

Enediolate-Dilithium Amide Mixed Aggregates in the  
Enantioselective Alkylation of Arylacetic Acids:  
Structural Studies and a Stereochemical Model

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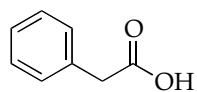
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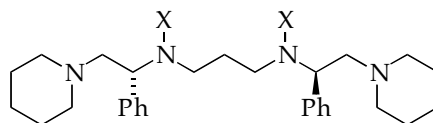
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## Structures

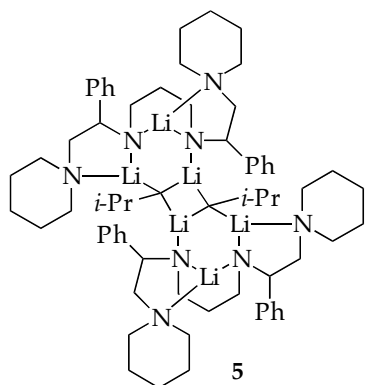


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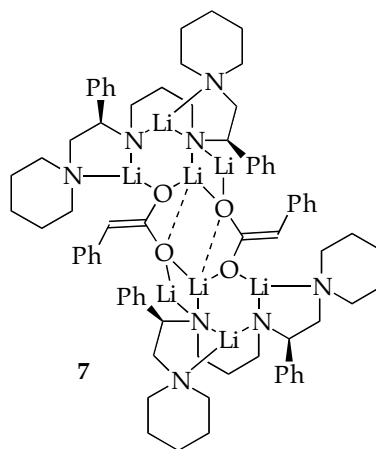


3; X = H

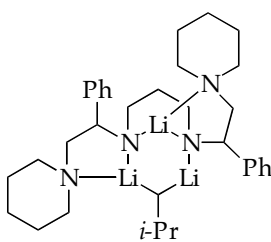
4; X = Li (R\*<sub>2</sub>NLi)



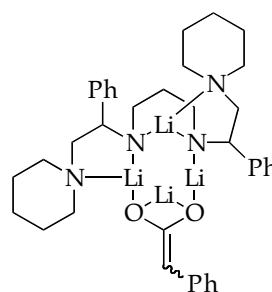
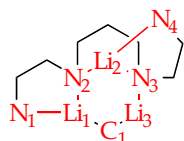
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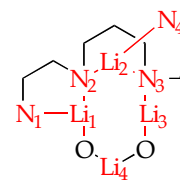
7



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Part 1:  $^1\text{H}$  and  $^{13}\text{C}$  NMR of "Substrates"

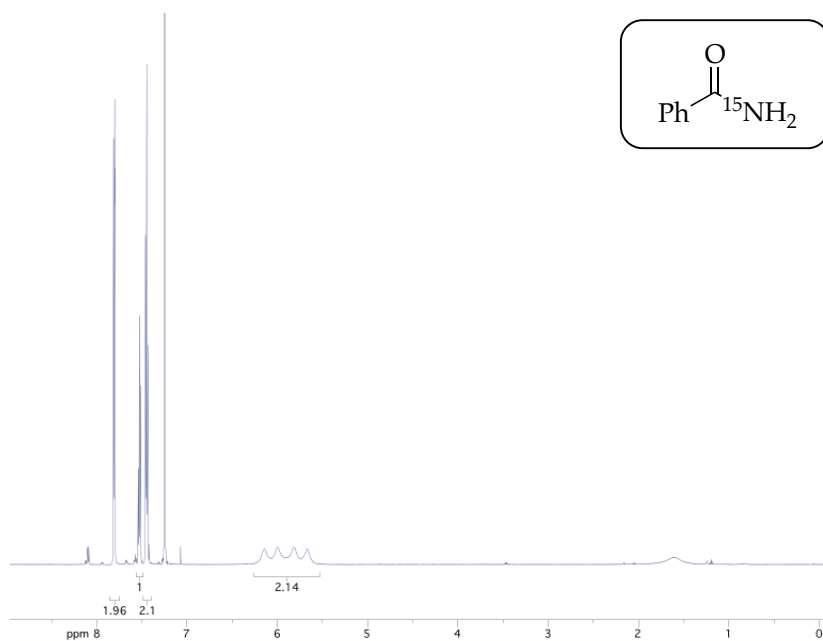


Figure 1.  $^1\text{H}$  NMR ( $\text{CDCl}_3$ ) of 12

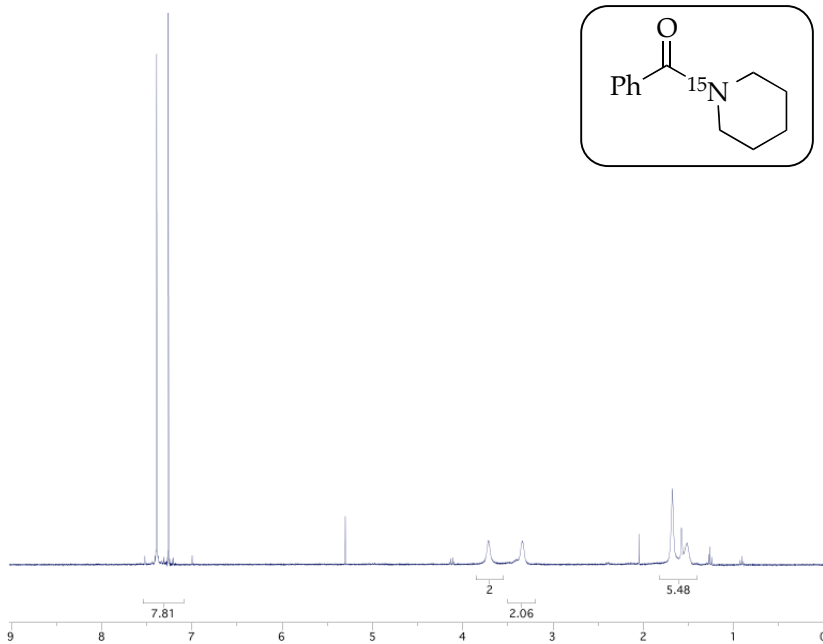
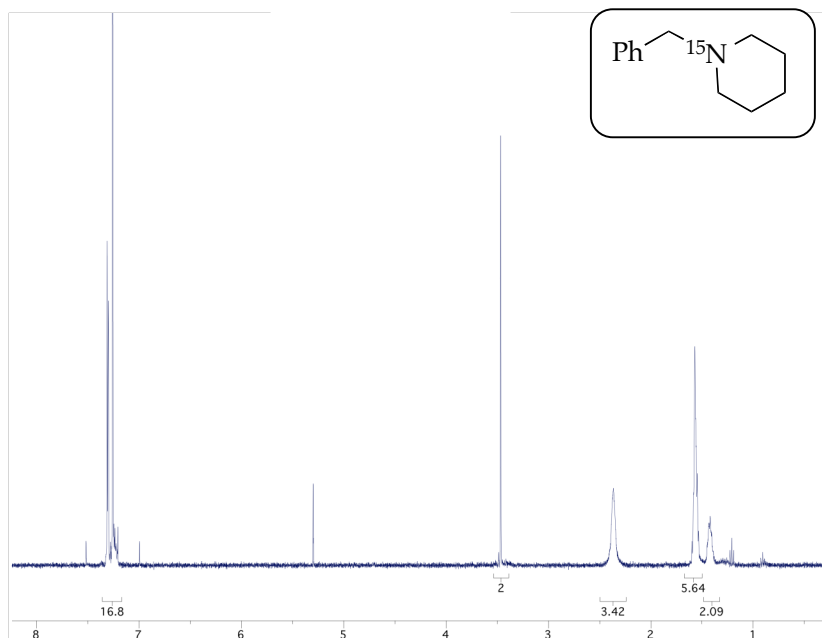
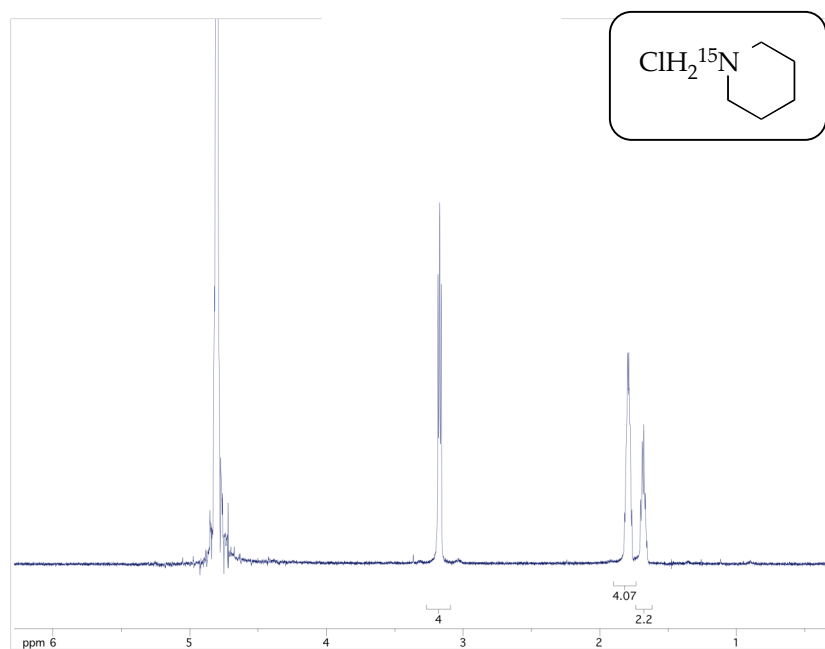


Figure 2.  $^1\text{H}$  NMR ( $\text{CDCl}_3$ ) of 13

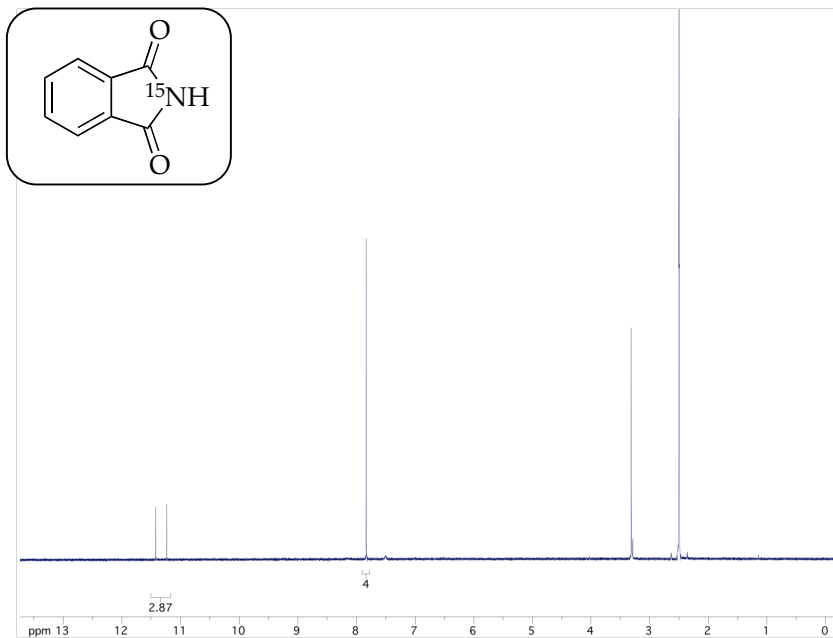


**Figure 3.**  $^1\text{H}$  NMR ( $\text{CDCl}_3$ ) of **14**

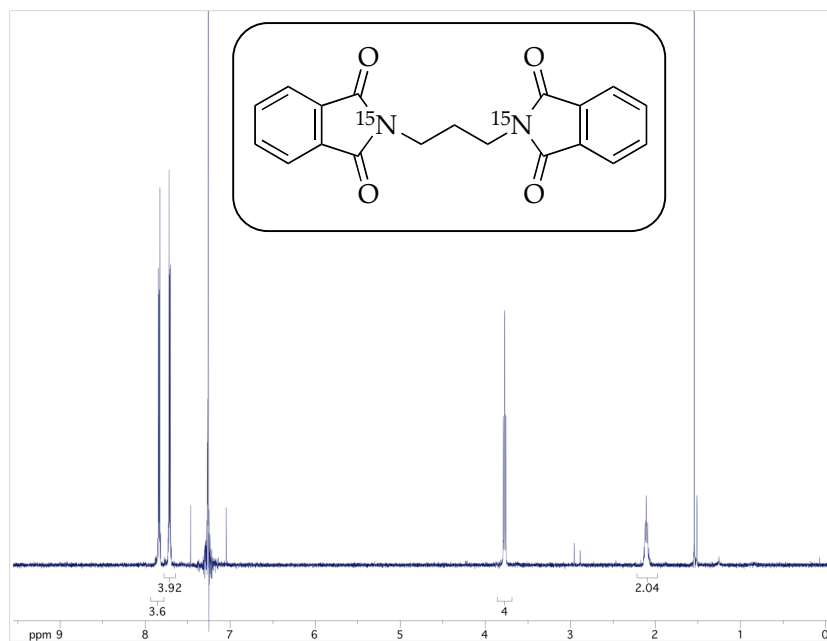


**Figure 4.**  $^1\text{H}$  NMR ( $\text{CDCl}_3$ ) of **15**





**Figure 5.** <sup>1</sup>H NMR (CDCl<sub>3</sub>) of **9**



**Figure 6.** <sup>1</sup>H NMR (CDCl<sub>3</sub>) of **10**

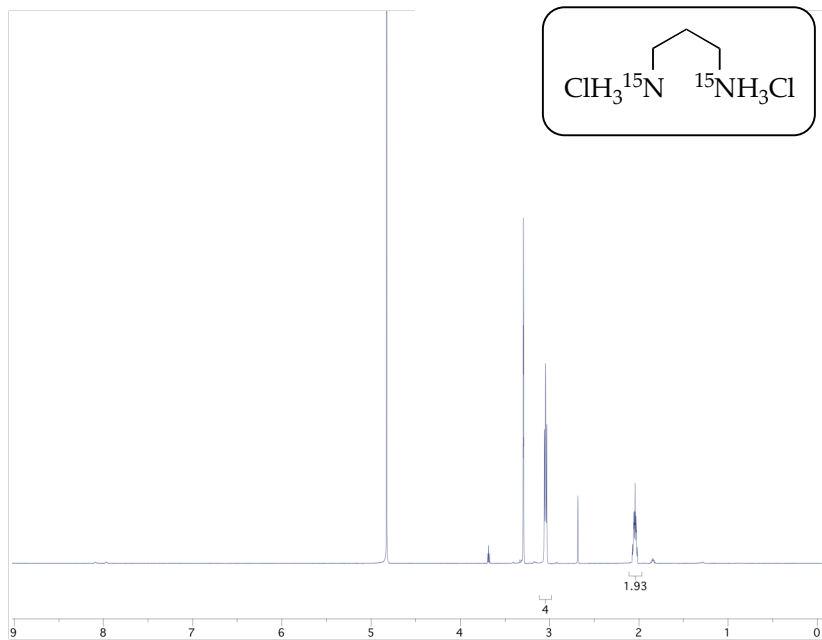


Figure 7.  $^1\text{H}$  NMR ( $\text{CDCl}_3$ ) of **11**

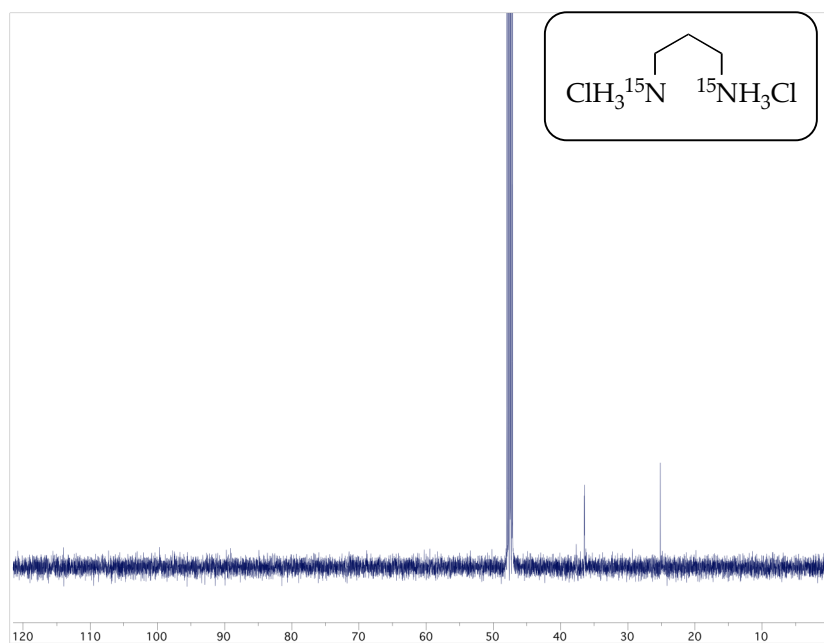
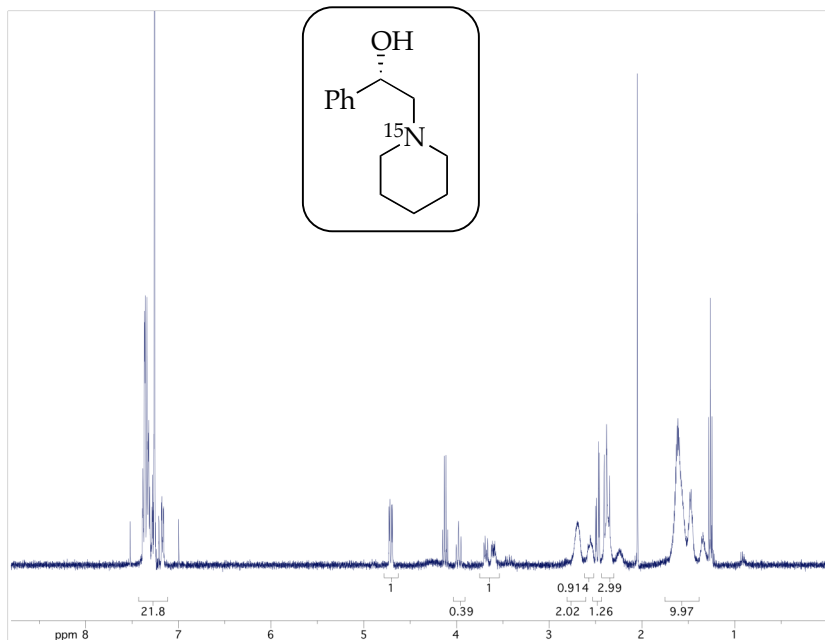
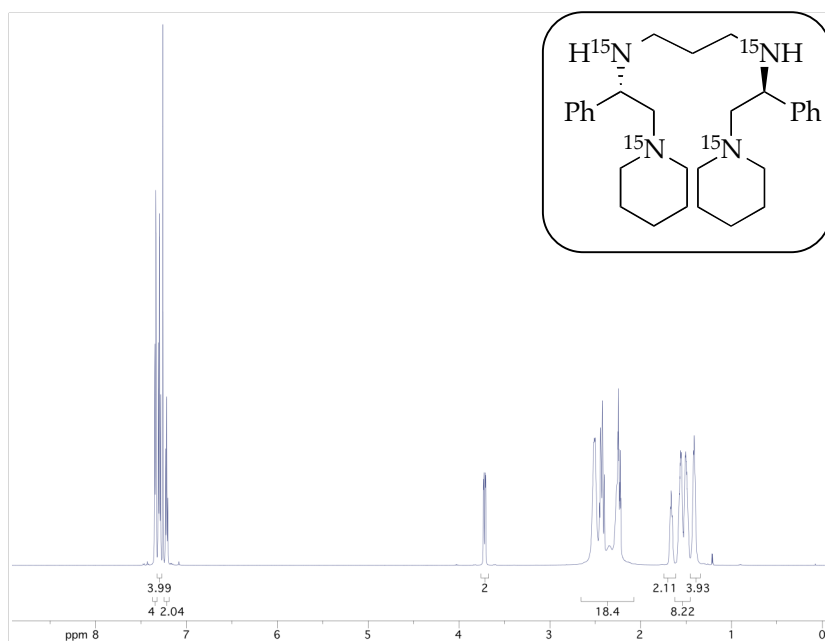


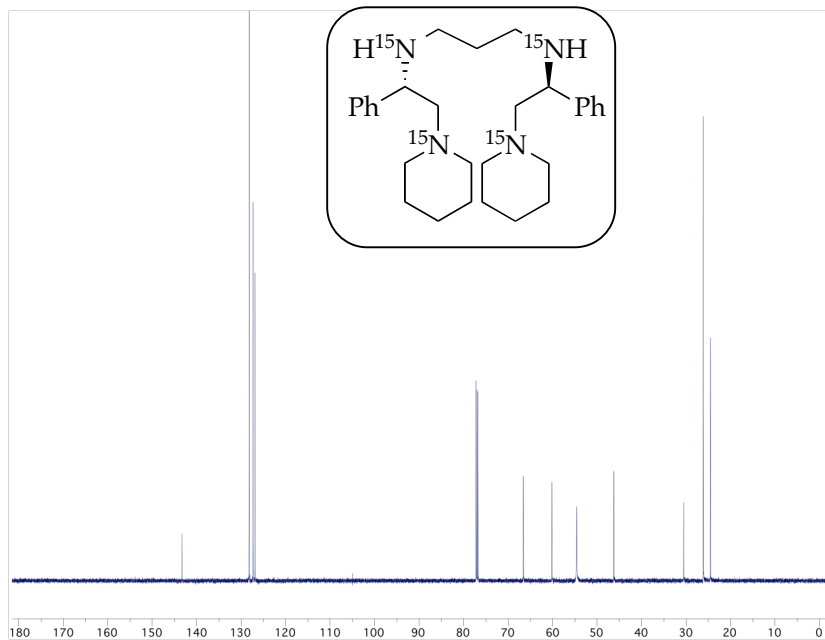
Figure 8.  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ ) of **11**



**Figure 9.**  $^1\text{H}$  NMR ( $\text{CDCl}_3$ ) of **16**

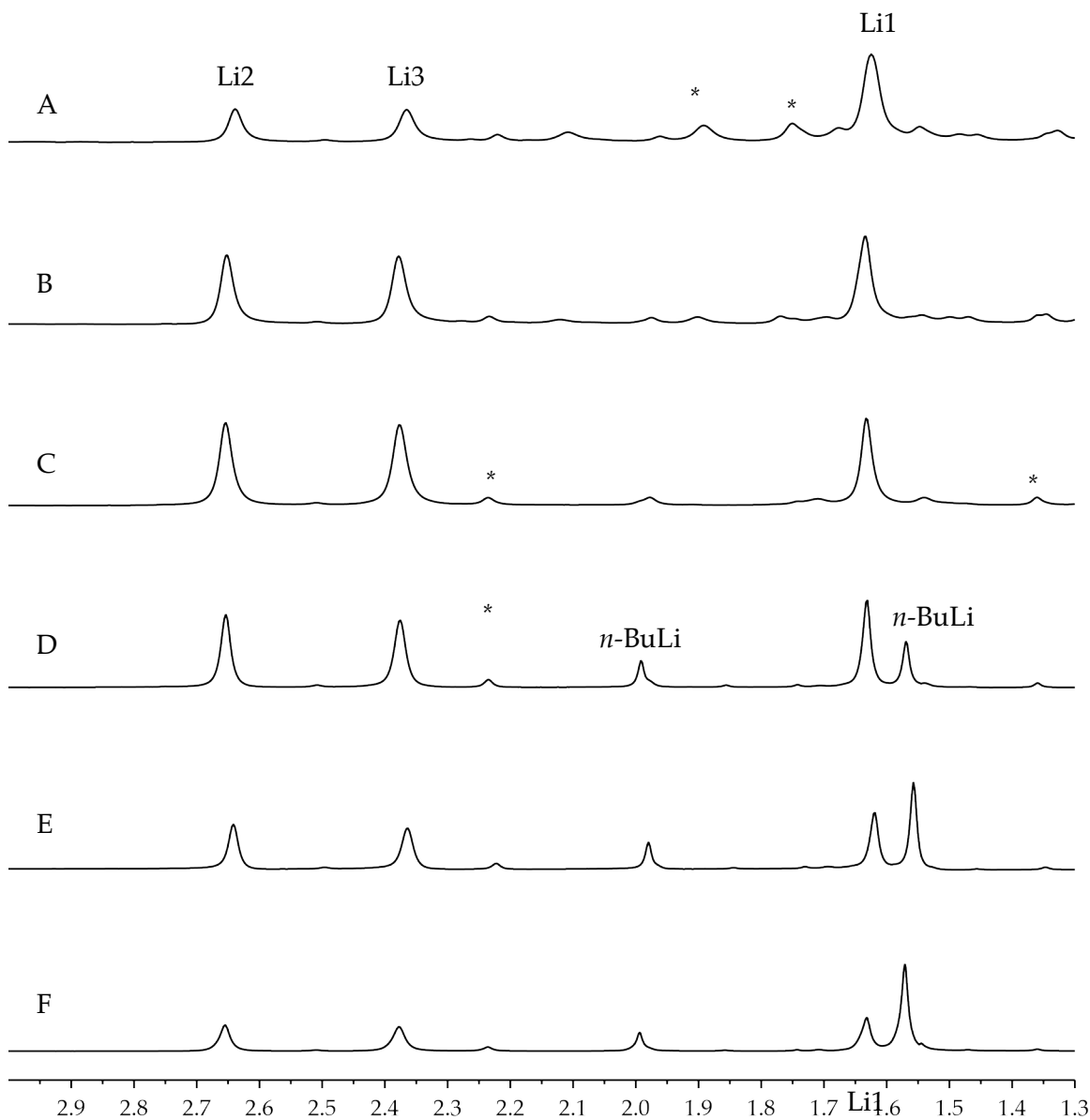


**Figure 10.**  $^1\text{H}$  NMR ( $\text{CDCl}_3$ ) of **3**

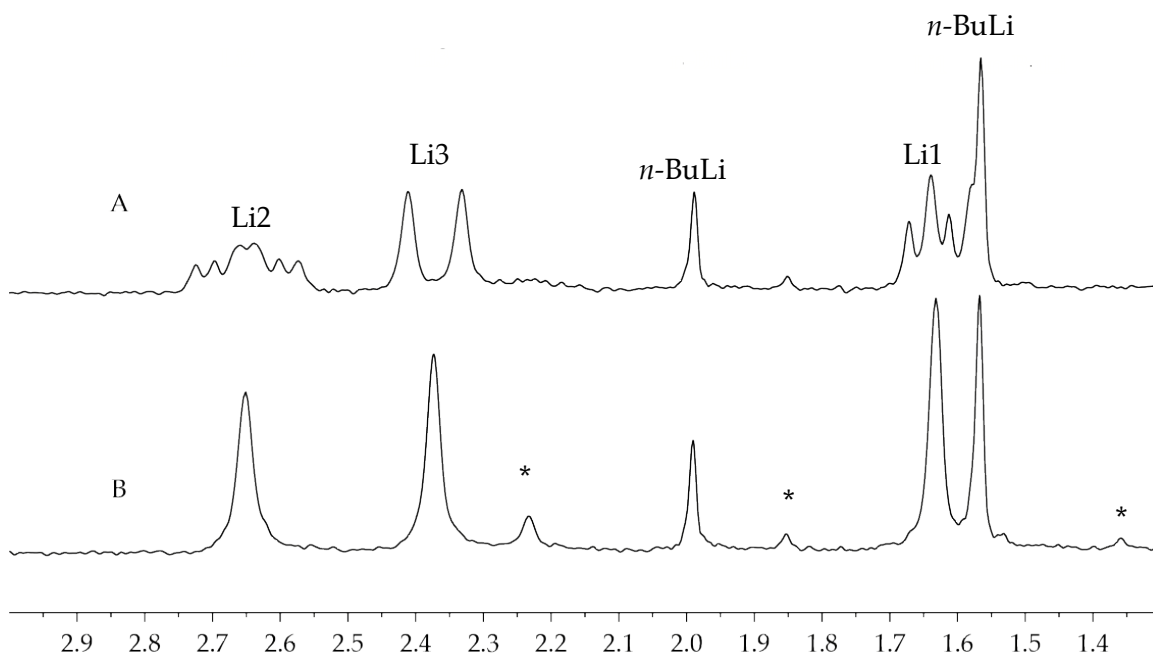


**Figure 11.**  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ ) of **3**

## Part 2: 1D NMR [ $^6\text{Li}$ , $^{13}\text{C}$ , $^{15}\text{N}$ ] Spectroscopic Studies

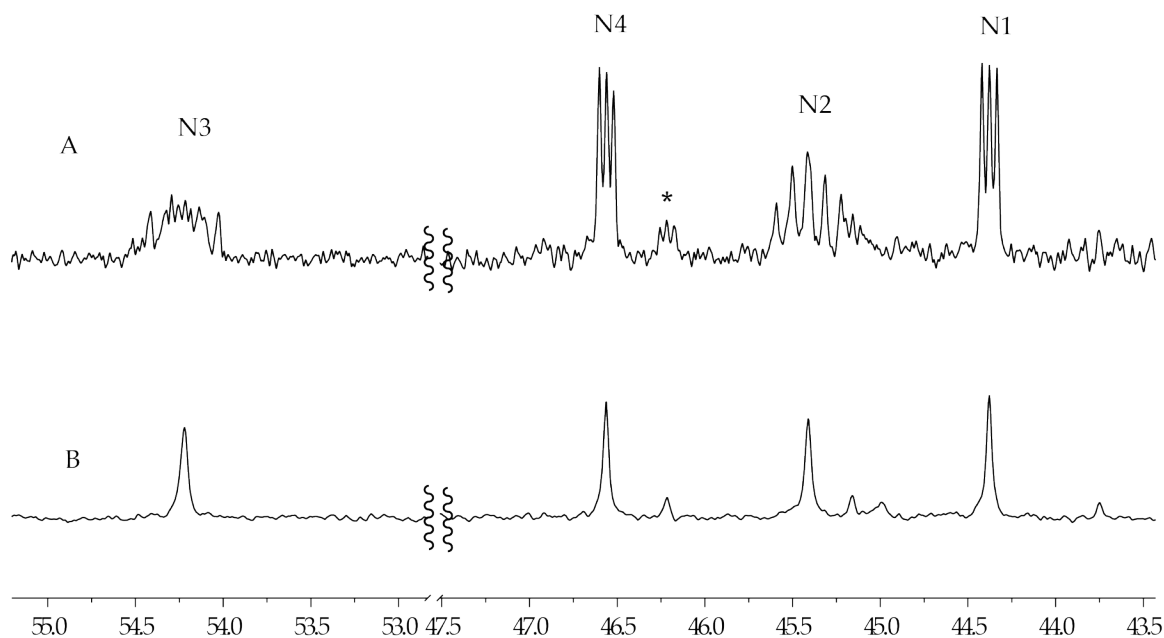


**Figure 12.**  $^6\text{Li}$  NMR spectra of amine 3 with varying equiv of  $n\text{-BuLi}$  in THF-pentane *per diamine* recorded at  $-90\text{ }^\circ\text{C}$  at after aging at  $-78\text{ }^\circ\text{C}$  for 2 hrs: (A) 0.5 equiv  $n\text{-BuLi}$ ; (B) 1.0 equiv  $n\text{-BuLi}$ ; (C) 2.0 equiv  $n\text{-BuLi}$ ; (D) 3.0 equiv  $n\text{-BuLi}$ ; (E) 4.0 equiv  $n\text{-BuLi}$ ; (F) 5.0 equiv  $n\text{-BuLi}$ .



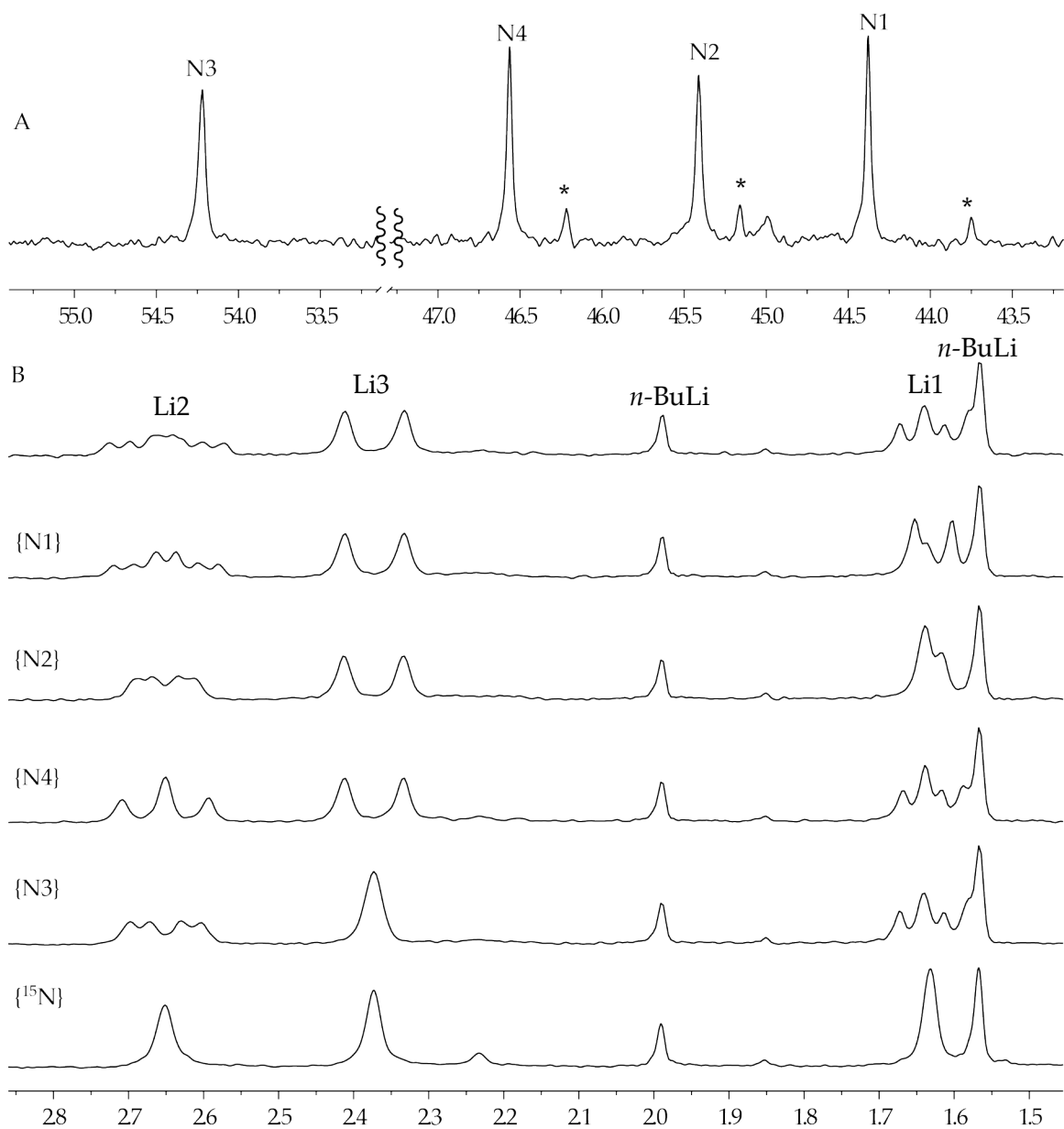
**Figure 13.**  ${}^6\text{Li}$  NMR spectra of 0.10 M  $[{}^6\text{Li}, {}^{15}\text{N}]6$  prepared from  $[{}^{15}\text{N}_4]3$  with 4.0 equiv  $n\text{-BuLi}$  in 6.10 M THF-pentane recorded at  $-90\text{ }^\circ\text{C}$  after aging at  $-78\text{ }^\circ\text{C}$  for 2.0 hrs: (A) fully coupled; (B) broad-band  ${}^{15}\text{N}$  decoupled.

| ${}^6\text{Li}$ | $\delta$ (ppm)   |
|-----------------|--|
| 1               | 1.63 (dd, $J[\text{Li}_1\text{-N}_2] = 4.3$ , $J[\text{Li}_1\text{-N}_1] = 2.1$ Hz)                                      |
| 2               | 2.65 (ddd, $J[\text{Li}_2\text{-N}_2] = 4.9$ , $J[\text{Li}_2\text{-N}_3] = 4.3$ , $J[\text{Li}_2\text{-N}_4] = 2.1$ Hz) |
| 3               | 2.37 (d, $J[\text{Li}_3\text{-N}_3] = 5.8$ Hz)   |



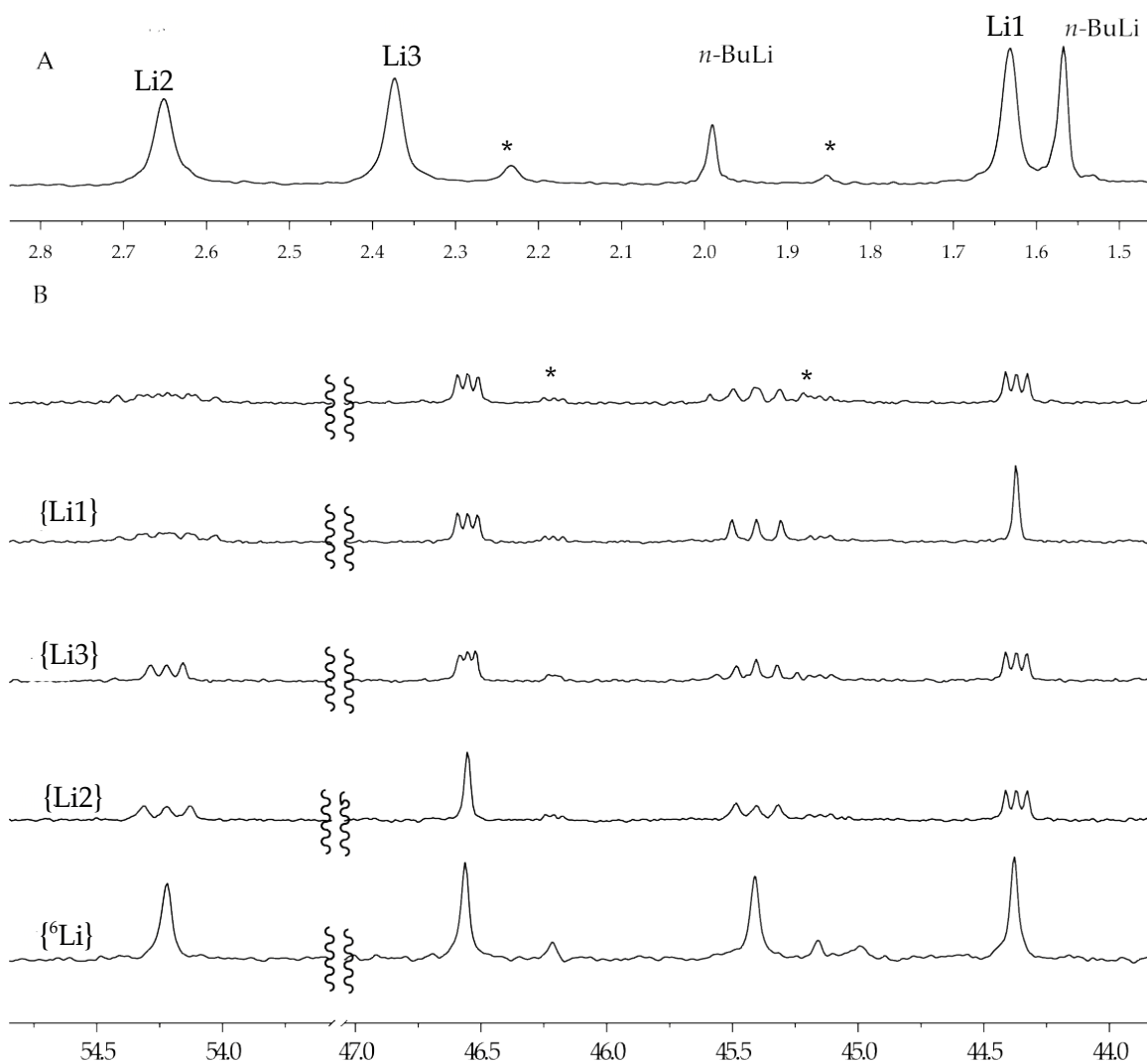
**Figure 14.**  $^{15}\text{N}$  NMR spectra of 0.10 M  $[\text{}^6\text{Li}, \text{}^{15}\text{N}]\mathbf{6}$  prepared from  $[\text{}^{15}\text{N}_4]\mathbf{3}$  with 4.0 equiv *n*-BuLi in 6.10 M THF-pentane recorded at  $-90\text{ }^\circ\text{C}$  after aging at  $-78\text{ }^\circ\text{C}$  for overnight: (A) fully coupled; (B) broadband  $^{15}\text{N}$  decoupled. \*Unknown impurities that appear sporadically.

| $^{15}\text{N}$ | $\delta$ (ppm)   |
|-----------------|--|
| 1               | 44.4 (t, $J[\text{N}_1\text{-Li}_1] = 2.1\text{ Hz}$ )                                   |
| 2               | 45.4 (tt, $J[\text{N}_2\text{-Li}_2] = 4.9, J[\text{N}_2\text{-Li}_1] = 4.3\text{ Hz}$ ) |
| 3               | 54.2 (tt, $J[\text{N}_3\text{-Li}_3] = 5.8, J[\text{N}_3\text{-Li}_2] = 4.3\text{ Hz}$ ) |
| 4               | 46.6 (t, $J[\text{N}_4\text{-Li}_2] = 2.1\text{ Hz}$ )                                   |

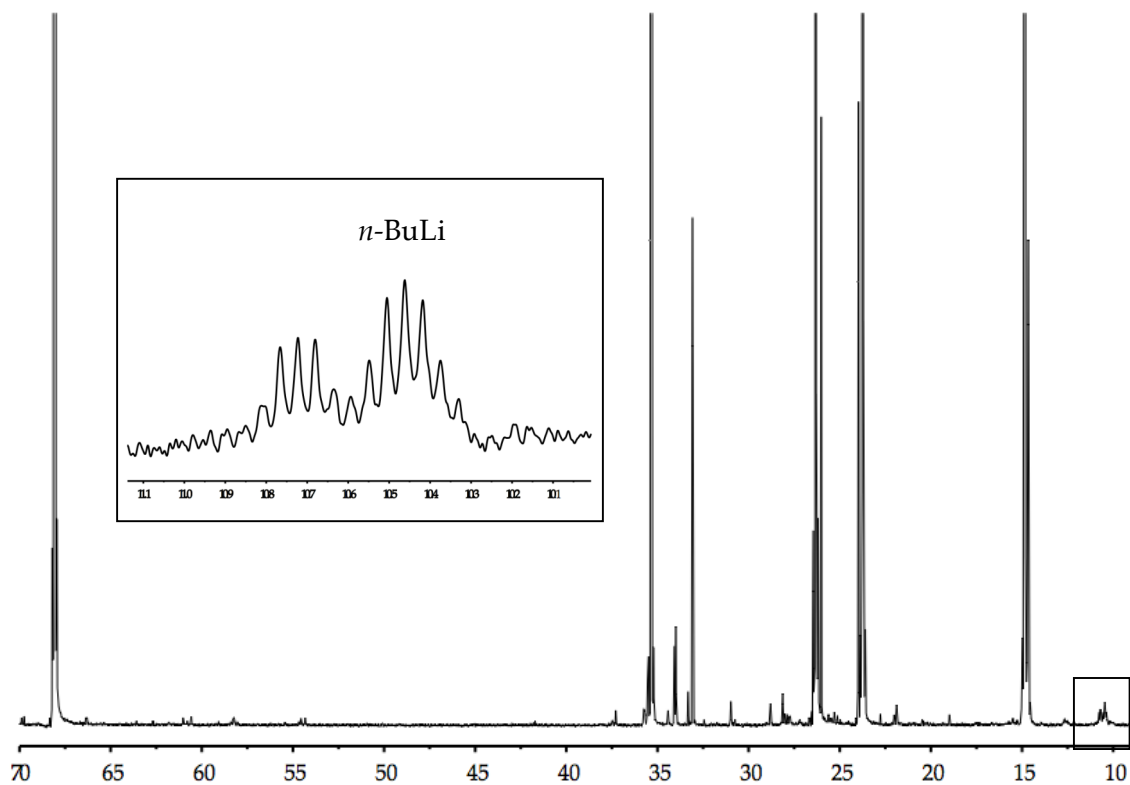


**Figure 15.** NMR spectra of 0.10 M  $[\text{}^6\text{Li}, \text{}^{15}\text{N}]\mathbf{6}$  prepared from  $[\text{}^{15}\text{N}_4]\mathbf{3}$  with 4.0 equiv *n*-BuLi in 6.10 M THF-pentane recorded at  $-90\text{ }^\circ\text{C}$  after aging at  $-78\text{ }^\circ\text{C}$  overnight showing effects of single-frequency  $^{15}\text{N}$  decoupling. Resonance labels refer to those used on structure **6** (pg S4). (A) broad band  $^6\text{Li}$  decoupled  $^{15}\text{N}$  spectrum with resonance labels (N1-N4); (B)  $^6\text{Li}$  NMR spectra with selective  $^{15}\text{N}$  decoupling at 44.3 ppm (N1), 45.4 ppm (N2), 46.4 ppm (N4), 54.2 ppm (N3), and broadband. \*Indicate unassigned resonances.

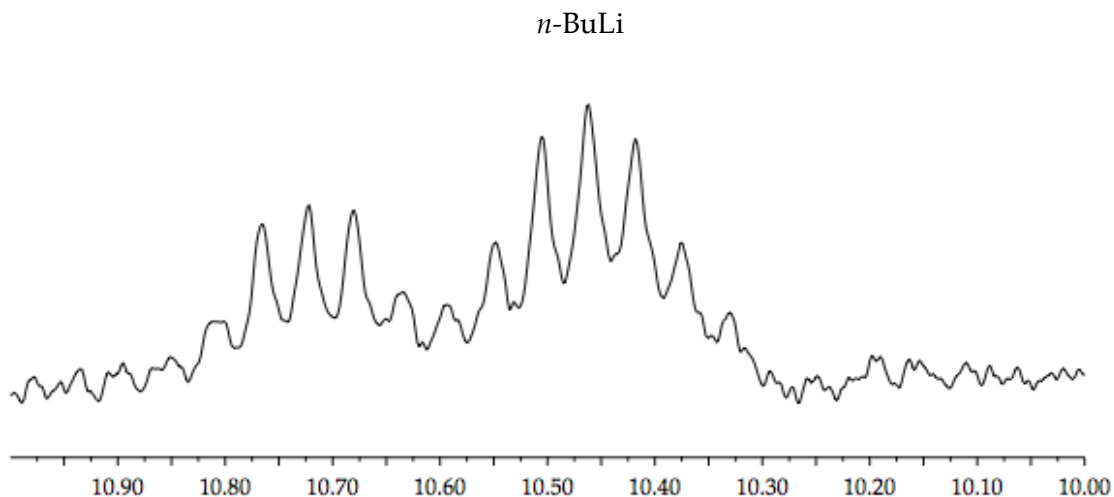




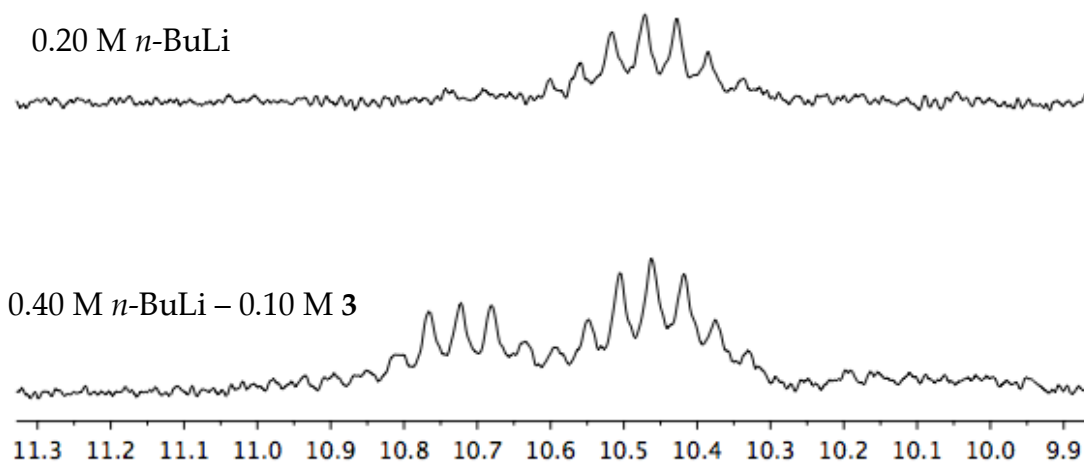
**Figure 16.** NMR spectra of 0.10 M  $[^6\text{Li}, ^{15}\text{N}]\mathbf{6}$  prepared from  $[^{15}\text{N}_4]\mathbf{3}$  with 4.0 equiv *n*-BuLi in 6.10 M THF-pentane recorded at  $-90\text{ }^\circ\text{C}$  after aging at  $-78\text{ }^\circ\text{C}$  overnight showing effects of single-frequency  $^{15}\text{N}$  decoupling. Resonance labels refer to those used on structure **6** (pg S4). (A) broadband  $^{15}\text{N}$  decoupled  $^6\text{Li}$  spectrum with resonance labels (Li1-Li3); (B)  $^{15}\text{N}$  NMR spectra with selective  $^6\text{Li}$  decoupling at 1.63 ppm (Li1), 2.65 ppm (Li2), 2.37 ppm (Li3), and broadband  $^6\text{Li}$  decoupled  $^{15}\text{N}$  spectrum. \*Indicate unassigned resonances.



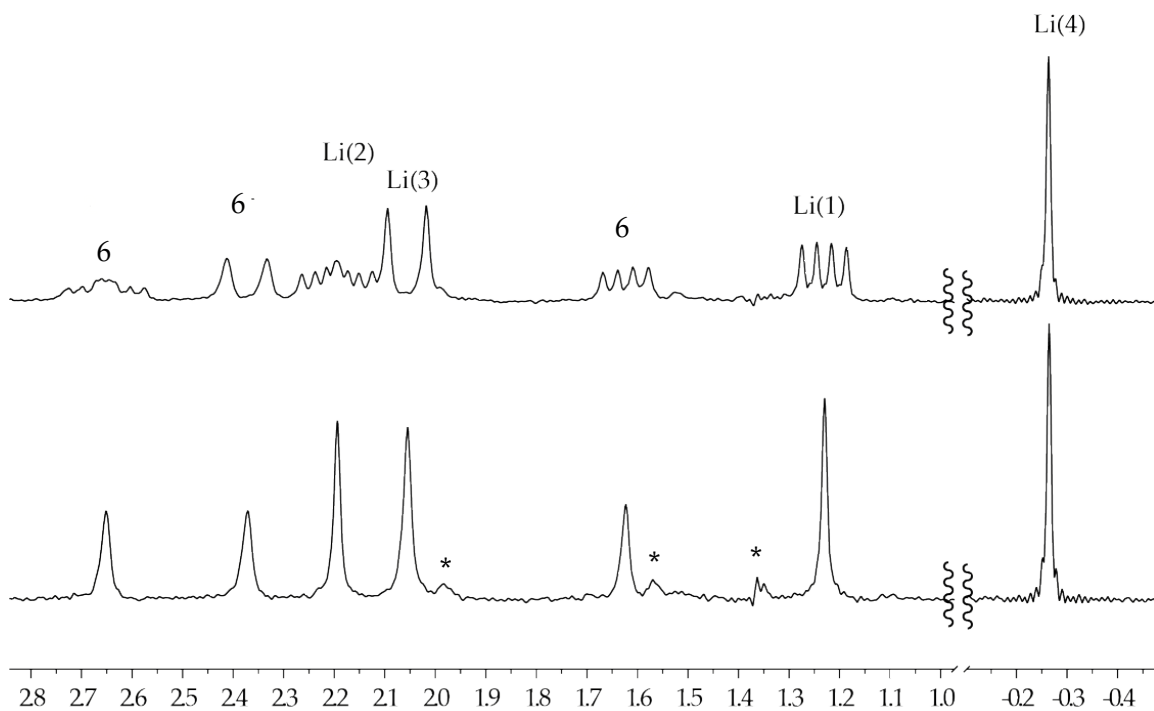
**Figure 17.**  $^{13}\text{C}$  NMR spectra of 0.10 M  $[\text{}^6\text{Li}, \text{}^{15}\text{N}]6$  prepared from  $[\text{}^{15}\text{N}_4]3$  with 4.0 equiv *n*-BuLi in 6.10 M THF-pentane recorded at  $-90\text{ }^\circ\text{C}$  after aging at  $-78\text{ }^\circ\text{C}$  for overnight.



**Figure 18.**  $^{13}\text{C}$  NMR spectra of 0.10 M  $[^6\text{Li},^{15}\text{N}]\mathbf{6}$  prepared from  $[^{15}\text{N}_4]\mathbf{3}$  with 4.0 equiv *n*-BuLi in 6.10 M THF-pentane recorded at  $-90\text{ }^\circ\text{C}$  after aging at  $-78\text{ }^\circ\text{C}$  for overnight. ( $^{13}\text{C}$  resonance of the *n*-BuLi dimer appears as a 1:2:1 triplet at 12.6 ppm.)

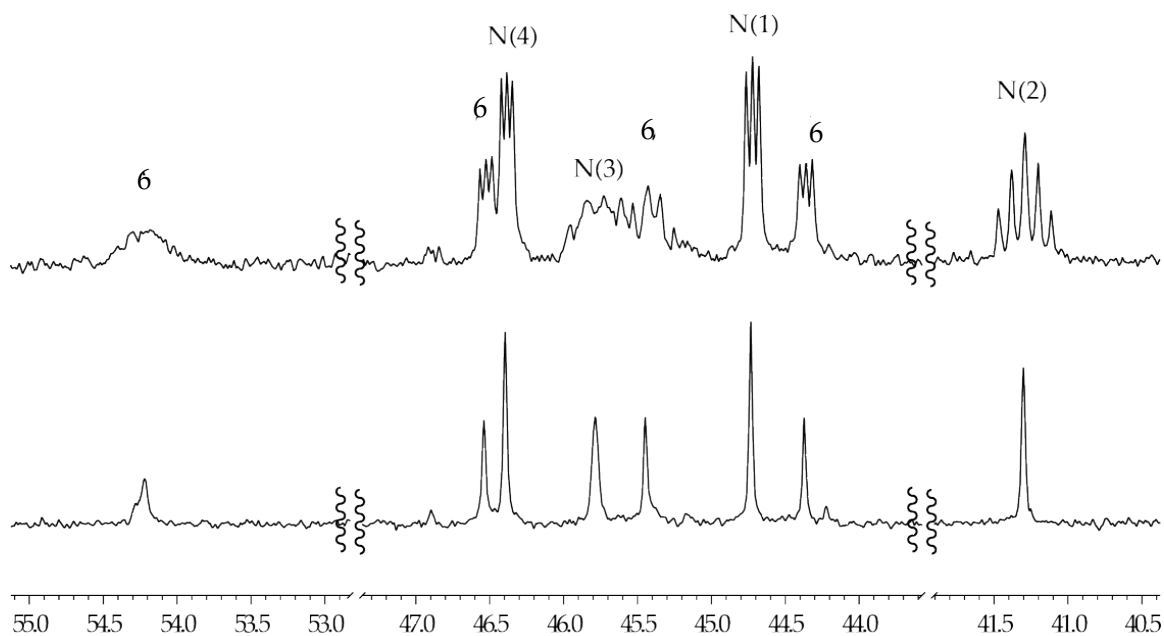


**Figure 19.**  $^{13}\text{C}$  NMR spectra of 0.10 M  $[^6\text{Li},^{15}\text{N}]\mathbf{6}$  prepared from  $[^{15}\text{N}_4]\mathbf{3}$  with 4.0 equiv *n*-BuLi in 6.10 M THF-pentane recorded at  $-90\text{ }^\circ\text{C}$  after aging at  $-78\text{ }^\circ\text{C}$  for overnight



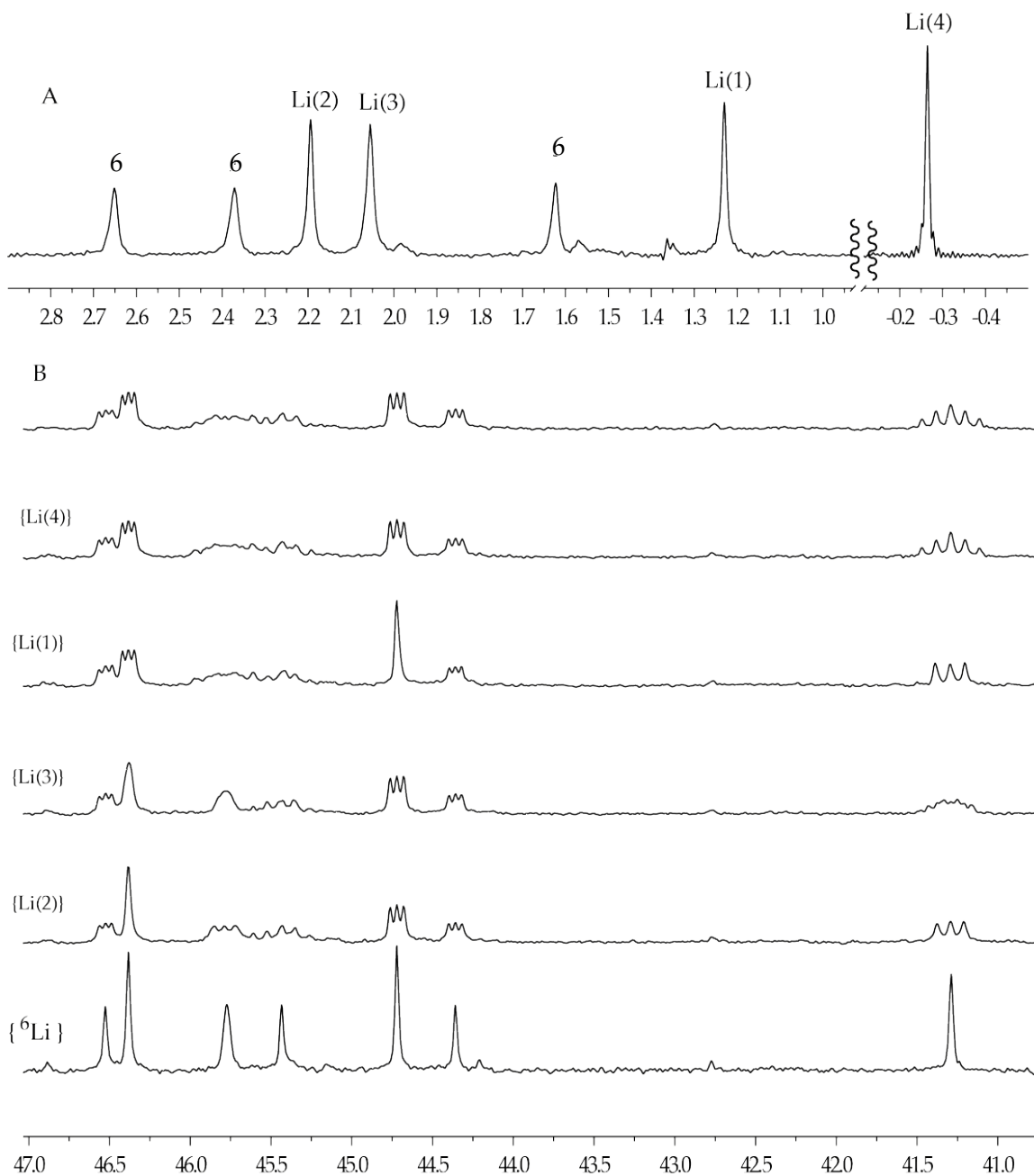
**Figure 20.**  ${}^6\text{Li}$  NMR spectra of 0.10 M  $[{}^6\text{Li}, {}^{15}\text{N}]\mathbf{8}$  prepared from  $[{}^{15}\text{N}_4]\mathbf{3}$  with 4.0 equiv *n*-BuLi and phenylacetic acid in 6.1 M THF-pentane recorded at  $-90\text{ }^\circ\text{C}$  after aging at  $-78\text{ }^\circ\text{C}$  for 2.0 hrs: (A) fully coupled  ${}^6\text{Li}$  spectrum; (B)  ${}^{15}\text{N}$  broad band decoupled. \*Indicate unassigned resonances.

| ${}^6\text{Li}$ | $\delta$ (ppm)   |
|-----------------|--|
| (1)             | 1.24 (dd, $J[\text{Li}_1\text{-N}_2]=4.3$ , $J[\text{Li}_1\text{-N}_1]=2.2$ Hz)                                    |
| (2)             | 2.20 (ddd, $J[\text{Li}_2\text{-N}_2]=4.8$ , $J[\text{Li}_2\text{-N}_3]=3.6$ , $J[\text{Li}_2\text{-N}_4]=1.9$ Hz) |
| (3)             | 2.06 (d, $J[\text{Li}_3\text{-N}_3]=5.6$ Hz)   |
| (4)             | -0.26 (s)  |

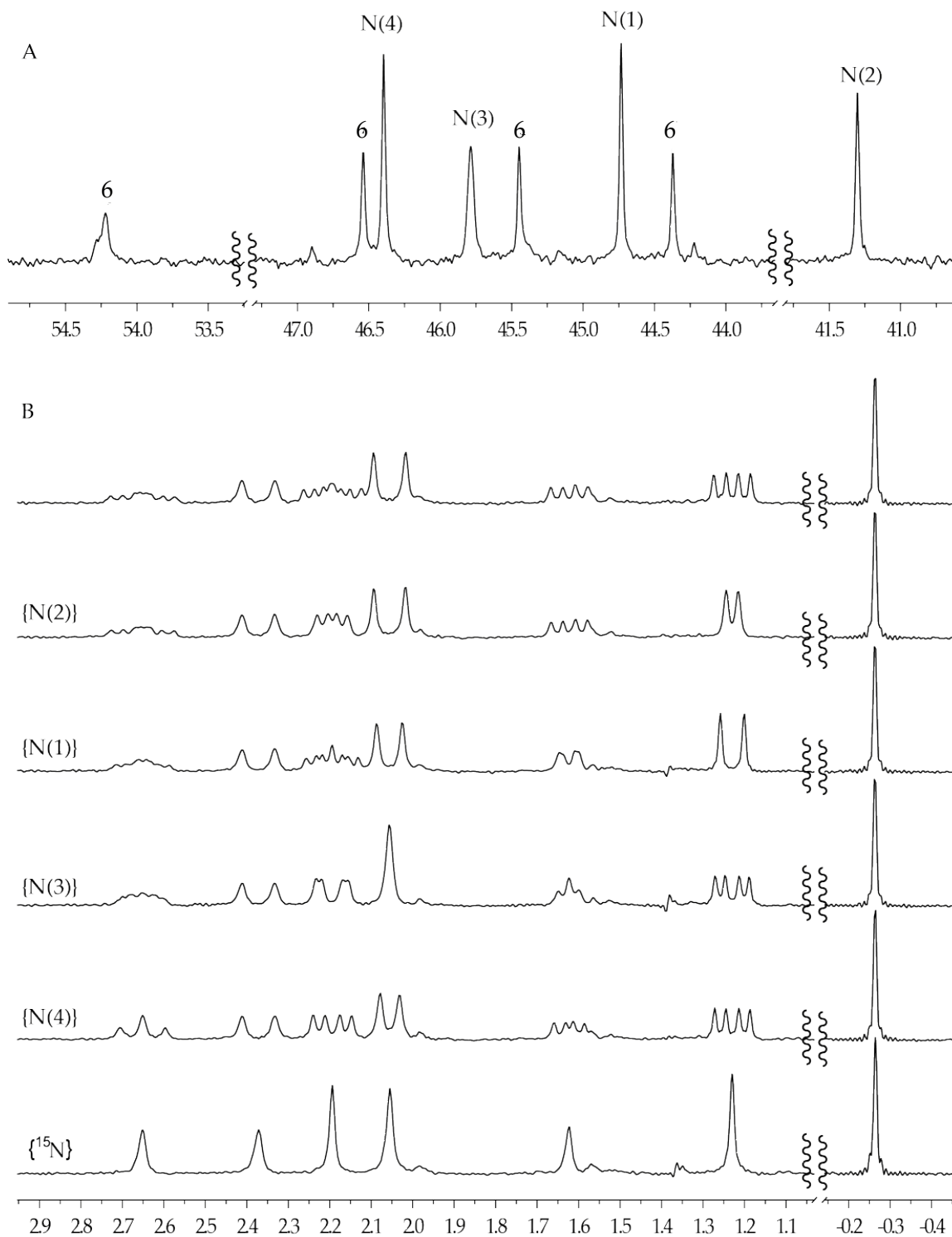


**Figure 21.**  $^{15}\text{N}$  NMR spectra of 0.10 M  $[\text{}^6\text{Li}, \text{}^{15}\text{N}]\mathbf{8}$  prepared from  $[\text{}^{15}\text{N}_4]\mathbf{3}$ , 4.0 equiv *n*-BuLi, and phenylacetic acid in 6.1 M THF-pentane recorded at  $-90\text{ }^\circ\text{C}$  after aging at  $-78\text{ }^\circ\text{C}$  for 2.0 hrs: (A) fully coupled; (B) broad band decoupled.

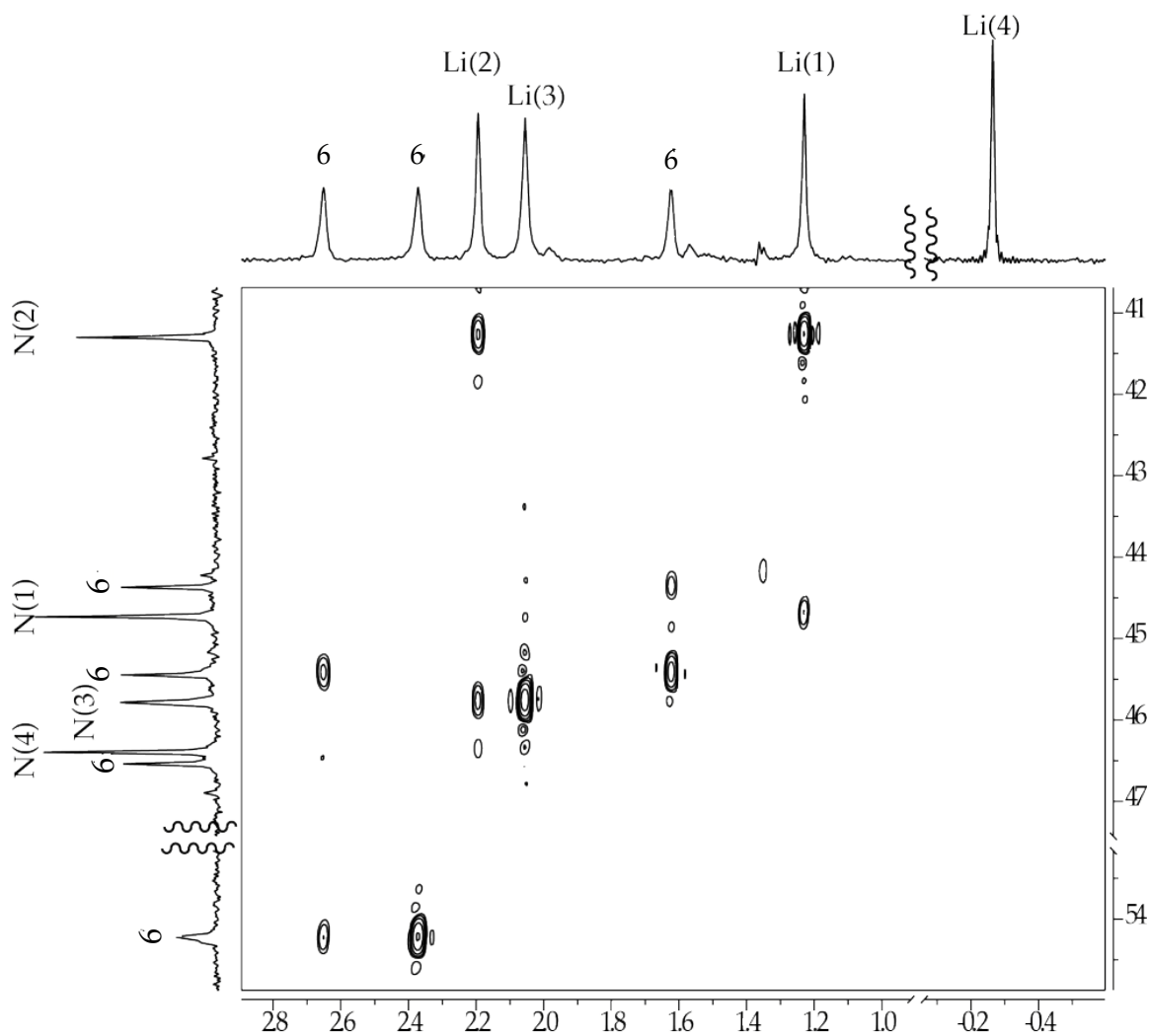
| $^{15}\text{N}$ | $\square$ (ppm)  |
|-----------------|--|
| 1               | 44.7 (t, $J[\text{N}_1\text{-Li}_1] = 2.2\text{ Hz}$ )                                     |
| 2               | 41.3 (p, $J[\text{N}_2\text{-Li}_2] = 4.8$ , $J[\text{N}_2\text{-Li}_1] = 4.3\text{ Hz}$ ) |
| 3               | 45.8 (m)   |
| 4               | 46.4 (t, , $J[\text{N}_4\text{-Li}_2] = 1.9\text{ Hz}$ )                                   |



**Figure 22.**  ${}^{15}\text{N}$  NMR spectra of 0.10 M  $[{}^6\text{Li}, {}^{15}\text{N}]\mathbf{8}$  prepared from  $[{}^{15}\text{N}_4]\mathbf{3}$ , 4.0 equiv *n*-BuLi, and phenylacetic acid in 6.1 M THF-pentane recorded at  $-90\text{ }^\circ\text{C}$  after aging at  $-78\text{ }^\circ\text{C}$  overnight: (A) fully coupled  ${}^6\text{Li}$  spectrum ; (B) selective decoupling of Li4 ( $-0.26\text{ ppm}$ ), Li1 ( $2.06\text{ ppm}$ ), Li3 ( $2.20\text{ ppm}$ ), Li2 ( $1.20\text{ ppm}$ ), and broadband decoupling.

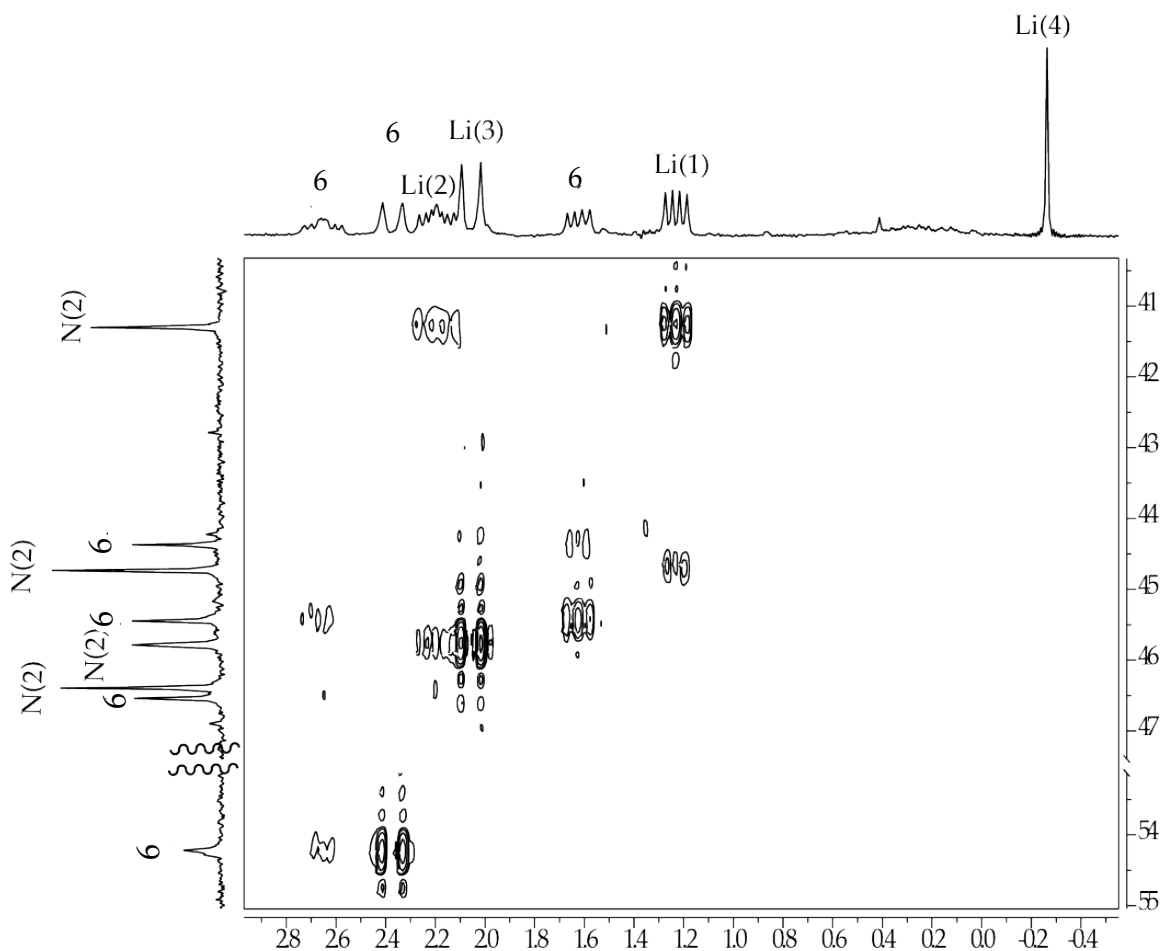


**Figure 23.**  ${}^6\text{Li}$  NMR spectra of 0.10 M  $[{}^6\text{Li}, {}^{15}\text{N}]\mathbf{8}$  prepared from  $[{}^{15}\text{N}_4]\mathbf{3}$ , 4.0 equiv *n*-BuLi, and phenylacetic acid in 6.1 M THF-pentane recorded at  $-90\text{ }^\circ\text{C}$  after aging at  $-78\text{ }^\circ\text{C}$  overnight: (A) fully coupled  ${}^{15}\text{N}$  spectrum ; (B) selective decoupling of N2 (41.3 ppm), N1 (44.7 ppm), N3 (45.8 ppm), N4 (46.4 ppm), and broadband decoupling.



**Figure 24.**  $[^6\text{Li}, ^{15}\text{N}]$ HMQC NMR spectrum of a mixture 0.10 M  $[^6\text{Li}, ^{15}\text{N}]$ 6 and  $[^6\text{Li}, ^{15}\text{N}]$ 8 prepared from  $[^{15}\text{N}_4]$ 3, 4.0 equiv *n*-BuLi, and phenylacetic acid in 0.10 M THF-pentane recorded at  $-90\text{ }^\circ\text{C}$  after aging at  $-78\text{ }^\circ\text{C}$  overnight. The spectrum was recorded with broadband  $^6\text{Li}$  and  $^{15}\text{N}$  decoupling.





**Figure 25.** [ $^6\text{Li}$ ,  $^{15}\text{N}$ ] HMQC NMR spectrum of 0.10 M mixture of [ $^6\text{Li}$ ,  $^{15}\text{N}$ ]6 and [ $^6\text{Li}$ ,  $^{15}\text{N}$ ]8 prepared from [ $^{15}\text{N}_4$ ]3, 4.0 equiv *n*-BuLi, and phenylacetic acid in 6.10 M THF-pentane recorded at  $-90\text{ }^\circ\text{C}$  after aging at  $-78\text{ }^\circ\text{C}$  overnight. The spectrum was recorded with broadband  $^6\text{Li}$  decoupling.

