400400	5.14647100	1.86851300
C	-0.08030900	-3.49950700	1.39905900
C	1.17286600	-4.31321200	1.56715400
H	1.25513500	-4.72279600	2.58403500
H	1.20058600	-5.17562100	0.88429300
H	2.07077500	-3.71274600	1.38649100
H	-1.02359800	-4.00293500	1.59214300
H	5.58086000	2.89667800	1.67928200
H	4.98640400	4.54844500	1.40027400
H	-3.19496300	-1.62803100	-0.22937200
C	-1.09633900	-0.67104800	3.17487900
H	-0.07902400	-0.29080900	3.04040300
H	-1.59213900	-0.05962500	3.93809700
H	-1.02271000	-1.69414900	3.55229400
H	-2.91471200	-0.99692500	2.11633300
C	-3.18220600	1.02455200	0.35098800
C	-4.52381000	1.04252800	0.75938200
C	-5.55988600	1.16644200	-0.16592500
C	-5.27374800	1.28161800	-1.52848300
C	-3.94414500	1.27283100	-1.95083700
C	-2.91027600	1.14827000	-1.01780500
H	-1.88089300	1.13376300	-1.36767200
H	-3.70694400	1.36335300	-3.00802800
H	-6.07861700	1.38347800	-2.25135200
H	-6.59125000	1.18278100	0.17735900
H	-4.75846700	0.96549100	1.81965900
H	-2.42161200	1.42175000	2.28680100
C	-2.41084300	-2.28972300	0.14562900
H	-1.98865800	-2.84515900	-0.69561400
H	-2.87581000	-3.01042100	0.83828300

Table 30. Geometric coordinates and thermally corrected MP2 energies for R_2S (using the same core as **5**)

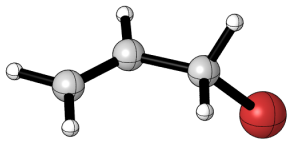


G = –2177.383382
G_{MP2} = –2170.227621

Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	H	-0.66618200	-4.02967500	-3.59055400
Li	-0.49236100	-2.39891500	-0.52533800	H	-3.43532100	-1.70380600	-3.22632000
O	0.98013100	-1.39527700	-1.08201900	C	-3.30306500	-3.55670200	-4.25592700
C	2.08701000	-1.61843600	-0.24713200	H	-4.36546900	-3.75768000	-4.09403700
C	2.03069000	-3.02797900	0.41571700	H	-3.18354300	-3.12690500	-5.25595800
N	0.65456400	-3.29887100	0.94577900	H	-2.78125800	-4.51998900	-4.23512500
C	0.14278400	-2.32710500	1.92267000	H	-2.16837200	-4.03334500	-1.71000300
O	-0.49911700	-1.31243400	1.33933500	C	-4.23163400	-3.65221100	-1.36377600
Li	-2.21418100	-1.13640000	0.73379500	C	-4.53284600	-5.01951500	-1.38759800
O	-2.08668300	0.59784600	-0.16575300	C	-5.81051500	-5.48315400	-1.06712000
Li	-1.31992400	1.36350000	-1.86155400	C	-6.81417300	-4.58109600	-0.71290800
O	-2.03343300	0.10892800	-3.09642600	C	-6.52790900	-3.21426400	-0.67833200
Li	-2.77287500	-0.49657000	-1.51500200	C	-5.24852200	-2.75796100	-0.99805400
O	-2.37991700	-2.17602300	-0.82352200	H	-5.04035000	-1.69115200	-0.94585800
C	-2.83649900	-3.14888400	-1.72614500	H	-7.29960100	-2.50196400	-0.39759100
C	-2.77723200	-2.57941200	-3.19221400	H	-7.80841900	-4.93859700	-0.45890600
N	-1.42512000	-2.08308700	-3.50695100	H	-6.01814100	-6.55000200	-1.08713100
C	-1.18006800	-0.70906700	-3.68050600	H	-3.75531300	-5.73129700	-1.65771000
C	-0.06142100	-0.24240600	-4.35882600	O	0.51769400	1.38807200	-1.26119900
C	0.04770600	1.21668500	-4.77043100	C	0.44103300	2.71887100	-1.13918900
H	0.02493500	1.92420200	-3.93007300	N	-0.93497800	3.15423200	-0.89204800
H	0.99842400	1.39091000	-5.28874000	C	-1.47693200	2.90498500	0.49226500
H	-0.75620200	1.52691000	-5.45681000	C	-2.53802000	1.74494700	0.51227900
H	0.49449800	-0.94580300	-4.97138100	H	-2.67872200	1.51804700	1.58568400
C	-0.44280800	-3.03732000	-3.99200600	C	-3.90276000	2.22549700	0.00758900

H	-0.41226000	-3.11348000	-5.09039600
H	0.55183600	-2.74971900	-3.63857100
C	-6.42906500	3.16011800	-0.84679800
C	-5.54136100	2.59130500	-1.76078700
C	-4.29162300	2.12731100	-1.33742300
H	-3.62819500	1.69593200	-2.08281500
H	-5.81544400	2.50632700	-2.80925300
H	-7.40163500	3.51608900	-1.17539000
H	-6.74133500	3.69498700	1.21994500
H	-4.53373000	2.87532200	1.96297600
H	-2.01752700	3.81732100	0.77046800
C	-0.39422100	2.71455400	1.56337900
H	-0.86060700	2.71058400	2.55477000
H	0.15857900	1.77591800	1.46122900
H	0.33433100	3.52908700	1.52790700
C	-1.27118500	4.49983500	-1.37344800
H	-0.83013300	5.30238000	-0.76060600
H	-0.91631700	4.61723700	-2.40011000
H	-2.35854100	4.61939100	-1.36157100
C	1.46189500	3.58669900	-1.29178800
C	2.86370600	3.19465400	-1.66629000
H	3.14305400	3.55761500	-2.66694400
H	3.59794200	3.61752700	-0.96642000
H	2.99109800	2.10802500	-1.65665200
H	1.26943100	4.64519600	-1.14503900
Li	1.06523400	-0.06677300	-2.37464500
C	0.27633800	-2.50635000	3.25315400
H	2.10492200	-0.88973600	0.59053500
C	-4.80896100	2.79788100	0.91258700
C	-6.05665300	3.26202500	0.49509400
H	-0.82551100	-0.75043700	3.82558400
H	0.83012100	-3.37143400	3.60664300
C	0.46085300	-4.70509200	1.31463400
H	0.70280200	-5.33530300	0.44960200
H	1.07907100	-5.04509900	2.15822100
H	-0.58765600	-4.86327200	1.58183800
H	2.16789400	-3.76219100	-0.39137800
C	3.14424400	-3.22029000	1.45486700
H	3.14298500	-4.23672700	1.86211600
H	4.12544200	-3.04863500	1.00252300
H	3.01979100	-2.52248100	2.28941600
C	3.39565700	-1.42053300	-1.01540500
C	4.39675600	-0.56185500	-0.54446700
C	5.57496800	-0.36332100	-1.26938800
C	5.76912300	-1.02232600	-2.48374200
C	4.77775300	-1.88076400	-2.96726200
C	3.60250800	-2.07470900	-2.24035100
H	2.83090800	-2.73681200	-2.62431200
C	-0.30439400	-1.59075800	4.29431300
H	-1.01826100	-2.11185800	4.94976900
H	0.47306200	-1.17507400	4.95152200
H	4.92169900	-2.40150700	-3.91082600
H	6.68338300	-0.86820100	-3.05071300
H	6.33687400	0.31088900	-0.88662300
H	4.24996900	-0.03914900	0.39817100

Table 31. Geometric coordinates and thermally corrected MP2 energies for allyl bromide.



G = –2688.957329
G_{MP2} = – 2686.820664

Atom	X	Y	Z	Atom	X	Y	Z
C	0.00000000	0.00000000	0.00000000	H	1.02321800	-1.27749700	1.46279300
C	1.10490300	-0.88775900	0.44963500	H	0.14734800	0.38227100	-1.00952900
C	2.15799100	-1.19767100	-0.30916900	H	-0.19578300	0.82059700	0.69089400
H	2.25777900	-0.83072700	-1.32844300	Br	-1.74098500	-0.99047000	-0.05511700
H	2.96065300	-1.82837200	0.06186800				

Scheme 1. Mechanism of alkylation of cubic mixed aggregates.

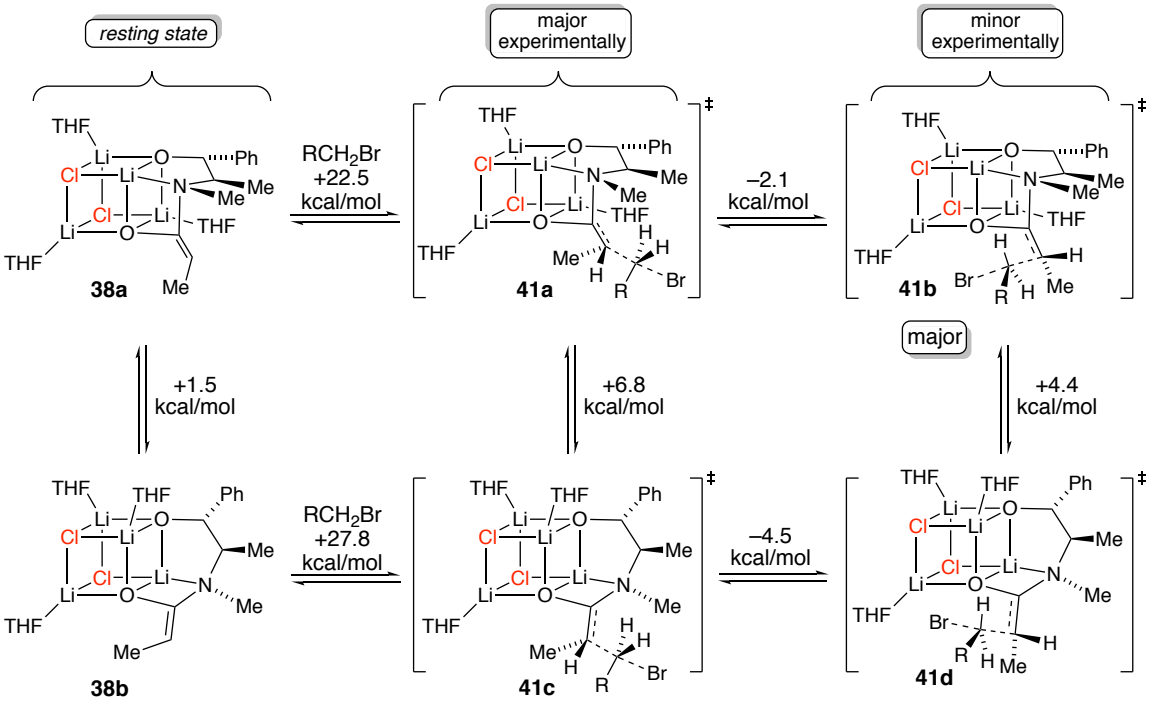
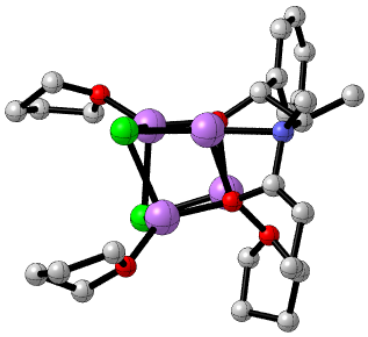
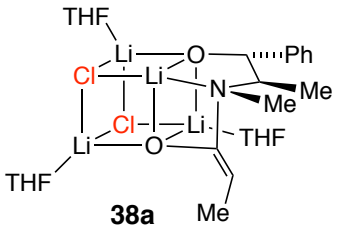


Table 32. Geometric coordinates and thermally corrected MP2 energies for **38a**.





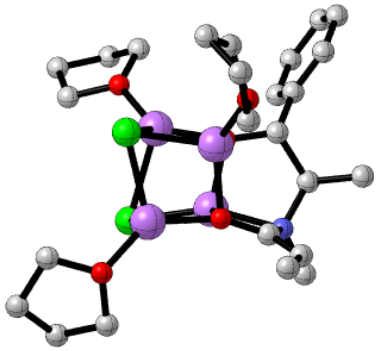
38a

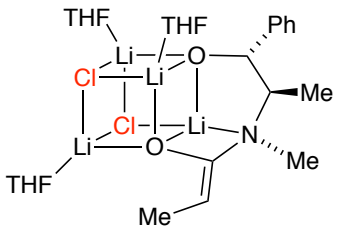
G = –2358.593477
G_{MP2} = –2352.599545

Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	H	6.37608900	0.51098600	-0.04508300
Li	-0.59856700	-0.22014300	2.54212100	H	6.75088500	-0.55600500	1.31905800
O	0.55467900	-1.31768400	1.40685400	H	4.78576200	-1.71406800	0.57803200
C	0.03815100	-2.27545200	0.62868100	H	4.08570100	-0.23409400	-0.13693400
N	-1.00525300	-1.74786400	-0.25008500	O	-0.45607600	4.13864100	1.37936300
C	-2.30401000	-1.40198500	0.44234400	C	-0.87093200	4.72056500	2.64541100
C	-2.49115600	0.15402400	0.42589400	C	-0.12873100	6.05834100	2.75895900
O	-1.38871900	0.74759700	1.06261600	C	1.11122200	5.82931000	1.87954300
Li	-0.26032300	2.21553000	1.29907100	C	0.53749200	4.98338200	0.74631000
Cl	0.95129800	1.38495400	3.33659800	H	1.26009800	4.32690200	0.25641100
Li	1.98674900	-0.08213900	1.70280300	H	0.04082000	5.60550300	-0.01050600
Cl	1.66370800	1.49855800	-0.24681500	H	1.87121400	5.26036900	2.42681200
O	3.88893800	-0.39973700	1.91401500	H	1.56426500	6.75877100	1.52134800
C	4.66267400	-0.63402600	0.70307300	H	0.11699500	6.30497800	3.79601200
C	5.99003100	0.11111100	0.89695300	H	-0.73786700	6.87398100	2.35194100
C	5.61717900	1.20506200	1.91068300	H	-1.95985500	4.82722700	2.63433800
C	4.62484800	0.47199200	2.80826100	H	-0.58433900	4.02252800	3.43950600
H	3.89787900	1.11807500	3.30583100	C	-3.81382000	0.60265000	1.04057300
H	5.13764000	-0.14371200	3.55988400	C	-4.78136800	1.24218800	0.25724000
H	5.12038600	2.04186800	1.40735900	C	-5.99008600	1.67258200	0.81080000
H	6.47805100	1.59208100	2.46445000	C	-6.25059600	1.46449700	2.16489100
C	-5.29343400	0.82583500	2.95843500	H	1.28376000	-4.89170000	2.07705400
C	-4.08644300	0.40201600	2.40279100	H	2.34221100	-4.59268600	0.70322600
H	-3.34997200	-0.09211700	3.03073700	H	2.10343500	-3.32726700	1.92311400
H	-5.48898700	0.65814700	4.01509400	H	-0.09413200	-4.24627800	-0.07538500
H	-7.18933100	1.79738700	2.60032000	O	-1.35173600	-1.16994700	4.11685200
H	-6.72440200	2.17219500	0.18361600	C	-1.35307800	-0.49047300	5.39211700
H	-4.58264900	1.41170400	-0.79915300	C	-0.23537700	-1.16516000	6.17851800
H	-2.52569200	0.44633200	-0.64355500	C	-0.39404600	-2.63797800	5.75893500