## Part 3: 2D NMR [ $^1\text{H}$ and $^{13}\text{C}$ ] Spectroscopic Studies

### 2D-NMR Experimental and Analysis

**2D-NMR analysis of the diamine-acid enolate complex:** A sample containing a 1:0.6 ratio of lithium diamide/acid enolate and lithium dimaide/ $n\text{BuLi}$  aggregates in THF- $d_8$ /pentane was studied by standard 2D NMR techniques (COSY, TOCSY, HSQC, HMBC and ROESY) at  $-80^\circ\text{C}$ . These experiments allowed the assignment of most  $^1\text{H}$  and  $^{13}\text{C}$  resonances for both aggregates. Signal overlap in both  $^1\text{H}$  and  $^{13}\text{C}$  dimensions prevented unambiguous assignment of some piperidyl and phenyl resonances. Scalar coupling constants derived from COSY and HSQC experiments yielded dihedral angle information for the diamide backbone. The ROESY experiment yielded a large number of interatomic distance constraints as well as information on exchange processes.

**Experimental:** 2D NMR spectra were acquired on a 500 MHz Varian INOVA spectrometer operating at 499.76 MHz for  $^1\text{H}$  observation using a 5 mm Varian DBG dual broadband probehead with single-axis pulsed field gradient. Sample temperature was maintained at  $-80^\circ\text{C}$  as calibrated with a neat methanol sample.  $^1\text{H}$  and  $^{13}\text{C}$  chemical shifts were referenced to the residual downfield THF- $d_5$  resonance at 3.58 ppm and 67.57 ppm, respectively. 2D experiments were acquired using standard pulse sequences supplied in VnmrJ 2.2D/Chempack 4.1 (Agilent Inc.) and processed and analyzed in MestReNova 8.0.2 (Mestrelab Research S.L.).

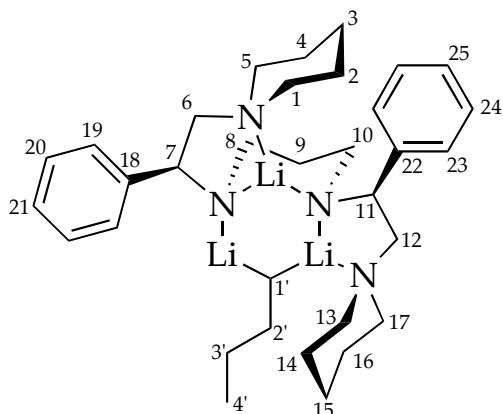
**Conformation of the amide backbone:** For the purposes of the following discussion, the Li-containing ring will be defined as the central plane of the aggregates. Bottom and below refer to the same side as the C-8–C-10 linker and top and above refer to the side opposite the linker. The diamide backbone appears to have very similar conformation in both mixed aggregates in solution and is also in agreement with the conformation observed in solid state and predicted by theory. We did not observe exchange for the diamide backbone in ROESY spectra—all diamide-related cross peaks with the same phase as the diagonal could be readily interpreted as relayed ROEs—indicating that no other conformations are accessed on the NMR time scale. The C-8 to C-10 linker adopts a fixed chair conformation with C-9 positioned under the central plane as evidenced by the large geminal and axial-axial couplings ( $\sim 12$  Hz) observed in the HSQC cross peaks, and ROEs observed between H-7 and H-8<sub>ax</sub> as well as H-11 and H-10<sub>eq</sub>. We observed large couplings ( $\sim 12$  Hz) between H-6<sub>top</sub> and H-7 as well as H-11<sub>top</sub> and H-12', consistent with dihedral angles approaching  $180^\circ$ , and allowing top/bottom assignment of the C-6 and C-12 methylene hydrogens. The large dihedral angle shows that one of two carbons of the five-membered rings must be puckered out of the plane, and that these rings are either conformationally rigid or such conformations dominate in a rapidly interconverting system. The piperidyl residues are most likely in chair conformations based on coupling patterns observed in HSQC. The Li-N bond occupies the axial position for both piperidines as evidenced by ROEs between H-6<sub>top</sub>/H-12<sub>top</sub> and both axial  $\alpha$ -hydrogens on the respective rings. Top/bottom assignment was based on ROEs between H-7/H-11 and the equatorial  $\alpha$ -

hydrogens on the top edge as well as H-6<sub>bottom</sub>/H-12<sub>bottom</sub> and both equatorial and axial  $\alpha$ -hydrogens on the bottom edge. The methine hydrogens (H-7 and H-11) gave 3-bond HMBC correlations to single carbon chemical-shifts in the ortho aromatic region indicating side-to-side equivalence of the phenyl rings on the diamide consistent with rapid rotation.

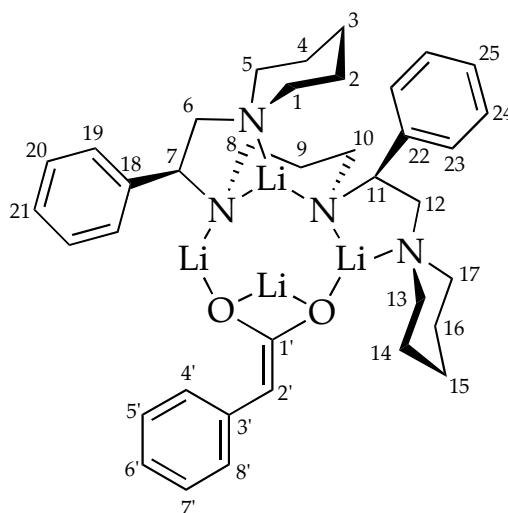
**Conformation of the acid enolate:** ROE correlations between the vinylic hydrogen and the equatorial  $\alpha$ -, and axial  $\beta$ -hydrogens of the *top* face of the proximal piperidine confirms the side-to-side orientation of the enolate and strongly suggests that the enolate projects above the central plane. The resonances corresponding to the ortho-hydrogens of the enolate appeared as very broad singlets at 6.30 and 7.51 ppm. Three-bond HMBC correlations from both vinylic and para-hydrogens indicated the presence of two distinct ortho-carbon environments at 119.16 and 121.79 ppm, with noticeable broadening in the carbon dimension. These results indicate that the rotation of the aromatic ring is restricted, either due to steric or electronic reasons, and is intermediate on these NMR time scales ( $\sim 1$  ms). The anomalously-high chemical shift of one ortho-hydrogen is likely due to the ring current effect of the proximal phenyl group of the diamide.

**Conformation of the *n*BuLi:** The 1D proton spectrum displayed two broadened triplets centered around -1 ppm instead of the AA'XX' multiplet usually observed in achiral *n*BuLi aggregates where restricted rotation around the C-1–C-2 bond causes magnetic non-equivalence of the  $\alpha$ -hydrogens. The presence of two unique chemical shifts for *n*BuLi  $\alpha$ -hydrogens is consistent with diastereotopicity induced by the diamide. In the ROESY spectrum strong exchange is observed between the  $\alpha$ -hydrogens indicating intermediate exchange on their NMR time scale ( $\sim 5$  ms). The fact that the diastereotopic hydrogens of the  $\beta$  and  $\gamma$  methylenes also display unique chemical shifts despite much longer time scales ( $\sim 1$ s) suggests that the exchange of the  $\alpha$ -hydrogens arises from an intramolecular process that intraconverts those hydrogens, consistent with the well-known racemization of chiral lithiated carbon atoms.

We observed four ROE correlations between the two *n*-butyl  $\alpha$ -hydrogens and the top equatorial  $\alpha$ -hydrogens of both piperidines. Careful examination of the cross peaks revealed an asymmetry of intensities, suggesting that one set arose from direct ROE, and the other from chemical exchange followed by ROE. This result contradicts the dimeric structure observed in solid state, which predicts that only a single set of ROEs would be observed between one butyl hydrogen and H-1<sub>eq</sub> of the diamide. The NMR results can be explained by exchanging the appropriate hydrogen and propyl substituents on the lithiated carbon, so the chain extends away from the central plane instead of above the plane as seen in the crystal structure, suggesting that the aggregate is monomeric in THF solutions.



Diamide *n*-Buli aggregate



Diamide-enolate aggregate

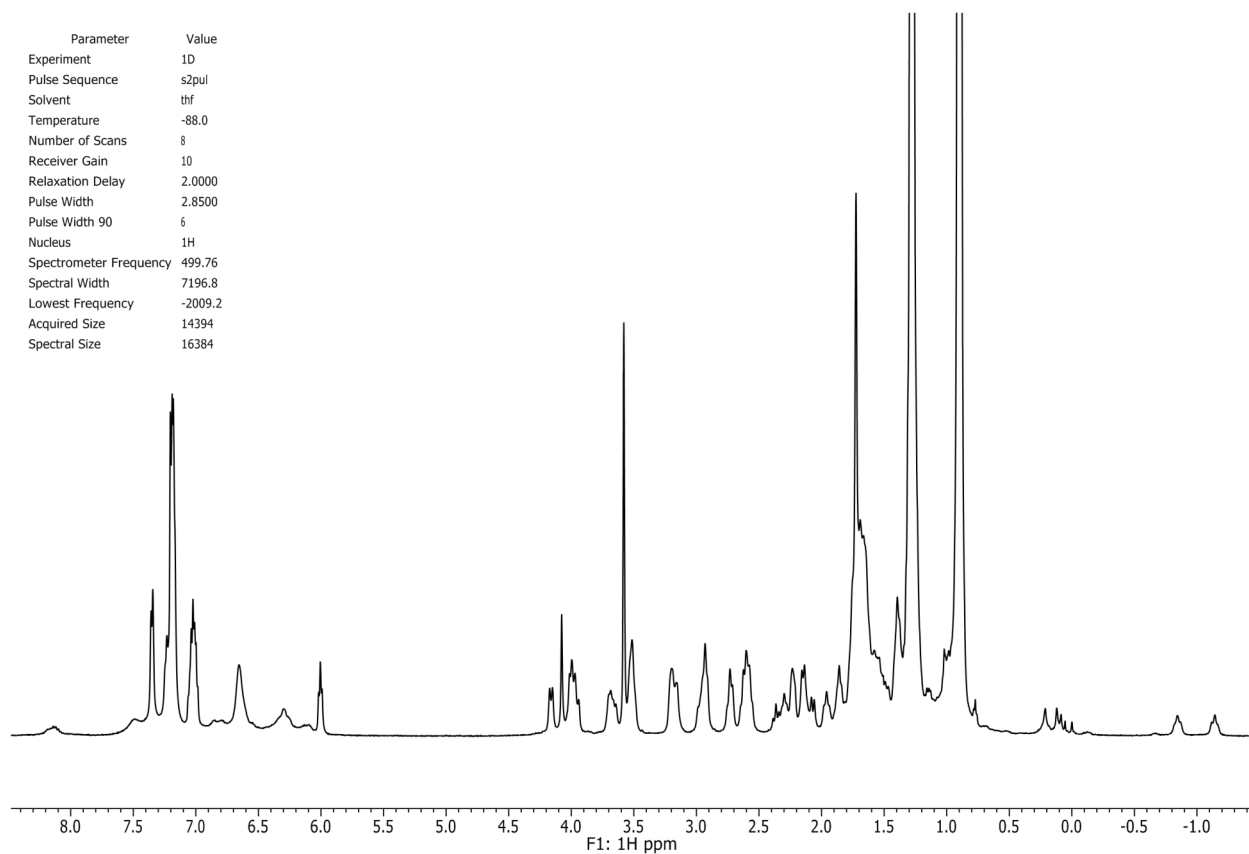
| Atom # | $\square$ $^{13}\text{C}$ (ppm) | $\square$ $^1\text{H}$ (ppm) | Multiplicity <sup>1</sup> | $\square$ $^{13}\text{C}$ (ppm) | $\square$ $^1\text{H}$ (ppm) | Multiplicity <sup>1</sup> |
|--------|---------------------------------|------------------------------|---------------------------|---------------------------------|------------------------------|---------------------------|
| 1      | 58.17                           | eq. 2.98<br>ax. 1.85         | d<br>t                    | 58.33                           | eq. 3.16<br>ax. 1.70         | d<br>t                    |
| 2      | n/d <sup>2</sup>                | n/d                          | n/d                       | n/d                             | n/d                          | n/d                       |
| 3      | n/d                             | n/d                          | n/d                       | 24.90                           | eq. 1.40<br>ax. 0.95         | d<br>q                    |
| 4      | n/d                             | n/d                          | n/d                       | 26.85                           | ax. 1.14<br>eq. 1.00         | q<br>d                    |
| 5      | 54.28                           | eq. 3.66<br>ax. 1.66         | d<br>t                    | 55.58                           | eq. 3.70<br>ax. 1.66         | d<br>q                    |
| 6      | 71.99                           | 2.61<br>2.07                 | t<br>d                    | 73.22                           | 2.59<br>2.15                 | t<br>d                    |
| 7      | 69.80                           | 3.95                         | d                         | 70.70                           | 4.17                         | d                         |
| 8      | 61.09                           | eq. 3.20<br>ax. 2.57         | d<br>t                    | 61.69                           | eq. 2.52<br>ax. 2.30         | d<br>t                    |
| 9      | 37.39                           | eq. 1.74<br>ax. 1.39         | d<br>q                    | 37.41                           | eq. 1.69<br>ax. 1.55         | d<br>q                    |
| 10     | 60.58                           | ax. 2.93<br>eq. 2.72         | t<br>d                    | 61.69                           | eq. 2.94<br>ax. 2.73         | d<br>t                    |
| 11     | 68.35                           | 3.99                         | d                         | 67.93                           | 4.00                         | d, J=12.5 Hz              |
| 12     | 74.15                           | 2.36<br>bot. 2.22            | t<br>d                    | 73.64                           | 2.63<br>2.23                 | t<br>d                    |
| 13     | 58.19                           | eq. 2.92<br>ax. 1.86         | d<br>t                    | 57.98                           | eq. 3.20<br>ax. 1.96         | d<br>t                    |
| 14     | n/d                             | n/d                          | n/d                       | 27.24                           | ax. 2.14<br>eq. 1.77         | q<br>d                    |
| 15     | n/d                             | n/d                          | n/d                       | n/d                             | n/d                          |                           |
| 16     | n/d                             | n/d                          | n/d                       | n/d                             | n/d                          |                           |
| 17     | n/d                             | n/d                          | n/d                       | 54.51                           | eq. 3.50<br>ax. 1.74         | d<br>t                    |

|    |                            |                            |        |                              |                            |             |
|----|----------------------------|----------------------------|--------|------------------------------|----------------------------|-------------|
| 18 | 150.17                     | —                          |        | 150.70                       | —                          |             |
| 19 | 127.72                     | ~                          |        | 128.56                       | 7.35                       | d           |
| 20 | 127–<br>128.1 <sup>3</sup> | 7.15–<br>7.21 <sup>3</sup> |        | 127.0–<br>128.1 <sup>3</sup> | 7.18                       | t           |
| 21 | 124.9–<br>126 <sup>3</sup> | 6.97–<br>7.07 <sup>3</sup> |        | 125.06                       | 7.02                       | t           |
| 22 | 148.52                     |                            |        | 150.08                       | —                          |             |
| 23 | 128.72                     | 7.24                       |        | 127.7–<br>128.1 <sup>3</sup> | 7.19                       |             |
| 24 | 127.0–<br>128.1            | 7.15–<br>7.21 <sup>3</sup> |        | 127.0–<br>128.1 <sup>3</sup> | 7.15–<br>7.21 <sup>3</sup> |             |
| 25 | 124.9–126                  | 6.97–<br>7.07 <sup>3</sup> |        | 124.9–<br>126 <sup>3</sup>   | 6.97–<br>7.07 <sup>3</sup> |             |
| 1' | 11.78                      | -0.86                      | t (br) | 179.83                       | —                          |             |
|    |                            | -1.14                      | t (br) |                              |                            |             |
| 2' | 34.47                      | 1.66                       | n/d    | 72.58                        | 4.08                       | s           |
|    |                            | 1.62                       |        |                              |                            |             |
| 3' | 34.94                      | 1.36                       | n/d    | 149.81                       | —                          |             |
|    |                            | 1.31                       |        |                              |                            |             |
| 4' | n/d                        | 0.92                       | n/d    | 119.16<br>(br)               | 7.51                       | s (br)      |
| 5' |                            |                            |        | 127.71                       | 6.65                       | s (br)      |
| 6' |                            |                            |        | 111.77                       | 6.01                       | t, J=9.6 Hz |
| 7' |                            |                            |        | 127.71                       | 6.65                       | s (br)      |
| 8' |                            |                            |        | 121.72                       | 6.30                       | s (br)      |

<sup>1</sup> Gross multiplicity as determined from cross peak profiles of 2D experiments and does not include small couplings.

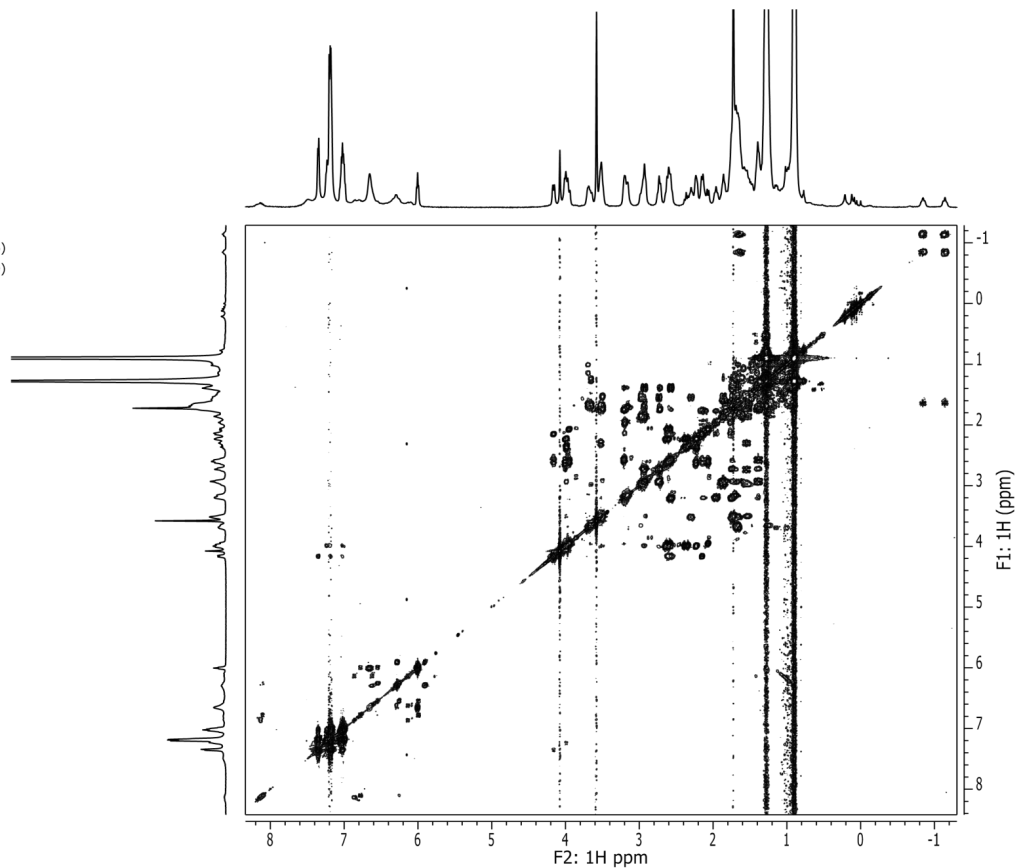
<sup>2</sup> Could not be determined.

<sup>3</sup> Could not be determined unambiguously, range or values given.

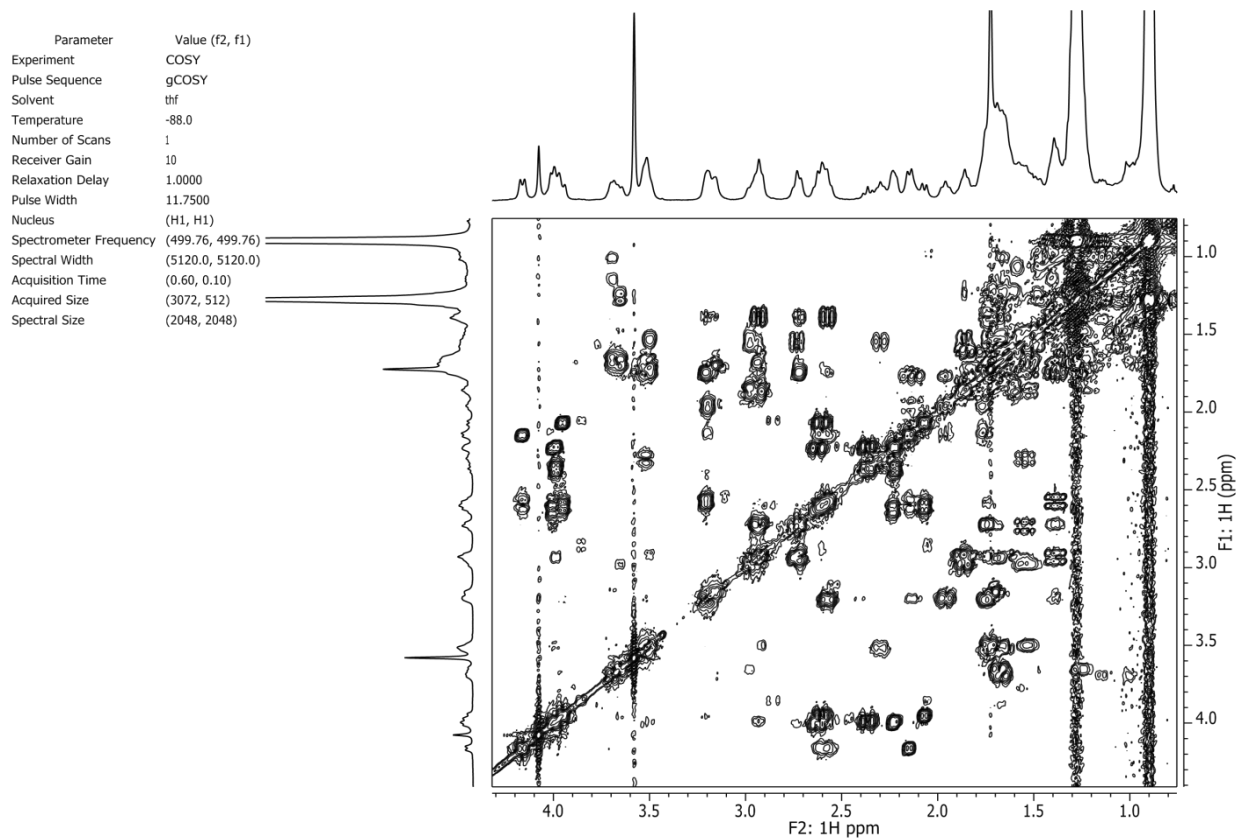


**Figure 26.** <sup>1</sup>H spectrum at -80°C of a sample in THF-*d*<sub>8</sub>/pentane containing a 1:0.6 ratio of diamide/acid enolate and diamide/*n*-BuLi aggregates.

| Parameter              | Value (f2, f1)   |
|------------------------|------------------|
| Experiment             | COSY             |
| Pulse Sequence         | gCOSY            |
| Solvent                | thf              |
| Temperature            | -88.0            |
| Number of Scans        | 1                |
| Receiver Gain          | 10               |
| Relaxation Delay       | 1.0000           |
| Pulse Width            | 11.7500          |
| Nucleus                | (H1, H1)         |
| Spectrometer Frequency | (499.76, 499.76) |
| Spectral Width         | (5120.0, 5120.0) |
| Acquisition Time       | (0.60, 0.10)     |
| Acquired Size          | (3072, 512)      |
| Spectral Size          | (2048, 2048)     |



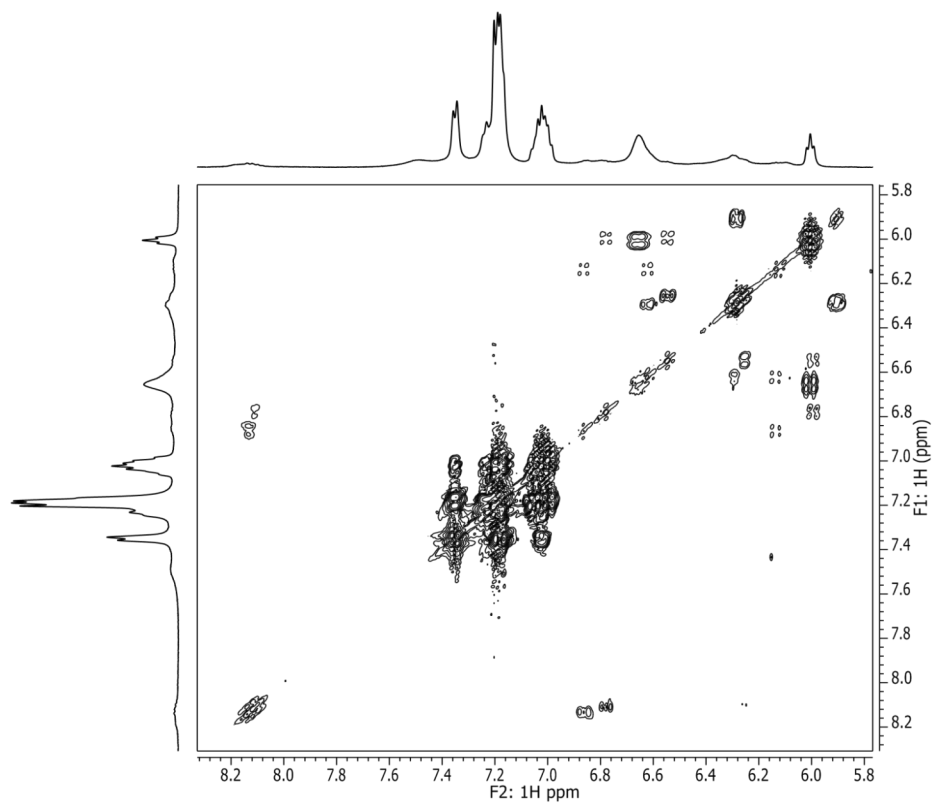
**Figure 27.** Full display of gradient-COSY spectrum at -80°C.



**Figure 28** Expansion of the aliphatic region of gradient-COSY spectrum at  $-80^{\circ}\text{C}$ .

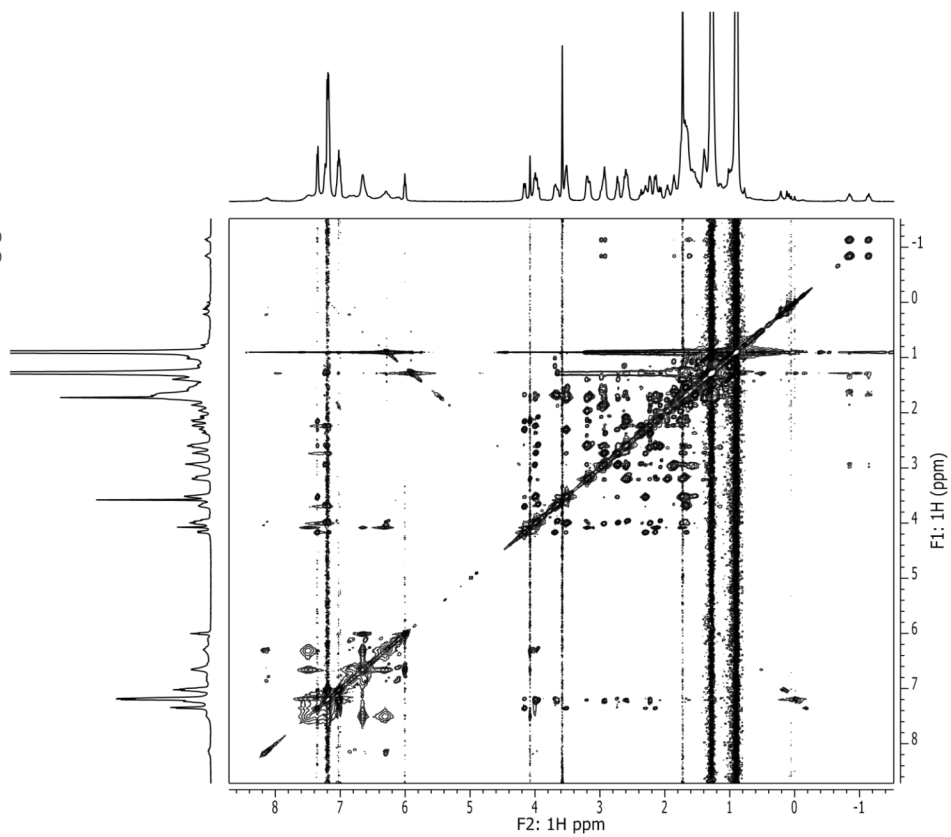


| Parameter              | Value (f2, f1)   |
|------------------------|------------------|
| Experiment             | COSY             |
| Pulse Sequence         | gCOSY            |
| Solvent                | thf              |
| Temperature            | -88.0            |
| Number of Scans        | 1                |
| Receiver Gain          | 10               |
| Relaxation Delay       | 1.0000           |
| Pulse Width            | 11.7500          |
| Nucleus                | (H1, H1)         |
| Spectrometer Frequency | (499.76, 499.76) |
| Spectral Width         | (5120.0, 5120.0) |
| Acquisition Time       | (0.60, 0.10)     |
| Acquired Size          | (3072, 512)      |
| Spectral Size          | (2048, 2048)     |

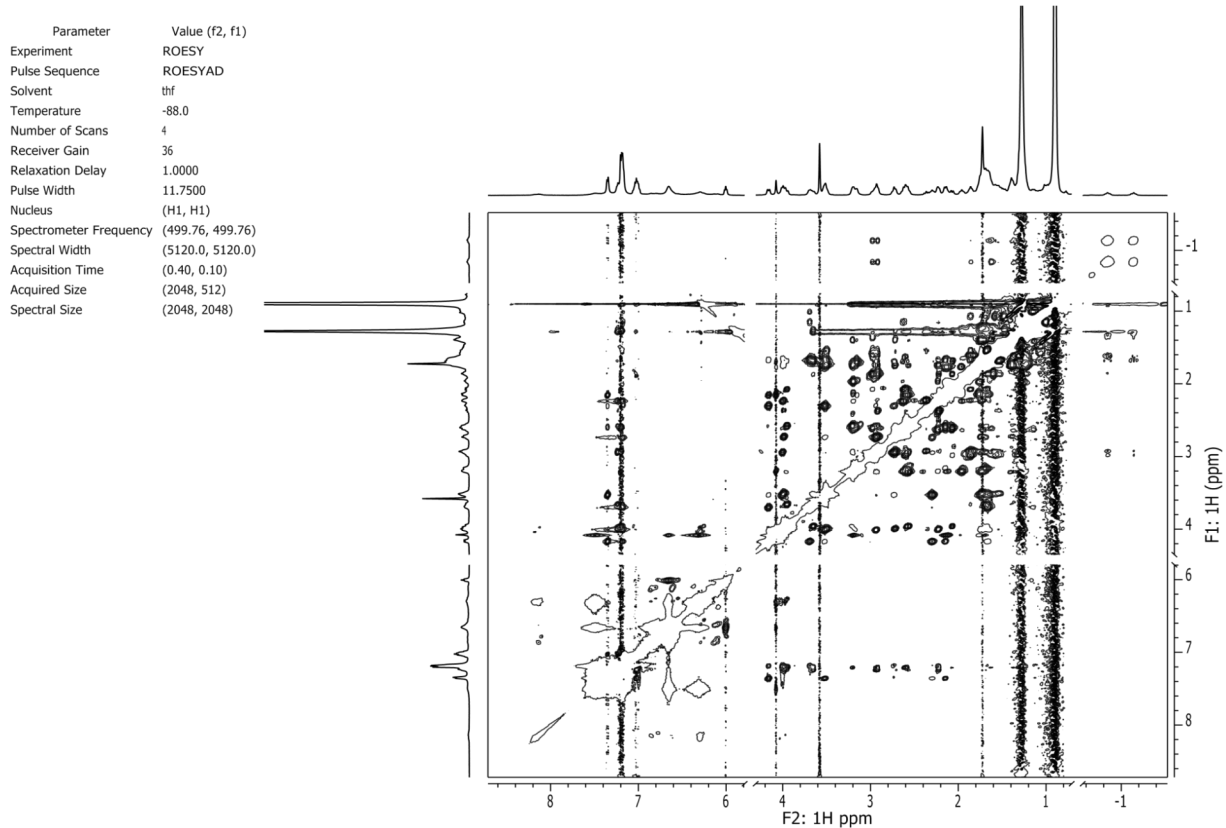


**Figure 29.** Expansion of the aromatic region of gradient-COSY spectrum at -80°C.

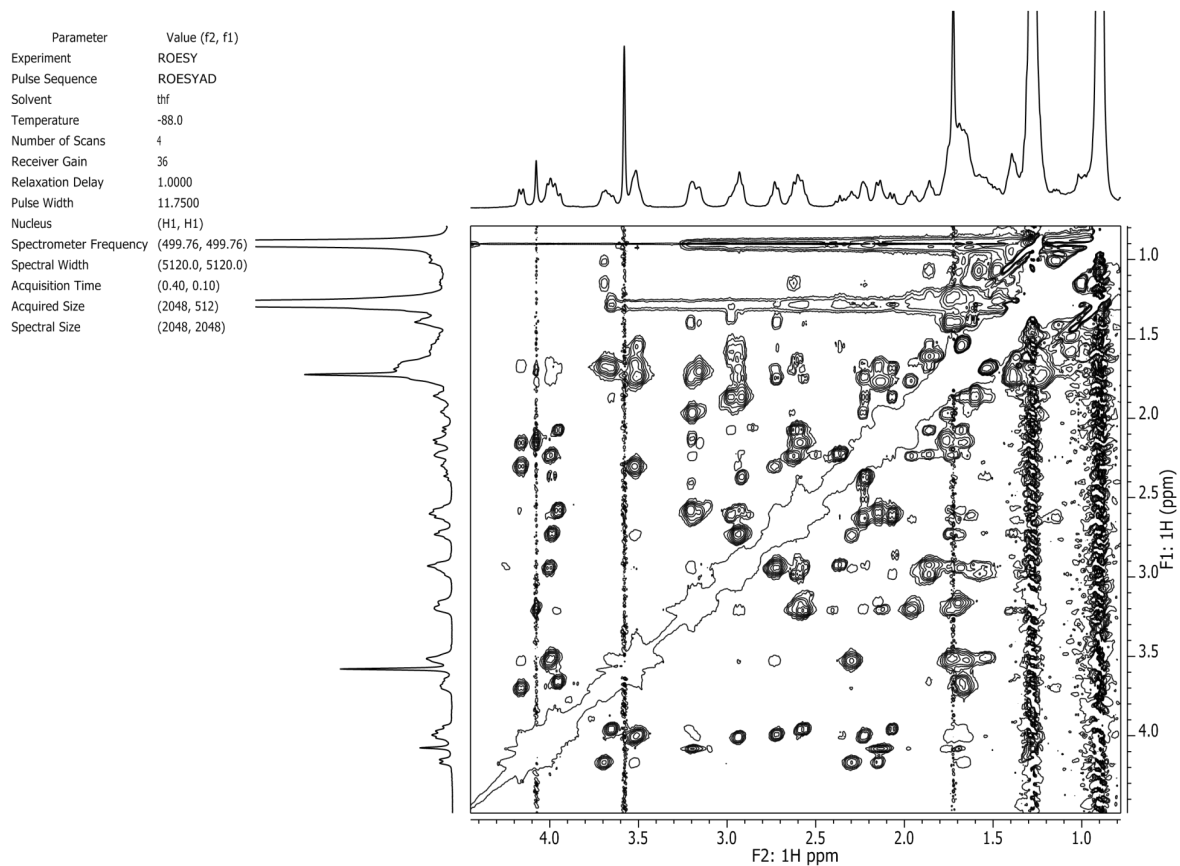
| Parameter              | Value (f2, f1)   |
|------------------------|------------------|
| Experiment             | ROESY            |
| Pulse Sequence         | ROESYAD          |
| Solvent                | thf              |
| Temperature            | -88.0            |
| Number of Scans        | 4                |
| Receiver Gain          | 36               |
| Relaxation Delay       | 1.0000           |
| Pulse Width            | 11.7500          |
| Nucleus                | (H1, H1)         |
| Spectrometer Frequency | (499.76, 499.76) |
| Spectral Width         | (5120.0, 5120.0) |
| Acquisition Time       | (0.40, 0.10)     |
| Acquired Size          | (2048, 512)      |
| Spectral Size          | (2048, 2048)     |



**Figure 30.** Full display of ROESY spectrum with 80 ms mixing time at -80°C.

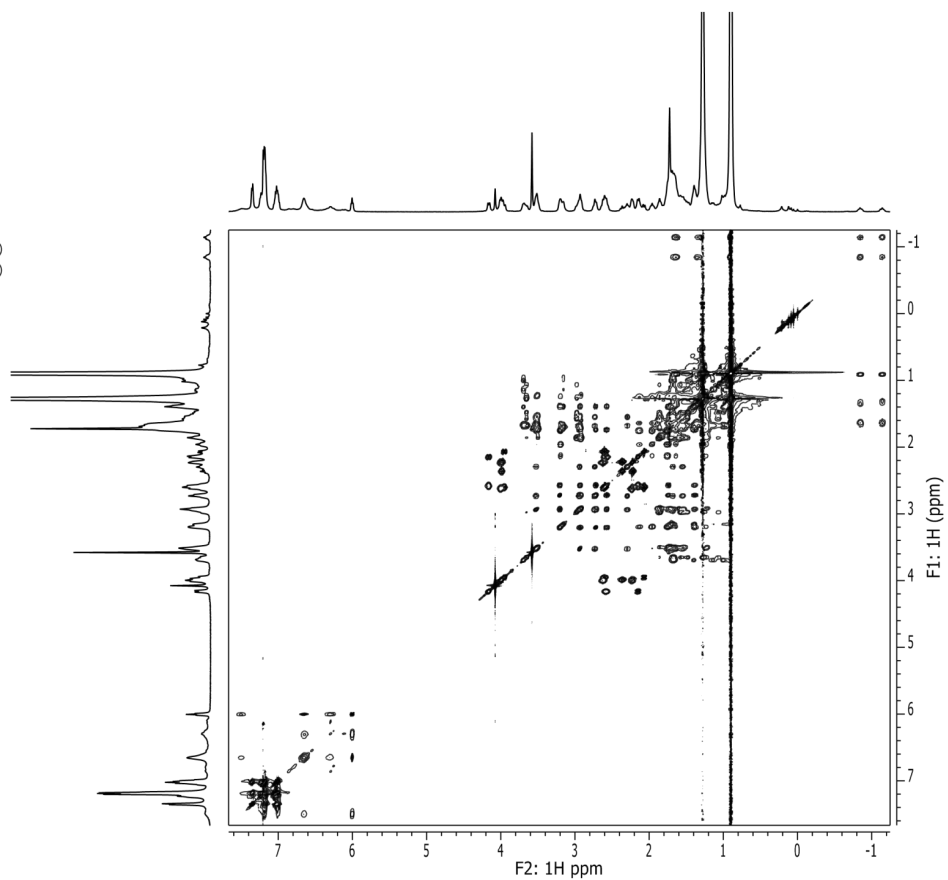


**Figure 31.** ROESY spectrum with 80 ms mixing time at  $-80^{\circ}\text{C}$  with regions of noise excised, ten positive contour levels (ROE's) and a single negative contour level (diagonal, exchange and relayed ROE's).

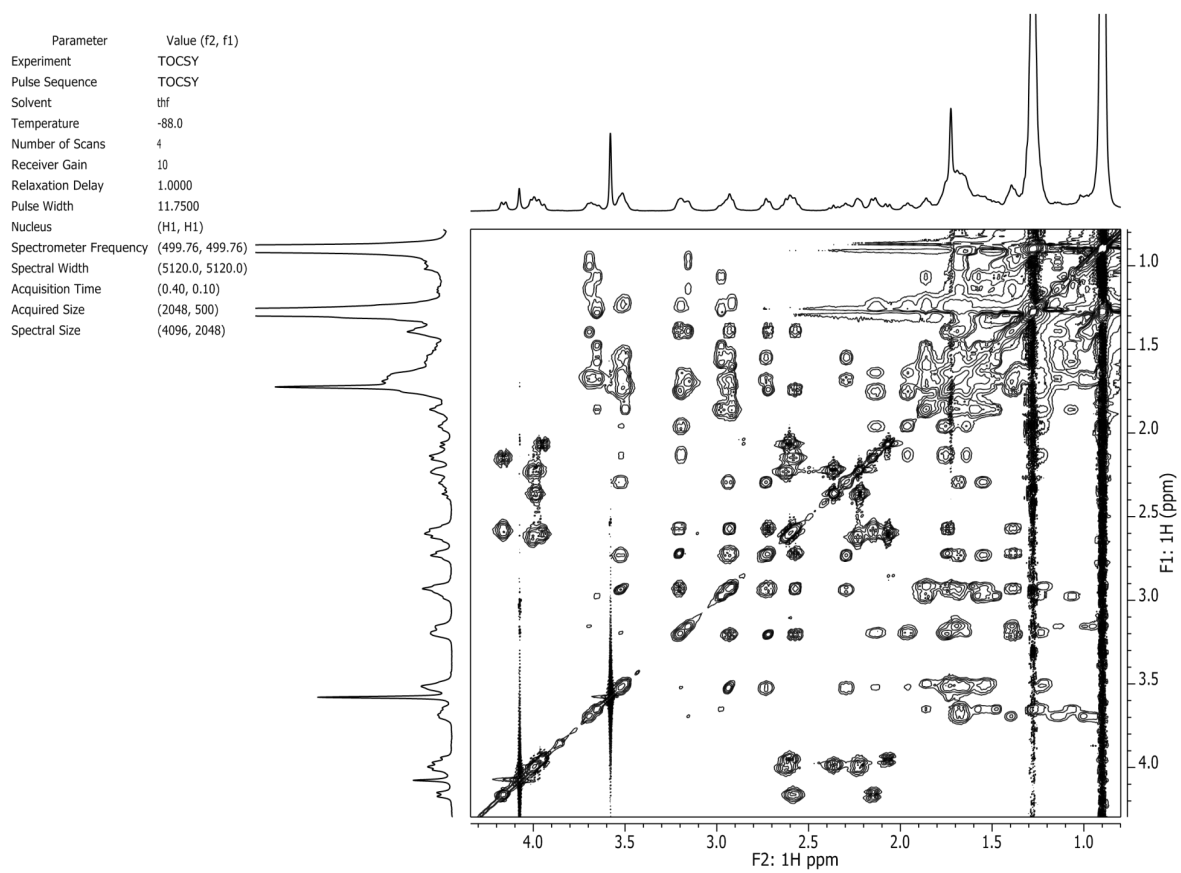


**Figure 32.** Expansion of the aliphatic region of ROESY spectrum with 80 ms mixing time at  $-80^{\circ}\text{C}$  with ten positive contour levels (ROE's) and a single negative contour level (diagonal and relayed ROE's).

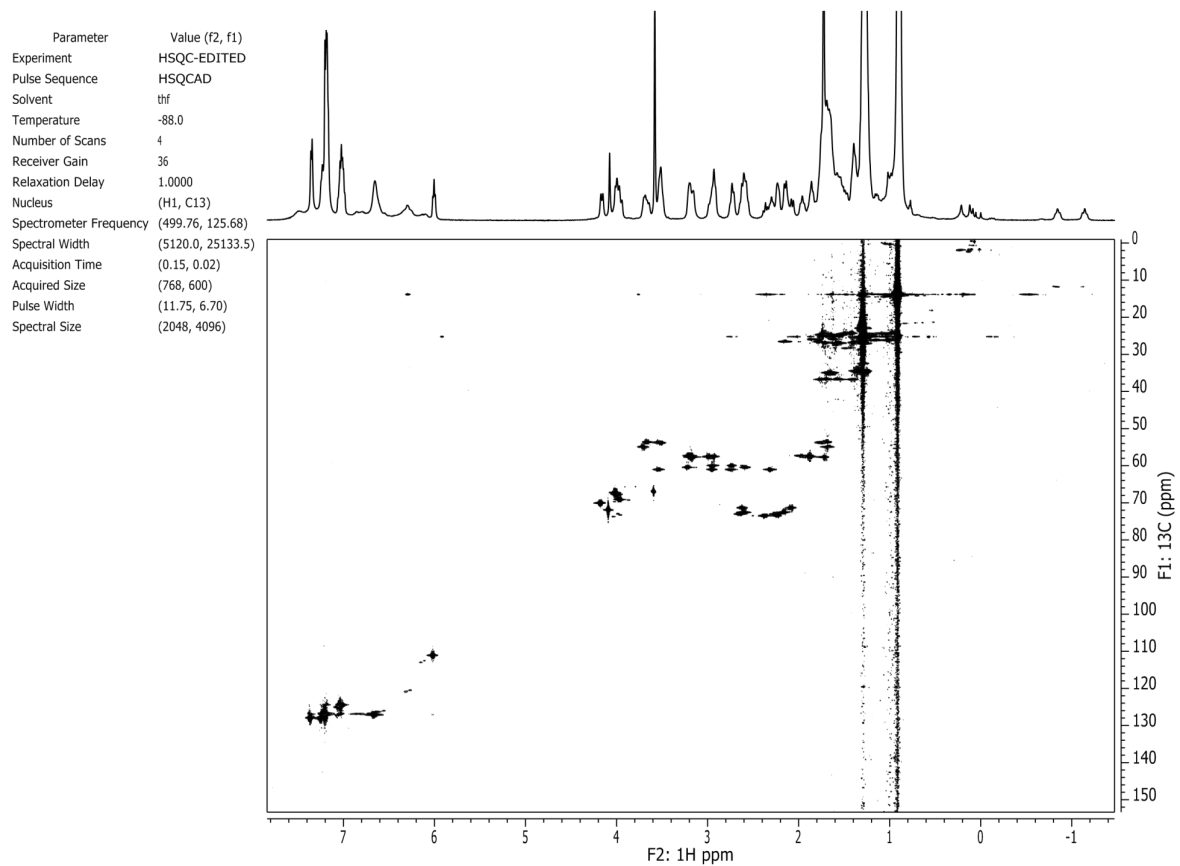
| Parameter              | Value (f2, f1)   |
|------------------------|------------------|
| Experiment             | TOCSY            |
| Pulse Sequence         | TOCSY            |
| Solvent                | thf              |
| Temperature            | -88.0            |
| Number of Scans        | 4                |
| Receiver Gain          | 10               |
| Relaxation Delay       | 1.0000           |
| Pulse Width            | 11.7500          |
| Nucleus                | (H1, H1)         |
| Spectrometer Frequency | (499.76, 499.76) |
| Spectral Width         | (5120.0, 5120.0) |
| Acquisition Time       | (0.40, 0.10)     |
| Acquired Size          | (2048, 500)      |
| Spectral Size          | (4096, 2048)     |



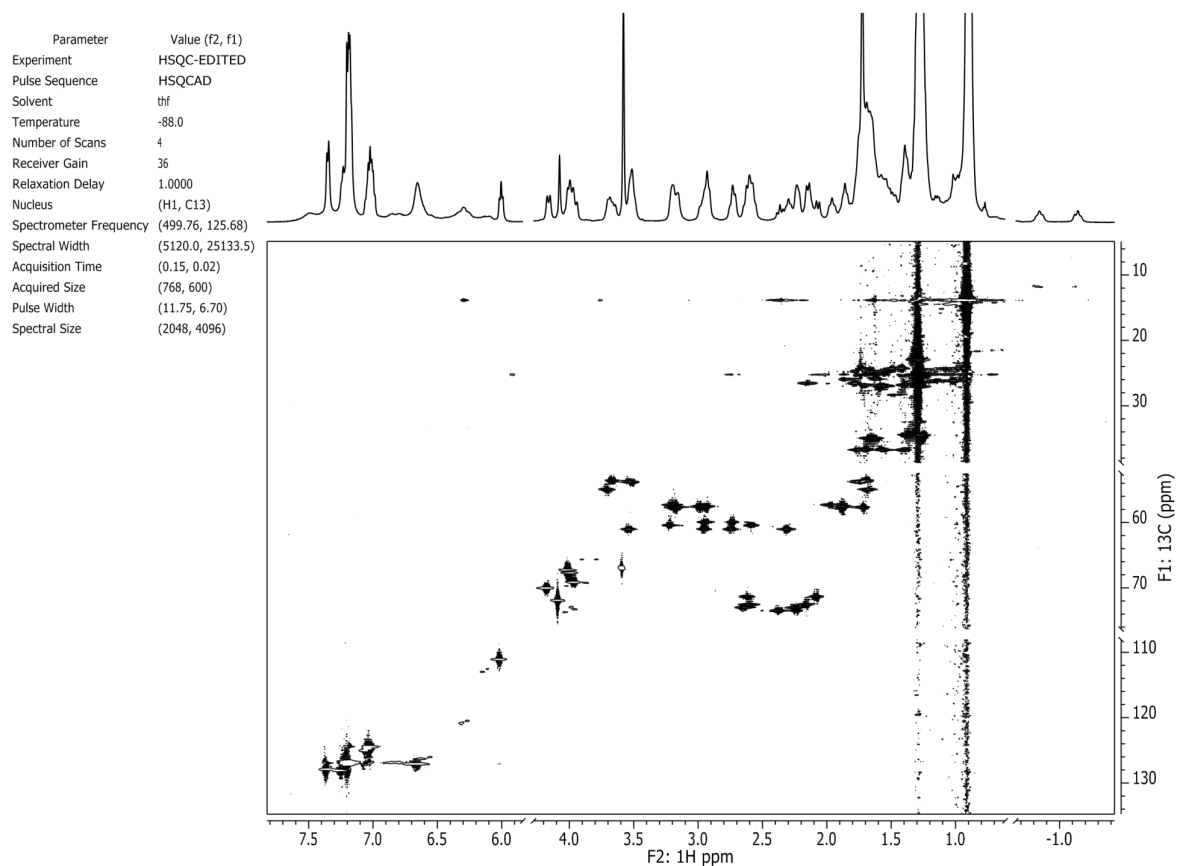
**Figure 33.** Full display of TOCSY spectrum at -80°C.



**Figure 34.** Expansion of the aliphatic region of TOCSY spectrum at  $-80^{\circ}\text{C}$ .

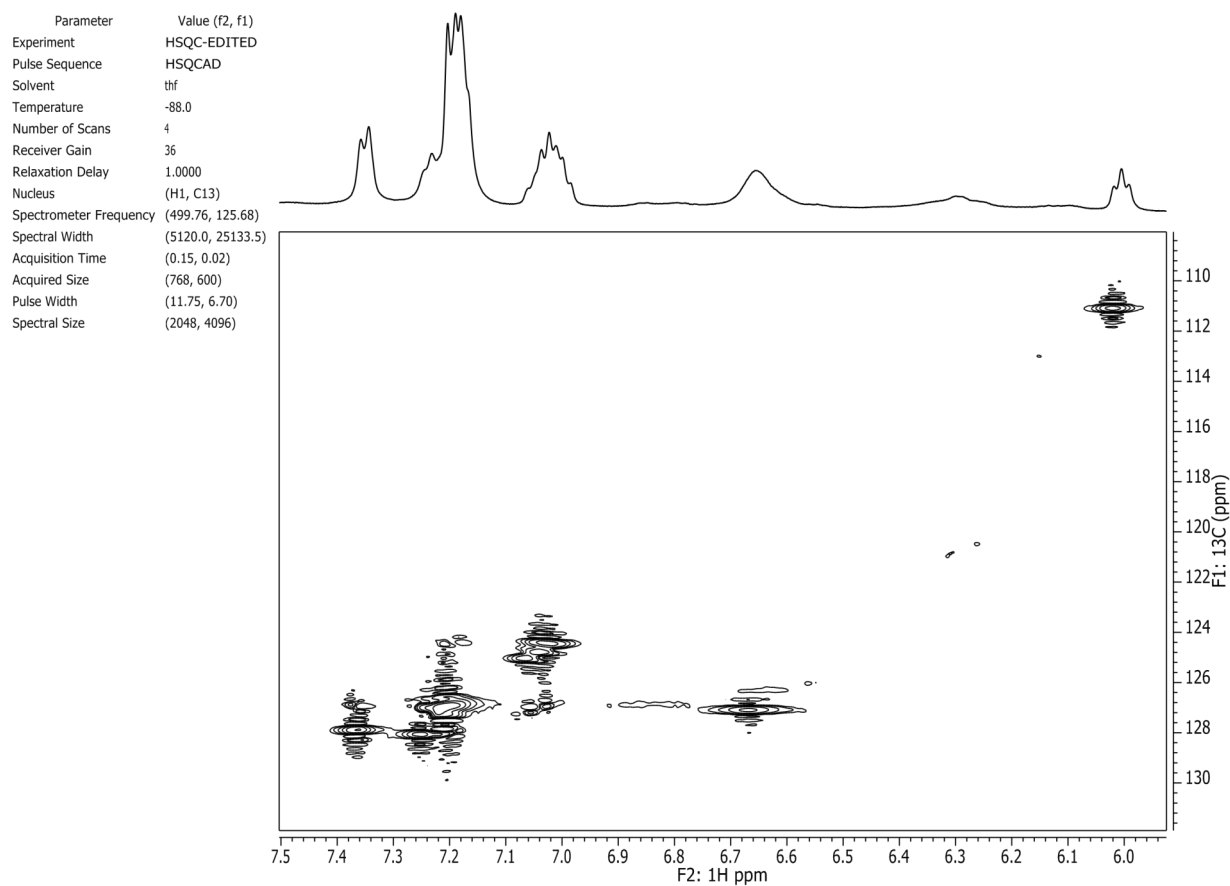


**Figure 35.** Full display of multiplicity-edited HSQC spectrum at  $-80^{\circ}\text{C}$ .



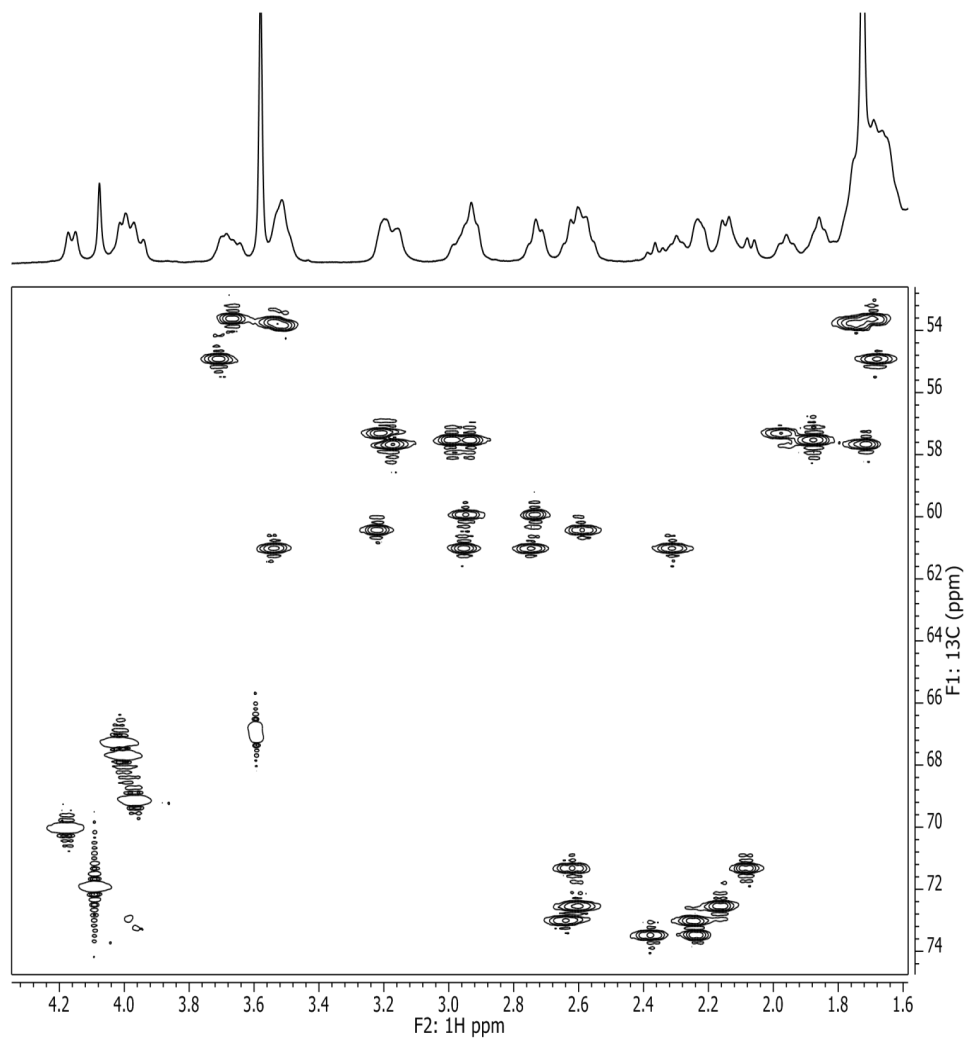
**Figure 36.** Multiplicity-edited HSQC spectrum at  $-80^{\circ}\text{C}$  with regions of noise excised, ten negative contour levels ( $\text{CH}_2$ ) and a single positive contour ( $\text{CH}_3$  and  $\text{CH}$ ).



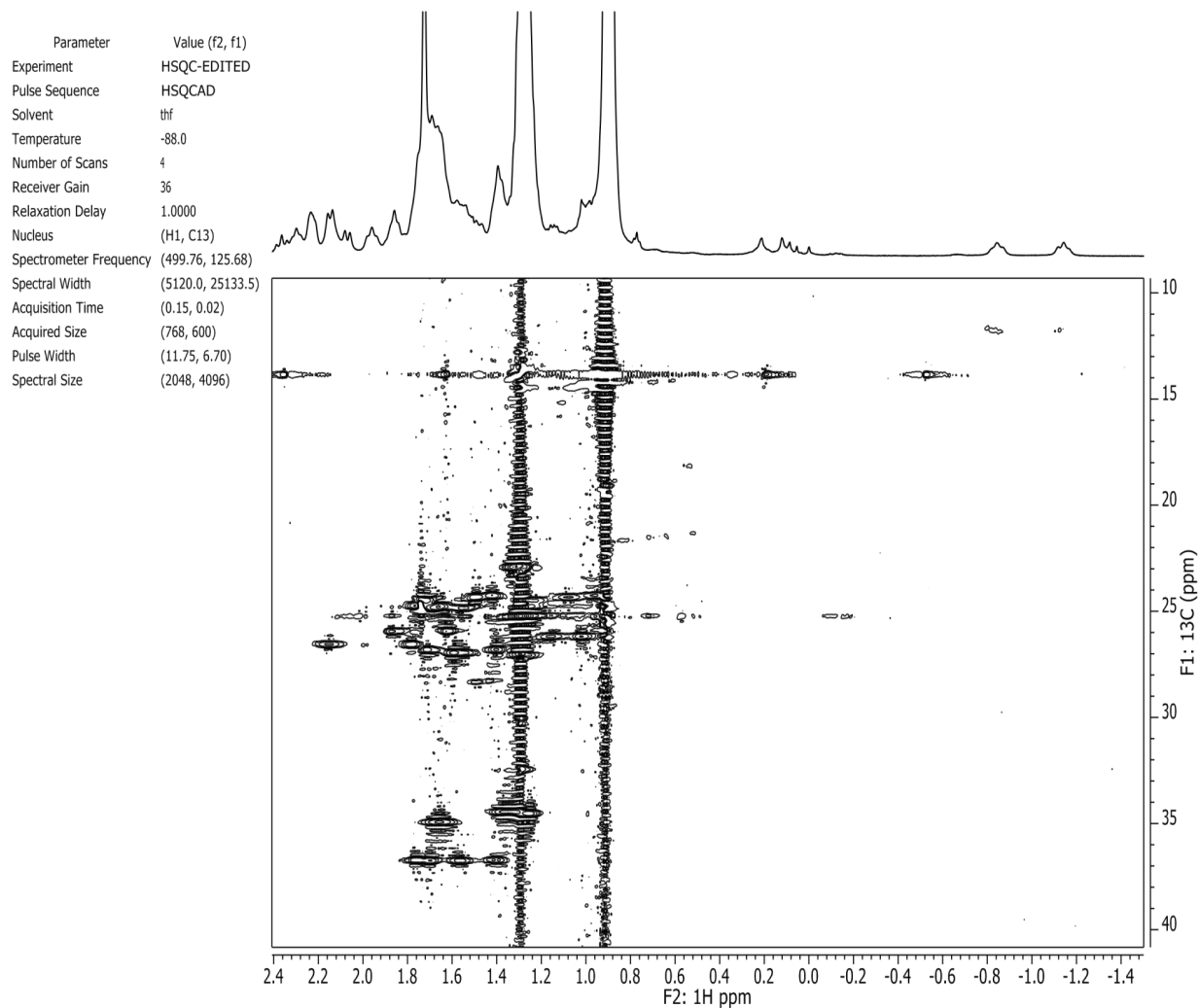


**Figure 37.** Expansion of the aromatic region of multiplicity-edited HSQC spectrum at  $-80^{\circ}\text{C}$ . No correlations were observed for the exchange broadened ortho-hydrogens of the acid enolate. Note the low  $^1\text{H}$  chemical shift of the para-hydrogen of the acid enolate (6.13 ppm), likely due to the ring current of the amide phenyl in close proximity.

| Parameter              | Value (f2, f1)    |
|------------------------|-------------------|
| Experiment             | HSQC-EDITED       |
| Pulse Sequence         | HSQCAD            |
| Solvent                | thf               |
| Temperature            | -88.0             |
| Number of Scans        | 4                 |
| Receiver Gain          | 36                |
| Relaxation Delay       | 1.0000            |
| Nucleus                | (H1, C13)         |
| Spectrometer Frequency | (499.76, 125.68)  |
| Spectral Width         | (5120.0, 25133.5) |
| Acquisition Time       | (0.15, 0.02)      |
| Acquired Size          | (768, 600)        |
| Pulse Width            | (11.75, 6.70)     |
| Spectral Size          | (2048, 4096)      |

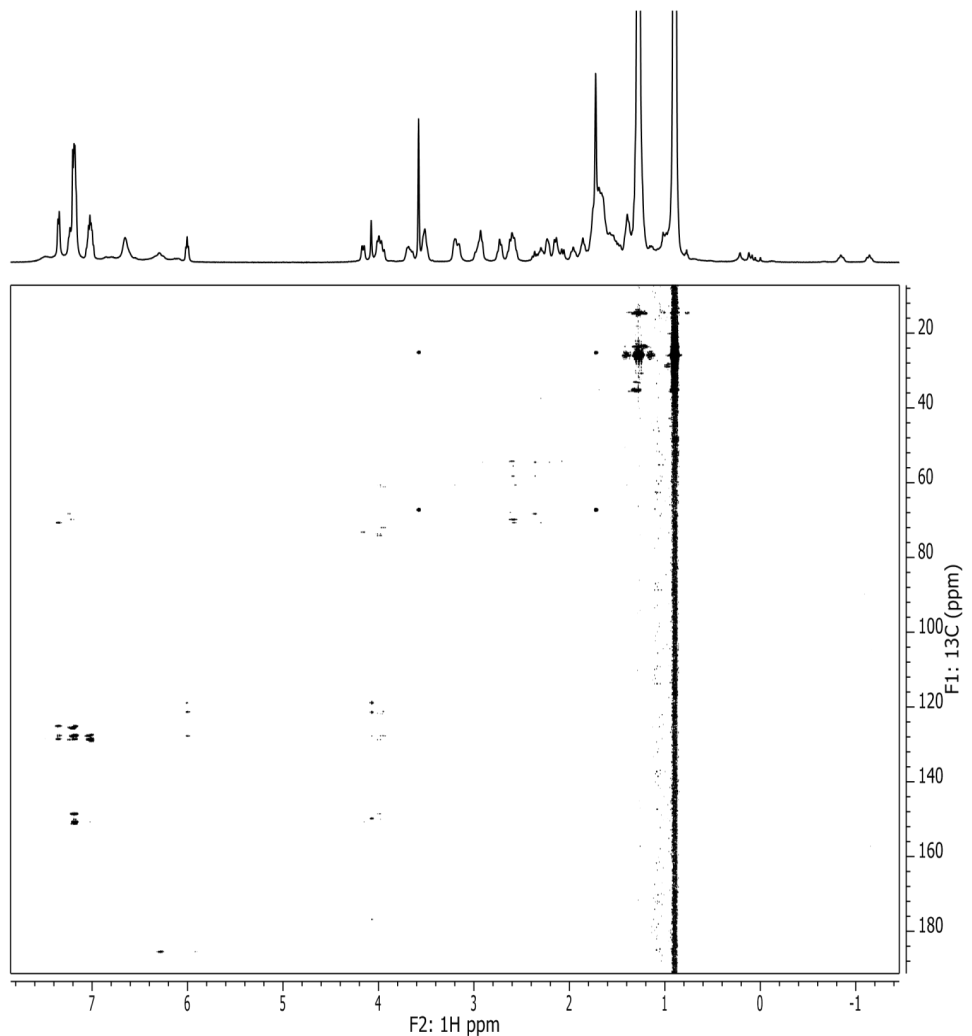


**Figure 38.** Expansion of multiplicity-edited HSQC spectrum at  $-80^{\circ}\text{C}$  with ten negative contour levels ( $\text{CH}_2$ ) and a single positive contour ( $\text{CH}_3$  and  $\text{CH}$ ).



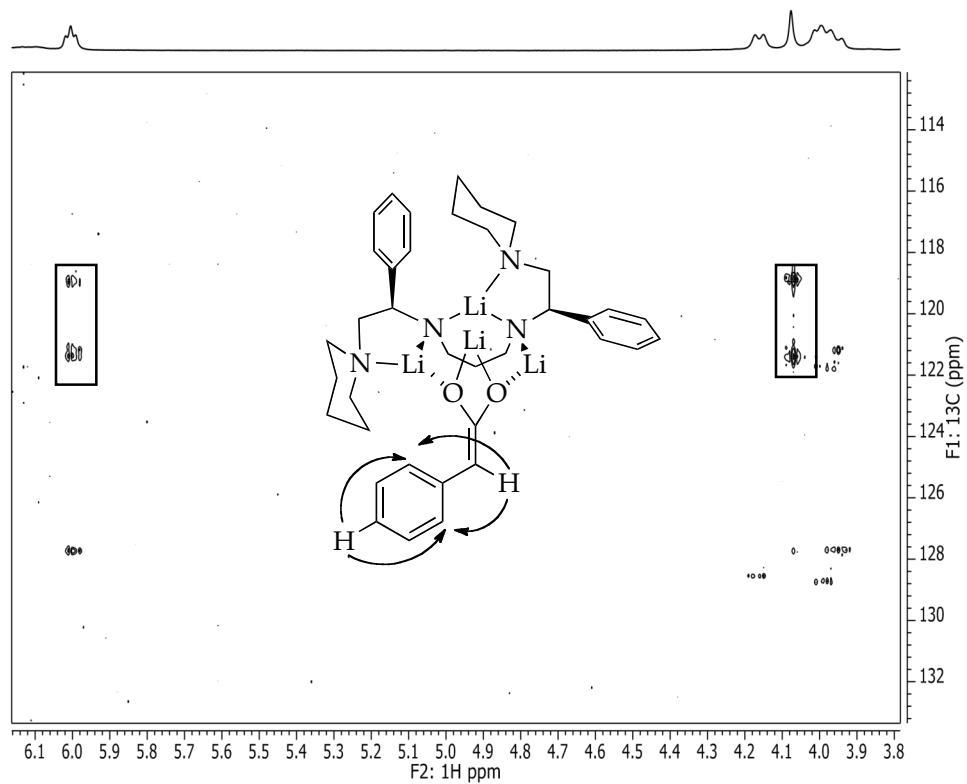
**Figure 39.** High-field expansion of multiplicity-edited HSQC spectrum at  $-80^{\circ}\text{C}$  with ten negative contour levels ( $\text{CH}_2$ ) and a single positive contour ( $\text{CH}_3$  and  $\text{CH}$ ).

| Parameter              | Value (f2, f1)    |
|------------------------|-------------------|
| Experiment             | HMBC              |
| Pulse Sequence         | gHMBCAD           |
| Solvent                | thf               |
| Temperature            | -88.0             |
| Number of Scans        | 4                 |
| Receiver Gain          | 36                |
| Relaxation Delay       | 1.0000            |
| Nucleus                | (H1, C13)         |
| Spectrometer Frequency | (499.76, 125.68)  |
| Spectral Width         | (5120.0, 30154.5) |
| Acquisition Time       | (0.30, 0.03)      |
| Acquired Size          | (1536, 1000)      |
| Pulse Width            | (11.75, 6.70)     |
| Spectral Size          | (1024, 4096)      |



**Figure 40.** Full display of HMBC spectrum at -80°C.

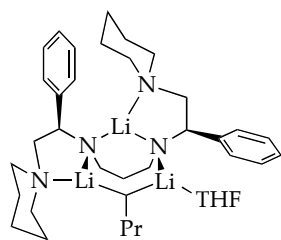
| Parameter              | Value (f2, f1)    |
|------------------------|-------------------|
| Experiment             | HMBC              |
| Pulse Sequence         | gHMBCAD           |
| Solvent                | thf               |
| Temperature            | -88.0             |
| Number of Scans        | 4                 |
| Receiver Gain          | 36                |
| Relaxation Delay       | 1.0000            |
| Nucleus                | (H1, C13)         |
| Spectrometer Frequency | (499.76, 125.68)  |
| Spectral Width         | (5120.0, 30154.5) |
| Acquisition Time       | (0.30, 0.03)      |
| Acquired Size          | (1536, 1000)      |
| Pulse Width            | (11.75, 6.70)     |
| Spectral Size          | (1024, 4096)      |



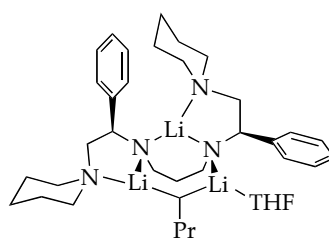
**Figure 41.** Expansion of HMBC spectrum showing 3-bond correlations to the non-equivalent ortho carbon atoms of the acid enolate.

## Part 4: Computational Studies

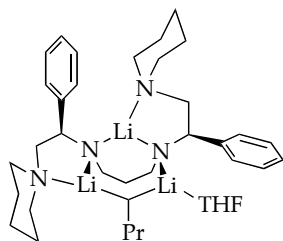
### Chart 1



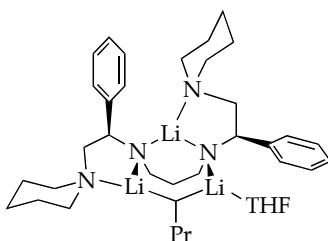
**6c, 6j**



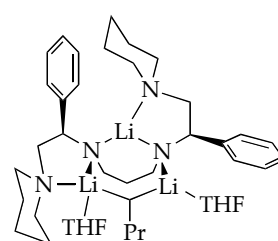
**6d, 6k**



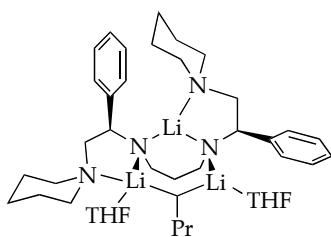
**6e, 6l**



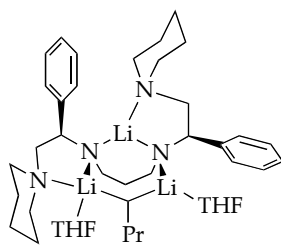
**6f, 6m**



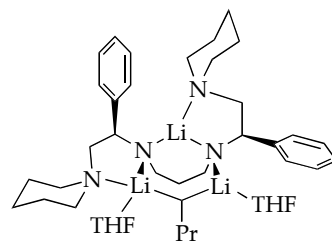
**6a, 6n, 6r**



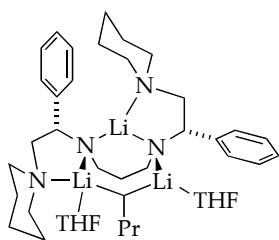
**6g, 6o**



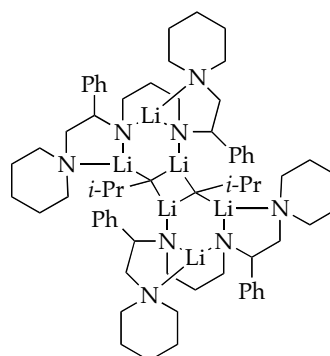
**6h, 6p**



**6i, 6q**

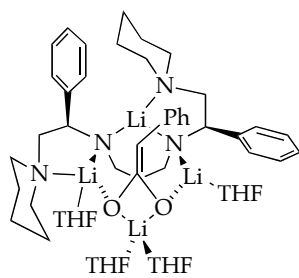


**6b**

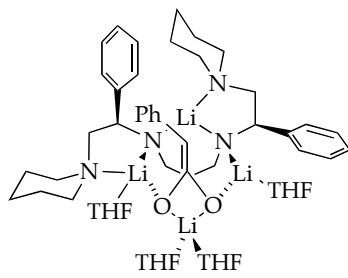


**5**

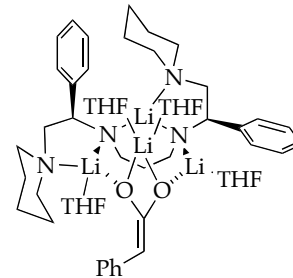
Chart 2



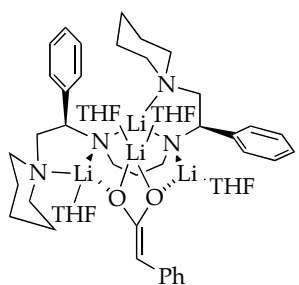
8a



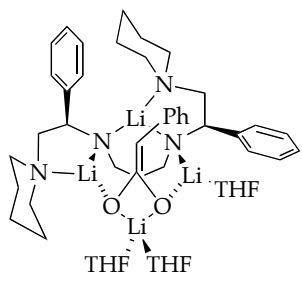
8c



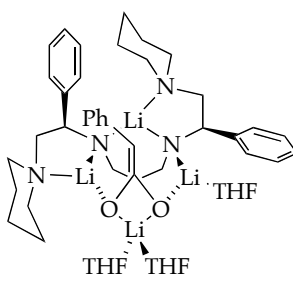
8d



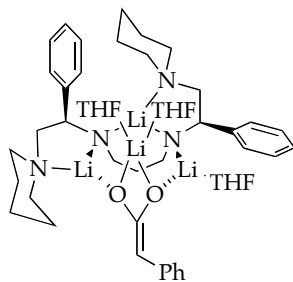
8b



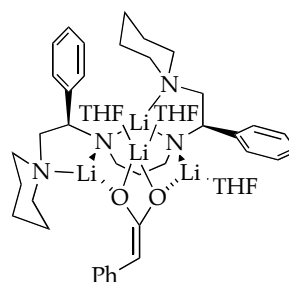
8e, 8g



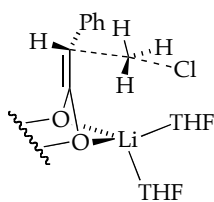
8f, 8h



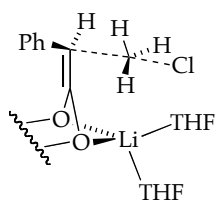
8i



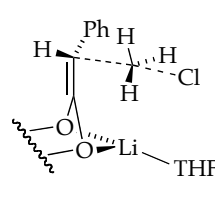
8j



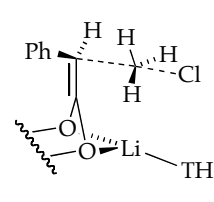
17a



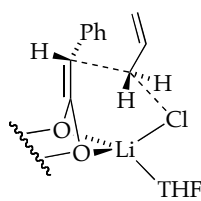
17b



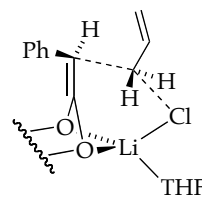
17c



17d



17e

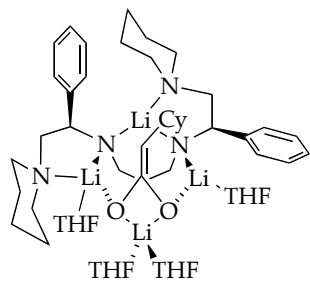


17f

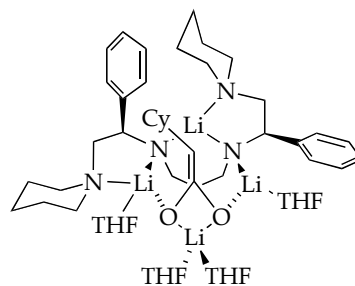




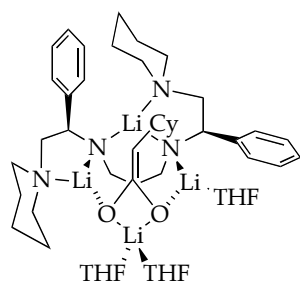
### Chart 4



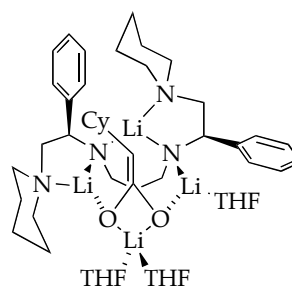
**20a**



**20b**

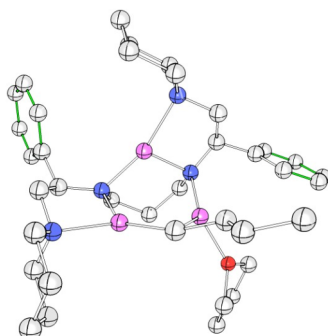
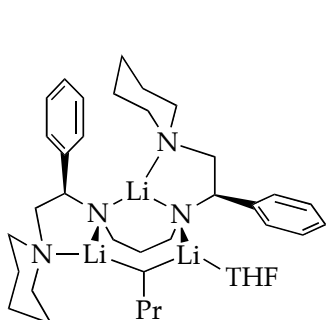


**20c, 20e**



**20d, 20f**

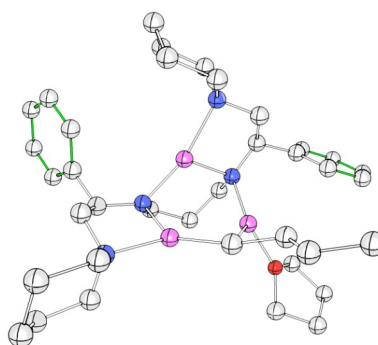
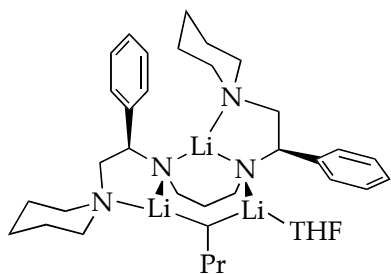
**Table 1.** Optimized geometries at B3LYP level of theory with 6-31G(d) basis set for the mono-solvated BuLi-ligand aggregation conformers at -78 °C with free energies (Hartrees) and cartesian coordinates (X, Y, Z) (Note:  $G_{\text{MP2}}$  includes single point MP2 corrections to B3LYP/6-31G(d) optimized structures).