C	-3.51249500	-2.18518500	-0.08417300	C	-0.91630200	-2.54505400	4.31130300
H	-4.37854900	-1.99168200	0.55419400	H	-1.76678800	-3.21166700	4.13025100
H	-3.78653200	-1.89610500	-1.10458400	H	-0.14637200	-2.74113600	3.56188600
H	-3.32051700	-3.26316400	-0.07189400	H	-1.12582500	-3.14142200	6.40068100
H	-2.17584800	-1.68964800	1.49312600	H	0.54310100	-3.19864800	5.81980600
C	-1.11078500	-2.36080600	-1.57591800	H	-0.32623500	-1.01563500	7.25882300
H	-1.72594100	-1.72837000	-2.22457300	H	0.72863100	-0.76416400	5.84837300
H	-0.10921400	-2.42448700	-2.00890400	H	-1.18107600	0.56922600	5.19520700
H	-1.54564600	-3.37095000	-1.57729800	H	-2.33211300	-0.62564700	5.87462300
C	1.59818200	-4.11816700	1.35991500	C	0.43871400	-3.56320100	0.58019700

Table 33. Geometric coordinates and thermally corrected MP2 energies for **38b**





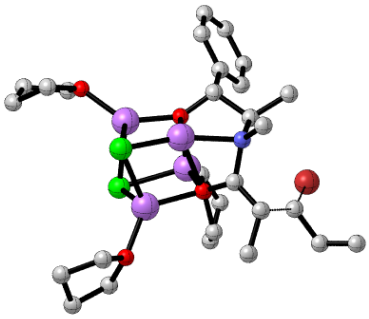
38b

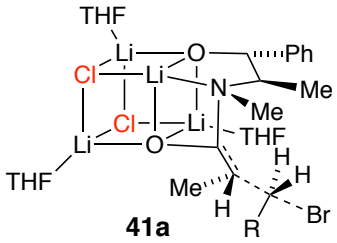
G = –2358.590869
G_{MP2} = –2352.597211

Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	H	3.20936600	3.80734900	-0.61047300
Li	-0.23645200	1.06724500	-2.44711900	H	3.67442700	6.51196900	-0.44010700
O	-1.22276000	-0.39122100	-1.44330100	H	2.65149500	5.89842900	-1.75667000
C	-0.73122200	-1.29103500	-2.29981200	H	1.73016700	7.03187800	0.93824600
N	0.24456900	-0.69929700	-3.23500700	H	1.11156100	7.45999200	-0.66353300
C	1.70424800	-0.74103100	-2.88899400	H	-0.18978200	5.42936100	-0.80734400
C	2.03704000	-0.04354400	-1.51497500	H	-0.07745500	5.47680600	0.96870500
O	1.17890900	1.01951100	-1.20665800	H	1.95473300	-0.83939600	-0.74847600
Li	0.46362400	2.58809600	-0.46529200	C	3.50233700	0.39805400	-1.51026900
Cl	-1.40189100	2.97573900	-2.21673700	C	4.47026600	-0.28828200	-0.76929400
Li	-2.31453000	1.05140900	-0.84577200	C	5.80502700	0.12821800	-0.76563700
Cl	-1.15060000	1.67915800	1.17513100	C	6.19105600	1.24319200	-1.50844500
O	-4.23777100	1.25813600	-0.87198100	C	5.23279200	1.94029400	-2.25135300
C	-4.88119000	1.22384700	-2.16904700	C	3.90220600	1.52236600	-2.24834500
C	-5.46293400	2.62129500	-2.36567000	H	3.15612900	2.07519500	-2.81417100
C	-5.87164900	2.99495100	-0.93178600	H	5.52545000	2.80952800	-2.83580700
C	-4.74439500	2.38133400	-0.09479800	H	7.22788800	1.56938000	-1.50955600
H	-5.07476100	2.00030400	0.87545600	H	6.54008500	-0.41872500	-0.18027300
H	-3.91573300	3.07949500	0.06133900	H	4.17630500	-1.15972000	-0.18746200
H	-6.83546200	2.53798700	-0.67735300	C	2.31324500	-2.14945900	-2.93432000
H	-5.95714500	4.07443200	-0.77656400	H	3.38295900	-2.10979600	-2.70521800
H	-6.29977600	2.63114300	-3.07077800	H	1.82652800	-2.80253100	-2.20201800
H	-4.68444700	3.29847200	-2.73246800	H	2.20597300	-2.60734200	-3.92321900
H	-4.12511700	0.95267200	-2.91095600	H	2.17384300	-0.13446800	-3.67525400
H	-5.66206200	0.45187200	-2.15451000	C	0.00208800	-1.03267700	-4.64394000
O	1.29855800	4.25554400	0.00143000	H	0.61529300	-0.37932100	-5.27669000
C	0.50081100	5.47090700	0.03979900	H	0.23599000	-2.07465000	-4.90752700
C	1.49953500	6.63617800	-0.05758100	H	-1.05114300	-0.85519200	-4.87730400
C	2.74816200	5.97553700	-0.66744400	C	-1.10239200	-2.58546400	-2.38615900
C	2.70091200	4.58612100	-0.03785000	C	-2.18622000	-3.21511200	-1.55708800

H	3.10226000	4.59601000	0.98566900	H	-2.97167100	-3.65849500	-2.18654700
H	-1.80351400	-4.02943300	-0.92356100	H	2.25766100	-1.17159700	2.58810900
H	-2.65618200	-2.47375600	-0.90425600	H	1.36101300	0.35897100	2.35836300
H	-0.61176000	-3.21267500	-3.12537400	H	0.98363400	-1.11514700	4.66497900
O	0.56970800	-1.28548600	1.38449100	H	-0.38273900	-0.30326600	3.86677400
C	-0.46895100	-2.19566300	1.83474000	H	0.49735000	-3.22218900	3.48890200
C	-0.21668500	-2.40532000	3.32852700	H	-1.13527800	-2.64510000	3.87232500
C	0.39928400	-1.05953400	3.74147600	H	-1.44200300	-1.72497300	1.65126200
C	1.26096600	-0.71609900	2.52733700	H	-0.39793000	-3.10929700	1.23899900

Table 34. Geometric coordinates and thermally corrected MP2 energies for transition state **41a**





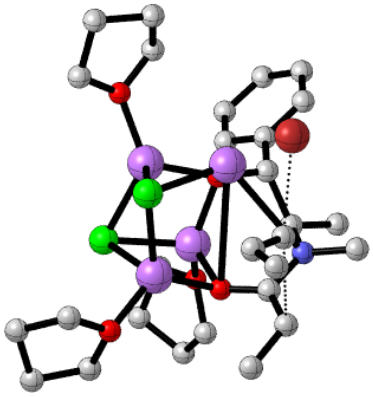
41a

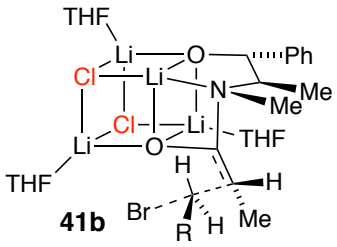
G = –5047.511284
G_{MP2} = –5039.384398

Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	H	-3.66129300	2.24917300	2.14302200
Li	-0.91075000	0.30612900	2.56733600	H	-4.43676200	4.34801000	3.13343200
O	-0.87835900	-1.34175300	1.30949600	H	-3.43473700	6.52380800	2.45427700
C	-1.69545600	-1.58067500	0.32691800	H	-1.63086900	6.56005800	0.73620900
N	-1.92227200	-0.45904000	-0.54271200	H	-0.83653200	4.44082000	-0.26782200
C	-2.60513500	0.76437800	0.06934100	H	-1.20253300	2.18409000	-0.73919200
C	-1.56944800	1.91363400	0.27252300	C	-3.84009600	1.19938700	-0.72927400
O	-0.49452500	1.45008200	1.06050100	H	-4.39448000	1.94381200	-0.15612500
Li	1.30277000	1.59410700	1.55826500	H	-3.57537700	1.64876300	-1.69277100
Cl	1.33582400	0.08052600	3.44065500	H	-4.52111300	0.36329200	-0.91344500
Li	1.06987100	-1.61238900	1.80244500	H	-2.95599700	0.45444700	1.05853600
Cl	2.16765900	-0.45030100	-0.07088500	C	-2.22601400	-0.76524500	-1.94668000
O	1.91547400	-3.29758400	2.23477000	H	-2.04548500	0.12440000	-2.55605700
C	2.96749900	-3.81058100	1.38124500	H	-1.54812200	-1.55092000	-2.28903900
C	4.19925300	-3.85797200	2.27905400	H	-3.25798800	-1.09556800	-2.12371900
C	3.59228400	-4.29345500	3.62341400	C	-2.34523300	-2.79978100	0.14471000
C	2.22219100	-3.59664000	3.62650800	C	-1.86135100	-4.06667700	0.79958900
H	2.23293600	-2.64497600	4.16602600	H	-1.08977900	-4.56489300	0.19429200
H	1.42430400	-4.22883200	4.02968400	H	-1.42503400	-3.86484100	1.78248600
H	4.20127000	-4.00218200	4.48397800	H	-2.68495600	-4.77823000	0.92380600
H	3.47171900	-5.38255100	3.64985100	H	-2.95791200	-2.91619200	-0.74324800
H	4.64086000	-2.85816800	2.35806000	O	-1.93482500	0.26773400	4.19586200
H	4.96451500	-4.54685800	1.90896800	C	-2.23658500	1.42384700	5.01275900
H	2.68495800	-4.81169800	1.02734800	C	-3.13828900	0.90016000	6.12802400
H	3.05394400	-3.13246900	0.52968200	C	-2.58101100	-0.51535300	6.34238300
O	2.63409900	2.98122700	1.67414700	C	-2.26855300	-0.94924900	4.90904500
C	2.72136900	3.69328400	2.94039700	H	-3.15407900	-1.38034200	4.43228700
C	4.21008200	3.99344700	3.15302800	H	-1.41563300	-1.63102100	4.83190000
C	4.89488400	2.87861300	2.34597700	H	-3.29387900	-1.18935700	6.82691000
C	3.96401800	2.74560400	1.14399600	H	-1.66727000	-0.48458200	6.94818800

H	3.96142300	1.75770900	0.67762200
H	4.17693400	3.50575800	0.38055900
H	4.90909300	1.94336200	2.91687700
H	5.92098700	3.12394700	2.05587000
H	4.48247700	3.98928800	4.21238000
H	4.46840000	4.97564400	2.74025400
H	2.10107000	4.59176200	2.87183100
H	2.31915200	3.03567400	3.71905100
C	-2.16353300	3.18729500	0.87222200
C	-1.62080700	4.42035300	0.48662700
C	-2.06634100	5.61550400	1.05306200
C	-3.07730700	5.59573300	2.01552800
C	-3.63530700	4.37515100	2.39942400
C	-3.18246600	3.17816800	1.83788600
H	-4.17100200	0.84558900	5.76921000
H	-3.09838500	1.52423500	7.02635100
H	-1.29316600	1.82909200	5.40329600
H	-2.71343600	2.17039900	4.37559700
C	-4.82633800	-3.21197100	1.78963400
H	-4.55020000	-3.75805300	2.68919200
C	-5.81718400	-3.67803500	1.01143900
H	-6.36010400	-4.58422300	1.26207200
H	-6.13009600	-3.15277600	0.11205700
C	-4.06719500	-2.01011700	1.50405500
H	-3.29507900	-1.68635400	2.17511400
H	-4.38778900	-1.35483800	0.71352100
Br	-5.28818300	-0.14091600	2.95374600

Table 35. Geometric coordinates and thermally corrected MP2 energies for transition state **41b**





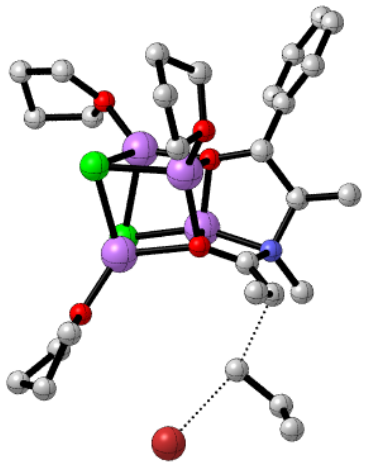
41b

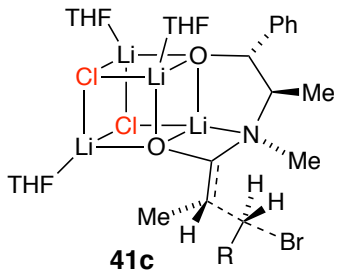
G = –5047.520262
G_{MP2} = –5039.387754

Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	C	4.97618400	-3.75511200	0.73871200
Li	0.45992800	-3.38883000	-0.21923900	C	5.95984400	-3.87967300	1.91161600
O	1.76990400	-2.61261500	-1.33661300	C	5.53933900	-2.72117500	2.83155700
C	1.56099500	-1.92895700	-2.42884300	C	5.14917100	-1.64857100	1.81986600
N	0.22285900	-1.70084100	-2.80321500	H	6.03100000	-1.12422500	1.42603600
C	-0.89163100	-2.52843400	-2.28011900	H	4.42631400	-0.91712400	2.18635100
C	-1.58847100	-1.81602300	-1.05833100	H	6.33785700	-2.39473000	3.50488800
O	-0.69092000	-1.74746700	0.02399500	H	4.66722700	-3.00277600	3.43153100
Li	-0.10182500	-1.84739500	1.83805000	H	6.99150200	-3.73860200	1.56850100
Cl	1.40150900	-3.68634100	1.88767200	H	5.89645600	-4.85800400	2.39679000
Li	2.61709600	-2.10038400	0.36083900	H	4.09595000	-4.39150100	0.87380600
Cl	1.76016200	-0.14857800	1.48058500	H	5.43321600	-3.96726800	-0.23301700
O	4.51621500	-2.37611300	0.73853900	O	-1.22021400	-1.17633200	3.26043400
C	-2.54758000	-0.66423100	3.01291300	H	-1.08783400	-0.43614700	-3.83860000
C	-2.46340400	0.80550400	3.41205300	H	0.60611100	-0.02512900	-4.01000100
C	-1.56162700	0.74199100	4.65881100	C	2.60712000	-1.34808300	-3.15605900
C	-0.61602400	-0.43751800	4.35921500	C	4.05316500	-1.59280100	-2.82712200
H	-0.50036400	-1.11386700	5.21268600	H	4.67547000	-0.74837400	-3.15104700
H	0.37103400	-0.11519600	4.01818800	H	4.21929200	-1.73154800	-1.75484700
H	-2.16250800	0.53718700	5.55205500	H	4.45322100	-2.48967500	-3.33074800
H	-1.01245500	1.67181200	4.83047100	H	2.40334100	-0.97338400	-4.15214800
H	-3.44468000	1.24489700	3.61520900	O	0.16361700	-5.34239600	-0.77393200
H	-1.98419600	1.38548000	2.61503300	C	-0.26639000	-6.34770400	0.18068600
H	-2.77492500	-0.84522500	1.96047700	C	0.72672000	-7.50224700	0.04157400
H	-3.27017200	-1.21193800	3.63434600	C	1.13367300	-7.40342700	-1.43653600
C	-2.92096500	-2.45154700	-0.66348100	C	1.18090100	-5.89069100	-1.65019600
C	-4.12809100	-1.91145300	-1.12734300	H	0.94964600	-5.58069000	-2.67323800

C	-5.35515100	-2.47984800	-0.77874600
C	-5.39601600	-3.60170500	0.04998000
C	-4.20125300	-4.14214000	0.53228200
C	-2.97771400	-3.56884800	0.18202600
H	-2.05829900	-3.98184400	0.58626500
H	-4.22190700	-5.00740900	1.19047100
H	-6.34902600	-4.04479000	0.32686900
H	-6.27819900	-2.03950500	-1.14752300
H	-4.10601300	-1.02904600	-1.76374300
H	-1.83168300	-0.79910700	-1.42371500
C	-1.86714500	-2.96210600	-3.38855000
H	-2.53343200	-3.73678400	-3.00083100
H	-2.49716400	-2.14575200	-3.75472400
H	-1.31974700	-3.38059900	-4.23990000
H	-0.45719900	-3.46381000	-1.92590900
C	-0.08749000	-0.86029300	-3.95262000
H	-0.04301900	-1.40189400	-4.90940000
H	2.15017200	-5.46482100	-1.36791800
H	0.36902300	-7.85926400	-2.07688300
H	2.09210600	-7.88335100	-1.65666900
H	0.28409200	-8.46701000	0.30713500
H	1.59406200	-7.33187600	0.68918200
H	-0.26007400	-5.88988700	1.17245000
H	-1.28719500	-6.65375600	-0.08064900
C	1.89857700	1.14226800	-1.99067100
C	3.03585200	1.79006900	-1.39627100
H	3.28564600	1.49700700	-0.37968800
C	3.76838600	2.71832100	-2.04334100
H	4.63043700	3.18871900	-1.57997100
H	3.52271600	3.03396800	-3.05477800
H	1.60369900	1.39695900	-2.99739200
H	1.52563500	0.22950700	-1.58251900
Br	-0.21277700	2.18552100	-1.03940000

Table 36. Geometric coordinates and thermally corrected MP2 energies for transition state **41c**





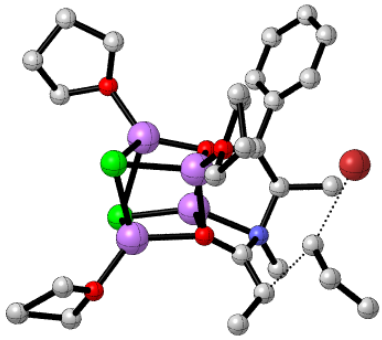
41c

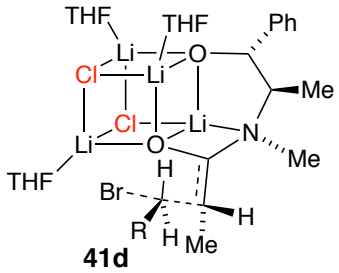
G = –5047.501025
G_{MP2} = –5039.373623

Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	H	2.12905000	3.99277400	-0.24594000
Li	-0.72979600	0.17020000	-2.66439500	H	3.82858800	3.62806900	-0.64610600
O	-1.70991900	-0.38437200	-0.83559200	H	2.69321000	6.19639000	-1.03359600
C	-1.93905000	-1.53689700	-1.36422200	H	4.06525000	5.58632400	-1.97042100
N	-1.24548200	-1.76299000	-2.63347800	H	1.09753900	5.43284800	-2.73071500
C	0.16366700	-2.32410700	-2.56426900	H	2.44966100	5.96242000	-3.75618300
C	1.15580300	-1.45600300	-1.70039100	H	3.32691800	3.66418700	-3.87491900
O	0.87214400	-0.08757600	-1.74652200	H	1.55954200	3.37712200	-3.93446500
Li	1.03219700	1.81064000	-1.68970300	H	1.05807100	-1.84157000	-0.66490100
Cl	-0.10736900	2.24801200	0.48989700	C	2.59469800	-1.75402200	-2.12981800
Li	-2.02752900	1.71920200	-0.84802100	C	3.41300600	-2.62028600	-1.39619400
Cl	-1.01558400	2.36062700	-2.99708800	C	4.72616600	-2.88094500	-1.79780400
O	-3.74029600	2.43012000	-0.53509900	C	5.23932200	-2.27300000	-2.94313200
C	-4.46557500	3.22058000	-1.52868700	C	4.43320600	-1.40081600	-3.68041400
C	-5.57666800	3.90654700	-0.73969300	C	3.12438000	-1.14270200	-3.27485300
C	-5.92647500	2.83457900	0.30488000	H	2.50724200	-0.44644900	-3.83641700
C	-4.55250300	2.25646500	0.65162200	H	4.82720200	-0.91831000	-4.57132100
H	-4.58546700	1.18892400	0.89432100	H	6.26051000	-2.47148100	-3.25748900
H	-4.06820400	2.79439300	1.47688900	H	5.34673500	-3.55468000	-1.21236500
H	-6.54442100	2.06094300	-0.16170600	H	3.02135600	-3.09575300	-0.49883500
H	-6.44070600	3.23389500	1.18482900	C	0.20636400	-3.79518500	-2.13113900
H	-6.42648100	4.16452200	-1.37820500	H	1.23461600	-4.16583600	-2.17092300
H	-5.20949800	4.82222400	-0.25907700	H	-0.15850400	-3.91466500	-1.10457900
H	-3.74510100	3.90078200	-1.98886500	H	-0.39686800	-4.43292400	-2.78427100
H	-4.87780900	2.53351400	-2.27302100	H	0.50645800	-2.25331500	-3.60420700
O	2.41875400	3.10492800	-2.08447700	C	-2.03438800	-2.43302400	-3.68159200

C	2.37329500	3.80946100	-3.34839600
C	2.15506300	5.26802600	-2.96360800
C	3.02124200	5.39255500	-1.69872000
C	2.88045700	4.00889500	-1.04036100
C	-3.20837400	-2.45294500	0.61997600
H	-4.16085500	-2.96552200	0.79302500
H	-2.44380400	-2.98208300	1.20622900
H	-3.28128400	-1.43439300	1.01235200
H	-2.88251100	-3.42929900	-1.33207100
O	0.60468400	-0.88112900	1.66139900
C	-0.22160200	-0.63097400	2.83381600
C	0.74997400	-0.50972000	4.00896200
C	2.00749400	0.05653400	3.33086000
C	2.00452900	-0.68042700	1.99314700
H	2.48714400	-1.66330500	2.06683400
H	2.46851200	-0.11850100	1.17760900
H	2.92432500	-0.12058400	3.90097800
H	0.95742500	-1.49459700	4.44409300
H	-1.44521100	-2.43529000	-4.60391300
H	-2.30379200	-3.47145800	-3.44824500
H	-2.94990000	-1.87037800	-3.87208600
C	-2.86132300	-2.45601800	-0.85058500
H	1.89938700	1.13382900	3.16699900
H	0.35966000	0.13696100	4.79999000
H	-0.77014500	0.30236100	2.66561900
H	-0.92929300	-1.45898600	2.92825800
C	-6.26620400	-3.34882600	-0.99239500
H	-6.82395200	-4.24665300	-1.24097300
H	-6.42226400	-2.93534000	0.00035900
C	-5.47945200	-2.74141500	-1.89473900
H	-5.39385800	-3.16292400	-2.89488700
C	-4.68825400	-1.54642600	-1.63439300
H	-4.80760900	-0.99845600	-0.71281600
H	-4.23636500	-1.01402700	-2.45009000
Br	-6.53325500	0.24713900	-2.42947900

Table 37. Geometric coordinates and thermally corrected MP2 energies for transition state **41d**





41d

G = –5047.506569
G_{MP2} = –5039.373623

Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	O	3.26458200	3.04390700	-0.67105500
Li	0.78845900	0.02610600	-2.66658300	C	4.24513100	3.39266400	-1.67867800
O	0.16134200	1.47722900	-1.33218100	C	5.58220700	3.33858900	-0.94777700
C	-0.71749500	1.82869900	-2.22189900	C	5.20821000	3.89703400	0.43554400
N	-0.98117500	0.85374900	-3.25346000	C	3.78327400	3.36260800	0.65212100
C	-1.69457000	-0.48330400	-3.05314000	H	3.11823100	4.09725200	1.11744000
C	-1.31448300	-1.22085800	-1.72629400	H	3.76113100	2.43956200	1.23905400
O	0.07204800	-1.24368400	-1.50949000	H	5.21043200	4.99282300	0.41508300
Li	1.81818700	-1.66714000	-1.02882600	H	5.89058900	3.57489900	1.22728200
Cl	2.19651700	-0.11176700	0.85643800	H	6.36055600	3.92057800	-1.45029600
Li	2.16676100	1.47627200	-0.90281500	H	5.92226100	2.29988200	-0.86964300
Cl	3.00889500	0.01067900	-2.67485700	H	4.14657800	2.66990100	-2.49145300
H	4.02815300	4.40228900	-2.05391900	O	-1.15479400	0.17561600	1.52550600
O	2.77904000	-3.30149000	-0.72541400	C	-1.12045400	1.32344500	2.40291400
C	4.22884900	-3.21489600	-0.69072100	C	-2.22723000	1.07018500	3.42227000
C	4.62908700	-3.75182300	0.68160600	C	-2.13358100	-0.45283400	3.60478400
C	3.55520900	-4.82323300	0.93046000	C	-1.83549500	-0.93318100	2.18155200
C	2.30352600	-4.17147400	0.33697300	H	-2.75352100	-1.12523400	1.62241900
H	1.78044600	-3.55284400	1.07635900	H	-1.17606200	-1.80626100	2.14508000
H	1.59589200	-4.88256800	-0.09757500	H	-3.05611800	-0.89223400	3.99495000
H	3.42868200	-5.07146500	1.98826600	H	-1.31348400	-0.71088700	4.28577100
H	3.80161900	-5.74557000	0.39127600	H	-3.19597700	1.33127700	2.98448800
H	4.55812400	-2.95707800	1.43232400	H	-2.07954000	1.62983600	4.35128600
H	5.64797600	-4.15045200	0.69256300	H	-0.12793900	1.38377300	2.86942400
H	4.63053300	-3.83059000	-1.50525600	H	-1.27855100	2.21625500	1.79027700
H	4.50337700	-2.17140800	-0.86262400	C	-4.53365400	4.33410000	-1.11836300
H	-1.83793900	-0.66761800	-0.92245500	H	-4.92688900	5.26736000	-0.72704300
C	-1.91278300	-2.62982300	-1.72468100	H	-4.91891600	4.00566400	-2.08083300
C	-3.13585800	-2.89365800	-1.09320500	C	-3.63911300	3.60424300	-0.43234800

C	-3.66735400	-4.18587600	-1.09459200	H	-3.28815400	3.95935300	0.53422800
C	-2.98461400	-5.22808100	-1.72347200	C	-3.08249600	2.34835600	-0.90244500
C	-1.76362200	-4.97195700	-2.35285600	H	-3.49837900	1.87630300	-1.77371300
C	-1.23068100	-3.68210000	-2.34988200	H	-2.37708800	1.80392800	-0.30318200
H	-0.27119700	-3.48646500	-2.82105200	Br	-4.63452900	0.63357400	0.37913700
H	-1.22475200	-5.77803600	-2.84532300	H	-2.22020200	1.84074600	-4.73087100
H	-3.39857300	-6.23330300	-1.72204400	H	-0.47912300	2.18570800	-4.80156600
H	-4.61636300	-4.37526700	-0.59935400	C	-1.32718100	3.08293400	-2.21883300
H	-3.68027300	-2.08192800	-0.61344400	C	-0.72038800	4.24194300	-1.46904800
C	-3.22080500	-0.39704800	-3.23475000	H	0.10220800	4.70143800	-2.03703100
H	-3.61138100	-1.38685400	-3.48611100	H	-1.46862800	5.02034200	-1.28945000
H	-3.73206600	-0.07554400	-2.32145400	H	-0.31053200	3.92596000	-0.50485500
H	-3.49770800	0.27488400	-4.05230700	H	-1.96814800	3.33336100	-3.05725000
H	-1.28875300	-1.09560500	-3.87156700	H	-1.09687400	0.60795300	-5.32907600
C	-1.21983700	1.40980600	-4.59323600				

Scheme 2. Mechanism of alkylation of LiCl ate complexes.

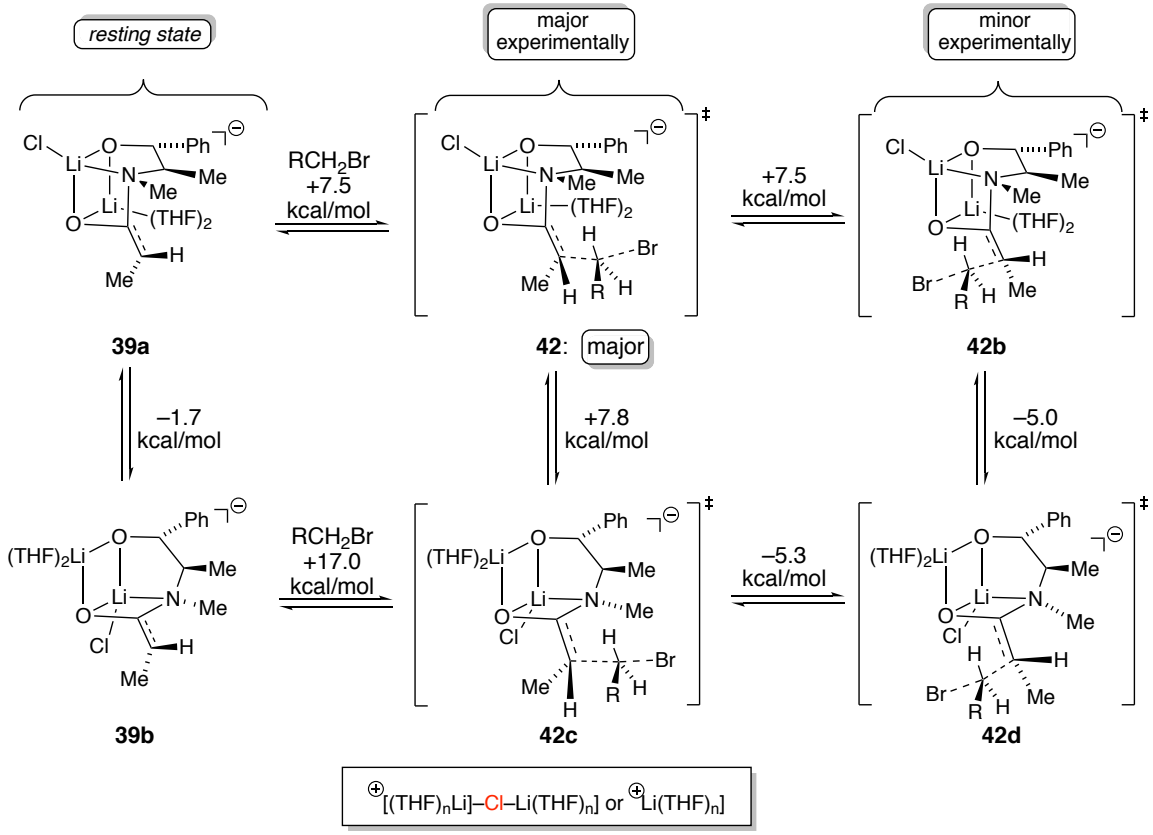
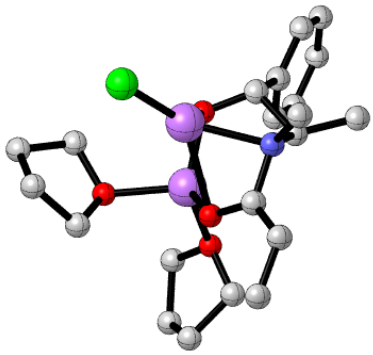
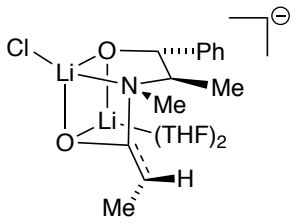