**6c**  
 $G = -1761.537572$   
 $G_{\text{MP2}} = -1756.295216$

| Atom | X         | Y         | Z         | Atom | X         | Y         | Z         |
|------|-----------|-----------|-----------|------|-----------|-----------|-----------|
| C    | 0         | 0         | 0         | C    | -5.511037 | -4.326064 | -1.931488 |
| Li   | 1.562427  | -0.355628 | -1.372622 | C    | -4.895519 | -3.49434  | -0.991496 |
| N    | 2.344642  | -1.784644 | -2.490619 | C    | -3.506981 | -3.494333 | -0.856138 |
| Li   | 1.297407  | -3.104933 | -1.405828 | H    | -3.049161 | -2.830554 | -0.126429 |
| N    | -0.533512 | -3.125591 | -2.07976  | H    | -5.499192 | -2.847586 | -0.358691 |
| Li   | -0.989195 | -1.28564  | -1.466147 | H    | -6.592736 | -4.325468 | -2.039538 |
| O    | -2.415384 | -0.247618 | -2.378206 | H    | -5.188383 | -5.80965  | -3.462829 |
| C    | -2.477474 | 1.185739  | -2.432574 | H    | -2.726941 | -5.823381 | -3.191206 |
| C    | -2.739478 | 1.522775  | -3.913135 | C    | -0.487971 | -3.152788 | -3.532523 |
| C    | -3.362528 | 0.218474  | -4.487797 | H    | -1.490977 | -3.078445 | -4.008318 |
| C    | -3.438374 | -0.720682 | -3.272265 | H    | -0.081261 | -4.119659 | -3.90975  |
| H    | -3.228291 | -1.768367 | -3.485901 | C    | 1.900989  | -2.116934 | -3.849764 |
| H    | -4.412803 | -0.650154 | -2.768947 | C    | 0.385768  | -2.027589 | -4.109299 |
| H    | -2.718023 | -0.20812  | -5.261704 | H    | 0.244746  | -2.024641 | -5.20039  |
| H    | -4.349613 | 0.382733  | -4.930142 | H    | 0.016184  | -1.051123 | -3.754862 |
| H    | -1.805171 | 1.764667  | -4.428276 | H    | 2.229433  | -3.126582 | -4.17695  |
| H    | -3.404781 | 2.385676  | -4.012793 | H    | 2.382879  | -1.426397 | -4.575109 |
| H    | -3.301663 | 1.533932  | -1.792924 | N    | 3.445179  | 0.54689   | -1.075814 |
| H    | -1.535233 | 1.565343  | -2.034415 | C    | 3.782678  | 1.136629  | 0.238002  |
| C    | -1.164967 | -4.313286 | -1.532251 | H    | 3.550137  | 0.393247  | 1.008986  |
| C    | -0.731371 | -4.472239 | -0.061107 | H    | 4.871282  | 1.332355  | 0.292468  |
| N    | 0.739336  | -4.600977 | 0.108188  | C    | 3.014457  | 2.432053  | 0.510084  |
| C    | 1.17578   | -5.972285 | -0.24377  | H    | 3.332625  | 2.834714  | 1.479894  |
| H    | 0.896247  | -6.167455 | -1.283151 | H    | 1.945415  | 2.20077   | 0.591954  |
| H    | 0.628267  | -6.703521 | 0.382013  | C    | 3.244847  | 3.457231  | -0.60646  |
| C    | 2.6816    | -6.169517 | -0.059832 | C    | 2.943911  | 2.819784  | -1.967562 |
| H    | 3.223846  | -5.539316 | -0.775049 | C    | 3.72747   | 1.517053  | -2.155323 |
| H    | 2.933307  | -7.209828 | -0.301356 | H    | 3.461567  | 1.058948  | -3.11135  |
| C    | 3.114795  | -5.825143 | 1.3704    | H    | 4.812058  | 1.738086  | -2.188299 |
| C    | 2.60823   | -4.428957 | 1.753612  | H    | 3.194037  | 3.505619  | -2.786609 |

| Table 1 (Continued). |           |           |           |   |           |           |           |
|----------------------|-----------|-----------|-----------|---|-----------|-----------|-----------|
| C                    | 1.102753  | -4.303994 | 1.511614  | H | 1.868124  | 2.607161  | -2.045333 |
| H                    | 0.762907  | -3.287501 | 1.739149  | H | 4.291972  | 3.793501  | -0.588006 |
| H                    | 0.564989  | -4.98784  | 2.196355  | H | 2.623943  | 4.347457  | -0.448687 |
| H                    | 2.82111   | -4.210683 | 2.807561  | H | 0.004235  | 1.097753  | -0.163394 |
| H                    | 3.131587  | -3.668052 | 1.158095  | H | 0.889873  | -0.169433 | 0.645838  |
| H                    | 2.69515   | -6.564813 | 2.067806  | C | -1.223135 | -0.312739 | 0.887913  |
| H                    | 4.205808  | -5.882348 | 1.469829  | H | -2.161219 | -0.143559 | 0.329397  |
| H                    | -1.244248 | -5.32966  | 0.408368  | H | -1.233657 | -1.386333 | 1.150668  |
| H                    | -1.035084 | -3.574653 | 0.487712  | C | -1.33275  | 0.479825  | 2.206442  |
| H                    | -0.829387 | -5.219364 | -2.080742 | H | -1.342231 | 1.553937  | 1.970771  |
| C                    | -2.699055 | -4.333678 | -1.640698 | H | -0.421282 | 0.30811   | 2.797025  |
| C                    | -3.33366  | -5.163078 | -2.574337 | C | -2.566119 | 0.125336  | 3.04549   |
| C                    | -4.723205 | -5.158755 | -2.726179 | H | -2.609476 | 0.708765  | 3.973245  |
| C                    | 5.961185  | -4.2125   | -4.159787 | H | -3.492771 | 0.318575  | 2.489374  |
| C                    | 6.318966  | -5.024867 | -3.08358  | H | -2.566003 | -0.936964 | 3.322249  |
| C                    | 5.864985  | -4.700111 | -1.803598 | C | 3.780309  | -1.516237 | -2.506532 |
| C                    | 5.053356  | -3.580965 | -1.606925 | C | 4.202023  | -0.714822 | -1.260332 |
| H                    | 4.714923  | -3.350624 | -0.59986  | H | 4.019999  | -1.314682 | -0.36013  |
| H                    | 6.148254  | -5.316684 | -0.953524 | H | 5.286897  | -0.510019 | -1.298208 |
| H                    | 6.948357  | -5.897529 | -3.23766  | H | 4.02681   | -0.886947 | -3.386847 |
| H                    | 6.309515  | -4.449846 | -5.162155 | C | 4.686747  | -2.749515 | -2.676063 |
| H                    | 4.904796  | -2.447827 | -4.793944 | C | 5.162709  | -3.086117 | -3.951616 |



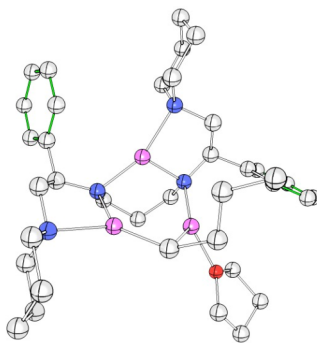
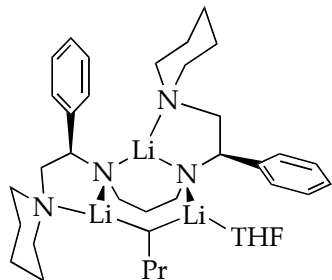
**6d**  
 $G = -1761.534084$   
 $G_{MP2} = -1756.290741$

| Atom | X         | Y         | Z         | Atom | X         | Y         | Z         |
|------|-----------|-----------|-----------|------|-----------|-----------|-----------|
| C    | 0         | 0         | 0         | H    | -3.136726 | -2.649867 | 0.135497  |
| H    | 0.220437  | 1.068534  | -0.214497 | H    | -5.571661 | -2.473703 | -0.142511 |
| Li   | 1.535477  | -0.530799 | -1.321329 | H    | -6.754497 | -3.886748 | -1.820169 |
| N    | 2.294972  | -2.029845 | -2.346445 | H    | -5.450911 | -5.507141 | -3.190855 |
| Li   | 1.187816  | -3.233193 | -1.190905 | H    | -3.004735 | -5.715503 | -2.873541 |
| N    | -0.633336 | -3.207123 | -1.879705 | C    | -0.585572 | -3.353812 | -3.325689 |
| Li   | -1.009613 | -1.30484  | -1.430825 | C    | 0.352358  | -2.327982 | -3.98226  |
| O    | -2.3078   | -0.282029 | -2.513985 | H    | 0.020513  | -1.307906 | -3.728269 |

**Table 1 (Continued).**

|   |           |           |           |   |           |           |           |
|---|-----------|-----------|-----------|---|-----------|-----------|-----------|
| C | -2.311815 | 1.144037  | -2.668141 | H | 0.231155  | -2.420456 | -5.07183  |
| C | -3.798823 | 1.520751  | -2.736167 | H | -0.233168 | -4.36964  | -3.620439 |
| C | -4.469292 | 0.253059  | -3.3359   | H | -1.58101  | -3.258317 | -3.811273 |
| C | -3.328384 | -0.784308 | -3.39693  | C | 1.858529  | -2.45481  | -3.683871 |
| H | -2.91184  | -0.864519 | -4.410598 | H | 2.155708  | -3.49833  | -3.922319 |
| H | -3.604376 | -1.777097 | -3.042893 | H | 2.377171  | -1.842916 | -4.451939 |
| H | -4.887365 | 0.436421  | -4.330287 | C | 3.729856  | -1.774002 | -2.374851 |
| H | -5.282541 | -0.09972  | -2.695664 | H | 3.98015   | -1.165719 | -3.270697 |
| H | -3.965374 | 2.416701  | -3.341649 | C | 4.628279  | -3.017468 | -2.509913 |
| H | -4.183042 | 1.720254  | -1.731211 | C | 5.271763  | -3.294143 | -3.722989 |
| H | -1.768739 | 1.565995  | -1.821102 | C | 6.074374  | -4.42665  | -3.880609 |
| H | -1.787997 | 1.409751  | -3.599123 | C | 6.260073  | -5.306415 | -2.814484 |
| C | -1.348243 | -4.295221 | -1.237475 | C | 5.629812  | -5.044782 | -1.595278 |
| C | -0.917411 | -4.362012 | 0.241261  | C | 4.820361  | -3.917207 | -1.451231 |
| N | 0.541269  | -4.584377 | 0.419777  | H | 4.335605  | -3.731843 | -0.495953 |
| C | 0.8778    | -6.003491 | 0.158523  | H | 5.773268  | -5.718311 | -0.753394 |
| H | 0.586908  | -6.244457 | -0.867853 | H | 6.888565  | -6.185721 | -2.929601 |
| H | 0.278282  | -6.652166 | 0.826131  | H | 6.555896  | -4.618741 | -4.836512 |
| C | 2.36497   | -6.29743  | 0.363916  | H | 5.138841  | -2.608995 | -4.557908 |
| C | 2.820162  | -5.894875 | 1.771582  | N | 3.406379  | 0.300235  | -0.970926 |
| C | 2.418708  | -4.443418 | 2.062282  | C | 3.610073  | 0.912308  | 0.36103   |
| C | 0.926925  | -4.222061 | 1.801984  | H | 2.811252  | 1.65278   | 0.503277  |
| H | 0.664492  | -3.16975  | 1.958277  | H | 3.458169  | 0.135239  | 1.118329  |
| H | 0.338521  | -4.815794 | 2.527953  | C | 4.976151  | 1.595097  | 0.542089  |
| H | 3.000087  | -3.761344 | 1.426187  | C | 5.209617  | 2.63958   | -0.560277 |
| H | 2.643642  | -4.176133 | 3.102333  | C | 5.001367  | 2.014442  | -1.94817  |
| H | 3.903511  | -6.027018 | 1.882638  | C | 3.634522  | 1.313552  | -2.028113 |
| H | 2.344329  | -6.554954 | 2.511371  | H | 3.495015  | 0.839493  | -3.003828 |
| H | 2.951287  | -5.756326 | -0.388602 | H | 2.841996  | 2.068952  | -1.921328 |
| H | 2.539833  | -7.366699 | 0.191035  | H | 5.058726  | 2.780237  | -2.732323 |
| H | -1.488736 | -5.136092 | 0.783144  | H | 5.803378  | 1.293779  | -2.156698 |
| H | -1.147426 | -3.400442 | 0.712642  | H | 6.213512  | 3.073899  | -0.477192 |
| H | -1.087429 | -5.266573 | -1.709931 | H | 4.496896  | 3.467476  | -0.428046 |
| C | -2.878967 | -4.201238 | -1.352061 | H | 5.776694  | 0.843651  | 0.51654   |
| C | -3.565273 | -4.995163 | -2.280886 | H | 5.016603  | 2.062766  | 1.534177  |
| C | -4.946971 | -4.881088 | -2.458212 | H | 0.813308  | -0.296064 | 0.698862  |
| C | -5.678307 | -3.972255 | -1.693096 | C | -1.295903 | -0.027327 | 0.836958  |
| C | -5.012534 | -3.177029 | -0.755583 | H | -2.163576 | 0.272574  | 0.222584  |
| C | -3.630337 | -3.286625 | -0.595079 | H | -1.517179 | -1.062567 | 1.155952  |
| H | -2.582895 | 1.421884  | 3.792448  | C | -1.306313 | 0.851367  | 2.103994  |
| H | -3.467836 | 1.108354  | 2.291522  | H | -1.105633 | 1.891994  | 1.810112  |
| C | 4.180899  | -0.95298  | -1.148271 | H | -0.465532 | 0.552067  | 2.746349  |
| H | 4.014688  | -1.540738 | -0.237106 | C | -2.61446  | 0.783436  | 2.901102  |
| H | 5.264981  | -0.774642 | -1.215986 | H | -2.822822 | -0.241245 | 3.235415  |

**Table 1 (Continued).**

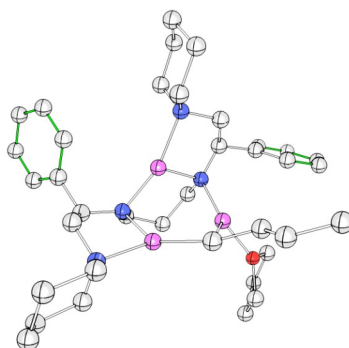
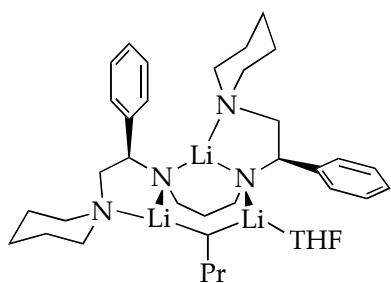


**6e**  
 $G = -1761.532691$   
 $G_{MP2} = -1756.292859$

| Atom | X         | Y         | Z         | Atom | X         | Y         | Z         |
|------|-----------|-----------|-----------|------|-----------|-----------|-----------|
| C    | 0         | 0         | 0         | C    | 0.902377  | -6.626662 | 1.343024  |
| H    | 0.910477  | 0.150406  | 0.615721  | C    | 1.226225  | -5.26795  | 0.698883  |
| H    | -0.222571 | 1.022765  | -0.364323 | H    | 0.870171  | -4.444388 | 1.327561  |
| Li   | 1.630801  | -0.530328 | -1.252322 | H    | 2.317927  | -5.166568 | 0.619419  |
| N    | 2.326247  | -1.885766 | -2.493723 | H    | 1.394263  | -6.687348 | 2.322462  |
| Li   | 1.187615  | -3.286448 | -1.670727 | H    | -0.17713  | -6.70312  | 1.529301  |
| N    | -0.631375 | -3.079003 | -2.308718 | H    | 2.458     | -7.781023 | 0.382677  |
| Li   | -0.976276 | -1.280455 | -1.476722 | H    | 1.060643  | -8.745551 | 0.852357  |
| O    | -2.427849 | -0.146109 | -2.270977 | H    | 1.208851  | -8.355204 | -1.664383 |
| C    | -2.641387 | 1.249104  | -1.941666 | H    | -0.294167 | -7.759606 | -0.972376 |
| C    | -3.901223 | 1.687529  | -2.706345 | H    | 2.204422  | -6.102523 | -1.648922 |
| C    | -4.605721 | 0.353343  | -3.001815 | H    | -1.346809 | -5.814556 | -0.40925  |
| C    | -3.41918  | -0.5767   | -3.230488 | H    | -1.010667 | -4.180159 | 0.158129  |
| H    | -3.012646 | -0.465214 | -4.245492 | H    | -1.154954 | -5.071454 | -2.762606 |
| H    | -3.626948 | -1.629727 | -3.041628 | C    | -2.865998 | -4.16657  | -1.914553 |
| H    | -5.276425 | 0.40137   | -3.865081 | C    | -3.671566 | -4.688132 | -2.935601 |
| H    | -5.184359 | 0.015272  | -2.134449 | C    | -5.058839 | -4.514284 | -2.929489 |
| H    | -3.628639 | 2.185825  | -3.643867 | C    | -5.672736 | -3.82043  | -1.886491 |
| H    | -4.51476  | 2.382288  | -2.125064 | C    | -4.88561  | -3.298612 | -0.855136 |
| H    | -2.766452 | 1.317507  | -0.856696 | C    | -3.500536 | -3.465184 | -0.875952 |
| H    | -1.751048 | 1.819861  | -2.223488 | H    | -2.9063   | -3.038545 | -0.071329 |
| C    | -1.336111 | -4.306325 | -1.979174 | H    | -5.352477 | -2.76468  | -0.030508 |
| C    | -0.802512 | -4.889047 | -0.650296 | H    | -6.751801 | -3.689805 | -1.87308  |
| N    | 0.670997  | -5.083939 | -0.661376 | H    | -5.6584   | -4.925241 | -3.738418 |
| C    | 1.116981  | -6.200758 | -1.533968 | H    | -3.201827 | -5.238018 | -3.748868 |
| H    | 0.679275  | -6.06238  | -2.526868 | C    | -0.593736 | -2.849835 | -3.747787 |
| C    | 0.792351  | -7.601059 | -0.984493 | C    | 0.40438   | -1.750402 | -4.15082  |
| C    | 1.358726  | -7.776783 | 0.432741  | H    | 0.285464  | -1.581375 | -5.231205 |
| H    | 5.079821  | 0.871596  | 0.435563  | H    | 0.134004  | -0.797061 | -3.667103 |
| C    | 3.322064  | 2.122047  | 0.660001  | H    | -0.299833 | -3.775361 | -4.293709 |
| H    | 3.673087  | 2.489851  | 1.632419  | H    | -1.580896 | -2.581062 | -4.182242 |
| H    | 2.236543  | 1.984018  | 0.739598  | C    | 1.895839  | -2.038673 | -3.887742 |
| C    | 3.635038  | 3.132177  | -0.45026  | H    | 2.475736  | -1.345891 | -4.534539 |
| C    | 3.276682  | 2.530306  | -1.813844 | H    | 2.113629  | -3.046309 | -4.306633 |
| C    | 3.949988  | 1.169769  | -2.013497 | C    | 3.779661  | -1.825172 | -2.42249  |

**Table 1 (Continued).**

|   |           |           |           |   |          |           |           |
|---|-----------|-----------|-----------|---|----------|-----------|-----------|
| H | 3.640208  | 0.740994  | -2.96957  | H | 4.174797 | -1.236981 | -3.275819 |
| H | 5.049103  | 1.301786  | -2.050631 | C | 4.489269 | -3.184909 | -2.536641 |
| H | 3.578021  | 3.199066  | -2.629795 | C | 5.119749 | -3.550258 | -3.733657 |
| H | 2.186941  | 2.406143  | -1.887504 | C | 5.729191 | -4.798339 | -3.88541  |
| H | 4.706925  | 3.378806  | -0.432911 | C | 5.73252  | -5.70858  | -2.82862  |
| H | 3.091651  | 4.070246  | -0.283714 | C | 5.115546 | -5.3596   | -1.6241   |
| C | -1.103763 | -0.391329 | 1.014381  | C | 4.495784 | -4.116501 | -1.486245 |
| H | -2.027834 | -0.729473 | 0.504177  | H | 4.019575 | -3.866813 | -0.540323 |
| H | -1.439606 | 0.458984  | 1.636384  | H | 5.124358 | -6.054897 | -0.787516 |
| C | -0.668118 | -1.508761 | 1.972802  | H | 6.213194 | -6.677271 | -2.938157 |
| H | -0.322171 | -2.369839 | 1.38226   | H | 6.205398 | -5.055961 | -4.82842  |
| H | 0.210143  | -1.163114 | 2.537787  | H | 5.13265  | -2.841188 | -4.558942 |
| C | -1.757887 | -1.955197 | 2.953505  | N | 3.592989 | 0.219462  | -0.939476 |
| H | -1.401053 | -2.743055 | 3.62821   | C | 3.978587 | 0.767641  | 0.377873  |
| H | -2.0977   | -1.11646  | 3.573904  | H | 3.684489 | 0.040244  | 1.143528  |
| H | -2.636527 | -2.346325 | 2.423977  | H | 3.974598 | -1.704319 | -0.259428 |
| C | 4.235431  | -1.100273 | -1.137541 | H | 5.335993 | -0.999667 | -1.141509 |


**6f**
 $G = -1761.532371$ 
 $G_{\text{MP2}} = -1756.287231$ 

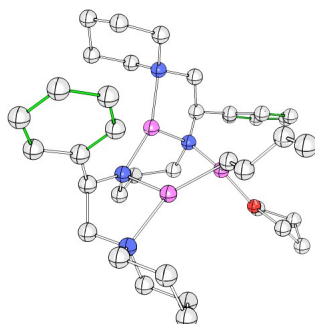
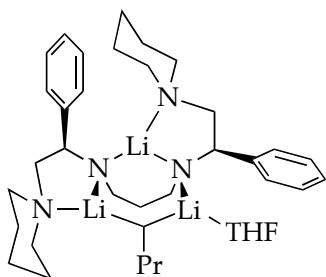
| Atom | X | Y | Z | Atom | X | Y | Z |
|------|---|---|---|------|---|---|---|
|------|---|---|---|------|---|---|---|

|    |           |           |           |   |           |           |           |
|----|-----------|-----------|-----------|---|-----------|-----------|-----------|
| C  | 0         | 0         | 0         | C | -3.970203 | 3.384501  | -2.874092 |
| Li | -1.438614 | 0.470491  | -1.443568 | C | -4.696599 | 3.699931  | -4.02863  |
| N  | -1.946487 | 1.878256  | -2.705645 | C | -5.197965 | 4.986576  | -4.244359 |
| Li | -0.65874  | 3.076241  | -1.79535  | C | -4.988779 | 5.987408  | -3.296131 |
| N  | 1.129711  | 2.681464  | -2.422075 | C | -4.269434 | 5.690173  | -2.135178 |
| Li | 1.238893  | 0.877545  | -1.575332 | C | -3.762515 | 4.406075  | -1.934417 |
| O  | 2.46386   | -0.482356 | -2.33012  | H | -3.199179 | 4.193327  | -1.027827 |
| C  | 3.588001  | -0.291715 | -3.206606 | H | -4.109478 | 6.459528  | -1.382953 |
| C  | 3.339744  | -1.252408 | -4.383074 | H | -5.381089 | 6.988218  | -3.456924 |
| C  | 2.403374  | -2.341913 | -3.785971 | H | -5.752229 | 5.204911  | -5.154078 |
| C  | 2.201026  | -1.893564 | -2.326518 | H | -4.868866 | 2.923738  | -4.771837 |
| H  | 2.915147  | -2.390773 | -1.653709 | N | -3.438747 | 0.039563  | -1.034724 |
| H  | 1.190774  | -2.033303 | -1.937862 | C | -3.760273 | -0.387204 | 0.345238  |
| H  | 2.836539  | -3.34527  | -3.839086 | H | -3.127382 | -1.256341 | 0.571636  |

**Table 1 (Continued).**

|   |           |           |           |   |           |           |           |
|---|-----------|-----------|-----------|---|-----------|-----------|-----------|
| H | 1.448441  | -2.364531 | -4.319261 | H | -3.454523 | 0.41245   | 1.028824  |
| H | 4.277032  | -1.667371 | -4.765538 | C | -5.235757 | -0.762338 | 0.564383  |
| H | 2.846064  | -0.72958  | -5.207066 | C | -5.678881 | -1.836658 | -0.440948 |
| H | 3.619673  | 0.76422   | -3.474057 | C | -5.346086 | -1.404108 | -1.877253 |
| H | 4.509243  | -0.548188 | -2.664826 | C | -3.865    | -1.005819 | -1.994096 |
| C | 1.954987  | 3.800801  | -2.005406 | H | -3.626555 | -0.667013 | -3.006089 |
| C | 1.520727  | 4.260363  | -0.595369 | H | -3.243298 | -1.891862 | -1.796636 |
| N | 0.079697  | 4.625274  | -0.535994 | H | -5.558173 | -2.214499 | -2.586383 |
| C | -0.21557  | 5.944377  | -1.151147 | H | -5.983406 | -0.558994 | -2.169488 |
| H | 0.222872  | 5.964692  | -2.15333  | H | -6.750856 | -2.045319 | -0.33736  |
| C | 0.262047  | 7.151529  | -0.324943 | H | -5.153167 | -2.777326 | -0.217719 |
| C | -0.290216 | 7.090476  | 1.107387  | H | -5.867946 | 0.129216  | 0.457272  |
| C | 0.023318  | 5.730266  | 1.7487    | H | -5.368162 | -1.117522 | 1.594384  |
| C | -0.459146 | 4.58538   | 0.843311  | H | -0.779048 | 0.536172  | 0.58739   |
| H | -0.210842 | 3.610309  | 1.277131  | H | -0.354541 | -1.0532   | 0.002416  |
| H | -1.555542 | 4.635521  | 0.766249  | C | 1.275289  | 0.039707  | 0.86763   |
| H | -0.459237 | 5.642971  | 2.730682  | H | 2.089823  | -0.522483 | 0.379708  |
| H | 1.104004  | 5.637536  | 1.920448  | H | 1.650447  | 1.07818   | 0.945598  |
| H | -1.381366 | 7.231447  | 1.080007  | C | 1.13832   | -0.501079 | 2.304943  |
| H | 0.115818  | 7.908975  | 1.714408  | H | 0.348659  | 0.064067  | 2.821115  |
| H | -0.058489 | 8.074036  | -0.825582 | H | 0.781879  | -1.540141 | 2.254665  |
| H | 1.3592    | 7.178596  | -0.297199 | C | 2.434444  | -0.439733 | 3.122057  |
| H | -1.304038 | 6.00486   | -1.281742 | H | 2.297116  | -0.837808 | 4.134902  |
| H | 2.17287   | 5.075766  | -0.249317 | H | 3.232782  | -1.021386 | 2.642991  |
| H | 1.654505  | 3.426597  | 0.10271   | H | 2.794862  | 0.592736  | 3.218895  |
| H | 1.810172  | 4.663987  | -2.690666 | C | -3.95267  | 1.396342  | -1.343741 |
| C | 3.466988  | 3.523295  | -2.038618 | H | -3.633921 | 2.034883  | -0.510236 |
| C | 4.253445  | 4.026858  | -3.083493 | H | -5.05238  | 1.439674  | -1.369828 |
| C | 5.617008  | 3.733781  | -3.175826 | C | -0.016135 | 1.563885  | -4.329783 |
| C | 6.22801   | 2.935039  | -2.209101 | C | -1.47575  | 1.996735  | -4.089496 |
| C | 5.460863  | 2.428501  | -1.155975 | H | -1.587001 | 3.024135  | -4.500056 |
| C | 4.097361  | 2.713999  | -1.07879  | H | -2.108138 | 1.36879   | -4.753069 |
| H | 3.520111  | 2.299061  | -0.255679 | H | 0.108443  | 1.414496  | -5.412543 |
| H | 5.926638  | 1.812446  | -0.390104 | H | 0.142309  | 0.575283  | -3.867853 |
| H | 7.289969  | 2.711311  | -2.271546 | H | 0.898001  | 3.512295  | -4.368829 |
| H | 6.201134  | 4.134813  | -4.000889 | H | 2.045767  | 2.184883  | -4.310098 |
| H | 3.786929  | 4.659868  | -3.835971 | C | -3.396444 | 1.970799  | -2.666361 |
| C | 1.085757  | 2.5346    | -3.868502 | H | -3.83935  | 1.368174  | -3.488646 |

Note: The following conformers have N-Li-N cyclohexane ring of the ligand backbone in the boat conformation and the left phenyl substituent pointing in the equatorial direction.



**6j**

$G = -1761.527261$

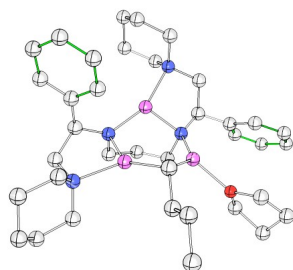
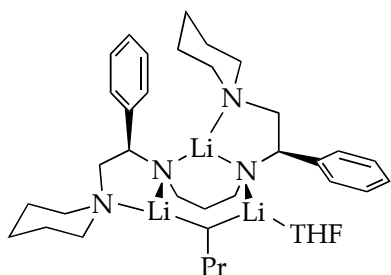
$G_{\text{MP2}} = -1756.288171$

| Atom | X         | Y         | Z         | Atom | X         | Y         | Z         |
|------|-----------|-----------|-----------|------|-----------|-----------|-----------|
| C    | 0         | 0         | 0         | H    | -1.687903 | 4.863695  | -0.388341 |
| H    | 0.996504  | -0.414815 | 0.277923  | H    | -0.258858 | 7.560799  | -0.702197 |
| H    | 0.071111  | 1.05491   | 0.347769  | H    | -1.850803 | 7.141326  | -1.336027 |
| Li   | -1.152858 | 0.178049  | -1.865582 | H    | 3.019611  | 4.558442  | -0.401858 |
| N    | -1.129294 | 1.745351  | -3.16589  | H    | 2.117162  | 3.127003  | 0.121329  |
| Li   | 0.131924  | 2.711493  | -2.044923 | H    | 3.104844  | 3.664147  | -2.717876 |
| N    | 1.927256  | 1.948814  | -2.302152 | C    | 4.254254  | 2.403366  | -1.468495 |
| Li   | 1.53805   | 0.254071  | -1.452156 | C    | 5.401083  | 2.665817  | -2.228896 |
| O    | 2.598783  | -1.366554 | -1.80982  | C    | 6.641937  | 2.117291  | -1.888973 |
| C    | 2.387814  | -2.630398 | -1.133866 | C    | 6.762337  | 1.303553  | -0.76314  |
| C    | 3.538635  | -3.542787 | -1.574596 | C    | 5.629828  | 1.039519  | 0.014952  |
| C    | 4.646522  | -2.535048 | -1.92014  | C    | 4.39287   | 1.577074  | -0.340273 |
| C    | 3.847802  | -1.394131 | -2.54375  | H    | 3.520741  | 1.349565  | 0.269327  |
| H    | 3.630897  | -1.585602 | -3.603268 | H    | 5.713499  | 0.418097  | 0.903926  |
| H    | 4.313733  | -0.412953 | -2.443725 | H    | 7.726315  | 0.882146  | -0.489648 |
| H    | 5.401652  | -2.939004 | -2.60113  | H    | 7.513909  | 2.332033  | -2.502402 |
| H    | 5.153416  | -2.187046 | -1.012841 | H    | 5.320506  | 3.310697  | -3.101869 |
| H    | 3.256011  | -4.116028 | -2.465459 | C    | 2.050876  | 1.570075  | -3.712124 |
| H    | 3.824496  | -4.253308 | -0.793362 | C    | 0.941336  | 2.13045   | -4.627169 |
| H    | 2.402451  | -2.444629 | -0.053651 | C    | -0.460604 | 1.51236   | -4.452707 |
| H    | 1.398943  | -3.010924 | -1.406218 | H    | -0.349657 | 0.431045  | -4.702994 |
| C    | 2.883448  | 2.962076  | -1.89102  | H    | -1.075577 | 1.92325   | -5.278276 |
| C    | 2.293045  | 3.793666  | -0.730953 | H    | 1.233831  | 1.96022   | -5.676134 |
| N    | 0.988595  | 4.42457   | -1.04768  | H    | 0.878808  | 3.223117  | -4.494745 |
| C    | 1.148003  | 5.515443  | -2.034426 | H    | 2.024091  | 0.467294  | -3.833328 |
| H    | 1.591575  | 5.099517  | -2.942942 | H    | 3.027484  | 1.869608  | -4.132764 |
| H    | 1.855322  | 6.272289  | -1.642477 | C    | -2.566034 | 1.801384  | -3.372019 |
| C    | -0.188413 | 6.183968  | -2.367785 | C    | -3.160087 | 0.423036  | -3.828123 |
| H    | -0.848044 | 5.449108  | -2.849454 | N    | -2.884962 | -0.697278 | -2.88529  |
| H    | -0.012694 | 6.984975  | -3.096961 | C    | -4.105058 | -1.03627  | -2.113389 |
| C    | -0.860452 | 6.731794  | -1.103413 | H    | -4.434384 | -0.136837 | -1.587326 |



**Table 1 (Continued).**

|   |           |           |           |   |           |           |           |
|---|-----------|-----------|-----------|---|-----------|-----------|-----------|
| C | -0.969501 | 5.620941  | -0.051999 | H | -4.913008 | -1.318991 | -2.815285 |
| C | 0.387467  | 4.956979  | 0.195209  | C | -3.876913 | -2.181337 | -1.124116 |
| H | 0.280388  | 4.124044  | 0.899632  | H | -4.827516 | -2.40845  | -0.625128 |
| H | 1.075719  | 5.688608  | 0.661524  | H | -3.177507 | -1.856639 | -0.346274 |
| H | -1.346733 | 6.0195    | 0.898391  | C | -3.323007 | -3.426026 | -1.828029 |
| C | -5.399523 | 3.359062  | -1.326565 | C | -2.090906 | -3.050908 | -2.660785 |
| C | -4.921847 | 3.27733   | -0.015739 | C | -2.407312 | -1.895469 | -3.613919 |
| C | -3.656038 | 2.740119  | 0.213014  | H | -1.513378 | -1.612654 | -4.181206 |
| C | -2.875984 | 2.285297  | -0.856883 | H | -3.167016 | -2.225243 | -4.34836  |
| H | -1.887138 | 1.889544  | -0.642627 | H | -1.736025 | -3.909649 | -3.244942 |
| H | -3.26457  | 2.67521   | 1.225221  | H | -1.270729 | -2.751557 | -1.992505 |
| H | -5.526484 | 3.634485  | 0.813669  | H | -4.092435 | -3.84804  | -2.491258 |
| H | -6.379201 | 3.787333  | -1.524226 | H | -3.074046 | -4.204864 | -1.096937 |
| H | -5.003569 | 2.969769  | -3.401964 | H | -4.241304 | 0.503222  | -4.017508 |
| C | -0.986098 | -0.71034  | 0.94791   | H | -2.692831 | 0.180426  | -4.787283 |
| H | -2.006287 | -0.316934 | 0.799684  | H | -2.820262 | 2.471729  | -4.222433 |
| H | -1.047831 | -1.780289 | 0.687044  | C | -3.345653 | 2.34344   | -2.176016 |
| C | -0.670951 | -0.611414 | 2.453839  | C | -4.620028 | 2.897364  | -2.386017 |
| H | 0.335832  | -1.018079 | 2.632267  | H | -1.732898 | -2.403839 | 3.110688  |
| H | -0.619937 | 0.4506    | 2.735961  | H | -1.423324 | -1.245172 | 4.413286  |
| C | -1.682931 | -1.333884 | 3.351227  | H | -2.692213 | -0.922311 | 3.221381  |



**6k**

$$G = -1761.527223$$

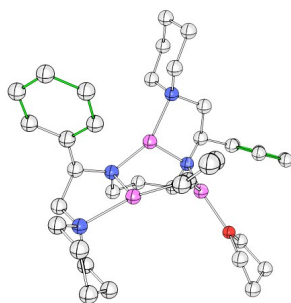
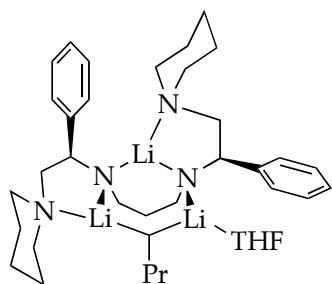
$$G_{\text{MP2}} = -1756.28878$$

Atom X Y Z Atom X Y Z

|    |           |           |           |   |           |          |           |
|----|-----------|-----------|-----------|---|-----------|----------|-----------|
| C  | 0         | 0         | 0         | C | -4.827561 | 2.555278 | 0.495795  |
| H  | -0.79082  | 0.22689   | -0.752628 | H | -4.140057 | 2.4619   | -0.341575 |
| H  | 0.910375  | 0.34135   | -0.537978 | H | -6.455792 | 1.649436 | -0.583471 |
| Li | 1.024474  | 0.973449  | 1.596426  | H | -8.046682 | 1.803078 | 1.326661  |
| N  | 1.156538  | 2.728934  | 2.576897  | H | -7.295447 | 2.833301 | 3.465972  |
| Li | -0.247811 | 3.570056  | 1.56309   | H | -4.992105 | 3.71618  | 3.675446  |
| N  | -1.933075 | 2.623025  | 1.931511  | C | -1.801977 | 2.077874 | 3.28742   |
| Li | -1.689102 | 0.91977   | 0.991038  | C | -0.789332 | 2.812187 | 4.201814  |
| O  | -3.145243 | -0.446335 | 1.015136  | C | 0.694809  | 2.488255 | 3.943578  |
| C  | -3.985557 | -0.672314 | 2.171976  | H | 0.838611  | 1.431878 | 4.277463  |
| C  | -4.814148 | -1.909327 | 1.828807  | H | 1.285814  | 3.084999 | 4.669885  |

| Table 1 (Continued). |           |           |           |   |           |           |           |
|----------------------|-----------|-----------|-----------|---|-----------|-----------|-----------|
| C                    | -5.012717 | -1.742689 | 0.314225  | H | -0.998865 | 2.557911  | 5.252817  |
| C                    | -3.668232 | -1.157002 | -0.130639 | H | -0.952535 | 3.897863  | 4.110482  |
| H                    | -3.761553 | -0.453319 | -0.964249 | H | -1.465268 | 1.02058   | 3.23848   |
| H                    | -2.949419 | -1.935982 | -0.409023 | H | -2.775521 | 2.03238   | 3.81058   |
| H                    | -5.821546 | -1.030277 | 0.119007  | C | 2.593479  | 2.90884   | 2.54624   |
| H                    | -5.247297 | -2.679771 | -0.199565 | C | 3.395336  | 1.624487  | 2.977474  |
| H                    | -5.755383 | -1.946624 | 2.385172  | N | 2.969329  | 0.392943  | 2.261464  |
| H                    | -4.249663 | -2.823951 | 2.045614  | C | 3.853589  | 0.029602  | 1.1246    |
| H                    | -3.331104 | -0.805572 | 3.037796  | H | 3.311619  | -0.706926 | 0.515758  |
| H                    | -4.61421  | 0.210129  | 2.330397  | H | 3.994117  | 0.91714   | 0.503449  |
| C                    | -2.948755 | 3.664713  | 1.85721   | C | 5.210589  | -0.562112 | 1.543661  |
| C                    | -2.611847 | 4.635348  | 0.704387  | C | 5.027639  | -1.75744  | 2.490549  |
| N                    | -1.29009  | 5.292501  | 0.845055  | C | 4.126976  | -1.368982 | 3.671441  |
| C                    | -1.309986 | 6.31778   | 1.912123  | C | 2.805163  | -0.774948 | 3.161225  |
| H                    | -1.609478 | 5.840204  | 2.848733  | H | 2.162962  | -0.474071 | 3.996377  |
| H                    | -2.075234 | 7.083767  | 1.678347  | H | 2.261395  | -1.546554 | 2.598254  |
| C                    | 0.056111  | 6.987442  | 2.081456  | H | 3.914313  | -2.240699 | 4.303862  |
| C                    | 0.518339  | 7.630026  | 0.76866   | H | 4.640737  | -0.634246 | 4.306946  |
| C                    | 0.46858   | 6.595863  | -0.3625   | H | 5.999396  | -2.123008 | 2.845167  |
| C                    | -0.902573 | 5.91875   | -0.437943 | H | 4.560305  | -2.587957 | 1.940651  |
| H                    | -0.895778 | 5.136998  | -1.206365 | H | 5.817361  | 0.208445  | 2.038358  |
| H                    | -1.666596 | 6.661725  | -0.739177 | H | 5.761886  | -0.859899 | 0.642494  |
| H                    | 1.239072  | 5.832703  | -0.20022  | H | 4.475198  | 1.803141  | 2.87798   |
| H                    | 0.68413   | 7.066425  | -1.330165 | H | 3.203767  | 1.472998  | 4.044295  |
| H                    | 1.530653  | 8.038815  | 0.871453  | H | 2.921316  | 3.660567  | 3.299093  |
| H                    | -0.14283  | 8.47495   | 0.525014  | C | 3.095035  | 3.428847  | 1.200013  |
| H                    | 0.786061  | 6.23281   | 2.404845  | C | 4.287869  | 4.168308  | 1.147199  |
| H                    | -0.011188 | 7.735308  | 2.881609  | C | 4.806457  | 4.632291  | -0.061678 |
| H                    | -3.407822 | 5.393232  | 0.593082  | C | 4.140725  | 4.364254  | -1.260237 |
| H                    | -2.577325 | 4.060983  | -0.228868 | C | 2.951463  | 3.635967  | -1.228843 |
| H                    | -2.971164 | 4.264424  | 2.787472  | C | 2.433685  | 3.180095  | -0.011787 |
| C                    | -4.388768 | 3.151536  | 1.689138  | H | 1.507214  | 2.612041  | -0.019192 |
| C                    | -5.304686 | 3.24449   | 2.745849  | H | 2.419265  | 3.418927  | -2.151874 |
| C                    | -6.608565 | 2.752921  | 2.626723  | H | 4.541965  | 4.722657  | -2.20454  |
| C                    | -7.02992  | 2.173368  | 1.430464  | H | 5.728803  | 5.208101  | -0.067383 |
| C                    | -6.132667 | 2.082632  | 0.360787  | H | 4.814023  | 4.388684  | 2.074147  |
| H                    | 1.156655  | -1.937623 | -1.735034 | C | 0.090524  | -1.536834 | 0.104481  |
| C                    | 0.345757  | -3.827766 | -1.054075 | H | 0.935974  | -1.815829 | 0.757499  |
| H                    | -0.554226 | -4.226608 | -0.567422 | H | -0.800809 | -1.931075 | 0.619737  |
| H                    | 0.45641   | -4.340857 | -2.017413 | C | 0.256574  | -2.30582  | -1.220916 |
| H                    | 1.203915  | -4.10816  | -0.429433 | H | -0.586896 | -2.057173 | -1.883128 |

**Table 1 (Continued).**



**6l**

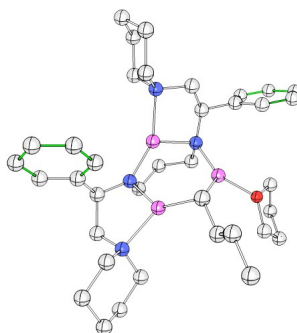
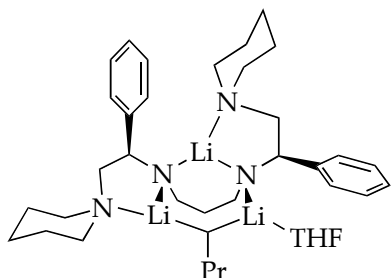
$G = -1761.522822$

$G_{MP2} = -1756.281377$

| Atom | X         | Y         | Z         | Atom | X         | Y         | Z         |
|------|-----------|-----------|-----------|------|-----------|-----------|-----------|
| C    | 0         | 0         | 0         | H    | 8.070825  | 1.143832  | -3.236553 |
| H    | 0.796951  | -0.668971 | 0.396048  | H    | 5.875631  | 2.204107  | -3.67429  |
| H    | 0.400464  | 1.016836  | 0.213883  | C    | 2.44652   | 0.450527  | -3.713066 |
| Li   | -1.016968 | 0.20332   | -1.945691 | C    | 1.573988  | 1.173161  | -4.763979 |
| N    | -0.556115 | 1.553282  | -3.39618  | C    | 0.049471  | 0.996993  | -4.611711 |
| Li   | 0.860418  | 2.22219   | -2.27592  | H    | -0.147023 | -0.09379  | -4.74377  |
| N    | 2.456893  | 1.069053  | -2.384555 | H    | -0.401255 | 1.466787  | -5.508738 |
| Li   | 1.667928  | -0.305665 | -1.296203 | H    | 1.839658  | 0.795968  | -5.764832 |
| O    | 2.337615  | -2.158436 | -1.278475 | H    | 1.819486  | 2.247727  | -4.763344 |
| C    | 3.495084  | -2.649392 | -2.00268  | H    | 2.057096  | -0.585061 | -3.644177 |
| C    | 3.758439  | -4.047944 | -1.444346 | H    | 3.467428  | 0.337773  | -4.122905 |
| C    | 2.341013  | -4.522826 | -1.087666 | C    | -1.908811 | 1.995198  | -3.680093 |
| C    | 1.699924  | -3.239192 | -0.557269 | C    | -2.87208  | 0.801124  | -4.000641 |
| H    | 1.892718  | -3.104517 | 0.514689  | N    | -2.934631 | -0.237083 | -2.933566 |
| H    | 0.621927  | -3.173491 | -0.727064 | C    | -4.189448 | -0.103518 | -2.153275 |
| H    | 2.32457   | -5.331121 | -0.350536 | H    | -4.217672 | 0.902098  | -1.726233 |
| H    | 1.817845  | -4.870734 | -1.986307 | H    | -5.055002 | -0.191292 | -2.837987 |
| H    | 4.381191  | -3.991195 | -0.543575 | C    | -4.312917 | -1.15676  | -1.050471 |
| H    | 4.264241  | -4.695681 | -2.166458 | H    | -5.279949 | -1.026806 | -0.548364 |
| H    | 3.247742  | -2.68021  | -3.071096 | H    | -3.536945 | -0.987794 | -0.296025 |
| H    | 4.313103  | -1.942769 | -1.850436 | C    | -4.181417 | -2.5761   | -1.61556  |
| C    | 3.546972  | 2.01335   | -2.226485 | C    | -2.90154  | -2.686899 | -2.453019 |
| C    | 3.213407  | 3.011876  | -1.093064 | C    | -2.854401 | -1.59397  | -3.523324 |
| N    | 1.954801  | 3.760595  | -1.340455 | H    | -1.921332 | -1.658739 | -4.094477 |
| C    | 2.098385  | 4.853536  | -2.333378 | H    | -3.68418  | -1.748652 | -4.23945  |
| H    | 2.579045  | 4.448593  | -3.229284 | H    | -2.83452  | -3.668015 | -2.940279 |
| C    | 2.863278  | 6.085319  | -1.816575 | H    | -2.023032 | -2.589859 | -1.798703 |
| C    | 2.235967  | 6.615095  | -0.518264 | H    | -5.049693 | -2.801459 | -2.252149 |
| C    | 2.099116  | 5.48515   | 0.513182  | H    | -4.181398 | -3.316557 | -0.806347 |
| C    | 1.347897  | 4.291352  | -0.097924 | H    | -3.884875 | 1.160104  | -4.240439 |
| H    | 1.27056   | 3.466612  | 0.619411  | H    | -2.487214 | 0.326258  | -4.908216 |
| H    | 0.323199  | 4.601809  | -0.344327 | H    | -1.941106 | 2.593426  | -4.617057 |
| H    | 1.559736  | 5.835086  | 1.402798  | C    | -2.505712 | 2.900882  | -2.604398 |
| H    | 3.093815  | 5.166335  | 0.853009  | C    | -3.559259 | 3.76528   | -2.946737 |

**Table 1 (Continued).**

|   |           |           |           |   |           |           |           |
|---|-----------|-----------|-----------|---|-----------|-----------|-----------|
| H | 1.237851  | 7.021786  | -0.739603 | C | -4.162327 | 4.592093  | -2.000069 |
| H | 2.829739  | 7.443404  | -0.112157 | C | -3.724905 | 4.575241  | -0.672959 |
| H | 2.859798  | 6.859593  | -2.594456 | C | -2.677004 | 3.728659  | -0.314101 |
| H | 3.915486  | 5.826003  | -1.639696 | C | -2.072298 | 2.906176  | -1.271807 |
| H | 1.083534  | 5.157149  | -2.626134 | H | -1.251603 | 2.26614   | -0.961412 |
| H | 4.071408  | 3.678875  | -0.920351 | H | -2.322464 | 3.702873  | 0.713383  |
| H | 3.06186   | 2.440455  | -0.169869 | H | -4.192469 | 5.217602  | 0.068607  |
| H | 3.69997   | 2.613309  | -3.14776  | H | -4.970804 | 5.254744  | -2.299291 |
| C | 4.91647   | 1.373756  | -1.937642 | H | -3.905568 | 3.793058  | -3.978113 |
| C | 6.003926  | 1.574074  | -2.79583  | C | -1.183878 | -0.213614 | 0.963895  |
| C | 7.245367  | 0.979745  | -2.547795 | H | -2.030491 | 0.435131  | 0.681815  |
| C | 7.423869  | 0.179349  | -1.420554 | H | -1.562569 | -1.244392 | 0.861814  |
| C | 6.349427  | -0.026144 | -0.548222 | C | -0.893975 | 0.034386  | 2.457838  |
| C | 5.110938  | 0.558718  | -0.811127 | H | -0.063207 | -0.615923 | 2.770255  |
| H | 4.277168  | 0.379282  | -0.135636 | H | -0.530444 | 1.065388  | 2.580667  |
| H | 6.480431  | -0.640896 | 0.339753  | C | -2.101178 | -0.197145 | 3.374479  |
| H | 8.388145  | -0.280871 | -1.220222 | H | -2.463468 | -1.230755 | 3.3       |
| H | -2.936105 | 0.46206   | 3.103959  | H | -1.856713 | -0.007368 | 4.426816  |



**6m**

$G = -1761.523166$

$G_{MP2} = -1756.279342$

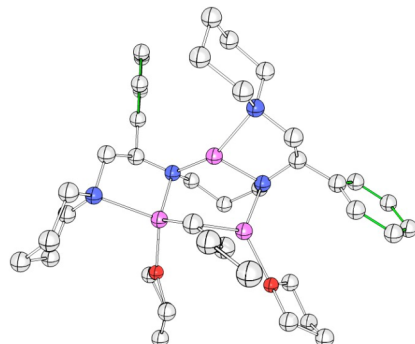
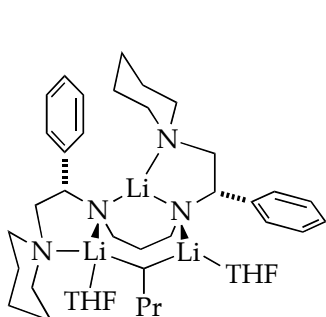
Atom X Y Z Atom X Y Z

|    |           |           |           |   |           |           |           |
|----|-----------|-----------|-----------|---|-----------|-----------|-----------|
| C  | 0         | 0         | 0         | H | 7.98029   | 0.760479  | -3.341715 |
| H  | 0.951149  | 0.119993  | 0.569554  | H | 5.884477  | 1.996907  | -3.80279  |
| H  | -0.54787  | 0.917591  | 0.312442  | C | 2.38249   | 0.747596  | -3.700391 |
| Li | -0.880832 | 0.593974  | -1.84811  | C | 1.484669  | 1.487654  | -4.719167 |
| N  | -0.536523 | 2.001067  | -3.254322 | C | -0.035886 | 1.379988  | -4.48407  |
| Li | 0.97297   | 2.628821  | -2.241183 | H | -0.286656 | 0.294137  | -4.568854 |
| N  | 2.476366  | 1.362655  | -2.372547 | H | -0.519248 | 1.84101   | -5.368698 |
| Li | 1.746168  | -0.088843 | -1.284748 | H | 1.685182  | 1.07949   | -5.722961 |
| O  | 2.541083  | -1.917004 | -1.44963  | H | 1.771532  | 2.551396  | -4.753479 |
| C  | 3.79112   | -2.183282 | -2.124821 | H | 1.968614  | -0.278082 | -3.6159   |
| C  | 3.461413  | -3.30758  | -3.100209 | H | 3.37883   | 0.60752   | -4.160311 |
| C  | 2.497111  | -4.170019 | -2.26804  | C | -1.890184 | 2.483817  | -3.447378 |
| C  | 1.753502  | -3.132911 | -1.404047 | C | -2.942817 | 1.323275  | -3.589324 |
| H  | 1.648413  | -3.451747 | -0.362042 | N | -2.884707 | 0.333479  | -2.48124  |

**Table 1 (Continued).**

|   |           |           |           |   |           |           |           |
|---|-----------|-----------|-----------|---|-----------|-----------|-----------|
| H | 0.75963   | -2.891088 | -1.79264  | C | -3.891291 | 0.577646  | -1.416    |
| H | 3.060541  | -4.863804 | -1.633943 | H | -3.590881 | -0.018272 | -0.543344 |
| H | 1.811803  | -4.762734 | -2.881049 | H | -3.830903 | 1.62807   | -1.123486 |
| H | 4.349419  | -3.854007 | -3.432011 | C | -5.330735 | 0.203149  | -1.80971  |
| H | 2.956906  | -2.900244 | -3.983899 | C | -5.412012 | -1.247955 | -2.305842 |
| H | 4.117416  | -1.25216  | -2.587314 | C | -4.379446 | -1.491984 | -3.415782 |
| H | 4.54427   | -2.495288 | -1.388659 | C | -2.978456 | -1.071884 | -2.944651 |
| C | 3.638298  | 2.229206  | -2.242963 | H | -2.239331 | -1.217764 | -3.740969 |
| C | 3.387832  | 3.291252  | -1.148106 | H | -2.678912 | -1.712602 | -2.102552 |
| N | 2.19127   | 4.128807  | -1.414098 | H | -4.362717 | -2.550175 | -3.707591 |
| C | 2.390768  | 5.135141  | -2.486179 | H | -4.6531   | -0.920832 | -4.313684 |
| H | 2.790303  | 4.628693  | -3.369983 | H | -6.424357 | -1.480773 | -2.658736 |
| C | 3.287256  | 6.320002  | -2.087994 | H | -5.206624 | -1.930362 | -1.467407 |
| C | 2.764464  | 6.996904  | -0.811645 | H | -5.69269  | 0.880886  | -2.59463  |
| C | 2.562538  | 5.959095  | 0.302934  | H | -5.986571 | 0.354875  | -0.942894 |
| C | 1.68375   | 4.798833  | -0.194304 | H | -3.954061 | 1.735019  | -3.717113 |
| H | 1.56498   | 4.037432  | 0.585239  | H | -2.701636 | 0.795247  | -4.517652 |
| H | 0.680968  | 5.1813    | -0.427345 | H | -1.984585 | 3.014295  | -4.419753 |
| H | 2.090219  | 6.419352  | 1.180412  | C | -2.332926 | 3.498416  | -2.394268 |
| H | 3.535994  | 5.5743    | 0.635602  | C | -3.331163 | 4.431562  | -2.71909  |
| H | 1.801184  | 7.48199   | -1.029334 | C | -3.793311 | 5.361347  | -1.787805 |
| H | 3.448774  | 7.789743  | -0.485116 | C | -3.265353 | 5.380834  | -0.494739 |
| H | 3.323137  | 7.034806  | -2.920077 | C | -2.270492 | 4.464835  | -0.153238 |
| H | 4.317566  | 5.975067  | -1.929515 | C | -1.808359 | 3.539338  | -1.09499  |
| H | 1.395646  | 5.513545  | -2.758509 | H | -1.036583 | 2.834742  | -0.799615 |
| H | 4.297894  | 3.89209   | -1.001635 | H | -1.850297 | 4.46377   | 0.849647  |
| H | 3.194841  | 2.769402  | -0.20366  | H | -3.622714 | 6.102699  | 0.2349    |
| H | 3.835088  | 2.778782  | -3.185897 | H | -4.561972 | 6.0752    | -2.073877 |
| C | 4.953463  | 1.495331  | -1.929485 | H | -3.745787 | 4.431985  | -3.725394 |
| C | 6.000194  | 1.466201  | -2.859528 | C | -0.740689 | -1.190444 | 0.644049  |
| C | 7.186873  | 0.773325  | -2.59807  | H | -1.732038 | -1.316309 | 0.173928  |
| C | 7.354006  | 0.106942  | -1.384952 | H | -0.206734 | -2.129109 | 0.426447  |
| C | 6.322053  | 0.132579  | -0.440741 | C | -0.955585 | -1.116047 | 2.167877  |
| C | 5.135568  | 0.810482  | -0.716634 | H | 0.024306  | -1.011316 | 2.657134  |
| H | 4.334807  | 0.803458  | 0.019826  | H | -1.509454 | -0.195511 | 2.404856  |
| H | 6.444548  | -0.376501 | 0.512653  | C | -1.694399 | -2.325205 | 2.754122  |
| H | 8.27767   | -0.425667 | -1.173116 | H | -1.146407 | -3.256594 | 2.560203  |
| H | -2.692243 | -2.434714 | 2.309189  | H | -1.824814 | -2.238292 | 3.839827  |

**Table 2.** Optimized geometries at B3LYP level of theory with 6-31G(d) basis set for the di-solvated BuLi-ligand aggregation conformers at -78 °C with free energies (Hartrees) and cartesian coordinates (X, Y, Z) (Note:  $G_{\text{MP2}}$  includes single point MP2 corrections to B3LYP/6-31G(d) optimized structures).

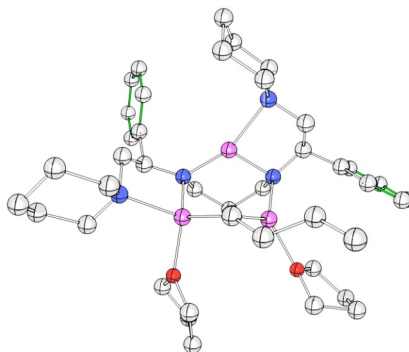
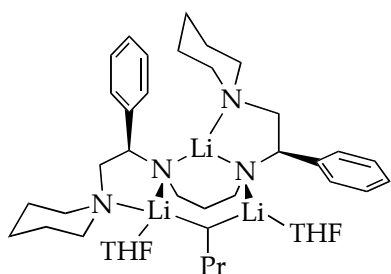


**6a**  
 $G = -1993.882182$   
 $G_{\text{MP2}} = -1987.993623$

| Atom | X         | Y         | Z         | Atom | X         | Y        | Z         |
|------|-----------|-----------|-----------|------|-----------|----------|-----------|
| N    | 0         | 0         | 0         | H    | -3.88998  | 1.285756 | 7.236108  |
| Li   | -0.63393  | 1.581872  | 1.103928  | H    | -4.668175 | 2.247061 | 5.969979  |
| Li   | -3.278993 | 0.568685  | 1.203493  | H    | -4.83803  | 0.485722 | 5.973468  |
| N    | -3.005893 | -1.16537  | 0.285743  | O    | -4.878148 | 1.686684 | 0.651361  |
| Li   | -1.217896 | -1.128334 | 1.103481  | C    | -5.855073 | 2.346255 | 1.493328  |
| N    | -1.842334 | -2.922631 | 2.352143  | C    | -7.175548 | 2.316568 | 0.71711   |
| C    | -3.295304 | -2.695223 | 2.165545  | C    | -6.699197 | 2.277941 | -0.742986 |
| C    | -3.686624 | -2.376065 | 0.709814  | C    | -5.466196 | 1.382947 | -0.642504 |
| H    | -3.371044 | -3.235656 | 0.082105  | H    | -4.708273 | 1.579972 | -1.404751 |
| C    | -5.216751 | -2.32532  | 0.554314  | H    | -5.72802  | 0.321284 | -0.667899 |
| C    | -5.81726  | -2.860614 | -0.59499  | H    | -6.424445 | 3.282571 | -1.087532 |
| C    | -7.196061 | -2.776147 | -0.806512 | H    | -7.448697 | 1.873678 | -1.429551 |
| C    | -8.01451  | -2.166291 | 0.144512  | H    | -7.810764 | 3.177368 | 0.947028  |
| C    | -7.436769 | -1.637848 | 1.302851  | H    | -7.733069 | 1.40356  | 0.951204  |
| C    | -6.056086 | -1.708484 | 1.497117  | H    | -5.902016 | 1.820625 | 2.450405  |
| H    | -5.63316  | -1.28646  | 2.405681  | H    | -5.511621 | 3.37269  | 1.676208  |
| H    | -8.06573  | -1.181928 | 2.064828  | O    | -1.240919 | 3.282885 | 0.143012  |
| H    | -9.089592 | -2.112085 | -0.00729  | C    | -2.280276 | 4.156327 | 0.650176  |
| H    | -7.63061  | -3.197806 | -1.709949 | C    | -2.411103 | 5.290448 | -0.373002 |
| H    | -5.190323 | -3.358675 | -1.331752 | C    | -1.962637 | 4.609568 | -1.675899 |
| H    | -3.867186 | -3.563614 | 2.540137  | C    | -0.839265 | 3.700318 | -1.1794   |
| H    | -3.559911 | -1.839383 | 2.796483  | H    | 0.111948  | 4.245979 | -1.10927  |
| C    | -1.457401 | -4.243615 | 1.805453  | H    | -0.688698 | 2.803263 | -1.783529 |
| H    | -1.685814 | -4.256156 | 0.736658  | H    | -1.625362 | 5.31506  | -2.441271 |
| H    | -2.075943 | -5.030743 | 2.280536  | H    | -2.778012 | 4.010478 | -2.098341 |
| C    | 0.024389  | -4.559123 | 2.017677  | H    | -1.734186 | 6.116616 | -0.124943 |
| H    | 0.626508  | -3.867265 | 1.418852  | H    | -3.428237 | 5.691358 | -0.420078 |
| H    | 0.226704  | -5.566885 | 1.633229  | H    | -3.200031 | 3.569615 | 0.735555  |
| C    | 0.418102  | -4.454043 | 3.49574   | H    | -1.986065 | 4.501228 | 1.646154  |
| C    | -0.035424 | -3.104125 | 4.064441  | C    | 1.452358  | 0.114804 | 0.030303  |

**Table 2 (Continued).**

|   |           |           |           |   |          |           |           |
|---|-----------|-----------|-----------|---|----------|-----------|-----------|
| C | -1.522988 | -2.869901 | 3.794517  | C | 1.920812 | 0.546427  | 1.433229  |
| H | -1.825233 | -1.887348 | 4.171434  | N | 1.458086 | 1.892644  | 1.844973  |
| H | -2.115653 | -3.627892 | 4.343893  | C | 1.65301  | 2.044131  | 3.303609  |
| H | 0.144859  | -3.053613 | 5.145669  | H | 1.058483 | 1.271493  | 3.801834  |
| H | 0.544845  | -2.291006 | 3.605991  | H | 2.715014 | 1.863709  | 3.563079  |
| H | -0.064354 | -5.26376  | 4.062772  | C | 1.240466 | 3.426355  | 3.815474  |
| H | 1.500466  | -4.584971 | 3.61922   | H | 1.437168 | 3.477032  | 4.893801  |
| C | -2.88928  | -1.084694 | -1.158984 | H | 0.157777 | 3.548901  | 3.682976  |
| C | -1.965358 | 0.05726   | -1.616079 | C | 1.983509 | 4.540596  | 3.070596  |
| C | -0.452282 | -0.122597 | -1.383515 | C | 1.805428 | 4.353328  | 1.560188  |
| H | 0.057774  | 0.638733  | -2.021587 | C | 2.21182  | 2.942091  | 1.127354  |
| H | -0.167696 | -1.089154 | -1.849101 | H | 2.042954 | 2.817033  | 0.054466  |
| H | -2.291844 | 1.001623  | -1.149623 | H | 3.298127 | 2.805864  | 1.299999  |
| H | -2.110813 | 0.18658   | -2.69941  | H | 2.406727 | 5.08265   | 1.002018  |
| H | -2.488621 | -2.031007 | -1.589867 | H | 0.755371 | 4.517091  | 1.288705  |
| H | -3.867575 | -0.946492 | -1.670964 | H | 3.054089 | 4.498246  | 3.319591  |
| C | -1.953545 | 1.09108   | 2.833032  | H | 1.624287 | 5.527911  | 3.387098  |
| H | -1.346143 | 0.232766  | 3.196491  | H | 3.021985 | 0.489748  | 1.502939  |
| H | -1.320129 | 1.967338  | 3.074809  | H | 1.514371 | -0.160764 | 2.165855  |
| C | -3.17218  | 1.203531  | 3.774722  | H | 1.782311 | 0.900288  | -0.686871 |
| H | -3.720174 | 2.135501  | 3.555344  | C | 2.232647 | -1.136242 | -0.418379 |
| H | -3.902561 | 0.391788  | 3.580255  | C | 2.68006  | -1.24059  | -1.742793 |
| C | -2.884167 | 1.184335  | 5.290204  | C | 3.369738 | -2.367732 | -2.194552 |
| H | -2.186402 | 2.001502  | 5.523692  | C | 3.643658 | -3.418157 | -1.318476 |
| H | -2.351374 | 0.254501  | 5.53816   | C | 3.216585 | -3.328315 | 0.008001  |
| C | -4.135783 | 1.307231  | 6.167368  | C | 2.515166 | -2.203629 | 0.44661   |
| H | 3.698011  | -2.421283 | -3.230024 | H | 2.196967 | -2.154832 | 1.48462   |
| H | 2.486068  | -0.418391 | -2.428703 | H | 3.434342 | -4.134006 | 0.705497  |
| H | 4.187367  | -4.294446 | -1.662247 |   |          |           |           |



**6g**

$G = -1993.873501$

$G_{MP2} = -1987.984874$

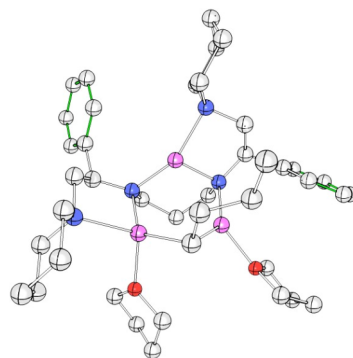
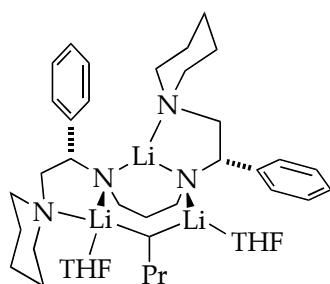
| Atom | X        | Y         | Z         |
|------|----------|-----------|-----------|
| C    | 0        | 0         | 0         |
| Li   | -1.26646 | -0.717779 | -1.637333 |

| Atom | X         | Y         | Z         |
|------|-----------|-----------|-----------|
| C    | -1.68824  | -3.705752 | -2.140519 |
| H    | -1.357892 | -4.55786  | -2.772482 |

| Table 2 (Continued). |           |           |           |   |           |           |           |
|----------------------|-----------|-----------|-----------|---|-----------|-----------|-----------|
| N                    | -1.021022 | -2.482517 | -2.556927 | C | -3.21792  | -3.679001 | -2.298167 |
| Li                   | 0.799151  | -2.580774 | -1.833346 | C | -3.808917 | -4.217115 | -3.450752 |
| N                    | 1.996462  | -1.388658 | -2.87641  | C | -5.188069 | -4.146631 | -3.665013 |
| Li                   | 1.440143  | 0.213346  | -1.767674 | C | -6.014866 | -3.54794  | -2.7139   |
| O                    | 1.041762  | 2.01651   | -2.628392 | C | -5.445941 | -3.018409 | -1.551686 |
| C                    | 0.134707  | 2.971755  | -2.024866 | C | -4.06543  | -3.076579 | -1.353435 |
| C                    | -0.372158 | 3.874992  | -3.16775  | H | -3.647344 | -2.651416 | -0.444685 |
| C                    | 0.017102  | 3.096583  | -4.437614 | H | -6.081177 | -2.568156 | -0.791772 |
| C                    | 1.298022  | 2.398071  | -3.990372 | H | -7.089989 | -3.503411 | -2.868849 |
| H                    | 2.160183  | 3.081243  | -4.030421 | H | -5.616097 | -4.56869  | -4.571354 |
| H                    | 1.537746  | 1.489874  | -4.54673  | H | -3.17455  | -4.703231 | -4.189209 |
| H                    | 0.165626  | 3.741467  | -5.309152 | H | -1.869264 | -4.877706 | -0.296286 |
| H                    | -0.744781 | 2.349246  | -4.685198 | H | -1.530843 | -3.155053 | -0.06359  |
| H                    | 0.13618   | 4.845517  | -3.147188 | C | 0.500355  | -5.637075 | -0.996237 |
| H                    | -1.447582 | 4.064092  | -3.097805 | H | 0.229452  | -5.712337 | -2.052764 |
| H                    | -0.656766 | 2.392821  | -1.544253 | H | -0.116837 | -6.37667  | -0.449473 |
| H                    | 0.67188   | 3.538646  | -1.255489 | C | 1.981296  | -5.974439 | -0.815427 |
| C                    | 1.514108  | -1.454153 | -4.256243 | C | 2.425241  | -5.791096 | 0.641227  |
| C                    | 0.001188  | -1.243929 | -4.456371 | C | 2.018623  | -4.400554 | 1.144137  |
| C                    | -0.925419 | -2.38465  | -4.003556 | C | 0.529067  | -4.143747 | 0.905773  |
| H                    | -0.537031 | -3.328296 | -4.45256  | H | 0.263422  | -3.132155 | 1.230019  |
| H                    | -1.909101 | -2.234458 | -4.50008  | H | -0.065259 | -4.851014 | 1.516841  |
| H                    | -0.160825 | -1.090992 | -5.534074 | H | 2.603289  | -3.629327 | 0.62287   |
| H                    | -0.308098 | -0.305114 | -3.967639 | H | 2.234018  | -4.293116 | 2.214686  |
| H                    | 2.026986  | -0.680643 | -4.876154 | H | 3.507998  | -5.939053 | 0.738743  |
| H                    | 1.774787  | -2.408143 | -4.759795 | H | 1.944602  | -6.555524 | 1.269202  |
| C                    | 3.452957  | -1.309319 | -2.880587 | H | 2.577919  | -5.333523 | -1.474015 |
| C                    | 3.982935  | -0.932191 | -1.482143 | H | 2.148723  | -7.007887 | -1.144381 |
| H                    | 3.619854  | -1.670631 | -0.757497 | O | -2.811431 | 0.424245  | -2.299614 |
| H                    | 5.08163   | -0.997377 | -1.478811 | C | -3.552053 | 1.438595  | -1.600804 |
| H                    | 3.780804  | -0.504875 | -3.578549 | C | -5.015335 | 1.070245  | -1.82653  |
| C                    | 4.187161  | -2.561553 | -3.395802 | C | -4.995412 | 0.588752  | -3.288117 |
| C                    | 4.616617  | -2.62207  | -4.728744 | C | -3.591091 | -0.027574 | -3.442461 |
| C                    | 5.261106  | -3.751415 | -5.238247 | H | -3.089328 | 0.29707   | -4.360836 |
| C                    | 5.505961  | -4.849202 | -4.41316  | H | -3.599543 | -1.116691 | -3.408921 |
| C                    | 5.096455  | -4.80399  | -3.078792 | H | -5.126263 | 1.436609  | -3.970252 |
| C                    | 4.441166  | -3.67566  | -2.582321 | H | -5.780816 | -0.140833 | -3.502192 |
| H                    | 4.136526  | -3.661083 | -1.539335 | H | -5.696036 | 1.91038   | -1.657264 |
| H                    | 5.292376  | -5.647463 | -2.420628 | H | -5.300126 | 0.251307  | -1.157267 |
| H                    | 6.013632  | -5.728089 | -4.802306 | H | -3.233739 | 1.42136   | -0.557095 |
| H                    | 5.575874  | -3.770307 | -6.279065 | H | -3.322673 | 2.428544  | -2.025905 |
| H                    | 4.44319   | -1.764573 | -5.375845 | H | 0.524127  | -0.880179 | 0.435595  |
| N                    | 0.164221  | -4.275084 | -0.521464 | H | 0.797419  | 0.772126  | -0.007521 |
| C                    | -1.289488 | -4.022478 | -0.686598 | C | -0.96969  | 0.504855  | 1.099018  |
| H                    | 2.998597  | 1.424086  | 0.727171  | H | -0.456478 | 0.744419  | 2.050548  |
| H                    | 3.098386  | -0.320437 | 0.920336  | H | -1.424641 | 1.460972  | 0.784776  |



| Table 2 (Continued). |          |           |           |   |           |           |           |
|----------------------|----------|-----------|-----------|---|-----------|-----------|-----------|
| C                    | 5.023122 | 0.715311  | 0.985664  | C | -2.106673 | -0.466236 | 1.451343  |
| C                    | 5.70793  | 1.904958  | 0.296539  | H | -1.670239 | -1.428968 | 1.756645  |
| C                    | 5.615265 | 1.7665    | -1.230321 | H | -2.705458 | -0.680102 | 0.552138  |
| C                    | 4.160415 | 1.530531  | -1.674357 | C | -3.031911 | 0.039422  | 2.56464   |
| H                    | 4.108781 | 1.38632   | -2.757267 | H | -3.51198  | 0.986221  | 2.283791  |
| H                    | 3.563409 | 2.423364  | -1.444695 | H | -3.826557 | -0.680794 | 2.794951  |
| H                    | 5.998779 | 2.667929  | -1.72612  | H | -2.47005  | 0.222242  | 3.488897  |
| H                    | 6.249417 | 0.935324  | -1.565756 | N | 3.494167  | 0.384634  | -1.013829 |
| H                    | 6.754043 | 1.992399  | 0.615619  | C | 3.590475  | 0.539167  | 0.454462  |
| H                    | 5.206577 | 2.834884  | 0.605223  | H | 4.989029  | 0.863842  | 2.072806  |
| H                    | 5.603855 | -0.201039 | 0.812569  |   |           |           |           |



**6h**

$G = -1993.87677$

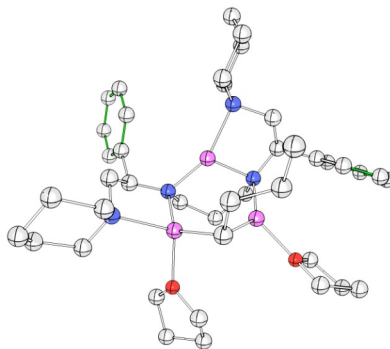
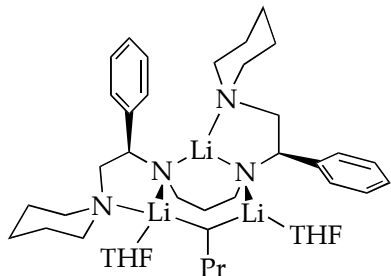
$G_{\text{MP2}} = -1987.988021$

| Atom | X         | Y         | Z         | Atom | X        | Y         | Z         |
|------|-----------|-----------|-----------|------|----------|-----------|-----------|
| C    | 0         | 0         | 0         | C    | 7.848512 | 0.462765  | 1.700996  |
| N    | -0.427984 | 0.10752   | 1.394309  | C    | 7.068799 | 0.250529  | 2.842262  |
| Li   | -0.149658 | -1.497459 | 2.602305  | C    | 5.733608 | 0.655532  | 2.868299  |
| O    | -0.124162 | -3.362593 | 1.652007  | H    | 5.145435 | 0.4692    | 3.7634    |
| C    | 0.86186   | -4.376653 | 1.972744  | H    | 7.505714 | -0.222919 | 3.719046  |
| C    | 0.661141  | -5.496622 | 0.946247  | H    | 8.888671 | 0.147444  | 1.679929  |
| C    | 0.100761  | -4.733643 | -0.264155 | H    | 7.873226 | 1.26963   | -0.298914 |
| C    | -0.78745  | -3.690848 | 0.413122  | H    | 5.515005 | 2.018475  | -0.225797 |
| H    | -1.781575 | -4.102594 | 0.637539  | H    | 4.014128 | 3.267362  | 3.228735  |
| H    | -0.906531 | -2.768536 | -0.159532 | H    | 3.375431 | 1.765476  | 3.89619   |
| H    | -0.454207 | -5.369159 | -0.961045 | C    | 1.647986 | 4.062123  | 2.110717  |
| H    | 0.909379  | -4.242416 | -0.817909 | H    | 2.018436 | 3.775531  | 1.122752  |
| H    | -0.072732 | -6.226939 | 1.307819  | C    | 2.262413 | 5.399848  | 2.557977  |
| H    | 1.590504  | -6.032429 | 0.729645  | C    | 1.784065 | 5.776329  | 3.968794  |
| H    | 1.854242  | -3.919841 | 1.898697  | C    | 2.026251 | 4.617826  | 4.948294  |
| H    | 0.703299  | -4.695819 | 3.006526  | C    | 1.419523 | 3.313768  | 4.402975  |
| H    | 1.482217  | -1.535005 | 0.374942  | H    | 1.621091 | 2.476183  | 5.079896  |
| C    | 1.404908  | -0.602889 | -0.207837 | H    | 0.326853 | 3.429331  | 4.349509  |
| C    | 2.604423  | 0.3108    | 0.101761  | H    | 1.58418  | 4.838738  | 5.928451  |
| N    | 2.736576  | 0.614747  | 1.518606  | H    | 3.103988 | 4.487096  | 5.113134  |

**Table 2 (Continued).**

|    |           |           |          |   |           |           |           |
|----|-----------|-----------|----------|---|-----------|-----------|-----------|
| Li | 1.00511   | 1.173589  | 2.20656  | H | 0.706765  | 5.998849  | 3.935575  |
| Li | 2.66986   | -1.069819 | 2.609672 | H | 2.281757  | 6.689798  | 4.317271  |
| C  | 1.415251  | -1.834786 | 4.217922 | H | 1.985703  | 6.177751  | 1.834894  |
| H  | 2.177136  | -2.633286 | 4.342248 | H | 3.358497  | 5.33672   | 2.541961  |
| H  | 0.484401  | -2.438186 | 4.230331 | H | 0.561413  | 4.178816  | 2.015493  |
| C  | 1.41888   | -1.024468 | 5.539015 | H | 2.472095  | 1.240078  | -0.498437 |
| H  | 0.810946  | -0.107594 | 5.436046 | H | 3.509142  | -0.166291 | -0.335685 |
| H  | 0.964427  | -1.571159 | 6.387658 | H | 1.483734  | -0.897932 | -1.265281 |
| C  | 2.823008  | -0.603401 | 5.994122 | C | -1.847115 | 0.414227  | 1.463488  |
| H  | 3.307745  | -0.026552 | 5.191475 | H | -2.424447 | -0.280351 | 0.813104  |
| H  | 3.436925  | -1.507685 | 6.126643 | C | -2.243207 | 1.815442  | 0.960448  |
| C  | 2.846634  | 0.212568  | 7.291361 | C | -2.851765 | 1.97103   | -0.291438 |
| H  | 3.868118  | 0.484159  | 7.585252 | C | -3.196487 | 3.23221   | -0.783924 |
| H  | 2.27291   | 1.142805  | 7.188019 | C | -2.949212 | 4.372783  | -0.020459 |
| H  | 2.401402  | -0.353361 | 8.119136 | C | -2.347873 | 4.237837  | 1.233688  |
| O  | 4.050523  | -2.489927 | 2.124674 | C | -1.993128 | 2.974925  | 1.710199  |
| C  | 4.689185  | -3.363228 | 3.085548 | H | -1.523365 | 2.891407  | 2.687721  |
| C  | 6.076735  | -3.664824 | 2.515858 | H | -2.161347 | 5.118435  | 1.844614  |
| C  | 5.821106  | -3.605985 | 1.002463 | H | -3.223187 | 5.355881  | -0.394662 |
| C  | 4.825367  | -2.45008  | 0.897655 | H | -3.661903 | 3.321662  | -1.76275  |
| H  | 4.129972  | -2.541268 | 0.058824 | H | -3.058612 | 1.085008  | -0.888728 |
| H  | 5.330472  | -1.481932 | 0.835591 | H | -0.02117  | 0.971053  | -0.539951 |
| H  | 5.369852  | -4.542646 | 0.652654 | H | -0.713915 | -0.63585  | -0.573497 |
| H  | 6.727325  | -3.42454  | 0.417251 | C | -2.35571  | 0.22864   | 2.906664  |
| H  | 6.467084  | -4.628665 | 2.85672  | H | -1.766046 | 0.876632  | 3.565863  |
| H  | 6.784936  | -2.881263 | 2.806588 | H | -3.407099 | 0.560437  | 2.983583  |
| H  | 4.711418  | -2.8547   | 4.052792 | N | -2.217582 | -1.148097 | 3.434869  |
| H  | 4.08446   | -4.274046 | 3.187307 | C | -2.398396 | -1.119089 | 4.903624  |
| N  | 1.886343  | 2.936338  | 3.049402 | H | -1.624202 | -0.468587 | 5.323383  |
| C  | 3.292334  | 2.455913  | 3.050044 | H | -3.378677 | -0.665185 | 5.151534  |
| C  | 3.662726  | 1.709744  | 1.748833 | C | -2.312873 | -2.508375 | 5.539931  |
| H  | 3.590761  | 2.448161  | 0.922998 | H | -2.488317 | -2.412756 | 6.618921  |
| C  | 5.145281  | 1.299437  | 1.767416 | H | -1.295579 | -2.899051 | 5.413652  |
| C  | 5.945846  | 1.512322  | 0.635847 | C | -3.322441 | -3.471687 | 4.906029  |
| C  | 7.278887  | 1.093732  | 0.594774 | C | -3.150313 | -3.466505 | 3.383316  |
| H  | -3.924821 | -4.076807 | 2.900652 | C | -3.22386  | -2.042323 | 2.825109  |
| H  | -2.177529 | -3.897968 | 3.11798  | H | -3.063893 | -2.056246 | 1.743568  |
| H  | -4.344388 | -3.152425 | 5.158501 | H | -4.239909 | -1.633099 | 2.995343  |
| H  | -3.198777 | -4.484736 | 5.308841 |   |           |           |           |

**Table 2 (Continued).**



**6i**

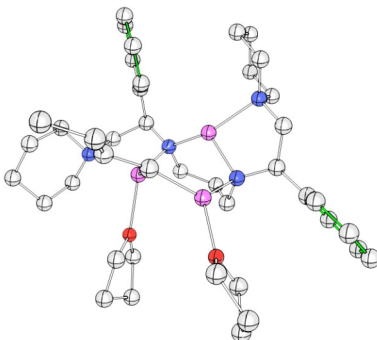
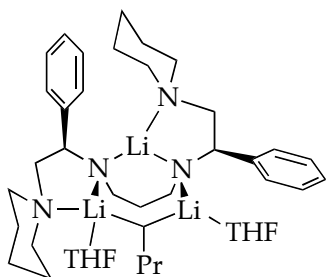
$G = -1993.872578$

$G_{MP2} = -1987.981698$

| Atom | X         | Y         | Z         | Atom | X         | Y        | Z         |
|------|-----------|-----------|-----------|------|-----------|----------|-----------|
| Li   | 0         | 0         | 0         | N    | -0.005638 | 1.649929 | -1.151581 |
| Li   | -2.799383 | -0.565873 | -0.061995 | C    | 0.835471  | 2.818594 | -0.952844 |
| N    | -3.138037 | 0.988883  | -1.320093 | C    | 0.408268  | 3.569016 | 0.327284  |
| C    | -4.573143 | 1.209264  | -1.284899 | N    | -1.021979 | 3.972061 | 0.297547  |
| C    | -5.100684 | 1.065304  | 0.158602  | C    | -1.30647  | 5.070807 | -0.660324 |
| N    | -4.839354 | -0.27033  | 0.742411  | H    | -0.909261 | 4.791445 | -1.639873 |
| C    | -4.874783 | -0.264356 | 2.221892  | C    | -0.76888  | 6.444673 | -0.224909 |
| H    | -4.443254 | -1.216431 | 2.560787  | C    | -1.285514 | 6.815704 | 1.173937  |
| H    | -4.20577  | 0.526091  | 2.575947  | C    | -0.999707 | 5.684293 | 2.173312  |
| C    | -6.281179 | -0.108717 | 2.823797  | C    | -1.530455 | 4.343577 | 1.637965  |
| C    | -7.214173 | -1.20802  | 2.295513  | H    | -1.298086 | 3.526814 | 2.33028   |
| C    | -7.190807 | -1.23646  | 0.760198  | H    | -2.626547 | 4.402248 | 1.564556  |
| C    | -5.746982 | -1.321619 | 0.2307    | H    | -1.467291 | 5.895769 | 3.143677  |
| H    | -5.740673 | -1.281478 | -0.862216 | H    | 0.08064   | 5.610741 | 2.355651  |
| H    | -5.313591 | -2.289009 | 0.519184  | H    | -2.372008 | 6.98352  | 1.123106  |
| H    | -7.762556 | -2.092471 | 0.378226  | H    | -0.839197 | 7.757663 | 1.516142  |
| H    | -7.681202 | -0.336228 | 0.366871  | H    | -1.075607 | 7.196856 | -0.962943 |
| H    | -8.237261 | -1.06394  | 2.664871  | H    | 0.328998  | 6.438529 | -0.225932 |
| H    | -6.875065 | -2.181599 | 2.680625  | H    | -2.396347 | 5.128647 | -0.770171 |
| H    | -6.688112 | 0.879558  | 2.569872  | H    | 1.081548  | 4.42243  | 0.498463  |
| H    | -6.213366 | -0.149544 | 3.918671  | H    | 0.515994  | 2.900434 | 1.188369  |
| H    | -6.167549 | 1.335619  | 0.187454  | H    | 0.704174  | 3.526139 | -1.798442 |
| H    | -4.57529  | 1.787634  | 0.794459  | C    | 2.345871  | 2.527184 | -0.935252 |
| H    | -5.095997 | 0.444692  | -1.904289 | C    | 3.099297  | 2.699976 | -2.106051 |
| C    | -5.045358 | 2.55455   | -1.867201 | C    | 4.459425  | 2.382642 | -2.153583 |
| C    | -5.648747 | 2.608486  | -3.130027 | C    | 5.105399  | 1.899025 | -1.015362 |
| C    | -6.059731 | 3.820029  | -3.691812 | C    | 4.374543  | 1.732589 | 0.164824  |
| C    | -5.886029 | 5.011952  | -2.988927 | C    | 3.012248  | 2.035043 | 0.199231  |
| C    | -5.292072 | 4.978278  | -1.724479 | H    | 2.466577  | 1.887789 | 1.127805  |
| C    | -4.871766 | 3.764901  | -1.178252 | H    | 4.869922  | 1.375591 | 1.065316  |
| H    | -4.408968 | 3.761257  | -0.193738 | H    | 6.166401  | 1.663791 | -1.042304 |
| H    | -5.16258  | 5.899253  | -1.160049 | H    | 5.015259  | 2.523914 | -3.077681 |
| H    | -6.210887 | 5.956496  | -3.417736 | H    | 2.607942  | 3.093581 | -2.993527 |
| H    | -6.518636 | 3.830478  | -4.677742 | C    | -0.102343 | 1.290252 | -2.558896 |

| Table 2 (Continued). |           |           |           |   |           |           |           |
|----------------------|-----------|-----------|-----------|---|-----------|-----------|-----------|
| H                    | -5.798099 | 1.681771  | -3.681005 | H | 0.834317  | 0.852957  | -2.969438 |
| Li                   | -1.781474 | 2.146614  | -0.52269  | H | -0.281641 | 2.189042  | -3.192452 |
| O                    | 1.490406  | -1.327975 | -0.372731 | C | -2.682825 | 0.823075  | -2.700027 |
| C                    | 2.125526  | -2.175058 | 0.608755  | C | -1.240848 | 0.296166  | -2.850417 |
| C                    | 3.594046  | -2.242385 | 0.193975  | H | -1.12114  | -0.602869 | -2.223996 |
| C                    | 3.488146  | -2.208589 | -1.338241 | H | -1.120638 | -0.041281 | -3.891176 |
| C                    | 2.317658  | -1.244952 | -1.56518  | H | -2.752848 | 1.756477  | -3.299204 |
| H                    | 1.700752  | -1.509303 | -2.429467 | H | -3.346378 | 0.108766  | -3.239025 |
| H                    | 2.651042  | -0.210286 | -1.67189  | O | -2.745251 | -2.47518  | -0.924918 |
| H                    | 3.254362  | -3.207398 | -1.726372 | C | -1.786442 | -3.469351 | -0.492436 |
| H                    | 4.403506  | -1.86079  | -1.825455 | C | -1.514956 | -4.337873 | -1.720976 |
| H                    | 4.09795   | -3.13527  | 0.576788  | C | -2.874122 | -4.308338 | -2.435491 |
| H                    | 4.12945   | -1.357518 | 0.555115  | C | -3.333706 | -2.868758 | -2.185461 |
| H                    | 1.957601  | -1.734705 | 1.594135  | H | -4.420139 | -2.76933  | -2.10774  |
| H                    | 1.656533  | -3.169214 | 0.587377  | H | -2.97518  | -2.186577 | -2.964416 |
| C                    | -1.258105 | -0.78844  | 1.608083  | H | -3.564896 | -5.020641 | -1.968523 |
| H                    | -0.514697 | -1.598975 | 1.760871  | H | -2.812268 | -4.545744 | -3.501812 |
| H                    | -2.205123 | -1.364678 | 1.668419  | H | -1.185031 | -5.347221 | -1.456158 |
| C                    | -1.20785  | 0.084399  | 2.889     | H | -0.742962 | -3.879206 | -2.350372 |
| H                    | -1.807357 | 1.003267  | 2.75929   | H | -0.91064  | -2.94062  | -0.113154 |
| H                    | -1.645193 | -0.414765 | 3.774781  | H | -2.228401 | -4.056344 | 0.323855  |
| C                    | 0.21376   | 0.506688  | 3.28644   | C | 0.281025  | 1.394508  | 4.534157  |
| H                    | 0.815834  | -0.399071 | 3.457513  | H | -0.159401 | 0.886289  | 5.401031  |
| H                    | 0.690978  | 1.028334  | 2.442107  | H | 1.313656  | 1.659754  | 4.792808  |
| H                    | -0.27482  | 2.329798  | 4.38816   |   |           |           |           |

Note: The following conformers have N-Li-N cyclohexane ring of the ligand backbone in the boat conformation and the left phenyl substituent pointing in the equatorial direction.



**6n**

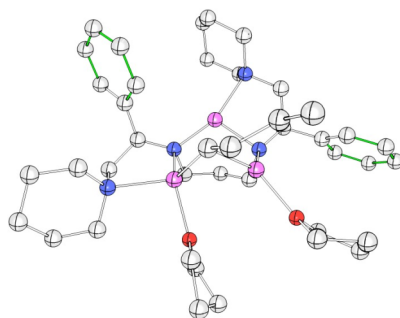
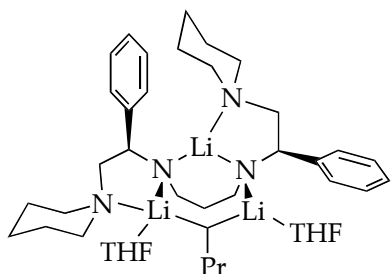
$G = -1993.865106$

$G_{MP2} = -1987.980069$

| Atom | X         | Y         | Z         | Atom | X         | Y         | Z         |
|------|-----------|-----------|-----------|------|-----------|-----------|-----------|
| N    | 0         | 0         | 0         | C    | 8.097261  | -0.212593 | 1.772129  |
| Li   | 0.054135  | -1.746607 | 1.12197   | C    | 7.131335  | -0.163598 | 2.783334  |
| N    | -2.380347 | -1.961589 | 0.324429  | C    | 5.836368  | 0.269289  | 2.498753  |
| C    | -3.465752 | -1.852397 | 1.324648  | H    | 5.096413  | 0.28712   | 3.295512  |
| H    | -3.300434 | -0.95387  | 1.92035   | H    | 7.393109  | -0.454073 | 3.798719  |
| H    | -4.435859 | -1.7222   | 0.803042  | H    | 9.106437  | -0.551164 | 1.99282   |
| C    | -3.54856  | -3.080616 | 2.235003  | H    | 8.494818  | 0.162237  | -0.313639 |
| H    | -4.384198 | -2.946783 | 2.933798  | H    | 6.208266  | 0.979455  | -0.793956 |
| H    | -2.635422 | -3.144657 | 2.838018  | C    | 3.018595  | -0.609878 | -0.453114 |
| C    | -3.723081 | -4.367396 | 1.420135  | C    | 2.058627  | 0.015769  | -1.496891 |
| C    | -2.636196 | -4.447151 | 0.341973  | C    | 0.556329  | -0.296326 | -1.320335 |
| C    | -2.601211 | -3.168897 | -0.497174 | H    | 0.417446  | -1.359483 | -1.625021 |
| H    | -1.796309 | -3.224985 | -1.236821 | H    | 0.028346  | 0.278905  | -2.109521 |
| H    | -3.551967 | -3.081021 | -1.061292 | H    | 2.34488   | -0.327854 | -2.504663 |
| H    | -2.805277 | -5.307049 | -0.319829 | H    | 2.206418  | 1.106855  | -1.494037 |
| H    | -1.65455  | -4.583266 | 0.812     | H    | 2.693585  | -1.658579 | -0.309884 |
| H    | -4.71186  | -4.365355 | 0.938016  | H    | 4.023169  | -0.687985 | -0.91139  |
| H    | -3.691159 | -5.249656 | 2.071941  | C    | 0.995098  | -1.755668 | 3.227541  |
| C    | -2.346369 | -0.768927 | -0.551854 | H    | 1.859128  | -2.385557 | 3.54213   |
| H    | -3.369346 | -0.384512 | -0.716181 | H    | 1.247561  | -0.748292 | 3.634982  |
| H    | -1.979017 | -1.095179 | -1.530597 | C    | -0.178245 | -2.280099 | 4.077205  |
| C    | -1.393202 | 0.391916  | -0.109466 | H    | -1.084556 | -1.683164 | 3.886249  |
| H    | -1.528091 | 1.122673  | -0.939272 | H    | -0.43862  | -3.306021 | 3.76084   |
| C    | -1.915775 | 1.103309  | 1.136914  | C    | 0.039872  | -2.311824 | 5.604148  |
| C    | -2.97527  | 2.017583  | 1.020231  | H    | 0.929142  | -2.922332 | 5.823012  |
| C    | -3.512107 | 2.657302  | 2.138075  | H    | 0.282122  | -1.294893 | 5.946831  |
| C    | -2.998604 | 2.395303  | 3.410717  | C    | -1.158577 | -2.848627 | 6.396303  |
| C    | -1.938958 | 1.497401  | 3.544573  | H    | -1.402469 | -3.876941 | 6.098696  |
| C    | -1.399816 | 0.86478   | 2.419132  | H    | -0.965907 | -2.854001 | 7.476354  |
| H    | -0.583353 | 0.159973  | 2.546712  | H    | -2.053634 | -2.237708 | 6.222316  |
| H    | -1.526095 | 1.282779  | 4.527418  | O    | 4.139379  | -2.833039 | 2.251542  |

**Table 2 (Continued).**

|    |           |           |           |   |          |           |           |
|----|-----------|-----------|-----------|---|----------|-----------|-----------|
| H  | -3.416332 | 2.888779  | 4.284506  | C | 4.576569 | -3.376375 | 3.521015  |
| H  | -4.330766 | 3.362454  | 2.014902  | C | 5.979801 | -3.944241 | 3.278797  |
| H  | -3.385217 | 2.230211  | 0.034608  | C | 5.948059 | -4.278512 | 1.779474  |
| Li | 1.309931  | 0.946353  | 1.067955  | C | 5.119842 | -3.121831 | 1.224203  |
| N  | 3.062308  | 0.072235  | 0.844741  | H | 4.574873 | -3.360828 | 0.306769  |
| Li | 2.695663  | -1.415411 | 2.031254  | H | 5.730856 | -2.230489 | 1.052579  |
| C  | 4.044372  | 1.145372  | 0.873338  | H | 5.442665 | -5.236749 | 1.607186  |
| C  | 3.604717  | 2.229599  | 1.880319  | H | 6.943633 | -4.330707 | 1.329063  |
| N  | 2.283009  | 2.828401  | 1.580986  | H | 6.192266 | -4.808989 | 3.914522  |
| C  | 2.351672  | 3.6982    | 0.385832  | H | 6.738485 | -3.178848 | 3.473469  |
| H  | 2.687825  | 3.09759   | -0.462796 | H | 4.55741  | -2.578114 | 4.26902   |
| H  | 3.109784  | 4.490377  | 0.545365  | H | 3.863546 | -4.15279  | 3.823919  |
| C  | 0.999978  | 4.340701  | 0.065515  | O | 0.834967 | -3.649335 | 0.356401  |
| H  | 0.276247  | 3.552153  | -0.180593 | C | 1.24682  | -4.62951  | 1.344463  |
| H  | 1.109321  | 4.969979  | -0.826906 | C | 1.463536 | -5.933105 | 0.572308  |
| C  | 0.48859   | 5.159848  | 1.255617  | C | 1.917962 | -5.417197 | -0.800812 |
| C  | 0.469907  | 4.283336  | 2.512962  | C | 1.039291 | -4.17727  | -0.971993 |
| C  | 1.828458  | 3.618512  | 2.747471  | H | 0.06599  | -4.440993 | -1.405712 |
| H  | 1.774736  | 2.943589  | 3.609644  | H | 1.493678 | -3.395089 | -1.585208 |
| H  | 2.581948  | 4.393556  | 2.989829  | H | 1.781164 | -6.142153 | -1.609054 |
| H  | 0.210952  | 4.87683   | 3.399034  | H | 2.977658 | -5.135457 | -0.772769 |
| H  | -0.298748 | 3.509755  | 2.410803  | H | 0.523589 | -6.489712 | 0.476695  |
| H  | 1.152035  | 6.022875  | 1.415153  | H | 2.195673 | -6.5868   | 1.056791  |
| H  | -0.511704 | 5.560199  | 1.051452  | H | 2.168956 | -4.274305 | 1.814032  |
| H  | 4.375329  | 3.018523  | 1.954898  | H | 0.467587 | -4.693379 | 2.107878  |
| H  | 3.519114  | 1.767209  | 2.870871  | C | 6.459144 | 0.644164  | 0.21044   |
| H  | 4.129207  | 1.635072  | -0.115496 | C | 7.753765 | 0.189621  | 0.481891  |
| C  | 5.474674  | 0.68743   | 1.207294  |   |          |           |           |



**60**

$G = -1993.860232$

$G_{MP2} = -1987.975152$

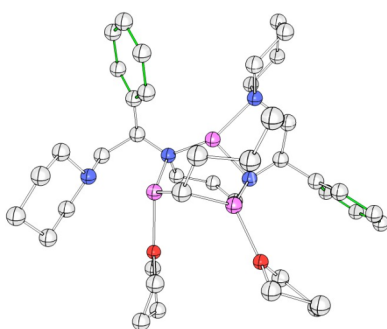
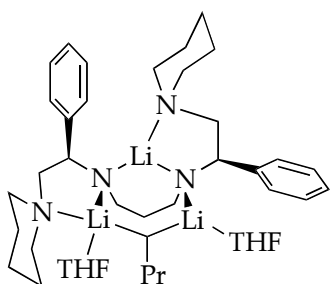
| Atom | X         | Y         | Z         | Atom | X         | Y         | Z         |
|------|-----------|-----------|-----------|------|-----------|-----------|-----------|
| C    | 0         | 0         | 0         | C    | -0.900452 | 0.868686  | -4.529557 |
| Li   | -1.025775 | -0.389248 | -2.061512 | H    | -0.929521 | -0.237484 | -4.683299 |

**Table 2 (Continued).**

|    |           |           |           |   |           |           |           |
|----|-----------|-----------|-----------|---|-----------|-----------|-----------|
| N  | -1.370142 | 1.280098  | -3.20324  | H | -1.574119 | 1.263335  | -5.317688 |
| Li | 0.003262  | 2.313998  | -2.287906 | H | 0.707365  | 0.934511  | -5.939393 |
| N  | 1.8026    | 1.602643  | -2.737657 | H | 0.544651  | 2.417575  | -5.00315  |
| Li | 1.671334  | 0.166604  | -1.398677 | H | 1.504703  | -0.209178 | -3.776518 |
| O  | 3.16798   | -1.263799 | -1.483748 | H | 2.612109  | 0.880236  | -4.583879 |
| C  | 3.632489  | -2.167534 | -0.469703 | C | -2.813084 | 1.450599  | -3.228711 |
| C  | 5.14988   | -2.007427 | -0.488289 | C | -3.612769 | 0.102116  | -3.35583  |
| C  | 5.44034   | -1.862081 | -1.99572  | N | -3.247062 | -0.943734 | -2.368286 |
| C  | 4.129876  | -1.276089 | -2.569776 | C | -4.025507 | -0.886179 | -1.104623 |
| H  | 3.733208  | -1.889358 | -3.388561 | H | -3.515792 | -1.542907 | -0.384621 |
| H  | 4.230234  | -0.24762  | -2.912773 | H | -3.968675 | 0.126298  | -0.705841 |
| H  | 5.656801  | -2.838765 | -2.442319 | C | -5.493767 | -1.329616 | -1.233779 |
| H  | 6.291742  | -1.206174 | -2.192395 | C | -5.601504 | -2.728508 | -1.85666  |
| H  | 5.672322  | -2.852138 | -0.028607 | C | -4.801518 | -2.788623 | -3.165755 |
| H  | 5.430528  | -1.094783 | 0.04816   | C | -3.359372 | -2.304802 | -2.937506 |
| H  | 3.154822  | -1.885906 | 0.469639  | H | -2.79122  | -2.330588 | -3.872494 |
| H  | 3.339422  | -3.199282 | -0.722671 | H | -2.863291 | -2.994691 | -2.24056  |
| C  | 2.648576  | 2.777476  | -2.885738 | H | -4.782279 | -3.811782 | -3.564513 |
| C  | 2.267536  | 3.840127  | -1.835482 | H | -5.28529  | -2.162885 | -3.928218 |
| N  | 0.862963  | 4.304658  | -1.917964 | H | -6.650814 | -3.000414 | -2.027026 |
| C  | 0.643222  | 5.117968  | -3.135049 | H | -5.195161 | -3.471108 | -1.152976 |
| H  | 0.859861  | 4.499267  | -4.009339 | H | -6.048687 | -0.607853 | -1.847499 |
| H  | 1.356433  | 5.966037  | -3.150818 | H | -5.958198 | -1.309626 | -0.239398 |
| C  | -0.789169 | 5.650308  | -3.220159 | H | -4.693632 | 0.311475  | -3.362338 |
| C  | -1.135468 | 6.492139  | -1.987432 | H | -3.371744 | -0.304023 | -4.344252 |
| C  | -0.857801 | 5.679844  | -0.717765 | H | -3.118301 | 1.97799   | -4.158902 |
| C  | 0.563932  | 5.115237  | -0.715806 | C | -3.374912 | 2.312367  | -2.099084 |
| H  | 0.716986  | 4.479267  | 0.163764  | C | -4.518528 | 3.090887  | -2.341326 |
| H  | 1.289386  | 5.949344  | -0.641545 | C | -5.111089 | 3.853345  | -1.333684 |
| H  | -1.575096 | 4.855437  | -0.648515 | C | -4.571863 | 3.85269   | -0.045645 |
| H  | -0.991249 | 6.298466  | 0.179163  | C | -3.431125 | 3.090935  | 0.212127  |
| H  | -2.18414  | 6.811295  | -2.016772 | C | -2.83629  | 2.338527  | -0.805469 |
| H  | -0.522456 | 7.40596   | -1.985202 | H | -1.956612 | 1.747423  | -0.576732 |
| H  | -1.48268  | 4.802738  | -3.297544 | H | -2.996078 | 3.079153  | 1.208826  |
| H  | -0.893119 | 6.239676  | -4.140112 | H | -5.031944 | 4.440775  | 0.744284  |
| H  | 2.956675  | 4.701961  | -1.901308 | H | -5.993351 | 4.449031  | -1.555905 |
| H  | 2.393246  | 3.401001  | -0.838874 | H | -4.949672 | 3.09955   | -3.340688 |
| H  | 2.517262  | 3.243647  | -3.88149  | O | -0.172866 | -2.238364 | -2.599781 |
| C  | 4.159472  | 2.500363  | -2.785324 | C | 0.023723  | -3.137042 | -1.478046 |
| C  | 4.980157  | 2.598122  | -3.916877 | C | 0.505094  | -4.468252 | -2.072759 |
| C  | 6.34934   | 2.31967   | -3.851507 | C | 1.11264   | -4.037438 | -3.416583 |
| C  | 6.931247  | 1.955479  | -2.637812 | C | 0.173573  | -2.905782 | -3.828057 |
| C  | 6.128749  | 1.861789  | -1.495043 | H | -0.735753 | -3.29941  | -4.304468 |
| C  | 4.760467  | 2.119606  | -1.573709 | H | 0.624881  | -2.166984 | -4.493787 |
| H  | 4.149071  | 2.025649  | -0.679236 | H | 1.150896  | -4.844081 | -4.155076 |
| H  | 6.574218  | 1.594246  | -0.539198 | H | 2.127786  | -3.65094  | -3.273359 |

**Table 2 (Continued).**

|   |          |           |           |   |           |           |           |
|---|----------|-----------|-----------|---|-----------|-----------|-----------|
| H | 7.997832 | 1.75376   | -2.577544 | H | -0.339922 | -5.146353 | -2.240391 |
| H | 6.960306 | 2.39786   | -4.74781  | H | 1.21779   | -4.979349 | -1.418206 |
| H | 4.539268 | 2.903621  | -4.863772 | H | 0.756541  | -2.673622 | -0.814802 |
| C | 1.674264 | 0.86249   | -3.995017 | H | -0.921767 | -3.232824 | -0.93378  |
| C | 0.521806 | 1.319715  | -4.92302  | H | -0.27038  | 1.058071  | 0.198127  |
| H | 1.548763 | 1.405003  | 1.829873  | H | -0.994251 | -0.501709 | -0.025003 |
| H | 2.633415 | 0.349243  | 0.944341  | C | 0.66035   | -0.490673 | 1.314112  |
| C | 2.51394  | -0.087874 | 3.058244  | H | -0.034    | -0.498233 | 2.175891  |
| H | 2.878551 | -1.12213  | 2.997802  | H | 0.991638  | -1.540441 | 1.216733  |
| H | 3.364453 | 0.548031  | 3.333276  | C | 1.870328  | 0.356872  | 1.739441  |
| H | 1.789119 | -0.048216 | 3.88067   |   |           |           |           |



**6p**  
 $G = -1993.863061$   
 $G_{MP2} = -1987.976685$

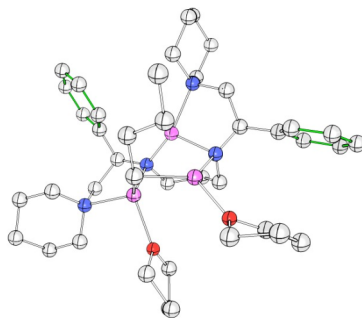
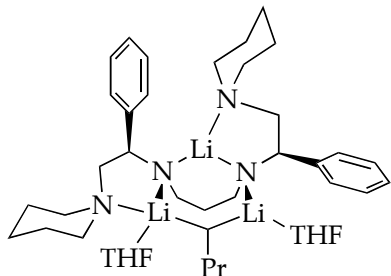
Atom X Y Z Atom X Y Z

|    |           |           |           |   |           |           |           |
|----|-----------|-----------|-----------|---|-----------|-----------|-----------|
| C  | 0         | 0         | 0         | H | -0.753852 | 1.530119  | -5.583546 |
| Li | -0.933278 | 0.012601  | -2.130049 | H | 1.37098   | 0.443107  | -5.968123 |
| N  | -0.71169  | 1.559154  | -3.46005  | H | 1.571689  | 1.983865  | -5.142993 |
| Li | 0.814394  | 2.257547  | -2.497904 | H | 1.584979  | -0.659163 | -3.617864 |
| N  | 2.382964  | 1.07468   | -2.732795 | H | 3.031828  | -0.076688 | -4.420036 |
| Li | 1.788322  | -0.07052  | -1.259549 | C | -2.014611 | 2.18928   | -3.582599 |
| O  | 2.879434  | -1.76409  | -0.935772 | C | -3.203305 | 1.170042  | -3.65463  |
| C  | 3.090148  | -2.510895 | 0.272069  | N | -3.333789 | 0.223186  | -2.520568 |
| C  | 4.601868  | -2.716764 | 0.324378  | C | -4.162604 | 0.801798  | -1.437232 |
| C  | 4.953386  | -2.956227 | -1.159599 | H | -3.700101 | 1.728391  | -1.099995 |
| C  | 3.811894  | -2.253086 | -1.93098  | H | -5.161111 | 1.066079  | -1.839953 |
| H  | 3.284701  | -2.94787  | -2.598055 | C | -4.335694 | -0.159847 | -0.258777 |
| H  | 4.140986  | -1.386667 | -2.503713 | H | -4.959725 | 0.323618  | 0.503427  |
| H  | 4.970945  | -4.027646 | -1.386134 | H | -3.356582 | -0.347952 | 0.201348  |
| H  | 5.929047  | -2.540827 | -1.423125 | C | -4.960374 | -1.48307  | -0.713834 |
| H  | 4.89433   | -3.547089 | 0.974495  | C | -4.154522 | -2.056302 | -1.885016 |
| H  | 5.084954  | -1.805478 | 0.692759  | C | -3.976533 | -1.020394 | -2.997352 |
| H  | 2.676373  | -1.928453 | 1.096689  | H | -3.358373 | -1.434724 | -3.799935 |
| H  | 2.55696   | -3.473427 | 0.215643  | H | -4.966967 | -0.790209 | -3.438649 |



| Table 2 (Continued). |           |           |           |   |           |                     |
|----------------------|-----------|-----------|-----------|---|-----------|---------------------|
| C                    | 3.473151  | 2.010644  | -2.960382 | H | -4.646981 | -2.945197 -2.301103 |
| C                    | 3.362566  | 3.205675  | -1.987881 | H | -3.164636 | -2.368511 -1.531879 |
| N                    | 2.077076  | 3.93435   | -2.114988 | H | -5.996518 | -1.305395 -1.037278 |
| C                    | 1.996044  | 4.801646  | -3.31617  | H | -5.006199 | -2.201167 0.114526  |
| H                    | 2.267806  | 4.208408  | -4.194167 | H | -4.159678 | 1.699126 -3.823095  |
| C                    | 2.852171  | 6.078129  | -3.237579 | H | -3.017707 | 0.567646 -4.550784  |
| C                    | 2.519258  | 6.884294  | -1.973354 | H | -2.100965 | 2.702983 -4.564651  |
| C                    | 2.611343  | 5.991075  | -0.7274   | C | -2.253973 | 3.287765 -2.549287  |
| C                    | 1.751193  | 4.728615  | -0.908869 | C | -3.060679 | 4.38783 -2.879171   |
| H                    | 1.835025  | 4.070627  | -0.036726 | C | -3.320698 | 5.403172 -1.957239  |
| H                    | 0.696777  | 5.021931  | -0.988923 | C | -2.778595 | 5.339034 -0.671957  |
| H                    | 2.271766  | 6.533616  | 0.164467  | C | -1.971939 | 4.253063 -0.32691   |
| H                    | 3.657726  | 5.710391  | -0.54515  | C | -1.708689 | 3.244426 -1.258406  |
| H                    | 1.495625  | 7.278794  | -2.056852 | H | -1.095251 | 2.396955 -0.966849  |
| H                    | 3.184288  | 7.752092  | -1.880808 | H | -1.547602 | 4.182672 0.671813   |
| H                    | 2.678219  | 6.679615  | -4.139155 | H | -2.981794 | 6.125214 0.050652   |
| H                    | 3.918605  | 5.815868  | -3.239717 | H | -3.945173 | 6.245876 -2.24441   |
| H                    | 0.94054   | 5.081577  | -3.436703 | H | -3.487592 | 4.450414 -3.878377  |
| H                    | 4.234842  | 3.865636  | -2.111474 | O | -0.633287 | -2.049058 -2.658782 |
| H                    | 3.397875  | 2.821263  | -0.962223 | C | -0.382694 | -3.004972 -1.598883 |
| H                    | 3.431533  | 2.432456  | -3.985031 | C | -0.655675 | -4.375262 -2.214469 |
| C                    | 4.877255  | 1.39169   | -2.852931 | C | -0.174185 | -4.165856 -3.657418 |
| C                    | 5.656105  | 1.189429  | -4.000375 | C | -0.611862 | -2.72493 -3.939405  |
| C                    | 6.919793  | 0.59452   | -3.929383 | H | -1.620632 | -2.687272 -4.368276 |
| C                    | 7.440981  | 0.205813  | -2.696056 | H | 0.068037  | -2.1886 -4.605497   |
| C                    | 6.681507  | 0.407704  | -1.538271 | H | -0.602907 | -4.876862 -4.370048 |
| C                    | 5.41299   | 0.981879  | -1.620494 | H | 0.917872  | -4.251981 -3.710008 |
| H                    | 4.830987  | 1.117181  | -0.711944 | H | -1.728869 | -4.599443 -2.196256 |
| H                    | 7.083983  | 0.123338  | -0.568212 | H | -0.129765 | -5.180901 -1.692652 |
| H                    | 8.428986  | -0.24335  | -2.633025 | H | 0.658272  | -2.903177 -1.276037 |
| H                    | 7.498434  | 0.444359  | -4.837875 | H | -1.032823 | -2.753329 -0.758017 |
| H                    | 5.267006  | 1.509557  | -4.964993 | H | 0.236865  | -0.999933 0.421571  |
| C                    | 2.102291  | 0.268247  | -3.924811 | H | -1.107989 | -0.049736 -0.08244  |
| C                    | 1.21807   | 0.95096   | -5.001564 | C | 0.278487  | 1.01878 1.13623     |
| C                    | -0.302111 | 0.972906  | -4.736973 | H | 0.024924  | 2.040634 0.810191   |
| H                    | -0.665862 | -0.070432 | -4.880053 | H | -0.34295  | 0.847672 2.035971   |
| C                    | 2.012535  | 2.054293  | 2.731415  | C | 1.739768  | 1.043629 1.611112   |
| H                    | 3.06189   | 2.0392    | 3.051     | H | 2.403265  | 1.26405 0.758719    |
| H                    | 1.778347  | 3.076664  | 2.407545  | H | 2.019338  | 0.038628 1.963133   |
| H                    | 1.392625  | 1.841197  | 3.611057  |   |           |                     |

**Table 2 (Continued).**

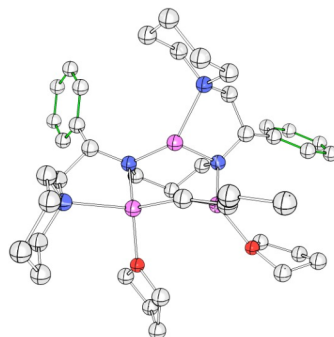
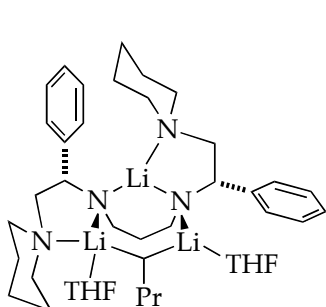


**6q**  
 $G = -1993.860348$   
 $G_{MP2} = -1987.973481$

| Atom | X         | Y         | Z         | Atom | X         | Y         | Z         |
|------|-----------|-----------|-----------|------|-----------|-----------|-----------|
| N    | 0         | 0         | 0         | C    | 3.907793  | -3.946394 | 3.592646  |
| Li   | -0.0987   | -1.518525 | 1.386405  | C    | 5.424457  | -4.088587 | 3.694741  |
| N    | -2.367135 | -1.485299 | 1.171975  | C    | 5.83355   | -4.299937 | 2.221203  |
| C    | -3.042881 | -1.006228 | 2.405225  | C    | 4.690479  | -3.635006 | 1.418481  |
| H    | -2.698023 | -1.648928 | 3.227775  | H    | 4.215851  | -4.342873 | 0.726751  |
| H    | -2.695478 | 0.002941  | 2.624651  | H    | 5.003386  | -2.750103 | 0.865171  |
| C    | -4.580539 | -1.042887 | 2.350446  | H    | 5.900136  | -5.367887 | 1.987362  |
| C    | -5.090537 | -2.442619 | 1.980197  | H    | 6.800559  | -3.845488 | 1.992137  |
| C    | -4.396445 | -2.939845 | 0.704162  | H    | 5.731002  | -4.911363 | 4.34801   |
| C    | -2.868729 | -2.839833 | 0.850034  | H    | 5.854966  | -3.160626 | 4.086298  |
| H    | -2.370582 | -3.180917 | -0.062424 | H    | 3.441546  | -3.391731 | 4.40874   |
| H    | -2.54823  | -3.508427 | 1.661594  | H    | 3.419493  | -4.930376 | 3.507332  |
| H    | -4.673693 | -3.980838 | 0.490225  | C    | 0.90396   | -1.403637 | 3.477877  |
| H    | -4.726073 | -2.342791 | -0.157124 | H    | 1.148568  | -2.377077 | 3.954316  |
| H    | -6.18087  | -2.441661 | 1.856788  | H    | -0.207005 | -1.447039 | 3.448253  |
| H    | -4.867967 | -3.137999 | 2.803843  | C    | 1.244964  | -0.325227 | 4.53955   |
| H    | -4.946148 | -0.310411 | 1.618675  | H    | 0.995455  | 0.681034  | 4.164648  |
| H    | -4.976611 | -0.729557 | 3.325015  | H    | 0.657978  | -0.432632 | 5.471629  |
| C    | -2.474429 | -0.557569 | 0.018757  | C    | 2.725083  | -0.303823 | 4.951999  |
| H    | -3.464979 | -0.079343 | -0.043657 | H    | 3.004697  | -1.297655 | 5.334779  |
| H    | -2.369184 | -1.169264 | -0.884398 | H    | 3.354394  | -0.131057 | 4.063651  |
| C    | -1.34707  | 0.534664  | -0.063217 | C    | 3.060861  | 0.749173  | 6.014716  |
| H    | -1.538477 | 0.983545  | -1.062023 | H    | 2.479403  | 0.5824    | 6.929916  |
| C    | -1.594373 | 1.672781  | 0.925871  | H    | 4.123477  | 0.732453  | 6.286925  |
| C    | -2.504362 | 2.690455  | 0.599541  | H    | 2.825122  | 1.760461  | 5.658697  |
| C    | -2.776602 | 3.736455  | 1.483004  | C    | 4.188906  | 0.60556   | 0.324741  |
| C    | -2.14361  | 3.786699  | 2.726551  | C    | 4.068279  | 1.822376  | 1.268734  |
| C    | -1.233823 | 2.784155  | 3.067537  | N    | 2.760671  | 2.513262  | 1.156412  |
| C    | -0.958915 | 1.745304  | 2.173393  | C    | 2.621643  | 3.338144  | -0.06923  |
| H    | -0.264638 | 0.962753  | 2.464577  | H    | 2.871229  | 2.720218  | -0.936687 |
| H    | -0.737519 | 2.802151  | 4.034918  | C    | 3.458274  | 4.629358  | -0.063896 |
| H    | -2.355612 | 4.596636  | 3.419767  | C    | 3.157335  | 5.47425   | 1.183713  |
| H    | -3.481766 | 4.513698  | 1.197959  | C    | 3.298702  | 4.62461   | 2.456106  |
| H    | -3.002739 | 2.664474  | -0.367813 | C    | 2.455095  | 3.343579  | 2.34335   |

| Table 2 (Continued). |           |           |           |   |          |           |           |
|----------------------|-----------|-----------|-----------|---|----------|-----------|-----------|
| O                    | 0.278783  | -3.601073 | 0.890568  | H | 2.575327 | 2.718457  | 3.235162  |
| C                    | 0.374155  | -4.553354 | 1.97416   | H | 1.393947 | 3.616583  | 2.283152  |
| C                    | 0.928328  | -5.832114 | 1.348992  | H | 2.976131 | 5.192539  | 3.338486  |
| C                    | 0.303669  | -5.78883  | -0.052834 | H | 4.354085 | 4.366332  | 2.617826  |
| C                    | 0.352434  | -4.292794 | -0.378513 | H | 2.127316 | 5.855763  | 1.120076  |
| H                    | -0.476056 | -3.959058 | -1.009747 | H | 3.815202 | 6.351413  | 1.225803  |
| H                    | 1.291556  | -4.014204 | -0.870204 | H | 3.243127 | 5.197438  | -0.978219 |
| H                    | -0.733462 | -6.142889 | -0.01699  | H | 4.528034 | 4.383326  | -0.095869 |
| H                    | 0.841269  | -6.391606 | -0.791025 | H | 1.557705 | 3.596448  | -0.159596 |
| H                    | 0.661886  | -6.728439 | 1.917574  | H | 4.918586 | 2.502159  | 1.10599   |
| H                    | 2.021641  | -5.778773 | 1.282894  | H | 4.140034 | 1.46594   | 2.302588  |
| H                    | 1.009469  | -4.115262 | 2.742989  | H | 4.110136 | 0.998546  | -0.709154 |
| H                    | -0.628485 | -4.719061 | 2.393171  | C | 5.613918 | 0.032942  | 0.415417  |
| Li                   | 1.538865  | 0.787215  | 0.862089  | C | 6.381893 | -0.157925 | -0.741002 |
| N                    | 3.133134  | -0.355598 | 0.603262  | C | 7.665486 | -0.710033 | -0.681517 |
| Li                   | 2.616175  | -1.502706 | 2.107967  | C | 8.217215 | -1.065552 | 0.548534  |
| O                    | 3.706814  | -3.194725 | 2.387019  | C | 7.468521 | -0.874242 | 1.715158  |
| C                    | 0.372721  | -0.619191 | -1.271563 | C | 6.180641 | -0.34344  | 1.644681  |
| H                    | 0.055095  | -1.684426 | -1.355167 | H | 5.606195 | -0.217335 | 2.559401  |
| H                    | -0.14703  | -0.118926 | -2.115056 | H | 7.894099 | -1.133272 | 2.682413  |
| H                    | 2.006388  | -1.111122 | -2.56938  | H | 9.220156 | -1.481606 | 0.602094  |
| H                    | 2.178134  | 0.460896  | -1.797032 | H | 8.235386 | -0.853121 | -1.596667 |
| H                    | 2.389621  | -2.143967 | -0.21948  | H | 5.96791  | 0.136422  | -1.703483 |
| H                    | 3.767392  | -1.501908 | -1.091814 | C | 2.843057 | -1.196414 | -0.562562 |
| C                    | 1.878077  | -0.582095 | -1.610789 |   |          |           |           |

**Table 3.** Optimized geometries at B3LYP level of theory with 6-31G(d) basis set for the Di-solvated SS diastereomer of BuLi-ligand aggregation conformer **6a** at -78 °C with free energies (Hartrees) and cartesian coordinates (X, Y, Z) (Note:  $G_{\text{MP2}}$  includes single point MP2 corrections to B3LYP/6-31G(d) optimized structures).



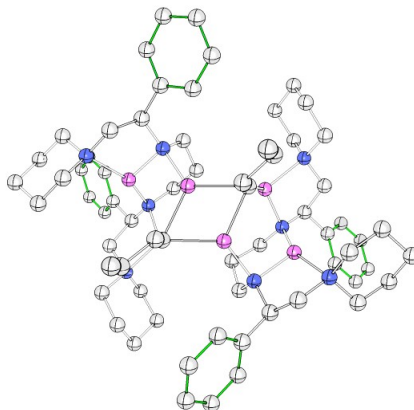
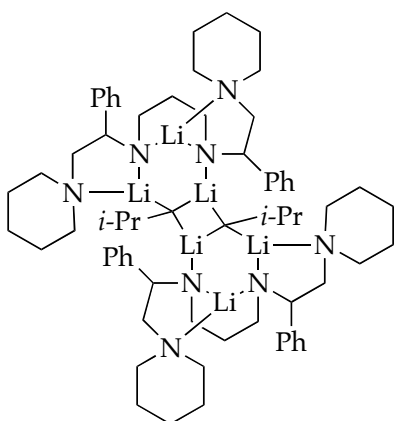
**6b**  
 $G = -1993.8722$   
 $G_{\text{MP2}} = -1987.978018$

| Atom | X         | Y         | Z         | Atom | X         | Y         | Z         |
|------|-----------|-----------|-----------|------|-----------|-----------|-----------|
| Li   | 0         | 0         | 0         | H    | -1.856845 | -5.959411 | 2.328499  |
| N    | 0.103857  | -1.925219 | -0.66142  | C    | -0.068085 | -4.86875  | 2.872869  |
| Li   | -1.347161 | -2.259245 | 0.602692  | H    | 0.56926   | -4.084985 | 2.441426  |
| Li   | -2.856294 | -0.176578 | 0.257246  | H    | 0.531561  | -5.787358 | 2.905697  |
| N    | -3.117672 | -2.026323 | -0.285307 | C    | -0.506063 | -4.449041 | 4.280315  |
| C    | -4.004584 | -2.888011 | 0.495453  | C    | -1.443376 | -3.240617 | 4.184229  |
| H    | -4.25879  | -2.316989 | 1.401461  | C    | -2.602812 | -3.516801 | 3.224303  |
| C    | -5.360951 | -3.214435 | -0.144319 | H    | -3.230407 | -2.625938 | 3.140415  |
| C    | -6.504785 | -2.509205 | 0.261048  | H    | -3.238154 | -4.323316 | 3.640781  |
| C    | -7.755261 | -2.74799  | -0.312204 | H    | -1.853412 | -2.983449 | 5.169019  |
| C    | -7.890316 | -3.708431 | -1.317029 | H    | -0.884624 | -2.362995 | 3.833433  |
| C    | -6.766111 | -4.423637 | -1.731559 | H    | -1.033174 | -5.284661 | 4.763651  |
| C    | -5.519309 | -4.180691 | -1.150753 | H    | 0.365043  | -4.219363 | 4.906235  |
| H    | -4.66033  | -4.753776 | -1.488326 | H    | -2.920502 | -4.740019 | 0.126525  |
| H    | -6.857915 | -5.177256 | -2.510181 | H    | -4.01754  | -4.851561 | 1.51044   |
| H    | -8.861175 | -3.901822 | -1.7661   | C    | 1.498253  | -2.315871 | -0.40899  |
| H    | -8.625419 | -2.195252 | 0.035269  | C    | 2.490194  | -1.139913 | -0.629475 |
| H    | -6.411656 | -1.767357 | 1.053049  | N    | 2.246616  | -0.004853 | 0.295048  |
| C    | -2.855495 | -2.483083 | -1.643994 | C    | 2.736756  | -0.324909 | 1.654189  |
| C    | -1.754831 | -1.649776 | -2.331951 | H    | 2.209555  | -1.211528 | 2.015556  |
| C    | -0.297929 | -2.065405 | -2.054329 | H    | 3.813052  | -0.584568 | 1.607538  |
| H    | 0.336355  | -1.470388 | -2.755462 | C    | 2.532338  | 0.83006   | 2.638125  |
| H    | -0.194114 | -3.104504 | -2.421352 | H    | 2.939487  | 0.537815  | 3.614445  |
| H    | -1.900758 | -0.588532 | -2.070884 | H    | 1.456804  | 0.995989  | 2.77508   |
| H    | -1.902398 | -1.718016 | -3.420262 | C    | 3.199675  | 2.114633  | 2.134385  |
| H    | -2.535348 | -3.547111 | -1.705601 | C    | 2.733947  | 2.411238  | 0.704044  |
| H    | -3.760093 | -2.435517 | -2.285973 | C    | 2.942001  | 1.198011  | -0.205377 |
| C    | -1.340317 | 0.239301  | 1.776817  | H    | 2.563499  | 1.411364  | -1.210213 |
| H    | -0.8231   | -0.597758 | 2.296015  | H    | 4.027361  | 0.997337  | -0.303243 |
| H    | -0.583274 | 1.051447  | 1.794051  | H    | 3.274917  | 3.270021  | 0.285874  |

**Table 3 (Continued).**

|   |           |           |           |   |           |           |           |
|---|-----------|-----------|-----------|---|-----------|-----------|-----------|
| C | -2.467076 | 0.707045  | 2.724533  | H | 1.667473  | 2.670725  | 0.710716  |
| H | -2.930183 | 1.625396  | 2.323147  | H | 4.292429  | 1.988959  | 2.141995  |
| H | -3.285365 | -0.038671 | 2.754928  | H | 2.973523  | 2.957298  | 2.79946   |
| C | -2.070642 | 1.001953  | 4.185847  | H | 3.540155  | -1.477507 | -0.54125  |
| H | -1.276856 | 1.763132  | 4.18579   | H | 2.360234  | -0.755797 | -1.647931 |
| H | -1.621221 | 0.097244  | 4.619458  | H | 1.562656  | -2.570114 | 0.659835  |
| C | -3.234661 | 1.471386  | 5.0668    | C | 2.004907  | -3.571666 | -1.13485  |
| H | -2.913846 | 1.668591  | 6.096983  | C | 1.953884  | -4.814173 | -0.487411 |
| H | -3.6794   | 2.396625  | 4.677008  | C | 2.390977  | -5.984014 | -1.11076  |
| H | -4.031228 | 0.716892  | 5.107302  | C | 2.897574  | -5.936172 | -2.410358 |
| O | -4.252447 | 1.116714  | -0.440972 | C | 2.959124  | -4.709259 | -3.072192 |
| C | -5.045704 | 2.137084  | 0.187621  | C | 2.518187  | -3.54464  | -2.441047 |
| C | -6.484411 | 1.655668  | 0.023211  | H | 2.570901  | -2.6031   | -2.980934 |
| C | -6.462371 | 1.045388  | -1.391553 | H | 3.350653  | -4.656416 | -4.085456 |
| C | -5.002994 | 0.57431   | -1.566402 | H | 3.242004  | -6.843188 | -2.900625 |
| H | -4.558134 | 0.946407  | -2.49717  | H | 2.34378   | -6.930997 | -0.577948 |
| H | -4.881938 | -0.508192 | -1.514531 | H | 1.57207   | -4.861259 | 0.529141  |
| H | -6.718587 | 1.803588  | -2.139742 | O | -0.312998 | 1.621775  | -1.247604 |
| H | -7.166517 | 0.216121  | -1.497776 | C | -1.049638 | 2.788869  | -0.800319 |
| H | -7.216386 | 2.46173   | 0.133258  | C | -1.122715 | 3.730533  | -2.007474 |
| H | -6.704385 | 0.886833  | 0.772014  | C | -1.043162 | 2.754241  | -3.190823 |
| H | -4.712173 | 2.222996  | 1.223603  | C | -0.055841 | 1.713367  | -2.665576 |
| H | -4.885515 | 3.100936  | -0.320368 | H | 0.982674  | 2.036967  | -2.824698 |
| N | -2.142648 | -3.899117 | 1.871182  | H | -0.185006 | 0.718015  | -3.095736 |
| C | -3.304168 | -4.186154 | 0.989921  | H | -0.705049 | 3.222626  | -4.120105 |
| C | -1.274919 | -5.093091 | 1.957255  | H | -2.019766 | 2.291299  | -3.375033 |
| H | -0.938924 | -5.337819 | 0.94393   | H | -0.264628 | 4.413144  | -2.020187 |
| H | -2.040081 | 2.456717  | -0.476072 | H | -2.033996 | 4.336364  | -2.004738 |
| H | -0.525629 | 3.223874  | 0.055976  |   |           |           |           |

**Table 4.** Optimized geometries at B3LYP level of theory with 6-31G(d) basis set for the BuLi-ligand dimer aggregate and its disolvated monomer generated from crystal structure coordinates at -78 °C with free energies (Hartrees) and cartesian coordinates (X, Y, Z) (Note:  $G_{\text{MP2}}$  includes single point MP2 corrections to B3LYP/6-31G(d) optimized structures).



5  
 $G = -3058.357797$   
 $G_{\text{MP2}} = \text{Not Calculated}$

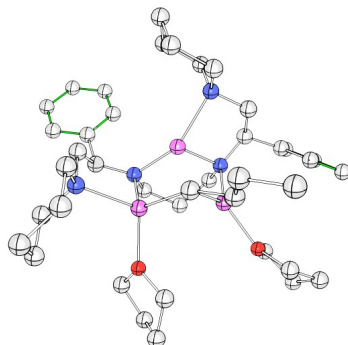
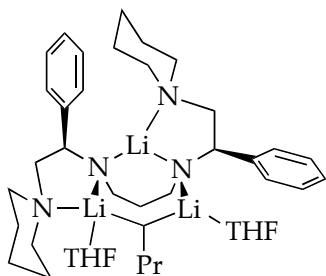
| Atom | X          | Y         | Z         | Atom | X          | Y         | Z         |
|------|------------|-----------|-----------|------|------------|-----------|-----------|
| N    | 0          | 0         | 0         | C    | -1.586064  | -5.135396 | 1.763684  |
| C    | -3.658539  | -2.237395 | 0.041201  | H    | -1.165567  | -4.521902 | 0.959439  |
| C    | -2.807642  | -0.265651 | 4.09774   | H    | -0.761429  | -5.751756 | 2.170109  |
| H    | -3.465288  | -0.763437 | 4.84294   | C    | -2.695106  | -5.009073 | 3.916357  |
| H    | -2.102604  | 0.332185  | 4.708581  | H    | -1.90906   | -5.61941  | 4.401493  |
| C    | 1.298887   | 0.493232  | 0.518581  | H    | -3.073809  | -4.315554 | 4.672643  |
| H    | 1.843921   | 1.013312  | -0.292526 | C    | -6.659529  | 5.075963  | 2.468038  |
| H    | 1.101315   | 1.237443  | 1.29646   | H    | -5.834478  | 5.693343  | 2.094398  |
| C    | -6.163354  | 0.561178  | 0.050895  | H    | -7.39297   | 5.759893  | 2.920158  |
| C    | -1.384003  | -2.170909 | 4.144999  | C    | 2.41349    | -1.72066  | 0.021788  |
| H    | -2.031463  | -2.524637 | 4.976627  | H    | 3.031947   | -1.313162 | -0.791215 |
| C    | -8.208965  | -3.679186 | 0.232843  | H    | 2.970452   | -2.561308 | 0.452735  |
| H    | -8.964093  | -4.154469 | 0.898154  | C    | -2.946362  | 1.732806  | 2.408301  |
| C    | -8.56903   | 0.297822  | 4.104787  | H    | -2.098365  | 2.156797  | 2.991587  |
| H    | -7.934612  | 0.628413  | 4.955719  | H    | -3.614524  | 2.601437  | 2.229432  |
| C    | -9.817034  | -0.310209 | 4.784812  | C    | -7.71805   | -6.168429 | -0.004643 |
| C    | -11.122267 | -2.410286 | 0.298895  | H    | -8.373881  | -6.332342 | 0.848531  |
| H    | -11.611241 | -2.902606 | -0.56358  | C    | -12.086376 | -1.393294 | 0.915687  |
| H    | -10.889543 | -3.19746  | 1.022877  | H    | -11.658026 | -0.995402 | 1.843872  |
| C    | -7.13085   | -1.593927 | 4.000389  | H    | -13.012261 | -1.911771 | 1.194159  |
| H    | -6.51885   | -1.125497 | 4.801006  | C    | -3.775681  | 4.524614  | -1.303035 |
| H    | -7.841835  | -2.246834 | 4.544736  | H    | -4.788375  | 4.577801  | -1.696212 |
| C    | 0.242295   | -1.010831 | -1.054849 | C    | -12.117544 | -1.357982 | 6.045935  |
| H    | -0.729785  | -1.357585 | -1.417654 | H    | -13.001042 | -1.762999 | 6.532538  |
| H    | 0.761287   | -0.54116  | -1.912296 | C    | -1.522218  | 1.963592  | 0.497358  |
| C    | -0.951398  | -3.415484 | 3.339786  | H    | -0.752495  | 2.318242  | 1.220254  |
| H    | -0.284237  | -4.057565 | 3.938586  | C    | -6.158168  | 4.089802  | 3.527913  |

**Table 4 (Continued).**

|   |            |           |           |   |            |           |           |
|---|------------|-----------|-----------|---|------------|-----------|-----------|
| H | -0.369213  | -3.067135 | 2.476979  | H | -5.322488  | 3.506676  | 3.121266  |
| C | -8.976137  | -2.813142 | -0.784401 | H | -5.774087  | 4.621068  | 4.407579  |
| H | -9.568954  | -3.442049 | -1.469891 | C | -6.055065  | -5.764158 | -2.193958 |
| H | -8.244287  | -2.271527 | -1.394145 | H | -5.415246  | -5.597316 | -3.057058 |
| C | 2.172675   | -0.633859 | 1.075473  | C | -7.317749  | 4.305094  | 1.318831  |
| H | 1.689595   | -1.070418 | 1.958455  | H | -7.777096  | 4.992967  | 0.597847  |
| H | 3.122823   | -0.20565  | 1.418101  | H | -6.555361  | 3.735068  | 0.773931  |
| C | -10.138703 | -0.716388 | -1.122749 | C | -12.377447 | -0.243035 | -0.054933 |
| H | -9.184105  | -0.277256 | -1.43064  | H | -12.946472 | -0.6229   | -0.915963 |
| H | -10.605124 | -1.147442 | -2.029222 | H | -13.00081  | 0.520595  | 0.4254    |
| C | -7.52622   | -4.862361 | -0.472389 | C | -11.568383 | -1.99763  | 4.935017  |
| C | -0.13502   | -1.604417 | 4.859384  | H | -12.019323 | -2.911485 | 4.555012  |
| C | 0.408083   | -2.280903 | 5.962007  | C | -2.677707  | -6.052109 | 1.208214  |
| H | -0.075488  | -3.188937 | 6.319739  | H | -2.231669  | -6.712167 | 0.453868  |
| C | -6.67736   | -4.679876 | -1.574205 | H | -3.434051  | -5.447627 | 0.692959  |
| H | -6.498168  | -3.677589 | -1.95583  | C | -3.688601  | -2.139412 | -1.503264 |
| C | -7.272801  | 3.143096  | 3.978107  | H | -3.259296  | -1.177345 | -1.832907 |
| H | -8.060508  | 3.725191  | 4.493978  | H | -4.728525  | -2.112521 | -1.866229 |
| H | -6.883647  | 2.420436  | 4.701144  | C | 1.626188   | 0.061797  | 5.097991  |
| C | -2.038642  | 3.258446  | -0.162301 | H | 2.085108   | 0.989637  | 4.764134  |
| C | -10.430049 | -1.475512 | 4.314127  | C | -6.042529  | 0.564995  | -1.492098 |
| H | -9.991028  | -1.991707 | 3.464706  | H | -6.393613  | -0.398039 | -1.900762 |
| C | -9.010304  | 1.564816  | 3.341804  | H | -4.984487  | 0.622307  | -1.796401 |
| H | -9.683436  | 2.180554  | 3.961312  | C | -3.820802  | -5.926276 | 3.434162  |
| H | -9.588328  | 1.241367  | 2.466484  | H | -4.6546    | -5.318292 | 3.062662  |
| C | -6.861939  | -3.491498 | 2.211613  | H | -4.200377  | -6.494207 | 4.292813  |
| H | -7.693535  | -4.00167  | 2.749343  | C | -3.018979  | -3.113802 | -3.789971 |
| H | -6.142637  | -4.306394 | 1.985243  | H | -4.054984  | -3.102659 | -4.152534 |
| C | -3.679533  | 0.739164  | 3.326771  | H | -2.551446  | -2.174251 | -4.111445 |
| H | -4.243641  | 1.312771  | 4.077384  | H | -2.498574  | -3.934007 | -4.299036 |
| H | -4.433974  | 0.182451  | 2.741658  | C | -6.79561   | 1.688383  | -2.230476 |
| C | -6.198465  | -2.5247   | 3.20818   | H | -6.439586  | 2.658328  | -1.85516  |
| H | -5.639088  | -3.119521 | 3.945694  | H | -7.862146  | 1.638039  | -1.96486  |
| H | -5.447145  | -1.908434 | 2.681998  | C | -1.197711  | 4.373942  | -0.278226 |
| C | 1.072467   | -2.192695 | -0.551548 | H | -0.189792  | 4.324533  | 0.132086  |
| H | 0.507125   | -2.726826 | 0.22476   | C | -7.087648  | -7.258835 | -0.610028 |
| H | 1.224188   | -2.899008 | -1.377247 | H | -7.252701  | -8.261913 | -0.223641 |
| C | 0.488433   | -0.423016 | 4.446523  | C | -2.923603  | 5.623947  | -1.420402 |
| H | 0.056611   | 0.133653  | 3.619373  | H | -3.266373  | 6.535381  | -1.903648 |
| C | -8.394616  | 3.349805  | 1.836697  | C | -2.967542  | -3.267875 | -2.265315 |
| H | -8.810084  | 2.765705  | 1.008101  | H | -3.415614  | -4.227394 | -1.97385  |
| H | -9.225568  | 3.937805  | 2.270991  | H | -1.919132  | -3.310976 | -1.935092 |
| C | -11.058377 | 0.362404  | -0.5483   | C | -6.255424  | -7.06062  | -1.711646 |
| H | -10.548729 | 0.865324  | 0.285574  | H | -5.768726  | -7.905381 | -2.192347 |
| H | -11.237969 | 1.12393   | -1.317386 | C | 2.164359   | -0.632713 | 6.181134  |
| C | -10.371505 | 0.310451  | 5.914279  | H | 3.047425   | -0.25672  | 6.691284  |

**Table 4 (Continued).**

|    |           |           |           |    |            |           |           |
|----|-----------|-----------|-----------|----|------------|-----------|-----------|
| H  | -9.896701 | 1.204217  | 6.316849  | C  | -3.339592  | -6.866791 | 2.324693  |
| C  | -3.334794 | 3.355267  | -0.678333 | H  | -2.613369  | -7.58208  | 2.738565  |
| H  | -4.002798 | 2.506642  | -0.568841 | H  | -4.176041  | -7.453103 | 1.926838  |
| C  | -0.787537 | 1.126615  | -0.572016 | C  | 1.547332   | -1.809403 | 6.613463  |
| H  | -0.135903 | 1.763461  | -1.193097 | H  | 1.94947    | -2.355019 | 7.463799  |
| H  | -1.547798 | 0.697242  | -1.235251 | C  | -11.511155 | -0.198676 | 6.536197  |
| Li | -1.403891 | -0.426242 | 1.634479  | H  | -11.922025 | 0.304274  | 7.408351  |
| N  | -9.850066 | -1.791471 | -0.14562  | C  | -6.641106  | 1.637224  | -3.754641 |
| N  | -2.087341 | -4.218943 | 2.816723  | H  | -5.587379  | 1.723718  | -4.047777 |
| N  | -7.880517 | 2.395418  | 2.848993  | H  | -7.018564  | 0.689728  | -4.160336 |
| N  | -7.331186 | -2.819257 | 1.008461  | H  | -7.1897    | 2.449891  | -4.24557  |
| N  | -2.116926 | -1.265647 | 3.278238  | C  | -1.629076  | 5.5448    | -0.902318 |
| N  | -7.814344 | -0.563751 | 3.212859  | H  | -0.958009  | 6.397167  | -0.978769 |
| N  | -2.489781 | 1.120382  | 1.167398  | Li | -3.957917  | -0.033617 | 0.48588   |
| H  | -5.885512 | 1.585499  | 0.375901  | Li | -3.204002  | -2.485144 | 2.154007  |
| H  | -7.261622 | 0.527611  | 0.241971  | Li | -8.500687  | -1.366774 | 1.536614  |
| H  | -2.573732 | -2.295142 | 0.291257  | Li | -6.724607  | 0.705996  | 2.147816  |
| H  | -4.024452 | -3.258227 | 0.279244  | Li | -5.84502   | -1.647022 | 0.415249  |



**6r**

$G = -1993.885961$

$G_{\text{MP2}} = -1987.996765$

Atom X Y Z Atom X Y Z

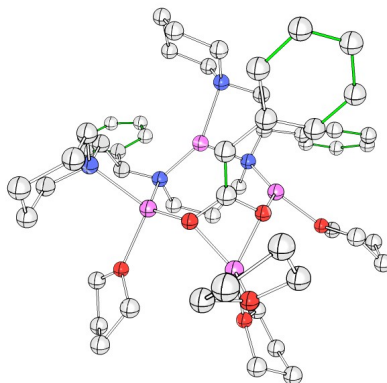
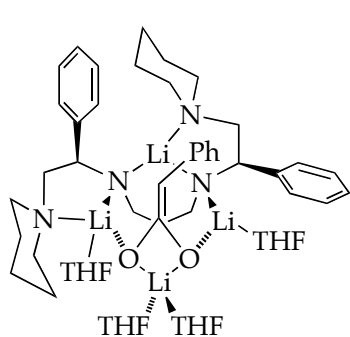
|    |           |           |           |   |           |           |           |
|----|-----------|-----------|-----------|---|-----------|-----------|-----------|
| Li | 0         | 0         | 0         | H | -4.275419 | -0.004013 | -2.45154  |
| N  | 0.430403  | -1.670575 | -1.056149 | H | -5.247792 | -1.189546 | -1.54744  |
| Li | -0.819257 | -2.509685 | 0.261931  | H | -5.988677 | 1.712252  | -2.224231 |
| Li | -2.782741 | -0.843844 | 0.200892  | H | -7.018482 | 0.273093  | -2.362029 |
| N  | -2.594761 | -2.652935 | -0.56557  | H | -7.267961 | 1.813797  | -0.118722 |
| C  | -3.239325 | -3.843825 | -0.046511 | H | -7.162937 | 0.05137   | 0.070661  |
| C  | -2.884685 | -4.017006 | 1.443253  | H | -5.261651 | 0.668832  | 1.416309  |
| N  | -1.431124 | -4.141854 | 1.712307  | H | -4.924371 | 2.10535   | 0.424927  |
| C  | -0.940759 | -5.480238 | 1.313981  | C | 1.875698  | -1.726145 | -1.078998 |
| H  | -1.10473  | -5.602698 | 0.239306  | C | 2.433678  | -1.353095 | 0.312756  |
| H  | -1.54016  | -6.260417 | 1.823608  | N | 2.115318  | 0.029331  | 0.744489  |
| C  | 0.541261  | -5.685439 | 1.641107  | C | 2.35396   | 0.1487    | 2.199347  |
| H  | 1.147102  | -5.006451 | 1.030125  | H | 1.692485  | -0.561968 | 2.705458  |



**Table 4 (Continued).**

|   |           |           |           |   |           |           |           |
|---|-----------|-----------|-----------|---|-----------|-----------|-----------|
| H | 0.826441  | -6.705328 | 1.353494  | H | 3.395959  | -0.144988 | 2.435403  |
| C | 0.829783  | -5.436676 | 3.125284  | C | 2.097307  | 1.562422  | 2.727668  |
| C | 0.282949  | -4.063717 | 3.531551  | H | 2.325997  | 1.585424  | 3.800663  |
| C | -1.194131 | -3.933897 | 3.158086  | H | 1.02952   | 1.793242  | 2.624491  |
| H | -1.564498 | -2.937594 | 3.418761  | C | 2.929017  | 2.602705  | 1.969251  |
| H | -1.781764 | -4.665746 | 3.746917  | C | 2.700694  | 2.443912  | 0.462095  |
| H | 0.394031  | -3.8991   | 4.610804  | C | 2.957058  | 1.00205   | 0.016628  |
| H | 0.853843  | -3.27211  | 3.026563  | H | 2.757267  | 0.898987  | -1.053596 |
| H | 0.343552  | -6.214636 | 3.732283  | H | 4.027511  | 0.758218  | 0.169139  |
| H | 1.905959  | -5.503966 | 3.32626   | H | 3.359842  | 3.113394  | -0.105665 |
| H | -3.424433 | -4.883007 | 1.867427  | H | 1.666604  | 2.712408  | 0.212263  |
| H | -3.224298 | -3.129791 | 1.988969  | H | 3.99568   | 2.455449  | 2.19388   |
| H | -2.876754 | -4.746805 | -0.583723 | H | 2.674753  | 3.618277  | 2.297856  |
| C | -4.767089 | -3.864401 | -0.240512 | H | 3.525127  | -1.514651 | 0.350026  |
| C | -5.325061 | -4.56246  | -1.320696 | H | 1.984228  | -2.037224 | 1.043642  |
| C | -6.700047 | -4.545063 | -1.570679 | H | 2.286354  | -0.989491 | -1.80857  |
| C | -7.556006 | -3.836329 | -0.728024 | C | 2.528309  | -3.061322 | -1.508537 |
| C | -7.020279 | -3.142048 | 0.361031  | C | 3.871087  | -3.089893 | -1.91319  |
| C | -5.64376  | -3.149513 | 0.592616  | C | 4.49088   | -4.281743 | -2.287886 |
| H | -5.251804 | -2.596248 | 1.442992  | C | 3.768432  | -5.477696 | -2.279995 |
| H | -7.67872  | -2.60333  | 1.039528  | C | 2.427032  | -5.462717 | -1.897493 |
| H | -8.627725 | -3.830063 | -0.910124 | C | 1.816182  | -4.264587 | -1.516194 |
| H | -7.101312 | -5.092742 | -2.420293 | H | 0.766857  | -4.244324 | -1.23656  |
| H | -4.667179 | -5.132575 | -1.973581 | H | 1.849854  | -6.384706 | -1.903527 |
| C | -2.505261 | -2.672101 | -2.015157 | H | 4.24459   | -6.408214 | -2.578907 |
| C | -1.601073 | -1.554947 | -2.568773 | H | 5.534954  | -4.277507 | -2.592747 |
| C | -0.083914 | -1.759041 | -2.418291 | H | 4.438199  | -2.160085 | -1.939674 |
| H | 0.414513  | -1.004689 | -3.073077 | O | -0.465806 | 1.738068  | -0.945912 |
| H | 0.154791  | -2.725471 | -2.907294 | C | -1.476862 | 2.655336  | -0.459454 |
| H | -1.886538 | -0.590058 | -2.115396 | C | -1.577305 | 3.762696  | -1.513666 |
| H | -1.809001 | -1.4556   | -3.644935 | C | -1.17319  | 3.025952  | -2.800408 |
| H | -2.100756 | -3.641263 | -2.387263 | C | -0.076911 | 2.090169  | -2.292048 |
| H | -3.495277 | -2.583267 | -2.514179 | H | 0.897499  | 2.59715   | -2.260065 |
| C | -1.364269 | -0.268116 | 1.748674  | H | 0.023139  | 1.166297  | -2.865905 |
| H | -0.781864 | -1.083476 | 2.228491  | H | -0.820851 | 3.694407  | -3.591743 |
| H | -0.700365 | 0.612572  | 1.86214   | H | -2.016629 | 2.445859  | -3.192952 |
| C | -2.56438  | 0.021655  | 2.677595  | H | -0.865235 | 4.568218  | -1.298304 |
| H | -3.079253 | 0.935507  | 2.336081  | H | -2.578675 | 4.201419  | -1.56061  |
| H | -3.326638 | -0.780401 | 2.605985  | H | -2.414634 | 2.100319  | -0.352716 |
| C | -2.253246 | 0.205801  | 4.177352  | H | -1.167734 | 3.017915  | 0.525419  |
| H | -1.518192 | 1.016593  | 4.284235  | O | -4.344794 | 0.293857  | -0.405085 |
| H | -1.756249 | -0.701003 | 4.551858  | C | -5.272404 | 1.064258  | 0.397767  |
| C | -3.485116 | 0.509298  | 5.038589  | C | -6.633455 | 0.939306  | -0.29162  |
| H | -3.223637 | 0.633966  | 6.096428  | C | -6.236486 | 0.748358  | -1.762824 |
| H | -4.223726 | -0.300596 | 4.974395  | C | -4.993495 | -0.129812 | -1.63764  |
| H | -3.980593 | 1.432356  | 4.709963  |   |           |           |           |

**Table 5.** Optimized geometries of dilithium amide-enediolate mixed aggregate **8** at B3LYP level of theory with 6-31G(d) basis set for the enolization of phenylacetic acid at -78 °C with free energies (Hartrees) and cartesian coordinates (X, Y, Z) (Note:  $G_{\text{MP2}}$  includes single point MP2 corrections to B3LYP/6-31G(d) optimized structures).