Table 38. Geometric coordinates and thermally corrected MP2 energies for **39a**



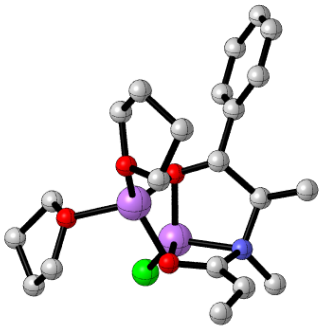


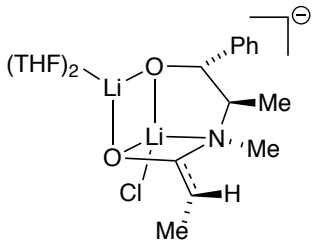
39a

G = –1650.786000
G_{MP2} = –1646.250660

Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	H	4.65947300	-4.97652600	0.57075400
O	-0.64750500	-1.16395500	1.87451600	H	6.78624900	-4.08501000	-0.37026100
Li	0.10374000	-2.39030500	0.66068800	H	6.91591100	-1.69005500	-1.04635000
O	1.31249400	-1.37696900	-0.32164200	H	4.94289000	-0.21582600	-0.77206000
C	2.45821500	-0.83033700	0.22599100	O	-1.35245800	-2.97713700	-0.63466500
C	2.20889200	-0.48558900	1.73793300	C	-1.08429000	-2.72175800	-2.04056700
N	1.02644700	0.42379200	1.83467800	C	-2.44921300	-2.44859300	-2.67213000
C	1.29871000	1.83999700	2.04512300	C	-3.20026500	-1.76100900	-1.52064800
H	1.99559400	2.19593000	1.27738200	C	-2.68543200	-2.51381600	-0.29098300
H	0.36143300	2.38946900	1.93199900	H	-3.30111000	-3.39716000	-0.06121600
H	1.72707700	2.08584000	3.03256800	H	-2.59602800	-1.88637000	0.60013400
C	-0.11848300	-0.15747100	2.52957600	H	-4.29013200	-1.82383200	-1.61705300
C	-0.56216500	0.36954100	3.70266200	H	-2.90332400	-0.70788800	-1.46513700
C	-1.82441200	-0.08119600	4.38241300	H	-2.94022900	-3.38881800	-2.95975100
H	-2.35376700	-0.79834700	3.74649900	H	-2.36753300	-1.81362500	-3.55949900
H	-1.64388100	-0.57199700	5.35540800	H	-0.41120800	-1.86267700	-2.11411400
H	-2.51367100	0.75494300	4.58663800	H	-0.57839800	-3.60574300	-2.44438300
H	-0.00610400	1.18307100	4.16008000	O	0.37028000	-4.15196800	1.73030000
H	1.90207100	-1.42912800	2.20525900	C	-0.18019800	-4.05275600	3.06299600
C	3.43980600	0.01716000	2.50555200	C	-1.40248800	-4.96755400	3.04083900
H	3.88453400	0.90808700	2.04617000	C	-0.91612300	-6.12365000	2.15077800
H	3.18078600	0.26256200	3.54224400	C	-0.01152300	-5.40877300	1.13003300
H	4.20961100	-0.76042800	2.52267900	H	-0.53869100	-5.17572700	0.20003400
H	2.72768200	0.13317700	-0.26406800	H	0.89316900	-5.98222300	0.89477400
C	3.67811800	-1.74300500	0.05718300	H	-1.73151400	-6.67176100	1.66739900
C	4.88238700	-1.25989400	-0.46991000	H	-0.33708600	-6.84098500	2.74559000
C	5.99534100	-2.09080500	-0.62559000	H	-2.24508800	-4.44614300	2.57261800
C	5.92387400	-3.43238100	-0.24971500	H	-1.70940500	-5.29131700	4.04091300
C	4.72782600	-3.93040500	0.27666600	H	0.56719400	-4.40175200	3.79177800
C	3.61859000	-3.09739500	0.42264100	H	-0.40834600	-2.99723700	3.22569700
H	2.68803200	-3.49598600	0.81747100	Cl	-1.22189000	1.34599100	-1.31068500

Table 39. Geometric coordinates and thermally corrected MP2 energies for **39b**.





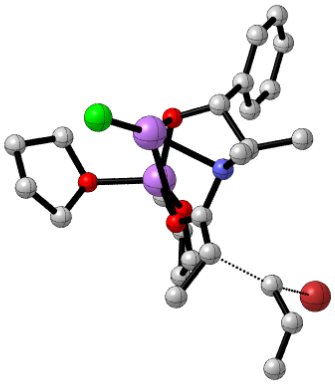
39b

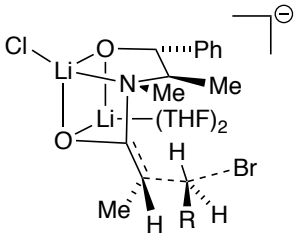
G = –1650.787232

G_{MP2} = –1646.253387

Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	H	2.80418600	-1.46814100	-1.78592900
O	-0.16198500	2.11898200	0.52263900	H	4.80044500	-2.50508600	-2.87564100
Li	0.43192200	2.07796100	-1.26732600	H	6.99499700	-1.32760900	-2.82072900
O	1.48106600	0.52047800	-1.12791700	H	7.17871200	0.86759900	-1.65743600
C	2.60773400	0.81630700	-0.39585100	H	5.19731500	1.85057100	-0.54433300
C	2.51745000	0.31751700	1.09595000	O	1.39753300	3.76447300	-1.85488700
N	1.15406300	0.55352600	1.64009400	C	1.87793300	4.66756300	-0.83152400
C	0.89838500	-0.14237600	2.89756500	C	3.34366100	4.94693800	-1.17989600
H	1.48003500	0.22980300	3.75888400	C	3.35518600	4.78986600	-2.70880200
H	-0.16335400	-0.05068000	3.14226500	C	2.37035000	3.63530200	-2.91236200
H	1.12677000	-1.20817400	2.76763000	H	2.86251500	2.65944400	-2.82267600
C	0.59690400	1.92372500	1.56743100	H	1.83913100	3.67540700	-3.86860700
C	0.84559400	2.81236300	2.57044800	H	4.34719300	4.56783000	-3.11508300
C	0.18605500	4.16096300	2.66536900	H	2.98385400	5.70321200	-3.19094600
H	-0.51626300	4.28968100	1.83551900	H	3.99157500	4.19311300	-0.71881200
H	-0.38045300	4.28446600	3.60385900	H	3.67312600	5.93460400	-0.84054000
H	0.90144900	5.00120500	2.63159100	H	1.27263000	5.58342100	-0.86894300
H	1.49028300	2.50697200	3.39051900	H	1.73745200	4.18869600	0.14062500
H	2.62159700	-0.77777900	1.06610900	O	-1.16837200	1.88746000	-2.44469000
C	3.64149900	0.88573400	1.97906900	C	-2.41623800	2.26243300	-1.80683600
H	3.58290500	0.49223500	3.00075700	C	-3.37791300	1.09706900	-2.05167000
H	4.62600100	0.62032300	1.58071100	C	-2.86503200	0.51727300	-3.37973700
H	3.56728800	1.97746600	2.03822700	C	-1.35236000	0.67685600	-3.22497400
H	2.78809100	1.91592500	-0.31880600	H	-0.82070100	0.81057100	-4.17324500
C	3.86952400	0.23521000	-1.06187300	H	-0.92298400	-0.16683300	-2.67612900
C	5.10784900	0.89051000	-1.05059800	H	-3.23539100	1.09907500	-4.23533400
C	6.22870500	0.33611700	-1.67668700	H	-3.14919400	-0.53007600	-3.51842600
C	6.12657800	-0.89224200	-2.33027100	H	-4.42315500	1.42408700	-2.09567400
C	4.89316100	-1.55153300	-2.35896700	H	-2.20618300	2.44069300	-0.74898100
C	3.77757700	-0.98921900	-1.73966600	H	-2.76946800	3.19358600	-2.27421500
H	-3.26357300	0.34558700	-1.26364100	Cl	-1.59642800	-1.58817400	-0.22086800

Table 40. Geometric coordinates and thermally corrected MP2 energies for transition state **42**





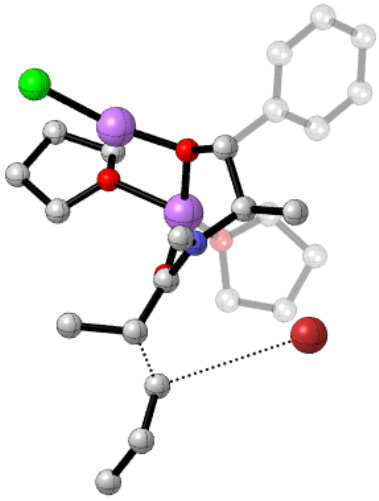
42

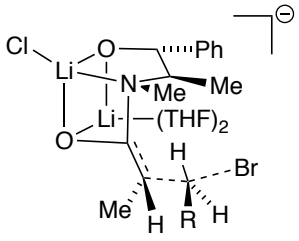
G = –4339.731431
G_{MP2} = –4333.059330

Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	C	-3.74353100	-2.69831600	0.84461200
Li	-1.15278100	1.13753500	2.12856700	H	-4.80407500	-2.99505300	0.86702400
O	-2.32206200	-0.19367800	1.43934000	H	-3.17013700	-3.59272000	0.55233800
C	-2.64340500	-0.49824700	0.23786800	H	-3.44197200	-2.43076000	1.86225300
N	-2.08865800	0.32922600	-0.79072000	H	-3.73137700	-1.72566000	-1.13850800
C	-2.18291600	1.81090500	-0.59686100	O	0.16248500	0.23682000	3.38323400
C	-0.74534100	2.38921700	-0.38266500	C	1.57559700	0.51009600	3.18102600
O	-0.12633300	1.73010500	0.67253900	C	2.31063600	-0.81545700	3.42653600
H	-0.20275400	2.21546200	-1.34049400	C	1.22025000	-1.86658100	3.15905600
C	-0.75708600	3.90721000	-0.18376000	C	-0.03461900	-1.16508800	3.67496900
C	-0.04359400	4.74736000	-1.04621400	H	-0.15219000	-1.28982000	4.76309000
C	-0.02104000	6.13223100	-0.85878900	H	-0.95520900	-1.47120200	3.17219000
C	-0.72513200	6.70497500	0.20008100	H	1.40691100	-2.81641300	3.67224500
C	-1.44624400	5.87908600	1.06780300	H	1.13984100	-2.05752900	2.08305900
C	-1.45870700	4.49689000	0.88051400	H	2.66385600	-0.87559000	4.46451800
H	-2.01991600	3.86643400	1.56495900	H	3.17227800	-0.93084200	2.76286100
H	-2.00715400	6.31596000	1.89174700	H	1.69362200	0.88233600	2.15955300
H	-0.71467600	7.78254300	0.34910600	H	1.87564700	1.29930900	3.88100200
H	0.54738300	6.76156000	-1.54083800	O	-2.25343800	2.25582800	3.40034500
H	0.50997500	4.30607100	-1.87295300	C	-3.47316400	1.66848800	3.93731900
H	-2.71895900	1.95142000	0.34641900	C	-3.66553600	2.28762000	5.33420500
C	-2.98712700	2.51185800	-1.70079000	C	-2.76489300	3.53492200	5.29468900
H	-2.45257900	2.52986900	-2.65787100	C	-1.61852300	3.05533700	4.40668900
H	-3.95725100	2.02814500	-1.86198600	H	-0.90009900	2.44327000	4.97246500
H	-3.17797400	3.54858100	-1.41006000	H	-1.07485900	3.85546900	3.89648100
C	-2.08024900	-0.16388400	-2.16629000	H	-2.42930800	3.86027400	6.28526800
H	-1.38097500	0.43651500	-2.75667300	H	-3.28611700	4.37093600	4.81387100
H	-1.71474200	-1.19279700	-2.17050900	H	-3.32167600	1.60102200	6.11753300

H	-3.06375400	-0.12905100	-2.66184900	H	-4.71564400	2.52329100	5.53047100
C	-3.50745200	-1.55181800	-0.09138200	H	-4.29105700	1.91147600	3.25371000
H	-3.35039600	0.58152600	3.96591900	H	-6.75880700	-1.90944100	1.95669200
Cl	1.25913300	-1.68433700	-0.62834900	C	-5.38539200	0.06945300	0.62436900
C	-6.46347100	-0.79002900	0.17522000	H	-4.87283800	-0.11270300	1.55447000
H	-6.81585400	-0.62271800	-0.84177400	H	-4.91886700	0.74372800	-0.06988700
C	-7.04957500	-1.74138100	0.92333900	Br	-6.55971600	1.99373500	1.57713100
H	-7.85805900	-2.35397400	0.53403000				

Table 41. Geometric coordinates and thermally corrected MP2 energies for optimized IRC of **42**





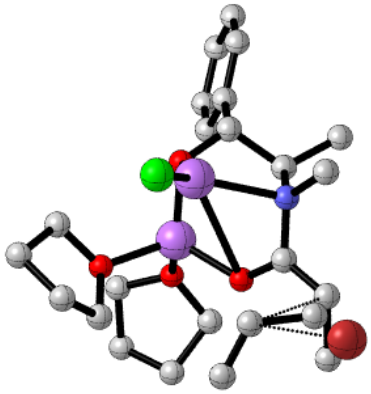
42

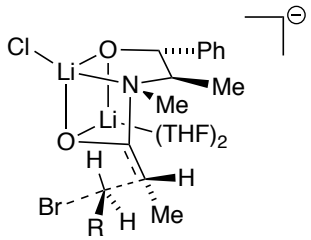
G = –4339.815795
G_{MP2} = –4333.161935

Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	C	3.28873700	-2.10970900	-2.69849000
Li	1.69750500	-1.50395100	1.54154700	H	2.33220700	-2.25628600	-3.20759300
O	3.41416700	-1.27400100	0.79661000	H	3.63657900	-1.10885900	-2.95791900
C	3.77650600	-1.46957300	-0.37757400	H	4.00171100	-2.85037700	-3.08375100
N	3.07074400	-2.22320200	-1.25933500	C	5.11776200	-0.86978900	-0.81364900
C	2.11686200	-3.27065600	-0.78996400	C	5.03217900	0.65987200	-0.93509700
C	0.65128800	-2.74614900	-0.78300200	H	6.01947000	1.08050400	-1.15485900
O	0.50595700	-1.71743300	0.13862900	H	4.34002400	0.97086400	-1.72736900
H	0.42849100	-2.39197300	-1.81208100	H	4.67808200	1.09064500	0.00773900
C	-0.36832200	-3.85267500	-0.48700200	H	5.41507200	-1.28750600	-1.78102300
C	-1.52367400	-3.97227800	-1.26739100	O	0.83117400	0.42362800	1.90838200
C	-2.50858100	-4.91740900	-0.96698700	C	-0.13542800	0.53449400	2.97023100
C	-2.34805700	-5.77140700	0.12395800	C	-0.58719000	1.99978200	2.93433100
C	-1.19547700	-5.66993300	0.90884200	C	0.64432900	2.75294800	2.36112300
C	-0.22036400	-4.71926800	0.60792500	C	1.62202300	1.63096400	1.96147700
H	0.67821500	-4.66439000	1.21699200	H	2.41855400	1.49127700	2.70549600
H	-1.05170500	-6.33900600	1.75460000	H	2.06753600	1.76290400	0.97469700
H	-3.10945600	-6.51156600	0.36005000	H	1.10036700	3.42795000	3.09342100
H	-3.40000700	-4.98531800	-1.58730500	H	0.35000100	3.32601600	1.47995300
H	-1.65654000	-3.30673800	-2.11827300	H	-0.88374500	2.35534300	3.92688600
H	2.43177200	-3.48571300	0.23606500	H	-1.43301700	2.11412800	2.25197500
C	2.35704500	-4.56794600	-1.57418300	H	-0.92550800	-0.19171500	2.76409700
H	2.08874500	-4.49131700	-2.63519900	H	0.35211000	0.27141800	3.91947300
H	3.40581500	-4.86011800	-1.46688900	O	1.92295400	-2.18778800	3.40087500
H	1.75354000	-5.36779000	-1.14037200	C	3.31261800	-2.36920200	3.83355900