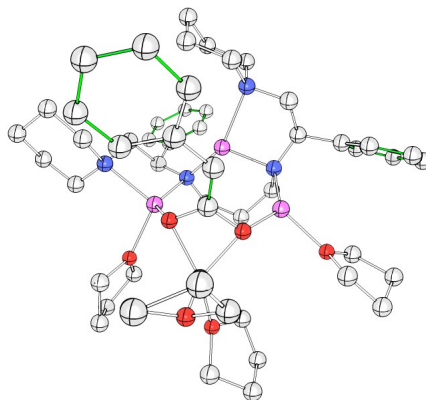
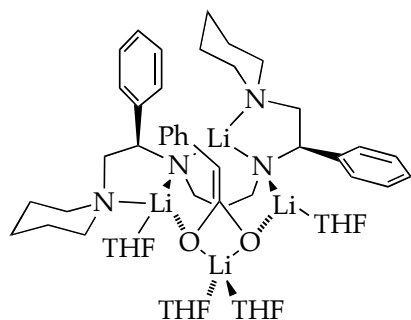
**8a**  
 $G = -2767.365419$   
 $G_{\text{MP2}} = -2759.347801$

| Atom | X        | Y         | Z         | Atom | X         | Y         | Z         |
|------|----------|-----------|-----------|------|-----------|-----------|-----------|
| Li   | 0        | 0         | 0         | C    | 5.388883  | -6.514296 | 2.741135  |
| O    | 1.701483 | -0.605298 | 0.727219  | C    | 4.388865  | -5.455794 | 3.218026  |
| Li   | 3.347787 | -0.965851 | -0.142494 | C    | 2.975415  | -5.77362  | 2.73057   |
| N    | 3.898754 | -2.735662 | -1.086704 | H    | 2.279346  | -4.992451 | 3.044198  |
| C    | 5.335442 | -2.549484 | -1.05828  | H    | 2.638593  | -6.718013 | 3.201094  |
| C    | 5.782976 | -2.350484 | 0.408794  | H    | 4.376914  | -5.389252 | 4.313253  |
| N    | 5.313992 | -1.070433 | 0.988845  | H    | 4.689727  | -4.468298 | 2.843181  |
| C    | 5.133547 | -1.183262 | 2.450418  | H    | 5.163536  | -7.47308  | 3.231107  |
| H    | 4.423824 | -1.993894 | 2.641258  | H    | 6.413067  | -6.244663 | 3.027946  |
| H    | 6.090482 | -1.459282 | 2.936598  | H    | 1.297756  | -7.306366 | 1.200777  |
| C    | 4.607099 | 0.121845  | 3.053084  | H    | 0.845249  | -5.619902 | 1.497314  |
| H    | 4.494113 | -0.003309 | 4.137506  | H    | 1.895761  | -6.624848 | -1.191896 |
| H    | 3.608722 | 0.313176  | 2.640177  | C    | -0.196551 | -6.713227 | -0.917027 |
| C    | 5.544112 | 1.294343  | 2.737061  | C    | -0.364002 | -7.407851 | -2.124057 |
| C    | 5.808433 | 1.362317  | 1.227748  | C    | -1.589532 | -7.982903 | -2.47208  |
| C    | 6.277628 | 0.006776  | 0.693117  | C    | -2.678595 | -7.887521 | -1.604524 |
| H    | 6.421159 | 0.051623  | -0.390535 | C    | -2.529087 | -7.204218 | -0.393563 |
| H    | 7.263257 | -0.239561 | 1.137078  | C    | -1.306903 | -6.616929 | -0.060375 |
| H    | 6.56848  | 2.121201  | 0.999457  | H    | -1.216361 | -6.093828 | 0.888805  |
| H    | 4.890347 | 1.647393  | 0.700649  | H    | -3.363872 | -7.140636 | 0.301326  |
| H    | 6.498077 | 1.153102  | 3.266229  | H    | -3.628961 | -8.348853 | -1.86166  |
| H    | 5.120567 | 2.239851  | 3.099316  | H    | -1.688388 | -8.51591  | -3.415062 |
| H    | 6.878195 | -2.43418  | 0.507003  | H    | 0.486407  | -7.505882 | -2.795947 |
| H    | 5.345857 | -3.16775  | 0.993009  | C    | 1.424759  | -4.399135 | -2.334138 |
| H    | 5.63287  | -1.625857 | -1.610857 | C    | 1.904455  | -2.961667 | -2.629024 |
| C    | 6.209631 | -3.654089 | -1.696698 | H    | 1.648461  | -2.720758 | -3.672587 |
| C    | 7.536132 | -3.37569  | -2.058222 | H    | 1.343867  | -2.25369  | -1.998334 |
| C    | 8.358515 | -4.354993 | -2.614859 | C    | 3.411735  | -2.69834  | -2.463353 |
| C    | 7.861009 | -5.641628 | -2.836253 | H    | 3.620697  | -1.710425 | -2.937608 |

**Table 5 (Continued).**

|    |           |           |           |   |           |           |           |
|----|-----------|-----------|-----------|---|-----------|-----------|-----------|
| C  | 6.539139  | -5.930388 | -2.496093 | H | 3.934491  | -3.423593 | -3.118096 |
| C  | 5.724669  | -4.944506 | -1.932109 | H | 2.170485  | -5.100554 | -2.770434 |
| H  | 4.690819  | -5.162089 | -1.680279 | H | 0.503144  | -4.579432 | -2.933159 |
| H  | 6.136077  | -6.924461 | -2.67681  | O | 3.544156  | 0.803806  | -1.372099 |
| H  | 8.495214  | -6.406902 | -3.27688  | C | 2.609406  | 1.893329  | -1.193535 |
| H  | 9.385116  | -4.113977 | -2.88166  | C | 3.134896  | 3.047031  | -2.053806 |
| H  | 7.929714  | -2.371704 | -1.901839 | C | 3.853042  | 2.297427  | -3.185804 |
| Li | 2.863993  | -4.019196 | 0.010865  | C | 4.472359  | 1.121858  | -2.430242 |
| N  | 1.236255  | -4.637432 | -0.907967 | H | 5.437688  | 1.404378  | -1.988308 |
| Li | -0.190118 | -3.376884 | -0.356995 | H | 4.613027  | 0.225698  | -3.038707 |
| O  | -0.186942 | -1.798542 | 0.629518  | H | 4.601671  | 2.903314  | -3.705216 |
| C  | 0.934565  | -1.529892 | 1.293586  | H | 3.130023  | 1.937745  | -3.927822 |
| C  | 1.257132  | -2.098341 | 2.525086  | H | 3.84954   | 3.658394  | -1.489809 |
| H  | 2.184742  | -1.746551 | 2.968051  | H | 2.332533  | 3.70366   | -2.405044 |
| C  | 0.444566  | -2.954841 | 3.364515  | H | 1.621648  | 1.559549  | -1.529334 |
| C  | 0.935599  | -3.324914 | 4.646993  | H | 2.556038  | 2.128564  | -0.126847 |
| C  | 0.215029  | -4.138035 | 5.514749  | O | -0.824083 | 1.260686  | 1.366122  |
| C  | -1.045503 | -4.62835  | 5.156735  | C | -1.777486 | 0.615429  | 2.258037  |
| C  | -1.560924 | -4.271257 | 3.908467  | C | -1.18542  | 0.739338  | 3.661889  |
| C  | -0.843814 | -3.45747  | 3.031929  | C | -0.403234 | 2.0584    | 3.569393  |
| H  | -1.279168 | -3.169427 | 2.083148  | C | 0.156106  | 1.99842   | 2.147595  |
| H  | -2.546872 | -4.626581 | 3.611017  | H | 1.101677  | 1.447528  | 2.100554  |
| H  | -1.608958 | -5.265596 | 5.832941  | H | 0.281611  | 2.983603  | 1.685416  |
| H  | 0.640509  | -4.390333 | 6.484437  | H | 0.388793  | 2.141478  | 4.319608  |
| H  | 1.911464  | -2.951652 | 4.954422  | H | -1.074907 | 2.91803   | 3.685404  |
| O  | -1.996089 | -3.302489 | -1.262658 | H | -0.508    | -0.098509 | 3.85291   |
| C  | -2.45062  | -4.036772 | -2.430737 | H | -1.956854 | 0.748218  | 4.437777  |
| C  | -3.980095 | -4.08685  | -2.330648 | H | -2.737296 | 1.142221  | 2.169025  |
| C  | -4.304257 | -2.856762 | -1.467581 | H | -1.886718 | -0.420491 | 1.93001   |
| C  | -3.129729 | -2.848987 | -0.49181  | O | -0.702305 | 0.691169  | -1.715218 |
| H  | -3.303232 | -3.544182 | 0.340817  | C | -0.913427 | -0.201752 | -2.846    |
| H  | -2.877331 | -1.869683 | -0.080384 | C | -1.959893 | 0.484261  | -3.735061 |
| H  | -5.271213 | -2.925544 | -0.95989  | C | -2.696771 | 1.404265  | -2.747774 |
| H  | -4.303234 | -1.943979 | -2.076985 | C | -1.558601 | 1.848303  | -1.832618 |
| H  | -4.292142 | -5.003547 | -1.819312 | H | -1.862563 | 2.130872  | -0.822942 |
| H  | -4.461365 | -4.06666  | -3.313186 | H | -0.98912  | 2.675481  | -2.280783 |
| H  | -2.115617 | -3.485947 | -3.318666 | H | -3.444345 | 0.84093   | -2.176359 |
| H  | -1.984117 | -5.022618 | -2.427185 | H | -3.200252 | 2.245648  | -3.233296 |
| C  | 1.155871  | -6.056497 | -0.589405 | H | -2.618545 | -0.237063 | -4.227557 |
| C  | 1.498928  | -6.26283  | 0.898578  | H | -1.474202 | 1.080739  | -4.515928 |
| N  | 2.893431  | -5.898113 | 1.255135  | H | 0.045445  | -0.358737 | -3.347867 |
| C  | 3.832602  | -6.945392 | 0.793179  | H | -1.26183  | -1.158614 | -2.446262 |
| H  | 3.774331  | -7.010441 | -0.29728  | H | 5.642591  | -5.771106 | 0.722938  |
| H  | 3.511031  | -7.9279   | 1.192062  | H | 5.908017  | -7.502652 | 0.868353  |
| C  | 5.277877  | -6.676562 | 1.221536  |   |           |           |           |

**Table 5 (Continued).**



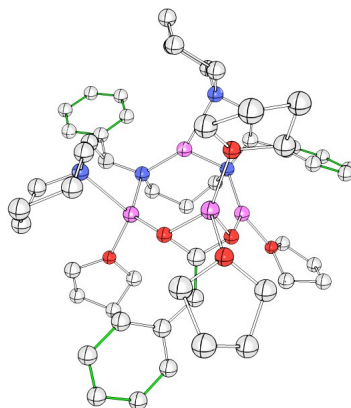
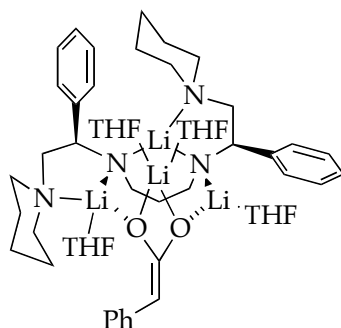
**8c**  
 $G = -2767.355533$   
 $G_{MP2} = -2759.336754$

| Atom | X         | Y         | Z         | Atom | X         | Y         | Z         |
|------|-----------|-----------|-----------|------|-----------|-----------|-----------|
| Li   | 0         | 0         | 0         | H    | -1.227557 | 6.921593  | 0.155403  |
| O    | -1.707838 | 0.575926  | 0.793178  | C    | 0.78472   | 6.812993  | 0.798319  |
| Li   | -2.983058 | 1.283083  | -0.493124 | C    | 1.174755  | 7.798757  | -0.119699 |
| N    | -3.191712 | 3.245199  | -1.225171 | C    | 2.452661  | 8.363937  | -0.085427 |
| C    | -4.590911 | 3.240731  | -1.605277 | C    | 3.369938  | 7.963108  | 0.886959  |
| H    | -4.762006 | 2.563524  | -2.476045 | C    | 2.997227  | 6.98679   | 1.815922  |
| C    | -5.200925 | 4.587055  | -2.067536 | C    | 1.72516   | 6.414221  | 1.763416  |
| C    | -6.376152 | 4.595546  | -2.833205 | H    | 1.459     | 5.655777  | 2.495941  |
| C    | -6.972814 | 5.789574  | -3.237919 | H    | 3.695573  | 6.679292  | 2.591541  |
| C    | -6.392461 | 7.012527  | -2.892631 | H    | 4.359471  | 8.411502  | 0.928145  |
| C    | -5.213682 | 7.021242  | -2.146283 | H    | 2.726456  | 9.125399  | -0.812146 |
| C    | -4.627366 | 5.819502  | -1.740016 | H    | 0.458871  | 8.130723  | -0.868984 |
| H    | -3.698433 | 5.825556  | -1.17707  | C    | -0.511951 | 5.046032  | -1.4551   |
| H    | -4.742524 | 7.96649   | -1.885606 | C    | -0.887556 | 3.741408  | -2.191096 |
| H    | -6.84903  | 7.946424  | -3.21093  | H    | -0.408406 | 3.750073  | -3.182322 |
| H    | -7.886169 | 5.766623  | -3.828198 | H    | -0.463677 | 2.88237   | -1.647986 |
| H    | -6.828523 | 3.647035  | -3.121699 | H    | -1.167596 | 5.857403  | -1.842811 |
| Li   | -2.415512 | 4.160974  | 0.352987  | H    | 0.509133  | 5.345133  | -1.782764 |
| N    | -0.630306 | 4.898303  | -0.010372 | C    | -2.3895   | 3.505814  | -2.421782 |
| Li   | 0.588056  | 3.397135  | 0.400541  | H    | -2.481742 | 2.67022   | -3.154313 |
| O    | 0.240618  | 1.668818  | 0.896314  | H    | -2.757126 | 4.389021  | -2.980001 |
| C    | -0.896638 | 1.333308  | 1.51461   | N    | -5.220243 | 1.260881  | -0.178598 |
| C    | -1.102469 | 1.70941   | 2.841128  | C    | -5.576628 | 0.870287  | 1.203644  |
| H    | -0.318637 | 2.338144  | 3.259961  | H    | -5.178984 | -0.140332 | 1.365206  |
| C    | -2.087633 | 1.226585  | 3.786203  | H    | -5.043245 | 1.524225  | 1.897833  |
| C    | -2.085535 | 1.736914  | 5.112674  | C    | -7.085933 | 0.862018  | 1.494613  |
| C    | -2.974654 | 1.285808  | 6.082823  | C    | -7.817007 | -0.057958 | 0.50572   |
| C    | -3.913722 | 0.292491  | 5.785774  | C    | -7.4566   | 0.316537  | -0.940132 |
| C    | -3.930698 | -0.235042 | 4.491258  | C    | -5.929123 | 0.377477  | -1.131308 |
| C    | -3.046672 | 0.215838  | 3.512969  | H    | -5.683237 | 0.69304   | -2.149541 |
| H    | -3.074142 | -0.202714 | 2.514368  | H    | -5.518209 | -0.632167 | -1.000748 |
| H    | -4.64571  | -1.016919 | 4.237542  | H    | -7.875524 | -0.412124 | -1.647099 |
| H    | -4.608761 | -0.061638 | 6.542563  | H    | -7.907198 | 1.28537   | -1.192465 |

**Table 5 (Continued).**

|   |           |           |           |   |           |           |           |
|---|-----------|-----------|-----------|---|-----------|-----------|-----------|
| H | -2.931142 | 1.71063   | 7.084226  | H | -8.902948 | -0.015142 | 0.6574    |
| H | -1.35419  | 2.500394  | 5.374391  | H | -7.514587 | -1.099311 | 0.694754  |
| O | 2.523156  | 3.373936  | -0.138253 | H | -7.487005 | 1.882146  | 1.42171   |
| C | 3.453507  | 2.602417  | 0.651432  | H | -7.250141 | 0.532878  | 2.528427  |
| C | 4.812511  | 2.805908  | -0.016646 | O | -2.802941 | -0.271048 | -1.921164 |
| C | 4.703967  | 4.259055  | -0.505072 | C | -2.752532 | -1.643047 | -1.486979 |
| C | 3.236204  | 4.358065  | -0.933044 | C | -2.195453 | -2.422328 | -2.676803 |
| H | 3.098767  | 4.097174  | -1.989922 | C | -2.816712 | -1.660139 | -3.858072 |
| H | 2.79562   | 5.33862   | -0.748244 | C | -2.78446  | -0.207341 | -3.364303 |
| H | 5.392086  | 4.495475  | -1.322259 | H | -3.639857 | 0.38528   | -3.702387 |
| H | 4.90193   | 4.954419  | 0.317666  | H | -1.867136 | 0.308514  | -3.670855 |
| H | 4.928384  | 2.121047  | -0.86622  | H | -3.849689 | -1.98978  | -4.020183 |
| H | 5.647402  | 2.639093  | 0.670833  | H | -2.271362 | -1.791904 | -4.797472 |
| H | 3.455378  | 2.983748  | 1.681652  | H | -2.467065 | -3.48223  | -2.652895 |
| H | 3.099358  | 1.569514  | 0.665576  | H | -1.102779 | -2.343332 | -2.701754 |
| C | -0.609039 | 6.170209  | 0.692618  | H | -2.140963 | -1.680256 | -0.583406 |
| C | -1.219858 | 5.968263  | 2.093012  | H | -3.767134 | -1.984135 | -1.234711 |
| N | -2.649725 | 5.575357  | 2.071517  | O | 0.948928  | -0.431098 | -1.697169 |
| C | -3.505622 | 6.759549  | 1.834534  | C | 1.794585  | -1.591384 | -1.863985 |
| H | -3.245003 | 7.189196  | 0.862698  | C | 3.126988  | -1.044153 | -2.369239 |
| H | -3.284808 | 7.530906  | 2.59856   | C | 2.663968  | 0.11608   | -3.265025 |
| C | -4.999001 | 6.424976  | 1.874214  | C | 1.462886  | 0.67522   | -2.492794 |
| C | -5.385565 | 5.759837  | 3.200033  | H | 0.660554  | 1.03862   | -3.140997 |
| C | -4.46825  | 4.560567  | 3.462178  | H | 1.747047  | 1.477118  | -1.804213 |
| C | -2.995851 | 4.960088  | 3.375889  | H | 2.353291  | -0.263819 | -4.245386 |
| H | -2.364187 | 4.078148  | 3.506734  | H | 3.436836  | 0.872861  | -3.42928  |
| H | -2.762909 | 5.668465  | 4.195285  | H | 3.717076  | -1.795929 | -2.901956 |
| H | -4.668172 | 3.77268   | 2.723956  | H | 3.725329  | -0.668658 | -1.530342 |
| H | -4.655408 | 4.118591  | 4.447682  | H | 1.843577  | -2.098772 | -0.898754 |
| H | -6.438395 | 5.45127   | 3.184951  | H | 1.339204  | -2.265464 | -2.603693 |
| H | -5.280664 | 6.486066  | 4.019849  | O | 0.672097  | -1.513162 | 1.219984  |
| H | -5.243062 | 5.7589    | 1.038153  | C | 1.578609  | -1.04922  | 2.259586  |
| H | -5.570193 | 7.348573  | 1.716172  | C | 0.916473  | -1.418817 | 3.586631  |
| H | -1.08422  | 6.870876  | 2.715162  | C | 0.136163  | -2.690887 | 3.2218    |
| H | -0.680976 | 5.149559  | 2.582044  | C | -0.342606 | -2.375961 | 1.804135  |
| H | 1.647563  | -1.577136 | 4.385637  | H | -1.288943 | -1.825636 | 1.809924  |
| H | 2.54213   | -1.560546 | 2.125028  | H | -0.43631  | -3.263646 | 1.168832  |
| H | 1.704149  | 0.027633  | 2.125116  | H | -0.698612 | -2.885614 | 3.900967  |
| C | -5.459174 | 2.697702  | -0.447388 | H | 0.795415  | -3.567747 | 3.22298   |
| H | -6.52029  | 2.910401  | -0.64031  | H | 0.228208  | -0.624851 | 3.890667  |
| H | -5.187835 | 3.250484  | 0.45957   |   |           |           |           |

**Table 5 (Continued).**



**8d**

$G = -2767.351929$

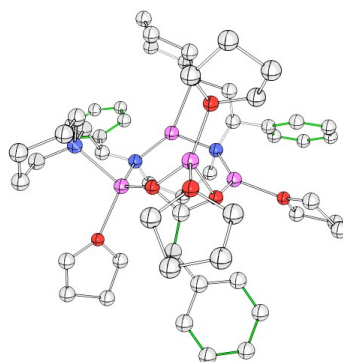
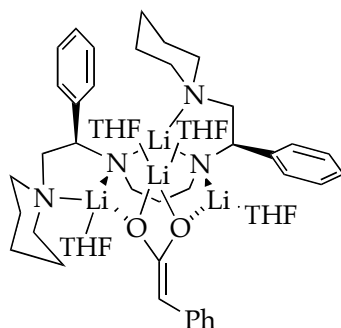
$G_{\text{MP2}} = -2759.3378964$

| Atom | X         | Y        | Z         | Atom | X        | Y         | Z         |
|------|-----------|----------|-----------|------|----------|-----------|-----------|
| Li   | 0         | 0        | 0         | H    | 6.614262 | 4.382395  | -0.224159 |
| O    | -0.733622 | 1.195198 | -1.375433 | C    | 5.326414 | 3.864577  | 1.454803  |
| Li   | -0.117283 | 2.786938 | -2.32564  | C    | 4.068329 | 3.022032  | 1.688899  |
| N    | 1.839853  | 3.365783 | -2.902903 | C    | 4.220426 | 1.625664  | 1.081584  |
| C    | 1.665736  | 4.785605 | -2.674156 | H    | 3.297289 | 1.054025  | 1.215132  |
| H    | 0.819095  | 5.186577 | -3.280308 | H    | 5.025544 | 1.087627  | 1.621467  |
| C    | 2.850823  | 5.713991 | -3.025861 | H    | 3.85849  | 2.921305  | 2.762176  |
| C    | 2.625177  | 7.074801 | -3.278455 | H    | 3.200504 | 3.522521  | 1.23916   |
| C    | 3.677345  | 7.945256 | -3.562993 | H    | 6.164746 | 3.432018  | 2.020726  |
| C    | 4.988147  | 7.464456 | -3.61328  | H    | 5.186313 | 4.887167  | 1.825493  |
| C    | 5.227949  | 6.11002  | -3.379311 | H    | 5.645839 | -0.154616 | -0.414878 |
| C    | 4.167621  | 5.247055 | -3.089577 | H    | 3.880222 | -0.322584 | -0.42688  |
| H    | 4.347479  | 4.187946 | -2.928028 | H    | 5.488313 | 0.755688  | -2.7848   |
| H    | 6.242351  | 5.720692 | -3.432546 | C    | 5.127625 | -1.325811 | -2.749259 |
| H    | 5.811006  | 8.136851 | -3.842893 | C    | 4.529394 | -2.459665 | -2.175681 |
| H    | 3.474829  | 8.996991 | -3.752389 | C    | 4.914311 | -3.748227 | -2.547087 |
| H    | 1.604989  | 7.456466 | -3.255002 | C    | 5.900817 | -3.935071 | -3.520503 |
| C    | 1.306327  | 5.014139 | -1.18906  | C    | 6.498218 | -2.820153 | -4.109528 |
| N    | -0.043685 | 4.522215 | -0.823956 | C    | 6.117447 | -1.532824 | -3.719637 |
| C    | -0.069718 | 4.096568 | 0.589481  | H    | 6.597728 | -0.668583 | -4.174427 |
| H    | 0.671815  | 3.298909 | 0.710608  | H    | 7.266029 | -2.950232 | -4.868608 |
| H    | 0.23964   | 4.933936 | 1.247288  | H    | 6.202186 | -4.938365 | -3.810974 |
| C    | -1.450893 | 3.593309 | 1.016557  | H    | 4.448338 | -4.609423 | -2.073204 |
| H    | -1.416126 | 3.316025 | 2.079352  | H    | 3.750822 | -2.336842 | -1.425444 |
| H    | -1.681929 | 2.689548 | 0.440882  | C    | 3.448345 | 0.907621  | -4.278365 |
| C    | -2.529007 | 4.656309 | 0.77384   | C    | 2.164387 | 1.633396  | -4.729681 |
| C    | -2.462752 | 5.130137 | -0.682546 | C    | 2.036395 | 3.115134  | -4.332292 |
| C    | -1.046315 | 5.584716 | -1.042287 | H    | 1.199391 | 3.546763  | -4.919448 |
| H    | -0.995935 | 5.890922 | -2.091163 | H    | 2.937856 | 3.623267  | -4.729342 |
| H    | -0.786286 | 6.475183 | -0.435273 | H    | 2.119684 | 1.589877  | -5.827958 |
| H    | -3.159469 | 5.960141 | -0.855961 | H    | 1.28279  | 1.077067  | -4.371867 |
| H    | -2.762004 | 4.310778 | -1.346917 | H    | 4.307122 | 1.590006  | -4.469136 |
| H    | -2.361811 | 5.511749 | 1.445135  | H    | 3.619889 | 0.055512  | -4.970108 |

**Table 5 (Continued).**

|    |           |           |           |   |           |           |           |
|----|-----------|-----------|-----------|---|-----------|-----------|-----------|
| H  | -3.524407 | 4.258887  | 1.007376  | O | -1.313171 | 3.241218  | -4.095953 |
| H  | 1.40698   | 6.076866  | -0.913178 | C | -2.238137 | 4.319767  | -4.345636 |
| H  | 2.042482  | 4.459911  | -0.594895 | C | -2.74392  | 4.133387  | -5.779366 |
| Li | 2.893024  | 2.097573  | -1.875934 | C | -2.65402  | 2.610075  | -5.951327 |
| N  | 3.391068  | 0.500817  | -2.875978 | C | -1.369556 | 2.288669  | -5.190971 |
| Li | 1.78751   | -0.716971 | -2.816743 | H | -0.48475  | 2.436747  | -5.822796 |
| O  | 0.26459   | -0.775291 | -1.743357 | H | -1.348344 | 1.285898  | -4.760645 |
| C  | -0.767696 | 0.033075  | -2.013244 | H | -2.602923 | 2.29815   | -6.999586 |
| C  | -1.819582 | -0.405914 | -2.814221 | H | -3.509819 | 2.115303  | -5.481782 |
| H  | -1.679219 | -1.383566 | -3.267458 | H | -2.080946 | 4.641123  | -6.49052  |
| C  | -3.123499 | 0.190155  | -3.011615 | H | -3.755663 | 4.528289  | -5.914606 |
| C  | -4.058159 | -0.462671 | -3.860385 | H | -3.062428 | 4.246288  | -3.626774 |
| C  | -5.34404  | 0.02679   | -4.065629 | H | -1.714141 | 5.269788  | -4.196806 |
| C  | -5.773397 | 1.198817  | -3.432795 | O | 1.188428  | -0.050549 | 1.600082  |
| C  | -4.874896 | 1.861726  | -2.590757 | C | 0.745692  | 0.627642  | 2.803514  |
| C  | -3.583355 | 1.379837  | -2.384756 | C | 0.772046  | -0.42436  | 3.912925  |
| H  | -2.898244 | 1.909939  | -1.73498  | C | 1.90604   | -1.352752 | 3.450147  |
| H  | -5.18655  | 2.772563  | -2.080563 | C | 1.706488  | -1.363816 | 1.934775  |
| H  | -6.77848  | 1.581292  | -3.589885 | H | 0.971149  | -2.117874 | 1.63009   |
| H  | -6.020421 | -0.512697 | -4.726399 | H | 2.628229  | -1.514062 | 1.36649   |
| H  | -3.749822 | -1.377643 | -4.364334 | H | 1.849056  | -2.355275 | 3.883952  |
| O  | 1.605888  | -2.18282  | -4.161553 | H | 2.882509  | -0.924835 | 3.705247  |
| C  | 2.479503  | -2.580963 | -5.241278 | H | -0.177855 | -0.969288 | 3.942766  |
| C  | 2.230658  | -4.091707 | -5.473306 | H | 0.94739   | 0.016111  | 4.898812  |
| C  | 1.201598  | -4.47042  | -4.38577  | H | 1.441186  | 1.451768  | 3.004864  |
| C  | 0.52874   | -3.131217 | -4.093239 | H | -0.249296 | 1.041067  | 2.618004  |
| H  | 0.081992  | -3.030905 | -3.103975 | O | -1.579112 | -1.000147 | 0.896182  |
| H  | -0.228357 | -2.888466 | -4.853992 | C | -1.799164 | -2.334806 | 0.35696   |
| H  | 1.709091  | -4.834909 | -3.485765 | C | -3.28625  | -2.412102 | 0.001141  |
| H  | 0.493815  | -5.237723 | -4.714853 | C | -3.91656  | -1.406537 | 0.97731   |
| H  | 3.154115  | -4.670385 | -5.387152 | C | -2.852531 | -0.312945 | 1.026602  |
| H  | 1.820258  | -4.265606 | -6.473631 | H | -2.835165 | 0.242255  | 1.970318  |
| H  | 2.237657  | -1.988015 | -6.132179 | H | -2.960245 | 0.388221  | 0.193251  |
| H  | 3.498953  | -2.353318 | -4.929721 | H | -4.056585 | -1.85712  | 1.967906  |
| C  | 4.692532  | 0.101161  | -2.371326 | H | -4.881244 | -1.024581 | 0.631327  |
| C  | 4.712752  | 0.260623  | -0.83741  | H | -3.685389 | -3.425593 | 0.108969  |
| N  | 4.52421   | 1.656665  | -0.366464 | H | -3.440337 | -2.080371 | -1.029577 |
| C  | 5.75345   | 2.450234  | -0.601275 | H | -1.139934 | -2.453274 | -0.506338 |
| H  | 5.940097  | 2.488565  | -1.678194 | H | -1.52756  | -3.059787 | 1.136427  |
| H  | 6.617965  | 1.931466  | -0.142161 | H | 4.894469  | 4.432437  | -0.586663 |
| C  | 5.660841  | 3.871629  | -0.039937 |   |           |           |           |

**Table 5 (Continued).**



**8b**

$G = -2767.351209$

$G_{\text{MP2}} = -2759.3295$

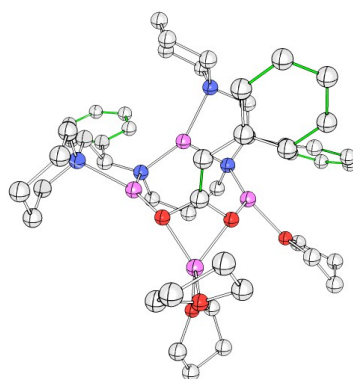
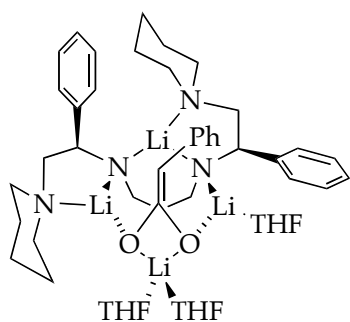
| Atom | X         | Y         | Z         | Atom | X         | Y         | Z         |
|------|-----------|-----------|-----------|------|-----------|-----------|-----------|
| Li   | 0         | 0         | 0         | C    | -5.521159 | 3.690833  | 0.967093  |
| O    | -1.02953  | -0.931669 | -1.327013 | C    | -4.281754 | 2.860264  | 1.315182  |
| Li   | -2.605841 | -1.106327 | -2.381047 | C    | -3.012949 | 3.486506  | 0.732622  |
| N    | -3.625749 | 0.510837  | -3.219757 | H    | -2.147324 | 2.849839  | 0.943645  |
| C    | -4.954695 | -0.056346 | -3.118487 | H    | -2.835419 | 4.461456  | 1.229909  |
| H    | -5.023915 | -1.019777 | -3.677067 | H    | -4.163742 | 2.767655  | 2.403024  |
| C    | -6.130742 | 0.7852    | -3.662248 | H    | -4.399553 | 1.844001  | 0.919229  |
| C    | -7.321495 | 0.157483  | -4.054211 | H    | -5.466253 | 4.66226   | 1.480316  |
| C    | -8.415322 | 0.894254  | -4.509015 | H    | -6.433212 | 3.195608  | 1.321797  |
| C    | -8.333989 | 2.28637   | -4.592884 | H    | -1.850693 | 5.411711  | -0.8284   |
| C    | -7.150595 | 2.925156  | -4.220207 | H    | -1.010602 | 3.857876  | -0.671636 |
| C    | -6.062304 | 2.179013  | -3.760796 | H    | -2.498003 | 4.681275  | -3.202478 |
| H    | -5.13228  | 2.670752  | -3.489505 | C    | -0.482973 | 5.285713  | -3.100985 |
| H    | -7.070024 | 4.007339  | -4.297434 | C    | 0.645567  | 5.541984  | -2.306684 |
| H    | -9.180393 | 2.86482   | -4.954804 | C    | 1.630846  | 6.443402  | -2.713458 |
| H    | -9.328591 | 0.382779  | -4.804689 | C    | 1.521471  | 7.099602  | -3.942393 |
| H    | -7.388428 | -0.928833 | -4.004576 | C    | 0.411995  | 6.849526  | -4.751446 |
| C    | -5.252484 | -0.366572 | -1.63411  | C    | -0.578651 | 5.960708  | -4.32724  |
| N    | -4.405243 | -1.442856 | -1.061103 | H    | -1.451584 | 5.790212  | -4.953685 |
| C    | -4.137392 | -1.175401 | 0.366418  | H    | 0.309481  | 7.356307  | -5.708137 |
| H    | -3.608918 | -0.218631 | 0.428804  | H    | 2.286777  | 7.803435  | -4.259762 |
| H    | -5.090228 | -1.063108 | 0.921917  | H    | 2.48202   | 6.641581  | -2.065328 |
| C    | -3.294187 | -2.272093 | 1.019346  | H    | 0.756591  | 5.041866  | -1.347776 |
| H    | -3.143912 | -2.023226 | 2.078706  | C    | -1.554659 | 2.691284  | -4.505109 |
| H    | -2.3099   | -2.284284 | 0.53606   | C    | -1.829572 | 1.216184  | -4.865006 |
| C    | -3.96651  | -3.641113 | 0.871689  | C    | -3.268334 | 0.718799  | -4.623856 |
| C    | -4.259343 | -3.899251 | -0.609969 | H    | -3.402338 | -0.218221 | -5.202021 |
| C    | -5.069429 | -2.751868 | -1.220969 | H    | -3.939474 | 1.441718  | -5.130113 |
| H    | -5.229255 | -2.920868 | -2.29114  | H    | -1.618023 | 1.090077  | -5.937077 |
| H    | -6.070403 | -2.72659  | -0.745829 | H    | -1.116325 | 0.563809  | -4.336013 |
| H    | -4.812966 | -4.837481 | -0.744654 | H    | -2.409294 | 3.289983  | -4.890203 |
| H    | -3.310055 | -4.002086 | -1.147572 | H    | -0.687775 | 3.03482   | -5.112224 |
| H    | -4.906586 | -3.655909 | 1.442757  | O    | -2.560386 | -2.772439 | -4.000508 |



**Table 5 (Continued).**

|    |           |           |           |   |           |           |           |
|----|-----------|-----------|-----------|---|-----------|-----------|-----------|
| H  | -3.331452 | -4.43475  | 1.284796  | C | -2.670688 | -4.196009 | -3.81982  |
| H  | -6.317468 | -0.609078 | -1.486926 | C | -2.396043 | -4.823881 | -5.187239 |
| H  | -5.056011 | 0.554717  | -1.073852 | C | -1.378639 | -3.840035 | -5.78064  |
| Li | -2.787479 | 1.91016   | -2.16147  | C | -1.890258 | -2.49498  | -5.261379 |
| N  | -1.364222 | 2.905461  | -3.070575 | H | -2.623532 | -2.053036 | -5.944849 |
| Li | 0.337208  | 1.922844  | -2.66164  | H | -1.091523 | -1.77681  | -5.068022 |
| O  | 0.764028  | 0.34209   | -1.754724 | H | -1.334356 | -3.869435 | -6.873689 |
| C  | 0.104376  | -0.783375 | -2.016414 | H | -0.373312 | -4.039861 | -5.396066 |
| C  | 0.569158  | -1.804661 | -2.837623 | H | -3.312225 | -4.841954 | -5.789972 |
| H  | -0.057731 | -2.692689 | -2.846455 | H | -2.020362 | -5.848991 | -5.108116 |
| C  | 1.796413  | -1.898239 | -3.598852 | H | -1.927654 | -4.525772 | -3.079058 |
| C  | 2.175015  | -3.159689 | -4.13367  | H | -3.669838 | -4.420897 | -3.435938 |
| C  | 3.331723  | -3.333138 | -4.886204 | O | -0.185843 | 1.332776  | 1.464331  |
| C  | 4.179855  | -2.252802 | -5.147318 | C | -0.533186 | 0.851004  | 2.789486  |
| C  | 3.832588  | -1.000915 | -4.63134  | C | 0.113625  | 1.831795  | 3.769564  |
| C  | 2.677344  | -0.819234 | -3.873368 | C | 1.361035  | 2.284849  | 2.994556  |
| H  | 2.425945  | 0.162064  | -3.491069 | C | 0.834621  | 2.358221  | 1.561001  |
| H  | 4.474546  | -0.144122 | -4.833357 | H | 1.591155  | 2.156822  | 0.79728   |
| H  | 5.082475  | -2.382189 | -5.738598 | H | 0.370192  | 3.329555  | 1.349762  |
| H  | 3.575499  | -4.321929 | -5.270905 | H | 2.153946  | 1.532147  | 3.074211  |
| H  | 1.537512  | -4.019766 | -3.932437 | H | 1.762487  | 3.242138  | 3.339671  |
| O  | 2.105771  | 2.688271  | -3.164614 | H | 0.34738   | 1.364075  | 4.730308  |
| C  | 2.492617  | 3.20712   | -4.460978 | H | -0.549909 | 2.683809  | 3.957292  |
| C  | 3.932496  | 3.701274  | -4.295857 | H | -1.624184 | 0.814447  | 2.85892   |
| C  | 4.472402  | 2.787312  | -3.183456 | H | -0.128554 | -0.161332 | 2.898298  |
| C  | 3.24562   | 2.61701   | -2.285897 | O | 1.244205  | -1.340969 | 0.927455  |
| H  | 3.173957  | 3.431761  | -1.550728 | C | 2.646771  | -1.109098 | 0.62782   |
| H  | 3.203021  | 1.655451  | -1.768049 | C | 3.308546  | -2.484312 | 0.673582  |
| H  | 5.324826  | 3.216357  | -2.647438 | C | 2.188225  | -3.382356 | 0.12765   |
| H  | 4.779027  | 1.818588  | -3.592348 | C | 0.932643  | -2.751149 | 0.73366   |
| H  | 3.935836  | 4.746979  | -3.969994 | H | 0.690063  | -3.17721  | 1.716004  |
| H  | 4.503744  | 3.630661  | -5.226341 | H | 0.061107  | -2.810287 | 0.078237  |
| H  | 2.423427  | 2.388301  | -5.187789 | H | 2.301561  | -4.434147 | 0.408252  |
| H  | 1.789659  | 3.996703  | -4.733951 | H | 2.151224  | -3.307167 | -0.963052 |
| C  | -1.589359 | 4.293118  | -2.693785 | H | 3.563672  | -2.756716 | 1.705381  |
| C  | -1.842593 | 4.363089  | -1.176444 | H | 4.220119  | -2.524247 | 0.070232  |
| N  | -3.083847 | 3.679665  | -0.733395 | H | 2.71341   | -0.65884  | -0.369072 |
| C  | -4.267486 | 4.505723  | -1.07052  | H | 3.036452  | -0.409272 | 1.37534   |
| H  | -4.314686 | 4.614492  | -2.15744  | H | -5.776834 | 2.96067   | -1.055973 |
| H  | -4.136159 | 5.52226   | -0.650054 | H | -6.39916  | 4.587006  | -0.814237 |
| C  | -5.577248 | 3.911151  | -0.547739 |   |           |           |           |

Table 5 (Continued).



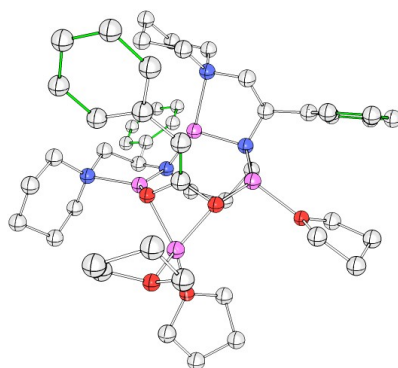
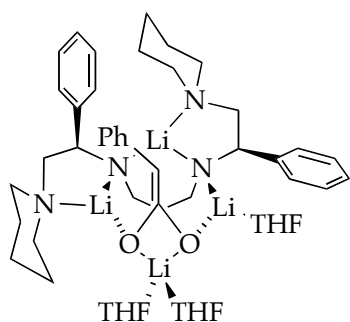
**8e**  
 $G = -2535.021549$   
 $G_{MP2} = -2527.653427$

| Atom | X        | Y         | Z         | Atom | X         | Y         | Z         |
|------|----------|-----------|-----------|------|-----------|-----------|-----------|
| Li   | 0        | 0         | 0         | C    | -1.340954 | -4.847568 | -1.501674 |
| O    | 1.713011 | 0.028367  | 0.88277   | C    | -2.816921 | -5.221745 | -1.335224 |
| Li   | 3.40825  | -0.340653 | 0.290608  | C    | -3.427308 | -3.926861 | -0.776708 |
| N    | 4.413968 | -1.751732 | -0.730386 | C    | -2.310173 | -3.426265 | 0.136981  |
| C    | 5.698182 | -1.099184 | -0.911064 | H    | -2.35761  | -3.906913 | 1.12317   |
| C    | 6.12129  | -0.396185 | 0.399232  | H    | -2.284043 | -2.344312 | 0.280086  |
| N    | 5.180879 | 0.674752  | 0.807313  | H    | -4.367233 | -4.085499 | -0.239283 |
| C    | 5.325922 | 0.986718  | 2.245089  | H    | -3.614144 | -3.208142 | -1.584582 |
| H    | 5.172803 | 0.059581  | 2.808397  | H    | -2.918353 | -6.036139 | -0.609791 |
| H    | 6.356367 | 1.332195  | 2.457779  | H    | -3.271707 | -5.5462   | -2.276077 |
| C    | 4.31857  | 2.047447  | 2.697985  | H    | -1.13757  | -4.425463 | -2.494251 |
| H    | 4.47485  | 2.25583   | 3.763925  | H    | -0.657361 | -5.678231 | -1.322476 |
| H    | 3.306521 | 1.639489  | 2.586203  | C    | 2.676153  | -5.558505 | 0.491536  |
| C    | 4.453317 | 3.329532  | 1.866982  | C    | 3.121721  | -5.404451 | 1.959411  |
| C    | 4.374907 | 2.992559  | 0.372795  | N    | 4.385856  | -4.639488 | 2.120173  |
| C    | 5.382703 | 1.899499  | 0.004953  | C    | 5.553195  | -5.495764 | 1.808746  |
| H    | 5.289374 | 1.641157  | -1.054092 | H    | 5.474964  | -5.827307 | 0.768414  |
| H    | 6.412475 | 2.279609  | 0.154423  | H    | 5.519934  | -6.405393 | 2.439702  |
| H    | 4.572155 | 3.880808  | -0.240811 | C    | 6.887251  | -4.77663  | 2.029983  |
| H    | 3.362044 | 2.645594  | 0.127023  | H    | 6.979931  | -3.95171  | 1.313884  |
| H    | 5.42024  | 3.808677  | 2.080919  | H    | 7.704047  | -5.475746 | 1.810141  |
| H    | 3.675301 | 4.052369  | 2.142294  | C    | 7.000867  | -4.236021 | 3.459579  |
| H    | 7.146275 | 0.003135  | 0.320717  | C    | 5.768235  | -3.386525 | 3.787524  |
| H    | 6.128989 | -1.150396 | 1.195413  | C    | 4.47795   | -4.162047 | 3.520779  |
| H    | 5.620733 | -0.306805 | -1.690428 | H    | 3.606026  | -3.535537 | 3.723374  |
| C    | 6.875368 | -1.974124 | -1.40153  | H    | 4.425728  | -5.024536 | 4.212898  |
| C    | 8.031174 | -1.36826  | -1.917137 | H    | 5.778113  | -3.065047 | 4.836521  |
| C    | 9.115223 | -2.127904 | -2.355835 | H    | 5.775436  | -2.474057 | 3.174447  |
| C    | 9.058842 | -3.522889 | -2.301725 | H    | 7.060486  | -5.075872 | 4.167462  |
| C    | 7.909087 | -4.140702 | -1.810014 | H    | 7.922747  | -3.653626 | 3.580147  |
| C    | 6.830218 | -3.370931 | -1.365655 | H    | 3.215617  | -6.391917 | 2.444465  |
| H    | 5.926709 | -3.851386 | -1.001224 | H    | 2.347639  | -4.849543 | 2.499114  |
| H    | 7.845996 | -5.22613  | -1.77903  | H    | 3.512481  | -6.028803 | -0.068981 |

**Table 5 (Continued).**

|    |           |           |           |   |           |           |           |
|----|-----------|-----------|-----------|---|-----------|-----------|-----------|
| H  | 9.898208  | -4.119976 | -2.649187 | C | 1.519894  | -6.566438 | 0.389215  |
| H  | 10.001062 | -1.632656 | -2.746828 | C | 1.511362  | -7.527098 | -0.632121 |
| H  | 8.078935  | -0.281918 | -1.983027 | C | 0.453912  | -8.429948 | -0.775566 |
| Li | 3.891929  | -3.16133  | 0.573259  | C | -0.618219 | -8.398711 | 0.117217  |
| N  | 2.382852  | -4.239283 | -0.054826 | C | -0.623994 | -7.451184 | 1.145683  |
| Li | 0.667026  | -3.30423  | 0.357412  | C | 0.427164  | -6.541173 | 1.272833  |
| O  | 0.213123  | -1.623673 | 1.046676  | H | 0.400396  | -5.813698 | 2.080897  |
| C  | 1.20779   | -0.961113 | 1.621929  | H | -1.444465 | -7.428645 | 1.859749  |
| C  | 1.682665  | -1.212089 | 2.906952  | H | -1.435096 | -9.109664 | 0.020793  |
| H  | 2.477604  | -0.5513   | 3.245773  | H | 0.474372  | -9.163884 | -1.577979 |
| C  | 1.167136  | -2.136445 | 3.897391  | H | 2.352879  | -7.569839 | -1.320913 |
| C  | 1.776611  | -2.178036 | 5.180237  | C | 2.449123  | -4.213908 | -1.511771 |
| C  | 1.338679  | -3.034518 | 6.184566  | C | 2.492105  | -2.771738 | -2.058442 |
| C  | 0.26099   | -3.899337 | 5.967568  | H | 2.154264  | -2.7894   | -3.105841 |
| C  | -0.367496 | -3.87107  | 4.720175  | H | 1.76545   | -2.151973 | -1.509655 |
| C  | 0.066301  | -3.0151   | 3.708118  | C | 3.861687  | -2.072954 | -2.049863 |
| H  | -0.459538 | -2.986267 | 2.761394  | H | 3.756958  | -1.146903 | -2.661911 |
| H  | -1.220555 | -4.521575 | 4.53159   | H | 4.546802  | -2.711214 | -2.642696 |
| H  | -0.081542 | -4.570633 | 6.750368  | H | 3.348527  | -4.748345 | -1.892673 |
| H  | 1.842114  | -3.025336 | 7.149592  | H | 1.597584  | -4.739481 | -1.998865 |
| H  | 2.612814  | -1.508841 | 5.37823   | O | -1.191957 | 1.296691  | 1.001984  |
| O  | -1.079439 | -3.812575 | -0.516963 | C | -0.491577 | 2.478298  | 1.480179  |
| C  | -0.773911 | -0.909021 | -2.778068 | C | -1.001394 | 2.725382  | 2.902502  |
| C  | -2.010776 | -0.531537 | -3.589434 | C | -1.357797 | 1.305934  | 3.370282  |
| C  | -1.840876 | 0.990531  | -3.726056 | C | -1.930338 | 0.687244  | 2.096382  |
| C  | -1.226935 | 1.385358  | -2.374833 | H | -2.99587  | 0.923095  | 1.968937  |
| H  | -1.980674 | 1.698255  | -1.645349 | H | -1.776632 | -0.392154 | 2.033857  |
| H  | -0.474197 | 2.175865  | -2.464134 | H | -2.071968 | 1.289997  | 4.199105  |
| H  | -2.780449 | 1.51521   | -3.92234  | H | -0.458214 | 0.759928  | 3.672718  |
| H  | -1.149578 | 1.220443  | -4.544694 | H | -1.893603 | 3.363371  | 2.888907  |
| H  | -2.923079 | -0.769534 | -3.028887 | H | -0.247811 | 3.209368  | 3.530915  |
| H  | -2.055353 | -1.047935 | -4.552934 | H | 0.58058   | 2.255376  | 1.463409  |
| H  | 0.114301  | -1.000626 | -3.416212 | H | -0.705891 | 3.303351  | 0.79233   |
| H  | -0.877473 | -1.819633 | -2.18355  | O | -0.587815 | 0.191396  | -1.858592 |

**Table 5 (Continued).**



**8f**

$G = -2535.021549$

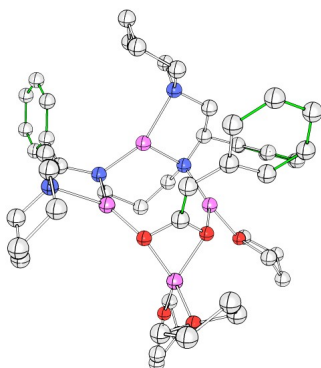
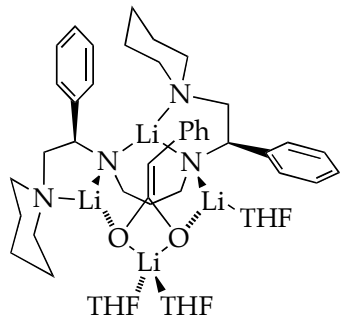
$G_{\text{MP2}} = -2527.653427$

| Atom | X         | Y         | Z         | Atom | X         | Y         | Z         |
|------|-----------|-----------|-----------|------|-----------|-----------|-----------|
| Li   | 0         | 0         | 0         | H    | -7.249273 | 4.001662  | 3.416061  |
| O    | -1.670606 | 0.344187  | 0.976152  | H    | -2.161483 | 6.275312  | 3.30892   |
| Li   | -3.007219 | 1.004003  | -0.113286 | H    | -1.509817 | 4.651479  | 3.0265    |
| N    | -3.602191 | 2.719674  | -1.001548 | H    | -2.236031 | 6.576062  | 0.768951  |
| C    | -4.93652  | 2.388129  | -1.472862 | C    | -0.241498 | 6.65518   | 1.475679  |
| C    | -5.617475 | 1.386933  | -0.514843 | C    | 0.003431  | 7.832448  | 0.755125  |
| N    | -4.900678 | 0.091033  | -0.409384 | C    | 1.195179  | 8.546952  | 0.908617  |
| C    | -5.462601 | -0.696011 | 0.711165  | C    | 2.16776   | 8.102285  | 1.805043  |
| H    | -5.351899 | -0.106108 | 1.626747  | C    | 1.938919  | 6.9328    | 2.536927  |
| H    | -6.546815 | -0.854599 | 0.550719  | C    | 0.753968  | 6.216001  | 2.36476   |
| C    | -4.769073 | -2.050877 | 0.874856  | H    | 0.598675  | 5.307453  | 2.942339  |
| H    | -5.240839 | -2.592596 | 1.703966  | H    | 2.681283  | 6.584498  | 3.251906  |
| H    | -3.721773 | -1.883095 | 1.152889  | H    | 3.089333  | 8.663045  | 1.939627  |
| C    | -4.829108 | -2.869244 | -0.419331 | H    | 1.358073  | 9.455937  | 0.334142  |
| C    | -4.283183 | -2.029518 | -1.578626 | H    | -0.756761 | 8.195733  | 0.066234  |
| C    | -5.002843 | -0.680881 | -1.667402 | C    | -1.261577 | 4.991556  | -0.999691 |
| H    | -4.575693 | -0.086146 | -2.478715 | C    | -1.415323 | 3.72962   | -1.872364 |
| H    | -6.068824 | -0.850803 | -1.916321 | H    | -0.959201 | 3.928882  | -2.853972 |
| H    | -4.397987 | -2.555195 | -2.53508  | H    | -0.837339 | 2.905618  | -1.425788 |
| H    | -3.207295 | -1.856002 | -1.433671 | C    | -2.85048  | 3.253238  | -2.144676 |
| H    | -5.870892 | -3.149863 | -0.633049 | H    | -2.788565 | 2.489807  | -2.954162 |
| H    | -4.264632 | -3.804112 | -0.314892 | H    | -3.377843 | 4.104705  | -2.619283 |
| H    | -6.66552  | 1.213658  | -0.811905 | H    | -2.033133 | 5.727387  | -1.321633 |
| H    | -5.638133 | 1.830766  | 0.489176  | H    | -0.297811 | 5.478883  | -1.266403 |
| H    | -4.873388 | 1.885953  | -2.46227  | O    | 0.823678  | -1.621724 | 0.866672  |
| C    | -5.908619 | 3.563463  | -1.738243 | C    | -0.129594 | -2.557152 | 1.450407  |
| C    | -7.090587 | 3.344482  | -2.462964 | C    | 0.463761  | -2.984859 | 2.795206  |
| C    | -7.985861 | 4.381132  | -2.723828 | C    | 1.305942  | -1.76065  | 3.186269  |
| C    | -7.707912 | 5.675057  | -2.275819 | C    | 1.858265  | -1.308787 | 1.835756  |
| C    | -6.528068 | 5.913536  | -1.571826 | H    | 2.770774  | -1.856125 | 1.560673  |
| C    | -5.640945 | 4.865826  | -1.307655 | H    | 2.042563  | -0.232875 | 1.782285  |
| H    | -4.712988 | 5.057255  | -0.776735 | H    | 2.098331  | -1.994888 | 3.904029  |
| H    | -6.290924 | 6.919108  | -1.231875 | H    | 0.668083  | -0.975994 | 3.605724  |

**Table 5 (Continued).**

|    |           |           |           |   |           |           |           |
|----|-----------|-----------|-----------|---|-----------|-----------|-----------|
| H  | -8.398949 | 6.488196  | -2.483014 | H | 1.099443  | -3.870851 | 2.676047  |
| H  | -8.896658 | 4.181865  | -3.283793 | H | -0.313736 | -3.217056 | 3.528402  |
| H  | -7.308863 | 2.345554  | -2.838371 | H | -1.077838 | -2.02486  | 1.570943  |
| Li | -3.082168 | 3.750901  | 0.632109  | H | -0.259669 | -3.388748 | 0.749602  |
| N  | -1.372789 | 4.673055  | 0.418004  | O | 0.538473  | -0.107876 | -1.879656 |
| Li | 0.128823  | 3.384767  | 0.702041  | C | 1.216149  | 0.99546   | -2.526249 |
| O  | 0.196981  | 1.574688  | 1.070599  | C | 2.430643  | 0.361906  | -3.199274 |
| C  | -0.861735 | 1.091238  | 1.723881  | C | 1.861344  | -0.988744 | -3.664114 |
| C  | -1.012822 | 1.319856  | 3.087018  | C | 0.887627  | -1.354974 | -2.533318 |
| H  | -0.230699 | 1.931888  | 3.53214   | H | 1.34344   | -2.003423 | -1.778497 |
| C  | -1.993843 | 0.786112  | 4.009354  | H | -0.02983  | -1.827926 | -2.899344 |
| C  | -1.926335 | 1.156309  | 5.378905  | H | 2.628973  | -1.7539   | -3.811854 |
| C  | -2.833109 | 0.681098  | 6.320286  | H | 1.323083  | -0.865133 | -4.61059  |
| C  | -3.857093 | -0.196748 | 5.947904  | H | 3.235932  | 0.211726  | -2.469982 |
| C  | -3.940328 | -0.585142 | 4.607798  | H | 2.820815  | 0.969719  | -4.02112  |
| C  | -3.037291 | -0.109243 | 3.658962  | H | 0.540012  | 1.452006  | -3.260378 |
| H  | -3.110461 | -0.426638 | 2.627337  | H | 1.452641  | 1.734052  | -1.7568   |
| H  | -4.721676 | -1.276377 | 4.29428   | C | -1.535787 | 5.85748   | 1.248009  |
| H  | -4.565451 | -0.570206 | 6.682657  | C | -2.147713 | 5.43101   | 2.597746  |
| H  | -2.738789 | 0.996806  | 7.357758  | N | -3.506353 | 4.843561  | 2.476277  |
| H  | -1.13665  | 1.836303  | 5.695067  | C | -4.526526 | 5.911521  | 2.372371  |
| O  | 2.00709   | 3.749455  | 0.084266  | H | -4.317417 | 6.507451  | 1.477569  |
| C  | 2.530387  | 4.900672  | -0.629262 | H | -4.433719 | 6.592453  | 3.240865  |
| C  | 4.021183  | 4.972068  | -0.279304 | C | -5.954513 | 5.359542  | 2.314756  |
| C  | 4.356077  | 3.511743  | 0.062498  | H | -6.089236 | 4.795539  | 1.384343  |
| C  | 3.077789  | 3.057948  | 0.764333  | H | -6.654802 | 6.203676  | 2.273865  |
| H  | 3.079692  | 3.349995  | 1.823334  | C | -6.255034 | 4.454718  | 3.515582  |
| H  | 2.870931  | 1.988168  | 0.70164   | C | -5.17095  | 3.378866  | 3.635763  |
| H  | 5.242245  | 3.406428  | 0.695913  | C | -3.778155 | 4.006309  | 3.671364  |
| H  | 4.51929   | 2.928322  | -0.852243 | H | -3.014932 | 3.226812  | 3.71775   |
| H  | 4.171514  | 5.613158  | 0.596136  | H | -3.68044  | 4.621689  | 4.586643  |
| H  | 4.621348  | 5.37445   | -1.100974 | H | -5.30554  | 2.770369  | 4.537309  |
| H  | 2.368526  | 4.730646  | -1.700756 | H | -5.233704 | 2.690098  | 2.781273  |
| H  | 1.971664  | 5.786094  | -0.321708 | H | -6.272152 | 5.057302  | 4.435815  |

Table 5 (Continued).



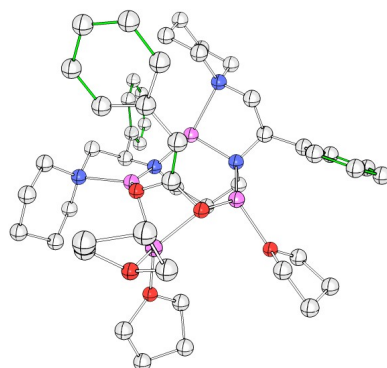
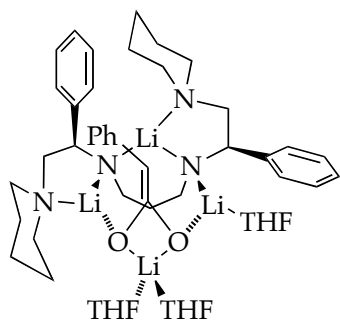
**8g**  
 $G = -2535.017614$   
 $G_{\text{MP2}} = -2527.649109$

| Atom | X         | Y         | Z         | Atom | X         | Y        | Z         |
|------|-----------|-----------|-----------|------|-----------|----------|-----------|
| Li   | 0         | 0         | 0         | C    | -0.738411 | 4.144857 | 5.762415  |
| O    | -1.748132 | -0.073629 | 0.806124  | C    | -0.031096 | 4.072692 | 4.559692  |
| Li   | -3.460488 | 0.183854  | 0.199661  | C    | -0.371645 | 3.149373 | 3.571453  |
| N    | -4.629863 | 1.439535  | -0.848477 | H    | 0.211549  | 3.089328 | 2.660329  |
| C    | -5.835107 | 0.617548  | -0.983885 | H    | 0.810733  | 4.742372 | 4.388679  |
| C    | -6.133877 | -0.11525  | 0.338419  | H    | -0.468222 | 4.86875  | 6.526468  |
| N    | -5.067748 | -1.068059 | 0.724273  | H    | -2.361929 | 3.278689 | 6.891648  |
| C    | -5.150224 | -1.391316 | 2.164576  | H    | -2.966847 | 1.641244 | 5.16433   |
| H    | -5.091446 | -0.451058 | 2.724277  | O    | 0.824517  | 3.725281 | -0.827795 |
| H    | -6.132381 | -1.848243 | 2.395837  | C    | 1.068012  | 4.693417 | -1.883136 |
| C    | -4.022772 | -2.330771 | 2.601344  | C    | 2.539251  | 5.10929  | -1.750874 |
| H    | -4.13835  | -2.553527 | 3.669645  | C    | 3.167544  | 3.911258 | -1.020882 |
| H    | -3.066661 | -1.809746 | 2.472481  | C    | 2.039631  | 3.502182 | -0.077653 |
| C    | -4.02589  | -3.621424 | 1.772647  | H    | 2.028428  | 4.132613 | 0.821963  |
| C    | -4.011034 | -3.28065  | 0.27721   | H    | 2.047005  | 2.455548 | 0.229851  |
| C    | -5.142488 | -2.309812 | -0.073369 | H    | 4.089743  | 4.163387 | -0.488353 |
| H    | -5.097767 | -2.046341 | -1.133976 | H    | 3.391135  | 3.100115 | -1.725348 |
| H    | -6.119657 | -2.803801 | 0.095093  | H    | 2.619334  | 6.012557 | -1.137085 |
| H    | -4.117843 | -4.186977 | -0.332471 | H    | 3.000078  | 5.316977 | -2.721396 |
| H    | -3.049002 | -2.821269 | 0.013092  | H    | 0.867445  | 4.195405 | -2.839789 |
| H    | -4.929008 | -4.205952 | 2.00278   | H    | 0.373462  | 5.526343 | -1.764785 |
| H    | -3.167023 | -4.251892 | 2.035     | C    | -2.936505 | 5.412886 | 0.159262  |
| H    | -7.109588 | -0.628986 | 0.28619   | C    | -3.414953 | 5.313912 | 1.621457  |
| H    | -6.200959 | 0.627585  | 1.142147  | N    | -4.734321 | 4.644651 | 1.749736  |
| H    | -5.658458 | -0.165788 | -1.754145 | C    | -5.816343 | 5.60283  | 1.427108  |
| C    | -7.093674 | 1.344793  | -1.488547 | H    | -5.675216 | 5.955567 | 0.401524  |
| C    | -7.401125 | 1.335127  | -2.856728 | H    | -5.728177 | 6.486812 | 2.088444  |
| C    | -8.520576 | 2.002624  | -3.357972 | C    | -7.210401 | 4.992899 | 1.57887   |
| C    | -9.373796 | 2.685911  | -2.49126  | H    | -7.343857 | 4.2131   | 0.82152   |
| C    | -9.093329 | 2.694156  | -1.123394 | H    | -7.958489 | 5.76832  | 1.369619  |
| C    | -7.964544 | 2.0349    | -0.632916 | C    | -7.415993 | 4.40593  | 2.980945  |
| H    | -7.771572 | 2.047581  | 0.436106  | C    | -6.257983 | 3.463953 | 3.332735  |
| H    | -9.757933 | 3.210321  | -0.43446  | C    | -4.906633 | 4.153698 | 3.136728  |

**Table 5 (Continued).**

|    |            |           |           |   |           |           |           |
|----|------------|-----------|-----------|---|-----------|-----------|-----------|
| H  | -10.250875 | 3.200945  | -2.874773 | H | -4.085888 | 3.466563  | 3.35996   |
| H  | -8.72877   | 1.982334  | -4.425169 | H | -4.822769 | 4.996866  | 3.848952  |
| H  | -6.752209  | 0.787915  | -3.537389 | H | -6.335771 | 3.119385  | 4.37154   |
| Li | -4.243219  | 3.043635  | 0.288301  | H | -6.301404 | 2.568214  | 2.696294  |
| N  | -2.670587  | 4.065008  | -0.333297 | H | -7.451217 | 5.222479  | 3.71704   |
| Li | -0.909079  | 3.228835  | 0.11193   | H | -8.378628 | 3.882918  | 3.045151  |
| O  | -0.343991  | 1.659609  | 0.958996  | H | -3.451468 | 6.310411  | 2.095044  |
| C  | -1.325739  | 0.968626  | 1.523734  | H | -2.692028 | 4.712907  | 2.182517  |
| C  | -1.868351  | 1.245631  | 2.775778  | H | -3.749331 | 5.882718  | -0.433382 |
| H  | -2.644531  | 0.559329  | 3.107969  | C | -1.75636  | 6.390642  | 0.047815  |
| C  | -1.452271  | 2.242307  | 3.742132  | C | -1.712657 | 7.327897  | -0.994429 |
| C  | -2.143384  | 2.330058  | 4.980274  | C | -0.639414 | 8.212308  | -1.135268 |
| C  | -1.798653  | 3.25436   | 5.960521  | C | 0.414417  | 8.184201  | -0.220517 |
| C  | 0.99677    | -2.555137 | 3.035769  | C | 0.38569   | 7.258923  | 0.827603  |
| C  | 1.248368   | -1.102335 | 3.467661  | C | -0.682489 | 6.368759  | 0.954489  |
| C  | 1.866545   | -0.501065 | 2.207467  | H | -0.68746  | 5.664641  | 1.78383   |
| H  | 2.947098   | -0.691695 | 2.149339  | H | 1.190733  | 7.24103   | 1.559149  |
| H  | 1.669631   | 0.567264  | 2.096398  | H | 1.242595  | 8.882382  | -0.314311 |
| H  | 1.906958   | -1.017422 | 4.337334  | H | -0.633527 | 8.930261  | -1.952274 |
| H  | 0.304418   | -0.594648 | 3.691766  | H | -2.540492 | 7.369225  | -1.699702 |
| H  | 1.920001   | -3.143502 | 3.103611  | C | -2.735695 | 3.98114   | -1.787382 |
| H  | 0.230658   | -3.056145 | 3.634977  | C | -2.800595 | 2.519304  | -2.272534 |
| H  | -0.513615  | -2.238323 | 1.481431  | H | -2.504141 | 2.500432  | -3.332447 |
| H  | 0.877562   | -3.222132 | 0.934408  | H | -2.051571 | 1.920445  | -1.730033 |
| O  | 0.636631   | -0.282949 | -1.832175 | H | -3.626499 | 4.51258   | -2.192623 |
| C  | 0.599631   | 0.722076  | -2.873372 | H | -1.875208 | 4.470459  | -2.297372 |
| C  | 1.804587   | 0.413848  | -3.759398 | C | -4.167837 | 1.815425  | -2.188149 |
| C  | 1.851287   | -1.121452 | -3.701884 | H | -4.095986 | 0.907933  | -2.832628 |
| C  | 1.439609   | -1.412527 | -2.253319 | H | -4.892962 | 2.466349  | -2.717723 |
| H  | 2.30115    | -1.48303  | -1.580933 | O | 1.219946  | -1.181092 | 1.097125  |
| H  | 0.841552   | -2.323925 | -2.151798 | C | 0.56719   | -2.38955  | 1.575008  |
| H  | 2.834481   | -1.535601 | -3.943698 | H | 1.68986   | 0.804511  | -4.774834 |
| H  | 1.123555   | -1.547698 | -4.401879 | H | -0.343362 | 0.629857  | -3.426932 |
| H  | 2.717087   | 0.84312   | -3.327753 | H | 0.631903  | 1.69944   | -2.38673  |

**Table 5 (Continued).**



**8h**

$G = -2535.015535$

$G_{MP2} = -2527.645802$

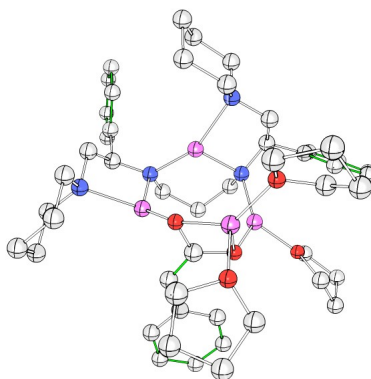
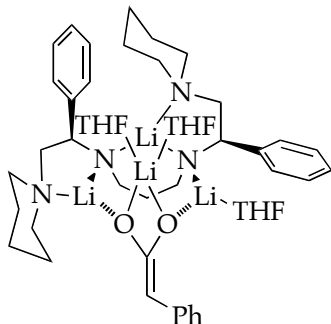
| Atom | X         | Y         | Z         | Atom | X         | Y        | Z         |
|------|-----------|-----------|-----------|------|-----------|----------|-----------|
| Li   | 0         | 0         | 0         | H    | -7.402181 | 3.673966 | 0.099237  |
| O    | -1.811067 | 0.001975  | 0.705868  | H    | -8.187172 | 5.11184  | 0.744181  |
| Li   | -3.132694 | 0.138431  | -0.578568 | C    | -7.785601 | 3.565798 | 2.227729  |
| N    | -4.329836 | 1.357916  | -1.634865 | C    | -6.63225  | 2.630784 | 2.611112  |
| C    | -5.419914 | 0.467034  | -2.048572 | C    | -5.311108 | 3.394775 | 2.701337  |
| C    | -5.543209 | -0.753497 | -1.115933 | H    | -4.492723 | 2.710581 | 2.938269  |
| N    | -4.297431 | -1.547482 | -1.012686 | H    | -5.371947 | 4.130898 | 3.526555  |
| C    | -4.450709 | -2.584266 | 0.028365  | H    | -6.820809 | 2.137457 | 3.571928  |
| H    | -4.737891 | -2.086249 | 0.959862  | H    | -6.533778 | 1.833444 | 1.861572  |
| H    | -5.275426 | -3.27198  | -0.243263 | H    | -7.971751 | 4.268318 | 3.053676  |
| C    | -3.159977 | -3.380607 | 0.232192  | H    | -8.714975 | 3.000794 | 2.080786  |
| H    | -3.32661  | -4.142468 | 1.004036  | H    | -3.841397 | 5.696446 | 2.250473  |
| H    | -2.38627  | -2.698632 | 0.60468   | H    | -3.015044 | 4.130683 | 2.107134  |
| C    | -2.698602 | -4.025669 | -1.080359 | H    | -3.804534 | 5.832642 | -0.304482 |
| C    | -2.613311 | -2.960968 | -2.180504 | C    | -1.878955 | 6.175812 | 0.498017  |
| C    | -3.922212 | -2.172764 | -2.296764 | C    | -1.755669 | 7.364196 | -0.235697 |
| H    | -3.811527 | -1.387476 | -3.0483   | C    | -0.66459  | 8.220311 | -0.0596   |
| H    | -4.731957 | -2.845156 | -2.642076 | C    | 0.328134  | 7.907453 | 0.870337  |
| H    | -2.388127 | -3.418873 | -3.152472 | C    | 0.220392  | 6.728274 | 1.614341  |
| H    | -1.796087 | -2.260937 | -1.956174 | C    | -0.86546  | 5.871969 | 1.423528  |
| H    | -3.417255 | -4.801874 | -1.381951 | H    | -0.931548 | 4.96212  | 2.017227  |
| H    | -1.731123 | -4.527053 | -0.948582 | H    | 0.97669   | 6.48231  | 2.356659  |
| H    | -6.381664 | -1.390847 | -1.449851 | H    | 1.169467  | 8.578722 | 1.023745  |
| H    | -5.779801 | -0.419686 | -0.097909 | H    | -0.596842 | 9.136471 | -0.641827 |
| H    | -5.187255 | 0.06185   | -3.054489 | H    | -2.534133 | 7.624579 | -0.95024  |
| C    | -6.800352 | 1.11952   | -2.242079 | C    | -2.66741  | 4.25194  | -1.925756 |
| C    | -7.193671 | 1.537899  | -3.522565 | C    | -2.603249 | 2.929921 | -2.70948  |
| C    | -8.436563 | 2.13336   | -3.746885 | H    | -2.290645 | 3.163276 | -3.738518 |
| C    | -9.331051 | 2.30445   | -2.69     | H    | -1.814262 | 2.287045 | -2.285497 |
| C    | -8.963351 | 1.883171  | -1.410735 | H    | -3.554975 | 4.817411 | -2.291001 |
| C    | -7.709788 | 1.308197  | -1.190802 | H    | -1.802522 | 4.877038 | -2.242507 |
| H    | -7.447209 | 0.993053  | -0.184431 | C    | -3.910495 | 2.123146 | -2.816985 |