C	3.34971400	-3.66625800	4.65179400
C	2.08355400	-4.40152100	4.18333900
C	1.11468600	-3.24754000	3.94555200
H	0.65282000	-2.90823900	4.88712300
H	0.32028500	-3.46279100	3.22487200
H	1.70405500	-5.12734300	4.91151400
H	2.31660200	-4.91202600	3.24235200
H	3.31459100	-3.46448800	5.73069700
H	4.25006900	-4.23700000	4.40952800
H	3.92138400	-2.46538600	2.93283100
H	3.60338600	-1.48275200	4.41026300
Cl	-0.77045600	1.86375000	-0.88139400
C	7.58515300	-1.08472300	-0.26189100
H	7.87037900	-1.64999400	-1.15279300
C	8.48980200	-0.27611300	0.29554100
H	9.49625000	-0.17524000	-0.10471500
H	8.26070500	0.30481500	1.18712600
C	6.18522500	-1.31178500	0.23017200
H	6.01286500	-0.76822600	1.16550600
H	6.02874200	-2.37842700	0.45851200
Br	4.63445700	-4.68445300	1.38612600

Table 42. Geometric coordinates and thermally corrected MP2 energies for transition state **42b**





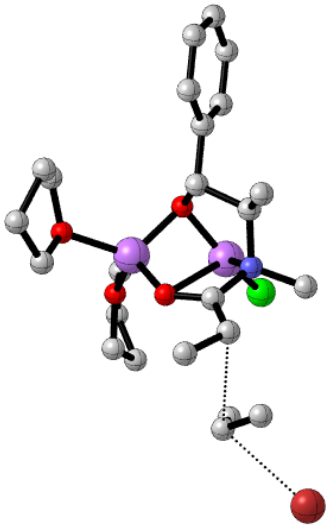
42b

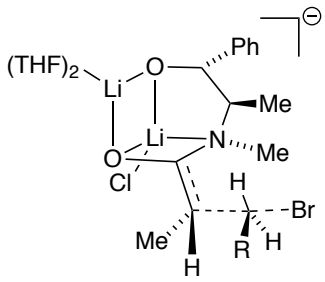
G = –4339.719461
G_{MP2} = –4333.047376

Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	C	-2.11853900	0.83619400	-4.65373800
Li	1.41660200	1.56683600	-1.61926100	H	-2.30693900	1.81892500	-4.20234800
O	-0.04979800	1.05383600	-2.75987400	H	-1.26421700	0.96304900	-5.33736000
C	-0.71078700	-0.03579300	-2.79672900	H	-2.99096000	0.57116000	-5.26335300
N	-0.20849600	-1.09800200	-1.96521400	H	-2.15040400	-1.22712200	-3.82512400
C	1.24279200	-1.41035600	-2.20447200	O	0.94602500	3.11641000	-0.42503500
C	2.04727900	-1.13789400	-0.88956000	C	1.28944300	3.07423200	0.98861300
O	1.79223400	0.15347900	-0.45756800	C	0.31208500	4.02604400	1.68123600
H	1.69446900	-1.89394200	-0.14972600	C	-0.92964900	3.92502000	0.78121700
C	3.54043000	-1.41396500	-1.08456500	C	-0.31003000	3.81526500	-0.61162400
C	4.13921200	-2.56866000	-0.56613200	H	-0.09516000	4.80584800	-1.04161300
C	5.50043700	-2.82511700	-0.74939400	H	-0.91161600	3.23954900	-1.31928800
C	6.29120800	-1.92305000	-1.46149400	H	-1.60091500	4.78588600	0.87103400
C	5.70739000	-0.76391800	-1.98091100	H	-1.48180800	3.01023300	1.02050600
C	4.34886300	-0.51023300	-1.79068800	H	0.70604200	5.05131100	1.69273600
H	3.90654400	0.40253600	-2.17995700	H	0.11081600	3.71978700	2.71173800
H	6.31695100	-0.05099400	-2.53307900	H	1.17558200	2.04544100	1.33886400
H	7.35220100	-2.11583000	-1.60471400	H	2.33950000	3.37088800	1.08632400
H	5.94282900	-3.72611500	-0.32926400	O	2.69504800	2.47054700	-2.97009600
H	3.53009500	-3.27240500	-0.00178300	C	2.17505700	2.64186400	-4.30598100
H	1.58994500	-0.65916300	-2.92029100	C	2.00287100	4.15082300	-4.45766000
C	1.46835700	-2.79032800	-2.83691500	C	3.23389400	4.68422100	-3.70511400
H	1.24735100	-3.61227300	-2.14645300	C	3.41238700	3.65979300	-2.56791400
H	0.84835500	-2.92078000	-3.73131600	H	2.96866000	3.99784300	-1.62710400
H	2.51631700	-2.88729700	-3.13531600	H	4.46350500	3.40113800	-2.39458100
C	-1.08278100	-2.24164900	-1.70268800	H	3.10086300	5.70239000	-3.32608300
H	-0.63698400	-2.85944200	-0.91721000	H	4.10965200	4.68516800	-4.36532600

H	-2.04002600	-1.87846400	-1.32779500
H	-1.26552500	-2.88030900	-2.58058600
C	-1.85992700	-0.20642600	-3.59403700
H	1.24727900	2.06975500	-4.35627000
Cl	-1.46500600	0.29346600	1.58701200
C	-3.62041100	1.15652000	-1.57318000
H	-3.22233200	0.91545700	-0.58816300
C	-3.80443900	2.44271300	-1.92072100
H	-3.57436900	3.25023900	-1.23133800
H	1.07754500	4.46970900	-3.96462400
H	1.96413300	4.47170800	-5.50369100
H	2.90158800	2.24819200	-5.03320200
H	-4.24291100	2.72116100	-2.87601300
C	-3.91565300	0.03347300	-2.44272700
H	-4.29434100	0.18618500	-3.43863300
H	-3.81609800	-0.97604100	-2.09002500
Br	-6.40176300	-0.38270000	-1.89833600

Table 43. Geometric coordinates and thermally corrected MP2 energies for transition state **42c**.





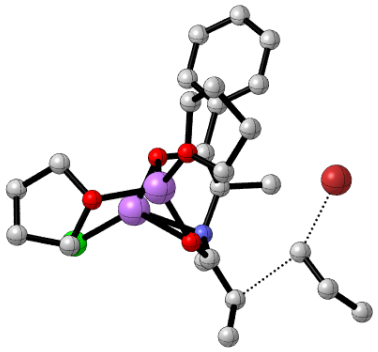
42c

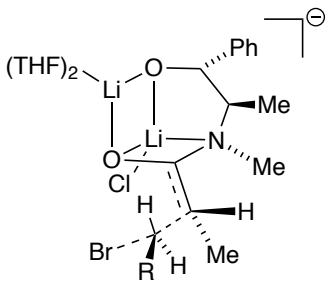
G = –4339.719435
G_{MP2} = –4333.046849

Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	C	5.28418000	-3.31831200	0.90446700
O	-0.58288800	-0.91051100	2.79159400	C	5.77257800	-2.76213800	-0.27824000
Li	0.80166800	0.37790800	2.49746800	C	4.99264700	-1.83104400	-0.97082600
O	1.58970200	-0.26868800	0.93205600	C	3.73756600	-1.46278700	-0.48684200
C	1.83812900	-1.60058900	1.19635500	H	3.14061300	-0.71276500	-0.99690600
C	0.73839400	-2.53563600	0.57569400	H	5.36947900	-1.38307600	-1.88799800
N	-0.63459100	-1.93846800	0.70837700	H	6.75451900	-3.04333000	-0.65256700
C	-1.56967800	-2.51702400	-0.26388200	H	5.88576400	-4.03436600	1.46099500
H	-1.79201800	-3.58406900	-0.10485400	H	3.65127200	-3.38671000	2.30669000
H	-2.50499100	-1.95894700	-0.23984900	O	1.86044100	0.45742800	4.22503300
H	-1.14324000	-2.40097100	-1.26537100	C	1.17471800	-0.02532100	5.40780200
C	-1.12125300	-1.81418000	2.08054000	C	2.21521200	-0.82023100	6.21526800
C	-2.14212100	-2.65246700	2.56128900	C	3.26868300	-1.18279400	5.15516800
C	-2.36171800	-2.71116900	4.05587600	C	3.23914800	0.04846700	4.25042000
H	-2.52368200	-1.71187100	4.47498700	H	3.54551000	-0.14224000	3.21916700
H	-3.23212100	-3.32922500	4.30881100	H	3.85566000	0.86158300	4.66320000
H	-1.49718200	-3.13890200	4.58996700	H	2.95659600	-2.06736500	4.58917900
H	-2.33795900	-3.56598700	2.00695500	H	4.26039400	-1.37531600	5.57721700
H	0.92091500	-2.54710500	-0.50785900	H	1.77647300	-1.69671100	6.70199100
C	0.81505500	-3.97959700	1.09515000	H	2.66324000	-0.19266400	6.99547800
H	1.78660600	-4.42228800	0.85517500	H	0.78174200	0.83583700	5.96018100
H	0.68150200	-4.01394800	2.18273300	H	0.33882800	-0.64054900	5.06316100
H	0.04196700	-4.61162000	0.64503900	O	0.19952100	2.23263900	2.15226800
H	1.83087400	-1.81811100	2.28757400	C	-1.11691000	2.73559800	2.45826900

C	3.22627600	-2.02729500	0.69031700
C	4.02262000	-2.95027100	1.38081100
H	-1.78338700	1.87504900	2.55139400
H	-1.08204500	3.27152400	3.41981800
Cl	-0.95126800	1.22825900	-1.55961000
C	-4.24317000	-0.44756800	2.21072500
H	-4.45845600	-0.13161100	3.22983600
C	-3.94455800	0.47694300	1.28266200
H	-3.72724400	0.22317400	0.24850600
H	-3.92406100	1.53424400	1.52863900
C	-4.32731100	-1.87459200	1.96158800
H	-4.55320800	-2.56334500	2.75206200
C	-1.46353700	3.67264600	1.30330600
C	-0.09227200	4.28466900	0.97387800
C	0.85726200	3.10031200	1.19007000
H	1.83011500	3.39040600	1.60205800
H	1.00415200	2.53181300	0.26821900
H	0.14278000	5.10599700	1.66368500
H	-0.03566900	4.66454900	-0.05011300
H	-2.21633800	4.41897700	1.57957000
H	-1.82163300	3.09278600	0.44635400
H	-4.22482900	-2.26489500	0.96311100
Br	-6.86854000	-2.06110900	1.66613600

Table 44. Geometric coordinates and thermally corrected MP2 energies for transition state **42d**.





42d

G = –4339.72642
G_{MP2} = –4333.055324

Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	H	1.57798400	5.69801800	-1.46901200
O	1.84984500	-1.20338200	1.60047900	H	3.92068000	6.41989900	-1.03033900
Li	1.19452800	0.40630500	2.33473500	H	5.51467000	4.83250600	0.03870500
O	0.97948100	1.39432300	0.74202200	H	4.77830100	2.54204200	0.64049300
C	2.28862600	1.39820700	0.28287200	O	2.34337700	1.20423700	3.79012700
C	2.46508100	0.44702400	-0.94632400	C	3.40606800	0.50376800	4.48240800
N	1.84728000	-0.90257400	-0.70833300	C	4.35762700	1.58465100	5.01507100
C	1.62615100	-1.64233500	-1.95277800	C	3.47208100	2.84086400	5.05245500
H	2.54896800	-1.99254900	-2.44297700	C	2.57858200	2.62503000	3.83212400
H	0.98980800	-2.50551400	-1.74953800	H	3.07551200	2.94480400	2.90850700
H	1.09603100	-0.99080700	-2.65626200	H	1.60474900	3.11907000	3.89403400
C	2.15739500	-1.69590300	0.46357900	H	4.04301500	3.77323800	4.99158100
C	2.76593300	-2.95148800	0.32642200	H	2.86842500	2.86655800	5.96888700
C	2.61228800	-4.02112600	1.37555000	H	5.18512800	1.70625300	4.30830800
H	2.46071600	-3.57572400	2.36371300	H	4.77752600	1.32342300	5.99209300
H	1.74306100	-4.67043600	1.17563700	H	2.94338800	-0.08793100	5.28207700
H	3.49325800	-4.67489000	1.42300900	H	3.91444500	-0.16029200	3.78005400
H	3.02817500	-3.29132200	-0.67088800	O	-0.63109600	0.22370900	3.16025800
H	1.84269700	0.87635200	-1.74557600	C	-1.40824300	-0.99839100	3.18550000
C	3.91592300	0.38508900	-1.46267200	C	-2.85167600	-0.55600400	3.42924800
H	4.06383200	-0.45441400	-2.15135800	C	-2.89246300	0.79288700	2.69228800
H	4.16024700	1.30257100	-2.00750000	C	-1.50353400	1.36679200	2.98442200
H	4.63769600	0.29782500	-0.64482100	H	-1.48934500	1.95256900	3.91523100
H	3.00314400	1.03402200	1.04829600	H	-1.09676600	1.97335100	2.17045000
C	2.76527000	2.81044100	-0.08654800	H	-3.69540200	1.45301200	3.03897300
C	4.07903100	3.23112200	0.16895500	H	-3.00580400	0.61732100	1.61774200
C	4.49257800	4.52266200	-0.17019100	H	-3.04268500	-0.42467000	4.50298700
C	3.59935600	5.41389100	-0.76767800	H	-3.57246300	-1.27728900	3.03248100
C	2.28506600	5.00637700	-1.01446300	H	-1.31121100	-1.50160800	2.21783900

C	1.87214300	3.71888600	-0.66983300	H	-0.99835200	-1.63624100	3.97523300
H	0.84434400	3.40238200	-0.82180700	Cl	-1.99370100	-0.76827600	-0.58179500
C	5.66553100	-2.96661200	1.67504700	C	4.92129900	-1.81683200	1.19291400
H	5.52329400	-3.22562800	2.72273400	H	5.03970200	-1.50850600	0.16923900
C	6.49107300	-3.71090400	0.92151600	H	4.11017600	-1.40697200	1.76577800
H	6.66457300	-3.48071200	-0.12712000	Br	6.26450100	0.08689300	1.98798600
H	7.02040300	-4.56727200	1.32993400				

Scheme 3. Mechanism of alkylation of dilithiated monomers.