**Table 5 (Continued).**

|    |            |           |           |   |           |           |           |
|----|------------|-----------|-----------|---|-----------|-----------|-----------|
| H  | -9.65485   | 1.99996   | -0.579524 | H | -3.778901 | 1.429705  | -3.678162 |
| H  | -10.305331 | 2.755232  | -2.860686 | H | -4.691509 | 2.833109  | -3.162472 |
| H  | -8.709677  | 2.452022  | -4.750144 | O | 1.188017  | -1.047383 | 1.248091  |
| H  | -6.51566   | 1.381107  | -4.358692 | C | 0.518947  | -2.103011 | 1.995327  |
| Li | -4.2536    | 2.797216  | -0.201746 | C | 1.155194  | -2.09508  | 3.384718  |
| N  | -2.725072  | 4.019112  | -0.490209 | C | 1.494546  | -0.608232 | 3.567857  |
| Li | -0.922591  | 3.244779  | -0.075524 | C | 1.940113  | -0.201729 | 2.162678  |
| O  | -0.377374  | 1.715244  | 0.79222   | H | 3.009918  | -0.390036 | 1.999587  |
| C  | -1.354514  | 1.039104  | 1.40271   | H | 1.700585  | 0.836667  | 1.921336  |
| C  | -1.770202  | 1.381834  | 2.68258   | H | 2.271126  | -0.430442 | 4.318283  |
| H  | -1.269098  | 2.247898  | 3.109927  | H | 0.597398  | -0.046788 | 3.847326  |
| C  | -2.721799  | 0.710187  | 3.544421  | H | 2.065829  | -2.706729 | 3.398503  |
| C  | -2.996519  | 1.257124  | 4.826205  | H | 0.473097  | -2.475947 | 4.150191  |
| C  | -3.89827   | 0.668016  | 5.706321  | H | -0.548435 | -1.863482 | 2.036193  |
| C  | -4.574126  | -0.506161 | 5.357859  | H | 0.663617  | -3.041771 | 1.450876  |
| C  | -4.313087  | -1.073207 | 4.107336  | O | 0.647644  | -0.3892   | -1.809346 |
| C  | -3.412644  | -0.487199 | 3.219401  | C | 0.860182  | 0.642615  | -2.802305 |
| H  | -3.21083   | -0.949333 | 2.261438  | C | 2.227999  | 0.327229  | -3.402195 |
| H  | -4.816589  | -1.995136 | 3.818583  | C | 2.221231  | -1.210302 | -3.407439 |
| H  | -5.278638  | -0.96832  | 6.044305  | C | 1.459788  | -1.551246 | -2.11801  |
| H  | -4.074148  | 1.128815  | 6.676739  | H | 2.126251  | -1.722622 | -1.266844 |
| H  | -2.481706  | 2.169838  | 5.122518  | H | 0.800291  | -2.418129 | -2.228979 |
| O  | 0.820977   | 3.846027  | -0.937405 | H | 3.223851  | -1.64738  | -3.422243 |
| C  | 1.033103   | 4.983674  | -1.816692 | H | 1.679393  | -1.581962 | -4.284543 |
| C  | 2.489952   | 5.427544  | -1.606633 | H | 3.025209  | 0.707824  | -2.752097 |
| C  | 3.149079   | 4.178082  | -0.999722 | H | 2.361297  | 0.760604  | -4.397897 |
| C  | 2.011205   | 3.614719  | -0.15382  | H | 0.065792  | 0.584     | -3.558054 |
| H  | 1.925394   | 4.147787  | 0.802567  | H | 0.798223  | 1.608377  | -2.295104 |
| H  | 2.066163   | 2.543893  | 0.047221  | H | 0.312598  | 5.764111  | -1.563768 |
| H  | 4.041733   | 4.40471   | -0.408505 | C | -3.063029 | 5.226483  | 0.254871  |
| H  | 3.430517   | 3.46524   | -1.784941 | C | -3.699729 | 4.816745  | 1.597421  |
| H  | 2.529652   | 6.25905   | -0.895251 | N | -4.982733 | 4.091583  | 1.434471  |
| H  | 2.961415   | 5.756187  | -2.537656 | C | -6.067788 | 5.040557  | 1.096095  |
| H  | 0.844043   | 4.642618  | -2.840604 | H | -5.813507 | 5.544388  | 0.15901   |
| C  | -7.425909  | 4.351068  | 0.960249  | H | -6.126374 | 5.822146  | 1.878934  |

**Table 5 (Continued).**



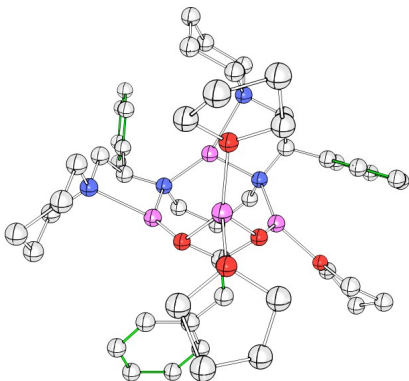
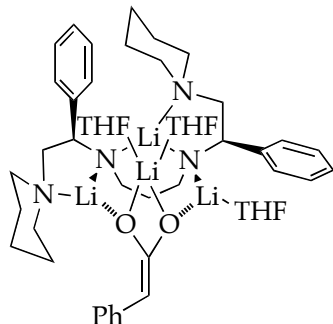
**8i**  
 $G = -2535.011204$   
 $G_{MP2} = -2527.639386$

| Atom | X         | Y         | Z         | Atom | X         | Y         | Z         |
|------|-----------|-----------|-----------|------|-----------|-----------|-----------|
| Li   | 0         | 0         | 0         | H    | 6.223917  | -3.416042 | 1.88558   |
| O    | 1.516065  | 0.607462  | -1.001054 | H    | 1.303899  | -5.237511 | -0.01609  |
| Li   | 2.976728  | 0.490142  | -2.220498 | H    | 0.823836  | -3.544351 | -0.243095 |
| N    | 3.975036  | -1.061971 | -3.062013 | H    | 2.254339  | -5.103986 | -2.432154 |
| C    | 5.345146  | -0.546408 | -3.068992 | C    | 0.159215  | -5.344445 | -2.422894 |
| H    | 5.46815   | 0.153646  | -3.923199 | C    | -1.061857 | -5.21216  | -1.743471 |
| C    | 6.446359  | -1.59785  | -3.290026 | C    | -2.171077 | -5.987198 | -2.085669 |
| C    | 6.924547  | -1.847456 | -4.584547 | C    | -2.090731 | -6.906238 | -3.135658 |
| C    | 7.896785  | -2.820346 | -4.827638 | C    | -0.887672 | -7.045079 | -3.829503 |
| C    | 8.43026   | -3.557857 | -3.770505 | C    | 0.222452  | -6.277417 | -3.468337 |
| C    | 7.981767  | -3.309963 | -2.471307 | H    | 1.162181  | -6.406077 | -4.001457 |
| C    | 7.000093  | -2.344843 | -2.239929 | H    | -0.808499 | -7.758813 | -4.64614  |
| H    | 6.675246  | -2.158535 | -1.219989 | H    | -2.953181 | -7.511565 | -3.403076 |
| H    | 8.402083  | -3.863836 | -1.634806 | H    | -3.098832 | -5.879756 | -1.527488 |
| H    | 9.192459  | -4.310878 | -3.954132 | H    | -1.149922 | -4.497339 | -0.928869 |
| H    | 8.241997  | -2.995951 | -5.84383  | C    | 1.745569  | -3.236962 | -4.127789 |
| H    | 6.530807  | -1.262432 | -5.412729 | C    | 2.159789  | -1.862809 | -4.688376 |
| Li   | 3.061494  | -2.381842 | -1.91112  | C    | 3.615114  | -1.429255 | -4.437966 |
| N    | 1.433861  | -3.173897 | -2.701123 | H    | 3.809688  | -0.57179  | -5.120185 |
| Li   | -0.113829 | -1.906865 | -2.635515 | H    | 4.255664  | -2.245369 | -4.829945 |
| O    | -0.376614 | -0.200681 | -1.899668 | H    | 2.028417  | -1.888587 | -5.779653 |
| C    | 0.636209  | 0.648838  | -2.004822 | H    | 1.477529  | -1.078896 | -4.325437 |
| C    | 0.82419   | 1.556438  | -3.046376 | H    | 2.574366  | -3.95179  | -4.33364  |
| H    | 1.636918  | 2.266639  | -2.893914 | H    | 0.899882  | -3.61916  | -4.740247 |
| C    | 0.035135  | 1.774225  | -4.24656  | N    | 4.795473  | 1.483712  | -1.674299 |
| C    | 0.39249   | 2.835572  | -5.115884 | C    | 4.782149  | 1.959488  | -0.275413 |
| C    | -0.316694 | 3.110219  | -6.279871 | H    | 4.389937  | 1.14987   | 0.349815  |
| C    | -1.425406 | 2.336683  | -6.637376 | H    | 5.815261  | 2.169276  | 0.065717  |
| C    | -1.796938 | 1.283716  | -5.798649 | C    | 3.917749  | 3.210605  | -0.107937 |
| C    | -1.090225 | 1.003657  | -4.629795 | H    | 3.944999  | 3.526704  | 0.943112  |
| H    | -1.396527 | 0.182872  | -3.994305 | H    | 2.88181   | 2.942256  | -0.346716 |
| H    | -2.656139 | 0.666603  | -6.05936  | C    | 4.392576  | 4.33998   | -1.029773 |
| H    | -1.981434 | 2.547956  | -7.547004 | C    | 4.471135  | 3.83056   | -2.473547 |

**Table 5 (Continued).**

|   |           |           |           |   |           |           |           |
|---|-----------|-----------|-----------|---|-----------|-----------|-----------|
| H | -0.001829 | 3.936221  | -6.914743 | C | 5.304861  | 2.549898  | -2.564443 |
| H | 1.251392  | 3.453654  | -4.858051 | H | 5.301999  | 2.175737  | -3.59144  |
| O | -1.8896   | -2.392533 | -3.392837 | H | 6.357429  | 2.77733   | -2.304233 |
| C | -2.099872 | -3.150917 | -4.610971 | H | 4.913446  | 4.58795   | -3.132762 |
| C | -3.617786 | -3.264151 | -4.767643 | H | 3.459746  | 3.630718  | -2.850392 |
| C | -4.114783 | -1.97745  | -4.089981 | H | 5.387518  | 4.682283  | -0.708484 |
| C | -3.134439 | -1.835235 | -2.924313 | H | 3.722735  | 5.206085  | -0.960438 |
| H | -3.471948 | -2.412387 | -2.050844 | C | 5.624047  | 0.260618  | -1.787629 |
| H | -2.943565 | -0.803588 | -2.620029 | H | 6.695478  | 0.517972  | -1.715827 |
| H | -5.155252 | -2.036441 | -3.755522 | H | 5.384164  | -0.366241 | -0.919676 |
| H | -4.023299 | -1.123205 | -4.770658 | O | -0.360466 | -1.298999 | 1.450677  |
| H | -3.987314 | -4.147346 | -4.234234 | C | -0.179532 | -0.854191 | 2.82138   |
| H | -3.921976 | -3.346034 | -5.815438 | C | -1.222296 | -1.609744 | 3.653347  |
| H | -1.644868 | -2.595458 | -5.440065 | C | -2.326963 | -1.890924 | 2.622087  |
| H | -1.597885 | -4.113589 | -4.501674 | C | -1.509326 | -2.173369 | 1.363613  |
| C | 1.393155  | -4.492124 | -2.084533 | H | -2.030478 | -1.949477 | 0.428644  |
| C | 1.54212   | -4.307674 | -0.56196  | H | -1.162384 | -3.214675 | 1.334726  |
| N | 2.890827  | -3.824874 | -0.175346 | H | -2.95305  | -1.00276  | 2.47804   |
| C | 3.828051  | -4.97022  | -0.108125 | H | -2.974433 | -2.728398 | 2.897936  |
| H | 3.856105  | -5.451865 | -1.08962  | H | -1.569565 | -1.024786 | 4.509757  |
| H | 3.436438  | -5.718129 | 0.609105  | H | -0.807112 | -2.550927 | 4.03152   |
| C | 5.237896  | -4.554688 | 0.31144   | H | 0.851596  | -1.069036 | 3.118086  |
| H | 5.674123  | -3.929476 | -0.474389 | H | -0.344145 | 0.228221  | 2.842803  |
| H | 5.862804  | -5.453717 | 0.384488  | O | -1.044151 | 1.616571  | 0.661544  |
| C | 5.223524  | -3.795786 | 1.643858  | C | -2.288339 | 1.841653  | -0.061076 |
| C | 4.206473  | -2.64889  | 1.585609  | C | -2.394803 | 3.355556  | -0.256887 |
| C | 2.83223   | -3.1556   | 1.141517  | C | -0.918364 | 3.776508  | -0.315609 |
| H | 2.120718  | -2.326807 | 1.067358  | C | -0.283978 | 2.853117  | 0.722817  |
| H | 2.439901  | -3.855908 | 1.906468  | H | -0.367932 | 3.262727  | 1.739064  |
| H | 4.111541  | -2.161489 | 2.564627  | H | 0.757468  | 2.604632  | 0.508728  |
| H | 4.551072  | -1.88112  | 0.879204  | H | -0.761567 | 4.834858  | -0.085501 |
| H | 4.942894  | -4.484784 | 2.454099  | H | -0.501803 | 3.56266   | -1.305305 |
| H | -2.216652 | 1.309888  | -1.015548 | H | -2.897123 | 3.823441  | 0.598728  |
| H | -3.106613 | 1.421584  | 0.534101  | H | -2.950181 | 3.613636  | -1.163085 |

**Table 5 (Continued).**



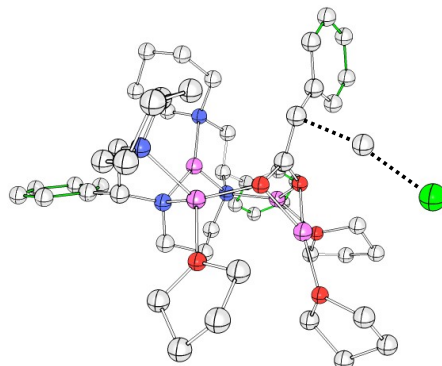
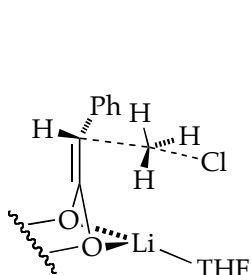
**8j**  
 $G = -2535.010975$   
 $G_{MP2} = -2527.63918$

| Atom | X         | Y         | Z         | Atom | X         | Y         | Z         |
|------|-----------|-----------|-----------|------|-----------|-----------|-----------|
| Li   | 0         | 0         | 0         | C    | 1.089688  | -3.124875 | -4.561188 |
| O    | 0.852032  | 0.269542  | -1.718964 | C    | 2.5951    | -2.828667 | -4.429584 |
| Li   | 2.336647  | -0.516195 | -2.547598 | H    | 2.842835  | -2.095594 | -5.228936 |
| N    | 3.0626    | -2.32638  | -3.127595 | H    | 3.128717  | -3.753155 | -4.727154 |
| C    | 4.484424  | -1.992711 | -3.238461 | H    | 0.903128  | -3.29035  | -5.632381 |
| H    | 4.647074  | -1.345559 | -4.128725 | H    | 0.513568  | -2.228448 | -4.289378 |
| C    | 5.43339   | -3.183324 | -3.463596 | H    | 1.255303  | -5.191828 | -3.942663 |
| C    | 5.824865  | -3.531312 | -4.764047 | H    | -0.384967 | -4.681564 | -4.301522 |
| C    | 6.658987  | -4.62502  | -5.006337 | N    | 4.300886  | 0.154383  | -1.926293 |
| C    | 7.136539  | -5.391237 | -3.942902 | C    | 4.331058  | 0.648819  | -0.534304 |
| C    | 6.771768  | -5.050387 | -2.638694 | H    | 3.799     | -0.078008 | 0.090878  |
| C    | 5.927973  | -3.962486 | -2.407579 | H    | 5.375454  | 0.691343  | -0.166781 |
| H    | 5.668301  | -3.707205 | -1.383969 | C    | 3.684282  | 2.02973   | -0.404124 |
| H    | 7.150714  | -5.628059 | -1.798534 | H    | 3.736587  | 2.351895  | 0.644775  |
| H    | 7.790825  | -6.239781 | -4.126041 | H    | 2.624835  | 1.945082  | -0.675621 |
| H    | 6.938722  | -4.874432 | -6.027155 | C    | 4.377693  | 3.047461  | -1.318036 |
| H    | 5.469715  | -2.930784 | -5.598666 | C    | 4.413154  | 2.514118  | -2.754895 |
| Li   | 2.117814  | -3.447053 | -1.803144 | C    | 5.010939  | 1.10632   | -2.811233 |
| N    | 0.346115  | -4.057329 | -2.375627 | H    | 4.971251  | 0.722348  | -3.834461 |
| Li   | -1.019654 | -2.586933 | -2.268584 | H    | 6.0793    | 1.148064  | -2.521913 |
| O    | -0.979136 | -0.963467 | -1.310729 | H    | 5.005452  | 3.174109  | -3.400937 |
| C    | -0.301251 | -0.212876 | -2.181962 | H    | 3.398068  | 2.489878  | -3.166556 |
| C    | -0.797601 | 0.02436   | -3.458568 | H    | 5.405429  | 3.215822  | -0.963767 |
| H    | -1.736    | -0.472    | -3.690871 | H    | 3.866216  | 4.017048  | -1.278087 |
| C    | -0.222787 | 0.815929  | -4.529367 | C    | 4.928062  | -1.186343 | -2.004762 |
| C    | -0.803738 | 0.747635  | -5.822054 | H    | 6.027067  | -1.093081 | -1.968673 |
| C    | -0.315808 | 1.486213  | -6.893584 | H    | 4.620332  | -1.737327 | -1.10789  |
| C    | 0.781163  | 2.33969   | -6.732778 | O    | 0.538679  | -0.616398 | 1.804727  |
| C    | 1.36492   | 2.437115  | -5.468089 | C    | 1.419728  | 0.207426  | 2.606091  |
| C    | 0.879205  | 1.697977  | -4.389212 | C    | 0.678801  | 0.446791  | 3.921168  |
| H    | 1.321363  | 1.814948  | -3.406408 | C    | -0.118326 | -0.857761 | 4.077752  |
| H    | 2.207239  | 3.109902  | -5.313463 | C    | -0.518308 | -1.166179 | 2.63309   |
| H    | 1.165004  | 2.916614  | -7.569926 | H    | -1.46141  | -0.677105 | 2.360695  |

**Table 5 (Continued).**

|   |           |           |           |   |           |           |           |
|---|-----------|-----------|-----------|---|-----------|-----------|-----------|
| H | -0.794613 | 1.395008  | -7.866784 | H | -0.597392 | -2.234703 | 2.415434  |
| H | -1.658988 | 0.090616  | -5.972327 | H | -0.986359 | -0.757718 | 4.73569   |
| O | -2.818554 | -2.770359 | -3.107262 | H | 0.521692  | -1.652779 | 4.477758  |
| C | -3.161457 | -3.572208 | -4.262777 | H | -0.000505 | 1.301142  | 3.824171  |
| C | -4.587684 | -3.161744 | -4.63833  | H | 1.360134  | 0.641464  | 4.754617  |
| C | -5.178897 | -2.780311 | -3.272562 | H | 2.359012  | -0.338562 | 2.762523  |
| C | -3.988732 | -2.102266 | -2.591433 | H | 1.630867  | 1.122793  | 2.046361  |
| H | -3.987869 | -2.204587 | -1.502606 | O | -1.031449 | 1.713069  | 0.437432  |
| H | -3.924899 | -1.035867 | -2.841136 | C | -2.452144 | 1.568312  | 0.171691  |
| H | -5.467289 | -3.682955 | -2.721954 | C | -2.736241 | 2.469524  | -1.02762  |
| H | -6.051381 | -2.123407 | -3.343139 | C | -1.758224 | 3.6305    | -0.791314 |
| H | -5.133816 | -3.967624 | -5.137674 | C | -0.530712 | 2.91062   | -0.226172 |
| H | -4.575922 | -2.292122 | -5.306023 | H | 0.017388  | 3.504947  | 0.512757  |
| H | -2.426604 | -3.368223 | -5.046494 | H | 0.152544  | 2.584014  | -1.015834 |
| H | -3.100029 | -4.628619 | -3.981854 | H | -2.16649  | 4.337252  | -0.058372 |
| C | 0.123132  | -5.261688 | -1.589305 | H | -1.522691 | 4.183447  | -1.705043 |
| C | 0.465659  | -4.941199 | -0.120599 | H | -3.782264 | 2.788653  | -1.07347  |
| N | 1.913032  | -4.68313  | 0.089247  | H | -2.483253 | 1.941601  | -1.953333 |
| C | 2.638275  | -5.971624 | 0.186727  | H | -2.639676 | 0.511304  | -0.031229 |
| H | 2.484449  | -6.525032 | -0.74353  | H | -3.009338 | 1.886139  | 1.064325  |
| H | 2.194629  | -6.577621 | 1.000933  | H | 0.804833  | -6.073646 | -1.923053 |
| C | 4.134506  | -5.793296 | 0.446433  | C | -1.284586 | -5.870054 | -1.702413 |
| H | 4.596019  | -5.323241 | -0.428353 | C | -2.381193 | -5.368692 | -0.983198 |
| H | 4.59317   | -6.784427 | 0.552407  | C | -3.653742 | -5.925093 | -1.120708 |
| C | 4.387042  | -4.94316  | 1.697692  | C | -3.864942 | -6.991706 | -1.999166 |
| C | 3.589761  | -3.636476 | 1.612472  | C | -2.788434 | -7.497354 | -2.729472 |
| C | 2.109494  | -3.909003 | 1.332918  | C | -1.514774 | -6.944172 | -2.573978 |
| H | 1.564136  | -2.963985 | 1.237057  | H | -0.677059 | -7.355578 | -3.133494 |
| H | 1.67413   | -4.455408 | 2.193921  | H | -2.936646 | -8.329228 | -3.414125 |
| H | 3.679534  | -3.063444 | 2.544748  | H | -4.855281 | -7.427262 | -2.106026 |
| H | 3.996295  | -3.005764 | 0.809719  | H | -4.481558 | -5.531612 | -0.534449 |
| H | 4.069337  | -5.5023   | 2.590059  | H | -2.242502 | -4.535162 | -0.29798  |
| H | 5.457874  | -4.73808  | 1.818955  | C | 0.544924  | -4.345649 | -3.793825 |
| H | 0.124587  | -5.742225 | 0.558636  | H | -0.067164 | -4.024174 | 0.156478  |

**Table 6.** Optimized geometries of transition state structures at B3LYP level of theory with 6-31G(d) basis set for the alkylation of phenylacetic acid with 3-chloropropene at -78 °C with free energies (Hartrees) and cartesian coordinates (X, Y, Z) (Note:  $G_{MP2}$  includes single point MP2 corrections to B3LYP/6-31G(d) optimized structures).



**17a**

$G = -3035.060045$

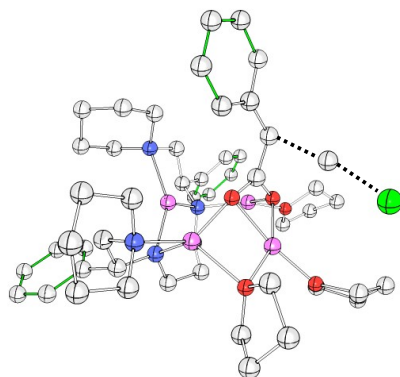
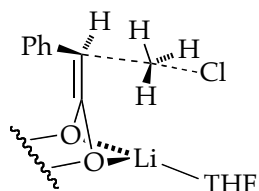
$G_{MP2} = -3026.969463$

| Atom | X        | Y         | Z         | Atom | X         | Y         | Z         |
|------|----------|-----------|-----------|------|-----------|-----------|-----------|
| Li   | 0        | 0         | 0         | H    | -2.976609 | -1.191149 | 0.17048   |
| O    | 1.628006 | -0.445503 | 0.96275   | H    | -5.459306 | -2.240339 | -0.430883 |
| Li   | 3.222884 | -0.799599 | -0.043209 | H    | -4.577142 | -1.327654 | -1.667682 |
| N    | 3.619144 | -2.585355 | -1.026703 | H    | -4.58357  | -4.375367 | -1.28229  |
| C    | 5.067723 | -2.49801  | -1.026103 | H    | -4.886998 | -3.497222 | -2.791361 |
| C    | 5.552377 | -2.324496 | 0.431847  | H    | -2.550783 | -2.89439  | -3.013771 |
| N    | 5.20443  | -1.004518 | 1.010535  | H    | -2.351578 | -4.445792 | -2.157707 |
| C    | 5.052272 | -1.10096  | 2.478195  | C    | 0.751942  | -5.803972 | -0.492291 |
| H    | 4.254983 | -1.821822 | 2.686959  | C    | 1.041091  | -5.984387 | 1.010067  |
| H    | 5.98151  | -1.495992 | 2.933967  | N    | 2.431726  | -5.639308 | 1.401131  |
| C    | 4.707225 | 0.250018  | 3.109729  | C    | 3.349425  | -6.747853 | 1.045337  |
| H    | 4.621607 | 0.123994  | 4.196332  | H    | 3.319611  | -6.889669 | -0.039187 |
| H    | 3.723428 | 0.569108  | 2.743116  | H    | 2.982557  | -7.686969 | 1.503328  |
| C    | 5.76227  | 1.308942  | 2.767904  | C    | 4.787857  | -6.492524 | 1.500948  |
| C    | 5.966902 | 1.366716  | 1.249378  | H    | 5.195252  | -5.632986 | 0.955195  |
| C    | 6.260028 | -0.023598 | 0.682587  | H    | 5.402717  | -7.358168 | 1.224834  |
| H    | 6.360702 | 0.020298  | -0.406535 | C    | 4.853015  | -6.234138 | 3.01031   |
| H    | 7.232093 | -0.379049 | 1.078621  | C    | 3.871919  | -5.118184 | 3.386299  |
| H    | 6.795827 | 2.038687  | 0.992281  | C    | 2.465079  | -5.418261 | 2.868673  |
| H    | 5.065091 | 1.763742  | 0.769345  | H    | 1.788884  | -4.591532 | 3.105152  |
| H    | 6.714311 | 1.047733  | 3.252793  | H    | 2.073882  | -6.314412 | 3.387096  |
| H    | 5.467629 | 2.290725  | 3.158173  | H    | 3.824324  | -4.983088 | 4.473776  |
| H    | 6.637582 | -2.499369 | 0.515448  | H    | 4.219209  | -4.166044 | 2.963821  |
| H    | 5.058126 | -3.098454 | 1.029742  | H    | 4.583176  | -7.152883 | 3.551309  |
| H    | 5.417291 | -1.601791 | -1.591818 | H    | 5.874339  | -5.975345 | 3.315524  |
| C    | 5.850061 | -3.669291 | -1.664504 | H    | 0.804558  | -7.012743 | 1.334821  |
| C    | 7.176543 | -3.479473 | -2.078506 | H    | 0.384483  | -5.309691 | 1.570656  |
| C    | 7.922939 | -4.522129 | -2.627094 | H    | 1.494485  | -6.405634 | -1.059259 |

**Table 6 (Continued).**

|    |           |           |           |   |           |           |           |
|----|-----------|-----------|-----------|---|-----------|-----------|-----------|
| C  | 7.347853  | -5.785525 | -2.785396 | C | -0.610147 | -6.416332 | -0.86169  |
| C  | 6.024587  | -5.986999 | -2.392679 | C | -0.775949 | -7.041172 | -2.10678  |
| C  | 5.286644  | -4.937338 | -1.838723 | C | -2.010775 | -7.559753 | -2.504537 |
| H  | 4.249464  | -5.090788 | -1.554129 | C | -3.111986 | -7.479766 | -1.650844 |
| H  | 5.560128  | -6.961462 | -2.526354 | C | -2.964177 | -6.871066 | -0.401452 |
| H  | 7.922819  | -6.599853 | -3.218876 | C | -1.731188 | -6.338618 | -0.017885 |
| H  | 8.950894  | -4.348357 | -2.936726 | H | -1.643484 | -5.876519 | 0.96264   |
| H  | 7.630639  | -2.494994 | -1.97084  | H | -3.807983 | -6.822671 | 0.283429  |
| Li | 2.579265  | -3.880159 | 0.028908  | H | -4.070674 | -7.896424 | -1.948939 |
| N  | 0.88864   | -4.391292 | -0.822718 | H | -2.108037 | -8.037641 | -3.476532 |
| Li | -0.443909 | -3.105683 | -0.177147 | H | 0.082433  | -7.128723 | -2.769579 |
| O  | -0.234564 | -1.651586 | 0.953517  | C | 1.068304  | -4.157171 | -2.251594 |
| C  | 0.809175  | -1.220781 | 1.624303  | C | 1.596101  | -2.736598 | -2.549284 |
| C  | 0.912051  | -1.343902 | 3.036588  | H | 1.338581  | -2.484555 | -3.589    |
| H  | 1.843891  | -0.960956 | 3.444399  | H | 1.060788  | -2.01038  | -1.914642 |
| C  | 0.212013  | -2.305537 | 3.892499  | C | 3.113674  | -2.525736 | -2.397582 |
| C  | 0.74524   | -2.580523 | 5.173064  | H | 3.356434  | -1.547519 | -2.874021 |
| C  | 0.126261  | -3.463872 | 6.053244  | H | 3.601124  | -3.270628 | -3.056526 |
| C  | -1.057477 | -4.111594 | 5.690597  | H | 1.784741  | -4.882336 | -2.69702  |
| C  | -1.609036 | -3.847719 | 4.435355  | H | 0.134296  | -4.304003 | -2.8374   |
| C  | -0.993462 | -2.96181  | 3.550837  | O | 3.261834  | 0.99489   | -1.111901 |
| H  | -1.445308 | -2.754978 | 2.58857   | C | 2.609008  | 2.181313  | -0.590338 |
| H  | -2.53883  | -4.330904 | 4.141428  | C | 3.249334  | 3.363209  | -1.320812 |
| H  | -1.54293  | -4.801812 | 6.375164  | C | 3.610327  | 2.74292   | -2.678734 |
| H  | 0.571293  | -3.647641 | 7.028582  | C | 4.053224  | 1.336354  | -2.271743 |
| H  | 1.666163  | -2.084553 | 5.474099  | H | 5.115593  | 1.318359  | -1.994604 |
| C  | -0.331256 | 0.58216   | 3.076031  | H | 3.880297  | 0.576838  | -3.038137 |
| H  | 0.484519  | 1.02649   | 2.534694  | H | 4.392927  | 3.288706  | -3.214178 |
| H  | -1.091226 | -0.005134 | 2.593162  | H | 2.726001  | 2.693978  | -3.32552  |
| H  | -0.362567 | 0.679299  | 4.151422  | H | 4.156256  | 3.692622  | -0.800385 |
| O  | -2.232401 | -2.748795 | -0.97     | H | 2.572852  | 4.219661  | -1.396904 |
| C  | -2.805111 | -3.45508  | -2.105263 | H | 1.537515  | 2.107569  | -0.803946 |
| C  | -4.314942 | -3.483778 | -1.858853 | H | 2.745419  | 2.200716  | 0.493333  |
| C  | -4.539765 | -2.21437  | -1.022796 | O | -0.700609 | 1.052665  | -1.406453 |
| C  | -3.288209 | -2.188526 | -0.147428 | C | -1.16923  | 0.432901  | -2.638867 |
| H  | -3.412296 | -2.813172 | 0.746248  | C | -2.195097 | 1.404431  | -3.235565 |
| H  | -2.997379 | 0.880364  | -3.763146 | C | -2.682313 | 2.185189  | -2.00409  |
| H  | -1.712076 | 2.082898  | -3.948051 | C | -1.405166 | 2.314005  | -1.183737 |
| H  | -0.305741 | 0.257318  | -3.28739  | H | -1.555621 | 2.428349  | -0.105747 |
| H  | -1.613279 | -0.532946 | -2.374491 | H | -0.771014 | 3.130396  | -1.553972 |
| Cl | -1.590577 | 2.470727  | 2.598483  | H | -3.43219  | 1.610867  | -1.447344 |
| H  | -3.115702 | 3.157667  | -2.254268 |   |           |           |           |

Table 6 (Continued).



**17b**

$G = -3035.060551$

$G_{\text{MP2}} = -3026.976046$

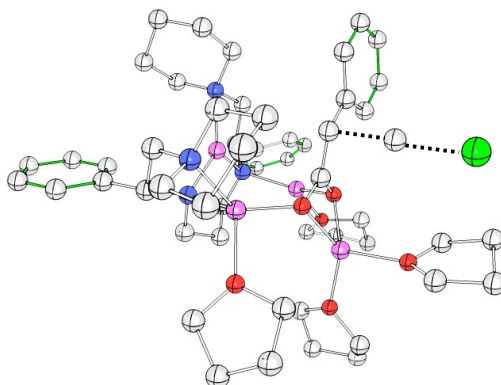
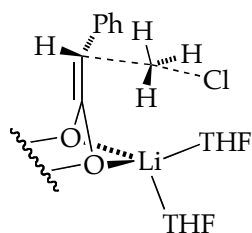
| Atom | X        | Y         | Z         | Atom | X         | Y         | Z         |
|------|----------|-----------|-----------|------|-----------|-----------|-----------|
| Li   | 0        | 0         | 0         | H    | 0.136408  | -6.353928 | 0.472926  |
| O    | 1.243113 | -0.803076 | 1.527439  | C    | -1.9018   | -6.11616  | 0.9782    |
| Li   | 2.472514 | -1.149587 | 0.151092  | C    | -2.306966 | -7.003756 | -0.02995  |
| N    | 2.523352 | -2.952854 | -0.793688 | C    | -3.613745 | -7.494271 | -0.088768 |
| C    | 3.934347 | -3.075325 | -1.109199 | C    | -4.54714  | -7.117856 | 0.878485  |
| H    | 4.198581 | -2.429861 | -1.979909 | C    | -4.160763 | -6.240039 | 1.895032  |
| C    | 4.44506  | -4.476147 | -1.523118 | C    | -2.858025 | -5.738752 | 1.935499  |
| C    | 5.646765 | -4.600824 | -2.235388 | H    | -2.583019 | -5.058887 | 2.738152  |
| C    | 6.150439 | -5.850318 | -2.596622 | H    | -4.872266 | -5.954945 | 2.667031  |
| C    | 5.448177 | -7.010257 | -2.260812 | H    | -5.56     | -7.511344 | 0.848081  |
| C    | 4.242503 | -6.902049 | -1.567131 | H    | -3.898023 | -8.18108  | -0.882509 |
| C    | 3.749414 | -5.646145 | -1.203506 | H    | -1.579349 | -7.319981 | -0.774492 |
| H    | 2.801011 | -5.559315 | -0.681288 | C    | -0.365992 | -4.410854 | -1.157041 |
| H    | 3.678067 | -7.797132 | -1.315455 | C    | 0.222607  | -3.173438 | -1.869639 |
| H    | 5.832241 | -7.986163 | -2.546617 | H    | -0.201201 | -3.123523 | -2.883673 |
| H    | 7.085967 | -5.919368 | -3.146821 | H    | -0.121449 | -2.262496 | -1.349842 |
| H    | 6.192811 | -3.701576 | -2.51909  | C    | 1.753041  | -3.140941 | -2.023368 |
| C    | 4.795482 | -2.591628 | 0.081123  | H    | 1.992727  | -2.344851 | -2.767993 |
| N    | 4.606622 | -1.148976 | 0.382624  | H    | 2.028017  | -4.078648 | -2.54424  |
| C    | 5.009868 | -0.799328 | 1.766147  | H    | 0.190741  | -5.302016 | -1.521578 |
| H    | 4.639911 | 0.216628  | 1.964361  | H    | -1.401124 | -4.564613 | -1.536266 |
| H    | 4.482571 | -1.466341 | 2.454067  | O    | 1.75888   | 0.688882  | -0.862273 |
| C    | 6.526529 | -0.837443 | 2.014698  | C    | 2.132678  | 1.964534  | -0.235373 |
| C    | 7.258647 | 0.078311  | 1.022453  | C    | 2.300312  | 2.956623  | -1.386366 |
| C    | 6.85078  | -0.256806 | -0.42032  | C    | 2.705633  | 2.053972  | -2.562381 |
| C    | 5.318932 | -0.265222 | -0.57127  | C    | 1.866478  | 0.803592  | -2.311231 |
| H    | 5.034148 | -0.54942  | -1.588973 | H    | 2.312679  | -0.121961 | -2.682056 |
| H    | 4.946394 | 0.754478  | -0.404178 | H    | 0.85403   | 0.904133  | -2.717838 |
| H    | 7.272749 | 0.473113  | -1.123297 | H    | 3.77421   | 1.815229  | -2.516726 |
| H    | 7.262846 | -1.233536 | -0.705041 | H    | 2.499046  | 2.499777  | -3.539952 |
| H    | 8.345549 | -0.002854 | 1.145183  | H    | 3.041599  | 3.72679   | -1.155591 |
| H    | 6.995946 | 1.124791  | 1.238775  | H    | 1.349749  | 3.459109  | -1.595737 |
| H    | 6.894102 | -1.867515 | 1.914689  | H    | 1.355157  | 2.257947  | 0.475195  |
| H    | 6.729625 | -0.530434 | 3.048415  | H    | 3.066443  | 1.800674  | 0.311513  |



**Table 6 (Continued).**

|    |           |           |           |    |           |           |           |
|----|-----------|-----------|-----------|----|-----------|-----------|-----------|
| H  | 5.851015  | -2.839268 | -0.094011 | O  | -1.289419 | 0.903747  | -1.200587 |
| H  | 4.482794  | -3.150879 | 0.970933  | C  | -1.677429 | 2.303291  | -1.102909 |
| Li | 1.539786  | -3.755406 | 0.743105  | C  | -3.201324 | 2.287062  | -1.12361  |
| N  | -0.297955 | -4.290255 | 0.294604  | C  | -3.49449  | 1.130794  | -2.09252  |
| Li | -1.478457 | -2.772318 | 0.742264  | C  | -2.380402 | 0.127032  | -1.766958 |
| O  | -0.95206  | -1.076282 | 1.291798  | H  | -2.007329 | -0.401273 | -2.650984 |
| C  | 0.085822  | -0.950726 | 2.096875  | H  | -2.689078 | -0.609252 | -1.018579 |
| C  | -0.144415 | -0.785154 | 3.490417  | H  | -3.41471  | 1.474632  | -3.130424 |
| H  | -1.165372 | -1.006323 | 3.793172  | H  | -4.490264 | 0.696321  | -1.9604   |
| C  | 0.842568  | -0.82391  | 4.568647  | H  | -3.623603 | 3.242211  | -1.448646 |
| C  | 0.402043  | -1.086951 | 5.886677  | H  | -3.586427 | 2.067058  | -0.121516 |
| C  | 1.281048  | -1.101192 | 6.96565   | H  | -1.252854 | 2.717402  | -0.184045 |
| C  | 2.642722  | -0.850042 | 6.774107  | H  | -1.272741 | 2.83982   | -1.973008 |
| C  | 3.09884   | -0.57952  | 5.481867  | Cl | -0.54216  | 3.601897  | 2.22691   |
| C  | 2.221426  | -0.564184 | 4.398059  | C  | -0.403559 | 1.472776  | 3.024666  |
| H  | 2.588248  | -0.348184 | 3.402972  | H  | -0.632706 | 1.717067  | 4.050656  |
| H  | 4.153661  | -0.369109 | 5.314504  | H  | 0.628486  | 1.413765  | 2.729908  |
| H  | 3.330892  | -0.857844 | 7.615164  | H  | -1.196052 | 1.157234  | 2.369413  |
| H  | 0.900837  | -1.310431 | 7.963175  | N  | 1.518102  | -5.131363 | 2.491788  |
| H  | -0.655117 | -1.283528 | 6.056098  | C  | 2.291052  | -6.384295 | 2.320362  |
| O  | -3.407385 | -2.599522 | 0.37065   | H  | 2.058614  | -6.805254 | 1.337515  |
| C  | -4.2355   | -1.861621 | 1.301712  | H  | 1.958628  | -7.124134 | 3.074299  |
| C  | -5.620104 | -1.822425 | 0.658558  | C  | 3.800295  | -6.171075 | 2.45646   |
| C  | -5.675428 | -3.184762 | -0.051493 | C  | 4.149016  | -5.526144 | 3.802418  |
| C  | -4.236192 | -3.363539 | -0.544258 | C  | 3.315766  | -4.254872 | 3.997381  |
| H  | -4.094186 | -2.948166 | -1.55024  | C  | 1.824369  | -4.536641 | 3.816817  |
| H  | -3.898171 | -4.401341 | -0.535129 | H  | 1.253839  | -3.608707 | 3.916024  |
| H  | -6.401502 | -3.218992 | -0.869186 | H  | 1.483713  | -5.219539 | 4.618753  |
| H  | -5.927659 | -3.977131 | 0.661318  | H  | 3.624776  | -3.494277 | 3.268075  |
| H  | -5.682454 | -1.003836 | -0.069089 | H  | 3.474043  | -3.817306 | 4.989488  |
| H  | -6.418205 | -1.683582 | 1.393872  | H  | 5.221704  | -5.302961 | 3.858592  |
| H  | -4.257506 | -2.398428 | 2.259662  | H  | 3.930235  | -6.233654 | 4.615628  |
| H  | -3.768509 | -0.887035 | 1.456706  | H  | 4.153246  | -5.5369   | 1.634182  |
| C  | -0.46475  | -5.566691 | 0.97721   | H  | 4.303255  | -7.139512 | 2.342314  |
| C  | 0.064176  | -5.418661 | 2.416842  | H  | -0.175977 | -6.312267 | 3.019069  |
| H  | -0.446912 | -4.568238 | 2.882257  |    |           |           |           |

**Table 6 (Continued).**



**17c**

$G = -3267.413799$

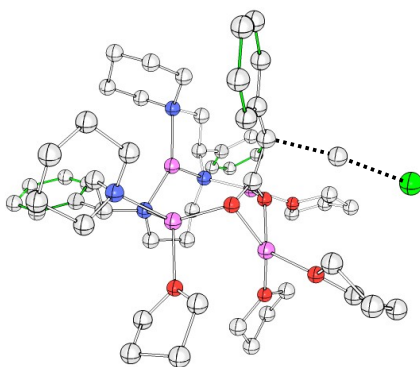
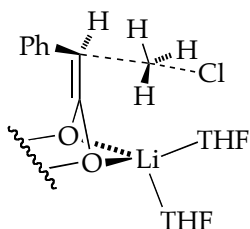
$G_{MP2} = -3258.675739$

| Atom | X         | Y         | Z         | Atom | X         | Y         | Z         |
|------|-----------|-----------|-----------|------|-----------|-----------|-----------|
| Li   | 0         | 0         | 0         | H    | -5.586152 | 4.561791  | 2.330764  |
| O    | -1.653478 | -0.685871 | 0.91617   | H    | -4.170463 | 3.503874  | 2.44487   |
| Li   | -3.253135 | -1.461424 | 0.18477   | H    | -5.743536 | 3.928256  | -0.138348 |
| N    | -4.87256  | -0.364694 | -0.523408 | C    | -4.148091 | 5.266823  | 0.214701  |
| C    | -5.84409  | -1.44166  | -0.535344 | C    | -4.558553 | 6.083025  | -0.849061 |
| C    | -5.970927 | -2.010734 | 0.896662  | C    | -3.976212 | 7.333414  | -1.075861 |
| N    | -4.759327 | -2.737753 | 1.344994  | C    | -2.972933 | 7.802303  | -0.226464 |
| C    | -4.637252 | -2.689237 | 2.817612  | C    | -2.554268 | 7.004201  | 0.84271   |
| H    | -4.592721 | -1.636468 | 3.116916  | C    | -3.128532 | 5.749183  | 1.05348   |
| H    | -5.540442 | -3.122718 | 3.290614  | H    | -2.787641 | 5.149425  | 1.894762  |
| C    | -3.393394 | -3.431194 | 3.312842  | H    | -1.787414 | 7.366576  | 1.523959  |
| H    | -3.350576 | -3.373972 | 4.407229  | H    | -2.529383 | 8.78168   | -0.387552 |
| H    | -2.50043  | -2.922689 | 2.929748  | H    | -4.315801 | 7.945022  | -1.908587 |
| C    | -3.394215 | -4.89152  | 2.844854  | H    | -5.354292 | 5.732972  | -1.503747 |
| C    | -3.595171 | -4.949642 | 1.326146  | C    | -4.092463 | 2.605937  | -1.523404 |
| C    | -4.829215 | -4.147932 | 0.907297  | C    | -3.581929 | 1.231007  | -2.003472 |
| H    | -4.947636 | -4.164353 | -0.180142 | H    | -3.309684 | 1.318594  | -3.066341 |
| H    | -5.734031 | -4.624548 | 1.334188  | H    | -2.656653 | 0.980511  | -1.461916 |
| H    | -3.71152  | -5.987409 | 0.987326  | C    | -4.563673 | 0.051712  | -1.889447 |
| H    | -2.714664 | -4.537463 | 0.818755  | H    | -4.126703 | -0.789664 | -2.476969 |
| H    | -4.211884 | -5.435495 | 3.340151  | H    | -5.469302 | 0.333508  | -2.461735 |
| H    | -2.460893 | -5.388356 | 3.134547  | H    | -5.14529  | 2.715303  | -1.865443 |
| H    | -6.85816  | -2.658368 | 0.991741  | H    | -3.543373 | 3.39109   | -2.090646 |
| H    | -6.12343  | -1.159265 | 1.569389  | O    | -2.316566 | -2.783436 | -1.18122  |
| H    | -5.502365 | -2.281721 | -1.185848 | C    | -0.917135 | -3.099664 | -0.998251 |
| C    | -7.259083 | -1.118985 | -1.067866 | C    | -0.681179 | -4.385187 | -1.790266 |
| C    | -8.103573 | -2.159471 | -1.482574 | C    | -1.642916 | -4.199274 | -2.973229 |
| C    | -9.394332 | -1.906911 | -1.946359 | C    | -2.845098 | -3.525029 | -2.304635 |
| C    | -9.866236 | -0.59387  | -2.018717 | H    | -3.558617 | -4.267932 | -1.927478 |
| C    | -9.033357 | 0.453428  | -1.624436 | H    | -3.379319 | -2.830358 | -2.958097 |
| C    | -7.744006 | 0.189823  | -1.153941 | H    | -1.91385  | -5.136495 | -3.468282 |
| H    | -7.089143 | 1.006003  | -0.862684 | H    | -1.19854  | -3.535554 | -3.724753 |
| H    | -9.384075 | 1.480981  | -1.690339 | H    | -0.966538 | -5.261148 | -1.196019 |

**Table 6 (Continued).**

|    |            |           |           |    |           |           |           |
|----|------------|-----------|-----------|----|-----------|-----------|-----------|
| H  | -10.868766 | -0.390422 | -2.386514 | H  | 0.36374   | -4.505713 | -2.092924 |
| H  | -10.03013  | -2.73283  | -2.256938 | H  | -0.316043 | -2.272723 | -1.397224 |
| H  | -7.740609  | -3.186037 | -1.442883 | H  | -0.727968 | -3.187224 | 0.07381   |
| Li | -4.865096  | 1.185066  | 0.692279  | O  | 0.591348  | 0.119701  | -1.92552  |
| N  | -3.981469  | 2.762929  | -0.074944 | C  | -0.062837 | 0.942277  | -2.932048 |
| Li | -2.019792  | 2.700617  | 0.276412  | C  | 0.945086  | 1.098137  | -4.081852 |
| O  | -0.883016  | 1.392917  | 1.062711  | C  | 2.292165  | 0.800824  | -3.403681 |
| C  | -1.525649  | 0.400348  | 1.628814  | C  | 1.896591  | -0.27643  | -2.398769 |
| C  | -1.948371  | 0.425064  | 2.992642  | H  | 2.545883  | -0.353203 | -1.526226 |
| C  | -1.926587  | 1.570938  | 3.902839  | H  | 1.824916  | -1.261834 | -2.882549 |
| C  | -2.615072  | 1.466598  | 5.13585   | H  | 2.668556  | 1.6873    | -2.879034 |
| C  | -2.596014  | 2.487119  | 6.082379  | H  | 3.063185  | 0.464079  | -4.103069 |
| C  | -1.883905  | 3.664983  | 5.841296  | H  | 0.900017  | 2.091554  | -4.537512 |
| C  | -1.184019  | 3.787085  | 4.639479  | H  | 0.749134  | 0.361442  | -4.869179 |
| C  | -1.197136  | 2.765241  | 3.688656  | H  | -0.989331 | 0.450948  | -3.238964 |
| H  | -0.625793  | 2.867829  | 2.774258  | H  | -0.311426 | 1.89493   | -2.456129 |
| H  | -0.606517  | 4.688111  | 4.440313  | H  | -2.667944 | -0.349368 | 3.242785  |
| H  | -1.866937  | 4.46343   | 6.577968  | C  | -0.290267 | -0.890926 | 3.793806  |
| H  | -3.139088  | 2.360105  | 7.016262  | H  | -0.50064  | -1.552769 | 2.973167  |
| H  | -3.16808   | 0.553208  | 5.34992   | H  | 0.41365   | -0.084678 | 3.67943   |
| O  | -0.67846   | 3.827981  | -0.687917 | H  | -0.83966  | -0.966004 | 4.716684  |
| C  | -0.912692  | 4.800152  | -1.741096 | O  | 1.771962  | -0.492261 | 0.783164  |
| C  | 0.253132   | 5.789801  | -1.665138 | C  | 2.295436  | -1.814765 | 1.099312  |
| C  | 1.379037   | 4.932716  | -1.066147 | C  | 2.552222  | 0.523151  | 1.466893  |
| C  | 0.611672   | 4.059047  | -0.074947 | C  | 3.682106  | -1.57401  | 1.691436  |
| H  | 0.463968   | 4.577667  | 0.881525  | H  | 1.640756  | -2.289214 | 1.835776  |
| H  | 1.064642   | 3.086031  | 0.124254  | H  | 2.304528  | -2.395433 | 0.17031   |
| H  | 2.163876   | 5.522299  | -0.582825 | C  | 3.488675  | -0.230848 | 2.412987  |
| H  | 1.847578   | 4.31305   | -1.841238 | H  | 3.110103  | 1.092459  | 0.709023  |
| H  | 0.001059   | 6.615387  | -0.991329 | H  | 1.856808  | 1.198149  | 1.973317  |
| H  | 0.502412   | 6.212986  | -2.642869 | H  | 4.440478  | -1.495094 | 0.901692  |
| H  | -0.927005  | 4.261646  | -2.697595 | H  | 3.96676   | -2.374934 | 2.378265  |
| H  | -1.887815  | 5.259595  | -1.577379 | H  | 4.425814  | 0.309023  | 2.580671  |
| C  | -4.782507  | 3.880218  | 0.414257  | H  | 3.004034  | -0.411754 | 3.37689   |
| C  | -5.109766  | 3.661284  | 1.904124  | Cl | 1.326092  | -2.328473 | 4.577182  |
| N  | -5.95795   | 2.470547  | 2.169208  | C  | -5.89041  | 2.171365  | 3.620296  |
| C  | -7.364623  | 2.740607  | 1.789214  | H  | -4.846226 | 1.979581  | 3.878666  |
| H  | -7.404454  | 2.939406  | 0.714147  | H  | -6.205414 | 3.063082  | 4.196209  |
| H  | -7.711626  | 3.659942  | 2.30023   | H  | -6.676043 | 0.831569  | 5.105982  |
| C  | -8.304466  | 1.582951  | 2.138605  | H  | -6.401366 | 0.074813  | 3.537663  |
| H  | -8.041885  | 0.706412  | 1.535386  | H  | -8.635512 | 2.059357  | 4.224771  |
| H  | -9.326095  | 1.863296  | 1.853044  | H  | -8.847177 | 0.349394  | 3.847511  |
| C  | -8.230279  | 1.229328  | 3.627581  | C  | -6.770017 | 0.988075  | 4.023982  |

**Table 6 (Continued).**



**17d**

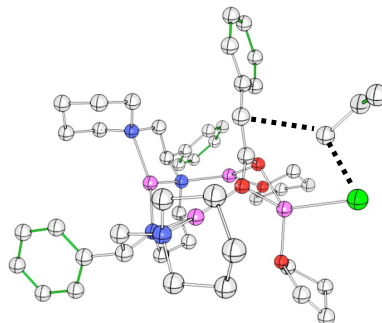
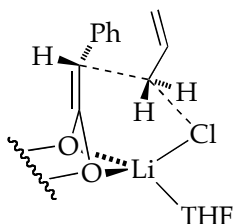
$G = -3267.405532$

$G_{\text{MP2}} = -3258.666802$

| Atom | X         | Y         | Z         | Atom | X         | Y         | Z         |
|------|-----------|-----------|-----------|------|-----------|-----------|-----------|
| Li   | 0         | 0         | 0         | C    | -0.565006 | 8.674472  | -0.148544 |
| O    | -1.610023 | -0.176882 | 1.216373  | C    | 0.432638  | 8.810591  | 0.818015  |
| Li   | -3.158941 | 0.098177  | 0.033102  | C    | 0.48032   | 7.905316  | 1.881246  |
| N    | -4.04835  | 1.887319  | -0.599535 | C    | -0.452425 | 6.869247  | 1.967271  |
| C    | -5.397805 | 1.405681  | -0.827697 | H    | -0.390817 | 6.17919   | 2.805113  |
| H    | -5.423323 | 0.666827  | -1.664978 | H    | 1.239343  | 8.011976  | 2.653159  |
| C    | -6.466818 | 2.449463  | -1.230337 | H    | 1.158063  | 9.617267  | 0.750601  |
| C    | -7.652455 | 2.028609  | -1.850797 | H    | -0.619615 | 9.375451  | -0.978163 |
| C    | -8.655063 | 2.934733  | -2.195374 | H    | -2.29698  | 7.567008  | -0.787621 |
| C    | -8.484869 | 4.29687   | -1.936005 | C    | -2.134848 | 4.470848  | -1.067704 |
| C    | -7.304605 | 4.734294  | -1.334477 | C    | -2.130904 | 3.092729  | -1.765273 |
| C    | -6.308772 | 3.817397  | -0.986995 | H    | -1.775936 | 3.237254  | -2.797648 |
| H    | -5.38169  | 4.163638  | -0.539315 | H    | -1.398693 | 2.433941  | -1.274876 |
| H    | -7.152272 | 5.794212  | -1.143349 | H    | -3.037791 | 5.021415  | -1.413802 |
| H    | -9.259551 | 5.008783  | -2.209208 | H    | -1.284988 | 5.062649  | -1.475646 |
| H    | -9.565889 | 2.579991  | -2.672196 | C    | -3.488127 | 2.371364  | -1.863398 |
| H    | -7.789643 | 0.970287  | -2.071177 | H    | -3.360998 | 1.535303  | -2.590991 |
| Li   | -3.527878 | 3.098067  | 0.866555  | H    | -4.175278 | 3.069756  | -2.379361 |
| N    | -2.102289 | 4.356122  | 0.386865  | N    | -5.156256 | -0.597459 | 0.677343  |
| Li   | -0.421685 | 3.394018  | 0.782461  | C    | -5.065105 | -0.952577 | 2.112118  |
| O    | -0.26118  | 1.585345  | 1.135899  | H    | -4.327787 | -1.759789 | 2.197223  |
| C    | -1.037152 | 0.805756  | 1.852388  | H    | -4.645347 | -0.101784 | 2.654278  |
| C    | -1.067951 | 0.997483  | 3.269297  | C    | -6.387252 | -1.41675  | 2.740448  |
| C    | -1.831063 | 0.237359  | 4.257975  | C    | -6.954291 | -2.613557 | 1.963059  |
| C    | -2.098203 | 0.816559  | 5.520615  | C    | -7.053061 | -2.280287 | 0.466828  |
| C    | -2.749231 | 0.112843  | 6.530931  | C    | -5.713933 | -1.744161 | -0.074017 |
| C    | -3.156367 | -1.207654 | 6.324693  | H    | -5.818527 | -1.45289  | -1.124126 |
| C    | -2.887567 | -1.806701 | 5.091209  | H    | -4.968363 | -2.55036  | -0.034854 |
| C    | -2.237926 | -1.104319 | 4.077074  | H    | -7.341127 | -3.167446 | -0.112719 |
| H    | -2.036438 | -1.582482 | 3.125533  | H    | -7.845495 | -1.537395 | 0.307626  |
| H    | -3.179809 | -2.840888 | 4.918195  | H    | -7.933895 | -2.911339 | 2.357061  |
| H    | -3.660434 | -1.761412 | 7.112244  | H    | -6.28564  | -3.477266 | 2.098225  |
| H    | -2.934142 | 0.59724   | 7.487337  | H    | -7.114211 | -0.592603 | 2.740566  |
| H    | -1.771629 | 1.838004  | 5.708929  | H    | -6.208592 | -1.680594 | 3.790037  |

| Table 6 (Continued). |           |           |           |    |           |           |           |
|----------------------|-----------|-----------|-----------|----|-----------|-----------|-----------|
| O                    | 1.44812   | 4.013915  | 0.533789  | O  | -2.596912 | -1.297816 | -1.489496 |
| C                    | 2.493926  | 3.54933   | 1.432699  | C  | -2.024295 | -2.566949 | -1.083357 |
| C                    | 3.766754  | 4.26614   | 0.983528  | C  | -2.174692 | -3.507324 | -2.284116 |
| C                    | 3.216534  | 5.594044  | 0.440657  | C  | -3.415024 | -2.941168 | -2.992063 |
| C                    | 1.915046  | 5.155715  | -0.22997  | C  | -3.238142 | -1.438507 | -2.777072 |
| H                    | 2.086622  | 4.829959  | -1.265271 | H  | -4.173378 | -0.875283 | -2.752469 |
| H                    | 1.13364   | 5.91693   | -0.218232 | H  | -2.592076 | -0.999031 | -3.548504 |
| H                    | 3.895583  | 6.094217  | -0.256515 | H  | -4.329815 | -3.292726 | -2.502216 |
| H                    | 2.999929  | 6.286658  | 1.261315  | H  | -3.470944 | -3.208603 | -4.051543 |
| H                    | 4.265586  | 3.701482  | 0.186537  | H  | -2.286585 | -4.552492 | -1.980908 |
| H                    | 4.479181  | 4.390334  | 1.80384   | H  | -1.297779 | -3.439946 | -2.939465 |
| H                    | 2.217941  | 3.824014  | 2.458025  | H  | -0.985266 | -2.399784 | -0.791524 |
| H                    | 2.545572  | 2.460969  | 1.368392  | H  | -2.578085 | -2.928966 | -0.209069 |
| C                    | -2.504797 | 5.585474  | 1.056625  | O  | 0.679172  | 0.524951  | -1.811828 |
| C                    | -2.880311 | 5.24451   | 2.510897  | C  | 0.132267  | 0.196509  | -3.109633 |
| N                    | -4.06486  | 4.356877  | 2.628982  | C  | 1.061234  | 0.854985  | -4.132296 |
| C                    | -5.308823 | 5.150864  | 2.486869  | C  | 1.557846  | 2.088567  | -3.362562 |
| H                    | -5.313034 | 5.616005  | 1.496904  | C  | 1.709458  | 1.536489  | -1.945282 |
| H                    | -5.303849 | 5.972711  | 3.229107  | H  | 1.559567  | 2.2776    | -1.157183 |
| C                    | -6.572982 | 4.309533  | 2.676699  | H  | 2.687356  | 1.056552  | -1.806427 |
| C                    | -6.566279 | 3.597745  | 4.034235  | H  | 0.802016  | 2.881308  | -3.38459  |
| C                    | -5.26125  | 2.811959  | 4.198973  | H  | 2.495482  | 2.494374  | -3.754205 |
| C                    | -4.043118 | 3.703693  | 3.960167  | H  | 0.542779  | 1.103999  | -5.062843 |
| H                    | -3.128013 | 3.108415  | 4.028085  | H  | 1.899912  | 0.191927  | -4.376014 |
| H                    | -3.995983 | 4.475568  | 4.752866  | H  | 0.087942  | -0.893658 | -3.196946 |
| H                    | -5.239941 | 1.977742  | 3.485952  | H  | -0.884324 | 0.600518  | -3.168756 |
| H                    | -5.182516 | 2.368291  | 5.198248  | C  | -5.904036 | 0.65775   | 0.42827   |
| H                    | -7.434951 | 2.934576  | 4.128404  | H  | -6.986415 | 0.483521  | 0.356035  |
| H                    | -6.647971 | 4.342777  | 4.839298  | H  | -5.749634 | 1.316086  | 1.290442  |
| H                    | -6.645179 | 3.573579  | 1.867005  | O  | 1.226211  | -1.563129 | 0.340753  |
| H                    | -7.44745  | 4.965298  | 2.581838  | C  | 1.072379  | -2.662352 | 1.269389  |
| H                    | -3.03674  | 6.161147  | 3.105606  | C  | 2.63551   | -1.462069 | -0.013906 |
| H                    | -2.037713 | 4.706388  | 2.960513  | C  | 2.129511  | -3.669288 | 0.833006  |
| H                    | -3.407319 | 6.011015  | 0.565402  | H  | 1.273591  | -2.313418 | 2.286961  |
| C                    | -1.469993 | 6.723193  | 1.010067  | H  | 0.039958  | -3.010554 | 1.195464  |
| C                    | -1.507243 | 7.648691  | -0.043789 | C  | 3.314013  | -2.74103  | 0.511246  |
| H                    | 3.864606  | -2.508274 | 1.426928  | H  | 2.681063  | -1.366965 | -1.103138 |
| H                    | -0.781826 | 2.000988  | 3.576986  | H  | 3.054025  | -0.56871  | 0.458548  |
| C                    | 1.081024  | 0.28805   | 3.543195  | H  | 1.795905  | -4.214491 | -0.059014 |
| H                    | 0.72509   | -0.720824 | 3.435823  | H  | 2.361746  | -4.396212 | 1.616837  |
| H                    | 1.281971  | 0.900204  | 2.684752  | H  | 4.007566  | -3.170742 | -0.218079 |
| H                    | 1.124149  | 0.705653  | 4.536714  | Cl | 3.27319   | -0.38769  | 3.550725  |

**Table 6 (Continued).**



**17e**

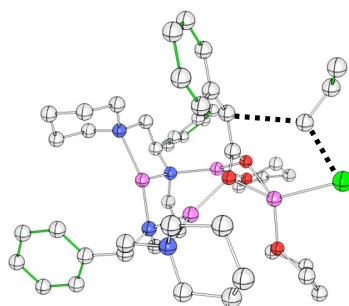
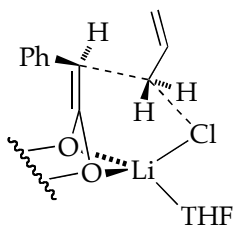
$G = -2880.08639$

$G_{MP2} = -2872.408896$

| Atom | X         | Y         | Z         | Atom | X         | Y         | Z         |
|------|-----------|-----------|-----------|------|-----------|-----------|-----------|
| C    | 0         | 0         | 0         | C    | 4.183351  | -2.759912 | 2.066556  |
| Li   | -0.763328 | 1.245009  | -1.770106 | C    | 2.815053  | -3.294967 | 1.640044  |
| O    | 0.755585  | 0.953792  | -0.501951 | H    | 2.060917  | -2.502921 | 1.683465  |
| Li   | 2.391543  | 0.67493   | -1.315514 | H    | 2.494493  | -4.083331 | 2.347163  |
| N    | 3.52202   | -0.639777 | -2.312615 | H    | 4.113728  | -2.376771 | 3.092275  |
| C    | 4.827343  | 0.028422  | -2.284812 | H    | 4.452982  | -1.907467 | 1.426007  |
| C    | 5.040329  | 0.763695  | -0.947669 | H    | 5.057811  | -4.626543 | 2.710465  |
| N    | 4.030623  | 1.816501  | -0.690841 | H    | 6.251518  | -3.43767  | 2.19368   |
| C    | 4.028276  | 2.190032  | 0.740582  | H    | 1.33946   | -5.342504 | 0.361708  |
| H    | 3.84424   | 1.28096   | 1.324459  | H    | 0.758231  | -3.671796 | 0.337302  |
| H    | 5.026347  | 2.569836  | 1.033476  | H    | 2.116319  | -4.967122 | -2.071976 |
| C    | 2.958388  | 3.238726  | 1.05525   | C    | 0.021013  | -5.231002 | -1.967294 |
| H    | 3.012661  | 3.49339   | 2.121383  | C    | 0.03337   | -6.092775 | -3.073892 |
| H    | 1.974126  | 2.793351  | 0.868137  | C    | -1.100473 | -6.821376 | -3.443022 |
| C    | 3.137928  | 4.489977  | 0.187156  | C    | -2.276003 | -6.71173  | -2.69845  |
| C    | 3.207472  | 4.091178  | -1.291735 | C    | -2.304798 | -5.862938 | -1.588104 |
| C    | 4.272099  | 3.014984  | -1.522996 | C    | -1.172552 | -5.126617 | -1.232852 |
| H    | 4.280697  | 2.713465  | -2.574354 | H    | -1.219401 | -4.481199 | -0.358302 |
| H    | 5.273751  | 3.43031   | -1.297944 | H    | -3.20781  | -5.784915 | -0.986588 |
| H    | 3.437158  | 4.960004  | -1.921425 | H    | -3.155756 | -7.28897  | -2.971657 |
| H    | 2.229483  | 3.708622  | -1.614511 | H    | -1.060798 | -7.482834 | -4.30538  |
| H    | 4.068631  | 5.00491   | 0.468017  | H    | 0.951622  | -6.199244 | -3.648057 |
| H    | 2.319513  | 5.200122  | 0.357067  | C    | 1.516989  | -2.958014 | -3.556716 |
| H    | 6.059069  | 1.186574  | -0.901846 | C    | 1.799385  | -1.511243 | -4.002446 |
| H    | 4.955     | 0.04069   | -0.12749  | H    | 1.664886  | -1.459902 | -5.093329 |
| H    | 4.857268  | 0.800998  | -3.082897 | H    | 1.044973  | -0.835337 | -3.569825 |
| C    | 6.039465  | -0.86717  | -2.592869 | C    | 3.204863  | -0.955156 | -3.712332 |
| C    | 6.572645  | -0.899891 | -3.889108 | H    | 3.316891  | -0.040405 | -4.337471 |
| C    | 7.653903  | -1.722696 | -4.212527 | H    | 3.926007  | -1.674024 | -4.151465 |
| C    | 8.240347  | -2.524518 | -3.233368 | H    | 2.393802  | -3.581481 | -3.846111 |
| C    | 7.733123  | -2.49444  | -1.932455 | H    | 0.687034  | -3.354235 | -4.182628 |
| C    | 6.643891  | -1.678632 | -1.621525 | O    | -0.377711 | 1.673095  | -3.645387 |
| H    | 6.272013  | -1.664631 | -0.600734 | C    | -1.165021 | 1.04261   | -4.679325 |
| H    | 8.190398  | -3.103012 | -1.155754 | C    | -2.064538 | 2.15722   | -5.202631 |
| H    | 9.086619  | -3.161371 | -3.47767  | C    | -1.106298 | 3.361803  | -5.187966 |
| H    | 8.040744  | -1.73165  | -5.22875  | C    | -0.204319 | 3.080522  | -3.971268 |

**Table 6 (Continued).**

|    |           |           |           |   |           |           |           |
|----|-----------|-----------|-----------|---|-----------|-----------|-----------|
| H  | 6.133067  | -0.264642 | -4.655245 | H | -0.505921 | 3.651835  | -3.089132 |
| Li | 2.860796  | -2.246592 | -1.311782 | H | 0.855557  | 3.2616    | -4.180507 |
| N  | 1.247171  | -3.034751 | -2.125359 | H | -1.629664 | 4.317152  | -5.094708 |
| Li | -0.445874 | -2.021537 | -1.886718 | H | -0.513956 | 3.389376  | -6.109469 |
| O  | -0.852218 | -0.545287 | -0.82766  | H | -2.896072 | 2.320722  | -4.509086 |
| O  | -2.107993 | -2.118192 | -2.991391 | H | -2.468931 | 1.944493  | -6.197135 |
| C  | -2.334238 | -2.978588 | -4.140063 | H | -0.494371 | 0.65807   | -5.460538 |
| C  | -3.851091 | -3.180538 | -4.225303 | H | -1.689094 | 0.199986  | -4.221546 |
| C  | -4.398065 | -1.921353 | -3.534478 | C | 0.023114  | -0.262856 | 1.389702  |
| C  | -3.375931 | -1.706737 | -2.421241 | H | 0.777483  | 0.28883   | 1.944575  |
| H  | -3.596293 | -2.338045 | -1.550392 | C | -0.682551 | -1.294305 | 2.125079  |
| H  | -3.272861 | -0.672948 | -2.086697 | C | -0.338565 | -1.514766 | 3.483097  |
| H  | -5.414508 | -2.04467  | -3.148961 | C | -0.975294 | -2.478903 | 4.256589  |
| H  | -4.396935 | -1.068276 | -4.223802 | C | -1.990768 | -3.27075  | 3.711555  |
| H  | -4.142407 | -4.078606 | -3.669923 | C | -2.354706 | -3.067811 | 2.377855  |
| H  | -4.196118 | -3.293797 | -5.257492 | C | -1.720475 | -2.103903 | 1.595955  |
| H  | -1.938635 | -2.463336 | -5.023928 | H | -2.029168 | -1.946081 | 0.569826  |
| H  | -1.782363 | -3.908774 | -3.992947 | H | -3.151929 | -3.665089 | 1.939202  |
| C  | 1.269288  | -4.405345 | -1.622777 | H | -2.489214 | -4.025067 | 4.314163  |
| C  | 1.495764  | -4.352622 | -0.099876 | H | -0.677388 | -2.614641 | 5.294062  |
| N  | 2.840177  | -3.83113  | 0.258798  | H | 0.447403  | -0.906277 | 3.926693  |
| C  | 3.837834  | -4.922932 | 0.168581  | C | -1.830182 | 1.833215  | 0.99375   |
| H  | 3.839845  | -5.306985 | -0.855954 | H | -2.173764 | 0.903209  | 0.576963  |
| H  | 3.524374  | -5.756917 | 0.825756  | H | -0.84111  | 2.181688  | 0.74461   |
| C  | 5.245026  | -4.471271 | 0.560762  | C | -2.540984 | 2.435992  | 2.084358  |
| H  | 5.608504  | -3.748397 | -0.177768 | H | -3.506192 | 2.01188   | 2.352309  |
| H  | 5.91819   | -5.336747 | 0.514328  | C | -2.054735 | 3.484848  | 2.779654  |
| C  | 5.260302  | -3.84691  | 1.961743  | H | -1.097892 | 3.934342  | 2.525586  |
| Cl | -2.545545 | 2.770369  | -1.152009 | H | -2.595896 | 3.918909  | 3.615108  |



**17f**

$G = -2880.085075$

$G_{MP2} = -2872.41204$

| Atom | X | Y | Z | Atom | X | Y | Z |
|------|---|---|---|------|---|---|---|
|------|---|---|---|------|---|---|---|

|    |           |          |           |   |          |          |           |
|----|-----------|----------|-----------|---|----------|----------|-----------|
| Li | 0         | 0        | 0         | H | 4.512683 | 3.941116 | -0.168649 |
| O  | -1.80965  | 0.209538 | 0.987624  | H | 3.735831 | 3.235756 | -1.599103 |
| Li | -3.131848 | 0.506057 | -0.295215 | H | 3.19983  | 5.999837 | -0.375494 |

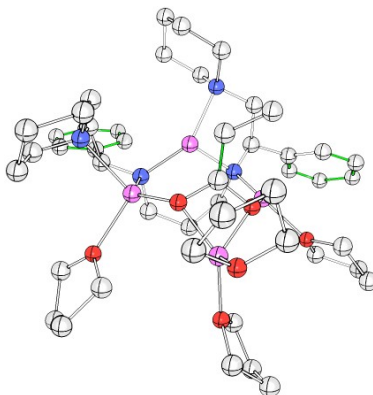
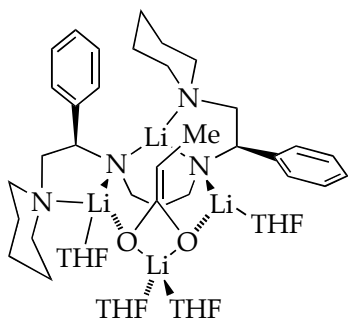
**Table 6 (Continued).**

|    |           |           |           |   |           |           |           |
|----|-----------|-----------|-----------|---|-----------|-----------|-----------|
| N  | -4.183802 | 1.92439   | -1.247337 | H | 3.53387   | 5.642019  | -2.078399 |
| C  | -5.377198 | 1.184374  | -1.672349 | H | 1.316958  | 4.748524  | -2.417194 |
| C  | -5.701191 | 0.034346  | -0.700017 | H | 0.926608  | 5.844115  | -1.066877 |
| N  | -4.607386 | -0.957571 | -0.571445 | C | -2.503167 | 5.517309  | 0.814557  |
| C  | -4.882886 | -1.864024 | 0.56505   | C | -3.099626 | 5.070304  | 2.163901  |
| H  | -5.01029  | -1.24868  | 1.461831  | N | -4.451488 | 4.473309  | 2.027713  |
| H  | -5.838831 | -2.396954 | 0.396565  | C | -5.464589 | 5.54539   | 1.891207  |
| C  | -3.757223 | -2.879431 | 0.774731  | H | -5.228564 | 6.137095  | 1.001783  |
| H  | -4.016838 | -3.530014 | 1.619182  | H | -5.392099 | 6.226537  | 2.761416  |
| H  | -2.840478 | -2.342132 | 1.046499  | C | -6.88994  | 5.000106  | 1.790236  |
| C  | -3.517118 | -3.704626 | -0.494856 | H | -6.996392 | 4.443419  | 0.852553  |
| C  | -3.300064 | -2.765448 | -1.686618 | H | -7.586272 | 5.846774  | 1.735894  |
| C  | -4.437525 | -1.747307 | -1.81054  | C | -7.228405 | 4.093601  | 2.981039  |
| H  | -4.232234 | -1.061936 | -2.636835 | C | -6.143509 | 3.024077  | 3.155026  |
| H  | -5.382019 | -2.273204 | -2.050838 | C | -4.753514 | 3.656938  | 3.227943  |
| H  | -3.227977 | -3.331456 | -2.624226 | H | -3.987518 | 2.882291  | 3.317792  |
| H  | -2.350162 | -2.22804  | -1.561573 | H | -4.686922 | 4.285754  | 4.136575  |
| H  | -4.391244 | -4.342985 | -0.690532 | H | -6.310596 | 2.433317  | 4.06346   |
| H  | -2.657028 | -4.372543 | -0.366195 | H | -6.174223 | 2.32042   | 2.310952  |
| H  | -6.637362 | -0.464185 | -1.00724  | H | -7.286093 | 4.699856  | 3.896922  |
| H  | -5.869109 | 0.444412  | 0.30367   | H | -8.214771 | 3.631601  | 2.847676  |
| H  | -5.177446 | 0.716079  | -2.658219 | H | -3.124893 | 5.906756  | 2.884244  |
| C  | -6.639016 | 2.028302  | -1.924391 | H | -2.450874 | 4.293937  | 2.583534  |
| C  | -6.964269 | 2.418708  | -3.231521 | H | -3.229863 | 6.202703  | 0.331442  |
| C  | -8.093826 | 3.193996  | -3.502482 | C | -1.241518 | 6.364868  | 1.037963  |
| C  | -8.939709 | 3.583183  | -2.463919 | C | -1.056709 | 7.565367  | 0.337565  |
| C  | -8.639599 | 3.193805  | -1.156841 | C | 0.105375  | 8.327057  | 0.490612  |
| C  | -7.499307 | 2.432476  | -0.892819 | C | 1.109438  | 7.905329  | 1.363619  |
| H  | -7.288953 | 2.13922   | 0.132335  | C | 0.941119  | 6.712997  | 2.074286  |
| H  | -9.298259 | 3.479135  | -0.339877 | C | -0.216251 | 5.951072  | 1.905954  |
| H  | -9.82586  | 4.178192  | -2.669244 | H | -0.326993 | 5.029144  | 2.47392   |
| H  | -8.315822 | 3.486133  | -4.526113 | H | 1.707722  | 6.382538  | 2.77169   |
| H  | -6.322554 | 2.10046   | -4.05045  | H | 2.007657  | 8.502625  | 1.498326  |
| Li | -3.942676 | 3.276705  | 0.228169  | H | 0.220564  | 9.254612  | -0.065306 |
| N  | -2.291661 | 4.332945  | -0.008891 | H | -1.842    | 7.91047   | -0.332149 |
| Li | -0.548235 | 3.394216  | 0.247007  | C | -2.270074 | 4.638311  | -1.433986 |
| O  | -0.18406  | 1.726684  | 0.969969  | C | -2.313258 | 3.354085  | -2.281461 |
| C  | -1.150821 | 1.135661  | 1.640252  | H | -1.989673 | 3.609595  | -3.301528 |
| C  | -1.301374 | 1.396343  | 3.021826  | H | -1.573235 | 2.634703  | -1.896001 |
| H  | -0.666994 | 2.193261  | 3.4014    | C | -3.677277 | 2.654124  | -2.418311 |
| C  | -2.260809 | 0.848702  | 3.95797   | H | -3.585269 | 1.955592  | -3.280448 |
| C  | -2.301401 | 1.369253  | 5.277115  | H | -4.392335 | 3.425677  | -2.771266 |
| C  | -3.194344 | 0.890371  | 6.229445  | H | -3.131829 | 5.276173  | -1.736314 |
| C  | -4.086854 | -0.139324 | 5.913705  | H | -1.377949 | 5.225471  | -1.747665 |
| C  | -4.054435 | -0.681378 | 4.626109  | O | 0.170488  | -0.183056 | -1.945119 |
| C  | -3.163581 | -0.204999 | 3.665774  | C | 0.732386  | 0.901549  | -2.719399 |



| <b>Table 6 (Continued).</b> |           |           |           |    |          |                     |
|-----------------------------|-----------|-----------|-----------|----|----------|---------------------|
| H                           | -3.144665 | -0.638116 | 2.674388  | C  | 1.9979   | 0.315443 -3.337505  |
| H                           | -4.732059 | -1.492261 | 4.364752  | C  | 1.545574 | -1.115097 -3.675853 |
| H                           | -4.785359 | -0.514547 | 6.656742  | C  | 0.572827 | -1.45436 -2.533371  |
| H                           | -3.194431 | 1.323421  | 7.227467  | H  | 1.041461 | -2.039053 -1.737563 |
| H                           | -1.614776 | 2.17091   | 5.542707  | H  | -0.3246  | -1.974009 -2.883894 |
| O                           | 1.224985  | 3.851208  | -0.557696 | H  | 2.376368 | -1.824224 -3.728434 |
| C                           | 1.552658  | 5.005196  | -1.377775 | H  | 1.028675 | -1.129647 -4.642123 |
| C                           | 3.051177  | 5.263409  | -1.172473 | H  | 2.806777 | 0.299278 -2.5983    |
| C                           | 3.576006  | 3.887495  | -0.731587 | H  | 2.338097 | 0.876478 -4.213422  |
| C                           | 2.415202  | 3.371937  | 0.113881  | H  | 0.01154  | 1.207083 -3.489934  |
| H                           | 2.446752  | 3.788797  | 1.129301  | H  | 0.900486 | 1.741871 -2.041386  |
| H                           | 2.341495  | 2.285598  | 0.184518  | Cl | 1.646815 | -1.56976 0.942982   |
| H                           | 2.173606  | -0.645331 | 4.431332  | C  | 0.668601 | -0.540433 2.871059  |
| C                           | 0.565465  | -1.9517   | 4.853148  | H  | 1.03692  | 0.376851 2.446463   |
| H                           | -0.394259 | -2.356395 | 4.542793  | H  | -0.28321 | -0.921948 2.541074  |
| H                           | 0.959795  | -2.293862 | 5.805483  | C  | 1.218205 | -1.045187 4.098051  |

**Table 7.** Optimized geometries of dilithium amide-enediolate complexes at B3LYP level of theory with 6-31G(d) basis set for the enolization of various acids at -78 °C with free energies (Hartrees) and cartesian coordinates (X, Y, Z) (Note:  $G_{\text{MP2}}$  includes single point MP2 corrections to B3LYP/6-31G(d) optimized structures).