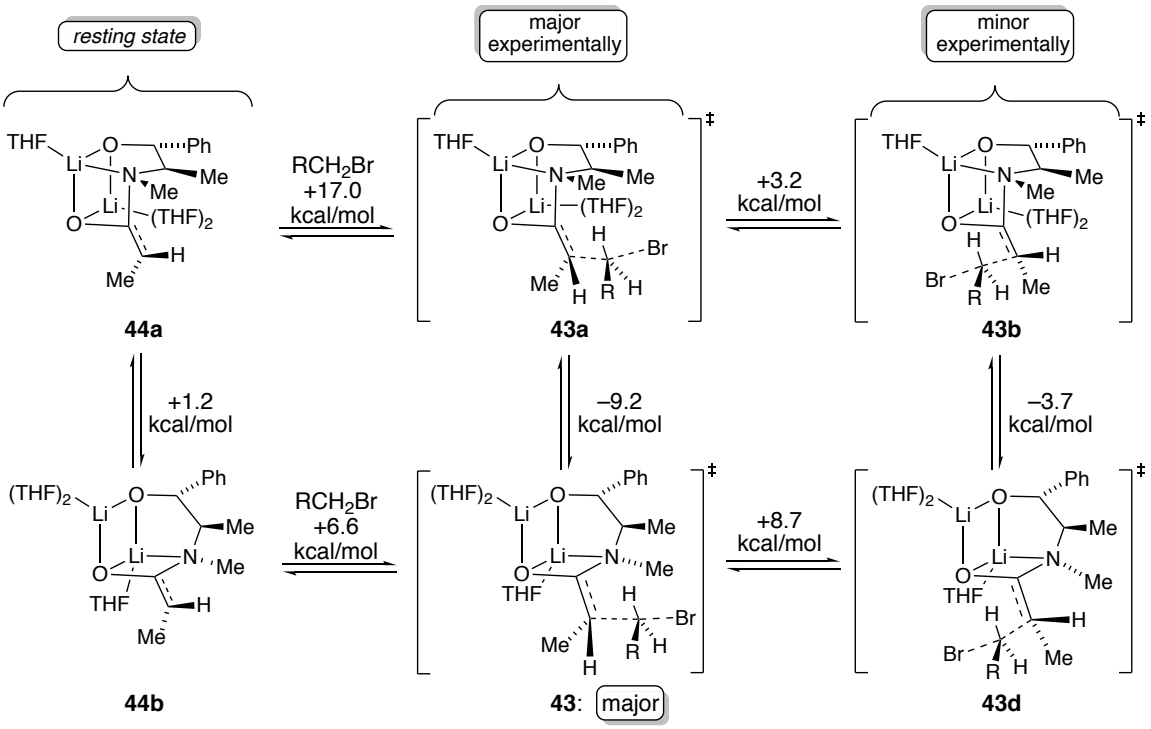
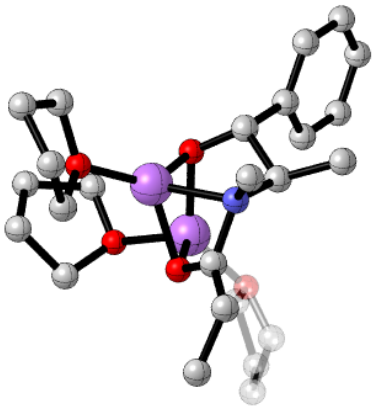
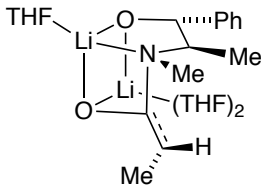


Table 45. Geometric coordinates and thermally corrected MP2 energies for **44a**





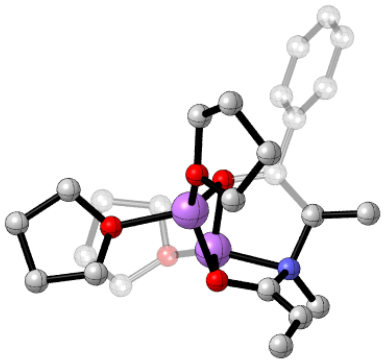
44a

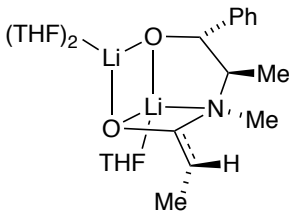
G = –1422.828600
G_{MP2} = –1418.117728

Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	C	5.86194000	-1.50034100	0.56198700
O	0.54092900	1.48862200	-1.16188200	C	4.57785200	-1.06299200	0.23767800
Li	1.98514400	1.36235500	0.10000100	H	4.40790300	-0.01497800	0.00580800
O	1.66685600	-0.43555000	0.67742500	H	6.68641300	-0.79057300	0.57781600
C	2.08660800	-1.48107400	-0.14354900	H	7.09500300	-3.18303300	1.12656900
C	1.96007100	-1.05191300	-1.64738300	H	5.19498600	-4.79175200	1.08732800
N	0.52520500	-0.69052100	-1.92581700	H	2.91959000	-4.00886700	0.50246900
C	-0.25050700	-1.66575600	-2.68296100	O	1.58259600	2.47986400	1.71892200
H	-0.18210100	-2.64663100	-2.19911000	C	1.65801600	1.77027200	2.98822500
H	-1.29800700	-1.35164300	-2.68694200	C	0.36724900	2.11644500	3.75267700
H	0.06167200	-1.78721000	-3.73203900	C	-0.57471200	2.62327500	2.64543800
C	0.28573700	0.72299200	-2.20901300	C	0.40136600	3.30464900	1.68822300
C	-0.23679300	1.13135100	-3.39466100	H	0.65351500	4.32002500	2.02978400
C	-0.63681300	2.55368800	-3.67597200	H	0.06164300	3.34200600	0.65023800
H	-0.56133700	3.15606100	-2.76528200	H	-1.34561600	3.30573000	3.01805500
H	-0.00142900	3.02873200	-4.44053700	H	-1.06843800	1.78514600	2.14086800
H	-1.67012100	2.63065900	-4.04880700	H	0.55102700	2.91005700	4.48641000
H	-0.35709100	0.40796500	-4.19602700	H	-0.03382300	1.25194200	4.29015900
H	2.53139900	-0.12195500	-1.74734000	H	1.74845700	0.70837800	2.74368500
C	2.55261800	-2.04721600	-2.65392100	H	2.55829000	2.10121300	3.51869400
H	2.11969500	-3.04946800	-2.55833000	O	3.59669900	2.29881900	-0.68654700
H	2.40372300	-1.70600300	-3.68442300	C	3.44299400	2.83069600	-2.02443400
H	3.62848300	-2.14125400	-2.48317500	C	3.73631400	4.32180500	-1.88464500
H	1.42663400	-2.37113300	-0.03460700	C	4.85610900	4.32429900	-0.83106600
C	3.49753900	-1.95880600	0.20493200	C	4.44963900	3.16833200	0.09684100
C	3.74657900	-3.30109700	0.51366600	H	3.86639300	3.50867400	0.95838600
C	5.02980000	-3.74445100	0.84460300	H	5.30699900	2.58926900	0.45713300
C	6.09459500	-2.84421200	0.86870600	H	4.94459100	5.27349900	-0.29392800

H	5.82204800	4.11591300	-1.30571100	C	-2.36981000	-1.32319500	1.26729100
H	2.84954300	4.84628000	-1.50971000	H	-1.80482200	-2.20411400	0.93906000
H	4.03332300	4.78395000	-2.83101900	H	-2.19053200	-1.17228200	2.33587900
H	4.16745100	2.34162400	-2.69086700	H	-4.21321100	-2.46065400	0.91846800
H	2.42814700	2.59455000	-2.34804800	H	-4.46417300	-0.84642300	1.60464000
O	-1.86636400	-0.16749100	0.55214100	H	-3.56804500	-1.50784000	-1.25549100
C	-2.87665900	0.34104300	-0.35933500	H	-4.88792500	-0.42483900	-0.77540300
C	-3.89516800	-0.78898300	-0.49500800	H	-3.32545100	1.23889400	0.08489000
C	-3.85452700	-1.42739400	0.90276700	H	-2.37775000	0.61457500	-1.29307900

Table 46. Geometric coordinates and thermally corrected MP2 energies for **44b**





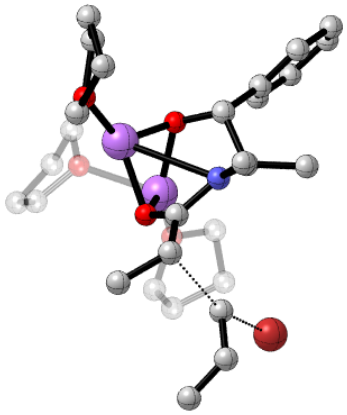
44b

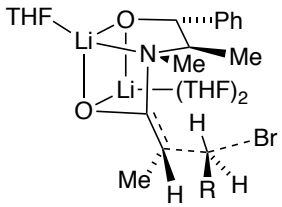
G = –1422.826052
G_{MP2} = –1418.115801

Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	C	3.41594000	-1.45334400	-2.31217400
O	0.05237800	1.89159300	0.53812800	H	2.47731600	-1.96645400	-2.12653700
Li	0.46185400	1.93470900	-1.32985200	H	4.21855200	-3.01749400	-3.55484100
O	1.25203600	0.20791700	-1.38718300	H	6.34063200	-1.80524500	-4.02609500
C	2.51672900	0.42842900	-0.85630800	H	6.70825300	0.45141500	-3.03983700
C	2.66051800	-0.08853300	0.62140900	H	4.97990100	1.46704900	-1.58933800
N	1.43890100	0.23915500	1.41838500	O	1.42985300	3.50685000	-2.10373400
C	1.40361000	-0.43158000	2.71804100	C	2.02911700	4.45362800	-1.18102200
H	2.16693800	-0.08783900	3.43292000	C	3.45335800	4.67785700	-1.69063500
H	0.42340100	-0.27010400	3.17704400	C	3.29195300	4.48762200	-3.20734500
H	1.54639600	-1.51016500	2.56930500	C	2.26057900	3.35886300	-3.28191900
C	0.98255500	1.64865700	1.44365400	H	2.73248000	2.37035300	-3.25340600
C	1.45514700	2.51600200	2.37232700	H	1.61512300	3.41655400	-4.16417100
C	0.92636600	3.91076000	2.56484700	H	4.22656900	4.22742600	-3.71288200
H	0.53081700	4.06298200	3.58120800	H	2.89848700	5.40182600	-3.66803700
H	1.69851000	4.68312400	2.42027500	H	4.12737000	3.91747500	-1.28030300
H	0.11470000	4.11135800	1.85882600	H	3.84363600	5.66252700	-1.41621900
H	2.21993800	2.17168800	3.06314400	H	1.44075600	5.38010900	-1.20492700
H	2.67306000	-1.18790200	0.57169300	H	1.97853400	4.02380600	-0.17780900
C	3.96818600	0.38318500	1.27618600	O	-1.42767200	2.14023700	-2.04824800
H	4.08170000	-0.02232500	2.28747000	C	-2.17786300	3.14714400	-1.34407300
H	4.83389000	0.05511100	0.69332600	C	-3.57623400	3.08178900	-1.97174100
H	3.99052800	1.47610600	1.34943500	C	-3.29936600	2.61979000	-3.43008700
H	2.75374200	1.51577400	-0.79991300	C	-1.79299100	2.27029300	-3.42782600
C	3.61144500	-0.18949400	-1.73847100	H	-1.20086200	3.07516000	-3.88762600
C	4.80865600	0.48134500	-2.01911700	H	-1.54671900	1.32744400	-3.92186700
C	5.78828300	-0.09171300	-2.83535000	H	-3.51861200	3.40396500	-4.16097000
C	5.58325500	-1.35527200	-3.38899500	H	-3.91058700	1.75067000	-3.69073300
C	4.39051900	-2.03416700	-3.12245600	H	-4.09248400	4.04521000	-1.92376000

H	-4.19513600	2.34792000	-1.44543300	H	-0.08859900	-1.73459900	-1.94329800
H	-2.11575500	2.90490800	-0.28324500	H	-0.81572000	-3.17929500	-1.16856400
H	-1.71042800	4.12913200	-1.51378000	H	-2.15550400	-1.23040800	-3.11454900
O	-1.37933900	-1.33555500	-0.39114700	H	-2.27380300	-3.00061200	-3.10953500
C	-2.80053300	-1.07110200	-0.40700200	H	-4.29118400	-1.57997700	-1.93596500
C	-3.38311100	-1.99110000	-1.48421600	H	-3.62992900	-2.97145900	-1.05987000
C	-2.21010400	-2.11538400	-2.46955300	H	-3.19840800	-1.26118000	0.59445500
C	-1.00634400	-2.16001400	-1.52956900	H	-2.95179100	-0.01345500	-0.65578100

Table 47. Geometric coordinates and thermally corrected MP2 energies for transition state **43a**





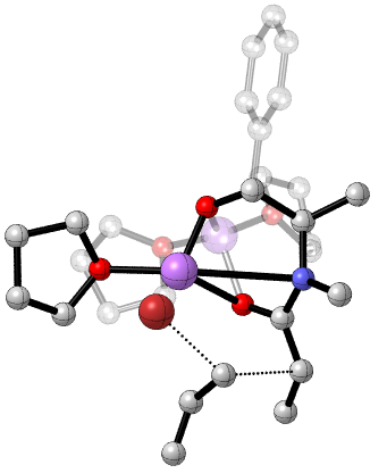
43a

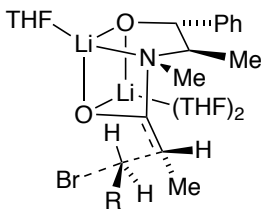
G = –4111.759145
G_{MP2} = –4104.911189

Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	H	-1.05720800	1.92097800	-4.70883700
O	-1.77734600	-0.68175500	-0.56799000	H	-2.68086900	1.25873100	-4.41780000
Li	-1.97546800	1.09347500	0.16079400	H	-2.25690700	2.87010300	-3.83403000
O	-0.31685000	1.74524800	-0.53135300	H	0.66539600	1.62985900	-2.35257900
C	-0.26354100	2.03028700	-1.88692800	C	-0.24350500	3.53734700	-2.16748700
C	-1.43764100	1.27823100	-2.62802700	C	0.45270800	4.05965800	-3.26590400
N	-1.14385900	-0.17999400	-2.72691000	C	0.46661800	5.43019700	-3.52997700
C	-0.57430400	-0.66896300	-3.97341500	C	-0.21737300	6.31099800	-2.69012600
H	0.19534400	0.02753100	-4.32196900	C	-0.90021100	5.80687500	-1.58132800
H	-0.09797000	-1.63665500	-3.79877100	C	-0.90449500	4.43550500	-1.32104600
H	-1.30780300	-0.79292500	-4.78473500	H	-1.40088700	4.04642100	-0.43830800
C	-1.66994900	-1.08516200	-1.79721600	H	-1.42340600	6.48589600	-0.91161100
C	-2.11616300	-2.35200500	-2.20704700	H	-0.20819700	7.37932400	-2.89083500
C	-2.32759200	-3.48151200	-1.24288700	H	1.01754100	5.81072900	-4.38696900
H	-2.33361900	-3.11340700	-0.21251500	H	1.00051300	3.38351100	-3.92044100
H	-3.28442100	-3.99381200	-1.42648800	O	-0.75061100	0.42403500	1.86511600
H	-1.54439100	-4.25266300	-1.32212800	C	-1.24740500	-0.53314200	2.82796100
H	-2.02848500	-2.61533200	-3.25611300	C	-1.59098800	0.27453500	4.10425400
H	-4.13926100	-1.11969200	-1.25298500	C	-1.19865600	1.72911300	3.74821700
C	-4.32806300	-1.22975300	-2.30757300	C	-0.20612600	1.54030300	2.60345000
C	-5.13193500	-2.32090500	-2.81074500	H	0.79480500	1.27384600	2.97522000
C	-5.72003000	-3.24689800	-2.03188400	H	-0.12300000	2.36676700	1.89674900
H	-5.65466400	-3.20094700	-0.94792800	H	-0.76785400	2.27167500	4.59493800
H	-6.31290200	-4.05322000	-2.45349700	H	-2.07001500	2.28523600	3.38864700
H	-5.25243100	-2.37733000	-3.89116800	H	-1.01035500	-0.09349400	4.95603500
H	-3.83821300	-0.56041300	-2.98856100	H	-2.64873500	0.19196200	4.36949800
H	-2.31630000	1.36959400	-1.97821500	H	-2.10078900	-1.03172600	2.36443800

C	-1.87380800	1.85778900	-3.98248300
O	-3.59979200	1.91613700	0.85438700
C	-4.71766500	1.12034800	1.33769100
C	-5.76969100	2.14118100	1.75756700
C	-5.59659800	3.21802700	0.67397700
C	-4.08195900	3.22733700	0.44112400
H	-3.56875700	3.97473500	1.05867100
H	-3.81243700	3.38535800	-0.60655900
H	-5.97266300	4.20067400	0.97501800
H	-6.10710200	2.90012500	-0.23951900
H	-5.55155500	2.54195300	2.75578100
H	-6.77528400	1.71093500	1.76725400
H	-5.08984500	0.49985000	0.51627900
H	-4.34408100	0.49574600	2.15516400
O	1.67443000	-0.98202600	-0.11853600
H	-0.46688500	-1.28016300	3.01985400
C	1.79834200	-2.27219900	-0.76179000
C	2.87550500	-2.07896900	-1.82641300
C	3.83417900	-1.09858900	-1.13092700
C	2.88073900	-0.19816400	-0.33338000
H	2.59469300	0.70559900	-0.88148700
H	3.28162500	0.09488400	0.64180800
H	4.44987900	-0.52787900	-1.83191800
H	4.50666300	-1.64059400	-0.45611700
H	2.44243500	-1.62418500	-2.72463700
H	3.35468700	-3.01932900	-2.11432800
H	2.10005900	-3.01745800	-0.01334100
H	0.81565100	-2.54142900	-1.15771100
Br	-5.98063800	0.68932800	-2.12880400

Table 48. Geometric coordinates and thermally corrected MP2 energies for transition state **43b**





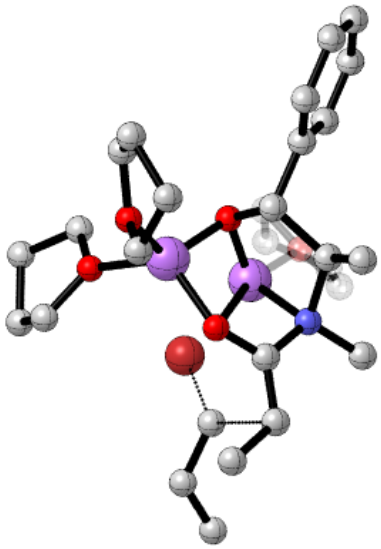
43b

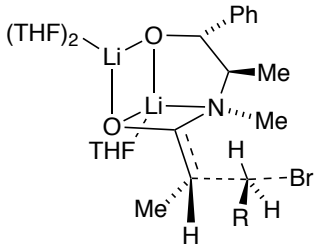
G = –4111.754234
G_{MP2} = –4104.906017

Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	H	1.21578200	2.30197400	4.43436100
Li	-2.20144400	1.35506900	0.09257700	H	-0.44204900	0.21646700	4.74927000
O	-1.04230700	1.33406200	1.67845300	O	-1.79761200	3.03012400	-0.96197800
C	-1.02192300	0.55066000	2.70795700	C	-1.41278700	3.15763800	-2.35189700
N	-1.58284700	-0.73185500	2.55461100	C	-0.82213800	4.56373400	-2.48914400
C	-2.75922500	-0.93152300	1.65673500	C	-0.22147600	4.79621700	-1.09350200
C	-2.31765700	-1.41466800	0.21919100	C	-1.25557200	4.12615100	-0.18825100
O	-1.71501100	-0.36600400	-0.46512800	H	-2.07213100	4.81884900	0.06101700
H	-1.60490400	-2.24696600	0.39471300	H	-0.84697900	3.70796500	0.73472700
C	-3.48378500	-2.01567400	-0.57413100	H	-0.07755300	5.85395500	-0.85296100
C	-3.72711300	-3.39529500	-0.56820400	H	0.74700000	4.29085700	-1.00549900
C	-4.79356800	-3.94638500	-1.28197900	H	-1.61025500	5.29881400	-2.69226200
C	-5.64006600	-3.12096100	-2.02331100	H	-0.08483600	4.62779700	-3.29506700
C	-5.40007700	-1.74486300	-2.05233900	H	-0.67290200	2.38250900	-2.56790700
C	-4.32918700	-1.20245700	-1.34095200	H	-2.30195400	2.99462100	-2.96907200
H	-4.12104400	-0.13799300	-1.39447200	O	-4.03725700	2.11219600	0.74297400
H	-6.04320200	-1.09483300	-2.64212000	C	-4.17221500	2.66205400	2.07473200
H	-6.46908100	-3.54586600	-2.58383800	C	-4.99494800	3.93822600	1.90258500
H	-4.95646400	-5.02157500	-1.26666300	C	-5.92908800	3.55451600	0.74423100
H	-3.06352600	-4.04904300	-0.00514600	C	-5.01069300	2.70740000	-0.14353900
H	-3.20218600	0.05580300	1.51271800	H	-4.47145200	3.31984800	-0.87634200
C	-3.85087900	-1.77857900	2.33199400	H	-5.53617400	1.90517100	-0.67092300
H	-3.59395400	-2.84007200	2.40599200	H	-6.34219600	4.41736700	0.21317400
H	-4.06746300	-1.40767800	3.34037700	H	-6.76640500	2.95250500	1.11572700
H	-4.76919800	-1.71410500	1.74314100	H	-4.34778100	4.77487200	1.61229800
C	-1.31296100	-1.76419800	3.54699200	H	-5.52768300	4.22054500	2.81554300

H	-1.51621300	-2.74498700	3.11241900
H	-0.25860800	-1.74509100	3.83087300
H	-1.90962300	-1.66241700	4.46670300
C	-0.34315200	0.87951700	3.89673700
C	0.14173500	2.26793900	4.18849300
H	-0.01656300	2.92342900	3.32728300
H	-0.38992900	2.70501200	5.04766500
H	2.12284600	2.47748500	-1.91239100
H	2.65080500	1.34175200	-0.63989800
H	3.78664600	1.24431600	-3.16502300
H	3.47360900	-0.23911300	-2.23469800
H	1.64153200	1.01840700	-4.35361400
H	2.17839700	-0.67035100	-4.27142000
H	0.80750100	-1.11901900	-2.31815700
H	-0.25129700	0.04410100	-3.14786800
C	2.19427000	0.94318400	2.24187700
H	-4.69482400	1.93338000	2.70918100
H	-3.16675600	2.81634900	2.47175300
O	0.89137500	0.83851200	-1.61847800
C	0.74284000	-0.10293000	-2.72070700
C	1.90116800	0.20040400	-3.66961600
C	3.00650900	0.63693300	-2.69530200
C	2.21906700	1.41644100	-1.64100600
H	1.54031500	1.59697700	1.67021400
C	3.37940600	1.40722200	2.69063100
H	3.70724500	2.42199900	2.48686300
H	4.05610000	0.77904500	3.26500700
C	1.70244600	-0.37555100	2.51453000
H	2.27312900	-1.02209500	3.17446900
H	0.71795000	-0.70042300	2.26999100
Br	2.08848700	-1.63707400	0.33823400

Table 49. Geometric coordinates and thermally corrected MP2 energies for transition state **43**





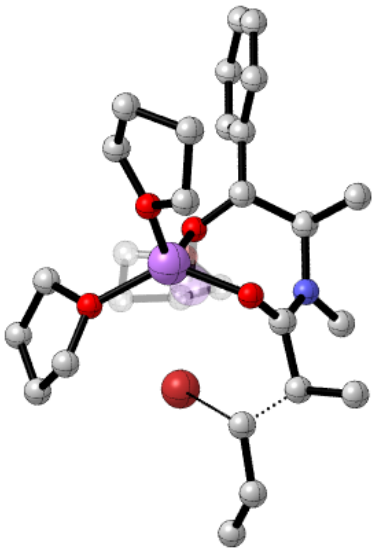
43

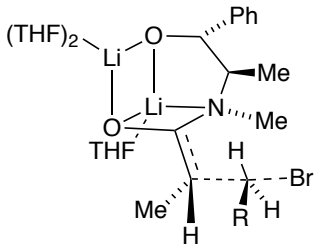
G = –4111.771181
G_{MP2} = –4104.925884

Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	C	-3.69385700	0.72225300	0.07566000
O	-1.14388800	-2.71875100	1.19760500	C	-5.06500200	0.44441900	0.11756000
Li	-1.58037700	-2.34050600	-0.61973300	C	-6.01431700	1.42037000	-0.20184800
O	-1.67310800	-0.45652200	-0.57072400	C	-5.60093100	2.69979600	-0.57001300
C	-2.64849300	-0.35221800	0.41205400	C	-4.23404900	2.99240000	-0.61490100
C	-2.06370700	-0.05725100	1.84397000	C	-3.29342500	2.01385900	-0.29804000
N	-0.68130200	-0.61205500	2.06482600	H	-2.23175900	2.23995200	-0.33943300
C	0.00393600	0.14033900	3.12496100	H	-3.90326900	3.98848300	-0.90140400
H	-0.38978500	-0.05822800	4.13282200	H	-6.33376900	3.46253600	-0.82134700
H	1.07180300	-0.09423600	3.13559900	H	-7.07409100	1.17844300	-0.16442100
H	-0.10337800	1.20982800	2.92192400	H	-5.39626000	-0.55197200	0.40563600
C	-0.58367800	-2.06503700	2.14568100	O	-3.19119600	-3.54803900	-0.94263800
C	0.20574200	-2.66607700	3.12205000	C	-3.59655700	-4.46593800	0.09426400
C	0.30987400	-4.16119800	3.23713800	C	-5.06815400	-4.14527400	0.34411700
H	1.31195400	-4.47402100	3.56138000	C	-5.56348200	-3.81371200	-1.07456800
H	-0.40100600	-4.57661300	3.97072000	C	-4.33972300	-3.13744200	-1.71871400
H	0.09212800	-4.63963200	2.27723600	H	-4.39637000	-2.04454600	-1.67605400
H	0.57224400	-2.08596600	3.96104100	H	-4.19173500	-3.43933200	-2.76171300
H	-1.91756300	1.02826100	1.89681000	H	-6.44514600	-3.16589600	-1.08398700
C	-3.04482900	-0.47035800	2.94919300	H	-5.82043900	-4.73528100	-1.60985900
H	-2.68491000	-0.18907300	3.94512800	H	-5.15594600	-3.27192400	1.00074500
H	-4.01360400	0.01641200	2.79615000	H	-5.61096300	-4.97629700	0.80530300
H	-3.20013300	-1.55475900	2.93726100	H	-3.47103500	-5.49837500	-0.26493000

H	-3.21730300	-1.29786000	0.51464600
C	0.76319100	-2.66181800	-4.22705700
C	-0.25048800	-1.96960400	-3.30568500
H	-1.21695900	-1.78480400	-3.78519800
H	0.13224600	-1.02417800	-2.91101600
H	0.24982900	-3.24727200	-4.99934400
H	1.41929200	-1.94355300	-4.72790200
H	1.99768100	-4.43766000	-3.75821200
H	2.27094300	-3.02312700	-2.70642400
H	0.74142300	-4.28884900	-1.30950600
H	-0.18159200	-4.86060600	-2.72198100
O	0.39221900	1.98426700	-0.19018600
C	0.47102200	2.38635800	-1.57862400
C	1.87537700	2.95868600	-1.74814000
C	2.10369700	3.64159400	-0.39002100
C	1.38627300	2.69686500	0.58518800
H	0.87759300	3.22847600	1.39664500
H	2.07031600	1.95827600	1.01814200
H	1.63802200	4.63391600	-0.37736700
H	-2.93481300	-4.29182500	0.94465200
H	3.16233700	3.76238000	-0.14256600
H	1.94968000	3.64728800	-2.59543500
H	2.59204500	2.14339000	-1.88963700
H	0.26838200	1.50550300	-2.19305400
H	-0.30548500	3.13742100	-1.77695200
C	4.28734000	-2.68726500	2.17731700
H	5.13527800	-3.35591900	2.29142900
H	4.29108500	-1.78303500	2.78158000
C	3.27617500	-2.96412000	1.33677300
H	3.30576100	-3.87534300	0.74234000
C	2.11173300	-2.11562100	1.17558700
H	1.21044500	-2.53355900	0.76050900
H	2.02598600	-1.24194700	1.79601500
Br	2.40628600	-0.75340700	-0.76944100
O	-0.45469400	-2.86732000	-2.18906800
C	0.39726000	-4.01975500	-2.31264000
C	1.51627500	-3.59013300	-3.26013700

Table 50. Geometric coordinates and thermally corrected MP2 energies for optimized IRC of **43**





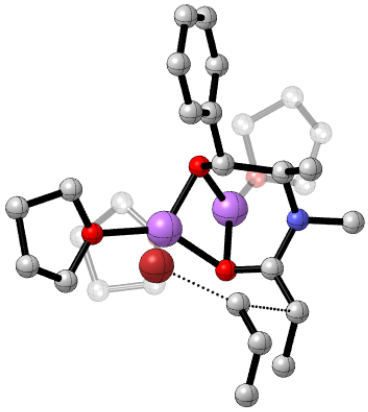
43

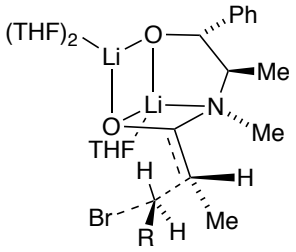
G = – 4111.876312
G_{MP2} = –4105.048570

Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	C	-4.99025600	-0.78401900	0.80968600
O	-0.74090000	-3.52979800	0.94326700	C	-6.08085700	0.08902200	0.76138300
Li	-1.09437500	-2.68647900	-0.81803000	C	-5.86852800	1.46116000	0.63188900
O	-1.51382200	-0.97688300	-0.16161600	C	-4.56072400	1.94762800	0.54712400
C	-2.47820000	-1.27429000	0.78385700	C	-3.47566900	1.07221000	0.59349200
C	-1.90749100	-1.28041300	2.24953800	H	-2.46305400	1.45561000	0.50329300
N	-0.50265700	-1.77316400	2.38471700	H	-4.38672100	3.01606500	0.43956500
C	0.33629400	-1.05899600	3.36291600	H	-6.71229700	2.14546800	0.59143800
H	0.58593400	-1.68210500	4.22860100	H	-7.09308300	-0.30426500	0.82058300
H	1.25709400	-0.69940200	2.89240300	H	-5.16505800	-1.85431700	0.90828400
H	-0.22166200	-0.19525000	3.72726900	O	-2.59601900	-3.84085500	-1.52082600
C	-0.06090000	-2.91051500	1.78961600	C	-3.04212200	-5.05203700	-0.87197600
C	1.28524900	-3.49942200	2.22731400	C	-4.56923200	-5.00894900	-0.93677400
C	1.00988200	-4.54519500	3.32881400	C	-4.81040900	-4.27909200	-2.26817000
H	1.94922400	-4.96553900	3.70131500	C	-3.67396500	-3.25133400	-2.28485100
H	0.47807900	-4.10812000	4.18238800	H	-3.96435400	-2.31123400	-1.80148000
H	0.39634700	-5.36324700	2.93470800	H	-3.30278200	-3.03022600	-3.29051900
H	1.92731700	-2.71760300	2.63647100	H	-5.79594600	-3.80858100	-2.33281300
H	-1.85312400	-0.22905200	2.55114700	H	-4.71197700	-4.97770600	-3.10756900
C	-2.81110800	-2.02849400	3.23831700	H	-4.96992800	-4.42295500	-0.10120400
H	-2.43689900	-1.93979500	4.26485300	H	-5.01956300	-6.00559400	-0.90089600
H	-3.82729600	-1.62359200	3.21333200	H	-2.64237500	-5.91531200	-1.42147100
H	-2.85633200	-3.09255300	2.98111700	H	-2.63184100	-5.05368400	0.13994300
H	-2.90068800	-2.28304200	0.62158200	O	0.05347800	-2.49696300	-2.43663200