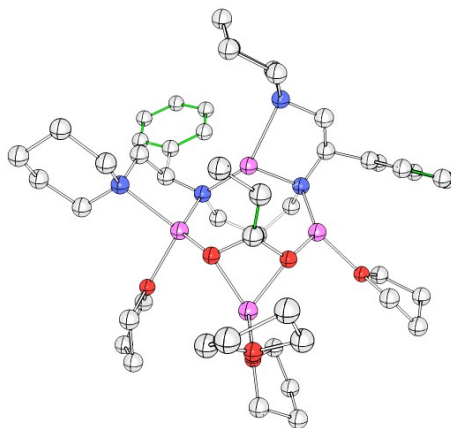
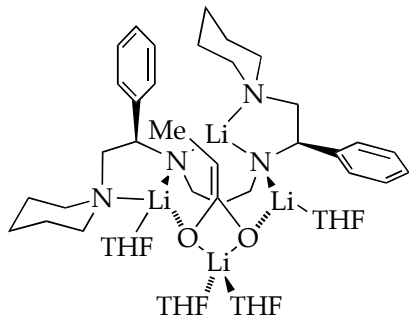
**18a**  
 $G = -2575.657905$   
 $G_{\text{MP2}} = -2568.18801$

| Atom | X         | Y         | Z         | Atom | X         | Y        | Z         |
|------|-----------|-----------|-----------|------|-----------|----------|-----------|
| Li   | 0         | 0         | 0         | C    | -4.161606 | 4.907775 | 2.930294  |
| O    | -1.82639  | 0.2386    | 0.559739  | H    | -3.36353  | 4.232431 | 3.246546  |
| Li   | -3.402603 | 0.42819   | -0.43807  | H    | -4.058697 | 5.84401  | 3.514917  |
| N    | -4.14102  | 2.185068  | -1.24634  | H    | -5.608379 | 4.11419  | 4.309965  |
| C    | -5.521166 | 1.780265  | -1.410576 | H    | -5.583832 | 3.29897  | 2.746876  |
| C    | -6.080183 | 1.344123  | -0.036167 | H    | -6.68608  | 6.105809 | 3.308111  |
| N    | -5.463815 | 0.096007  | 0.468529  | H    | -7.636818 | 4.686747 | 2.868379  |
| C    | -5.436723 | 0.072296  | 1.943925  | H    | -2.676872 | 6.872451 | 1.712832  |
| H    | -4.891277 | 0.957559  | 2.28389   | H    | -1.935586 | 5.279315 | 1.9354    |
| H    | -6.46612  | 0.138051  | 2.350573  | H    | -2.890723 | 6.321611 | -0.770581 |
| C    | -4.752541 | -1.191397 | 2.47131   | C    | -0.892268 | 6.76425  | -0.247576 |
| H    | -4.761088 | -1.173434 | 3.568732  | C    | -0.760017 | 7.626341 | -1.345769 |
| H    | -3.703356 | -1.169994 | 2.151044  | C    | 0.361148  | 8.447044 | -1.499324 |
| C    | -5.443532 | -2.455631 | 1.944595  | C    | 1.37447   | 8.435255 | -0.539899 |
| C    | -5.557302 | -2.394289 | 0.416167  | C    | 1.258296  | 7.586104 | 0.565245  |
| C    | -6.198836 | -1.079194 | -0.033435 | C    | 0.144948  | 6.755203 | 0.700286  |
| H    | -6.230403 | -1.023989 | -1.125818 | H    | 0.078958  | 6.098252 | 1.564458  |
| H    | -7.249725 | -1.045015 | 0.319574  | H    | 2.032641  | 7.579083 | 1.329631  |
| H    | -6.154319 | -3.234088 | 0.036489  | H    | 2.240062  | 9.084602 | -0.645527 |
| H    | -4.561038 | -2.468283 | -0.035532 | H    | 0.435937  | 9.103952 | -2.363023 |
| H    | -6.450971 | -2.530304 | 2.38039   | H    | -1.555327 | 7.656837 | -2.08787  |
| H    | -4.898991 | -3.356284 | 2.256496  | C    | -1.882842 | 4.359906 | -2.02386  |
| H    | -7.177996 | 1.24267   | -0.065183 | C    | -2.067676 | 2.904549 | -2.504009 |
| H    | -5.850908 | 2.146876  | 0.673189  | H    | -1.664304 | 2.82583  | -3.525709 |
| H    | -5.605713 | 0.893568  | -2.085373 | H    | -1.462729 | 2.230533 | -1.876962 |
| C    | -6.494973 | 2.806768  | -2.035509 | C    | -3.51644  | 2.387584 | -2.54999  |
| C    | -7.71429  | 2.37646   | -2.579025 | H    | -3.503983 | 1.441942 | -3.142756 |
| C    | -8.624073 | 3.27928   | -3.129316 | H    | -4.083344 | 3.093851 | -3.188884 |
| C    | -8.322295 | 4.643106  | -3.160063 | H    | -2.692572 | 4.969312 | -2.48285  |

**Table 7 (Continued).**

|    |           |          |           |   |           |           |           |
|----|-----------|----------|-----------|---|-----------|-----------|-----------|
| C  | -7.106666 | 5.085126 | -2.63684  | H | -0.951095 | 4.756875  | -2.488689 |
| C  | -6.204569 | 4.174067 | -2.080575 | O | -3.195446 | -1.199396 | -1.85092  |
| H  | -5.251643 | 4.511553 | -1.683693 | C | -2.118949 | -2.141784 | -1.64599  |
| H  | -6.854462 | 6.142949 | -2.668966 | C | -2.356855 | -3.275337 | -2.647735 |
| H  | -9.023836 | 5.350857 | -3.594916 | C | -3.038862 | -2.532811 | -3.806192 |
| H  | -9.565106 | 2.919395 | -3.539515 | C | -3.91688  | -1.529691 | -3.056123 |
| H  | -7.952739 | 1.313167 | -2.572357 | H | -4.882611 | -1.976902 | -2.783304 |
| Li | -3.394922 | 3.406258 | 0.140872  | H | -4.102762 | -0.604463 | -3.606504 |
| N  | -1.889176 | 4.472881 | -0.569839 | H | -3.618122 | -3.186955 | -4.465009 |
| Li | -0.324387 | 3.380016 | 0.009126  | H | -2.293646 | -2.007649 | -4.415803 |
| O  | -0.150125 | 1.718602 | 0.798075  | H | -3.034064 | -4.028908 | -2.22795  |
| C  | -1.3156   | 1.247524 | 1.274687  | H | -1.428661 | -3.778094 | -2.937689 |
| C  | -1.874517 | 1.743361 | 2.432137  | H | -1.167383 | -1.63239  | -1.835566 |
| H  | -2.741836 | 1.227483 | 2.834113  | H | -2.140982 | -2.462855 | -0.601192 |
| C  | -1.120812 | 2.6815   | 3.346738  | O | 0.868099  | -1.309472 | 1.324698  |
| H  | -1.748138 | 2.999619 | 4.189586  | C | 1.521804  | -0.605739 | 2.416839  |
| H  | -0.213425 | 2.232438 | 3.790085  | C | 0.695572  | -0.923326 | 3.662506  |
| H  | -0.776466 | 3.599039 | 2.846127  | C | 0.199014  | -2.345578 | 3.363338  |
| O  | 1.543127  | 3.76183  | -0.642516 | C | -0.083612 | -2.269506 | 1.861959  |
| C  | 2.003924  | 4.669119 | -1.676112 | H | -1.088487 | -1.885162 | 1.65612   |
| C  | 3.47476   | 4.96042  | -1.355488 | H | 0.065056  | -3.221548 | 1.340776  |
| C  | 3.901134  | 3.711913 | -0.566214 | H | -0.691979 | -2.620592 | 3.935755  |
| C  | 2.634973  | 3.404678 | 0.231449  | H | 0.982916  | -3.083318 | 3.575158  |
| H  | 2.582288  | 4.01685  | 1.142213  | H | -0.150672 | -0.231243 | 3.725128  |
| H  | 2.503643  | 2.357074 | 0.509082  | H | 1.282633  | -0.852901 | 4.583495  |
| H  | 4.771822  | 3.880013 | 0.075141  | H | 2.551643  | -0.979989 | 2.501327  |
| H  | 4.135322  | 2.884563 | -1.248237 | H | 1.526042  | 0.457107  | 2.164622  |
| H  | 3.551706  | 5.853592 | -0.726287 | O | 1.02359   | -0.366974 | -1.663828 |
| H  | 4.071221  | 5.129074 | -2.257309 | C | 1.236471  | 0.696538  | -2.634107 |
| H  | 1.889103  | 4.160064 | -2.641664 | C | 2.517108  | 0.323484  | -3.39653  |
| H  | 1.372696  | 5.558802 | -1.66733  | C | 3.241846  | -0.610257 | -2.412634 |
| C  | -2.118832 | 5.840305 | -0.133207 | C | 2.070571  | -1.352983 | -1.775282 |
| C  | -2.642587 | 5.840896 | 1.316674  | H | 2.260841  | -1.738486 | -0.771885 |
| N  | -3.964181 | 5.191712 | 1.491071  | H | 1.727107  | -2.176902 | -2.418093 |
| C  | -5.042259 | 6.082318 | 1.008218  | H | 3.779718  | -0.030243 | -1.653051 |
| H  | -4.891299 | 6.264132 | -0.059195 | H | 3.954922  | -1.282391 | -2.899508 |
| H  | -4.964377 | 7.063865 | 1.517559  | H | 3.105654  | 1.204562  | -3.669114 |
| C  | -6.439322 | 5.502531 | 1.243372  | H | 2.2759    | -0.215091 | -4.320337 |
| H  | -6.561832 | 4.597812 | 0.637444  | H | 0.354424  | 0.762595  | -3.277634 |
| H  | -7.184309 | 6.223074 | 0.883174  | H | 1.335264  | 1.632587  | -2.076586 |
| C  | -6.664879 | 5.174536 | 2.72277   | C | -5.525551 | 4.283599  | 3.228642  |

**Table 7 (Continued).**



**18b**

$G = -2575.652762$

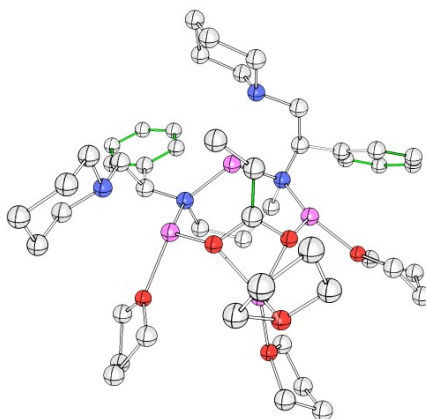
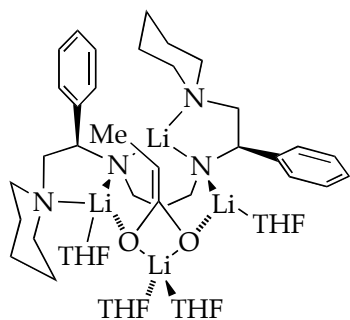
$G_{MP2} = -2568.17973$

| Atom | X         | Y         | Z         | Atom | X         | Y         | Z         |
|------|-----------|-----------|-----------|------|-----------|-----------|-----------|
| Li   | 0         | 0         | 0         | H    | -2.798786 | 4.428097  | 3.112472  |
| O    | -1.777536 | 0.402335  | 0.637687  | H    | -3.318818 | 6.089381  | 3.472828  |
| Li   | -3.235742 | 0.787175  | -0.530089 | H    | -5.108616 | 3.77553   | 2.556829  |
| N    | -3.742085 | 2.614836  | -1.429508 | H    | -5.053219 | 4.490101  | 4.167661  |
| C    | -5.150652 | 2.39815   | -1.690084 | H    | -6.9977   | 5.373068  | 2.771436  |
| H    | -5.292248 | 1.597483  | -2.455368 | H    | -5.894674 | 6.649928  | 3.285449  |
| C    | -5.953916 | 3.590693  | -2.26656  | H    | -5.931142 | 5.286267  | 0.535718  |
| C    | -7.1918   | 3.368956  | -2.888367 | H    | -6.371629 | 6.955282  | 0.871068  |
| C    | -7.949015 | 4.423263  | -3.39886  | H    | -1.817564 | 7.053024  | 1.721063  |
| C    | -7.471236 | 5.733177  | -3.310816 | H    | -1.262944 | 5.372978  | 1.84866   |
| C    | -6.233663 | 5.968619  | -2.711135 | H    | -2.102768 | 6.651695  | -0.794606 |
| C    | -5.485898 | 4.90632   | -2.195539 | C    | -0.063688 | 6.844514  | -0.270442 |
| H    | -4.514254 | 5.082955  | -1.743444 | C    | 0.168074  | 7.718913  | -1.341975 |
| H    | -5.84313  | 6.982295  | -2.651123 | C    | 1.377885  | 8.406403  | -1.475605 |
| H    | -8.053358 | 6.558191  | -3.714083 | C    | 2.384032  | 8.245651  | -0.522058 |
| H    | -8.907992 | 4.223178  | -3.871825 | C    | 2.169709  | 7.382217  | 0.556869  |
| H    | -7.566203 | 2.349506  | -2.979245 | C    | 0.966528  | 6.684009  | 0.671687  |
| C    | -5.867517 | 1.910859  | -0.409217 | H    | 0.825319  | 6.014817  | 1.517485  |
| N    | -5.43     | 0.560369  | 0.012785  | H    | 2.938146  | 7.261833  | 1.317836  |
| C    | -5.640893 | 0.312374  | 1.454123  | H    | 3.319914  | 8.79164   | -0.611755 |
| H    | -5.075119 | -0.59382  | 1.714213  | H    | 1.528352  | 9.076421  | -2.319115 |
| H    | -5.188586 | 1.135965  | 2.011453  | H    | -0.618989 | 7.86605   | -2.07895  |
| C    | -7.110985 | 0.118039  | 1.864265  | C    | -1.28943  | 4.622503  | -2.126613 |
| C    | -7.754292 | -1.013597 | 1.050412  | C    | -1.575211 | 3.19207   | -2.631932 |
| C    | -7.548641 | -0.769855 | -0.451664 | H    | -1.161976 | 3.094929  | -3.648083 |
| C    | -6.061838 | -0.524109 | -0.770255 | H    | -1.033817 | 2.466354  | -2.004654 |
| H    | -5.928811 | -0.30778  | -1.833805 | C    | -3.05755  | 2.791837  | -2.710551 |
| H    | -5.498846 | -1.443113 | -0.560203 | H    | -3.115084 | 1.862481  | -3.324399 |
| H    | -7.901823 | -1.628971 | -1.037624 | H    | -3.55007  | 3.555956  | -3.343949 |
| H    | -8.150569 | 0.091057  | -0.771398 | H    | -2.044794 | 5.300637  | -2.582623 |
| H    | -8.821414 | -1.110344 | 1.287213  | H    | -0.324357 | 4.957777  | -2.570671 |
| H    | -7.282387 | -1.968562 | 1.32824   | O    | -3.056924 | -0.900539 | -1.82734  |
| H    | -7.668093 | 1.051976  | 1.70772   | C    | -2.658388 | -2.147643 | -1.232543 |

**Table 7 (Continued).**

|    |           |           |           |   |           |           |           |
|----|-----------|-----------|-----------|---|-----------|-----------|-----------|
| H  | -7.160236 | -0.099611 | 2.93928   | C | -1.883518 | -2.875491 | -2.328402 |
| H  | -6.957683 | 1.969263  | -0.542199 | C | -2.687674 | -2.482111 | -3.578368 |
| H  | -5.610705 | 2.606284  | 0.398906  | C | -3.107323 | -1.036454 | -3.263807 |
| Li | -2.918372 | 3.763098  | -0.008541 | H | -4.118659 | -0.799699 | -3.611654 |
| N  | -1.307795 | 4.696689  | -0.672521 | H | -2.418131 | -0.302612 | -3.695035 |
| Li | 0.107373  | 3.431076  | -0.115646 | H | -3.568343 | -3.127099 | -3.680147 |
| O  | -0.00215  | 1.781096  | 0.64653   | H | -2.112682 | -2.554004 | -4.50665  |
| C  | -1.155054 | 1.420875  | 1.244266  | H | -1.832391 | -3.95728  | -2.168747 |
| C  | -1.586482 | 2.018228  | 2.40748   | H | -0.864315 | -2.478018 | -2.385147 |
| H  | -0.931436 | 2.780587  | 2.826939  | H | -2.082168 | -1.906396 | -0.337681 |
| C  | -2.673777 | 1.464419  | 3.29065   | H | -3.551916 | -2.719492 | -0.936789 |
| H  | -3.099592 | 0.563854  | 2.83812   | O | 0.952371  | -0.597518 | -1.645366 |
| H  | -2.294267 | 1.177524  | 4.287224  | C | 1.972794  | -1.621262 | -1.642999 |
| H  | -3.508837 | 2.157783  | 3.484848  | C | 3.174084  | -0.989012 | -2.342061 |
| O  | 2.003298  | 3.550124  | -0.790011 | C | 2.488508  | -0.1165   | -3.406018 |
| C  | 3.058418  | 3.060044  | 0.062887  | C | 1.246734  | 0.396627  | -2.666673 |
| C  | 4.349023  | 3.277716  | -0.725904 | H | 0.368689  | 0.501109  | -3.310293 |
| C  | 4.037164  | 4.580316  | -1.480057 | H | 1.426774  | 1.35039   | -2.160701 |
| C  | 2.54817   | 4.427507  | -1.809058 | H | 2.201051  | -0.729062 | -4.26863  |
| H  | 2.39163   | 3.946452  | -2.782965 | H | 3.118788  | 0.700294  | -3.770111 |
| H  | 1.99934   | 5.370254  | -1.786641 | H | 3.855613  | -1.733671 | -2.764281 |
| H  | 4.648886  | 4.719798  | -2.376567 | H | 3.739691  | -0.366209 | -1.638365 |
| H  | 4.189871  | 5.445922  | -0.826676 | H | 2.143391  | -1.908225 | -0.603743 |
| H  | 4.512436  | 2.452532  | -1.430796 | H | 1.605959  | -2.49507  | -2.20034  |
| H  | 5.228802  | 3.35019   | -0.079056 | O | 0.859865  | -1.216909 | 1.431083  |
| H  | 3.062735  | 3.636383  | 0.998298  | C | 1.655526  | -0.45191  | 2.376953  |
| H  | 2.835866  | 2.017319  | 0.29912   | C | 0.923877  | -0.559001 | 3.714476  |
| C  | -1.386137 | 6.061424  | -0.184026 | C | 0.286439  | -1.953502 | 3.623849  |
| C  | -1.902005 | 6.047745  | 1.268814  | C | -0.114292 | -2.024733 | 2.149158  |
| N  | -3.287719 | 5.542719  | 1.415498  | H | -1.101484 | -1.584745 | 1.971309  |
| C  | -4.258706 | 6.572015  | 0.983667  | H | -0.080556 | -3.039518 | 1.737696  |
| H  | -4.084242 | 6.793653  | -0.072638 | H | -0.573219 | -2.076687 | 4.289371  |
| H  | -4.075178 | 7.510217  | 1.544977  | H | 1.020393  | -2.732419 | 3.865431  |
| C  | -5.712092 | 6.138199  | 1.189532  | H | 0.150228  | 0.214065  | 3.76447   |
| C  | -5.97684  | 5.756182  | 2.649158  | H | 1.597393  | -0.445542 | 4.569867  |
| C  | -4.945325 | 4.716446  | 3.099302  | H | 2.660326  | -0.895351 | 2.420962  |
| C  | -3.51909  | 5.203275  | 2.83754   | H | 1.70944   | 0.573033  | 2.002801  |

**Table 7 (Continued).**



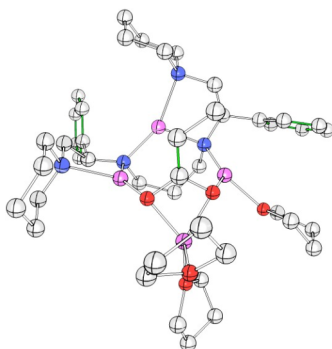
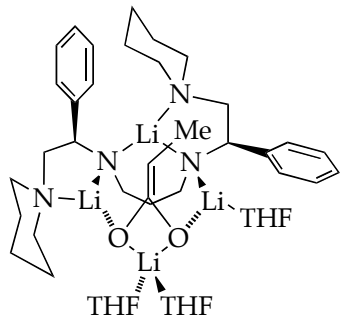
**18c**  
 $G = -2575.656449$   
 $G_{MP2} = -2568.184603$

| Atom | X         | Y         | Z         | Atom | X         | Y        | Z         |
|------|-----------|-----------|-----------|------|-----------|----------|-----------|
| Li   | 0         | 0         | 0         | H    | -5.428843 | 7.856648 | 0.743026  |
| O    | -1.743987 | 0.609724  | 0.561425  | C    | -5.193094 | 6.73469  | 2.598228  |
| Li   | -3.180972 | 1.134393  | -0.581117 | C    | -4.31937  | 5.585809 | 3.110851  |
| N    | -3.40637  | 3.022966  | -1.426335 | C    | -2.839822 | 5.841165 | 2.814341  |
| C    | -4.833336 | 3.038507  | -1.682892 | H    | -2.238153 | 4.989277 | 3.142725  |
| C    | -5.608757 | 2.687246  | -0.393392 | H    | -2.505614 | 6.726597 | 3.392987  |
| N    | -5.480592 | 1.26876   | 0.014069  | H    | -4.446481 | 5.442588 | 4.191568  |
| C    | -5.844052 | 1.120015  | 1.436911  | H    | -4.625815 | 4.650055 | 2.625609  |
| H    | -5.200822 | 1.778783  | 2.023435  | H    | -4.974673 | 7.646188 | 3.174427  |
| H    | -6.889952 | 1.451279  | 1.598371  | H    | -6.257238 | 6.51269  | 2.747515  |
| C    | -5.691238 | -0.326381 | 1.913556  | H    | -0.894626 | 7.332239 | 1.602421  |
| H    | -5.966131 | -0.387726 | 2.97428   | H    | -0.593329 | 5.595257 | 1.791881  |
| H    | -4.633914 | -0.611763 | 1.835441  | H    | -1.283714 | 6.876661 | -0.891768 |
| C    | -6.552669 | -1.276456 | 1.072158  | C    | 0.768264  | 6.827664 | -0.390322 |
| C    | -6.26266  | -1.060117 | -0.418456 | C    | 1.093352  | 7.635077 | -1.489931 |
| C    | -6.376281 | 0.419394  | -0.794673 | C    | 2.377776  | 8.161307 | -1.656505 |
| H    | -6.133687 | 0.561381  | -1.850984 | C    | 3.369113  | 7.903073 | -0.70907  |
| H    | -7.426333 | 0.750485  | -0.660738 | C    | 3.063116  | 7.104664 | 0.397782  |
| H    | -6.957212 | -1.642888 | -1.037973 | C    | 1.783594  | 6.566846 | 0.545526  |
| H    | -5.24762  | -1.401262 | -0.652463 | H    | 1.570388  | 5.946201 | 1.413074  |
| H    | -7.615709 | -1.073456 | 1.268714  | H    | 3.820762  | 6.910666 | 1.154441  |
| H    | -6.374008 | -2.321653 | 1.355664  | H    | 4.364558  | 8.324828 | -0.824465 |
| H    | -6.675863 | 2.952698  | -0.491842 | H    | 2.599057  | 8.782686 | -2.52141  |
| H    | -5.196625 | 3.304758  | 0.413612  | H    | 0.320492  | 7.860089 | -2.222259 |
| H    | -5.108267 | 2.26901   | -2.443377 | C    | -0.745095 | 4.7318   | -2.16219  |
| C    | -5.430818 | 4.344006  | -2.266385 | C    | -1.188385 | 3.329709 | -2.634714 |
| C    | -6.676208 | 4.320812  | -2.911155 | H    | -0.79     | 3.16529  | -3.648234 |
| C    | -7.246608 | 5.482165  | -3.432382 | H    | -0.731353 | 2.560357 | -1.992827 |
| C    | -6.568816 | 6.699696  | -3.330173 | C    | -2.706313 | 3.097672 | -2.707957 |
| C    | -5.321895 | 6.735665  | -2.705212 | H    | -2.864683 | 2.168895 | -3.307693 |
| C    | -4.761863 | 5.568293  | -2.179102 | H    | -3.108933 | 3.900496 | -3.355634 |
| H    | -3.784571 | 5.586087  | -1.706121 | H    | -1.427208 | 5.477031 | -2.628138 |

**Table 7 (Continued).**

|    |           |          |           |   |           |           |           |
|----|-----------|----------|-----------|---|-----------|-----------|-----------|
| H  | -4.777286 | 7.674841 | -2.633772 | H | 0.245783  | 4.950861  | -2.623027 |
| H  | -7.004608 | 7.606917 | -3.741594 | O | -3.171916 | -0.543725 | -1.945856 |
| H  | -8.21581  | 5.437066 | -3.924339 | C | -2.506816 | -1.766249 | -1.556534 |
| H  | -7.205738 | 3.373613 | -3.010176 | C | -2.959117 | -2.824755 | -2.565171 |
| Li | -2.388362 | 4.011663 | 0.037191  | C | -3.14764  | -1.982697 | -3.836206 |
| N  | -0.737412 | 4.843123 | -0.709613 | C | -3.73333  | -0.687613 | -3.268351 |
| Li | 0.535159  | 3.431042 | -0.170504 | H | -4.825859 | -0.752804 | -3.183834 |
| O  | 0.160981  | 1.79834  | 0.554381  | H | -3.481445 | 0.204781  | -3.846733 |
| C  | -1.057081 | 1.623083 | 1.09293   | H | -3.804594 | -2.44889  | -4.576773 |
| C  | -1.514183 | 2.415924 | 2.127936  | H | -2.179264 | -1.790284 | -4.313886 |
| H  | -0.79862  | 3.138486 | 2.518784  | H | -3.913093 | -3.270185 | -2.258492 |
| C  | -2.66601  | 2.030801 | 3.022484  | H | -2.228749 | -3.631979 | -2.680639 |
| H  | -3.462173 | 2.787198 | 3.101236  | H | -1.423692 | -1.607307 | -1.606979 |
| H  | -3.127738 | 1.107771 | 2.658599  | H | -2.782795 | -1.988671 | -0.522315 |
| H  | -2.339053 | 1.838887 | 4.059416  | O | 0.682144  | -1.255287 | 1.47081   |
| O  | 2.427559  | 3.302832 | -0.828583 | C | 1.454588  | -0.530949 | 2.466431  |
| C  | 3.057011  | 4.086163 | -1.876406 | C | 0.600083  | -0.535695 | 3.733163  |
| C  | 4.560123  | 4.051819 | -1.580383 | C | -0.132458 | -1.881452 | 3.62269   |
| C  | 4.719316  | 2.733638 | -0.806248 | C | -0.403823 | -1.975329 | 2.119532  |
| C  | 3.43055   | 2.700827 | 0.014724  | H | -1.338995 | -1.476792 | 1.842704  |
| H  | 3.532087  | 3.292784 | 0.934917  | H | -0.40276  | -3.003046 | 1.740349  |
| H  | 3.083131  | 1.699895 | 0.28102   | H | -1.055204 | -1.918276 | 4.209394  |
| H  | 5.616554  | 2.702178 | -0.180472 | H | 0.515574  | -2.702565 | 3.95325   |
| H  | 4.755706  | 1.881639 | -1.496994 | H | -0.111433 | 0.295672  | 3.695701  |
| H  | 4.836574  | 4.901864 | -0.947641 | H | 1.201534  | -0.444275 | 4.643085  |
| H  | 5.164205  | 4.096305 | -2.491672 | H | 2.408992  | -1.055731 | 2.613279  |
| H  | 2.817338  | 3.61216  | -2.836618 | H | 1.631097  | 0.472943  | 2.073175  |
| H  | 2.633784  | 5.091387 | -1.861115 | O | 0.913192  | -0.700518 | -1.618527 |
| C  | -0.641904 | 6.221906 | -0.264944 | C | 1.295864  | 0.234417  | -2.666141 |
| C  | -1.136468 | 6.333847 | 1.191796  | C | 2.437965  | -0.443345 | -3.433561 |
| N  | -2.576743 | 6.049773 | 1.375094  | C | 3.04243   | -1.380361 | -2.375441 |
| C  | -3.392052 | 7.179966 | 0.882305  | C | 1.795668  | -1.843556 | -1.625239 |
| H  | -3.199894 | 7.308871 | -0.185451 | H | 1.96649   | -2.130372 | -0.585629 |
| H  | -3.069917 | 8.115317 | 1.384202  | H | 1.303235  | -2.675069 | -2.14994  |
| C  | -4.890927 | 6.976182 | 1.116388  | H | 3.706576  | -0.824684 | -1.702234 |
| H  | -5.235283 | 6.122383 | 0.521597  | H | 3.609223  | -2.212144 | -2.804603 |
| H  | 0.416931  | 0.440547 | -3.283127 | H | 3.154786  | 0.281069  | -3.831504 |
| H  | 1.610419  | 1.164522 | -2.182734 | H | 2.047588  | -1.026147 | -4.276157 |

**Table 7 (Continued).**



**18d**

$G = -2343.3143$

$G_{MP2} = -2336.489847$

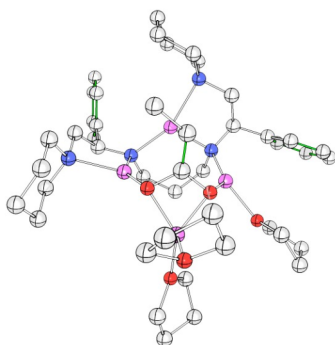
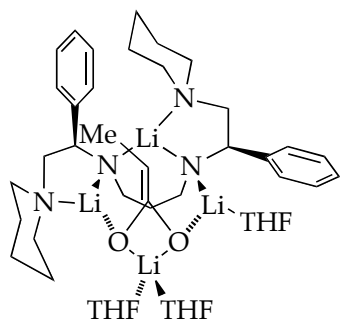
| Atom | X        | Y         | Z         | Atom | X         | Y        | Z         |
|------|----------|-----------|-----------|------|-----------|----------|-----------|
| Li   | 0        | 0         | 0         | H    | 7.645614  | 3.641382 | -0.784517 |
| O    | 1.744391 | -0.250609 | -0.730978 | H    | 8.342489  | 5.038169 | -1.599451 |
| Li   | 3.388671 | -0.027897 | 0.025207  | C    | 7.761593  | 3.421996 | -2.940522 |
| N    | 4.59745  | 1.180491  | 1.105349  | C    | 6.57078   | 2.474459 | -3.129316 |
| C    | 5.713022 | 0.281859  | 1.403162  | C    | 5.243163  | 3.235296 | -3.100426 |
| C    | 6.03644  | -0.609739 | 0.188456  | H    | 4.403462  | 2.536623 | -3.175431 |
| N    | 4.905395 | -1.46812  | -0.223405 | H    | 5.19299   | 3.914229 | -3.973737 |
| C    | 5.092879 | -1.953117 | -1.606478 | H    | 6.649878  | 1.930414 | -4.078897 |
| H    | 5.217138 | -1.078611 | -2.25501  | H    | 6.569163  | 1.720308 | -2.329827 |
| H    | 6.024359 | -2.548948 | -1.677897 | H    | 7.838711  | 4.083508 | -3.815806 |
| C    | 3.901071 | -2.787646 | -2.08212  | H    | 8.70211   | 2.859475 | -2.886786 |
| H    | 4.095165 | -3.136574 | -3.10448  | H    | 3.896085  | 5.653601 | -2.508127 |
| H    | 3.016452 | -2.140934 | -2.109096 | H    | 3.05385   | 4.099899 | -2.360732 |
| C    | 3.646154 | -3.971869 | -1.140887 | H    | 4.093997  | 5.60598  | 0.077587  |
| C    | 3.519178 | -3.468687 | 0.302386  | C    | 2.150223  | 6.150501 | -0.557834 |
| C    | 4.728213 | -2.613213 | 0.692974  | C    | 2.134292  | 7.248194 | 0.314199  |
| H    | 4.604452 | -2.229944 | 1.710125  | C    | 1.103767  | 8.19233  | 0.278798  |
| H    | 5.642661 | -3.23925  | 0.693095  | C    | 0.066585  | 8.062749 | -0.646084 |
| H    | 3.434978 | -4.308172 | 1.004631  | C    | 0.068053  | 6.976642 | -1.527041 |
| H    | 2.607493 | -2.864748 | 0.400312  | C    | 1.092644  | 6.030351 | -1.475597 |
| H    | 4.481659 | -4.685009 | -1.205959 | H    | 1.073395  | 5.194367 | -2.171997 |
| H    | 2.74235  | -4.517225 | -1.441029 | H    | -0.724847 | 6.873586 | -2.264718 |
| H    | 6.934333 | -1.220621 | 0.389641  | H    | -0.728084 | 8.803472 | -0.68857  |
| H    | 6.269585 | 0.034718  | -0.667009 | H    | 1.118155  | 9.034135 | 0.967359  |
| H    | 5.425795 | -0.39837  | 2.235298  | H    | 2.948883  | 7.366584 | 1.02612   |
| C    | 6.997922 | 0.960222  | 1.91124   | C    | 2.917289  | 3.968569 | 1.646133  |
| C    | 7.280952 | 0.986923  | 3.283656  | C    | 2.822609  | 2.581237 | 2.311488  |
| C    | 8.423115 | 1.618486  | 3.78134   | H    | 2.496525  | 2.724173 | 3.353053  |
| C    | 9.321727 | 2.229422  | 2.906921  | H    | 2.03131   | 1.995911 | 1.816953  |
| C    | 9.063566 | 2.202677  | 1.534432  | C    | 4.111221  | 1.74021  | 2.370751  |
| C    | 7.913381 | 1.579499  | 1.047936  | H    | 3.915047  | 0.917493 | 3.097293  |
| H    | 7.734687 | 1.565873  | -0.023445 | H    | 4.876071  | 2.367071 | 2.873098  |
| H    | 9.762507 | 2.663458  | 0.840052  | H    | 3.846716  | 4.461359 | 2.013394  |



**Table 7 (Continued).**

|    |           |          |           |   |           |           |           |
|----|-----------|----------|-----------|---|-----------|-----------|-----------|
| H  | 10.215365 | 2.717211 | 3.287906  | H | 2.097174  | 4.600055  | 2.055076  |
| H  | 8.611457  | 1.628976 | 4.852395  | O | -1.296112 | -1.181801 | -1.03688  |
| H  | 6.59206   | 0.501045 | 3.971845  | C | -0.697911 | -2.447374 | -1.429952 |
| Li | 4.414825  | 2.670136 | -0.205157 | C | -1.050727 | -2.643927 | -2.907723 |
| N  | 2.896122  | 3.861397 | 0.193288  | C | -1.181446 | -1.196051 | -3.40417  |
| Li | 1.097563  | 3.081587 | -0.236599 | C | -1.83567  | -0.510518 | -2.206474 |
| O  | 0.449104  | 1.55779  | -1.047592 | H | -2.927683 | -0.63604  | -2.208003 |
| C  | 1.422241  | 0.775702 | -1.541686 | H | -1.57789  | 0.54733   | -2.12096  |
| C  | 2.011496  | 0.966355 | -2.769245 | H | -1.777855 | -1.104128 | -4.317334 |
| H  | 2.719965  | 0.209015 | -3.100649 | H | -0.192715 | -0.757716 | -3.5781   |
| C  | 1.554134  | 1.993482 | -3.772807 | H | -2.004567 | -3.175791 | -3.011578 |
| H  | 2.376683  | 2.588689 | -4.200446 | H | -0.28422  | -3.214913 | -3.440298 |
| H  | 1.029133  | 1.549538 | -4.637286 | H | 0.383012  | -2.359727 | -1.277093 |
| H  | 0.852299  | 2.695328 | -3.307303 | H | -1.099757 | -3.232858 | -0.780574 |
| O  | -0.603113 | 3.792966 | 0.638387  | O | -0.699154 | -0.157071 | 1.838355  |
| C  | -0.785726 | 4.874061 | 1.589457  | C | -0.669514 | 0.900108  | 2.825154  |
| C  | -2.251875 | 5.3231   | 1.458799  | C | -1.924731 | 0.685057  | 3.667923  |
| C  | -2.924515 | 4.12404  | 0.768259  | C | -2.023284 | -0.848621 | 3.69442   |
| C  | -1.804824 | 3.632531 | -0.143813 | C | -1.555227 | -1.235818 | 2.285609  |
| H  | -1.735117 | 4.250677 | -1.050004 | H | -2.386472 | -1.320408 | 1.577948  |
| H  | -1.860655 | 2.58393  | -0.437789 | H | -0.982708 | -2.168946 | 2.265504  |
| H  | -3.83076  | 4.395727 | 0.218068  | H | -3.030631 | -1.216093 | 3.911336  |
| H  | -3.187073 | 3.349219 | 1.499352  | H | -1.344354 | -1.257101 | 4.451778  |
| H  | -2.317213 | 6.211194 | 0.821377  | H | -2.799766 | 1.118209  | 3.167891  |
| H  | -2.69786  | 5.570153 | 2.426972  | H | -1.844059 | 1.130453  | 4.664041  |
| H  | -0.560647 | 4.471811 | 2.583728  | H | 0.242247  | 0.803373  | 3.428691  |
| H  | -0.07593  | 5.671941 | 1.362388  | H | -0.640012 | 1.850234  | 2.286905  |
| C  | 3.270466  | 5.102327 | -0.471867 | C | 6.19669   | 4.956995  | -1.683165 |
| C  | 3.790609  | 4.751017 | -1.881199 | H | 6.050339  | 5.507274  | -0.749063 |
| N  | 5.074496  | 4.005381 | -1.84654  | H | 6.165716  | 5.699344  | -2.504444 |
| C  | 7.562565  | 4.270006 | -1.678021 |   |           |           |           |

**Table 7 (Continued).**



**18e**

$G = -2343.31295$

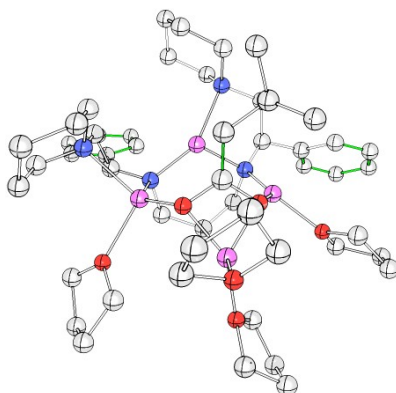
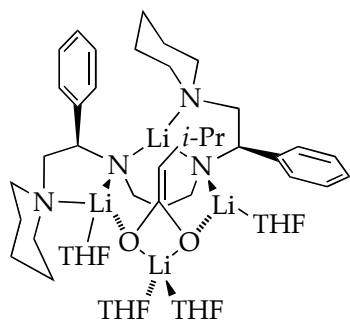
$G_{\text{MP2}} = -2336.487764$

| Atom | X         | Y         | Z         | Atom | X         | Y        | Z         |
|------|-----------|-----------|-----------|------|-----------|----------|-----------|
| Li   | 0         | 0         | 0         | C    | -3.788972 | 4.871206 | 1.596392  |
| O    | -1.757742 | -0.282225 | 0.704321  | N    | -5.041787 | 4.079239 | 1.626579  |
| Li   | -3.301221 | -0.135159 | -0.274007 | C    | -6.19997  | 4.95726  | 1.34739   |
| N    | -4.541793 | 1.113307  | -1.288289 | H    | -6.068314 | 5.402924 | 0.357316  |
| C    | -5.673364 | 0.2276    | -1.583424 | H    | -6.211452 | 5.789764 | 2.078575  |
| C    | -5.872114 | -0.820403 | -0.47241  | C    | -7.532199 | 4.209758 | 1.406878  |
| N    | -4.704154 | -1.710182 | -0.289379 | H    | -7.570404 | 3.482827 | 0.589042  |
| C    | -4.833854 | -2.470894 | 0.970894  | H    | -8.346064 | 4.925487 | 1.23325   |
| H    | -4.961021 | -1.751883 | 1.786575  | C    | -7.714291 | 3.496477 | 2.752205  |
| H    | -5.745924 | -3.099231 | 0.941141  | C    | -6.483234 | 2.635903 | 3.06225   |
| C    | -3.60641  | -3.346867 | 1.23324   | C    | -5.196842 | 3.457713 | 2.960811  |
| H    | -3.753049 | -3.896576 | 2.171737  | H    | -4.321797 | 2.824774 | 3.134027  |
| H    | -2.738761 | -2.688869 | 1.363251  | H    | -5.203247 | 4.240622 | 3.744784  |
| C    | -3.359719 | -4.312809 | 0.068407  | H    | -6.552036 | 2.201602 | 4.067483  |
| C    | -3.300075 | -3.530358 | -1.248508 | H    | -6.427839 | 1.794711 | 2.356737  |
| C    | -4.537531 | -2.644038 | -1.421707 | H    | -7.840691 | 4.244269 | 3.549022  |
| H    | -4.451566 | -2.065455 | -2.344931 | H    | -8.625964 | 2.885579 | 2.747333  |
| H    | -5.439494 | -3.280095 | -1.519812 | H    | -3.917541 | 5.804981 | 2.172502  |
| H    | -3.227182 | -4.210544 | -2.106851 | H    | -3.024949 | 4.271749 | 2.102618  |
| H    | -2.402655 | -2.896592 | -1.259125 | H    | -4.126593 | 5.644547 | -0.391506 |
| H    | -4.177125 | -5.047387 | 0.017924  | C    | -2.179684 | 6.223612 | 0.197407  |
| H    | -2.433975 | -4.881129 | 0.223959  | C    | -2.189647 | 7.293238 | -0.708919 |
| H    | -6.782669 | -1.413881 | -0.670441 | C    | -1.168156 | 8.24769  | -0.722493 |
| H    | -6.024277 | -0.305233 | 0.484213  | C    | -0.11383  | 8.158119 | 0.187527  |
| H    | -5.452608 | -0.338146 | -2.513122 | C    | -0.088728 | 7.10027  | 1.101884  |
| C    | -7.012774 | 0.91837   | -1.897919 | C    | -1.104063 | 6.142722 | 1.09817   |
| C    | -7.368781 | 1.167414  | -3.231875 | H    | -1.063505 | 5.328261 | 1.818747  |
| C    | -8.570555 | 1.797152  | -3.56254  | H    | 0.717699  | 7.028702 | 1.828647  |
| C    | -9.460629 | 2.176735  | -2.557769 | H    | 0.67369   | 8.907627 | 0.192634  |
| C    | -9.131975 | 1.9235    | -1.224558 | H    | -1.203111 | 9.066582 | -1.437428 |
| C    | -7.919967 | 1.30953   | -0.901885 | H    | -3.018003 | 7.381346 | -1.409258 |
| H    | -7.689927 | 1.119624  | 0.143369  | C    | -2.929053 | 3.972264 | -1.9106   |
| H    | -9.823234 | 2.200609  | -0.431968 | C    | -2.833521 | 2.569815 | -2.539225 |

**Table 7 (Continued).**

|    |            |           |           |   |           |           |           |
|----|------------|-----------|-----------|---|-----------|-----------|-----------|
| H  | -10.402618 | 2.657491  | -2.809123 | H | -2.525655 | 2.690039  | -3.589111 |
| H  | -8.81452   | 1.981592  | -4.60617  | H | -2.030049 | 1.999874  | -2.04557  |
| H  | -6.693959  | 0.85002   | -4.023875 | C | -4.120968 | 1.725612  | -2.554905 |
| Li | -4.339104  | 2.625047  | 0.0459    | H | -3.965773 | 0.929855  | -3.320299 |
| N  | -2.92217   | 3.904182  | -0.457317 | H | -4.910816 | 2.369615  | -2.99314  |
| Li | -1.139556  | 3.131917  | 0.001262  | H | -3.853669 | 4.456492  | -2.299625 |
| O  | -0.569228  | 1.620293  | 0.854053  | H | -2.103553 | 4.590958  | -2.328914 |
| C  | -1.517856  | 0.841738  | 1.40573   | O | 1.348442  | -0.962829 | 1.181212  |
| C  | -2.137546  | 1.149045  | 2.592488  | C | 0.7925    | -2.170615 | 1.769917  |
| H  | -1.810459  | 2.058698  | 3.092652  | C | 1.216007  | -2.156016 | 3.240111  |
| C  | -3.052992  | 0.216079  | 3.342642  | C | 1.293987  | -0.650468 | 3.535895  |
| H  | -2.696914  | 0.016586  | 4.367101  | C | 1.861041  | -0.096173 | 2.229369  |
| H  | -4.088984  | 0.581038  | 3.457623  | H | 2.958875  | -0.137703 | 2.20632   |
| H  | -3.109051  | -0.749604 | 2.829663  | H | 1.515671  | 0.916998  | 2.011471  |
| O  | 0.578278   | 3.800154  | -0.866851 | H | 1.922991  | -0.41127  | 4.399171  |
| C  | 0.772361   | 4.840752  | -1.860356 | H | 0.293412  | -0.23692  | 3.701915  |
| C  | 2.223956   | 5.322462  | -1.703154 | H | 2.199133  | -2.626488 | 3.365647  |
| C  | 2.901183   | 4.150359  | -0.972886 | H | 0.501823  | -2.684212 | 3.878918  |
| C  | 1.772388   | 3.662521  | -0.069356 | H | -0.295877 | -2.120364 | 1.659063  |
| H  | 1.685504   | 4.290711  | 0.828291  | H | 1.181169  | -3.029714 | 1.212724  |
| H  | 1.83809    | 2.61839   | 0.239075  | O | 0.726726  | -0.259316 | -1.8149   |
| H  | 3.792932   | 4.447847  | -0.412472 | C | 0.708252  | 0.752711  | -2.84808  |
| H  | 3.188905   | 3.363597  | -1.681407 | C | 1.999481  | 0.533963  | -3.63391  |
| H  | 2.255334   | 6.22377   | -1.081999 | C | 2.137758  | -0.996316 | -3.588258 |
| H  | 2.688576   | 5.559343  | -2.665094 | C | 1.622974  | -1.335231 | -2.183016 |
| H  | 0.588994   | 4.390621  | -2.842844 | H | 2.42742   | -1.370986 | -1.440783 |
| H  | 0.040252   | 5.632827  | -1.692173 | H | 1.070511  | -2.279967 | -2.145581 |
| C  | -3.294778  | 5.164824  | 0.165954  | H | 3.162063  | -1.345155 | -3.749313 |
| H  | 1.945404   | 0.932837  | -4.651283 | H | 1.500725  | -1.45549  | -4.352925 |
| H  | -0.177178  | 0.605636  | -3.480306 | H | 2.843812  | 1.011918  | -3.122044 |
| H  | 0.635034   | 1.724922  | -2.355325 |   |           |           |           |

**Table 7 (Continued).**



**19a**

$G = -2654.226423$

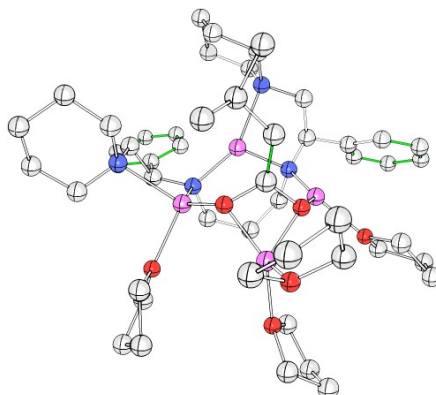
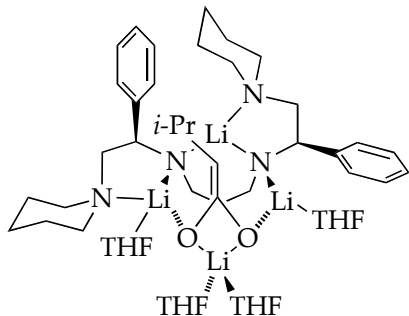
$G_{\text{MP2}} = -2646.519504$

| Atom | X         | Y         | Z         | Atom | X         | Y        | Z         |
|------|-----------|-----------|-----------|------|-----------|----------|-----------|
| Li   | 0         | 0         | 0         | N    | -4.33861  | 4.868299 | 1.547182  |
| O    | -1.801982 | 0.010218  | 0.671399  | C    | -5.498829 | 5.657151 | 1.074219  |
| Li   | -3.419912 | 0.105857  | -0.284712 | H    | -5.389397 | 5.82968  | 0.000131  |
| N    | -4.337029 | 1.792017  | -1.109374 | H    | -5.490621 | 6.651287 | 1.563749  |
| C    | -5.686088 | 1.279835  | -1.225901 | C    | -6.835941 | 4.966468 | 1.356457  |
| C    | -6.159273 | 0.806522  | 0.16869   | H    | -6.895173 | 4.041258 | 0.772509  |
| N    | -5.432217 | -0.391662 | 0.645417  | H    | -7.647485 | 5.613131 | 1.000135  |
| C    | -5.359577 | -0.424925 | 2.119642  | C    | -6.999487 | 4.652148 | 2.847144  |
| H    | -4.87008  | 0.495234  | 2.453211  | C    | -5.777008 | 3.872239 | 3.342554  |
| H    | -6.378555 | -0.440292 | 2.556376  | C    | -4.481028 | 4.60666  | 2.997494  |
| C    | -4.56719  | -1.638589 | 2.613114  | H    | -3.617907 | 4.018448 | 3.315345  |
| H    | -4.54656  | -1.630976 | 3.710403  | H    | -4.450961 | 5.564195 | 3.554442  |
| H    | -3.531834 | -1.535098 | 2.265507  | H    | -5.819503 | 3.720696 | 4.428657  |
| C    | -5.172767 | -2.947495 | 2.090837  | H    | -5.761137 | 2.875359 | 2.882813  |
| C    | -5.328997 | -2.880941 | 0.566535  | H    | -7.086979 | 5.590022 | 3.415375  |
| C    | -6.086674 | -1.617399 | 0.151811  | H    | -7.922617 | 4.086632 | 3.024723  |
| H    | -6.156166 | -1.555044 | -0.938166 | H    | -3.188221 | 6.653702 | 1.699922  |
| H    | -7.125346 | -1.670135 | 0.537038  | H    | -2.314683 | 5.132744 | 1.947209  |
| H    | -5.866633 | -3.761917 | 0.191315  | H    | -3.408625 | 6.009754 | -0.764272 |
| H    | -4.342124 | -2.868474 | 0.088381  | C    | -1.448244 | 6.641329 | -0.302813 |
| H    | -6.160674 | -3.103838 | 2.549349  | C    | -1.404024 | 7.452023 | -1.446339 |
| H    | -4.552608 | -3.8058   | 2.379983  | C    | -0.371196 | 8.370916 | -1.65166  |
| H    | -7.246889 | 0.623768  | 0.181929  | C    | 0.639606  | 8.512133 | -0.699868 |
| H    | -5.963807 | 1.624113  | 0.871632  | C    | 0.61059   | 7.716154 | 0.449254  |
| H    | -5.722634 | 0.385672  | -1.892607 | C    | -0.413629 | 6.786193 | 0.636748  |
| C    | -6.756725 | 2.220963  | -1.827045 | H    | -0.410889 | 6.176837 | 1.537534  |
| C    | -7.970069 | 1.694748  | -2.295329 | H    | 1.382577  | 7.827866 | 1.207812  |
| C    | -8.961085 | 2.517149  | -2.830853 | H    | 1.435726  | 9.238013 | -0.84564  |
| C    | -8.750421 | 3.895241  | -2.924123 | H    | -0.364472 | 8.9847   | -2.549546 |
| C    | -7.542893 | 4.432393  | -2.477309 | H    | -2.20027  | 7.364621 | -2.182913 |
| C    | -6.559059 | 3.601149  | -1.934317 | C    | -2.242839 | 4.101367 | -1.978089 |
| H    | -5.613102 | 4.014609  | -1.597345 | C    | -2.343965 | 2.625143 | -2.418554 |
| H    | -7.360691 | 5.501827  | -2.558813 | H    | -1.948763 | 2.547274 | -3.443441 |

**Table 7 (Continued).**

|    |           |           |           |   |           |           |           |
|----|-----------|-----------|-----------|---|-----------|-----------|-----------|
| H  | -9.516    | 4.540099  | -3.348492 | H | -1.690704 | 2.007134  | -1.782699 |
| H  | -9.894983 | 2.083268  | -3.181297 | C | -3.756221 | 2.013557  | -2.430622 |
| H  | -8.139178 | 0.619604  | -2.241986 | H | -3.690244 | 1.06129   | -3.006761 |
| Li | -3.712808 | 3.141389  | 0.186731  | H | -4.381837 | 2.669237  | -3.068851 |
| N  | -2.254794 | 4.257323  | -0.526932 | H | -3.08615  | 4.65113   | -2.452037 |
| Li | -0.61906  | 3.286675  | 0.084817  | H | -1.335776 | 4.537541  | -2.455543 |
| O  | -0.298073 | 1.664903  | 0.899642  | O | -3.170004 | -1.501478 | -1.787968 |
| C  | -1.348393 | 1.016293  | 1.436547  | C | -1.949338 | -2.277792 | -1.787594 |
| C  | -1.859086 | 1.31046   | 2.680968  | C | -2.036522 | -3.22955  | -2.991479 |
| H  | -2.655434 | 0.666151  | 3.04466   | C | -3.024351 | -2.50407  | -3.917725 |
| C  | -1.327921 | 2.355115  | 3.648114  | C | -3.988706 | -1.890475 | -2.905863 |
| H  | -1.459724 | 3.372079  | 3.2314    | H | -4.735388 | -2.628534 | -2.577235 |
| C  | -2.121801 | 2.302285  | 4.964968  | H | -4.505507 | -0.999048 | -3.266223 |
| H  | -1.80426  | 3.087752  | 5.662613  | H | -3.523282 | -3.169572 | -4.628915 |
| H  | -3.199757 | 2.41239   | 4.795938  | H | -2.517478 | -1.713087 | -4.483103 |
| H  | -1.969954 | 1.333545  | 5.459824  | H | -2.44525  | -4.201408 | -2.690322 |
| C  | 0.176775  | 2.235829  | 3.967287  | H | -1.059126 | -3.40632  | -3.451633 |
| H  | 0.514376  | 3.062139  | 4.610301  | H | -1.108657 | -1.583224 | -1.875724 |
| H  | 0.388099  | 1.296555  | 4.495344  | H | -1.868285 | -2.805236 | -0.832382 |
| H  | 0.759341  | 2.250903  | 3.0429    | O | 0.992855  | -1.444214 | 1.085968  |
| O  | 1.219912  | 3.818908  | -0.556329 | C | 1.630231  | -0.928991 | 2.285415  |
| C  | 1.621953  | 4.750681  | -1.592227 | C | 0.877571  | -1.562037 | 3.45457   |
| C  | 3.050962  | 5.177702  | -1.241171 | C | 0.482184  | -2.928826 | 2.877586  |
| C  | 3.574888  | 3.96942   | -0.448593 | C | 0.138057  | -2.56907  | 1.431422  |
| C  | 2.329495  | 3.547469  | 0.329229  | H | -0.899638 | -2.234496 | 1.330045  |
| H  | 2.212444  | 4.144801  | 1.243522  | H | 0.33987   | -3.378071 | 0.720786  |
| H  | 2.284698  | 2.490585  | 0.598399  | H | -0.362554 | -3.388829 | 3.399152  |
| H  | 4.416656  | 4.211624  | 0.207439  | H | 1.327968  | -3.626604 | 2.915161  |
| H  | 3.892881  | 3.169054  | -1.128871 | H | -0.015468 | -0.968251 | 3.675526  |
| H  | 3.029661  | 6.070037  | -0.606408 | H | 1.490077  | -1.631322 | 4.358864  |
| H  | 3.646519  | 5.40775   | -2.129945 | H | 2.688295  | -1.226057 | 2.27048   |
| H  | 1.580141  | 4.222226  | -2.553868 | H | 1.552217  | 0.159539  | 2.259681  |
| H  | 0.91171   | 5.578072  | -1.612018 | O | 0.97979   | -0.192806 | -1.73742  |
| C  | -2.585025 | 5.61706   | -0.130144 | C | 1.088099  | 0.910925  | -2.679293 |
| C  | -3.077966 | 5.618544  | 1.329185  | C | 2.377479  | 0.663953  | -3.482277 |
| H  | 3.893295  | -0.909062 | -3.134878 | C | 3.168519  | -0.301978 | -2.583918 |
| H  | 2.915157  | 1.592894  | -3.694165 | C | 2.047871  | -1.133209 | -1.967389 |
| H  | 2.149894  | 0.185801  | -4.441861 | H | 2.285622  | -1.589165 | -1.005205 |
| H  | 0.191637  | 0.927347  | -3.305986 | H | 1.705437  | -1.913496 | -2.66385  |
| H  | 1.123142  | 1.832023  | -2.091683 | H | 3.70471   | 0.246506  | -1.800111 |

**Table 7 (Continued).**



**19b**

$G = -2654.219649$

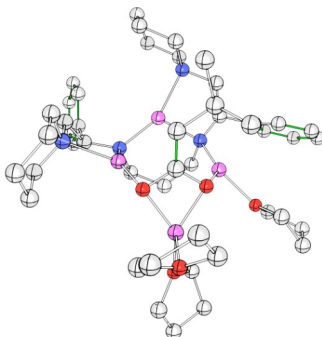
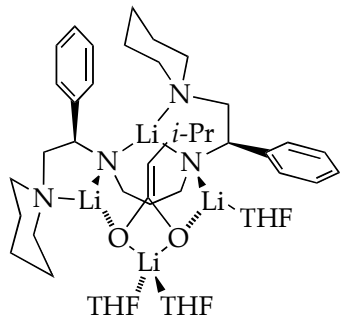
$G_{MP2} = -2646.512427$

| Atom | X         | Y         | Z         | Atom | X         | Y         | Z         |
|------|-----------|-----------|-----------|------|-----------|-----------|-----------|
| Li   | 0         | 0         | 0         | H    | -2.937466 | 3.884474  | 3.265453  |
| O    | -1.771088 | 0.3282    | 0.768126  | H    | -3.486965 | 5.470385  | 3.8526    |
| Li   | -3.224899 | 0.682348  | -0.403928 | H    | -5.239575 | 3.257715  | 2.657813  |
| N    | -3.84867  | 2.495193  | -1.276226 | H    | -5.182393 | 3.762405  | 4.344798  |
| C    | -5.240311 | 2.205544  | -1.553261 | H    | -7.161012 | 4.76691   | 3.083621  |
| H    | -5.331531 | 1.419825  | -2.340885 | H    | -6.085102 | 5.99511   | 3.750374  |
| C    | -6.107247 | 3.368133  | -2.096178 | H    | -6.116749 | 4.997417  | 0.846992  |
| C    | -7.296365 | 3.093461  | -2.78738  | H    | -6.592672 | 6.597405  | 1.401661  |
| C    | -8.118415 | 4.117966  | -3.256754 | H    | -2.046657 | 6.728007  | 2.185646  |
| C    | -7.757215 | 5.452102  | -3.053644 | H    | -1.440968 | 5.061355  | 2.173993  |
| C    | -6.568664 | 5.742425  | -2.382936 | H    | -2.317603 | 6.522006  | -0.360526 |
| C    | -5.754956 | 4.708849  | -1.911321 | C    | -0.284375 | 6.733008  | 0.178488  |
| H    | -4.818532 | 4.932253  | -1.407852 | C    | -0.082003 | 7.696299  | -0.820239 |
| H    | -6.267841 | 6.777117  | -2.233339 | C    | 1.104905  | 8.43053   | -0.897185 |
| H    | -8.390398 | 6.254767  | -3.423538 | C    | 2.116583  | 8.226807  | 0.042188  |
| H    | -9.037033 | 3.876489  | -3.786924 | C    | 1.931115  | 7.274362  | 1.049074  |
| H    | -7.579574 | 2.056244  | -2.96485  | C    | 0.750744  | 6.531512  | 1.106957  |
| C    | -5.935771 | 1.646996  | -0.290138 | H    | 0.631632  | 5.794738  | 1.898283  |
| N    | -5.41763  | 0.319695  | 0.112215  | H    | 2.703926  | 7.118157  | 1.798892  |
| C    | -5.609434 | 0.035807  | 1.549669  | H    | 3.034446  | 8.807766  | -0.002569 |
| H    | -4.997405 | -0.842998 | 1.79306   | H    | 1.232811  | 9.169981  | -1.684506 |
| H    | -5.194909 | 0.87083   | 2.120955  | H    | -0.874117 | 7.877013  | -1.544302 |
| C    | -7.066418 | -0.237622 | 1.960647  | C    | -1.450332 | 4.609943  | -1.83613  |
| C    | -7.652794 | -1.38845  | 1.130099  | C    | -1.700647 | 3.211048  | -2.438348 |
| C    | -7.461856 | -1.114562 | -0.369073 | H    | -1.287476 | 3.194599  | -3.45883  |
| C    | -5.99063  | -0.785871 | -0.686023 | H    | -1.136031 | 2.462278  | -1.861246 |
| H    | -5.870666 | -0.5471   | -1.746533 | C    | -3.170068 | 2.76987   | -2.54342  |
| H    | -5.379111 | -1.675956 | -0.488801 | H    | -3.197245 | 1.876262  | -3.209654 |
| H    | -7.77002  | -1.983624 | -0.965697 | H    | -3.688246 | 3.553369  | -3.131469 |
| H    | -8.109307 | -0.282927 | -0.677179 | H    | -2.222396 | 5.299114  | -2.246058 |
| H    | -8.713611 | -1.541684 | 1.365325  | H    | -0.494072 | 4.997244  | -2.254255 |
| H    | -7.133878 | -2.322324 | 1.395127  | O    | -2.955999 | -0.949805 | -1.743837 |
| H    | -7.671434 | 0.668781  | 1.820173  | C    | -2.543013 | -2.214345 | -1.195807 |

**Table 7 (Continued).**

|    |           |           |           |   |           |           |           |
|----|-----------|-----------|-----------|---|-----------|-----------|-----------|
| H  | -7.101043 | -0.475012 | 3.031918  | C | -1.800866 | -2.914278 | -2.331949 |
| H  | -7.025658 | 1.63781   | -0.436191 | C | -2.62905  | -2.474657 | -3.550192 |
| H  | -5.734228 | 2.342676  | 0.533135  | C | -3.017822 | -1.033663 | -3.183631 |
| Li | -3.118134 | 3.653993  | 0.148646  | H | -4.026165 | -0.763528 | -3.514306 |
| N  | -1.471745 | 4.582578  | -0.38003  | H | -2.315415 | -0.300567 | -3.595263 |
| Li | -0.020109 | 3.329902  | 0.149461  | H | -3.522002 | -3.10323  | -3.647709 |
| O  | 0.02992   | 1.665839  | 0.89921   | H | -2.078022 | -2.528341 | -4.49408  |
| C  | -1.078643 | 1.197105  | 1.515754  | H | -1.756947 | -4.000813 | -2.206629 |
| C  | -1.372394 | 1.546239  | 2.814247  | H | -0.77921  | -2.526051 | -2.403408 |
| H  | -0.669664 | 2.228877  | 3.289197  | H | -1.944341 | -2.000339 | -0.308408 |
| C  | -2.499354 | 1.013993  | 3.681187  | H | -3.429462 | -2.79211  | -0.892073 |
| H  | -3.478622 | 1.360942  | 3.305764  | O | 0.909123  | -0.406907 | -1.760797 |
| C  | -2.366344 | 1.556601  | 5.11483   | C | 1.952139  | -1.395798 | -1.905197 |
| H  | -3.190868 | 1.214352  | 5.753426  | C | 3.113715  | -0.655997 | -2.562751 |
| H  | -1.426277 | 1.213362  | 5.567623  | C | 2.372649  | 0.296096  | -3.514875 |
| H  | -2.355435 | 2.653242  | 5.135509  | C | 1.126722  | 0.679534  | -2.704113 |
| C  | -2.583511 | -0.524549 | 3.728538  | H | 0.228788  | 0.792855  | -3.318124 |
| H  | -1.698348 | -0.941818 | 4.228369  | H | 1.274928  | 1.595387  | -2.124057 |
| H  | -3.469612 | -0.862858 | 4.285719  | H | 2.091452  | -0.231703 | -4.433744 |
| H  | -2.628837 | -0.929422 | 2.71415   | H | 2.963507  | 1.171544  | -3.800342 |
| O  | 1.8633    | 3.591476  | -0.540549 | H | 3.807035  | -1.329514 | -3.075765 |
| C  | 2.937824  | 3.125887  | 0.302128  | H | 3.677355  | -0.090053 | -1.811092 |
| C  | 4.21155   | 3.373968  | -0.503221 | H | 2.161785  | -1.789739 | -0.909742 |
| C  | 3.868257  | 4.685788  | -1.227618 | H | 1.590765  | -2.211494 | -2.548486 |
| C  | 2.372065  | 4.525654  | -1.52673  | O | 1.070644  | -1.327349 | 1.178718  |
| H  | 2.196078  | 4.089901  | -2.518346 | C | 1.916663  | -0.630955 | 2.137245  |
| H  | 1.813574  | 5.45971   | -1.446886 | C | 1.504379  | -1.152468 | 3.514067  |
| H  | 4.4583    | 4.848302  | -2.134763 | C | 1.025383  | -2.578015 | 3.199724  |
| H  | 4.028026  | 5.540652  | -0.561967 | C | 0.344077  | -2.390768 | 1.843213  |
| H  | 4.37368   | 2.563049  | -1.224834 | H | -0.698591 | -2.07578  | 1.955678  |
| H  | 5.101462  | 3.4483    | 0.129479  | H | 0.389222  | -3.280776 | 1.20587   |
| H  | 2.941846  | 3.705311  | 1.235924  | H | 0.339897  | -2.978152 | 3.952755  |
| H  | 2.736113  | 2.080813  | 0.542335  | H | 1.877162  | -3.263882 | 3.113025  |
| C  | -1.582961 | 5.908105  | 0.204537  | H | 0.678286  | -0.54554  | 3.896959  |
| C  | -2.097959 | 5.763556  | 1.649589  | H | 2.32739   | -1.123247 | 4.235094  |
| N  | -3.469727 | 5.205722  | 1.739844  | H | 2.96307   | -0.872816 | 1.903701  |
| C  | -4.470341 | 6.256943  | 1.449914  | H | 1.733605  | 0.438146  | 2.008515  |
| H  | -4.306951 | 6.620665  | 0.431239  | C | -6.151092 | 5.188379  | 3.005413  |
| H  | -4.306755 | 7.116787  | 2.129266  | C | -5.090947 | 4.125598  | 3.313724  |
| C  | -5.91059  | 5.762203  | 1.605059  | C | -3.67808  | 4.673834  | 3.106437  |

**Table 7 (Continued).**



**19c**  
 $G = -2421.883415$   
 $G_{MP2} = -2414.824252$

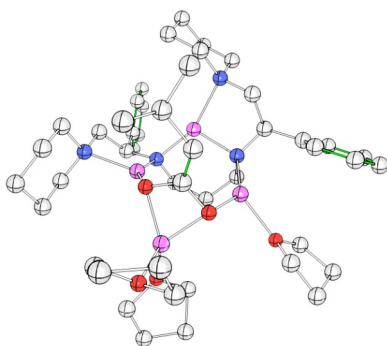
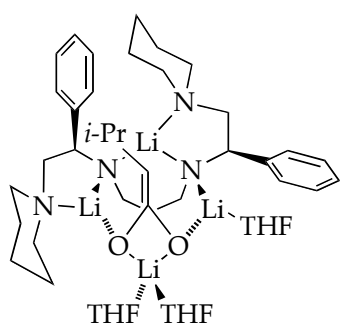
| Atom | X         | Y         | Z         | Atom | X         | Y         | Z         |
|------|-----------|-----------|-----------|------|-----------|-----------|-----------|
| Li   | 0         | 0         | 0         | C    | 8.211863  | 3.40249   | -2.725219 |
| O    | 1.639082  | -0.475164 | -0.826728 | C    | 7.014945  | 2.565568  | -3.193394 |
| Li   | 3.392062  | -0.228813 | -0.337006 | C    | 5.731095  | 3.397766  | -3.1997   |
| N    | 4.671693  | 0.912353  | 0.765336  | H    | 4.87801   | 2.779007  | -3.493445 |
| C    | 5.738821  | -0.053727 | 1.031761  | H    | 5.82328   | 4.205461  | -3.951723 |
| C    | 6.014157  | -0.915436 | -0.215786 | H    | 7.186787  | 2.164559  | -4.200187 |
| N    | 4.851061  | -1.727773 | -0.632181 | H    | 6.879561  | 1.703959  | -2.525056 |
| C    | 5.020154  | -2.199042 | -2.022489 | H    | 8.426256  | 4.175772  | -3.477475 |
| H    | 5.157685  | -1.319001 | -2.660796 | H    | 9.113317  | 2.781937  | -2.646164 |
| H    | 5.939602  | -2.811786 | -2.106541 | H    | 4.390267  | 5.735167  | -2.448958 |
| C    | 3.813179  | -3.008641 | -2.504612 | H    | 3.47973   | 4.218593  | -2.551238 |
| H    | 3.999609  | -3.34691  | -3.53193  | H    | 4.325906  | 5.45327   | 0.106963  |
| H    | 2.935781  | -2.3523   | -2.523996 | C    | 2.46881   | 6.098417  | -0.667438 |
| C    | 3.538827  | -4.198956 | -1.57749  | C    | 2.457104  | 7.19031   | 0.211413  |
| C    | 3.418983  | -3.705885 | -0.130713 | C    | 1.476802  | 8.183754  | 0.126804  |
| C    | 4.646011  | -2.881842 | 0.268962  | C    | 0.488331  | 8.109512  | -0.855613 |
| H    | 4.529676  | -2.509871 | 1.290762  | C    | 0.486173  | 7.028973  | -1.743527 |
| H    | 5.5469    | -3.527328 | 0.260846  | C    | 1.459881  | 6.034413  | -1.643069 |
| H    | 3.316285  | -4.549424 | 0.564219  | H    | 1.44072   | 5.203589  | -2.345647 |
| H    | 2.522671  | -3.080914 | -0.029205 | H    | -0.269441 | 6.967435  | -2.523708 |
| H    | 4.363053  | -4.924373 | -1.649986 | H    | -0.266351 | 8.887929  | -0.936126 |
| H    | 2.626549  | -4.725757 | -1.884833 | H    | 1.492761  | 9.019825  | 0.822227  |
| H    | 6.895896  | -1.559835 | -0.050571 | H    | 3.235662  | 7.265132  | 0.968301  |
| H    | 6.250732  | -0.251631 | -1.05615  | C    | 3.048065  | 3.728465  | 1.438184  |
| H    | 5.409151  | -0.747394 | 1.836176  | C    | 2.913694  | 2.30144   | 2.005807  |
| C    | 7.056584  | 0.528157  | 1.576355  | H    | 2.563573  | 2.388045  | 3.045766  |
| C    | 7.26922   | 0.588448  | 2.961511  | H    | 2.126977  | 1.757495  | 1.459786  |
| C    | 8.442727  | 1.121945  | 3.498279  | C    | 4.187444  | 1.435438  | 2.046619  |
| C    | 9.447097  | 1.594687  | 2.653329  | H    | 3.967935  | 0.590909  | 2.740437  |
| C    | 9.261229  | 1.529849  | 1.271048  | H    | 4.958595  | 2.029781  | 2.579142  |
| C    | 8.077894  | 1.008838  | 0.743516  | H    | 3.957687  | 4.187713  | 1.887446  |
| H    | 7.960228  | 0.962997  | -0.335675 | H    | 2.209183  | 4.336202  | 1.847642  |
| H    | 10.042072 | 1.880412  | 0.599939  | O    | -1.425238 | -1.223059 | -0.820651 |