C	-3.67475900	-0.30944200	0.73217000
C	2.18698000	-2.10852200	-3.34828400
C	1.25237900	-0.96135700	-3.81436100
C	-0.15195400	-1.40350400	-3.34627400
H	-0.76165500	-1.75219600	-4.19340100
H	-0.71490700	-0.64148700	-2.80226200
H	1.27210700	-0.82162700	-4.90000400
H	1.55031800	-0.01942900	-3.34594400
H	2.85784100	-2.45875300	-4.13885400
H	2.78083600	-1.76886000	-2.49696000
H	1.58417200	-3.80027700	-2.05297800
H	0.93554600	-3.87628300	-3.71587300
O	-0.15416800	2.01327700	0.04417200
C	0.02153100	2.58244300	-1.27420300
C	1.31375900	3.39230800	-1.20096300
C	1.27716800	3.91478100	0.24398900
C	0.66265000	2.73566000	1.00648800
H	0.01505200	3.04614000	1.83318900
C	1.21740600	-3.20382200	-2.89051700
H	1.42935800	2.04483400	1.37134300
H	0.63648800	4.80194400	0.31601700
H	2.26705200	4.17805800	0.62768700
H	1.34941100	4.19122500	-1.94825200
H	2.17384700	2.73098700	-1.34561700
H	0.06351300	1.75960300	-1.99486300
H	-0.84836300	3.21132100	-1.50750400
C	4.53567000	-3.96399900	1.07428700
H	5.50920700	-4.36659900	1.34404700
H	4.52070400	-2.99778400	0.57372200
C	3.40421600	-4.61533700	1.35249400
H	3.45841500	-5.57838900	1.86290300
C	2.03163000	-4.09572700	1.00981600
H	1.41546900	-4.89289500	0.57570100
H	2.12895700	-3.29677900	0.26788100
Br	2.32639700	-0.40188300	-0.00301700

Table 51. Geometric coordinates and thermally corrected MP2 energies for transition state **43d**





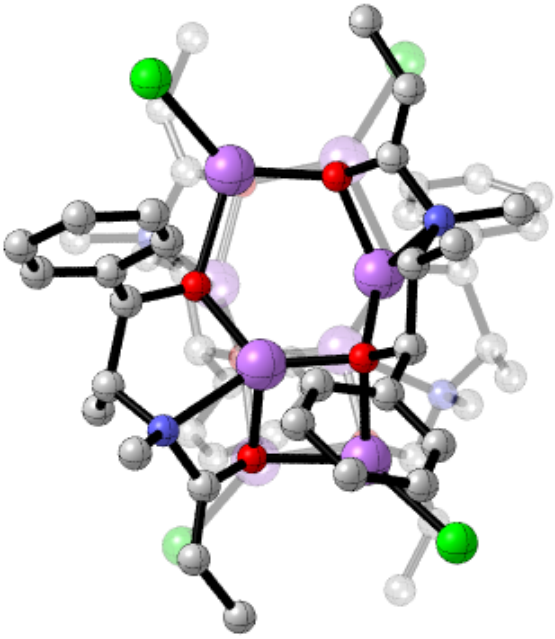
43d

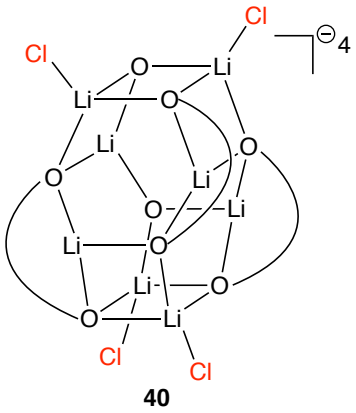
G = –4111.754713
G_{MP2} = –4104.911694

Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	H	-1.50962100	3.81365400	2.73627700
O	-1.68786600	-0.57909400	0.95439500	H	-1.98130400	4.48760200	1.17598800
Li	-2.12871100	-0.24024300	-0.92429800	H	-2.95956800	3.22086000	1.91150800
O	-0.92264800	1.20417000	-1.05869200	H	-2.71308600	1.74333200	-0.14835300
C	-1.69639600	2.13422300	-0.37469500	C	-1.93585200	3.39486500	-1.21452400
C	-1.08124900	2.52025500	1.00983600	C	-3.22937600	3.89870700	-1.40644500
N	-0.74495300	1.32741800	1.86855900	C	-3.44129400	5.03801200	-2.18859000
C	0.00110200	1.69780900	3.07157900	C	-2.36326600	5.68986100	-2.78828800
H	-0.58593900	2.22923000	3.83513800	C	-1.07019800	5.18986200	-2.60796400
H	0.41511500	0.79853300	3.53623700	C	-0.86215800	4.04948100	-1.83280600
H	0.82998400	2.35482000	2.78034300	H	0.14041700	3.64683500	-1.71457000
C	-1.59260500	0.17295200	1.99626900	H	-0.22493500	5.68752900	-3.07859500
C	-2.22176300	-0.12980800	3.20966000	H	-2.52700700	6.57617200	-3.39657400
C	-2.57582000	-1.53653700	3.60208300	H	-4.45275800	5.41143100	-2.33033600
H	-1.83082600	-1.96076100	4.29329500	H	-4.07353800	3.38573100	-0.94806600
H	-3.54494900	-1.58470900	4.11756300	O	-3.42538500	-0.70730700	-2.30144300
H	-2.62135800	-2.18677700	2.72314300	C	-4.51666500	-1.65216600	-2.14843700
C	-5.25396600	0.47929800	3.20190600	C	-5.68606200	-1.08944300	-2.96041000
C	-5.91317000	-0.61698000	3.61953000	C	-4.97779200	-0.23460600	-4.02355200
H	-6.60454100	-0.58177200	4.45631200	C	-3.80504400	0.34304500	-3.23578500
H	-5.80826500	-1.57074700	3.10941000	H	-4.09733000	1.23074800	-2.66732700
H	-5.41657400	1.42732600	3.71143200	H	-2.92536700	0.57625800	-3.84126800
C	-4.32299000	0.49135700	2.09760500	H	-5.61973000	0.54962900	-4.43574900
H	-3.83641600	1.40280100	1.81834100	H	-4.61914900	-0.85662600	-4.85353600
H	-4.07825900	-0.40642300	1.55618700	H	-6.29899200	-0.45574600	-2.31310900
H	-2.11680300	0.58390400	4.02163900	H	-6.31192900	-1.87986100	-3.38661200
H	-0.10456500	2.97686100	0.79163000	H	-4.17566800	-2.62281100	-2.53318400

C	-1.93107800	3.56379400	1.75774000
O	-0.47438500	-1.63565600	-1.32376800
C	-0.47544800	-2.99071500	-0.84195500
C	-0.98415400	-3.80606700	-2.02978100
C	-0.35799400	-3.07279400	-3.23977800
C	-0.03015200	-1.65945300	-2.69885500
H	-0.55359800	-0.85011900	-3.20969000
H	1.04774900	-1.45724700	-2.72573400
H	-1.04329300	-3.03566500	-4.09087800
H	0.55488600	-3.57610900	-3.57414500
H	-2.07686200	-3.75599800	-2.07099600
H	-0.69355300	-4.85943900	-1.97313000
H	0.54897000	-3.28270900	-0.56388700
H	-1.10948800	-3.01129900	0.04574600
O	1.99128400	0.03297400	-0.12230300
H	-4.74927000	-1.74433700	-1.08381300
C	2.94099700	0.06928100	0.96983100
C	4.05182500	1.03834000	0.54126900
C	3.33342400	1.94260200	-0.47332000
C	2.40133300	0.95445800	-1.16835400
H	2.92822300	0.39004300	-1.95046600
H	1.48738000	1.39260300	-1.57791100
H	4.01728500	2.43752000	-1.16924600
H	2.74916800	2.71450600	0.04130400
H	4.86857500	0.49472400	0.05246400
H	4.47296800	1.58587600	1.38954700
H	2.41410000	0.42104300	1.86384200
H	3.30447200	-0.94725500	1.15359800
Br	-5.77035600	1.11631500	0.05548500

Table 52. Geometric coordinates and thermally corrected MP2 energies for **40**





40

G = –4744.022592
G_{MP2} = –4732.134562

Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000
O	2.01636700	-0.26014900	-0.24546900
C	2.56510100	0.02365900	-1.41310300
N	2.75275000	-1.18653400	-2.22377500
C	4.02448400	-1.89799100	-1.92518300
C	5.14059000	-1.57951300	-2.93593900
H	6.10494300	-1.94910700	-2.57522200
H	5.21544900	-0.49366900	-3.07180800
H	4.95565100	-2.04066400	-3.91510500
C	3.74289300	-3.42171000	-1.69498100
O	2.83121900	-3.58499300	-0.65105100
Li	1.50044400	-2.11630300	-0.79621100
O	-0.43497500	-2.06889200	-0.71042700
C	-1.19276100	-2.23854700	-1.86094400
C	-1.28939800	-3.75233300	-2.29489000
N	-1.85060500	-4.60060700	-1.19353400
C	-1.04347300	-5.71933900	-0.70787200
O	-0.00367300	-5.31885700	0.00417300
Li	1.94236800	-5.50307300	-0.36742700
O	2.25798700	-5.31948800	1.69569700
C	3.29779000	-5.72021000	2.40758100
N	4.10484300	-4.60164500	2.89376800
C	3.54355400	-3.75386000	3.99549000
C	3.44670300	-2.23989700	3.56222000
O	2.68889000	-2.06976400	2.41182400
Li	0.75371400	-2.11687700	2.49811800
O	-0.57695900	-3.58563000	2.35177700
Li	-0.74976700	-3.57476400	0.47351800
Li	0.31191500	-5.50345500	2.06692200
Cl	-0.39076100	-7.07894800	3.78178400
C	-1.48863500	-3.42313100	3.39579000
C	-1.77077700	-1.89956300	3.62663500
N	-0.49932000	-1.18779300	3.92539700
C	-0.31183200	0.02264500	3.11503500
O	0.23733700	-0.26062700	1.94749900
Li	2.25332100	0.00077800	1.70153800
Cl	3.39104800	1.78335800	2.79096000
C	-0.67062900	1.24024400	3.58108400
C	-0.41804300	2.52443600	2.83188400
H	-0.68909200	2.43457900	1.77255600
H	0.64463500	2.80491600	2.86772900
H	-1.00676900	3.34993500	3.26310300
H	-1.09124400	1.29956700	4.58372200
C	-0.12444100	-1.09513400	5.32711900

H	0.88017100	-0.66740900	5.38848000	H	1.95518400	-8.33275400	2.46224800
H	-0.10265200	-2.10007400	5.76802000	H	4.51500800	-7.20978200	3.26950100
H	-0.79510100	-0.47013700	5.94628600	Cl	2.64494900	-7.07721200	-2.08324900
C	-2.88693100	-1.58189400	4.63759700	C	-1.41596400	-7.00490900	-0.91736000
H	-2.96223500	-0.49612600	4.77383000	C	-0.68948100	-8.17798200	-0.30853200
H	-2.70171100	-2.04327900	5.61660100	H	-0.53123600	-8.03833600	0.76925300
H	-3.85115500	-1.95178900	4.27684400	H	0.29846400	-8.33303600	-0.76489500
H	-2.08979100	-1.51340200	2.65273900	H	-1.27223100	-9.10395500	-0.43740100
C	-2.82107200	-4.15581700	3.18386400	H	-2.26045000	-7.20847500	-1.57079000
C	-3.27532400	-5.09454800	4.12012900	C	-3.26131100	-4.89681700	-1.40495400
C	-4.53067700	-5.69320200	3.99405300	H	-3.64522800	-5.44834700	-0.54472000
C	-5.36053100	-5.37034600	2.91875200	H	-3.44781100	-5.50207500	-2.31611100
C	-4.90979000	-4.45779500	1.96156900	H	-3.82085000	-3.96340600	-1.51190700
C	-3.65253400	-3.86417400	2.09251400	C	0.04939600	-4.24616200	-2.85198100
H	-3.31891600	-3.16446400	1.33232900	H	0.25360500	-3.72088700	-3.79497100
H	-5.53324100	-4.20485200	1.10597700	H	0.88156200	-4.05599600	-2.17310400
H	-6.33929600	-5.83932300	2.81492900	H	0.03656300	-5.32242400	-3.04492300
H	-4.85031700	-6.43145800	4.72915500	H	-2.00845800	-3.81211200	-3.12940100
H	-2.61123500	-5.38734200	4.92718100	C	-2.60339000	-1.62897800	-1.76738700
H	-1.06944400	-3.82876800	4.33707600	C	-3.11315500	-1.15354300	-0.55621600
Li	3.00433000	-3.57530600	1.22711300	C	-4.41138900	-0.64584800	-0.46847500
C	4.85723300	-1.63001500	3.46895100	C	-5.22599500	-0.58675800	-1.59996700
C	5.36672800	-1.15365100	2.25802400	C	-4.71858400	-1.02512100	-2.82660700
C	6.66482300	-0.64558100	2.17045100	C	-3.42235900	-1.53421700	-2.90377700
C	7.47956300	-0.58703900	3.30188200	H	-3.03477400	-1.86366600	-3.86723100
C	6.97241600	-1.02631800	4.52829600	H	-5.33225300	-0.96447500	-3.72628500
C	5.67631700	-1.53578200	4.60529700	H	-6.23640100	-0.18360200	-1.53327000
H	5.28894600	-1.86595400	5.56858900	H	-4.77564800	-0.27576100	0.48761200
H	7.58617800	-0.96611500	5.42794000	H	-2.46280900	-1.16228800	0.31152700
H	8.48986000	-0.18358800	3.23531100	H	-0.72095300	-1.72668900	-2.72740100
H	7.02887400	-0.27475800	1.21457000	C	5.07554100	-4.15410100	-1.48323500
H	4.71623200	-1.16198000	1.39038800	C	5.52948500	-5.09330500	-2.41917900
H	2.97484800	-1.72855200	4.42897300	C	6.78489600	-5.69187400	-2.29319500
C	2.20481900	-4.24808600	4.55238000	C	7.61511500	-5.36844400	-1.21835200
H	2.00054300	-3.72324300	5.49560100	C	7.16469300	-4.45539500	-0.26149000
H	2.21778100	-5.32443000	4.74486200	C	5.90738300	-3.86187000	-0.39232200
H	1.37264500	-4.05772300	3.87356900	H	5.57405300	-3.16172600	0.36759100
H	4.26263200	-3.81393100	4.82996300	H	7.78843700	-4.20197900	0.59375100
C	5.51555600	-4.89783800	3.10512500	H	8.59392800	-5.83734400	-1.11462500
H	6.07497300	-3.96442800	3.21271300	H	7.10429700	-6.43050100	-3.02802600
H	5.89963200	-5.44878200	2.24458100	H	4.86508600	-5.38660000	-3.22579000
H	5.70203100	-5.50364300	4.01592300	H	3.32387500	-3.82714000	-2.63642600
C	3.67036400	-7.00586900	2.61639500	H	4.34325200	-1.51206200	-0.95111900
C	2.94376300	-8.17858100	2.00697900	C	2.37803400	-1.09352800	-3.62552800
H	3.52565500	-9.10494700	2.13685400	H	3.04857300	-0.46811000	-4.24438200
H	2.78686400	-8.03915600	0.92894900	H	1.37328400	-0.66613000	-3.68688000

H	2.35664600	-2.09833300	-4.06673800	H	2.94088000	2.43513500	-0.06997800
C	2.92330300	1.24150900	-1.87894100	H	3.25969500	3.35099900	-1.55993900
H	3.34349700	1.30124100	-2.88173100	H	1.60790300	2.80619600	-1.16582500
C	2.67049900	2.52546200	-1.12942900	Cl	-1.13807400	1.78322100	-1.08854800