**Table 7 (Continued).**

|    |           |           |           |   |           |           |           |
|----|-----------|-----------|-----------|---|-----------|-----------|-----------|
| H  | 10.366729 | 2.00248   | 3.065235  | C | -0.891965 | -2.53393  | -1.157679 |
| H  | 8.574656  | 1.159949  | 4.577126  | C | -1.487867 | -2.889403 | -2.521245 |
| H  | 6.501484  | 0.201037  | 3.627838  | C | -1.648503 | -1.506059 | -3.168826 |
| Li | 4.580588  | 2.486575  | -0.447896 | C | -2.078094 | -0.645999 | -1.980351 |
| N  | 3.105556  | 3.731262  | -0.020036 | H | -3.164822 | -0.682162 | -1.821568 |
| Li | 1.277763  | 3.022679  | -0.477598 | H | -1.752342 | 0.393815  | -2.060312 |
| O  | 0.553438  | 1.465751  | -1.158627 | H | -2.380456 | -1.489323 | -3.982286 |
| C  | 1.422462  | 0.569445  | -1.646244 | H | -0.688105 | -1.149931 | -3.555303 |
| C  | 2.037203  | 0.682521  | -2.873049 | H | -2.463487 | -3.377276 | -2.404579 |
| H  | 2.641388  | -0.162443 | -3.197667 | H | -0.838515 | -3.559601 | -3.092553 |
| C  | 1.76838   | 1.770778  | -3.895501 | H | 0.198556  | -2.443494 | -1.196635 |
| H  | 2.012559  | 2.761911  | -3.470246 | H | -1.178128 | -3.230241 | -0.362237 |
| C  | 2.661383  | 1.57449   | -5.13148  | O | -0.627841 | 0.046437  | 1.872955  |
| H  | 2.527732  | 2.381869  | -5.862544 | C | -0.672882 | 1.208247  | 2.725891  |
| H  | 3.723375  | 1.530909  | -4.861457 | C | -1.988949 | 1.067386  | 3.485677  |
| H  | 2.415832  | 0.627913  | -5.631721 | C | -2.040783 | -0.449446 | 3.740043  |
| C  | 0.293326  | 1.852573  | -4.341544 | C | -1.364135 | -1.038417 | 2.487673  |
| H  | 0.125438  | 2.692777  | -5.031864 | H | -2.081079 | -1.400072 | 1.745558  |
| H  | -0.00307  | 0.930523  | -4.859299 | H | -0.667465 | -1.848581 | 2.731198  |
| H  | -0.355702 | 1.981587  | -3.470935 | H | -3.058259 | -0.827607 | 3.875464  |
| O  | -0.42263  | 3.871277  | 0.291664  | H | -1.469136 | -0.700194 | 4.64051   |
| C  | -0.61571  | 4.96508   | 1.225559  | H | -2.826719 | 1.38322   | 2.852217  |
| C  | -2.037984 | 5.493002  | 0.98193   | H | -2.012787 | 1.657469  | 4.40687   |
| C  | -2.737981 | 4.298443  | 0.312742  | H | 0.188334  | 1.198045  | 3.407679  |
| C  | -1.604278 | 3.711391  | -0.522973 | H | -0.605294 | 2.086304  | 2.080395  |
| H  | -1.476032 | 4.270538  | -1.460393 | N | 5.436683  | 3.971974  | -1.868599 |
| H  | -1.692138 | 2.650218  | -0.75817  | C | 6.565959  | 4.827365  | -1.436926 |
| H  | -3.602225 | 4.587837  | -0.29319  | H | 6.332585  | 5.239623  | -0.451494 |
| H  | -3.07502  | 3.573286  | 1.064146  | H | 6.659251  | 5.683354  | -2.133614 |
| H  | -2.008237 | 6.346592  | 0.296618  | C | 7.892981  | 4.070036  | -1.381647 |
| H  | -2.523932 | 5.81841   | 1.906789  | H | 7.843762  | 3.315636  | -0.589192 |
| H  | -0.495365 | 4.558099  | 2.23689   | H | 8.687085  | 4.773547  | -1.100583 |
| H  | 0.155221  | 5.71802   | 1.053849  | C | 4.192966  | 4.777351  | -1.936035 |
| C  | 3.55065   | 5.011549  | -0.552638 |   |           |           |           |

**Table 7 (Continued).**



**19d**

$G = -2421.881353$

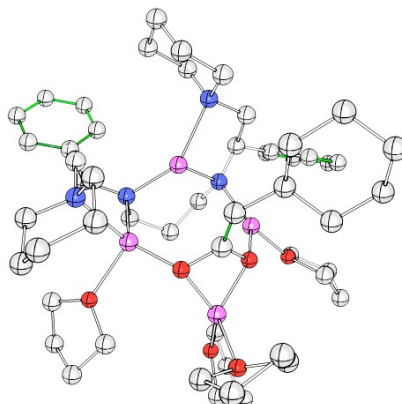
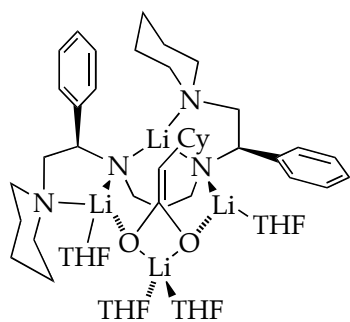
$G_{MP2} = -2414.82311$

| Atom | X         | Y         | Z         | Atom | X         | Y        | Z         |
|------|-----------|-----------|-----------|------|-----------|----------|-----------|
| Li   | 0         | 0         | 0         | H    | -2.81159  | 1.326315 | 6.017912  |
| O    | -1.530375 | -0.008599 | 1.207764  | H    | -1.251981 | 2.113298 | 5.729974  |
| Li   | -3.073782 | 0.03588   | 0.221074  | H    | -2.691624 | 2.69235  | 4.887454  |
| N    | -4.379365 | 1.076416  | -0.934999 | O    | 0.631205  | 3.965059 | -0.936647 |
| C    | -5.429961 | 0.091581  | -1.192803 | C    | 0.638883  | 5.081307 | -1.863699 |
| C    | -5.646668 | -0.812842 | 0.034581  | C    | 2.059619  | 5.664491 | -1.826713 |
| N    | -4.439404 | -1.572496 | 0.424111  | C    | 2.898211  | 4.486905 | -1.304605 |
| C    | -4.582912 | -2.096512 | 1.799163  | C    | 1.930327  | 3.83775  | -0.319024 |
| H    | -4.770353 | -1.246567 | 2.464856  | H    | 1.927699  | 4.368271 | 0.642593  |
| H    | -5.466216 | -2.762577 | 1.860856  | H    | 2.096876  | 2.776832 | -0.130298 |
| C    | -3.327989 | -2.843832 | 2.254496  | H    | 3.834683  | 4.799021 | -0.83182  |
| H    | -3.484985 | -3.220162 | 3.273115  | H    | 3.140608  | 3.791317 | -2.117774 |
| H    | -2.500145 | -2.126799 | 2.285783  | H    | 2.10323   | 6.502086 | -1.122383 |
| C    | -2.991063 | -3.991276 | 1.294755  | H    | 2.384288  | 6.028594 | -2.806279 |
| C    | -2.907196 | -3.456717 | -0.139958 | H    | 0.378449  | 4.688967 | -2.853785 |
| C    | -4.175704 | -2.684095 | -0.513218 | H    | -0.123155 | 5.800575 | -1.557022 |
| H    | -4.082632 | -2.273446 | -1.522552 | C    | -3.175903 | 5.065036 | 0.61339   |
| H    | -5.040038 | -3.37713  | -0.524352 | C    | -3.725374 | 4.678434 | 2.003448  |
| H    | -2.765752 | -4.275412 | -0.857456 | N    | -5.006152 | 3.928703 | 1.925537  |
| H    | -2.0401   | -2.788542 | -0.231571 | C    | -6.127149 | 4.862419 | 1.670842  |
| H    | -3.773084 | -4.763244 | 1.349349  | H    | -5.937974 | 5.384151 | 0.728652  |
| H    | -2.049357 | -4.474949 | 1.583562  | H    | -6.148953 | 5.630823 | 2.467969  |
| H    | -6.495458 | -1.497404 | -0.1413   | C    | -7.481925 | 4.155045 | 1.610991  |
| H    | -5.912961 | -0.184981 | 0.893335  | H    | -7.505406 | 3.493789 | 0.737342  |
| H    | -5.115074 | -0.569823 | -2.029388 | H    | -8.265736 | 4.908183 | 1.459729  |
| C    | -6.780941 | 0.659181  | -1.666149 | C    | -7.745357 | 3.348233 | 2.888737  |
| C    | -7.103596 | 0.651048  | -3.030177 | C    | -6.555092 | 2.428069 | 3.185489  |
| C    | -8.310752 | 1.174703  | -3.498504 | C    | -5.239345 | 3.20955  | 3.198044  |
| C    | -9.235996 | 1.708997  | -2.601903 | H    | -4.395507 | 2.532652 | 3.361919  |
| C    | -8.937788 | 1.716417  | -1.23748  | H    | -5.249113 | 3.926413 | 4.041768  |
| C    | -7.722928 | 1.202597  | -0.780374 | H    | -6.68068  | 1.925158 | 4.152466  |
| H    | -7.514261 | 1.215283  | 0.285678  | H    | -6.496431 | 1.639433 | 2.42233   |
| H    | -9.655621 | 2.118005  | -0.525881 | H    | -7.886906 | 4.0383   | 3.73341   |

**Table 7 (Continued).**

|    |           |           |           |   |           |           |           |
|----|-----------|-----------|-----------|---|-----------|-----------|-----------|
| H  | -10.18028 | 2.111454  | -2.959616 | H | -8.672168 | 2.768042  | 2.798006  |
| H  | -8.528854 | 1.160254  | -4.563827 | H | -3.847581 | 5.56631   | 2.648544  |
| H  | -6.393893 | 0.222956  | -3.735291 | H | -2.994234 | 4.015435  | 2.479335  |
| Li | -4.308935 | 2.629538  | 0.305731  | H | -3.975637 | 5.609132  | 0.07002   |
| N  | -2.81478  | 3.841418  | -0.091866 | C | -2.033345 | 6.080066  | 0.767755  |
| Li | -0.920376 | 3.184165  | 0.163197  | C | -2.026966 | 7.272145  | 0.030644  |
| O  | -0.098284 | 1.689251  | 0.848457  | C | -0.975986 | 8.188183  | 0.137563  |
| C  | -0.913849 | 1.069704  | 1.725348  | C | 0.091203  | 7.93145   | 0.999473  |
| C  | -1.048391 | 1.491081  | 3.024205  | C | 0.099155  | 6.748851  | 1.746129  |
| H  | -0.422988 | 2.328507  | 3.331348  | C | -0.947379 | 5.833282  | 1.625706  |
| C  | -1.87688  | 0.814804  | 4.095386  | H | -0.923986 | 4.920018  | 2.217848  |
| H  | -2.837977 | 0.488815  | 3.662699  | H | 0.916712  | 6.545128  | 2.434152  |
| C  | -1.21154  | -0.452126 | 4.679167  | H | 0.902744  | 8.648253  | 1.097854  |
| H  | -0.265952 | -0.194013 | 5.17494   | H | -0.997149 | 9.106075  | -0.445591 |
| H  | -1.853747 | -0.949786 | 5.421447  | H | -2.863544 | 7.487179  | -0.631612 |
| H  | -0.991641 | -1.171735 | 3.884592  | C | -2.918452 | 3.968181  | -1.540314 |
| C  | -2.183651 | 1.790089  | 5.245816  | C | -2.761762 | 2.596607  | -2.225831 |
| H  | 1.588408  | 0.009502  | 3.30325   | H | -2.507802 | 2.769354  | -3.282784 |
| H  | 2.908037  | -2.711245 | 2.762216  | H | -1.903083 | 2.069791  | -1.782876 |
| H  | 1.499304  | -2.39334  | 3.79275   | C | -3.985272 | 1.662595  | -2.222004 |
| H  | 0.060607  | -2.015166 | 1.889784  | H | -3.760866 | 0.850987  | -2.952077 |
| H  | 1.214815  | -3.140779 | 1.117148  | H | -4.815201 | 2.227485  | -2.694169 |
| O  | 0.158112  | -0.344397 | -1.944423 | H | -3.897131 | 4.399668  | -1.856438 |
| C  | 0.46854   | 0.717283  | -2.877199 | H | -2.166503 | 4.658314  | -1.981656 |
| C  | 1.681075  | 0.209155  | -3.652366 | O | 1.528075  | -1.121043 | 0.747561  |
| C  | 1.359407  | -1.288919 | -3.782203 | C | 1.113488  | -2.186817 | 1.646449  |
| C  | 0.674617  | -1.604334 | -2.443516 | C | 2.016678  | -2.083061 | 2.880495  |
| H  | 1.37688   | -1.986577 | -1.696312 | C | 2.399828  | -0.595132 | 2.884775  |
| H  | -0.157935 | -2.308493 | -2.54547  | C | 2.533632  | -0.299039 | 1.393578  |
| H  | 2.245007  | -1.909205 | -3.948516 | H | 3.522372  | -0.580716 | 1.003988  |
| H  | 0.669892  | -1.455473 | -4.617637 | H | 2.312598  | 0.740364  | 1.141408  |
| H  | 2.597407  | 0.358203  | -3.068551 | H | 3.321183  | -0.388587 | 3.43851   |
| H  | 1.803503  | 0.708535  | -4.618294 | H | 0.639878  | 1.627487  | -2.29743  |
| H  | -0.392457 | 0.877189  | -3.538994 |   |           |           |           |

**Table 7 (Continued).**



**20a**

$G = -2770.897292$

$G_{MP2} = -2762.855052$

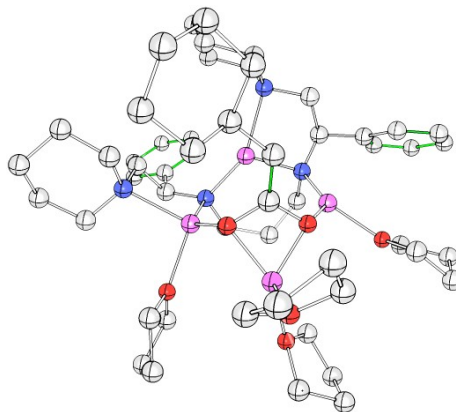
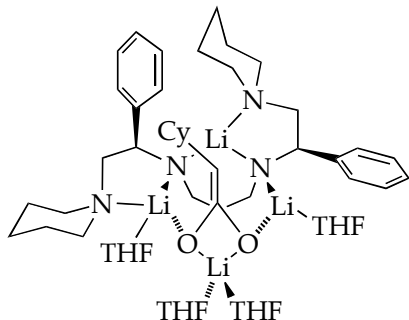
Atom X Y Z Atom X Y Z

|    |          |           |           |   |           |           |           |
|----|----------|-----------|-----------|---|-----------|-----------|-----------|
| Li | 0        | 0         | 0         | H | -0.819786 | -6.199457 | 0.891891  |
| O  | 1.672196 | -0.387073 | 0.872251  | H | -2.845321 | -7.422071 | 0.22022   |
| Li | 3.36026  | -0.690714 | 0.087673  | H | -2.926588 | -8.624156 | -1.961277 |
| N  | 4.086085 | -2.426198 | -0.833007 | H | -0.924409 | -8.602859 | -3.443862 |
| C  | 5.502694 | -2.140629 | -0.745108 | H | 1.131422  | -7.418526 | -2.735804 |
| C  | 5.867534 | -1.898102 | 0.738559  | C | 1.760696  | -4.233173 | -2.177489 |
| N  | 5.287162 | -0.646441 | 1.275449  | C | 2.160809  | -2.76435  | -2.434079 |
| C  | 5.033665 | -0.753231 | 2.726655  | H | 1.91606   | -2.522668 | -3.480219 |
| H  | 4.357064 | -1.598055 | 2.888845  | H | 1.544293  | -2.101522 | -1.806644 |
| H  | 5.976775 | -0.969393 | 3.267839  | C | 3.644606  | -2.41255  | -2.224912 |
| C  | 4.399751 | 0.525159  | 3.281242  | H | 3.805786  | -1.411533 | -2.688319 |
| H  | 4.241914 | 0.406835  | 4.360895  | H | 4.229324  | -3.102118 | -2.86644  |
| H  | 3.412726 | 0.645605  | 2.817889  | H | 2.549698  | -4.879325 | -2.622804 |
| C  | 5.274271 | 1.751468  | 2.991995  | H | 0.856809  | -4.451062 | -2.791103 |
| C  | 5.605825 | 1.816846  | 1.495955  | O | 3.568947  | 1.068928  | -1.247652 |
| C  | 6.190218 | 0.488761  | 1.009458  | C | 2.513167  | 2.057507  | -1.256243 |
| H  | 6.385028 | 0.528351  | -0.066339 | C | 2.941474  | 3.140382  | -2.256416 |
| H  | 7.167021 | 0.315498  | 1.505376  | C | 3.871909  | 2.364113  | -3.199998 |
| H  | 6.324006 | 2.621888  | 1.290836  | C | 4.568881  | 1.418768  | -2.22379  |
| H  | 4.69717  | 2.031889  | 0.920544  | H | 5.408964  | 1.921843  | -1.723253 |
| H  | 6.209478 | 1.680216  | 3.567283  | H | 4.930625  | 0.494796  | -2.679389 |
| H  | 4.773679 | 2.672104  | 3.318613  | H | 4.574414  | 3.00322   | -3.743646 |
| H  | 6.96003  | -1.90691  | 0.889024  | H | 3.290454  | 1.791128  | -3.932081 |
| H  | 5.458662 | -2.736302 | 1.313751  | H | 3.497067  | 3.939311  | -1.750943 |
| H  | 5.759847 | -1.202033 | -1.290951 | H | 2.086875  | 3.597048  | -2.765831 |
| C  | 6.479921 | -3.182806 | -1.337742 | H | 1.587575  | 1.561861  | -1.565069 |
| C  | 7.810792 | -2.825059 | -1.6015   | H | 2.384043  | 2.437567  | -0.239008 |
| C  | 8.722477 | -3.744645 | -2.119235 | O | -0.881771 | 1.490681  | 1.12159   |
| C  | 8.313733 | -5.050514 | -2.401826 | C | -1.780103 | 1.004985  | 2.154155  |
| C  | 6.989639 | -5.417602 | -2.160881 | C | -1.123405 | 1.382847  | 3.481032  |
| C  | 6.085118 | -4.491188 | -1.634072 | C | -0.409919 | 2.694036  | 3.122265  |
| H  | 5.050629 | -4.771066 | -1.457865 | C | 0.092172  | 2.397779  | 1.708554  |
| H  | 6.655051 | -6.426959 | -2.390547 | H | 1.056486  | 1.879059  | 1.715929  |
| H  | 9.018027 | -5.769441 | -2.81309  | H | 0.152374  | 3.287679  | 1.072397  |

**Table 7 (Continued).**

|    |           |           |           |   |           |           |           |
|----|-----------|-----------|-----------|---|-----------|-----------|-----------|
| H  | 9.750049  | -3.441895 | -2.30811  | H | 0.407618  | 2.940836  | 3.80626   |
| H  | 8.137444  | -1.805503 | -1.398365 | H | -1.116783 | 3.533032  | 3.117263  |
| Li | 3.104077  | -3.77295  | 0.216059  | H | -0.392264 | 0.615927  | 3.756498  |
| N  | 1.570799  | -4.522792 | -0.76013  | H | -1.849526 | 1.488367  | 4.292993  |
| Li | 0.057421  | -3.331844 | -0.227308 | H | -2.754266 | 1.497565  | 2.025544  |
| O  | -0.098657 | -1.764781 | 0.73136   | H | -1.891918 | -0.072636 | 2.016974  |
| C  | 0.961426  | -1.363895 | 1.459159  | O | -0.675452 | 0.547918  | -1.806836 |
| C  | 1.243478  | -1.859001 | 2.712257  | C | -0.829743 | -0.408851 | -2.891741 |
| H  | 2.076828  | -1.403796 | 3.241505  | C | -1.893469 | 0.17987   | -3.833618 |
| O  | -1.740881 | -3.45794  | -1.140508 | C | -2.641477 | 1.176925  | -2.932606 |
| C  | -2.156441 | -4.187392 | -2.323626 | C | -1.511705 | 1.69754   | -2.049102 |
| C  | -3.683111 | -4.311708 | -2.231182 | H | -1.823282 | 2.078807  | -1.075652 |
| C  | -4.066826 | -3.126454 | -1.329789 | H | -0.927639 | 2.471321  | -2.5699   |
| C  | -2.894943 | -3.095058 | -0.351995 | H | -3.391785 | 0.661856  | -2.320711 |
| H  | -3.032723 | -3.833314 | 0.450209  | H | -3.143024 | 1.972509  | -3.49198  |
| H  | -2.687044 | -2.124093 | 0.100405  | H | -2.543745 | -0.592584 | -4.254721 |
| H  | -5.030284 | -3.257982 | -0.827668 | H | -1.420723 | 0.708458  | -4.669343 |
| H  | -4.108393 | -2.195136 | -1.908941 | H | 0.140738  | -0.549581 | -3.376121 |
| H  | -3.95382  | -5.257778 | -1.750048 | H | -1.138736 | -1.356619 | -2.442961 |
| H  | -4.162796 | -4.283607 | -3.214353 | C | 0.423619  | -2.88263  | 3.475256  |
| H  | -1.845476 | -3.603553 | -3.19928  | C | 1.042401  | -3.147638 | 4.864993  |
| H  | -1.644618 | -5.15041  | -2.340783 | C | -1.068667 | -2.518902 | 3.671827  |
| C  | 1.597993  | -5.950903 | -0.487545 | H | 0.418958  | -3.853137 | 2.939606  |
| C  | 1.913346  | -6.179044 | 1.002861  | C | 0.291838  | -4.229666 | 5.655694  |
| N  | 3.253012  | -5.700825 | 1.42249   | H | 1.028802  | -2.204872 | 5.434194  |
| C  | 4.302759  | -6.644275 | 0.975421  | H | 2.101308  | -3.42018  | 4.762081  |
| H  | 4.288061  | -6.689426 | -0.117143 | C | -1.841545 | -3.605389 | 4.436718  |
| H  | 4.063326  | -7.661336 | 1.344383  | H | -1.126512 | -1.574426 | 4.234162  |
| C  | 5.69893   | -6.245883 | 1.461206  | H | -1.51995  | -2.338474 | 2.691486  |
| H  | 5.987043  | -5.297698 | 0.993829  | C | -1.200212 | -3.894107 | 5.802328  |
| H  | 6.419417  | -6.996869 | 1.113727  | H | 0.748137  | -4.364559 | 6.646035  |
| C  | 5.74275   | -6.109236 | 2.986726  | H | 0.3928    | -5.193756 | 5.13436   |
| C  | 4.628869  | -5.163549 | 3.44855   | H | -2.892401 | -3.310452 | 4.567278  |
| C  | 3.271573  | -5.604535 | 2.899573  | H | -1.852798 | -4.531996 | 3.841108  |
| H  | 2.496763  | -4.893468 | 3.194342  | H | -1.727832 | -4.710664 | 6.313908  |
| H  | 3.005571  | -6.585139 | 3.341811  | H | -1.30638  | -3.004577 | 6.441849  |
| H  | 4.572232  | -5.126034 | 4.543883  | H | 2.401014  | -6.438402 | -1.080835 |
| H  | 4.842814  | -4.142605 | 3.106246  | C | 0.316841  | -6.712157 | -0.875361 |
| H  | 5.59781   | -7.096141 | 3.450627  | C | 0.252756  | -7.403185 | -2.093934 |
| H  | 6.724575  | -5.746173 | 3.314891  | C | -0.905519 | -8.076628 | -2.492169 |
| H  | 1.796097  | -7.245964 | 1.265635  | C | -2.029069 | -8.087258 | -1.664379 |
| H  | 1.182824  | -5.617263 | 1.595093  | C | -1.982902 | -7.408273 | -0.442939 |
| C  | -0.828638 | -6.721779 | -0.061898 |   |           |           |           |

**Table 7 (Continued).**



**20b**

$G = -2770.891398$

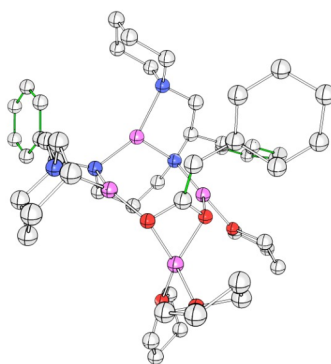
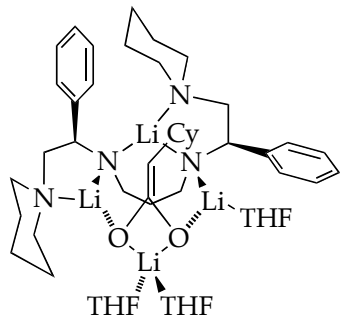
$G_{\text{MP2}} = -2762.848334$

| Atom | X         | Y        | Z         | Atom | X         | Y         | Z         |
|------|-----------|----------|-----------|------|-----------|-----------|-----------|
| Li   | 0         | 0        | 0         | H    | -2.573625 | 2.663     | -3.043893 |
| O    | -1.743506 | 0.432047 | 0.786875  | H    | -2.896267 | 4.36104   | -2.769856 |
| Li   | -3.007395 | 1.116302 | -0.454559 | N    | -5.246328 | 0.95762   | -0.160857 |
| N    | -3.337286 | 3.095209 | -1.10061  | C    | -5.557829 | 0.508903  | 1.211942  |
| C    | -4.721094 | 3.012417 | -1.51941  | H    | -5.065523 | -0.462484 | 1.356247  |
| H    | -4.826035 | 2.35044  | -2.412507 | H    | -5.085215 | 1.202807  | 1.912642  |
| C    | -5.406144 | 4.328822 | -1.961386 | C    | -7.058907 | 0.36129   | 1.512427  |
| C    | -6.557983 | 4.284121 | -2.760558 | C    | -7.71973  | -0.585163 | 0.499659  |
| C    | -7.219668 | 5.448567 | -3.150193 | C    | -7.407499 | -0.133206 | -0.934788 |
| C    | -6.729461 | 6.695764 | -2.755336 | C    | -5.891291 | 0.049959  | -1.134582 |
| C    | -5.574597 | 6.758477 | -1.97497  | H    | -5.676849 | 0.413731  | -2.143738 |
| C    | -4.922542 | 5.585631 | -1.584438 | H    | -5.403155 | -0.928268 | -1.037896 |
| H    | -4.01178  | 5.633937 | -0.994366 | H    | -7.778645 | -0.866138 | -1.663581 |
| H    | -5.173043 | 7.724202 | -1.675586 | H    | -7.932534 | 0.807563  | -1.146749 |
| H    | -7.236603 | 7.607307 | -3.061755 | H    | -8.803461 | -0.639364 | 0.66283   |
| H    | -8.113205 | 5.3841   | -3.767167 | H    | -7.327673 | -1.602591 | 0.650942  |
| H    | -6.939535 | 3.317273 | -3.087993 | H    | -7.546191 | 1.345278  | 1.474544  |
| Li   | -2.621906 | 3.943299 | 0.533914  | H    | -7.188171 | -0.014005 | 2.536015  |
| N    | -0.849881 | 4.743357 | 0.273972  | O    | -2.77349  | -0.366478 | -1.960955 |
| Li   | 0.40342   | 3.253606 | 0.699175  | C    | -2.630712 | -1.743647 | -1.561539 |
| O    | 0.204738  | 1.49391  | 1.144175  | C    | -1.979957 | -2.448942 | -2.751132 |
| C    | -0.978425 | 1.093206 | 1.663636  | C    | -2.588877 | -1.680629 | -3.934763 |
| C    | -1.27809  | 1.299902 | 2.990749  | C    | -2.643489 | -0.247313 | -3.393198 |
| H    | -0.50967  | 1.804586 | 3.574518  | H    | -3.488962 | 0.332821  | -3.774791 |
| O    | 2.358048  | 3.380626 | 0.168644  | H    | -1.720534 | 0.303294  | -3.611978 |
| C    | 3.313385  | 2.612242 | 0.930509  | H    | -3.59856  | -2.050752 | -4.14867  |
| C    | 4.66468   | 2.88311  | 0.270665  | H    | -2.000367 | -1.756637 | -4.854196 |
| C    | 4.509629  | 4.349164 | -0.16333  | H    | -2.193417 | -3.522187 | -2.7734   |
| C    | 3.037227  | 4.418747 | -0.583244 | H    | -0.893338 | -2.3116   | -2.726582 |
| H    | 2.905207  | 4.199632 | -1.650571 | H    | -2.049357 | -1.759006 | -0.637321 |
| H    | 2.566799  | 5.37672  | -0.35789  | H    | -3.624861 | -2.164914 | -1.353527 |
| H    | 5.187109  | 4.637644 | -0.972804 | O    | 1.001956  | -0.230957 | -1.751472 |
| H    | 4.689447  | 5.018711 | 0.684585  | C    | 1.876808  | -1.346843 | -2.025019 |

**Table 7 (Continued).**

|   |           |               |           |   |           |           |           |
|---|-----------|---------------|-----------|---|-----------|-----------|-----------|
| H | 4.801824  | 2.233718      | -0.603433 | C | 3.201972  | -0.718695 | -2.448016 |
| H | 5.505329  | 2.717732      | 0.951625  | C | 2.721402  | 0.506967  | -3.240569 |
| H | 3.303987  | 2.957601      | 1.973395  | C | 1.480578  | 0.951153  | -2.453229 |
| H | 2.991321  | 1.569798      | 0.908501  | H | 0.67641   | 1.327162  | -3.091782 |
| C | -0.879971 | 5.979377      | 1.037917  | H | 1.715473  | 1.709873  | -1.700661 |
| C | -1.548639 | 5.70193       | 2.398216  | H | 2.450042  | 0.214199  | -4.261644 |
| N | -2.971065 | 5.292603      | 2.293171  | H | 3.471167  | 1.300803  | -3.309171 |
| C | -3.830106 | 6.4742.054142 |           | H | 3.824119  | -1.399953 | -3.036504 |
| H | -3.533867 | 6.932231      | 1.106051  | H | 3.772662  | -0.408285 | -1.564394 |
| H | -3.649251 | 7.226132      | 2.847353  | H | 1.924559  | -1.950059 | -1.117231 |
| C | -5.320259 | 6.125066      | 2.022454  | H | 1.451487  | -1.95113  | -2.839954 |
| C | -5.752883 | 5.419498      | 3.311918  | O | 0.835845  | -1.623557 | 0.994122  |
| C | -4.838137 | 4.217322      | 3.569702  | C | 1.750205  | -1.176863 | 2.035662  |
| C | -3.365454 | 4.628569      | 3.556813  | C | 1.25763   | -1.823193 | 3.331134  |
| H | -2.723634 | 3.751128      | 3.677611  | C | 0.59459   | -3.114342 | 2.82766   |
| H | -3.172833 | 5.305532      | 4.412634  | C | -0.043013 | -2.650096 | 1.517799  |
| H | -5.00548  | 3.455816      | 2.796505  | H | -1.029949 | -2.206192 | 1.684283  |
| H | -5.066412 | 3.74589       | 4.533747  | H | -0.121696 | -3.443003 | 0.765834  |
| H | -6.802186 | 5.105411      | 3.248596  | H | -0.144782 | -3.519508 | 3.524986  |
| H | -5.681891 | 6.119891      | 4.157335  | H | 1.347456  | -3.889295 | 2.637418  |
| H | -5.524504 | 5.480937      | 1.159243  | H | 0.515928  | -1.170075 | 3.800943  |
| H | -5.894133 | 7.047534      | 1.868389  | H | 2.069709  | -2.00363  | 4.042479  |
| H | -1.456553 | 6.575646      | 3.068083  | H | 2.760549  | -1.51551  | 1.766506  |
| H | -1.019525 | 4.867837      | 2.87168   | H | 1.705551  | -0.085618 | 2.055864  |
| H | -1.486272 | 6.747271      | 0.510419  | C | -5.580967 | 2.379947  | -0.400638 |
| C | 0.493491  | 6.641036      | 1.243493  | H | -6.648922 | 2.521669  | -0.620968 |
| C | 0.892211  | 7.705017      | 0.421907  | H | -5.375339 | 2.929819  | 0.525195  |
| C | 2.151521  | 8.297207      | 0.553405  | C | -2.494789 | 0.810976  | 3.752283  |
| C | 3.039999  | 7.84392       | 1.529405  | C | -2.746686 | -0.713319 | 3.660016  |
| C | 2.658183  | 6.787491      | 2.362301  | C | -2.383439 | 1.201356  | 5.242563  |
| C | 1.405797  | 6.189815      | 2.212144  | H | -3.416057 | 1.290634  | 3.370745  |
| H | 1.133305  | 5.367162      | 2.869443  | C | -3.97294  | -1.163408 | 4.471173  |
| H | 3.334007  | 6.435414      | 3.138895  | H | -1.854802 | -1.235466 | 4.041307  |
| H | 4.014251  | 8.311903      | 1.646886  | H | -2.851377 | -0.9901   | 2.605823  |
| H | 2.432691  | 9.119925      | -0.100103 | C | -3.599143 | 0.762984  | 6.072052  |
| H | 0.198168  | 8.077439      | -0.329099 | H | -1.474959 | 0.734496  | 5.65501   |
| C | -0.694694 | 4.971493      | -1.156729 | H | -2.234937 | 2.285372  | 5.337417  |
| C | -1.02847  | 3.70589       | -1.97498  | C | -3.856879 | -0.745638 | 5.944716  |
| H | -0.524332 | 3.7804        | -2.951015 | H | -4.105604 | -2.251962 | 4.394872  |
| H | -0.601091 | 2.826297      | -1.469284 | H | -4.880671 | -0.711447 | 4.042481  |
| H | -1.35442  | 5.793051      | -1.516184 | H | -3.459359 | 1.03623   | 7.127034  |
| H | 0.328872  | 5.304919      | -1.438975 | H | -4.490465 | 1.309016  | 5.726359  |
| C | -2.518585 | 3.453297      | -2.258921 | H | -4.761492 | -1.029173 | 6.499902  |
| H | -3.021465 | -1.29247      | 6.408074  |   |           |           |           |

**Table 7 (Continued).**



**20c**

$G = -2538.553879$

$G_{MP2} = -2531.159552$

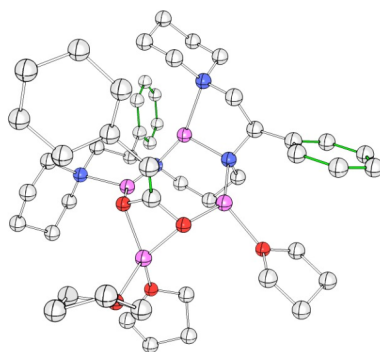
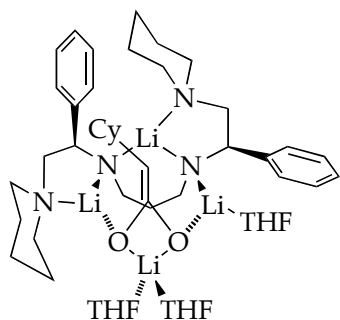
| Atom | X         | Y         | Z         | Atom | X         | Y        | Z         |
|------|-----------|-----------|-----------|------|-----------|----------|-----------|
| Li   | 0         | 0         | 0         | H    | -1.689759 | 1.381508 | 5.730679  |
| O    | -1.585225 | -0.223512 | 1.027677  | H    | -2.931081 | 2.396213 | 5.015428  |
| Li   | -3.334787 | 0.067665  | 0.579741  | H    | -1.259367 | 3.238319 | 3.346068  |
| N    | -4.615235 | 1.24441   | -0.473042 | O    | 0.730401  | 3.791144 | -0.706734 |
| C    | -5.781188 | 0.36157   | -0.541028 | C    | 0.935361  | 4.763786 | -1.763742 |
| C    | -5.998639 | -0.339922 | 0.814013  | C    | 2.407741  | 5.193352 | -1.673519 |
| N    | -4.884454 | -1.241532 | 1.180495  | C    | 3.063354  | 4.018531 | -0.928487 |
| C    | -4.892405 | -1.524652 | 2.631225  | C    | 1.955009  | 3.615757 | 0.039604  |
| H    | -4.836934 | -0.566742 | 3.160544  | H    | 1.940569  | 4.276032 | 0.917962  |
| H    | -5.848346 | -2.004816 | 2.920005  | H    | 1.978143  | 2.580505 | 0.381289  |
| C    | -3.716742 | -2.415338 | 3.042468  | H    | 3.990327  | 4.294866 | -0.416505 |
| H    | -3.776675 | -2.608587 | 4.121161  | H    | 3.28666   | 3.195452 | -1.618908 |
| H    | -2.785163 | -1.869891 | 2.852064  | H    | 2.495021  | 6.111925 | -1.083679 |
| C    | -3.715128 | -3.729722 | 2.252104  | H    | 2.845872  | 5.381418 | -2.658479 |
| C    | -3.772246 | -3.430496 | 0.749117  | H    | 0.710398  | 4.267061 | -2.715457 |
| C    | -4.948805 | -2.507173 | 0.421054  | H    | 0.238183  | 5.591656 | -1.624994 |
| H    | -4.955699 | -2.273272 | -0.647198 | C    | -3.058179 | 5.32092  | 0.349441  |
| H    | -5.901614 | -3.027674 | 0.643304  | C    | -3.547875 | 5.255883 | 1.810893  |
| H    | -3.873561 | -4.356272 | 0.168131  | N    | -4.848187 | 4.55601  | 1.951894  |
| H    | -2.839187 | -2.945384 | 0.434147  | C    | -5.952097 | 5.468987 | 1.576127  |
| H    | -4.589482 | -4.334386 | 2.535942  | H    | -5.804446 | 5.78307  | 0.539408  |
| H    | -2.826638 | -4.326175 | 2.495218  | H    | -5.898548 | 6.381075 | 2.202388  |
| H    | -6.956879 | -0.888695 | 0.819156  | C    | -7.32989  | 4.825631 | 1.732197  |
| H    | -6.058723 | 0.425775  | 1.596917  | H    | -7.428634 | 4.01024  | 1.007817  |
| H    | -5.59029  | -0.437293 | -1.291379 | H    | -8.095979 | 5.569569 | 1.478966  |
| C    | -7.091071 | 1.007245  | -1.027174 | C    | -7.539967 | 4.294624 | 3.155531  |
| C    | -7.434834 | 0.943284  | -2.385408 | C    | -6.364436 | 3.396874 | 3.560328  |
| C    | -8.604228 | 1.531386  | -2.87157  | C    | -5.027139 | 4.11062  | 3.35106   |
| C    | -9.472994 | 2.186672  | -1.998646 | H    | -4.197646 | 3.44093  | 3.597611  |
| C    | -9.156536 | 2.247794  | -0.640043 | H    | -4.964544 | 4.977001 | 4.038193  |
| C    | -7.977464 | 1.669523  | -0.165352 | H    | -6.446727 | 3.09373  | 4.611641  |
| H    | -7.756238 | 1.723446  | 0.897085  | H    | -6.376871 | 2.475501 | 2.961406  |
| H    | -9.832251 | 2.741986  | 0.054321  | H    | -7.605377 | 5.140361 | 3.855823  |



**Table 7 (Continued).**

|    |            |           |           |   |           |           |           |
|----|------------|-----------|-----------|---|-----------|-----------|-----------|
| H  | -10.389251 | 2.638727  | -2.369826 | H | -8.48929  | 3.749619  | 3.230855  |
| H  | -8.839399  | 1.470086  | -3.931608 | H | -3.61204  | 6.265042  | 2.254722  |
| H  | -6.774413  | 0.414953  | -3.069811 | H | -2.811142 | 4.68989   | 2.391553  |
| Li | -4.267449  | 2.893317  | 0.580609  | H | -3.876928 | 5.75629   | -0.260446 |
| N  | -2.75925   | 3.968366  | -0.101123 | C | -1.905485 | 6.331398  | 0.230213  |
| Li | -0.954849  | 3.157961  | 0.267022  | C | -1.917922 | 7.30656   | -0.776725 |
| O  | -0.293975  | 1.616512  | 1.040881  | C | -0.876451 | 8.229375  | -0.911163 |
| C  | -1.172407  | 0.858786  | 1.713915  | C | 0.201146  | 8.201827  | -0.024752 |
| C  | -1.598027  | 1.132727  | 2.993246  | C | 0.22983   | 7.237385  | 0.987596  |
| H  | -2.233202  | 0.389581  | 3.471747  | C | -0.806829 | 6.310352  | 1.10561   |
| C  | -1.090018  | 2.269691  | 3.85577   | H | -0.765584 | 5.568906  | 1.901102  |
| C  | -1.849904  | 2.331803  | 5.197068  | H | 1.056357  | 7.215064  | 1.694516  |
| C  | -1.392625  | 3.495902  | 6.08886   | H | 1.005333  | 8.927964  | -0.113975 |
| C  | 0.122112   | 3.45658   | 6.342732  | H | -0.913361 | 8.97548   | -1.701624 |
| C  | 0.904941   | 3.386705  | 5.022846  | H | -2.763986 | 7.346357  | -1.460178 |
| C  | 0.429476   | 2.212998  | 4.151898  | C | -2.850178 | 3.834843  | -1.551229 |
| H  | 0.648476   | 1.266143  | 4.669237  | C | -2.883285 | 2.357879  | -1.992787 |
| H  | 0.971838   | 2.191821  | 3.201094  | H | -2.629498 | 2.323183  | -3.063266 |
| H  | 1.982285   | 3.306124  | 5.224605  | H | -2.092048 | 1.798139  | -1.469672 |
| H  | 0.763026   | 4.329869  | 4.471711  | C | -4.218848 | 1.605218  | -1.837522 |
| H  | 0.433642   | 4.329251  | 6.932764  | H | -4.134088 | 0.686109  | -2.463087 |
| H  | 0.361523   | 2.568641  | 6.947335  | H | -4.988731 | 2.214554  | -2.354234 |
| H  | -1.936136  | 3.48087   | 7.043597  | H | -3.763074 | 4.329251  | -1.954048 |
| H  | -1.650536  | 4.448444  | 5.601155  | H | -2.013083 | 4.33139   | -2.092831 |
| O  | 0.458503   | -0.174071 | -1.917081 | O | 1.352279  | -1.315647 | 0.79559   |
| C  | 0.537036   | 0.920632  | -2.854606 | C | 0.707732  | -2.538602 | 1.250346  |
| C  | 1.759083   | 0.603233  | -3.712208 | C | 1.317828  | -2.85377  | 2.618882  |
| C  | 1.655103   | -0.925472 | -3.845642 | C | 1.676559  | -1.454357 | 3.140242  |
| C  | 1.084169   | -1.352083 | -2.482554 | C | 2.153469  | -0.757397 | 1.867268  |
| H  | 1.858423   | -1.676484 | -1.78139  | H | 3.212303  | -0.966918 | 1.659238  |
| H  | 0.33285    | -2.144751 | -2.569912 | H | 1.988442  | 0.322579  | 1.875575  |
| H  | 2.613904   | -1.406311 | -4.060656 | H | 2.441109  | -1.4651   | 3.9233    |
| H  | 0.961155   | -1.186058 | -4.652694 | H | 0.785506  | -0.947303 | 3.524656  |
| H  | 2.678024   | 0.884185  | -3.183301 | H | 2.219438  | -3.469434 | 2.511498  |
| H  | 1.745427   | 1.120904  | -4.67616  | H | 0.617227  | -3.388127 | 3.267575  |
| H  | -0.379865  | 0.95161   | -3.458157 | H | -0.365285 | -2.332485 | 1.318707  |
| H  | 0.611086   | 1.841346  | -2.272402 | H | 0.89105   | -3.318281 | 0.503163  |

**Table 7 (Continued).**



**20d**

$G = -2538.553114$

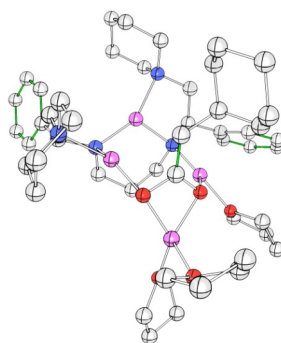
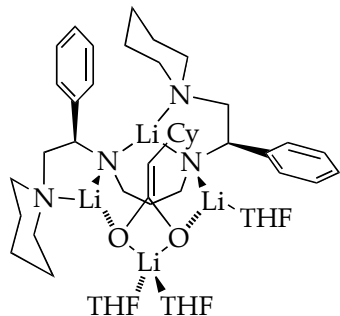
$G_{\text{MP2}} = -2531.158097$

| Atom | X          | Y         | Z         | Atom | X         | Y        | Z         |
|------|------------|-----------|-----------|------|-----------|----------|-----------|
| Li   | 0          | 0         | 0         | C    | -6.281106 | 4.332903 | 2.253723  |
| O    | -1.651802  | -0.27189  | 0.990095  | H    | -6.104882 | 5.014565 | 1.417053  |
| Li   | -3.079736  | -0.064181 | -0.139025 | H    | -6.336164 | 4.952082 | 3.170405  |
| N    | -4.412895  | 1.183378  | -1.019732 | C    | -7.607467 | 3.59834  | 2.054732  |
| C    | -5.446268  | 0.257     | -1.48832  | H    | -7.600145 | 3.096481 | 1.080667  |
| C    | -5.563331  | -0.961129 | -0.551675 | H    | -8.418137 | 4.337553 | 2.024427  |
| N    | -4.314293  | -1.748481 | -0.461692 | C    | -7.850702 | 2.574456 | 3.170272  |
| C    | -4.365085  | -2.668367 | 0.694355  | C    | -6.630199 | 1.657262 | 3.318381  |
| H    | -4.545019  | -2.069409 | 1.593685  | C    | -5.345098 | 2.471182 | 3.483889  |
| H    | -5.217924  | -3.367566 | 0.586499  | H    | -4.476636 | 1.808669 | 3.537396  |
| C    | -3.060179  | -3.452256 | 0.8496    | H    | -5.388928 | 3.029469 | 4.439254  |
| H    | -3.148211  | -4.126408 | 1.710854  | H    | -6.743335 | 0.989899 | 4.181919  |
| H    | -2.262093  | -2.733695 | 1.06851   | H    | -6.536965 | 1.016259 | 2.430687  |
| C    | -2.729477  | -4.236941 | -0.425359 | H    | -8.021737 | 3.101959 | 4.120137  |
| C    | -2.748207  | -3.292849 | -1.633221 | H    | -8.756032 | 1.988097 | 2.968665  |
| C    | -4.063076  | -2.511022 | -1.701286 | H    | -4.038704 | 4.927699 | 3.385749  |
| H    | -4.037929  | -1.813195 | -2.542179 | H    | -3.129088 | 3.463107 | 2.952095  |
| H    | -4.90077   | -3.21215  | -1.886948 | H    | -4.142931 | 5.449009 | 0.865751  |
| H    | -2.61658   | -3.849571 | -2.570134 | C    | -2.217915 | 5.829072 | 1.65646   |
| H    | -1.914349  | -2.580923 | -1.558437 | C    | -2.237448 | 7.13416  | 1.1454    |
| H    | -3.474723  | -5.032133 | -0.576063 | C    | -1.212136 | 8.041892 | 1.427312  |
| H    | -1.754364  | -4.732483 | -0.33494  | C    | -0.145299 | 7.661908 | 2.243035  |
| H    | -6.404585  | -1.604136 | -0.866558 | C    | -0.111139 | 6.364757 | 2.764936  |
| H    | -5.788675  | -0.611972 | 0.463878  | C    | -1.130947 | 5.459501 | 2.467734  |
| H    | -5.153845  | -0.136564 | -2.485026 | H    | -1.085973 | 4.455422 | 2.885936  |
| C    | -6.837563  | 0.866819  | -1.736964 | H    | 0.70599   | 6.061268 | 3.415719  |
| C    | -7.206332  | 1.253068  | -3.033765 | H    | 0.645435  | 8.369827 | 2.478924  |
| C    | -8.454558  | 1.819952  | -3.300179 | H    | -1.253274 | 9.048563 | 1.017522  |
| C    | -9.376464  | 1.99783   | -2.26858  | H    | -3.074601 | 7.443855 | 0.522614  |
| C    | -9.03294   | 1.608123  | -0.972333 | C    | -3.004701 | 4.186644 | -1.010033 |
| C    | -7.776665  | 1.056791  | -0.712716 | C    | -2.836369 | 2.982895 | -1.955192 |
| H    | -7.532921  | 0.759056  | 0.303467  | H    | -2.581708 | 3.368087 | -2.95432  |
| H    | -9.746987  | 1.728296  | -0.160806 | H    | -1.973577 | 2.383084 | -1.626402 |
| H    | -10.353209 | 2.429644  | -2.471296 | C    | -4.052189 | 2.057255 | -2.143213 |

**Table 7 (Continued).**

|    |           |           |           |   |           |           |           |
|----|-----------|-----------|-----------|---|-----------|-----------|-----------|
| H  | -8.70827  | 2.114964  | -4.3157   | H | -3.83526  | 1.437819  | -3.043771 |
| H  | -6.50242  | 1.097724  | -3.848702 | H | -4.896956 | 2.70401   | -2.458843 |
| Li | -4.372384 | 2.439965  | 0.53563   | H | -3.97525  | 4.67877   | -1.25253  |
| N  | -2.935667 | 3.774539  | 0.385218  | H | -2.241494 | 4.946661  | -1.288628 |
| Li | -1.055377 | 3.082739  | 0.601134  | O | 1.578862  | -1.075334 | 0.697616  |
| O  | -0.280859 | 1.505339  | 1.122758  | C | 1.289038  | -2.382424 | 1.257862  |
| C  | -1.129298 | 0.685403  | 1.777453  | C | 2.173442  | -2.515616 | 2.499733  |
| C  | -1.372    | 0.798659  | 3.12278   | C | 2.301753  | -1.055877 | 2.961265  |
| H  | -0.81998  | 1.571533  | 3.655274  | C | 2.379138  | -0.301807 | 1.634998  |
| C  | -2.243753 | -0.125301 | 3.944378  | H | 3.407031  | -0.252409 | 1.2498    |
| C  | -1.6436   | -1.538213 | 4.157829  | H | 1.941032  | 0.697576  | 1.682457  |
| C  | -2.554758 | -2.449792 | 4.995608  | H | 3.176839  | -0.878506 | 3.594293  |
| C  | -2.880513 | -1.816477 | 6.356314  | H | 1.403956  | -0.74464  | 3.504758  |
| C  | -3.463282 | -0.405221 | 6.187241  | H | 3.155414  | -2.925488 | 2.233173  |
| C  | -2.55408  | 0.486467  | 5.327473  | H | 1.725227  | -3.167941 | 3.25491   |
| H  | -1.60107  | 0.646588  | 5.856436  | H | 0.224663  | -2.413953 | 1.51336   |
| H  | -3.002436 | 1.48113   | 5.208101  | H | 1.499054  | -3.136077 | 0.491155  |
| H  | -3.629897 | 0.055555  | 7.170662  | O | 0.311847  | -0.012905 | -1.96007  |
| H  | -4.452667 | -0.480827 | 5.709587  | C | 0.533503  | 1.210807  | -2.700287 |
| H  | -3.574398 | -2.452377 | 6.922849  | C | 1.833408  | 0.972581  | -3.464093 |
| H  | -1.957217 | -1.753465 | 6.952152  | C | 1.707964  | -0.514284 | -3.834549 |
| H  | -2.090763 | -3.435961 | 5.137683  | C | 1.005567  | -1.110757 | -2.605212 |
| H  | -3.493627 | -2.625616 | 4.44743   | H | 1.713675  | -1.520924 | -1.878337 |
| H  | -0.67278  | -1.430064 | 4.666696  | H | 0.273851  | -1.882696 | -2.866118 |
| H  | -1.443476 | -1.989861 | 3.180537  | H | 2.670889  | -0.993994 | -4.032967 |
| H  | -3.210217 | -0.283108 | 3.429636  | H | 1.084407  | -0.628707 | -4.728516 |
| O  | 0.543491  | 4.012486  | -0.277783 | H | 2.69695   | 1.135526  | -2.807904 |
| C  | 0.586968  | 5.290806  | -0.964809 | H | 1.935569  | 1.626457  | -4.335477 |
| C  | 1.994274  | 5.854937  | -0.731118 | H | -0.309308 | 1.375175  | -3.384307 |
| C  | 2.823758  | 4.589166  | -0.464985 | H | 0.568774  | 2.032317  | -1.98083  |
| C  | 1.83066   | 3.731817  | 0.315845  | H | 2.353911  | 6.439728  | -1.583273 |
| H  | 1.807967  | 4.013614  | 1.37666   | H | 0.389503  | 5.10364   | -2.027266 |
| H  | 1.996511  | 2.655807  | 0.248033  | H | -0.202372 | 5.930549  | -0.565757 |
| H  | 3.743346  | 4.783111  | 0.095898  | C | -3.332726 | 4.831882  | 1.305672  |
| H  | 3.095467  | 4.098832  | -1.408222 | C | -3.878406 | 4.176884  | 2.591669  |
| H  | 1.996462  | 6.503007  | 0.15175   | N | -5.128998 | 3.408851  | 2.359818  |

**Table 7 (Continued).**



**20e**

$G = -2538.551938$

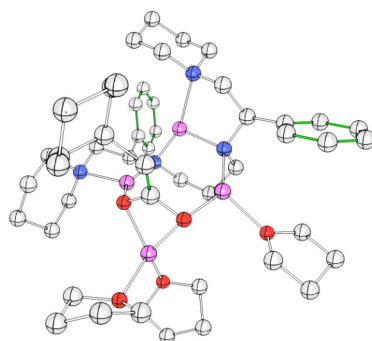
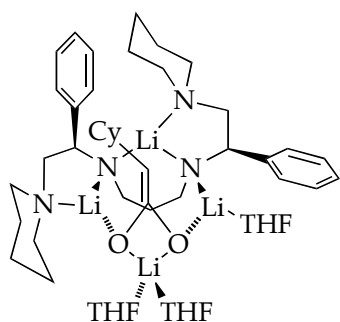
$G_{MP2} = -2531.158348$

| Atom | X          | Y         | Z         | Atom | X         | Y        | Z         |
|------|------------|-----------|-----------|------|-----------|----------|-----------|
| Li   | 0          | 0         | 0         | N    | -5.657763 | 3.718375 | 2.310398  |
| O    | -1.549695  | -0.663345 | 0.857238  | C    | -6.749185 | 4.512623 | 1.700359  |
| Li   | -3.381529  | -0.407042 | 0.698318  | H    | -6.4256   | 4.849609 | 0.712339  |
| N    | -4.750241  | 0.71796   | -0.326516 | H    | -6.926354 | 5.419173 | 2.312177  |
| C    | -5.763661  | -0.297872 | -0.612325 | C    | -8.048816 | 3.718038 | 1.568412  |
| C    | -5.974196  | -1.211584 | 0.610343  | H    | -7.900314 | 2.907943 | 0.847162  |
| N    | -4.771991  | -1.99088  | 0.978663  | H    | -8.822004 | 4.375404 | 1.150667  |
| C    | -4.924859  | -2.541282 | 2.341605  | C    | -8.498405 | 3.139958 | 2.915539  |
| H    | -5.084495  | -1.700863 | 3.026475  | C    | -7.342201 | 2.374395 | 3.569799  |
| H    | -5.828889  | -3.180238 | 2.392025  | C    | -6.086442 | 3.244424 | 3.644124  |
| C    | -3.703101  | -3.351116 | 2.784922  | H    | -5.258414 | 2.683502 | 4.086834  |
| H    | -3.891448  | -3.753496 | 3.788626  | H    | -6.282228 | 4.109879 | 4.307518  |
| H    | -2.837533  | -2.682632 | 2.856462  | H    | -7.611667 | 2.046838 | 4.581857  |
| C    | -3.392685  | -4.477781 | 1.792165  | H    | -7.117415 | 1.468719 | 2.989347  |
| C    | -3.27609   | -3.895132 | 0.379004  | H    | -8.811591 | 3.957439 | 3.581807  |
| C    | -4.526135  | -3.088415 | 0.017894  | H    | -9.372014 | 2.489049 | 2.784698  |
| H    | -4.415448  | -2.657457 | -0.980755 | H    | -4.68565  | 5.496946 | 2.965831  |
| H    | -5.407434  | -3.759661 | -0.014854 | H    | -3.751066 | 3.997469 | 3.107766  |
| H    | -3.141948  | -4.692244 | -0.363845 | H    | -4.450928 | 5.306991 | 0.440387  |
| H    | -2.401811  | -3.234834 | 0.323491  | C    | -2.644639 | 5.899703 | 1.35574   |
| H    | -4.199707  | -5.225339 | 1.816007  | C    | -2.649303 | 7.092544 | 0.619856  |
| H    | -2.46991   | -4.999153 | 2.076392  | C    | -1.686937 | 8.084406 | 0.832365  |
| H    | -6.831104  | -1.887776 | 0.440604  | C    | -0.700419 | 7.904721 | 1.802981  |
| H    | -6.220819  | -0.585634 | 1.476749  | C    | -0.681629 | 6.721767 | 2.549024  |
| H    | -5.40399   | -0.945816 | -1.441904 | C    | -1.638109 | 5.731431 | 2.321348  |
| C    | -7.122177  | 0.215288  | -1.129141 | H    | -1.60864  | 4.819408 | 2.914819  |
| C    | -7.334425  | 0.340994  | -2.510507 | H    | 0.072805  | 6.576619 | 3.319207  |
| C    | -8.546844  | 0.804059  | -3.025029 | H    | 0.040503  | 8.679498 | 1.983931  |
| C    | -9.592236  | 1.136074  | -2.162671 | H    | -1.7152   | 9.000234 | 0.246413  |
| C    | -9.406702  | 1.004078  | -0.785472 | H    | -3.426226 | 7.247906 | -0.126496 |
| C    | -8.184436  | 0.556392  | -0.279002 | C    | -3.212453 | 3.615621 | -0.914917 |
| H    | -8.06764   | 0.458853  | 0.797088  | C    | -3.063776 | 2.214576 | -1.541761 |
| H    | -10.217335 | 1.245235  | -0.10146  | H    | -2.743501 | 2.355188 | -2.585473 |

**Table 7 (Continued).**

|    |           |           |           |   |           |           |           |
|----|-----------|-----------|-----------|---|-----------|-----------|-----------|
| H  | -10.54232 | 1.486545  | -2.55797  | H | -2.25106  | 1.664693  | -1.042591 |
| H  | -8.677399 | 0.894869  | -4.100934 | C | -4.316218 | 1.317037  | -1.59147  |
| H  | -6.535112 | 0.05864   | -3.192134 | H | -4.088857 | 0.514024  | -2.330494 |
| Li | -4.667602 | 2.237692  | 0.952099  | H | -5.117144 | 1.91319   | -2.076923 |
| N  | -3.256491 | 3.567729  | 0.544619  | H | -4.130725 | 4.079893  | -1.339502 |
| Li | -1.376534 | 2.901893  | 0.874248  | H | -2.383937 | 4.247939  | -1.310705 |
| O  | -0.563328 | 1.299939  | 1.344612  | O | 1.563804  | -1.193007 | 0.566135  |
| C  | -1.396098 | 0.33134   | 1.743013  | C | 1.154174  | -2.554829 | 0.859549  |
| C  | -2.077425 | 0.348336  | 2.943688  | C | 2.080873  | -3.025944 | 1.979065  |
| H  | -2.617924 | -0.557846 | 3.205197  | C | 2.307445  | -1.727496 | 2.768917  |
| C  | -1.886544 | 1.393223  | 4.025138  | C | 2.360415  | -0.671176 | 1.660225  |
| C  | -2.924665 | 1.234552  | 5.161354  | H | 3.38316   | -0.515105 | 1.292438  |
| H  | -3.931718 | 1.155108  | 4.731253  | H | 1.93125   | 0.288467  | 1.962081  |
| C  | -2.659175 | 0.018066  | 6.065885  | H | 3.219837  | -1.741405 | 3.372945  |
| C  | -1.236834 | 0.046274  | 6.644349  | H | 1.460178  | -1.533734 | 3.43433   |
| C  | -0.192974 | 0.172593  | 5.525511  | H | 3.026965  | -3.398055 | 1.567155  |
| C  | -0.461789 | 1.403218  | 4.647428  | H | 1.633631  | -3.822906 | 2.580749  |
| H  | 0.272491  | 1.467871  | 3.837245  | H | 0.103009  | -2.532553 | 1.16711   |
| H  | -0.342805 | 2.309441  | 5.265362  | H | 1.250168  | -3.13686  | -0.062727 |
| H  | -0.232525 | -0.728212 | 4.896462  | O | 0.499404  | 0.284752  | -1.897908 |
| H  | 0.818576  | 0.220303  | 5.952215  | C | 0.517831  | 1.551817  | -2.586205 |
| H  | -1.140439 | 0.904625  | 7.327237  | C | 1.766721  | 1.491735  | -3.461525 |
| H  | -1.05188  | -0.853624 | 7.246766  | C | 1.752924  | 0.022433  | -3.917116 |
| H  | -2.793107 | -0.908081 | 5.489747  | C | 1.184882  | -0.714207 | -2.690759 |
| H  | -3.399583 | -0.012042 | 6.877041  | H | 1.965917  | -1.147867 | -2.059522 |
| H  | -2.915037 | 2.139693  | 5.787892  | H | 0.472259  | -1.500295 | -2.963882 |
| H  | -2.036084 | 2.396016  | 3.589418  | H | 2.741353  | -0.350246 | -4.201454 |
| O  | 0.270528  | 3.889074  | 0.148804  | H | 1.088841  | -0.097744 | -4.780345 |
| C  | 0.389378  | 5.072913  | -0.682155 | H | 2.660974  | 1.70299   | -2.862574 |
| C  | 1.79444   | 5.640852  | -0.425994 | H | 1.73503   | 2.200381  | -4.29469  |
| C  | 2.560929  | 4.429494  | 0.130632  | H | -0.392447 | 1.653507  | -3.192097 |
| C  | 1.471383  | 3.723849  | 0.932982  | H | 0.525159  | 2.333793  | -1.824272 |
| H  | 1.33268   | 4.202611  | 1.912357  | H | 2.243729  | 6.059553  | -1.331715 |
| H  | 1.613101  | 2.653     | 1.081989  | H | 0.255822  | 4.755945  | -1.723347 |
| H  | 3.422726  | 4.708958  | 0.744706  | H | -0.407556 | 5.770811  | -0.420964 |
| H  | 2.916063  | 3.784278  | -0.68274  | C | -3.719012 | 4.82436   | 1.117778  |
| H  | 1.74541   | 6.435824  | 0.325455  | C | -4.438588 | 4.548159  | 2.455755  |

**Table 7 (Continued).**



**20f**

$G = -2538.550208$

$G_{MP2} = -2531.155438$

| Atom | X         | Y         | Z         | Atom | X         | Y        | Z         |
|------|-----------|-----------|-----------|------|-----------|----------|-----------|
| Li   | 0         | 0         | 0         | O    | 0.125439  | 4.032904 | -0.662876 |
| O    | -1.3631   | -0.274686 | 1.35271   | C    | -0.053423 | 5.208529 | -1.494276 |
| Li   | -3.002568 | -0.363939 | 0.543374  | C    | 1.304855  | 5.922524 | -1.526478 |
| N    | -4.536684 | 0.573592  | -0.394044 | C    | 2.290369  | 4.785144 | -1.216538 |
| C    | -5.487969 | -0.517723 | -0.608931 | C    | 1.495055  | 3.960676 | -0.207173 |
| C    | -5.451557 | -1.517651 | 0.562212  | H    | 1.564307  | 4.392863 | 0.799989  |
| N    | -4.126507 | -2.144844 | 0.753733  | H    | 1.763835  | 2.905633 | -0.148371 |
| C    | -4.040015 | -2.777601 | 2.086989  | H    | 3.245019  | 5.137006 | -0.812996 |
| H    | -4.254086 | -2.009309 | 2.838448  | H    | 2.497092  | 4.194501 | -2.117923 |
| H    | -4.817995 | -3.560388 | 2.186222  | H    | 1.346849  | 6.684354 | -0.740711 |
| C    | -2.655014 | -3.376729 | 2.33968   | H    | 1.49337   | 6.413648 | -2.486115 |
| H    | -2.643271 | -3.8443   | 3.332255  | H    | -0.362327 | 4.866827 | -2.489621 |
| H    | -1.927693 | -2.557116 | 2.347093  | H    | -0.848921 | 5.823381 | -1.068688 |
| C    | -2.287115 | -4.395107 | 1.253775  | C    | -3.633722 | 4.615125 | 1.243519  |
| C    | -2.447382 | -3.757052 | -0.13135  | C    | -4.026159 | 4.122593 | 2.65331   |
| C    | -3.841069 | -3.143764 | -0.295997 | N    | -5.215168 | 3.231942 | 2.64231   |
| H    | -3.923758 | -2.657662 | -1.271991 | C    | -6.450857 | 4.033846 | 2.491014  |
| H    | -4.604734 | -3.946192 | -0.268574 | H    | -6.390177 | 4.592459 | 1.553176  |
| H    | -2.287179 | -4.496805 | -0.926553 | H    | -6.504154 | 4.778831 | 3.308804  |
| H    | -1.693564 | -2.968559 | -0.261033 | C    | -7.715479 | 3.174268 | 2.502219  |
| H    | -2.947043 | -5.272493 | 1.326899  | H    | -7.724296 | 2.533272 | 1.613418  |
| H    | -1.261833 | -4.759826 | 1.395824  | H    | -8.589681 | 3.83337  | 2.42605   |
| H    | -6.230685 | -2.289395 | 0.429191  | C    | -7.794231 | 2.316588 | 3.771386  |
| H    | -5.682931 | -0.983636 | 1.491771  | C    | -6.487597 | 1.536648 | 3.964019  |
| H    | -5.195235 | -1.08233  | -1.520849 | C    | -5.27339  | 2.466406 | 3.907354  |
| C    | -6.941882 | -0.098036 | -0.894183 | H    | -4.34788  | 1.889578 | 3.995107  |
| C    | -7.404676 | -0.04084  | -2.216422 | H    | -5.305823 | 3.160805 | 4.769243  |
| C    | -8.710488 | 0.352658  | -2.517227 | H    | -6.486452 | 1.006953 | 4.924878  |
| C    | -9.594527 | 0.685372  | -1.490876 | H    | -6.391053 | 0.772441 | 3.180201  |
| C    | -9.156021 | 0.623939  | -0.166369 | H    | -7.955957 | 2.968168 | 4.642645  |
| C    | -7.844598 | 0.243046  | 0.123765  | H    | -8.651459 | 1.633137 | 3.726548  |
| H    | -7.527802 | 0.199289  | 1.162072  | H    | -4.197051 | 4.971154 | 3.339128  |
| H    | -9.838708 | 0.86763   | 0.644486  | H    | -3.189689 | 3.536502 | 3.050034  |

**Table 7 (Continued).**

|    |            |           |           |   |           |           |           |
|----|------------|-----------|-----------|---|-----------|-----------|-----------|
| H  | -10.614541 | 0.984625  | -1.718083 | H | -4.524589 | 5.096713  | 0.790974  |
| H  | -9.037383  | 0.393267  | -3.553653 | C | -2.590071 | 5.736214  | 1.360972  |
| H  | -6.726733  | -0.314735 | -3.022263 | C | -2.779224 | 6.965757  | 0.715401  |
| Li | -4.510246  | 2.067181  | 0.922088  | C | -1.823564 | 7.983444  | 0.793563  |
| N  | -3.212777  | 3.465642  | 0.45203   | C | -0.656007 | 7.791992  | 1.533834  |
| Li | -1.235863  | 3.023496  | 0.506976  | C | -0.452491 | 6.572585  | 2.187999  |
| O  | -0.173881  | 1.601528  | 0.997887  | C | -1.40559  | 5.557226  | 2.0964    |
| C  | -0.824736  | 0.832853  | 1.895348  | H | -1.230346 | 4.616639  | 2.616297  |
| C  | -0.88309   | 1.147884  | 3.229155  | H | 0.445268  | 6.416698  | 2.782078  |
| H  | -0.332781  | 2.032981  | 3.540663  | H | 0.082746  | 8.586014  | 1.610049  |
| C  | -1.544367  | 0.294674  | 4.290897  | H | -1.996752 | 8.928192  | 0.283175  |
| C  | -0.690498  | -0.922996 | 4.747667  | H | -3.694263 | 7.129243  | 0.149081  |
| H  | -0.376354  | -1.488324 | 3.862942  | C | -3.454216 | 3.643863  | -0.974516 |
| C  | 0.531974   | -0.508507 | 5.578797  | C | -3.233634 | 2.326945  | -1.743136 |
| C  | 0.116681   | 0.305938  | 6.812751  | H | -3.10598  | 2.572487  | -2.808486 |
| C  | -0.724065  | 1.524991  | 6.405491  | H | -2.286977 | 1.872847  | -1.413982 |
| C  | -1.933105  | 1.114031  | 5.547423  | C | -4.350963 | 1.270025  | -1.673139 |
| H  | -2.491386  | 2.010273  | 5.249785  | H | -4.128066 | 0.528437  | -2.474332 |
| H  | -2.608911  | 0.510934  | 6.174258  | H | -5.28089  | 1.76754   | -2.018144 |
| H  | -0.092445  | 2.226176  | 5.842668  | H | -4.492113 | 3.993237  | -1.183921 |
| H  | -1.066455  | 2.065936  | 7.298408  | H | -2.809805 | 4.421437  | -1.44089  |
| H  | -0.47553   | -0.33432  | 7.484792  | O | 1.716119  | -1.003679 | 0.437887  |
| H  | 1.000822   | 0.623147  | 7.382608  | C | 1.586238  | -2.231677 | 1.195136  |
| H  | 1.194686   | 0.106894  | 4.953934  | C | 2.85451   | -2.32246  | 2.041442  |
| H  | 1.108725   | -1.393316 | 5.883033  | C | 3.126276  | -0.843531 | 2.358606  |
| H  | -1.314476  | -1.601422 | 5.353795  | C | 2.70318   | -0.137963 | 1.066073  |
| H  | -2.472552  | -0.125473 | 3.871088  | H | 3.542122  | -0.026167 | 0.367049  |
| C  | 1.097749   | -0.806765 | -3.99622  | H | 2.22947   | 0.832318  | 1.238285  |
| C  | 0.544854   | -1.31215  | -2.653551 | H | 4.170455  | -0.642847 | 2.617466  |
| H  | 1.329437   | -1.713744 | -2.005143 | H | 2.496859  | -0.513681 | 3.190515  |
| H  | -0.24082   | -2.065698 | -2.774725 | H | 3.676967  | -2.752646 | 1.456845  |
| H  | 2.020833   | -1.319883 | -4.281453 | H | 2.713809  | -2.935169 | 2.936827  |
| H  | 0.366394   | -0.961098 | -4.797621 | H | 0.683562  | -2.166512 | 1.813094  |
| H  | 2.236985   | 0.881408  | -3.214522 | H | 1.473733  | -3.053378 | 0.480474  |
| H  | 1.287255   | 1.29338   | -4.657833 | O | -0.01616  | -0.156568 | -1.981682 |
| H  | -0.817357  | 1.135955  | -3.405903 | C | 0.10815   | 1.008553  | -2.82945  |
| H  | 0.239432   | 1.876791  | -2.179499 | C | 1.292338  | 0.697165  | -3.740252 |

## Part 5: X-ray Crystallography

### Crystallographic information for BuLi-ligand Dimer (5)

**Table 8.** Crystal data and structure refinement for 5.

|                                   |  |          |
|-----------------------------------|--|----------|
| Identification code               | 5  |          |
| Empirical formula                 | C <sub>66</sub> H <sub>98</sub> Li <sub>6</sub> N <sub>8</sub> |          |
| Formula weight                    | 1045.16  |          |
| Temperature                       | 100(2) K   |          |
| Wavelength                        | 0.71073 Å  |          |
| Crystal system                    | Orthorhombic   |          |
| Space group                       | P2(1)2(1)2(1)  |          |
| Unit cell dimensions              | a = 15.4882(8) Å   | a = 90°. |
|                                   | b = 19.7919(11) Å  | b = 90°. |
|                                   | c = 24.4546(14) Å  | g = 90°. |
| Volume                            | 7496.3(7) Å <sup>3</sup>                                       |          |
| Z                                 | 4  |          |
| Density (calculated)              | 0.926 Mg/m <sup>3</sup>  |          |
| Absorption coefficient            | 0.053 mm <sup>-1</sup>   |          |
| F(000)                            | 2272   |          |
| Crystal size                      | 0.15 x 0.10 x 0.10 mm <sup>3</sup>                             |          |
| Theta range for data collection   | 1.67 to 24.81°.  |          |
| Index ranges                      | -18<=h<=11, -23<=k<=23, -24<=l<=28                             |          |
| Reflections collected             | 37167  |          |
| Independent reflections           | 7035 [R(int) = 0.0653]   |          |
| Completeness to theta = 24.81°    | 99.2 %   |          |
| Absorption correction             | Semi-empirical from equivalents                                |          |
| Max. and min. transmission        | 0.9940 and 0.9911  |          |
| Refinement method                 | Full-matrix least-squares on F <sup>2</sup>                    |          |
| Data / restraints / parameters    | 7035 / 0 / 723   |          |
| Goodness-of-fit on F <sup>2</sup> | 0.890  |          |
| Final R indices [I>2sigma(I)]     | R1 = 0.0419, wR2 = 0.0950                                      |          |
| R indices (all data)              | R1 = 0.0624, wR2 = 0.0995                                      |          |
| Absolute structure parameter      | 0(10)  |          |
| Largest diff. peak and hole       | 0.319 and -0.129 e.Å <sup>-3</sup>                             |          |



**Table 9.** Atomic coordinates ( $\times 10^4$ ) and equivalent isotropic displacement parameters ( $\text{\AA}^2 \times 10^3$ ) for **5**.  $U(\text{eq})$  is defined as one third of the trace of the orthogonalized  $U^{ij}$  tensor.

|       | x        | y        | z       | U(eq) |
|-------|----------|----------|---------|-------|
| N(4A) | 11275(1) | 10283(1) | 6521(1) | 29(1) |
| C(1A) | 9616(1)  | 9218(1)  | 7425(1) | 29(1) |
| C(14) | 10303(1) | 8012(1)  | 5926(1) | 34(1) |
| C(29) | 12097(1) | 10323(1) | 6214(1) | 35(1) |
| C(1)  | 7632(1)  | 9447(1)  | 6624(1) | 28(1) |
| C(7)  | 11534(1) | 7918(1)  | 6510(1) | 31(1) |
| C(52) | 7227(2)  | 8027(1)  | 8099(1) | 33(1) |
| C(36) | 6719(1)  | 7393(1)  | 5969(1) | 29(1) |
| C(37) | 6096(2)  | 6837(1)  | 6181(1) | 32(1) |
| C(58) | 5257(2)  | 8038(1)  | 7749(1) | 38(1) |
| C(43) | 7977(1)  | 7189(1)  | 6495(1) | 32(1) |
| C(25) | 11379(2) | 10635(1) | 7053(1) | 34(1) |
| C(6)  | 11842(1) | 8101(1)  | 7082(1) | 33(1) |
| C(53) | 6549(2)  | 8593(1)  | 8098(1) | 35(1) |
| C(28) | 12834(2) | 9996(1)  | 6537(1) | 39(1) |
| C(54) | 5541(2)  | 9203(1)  | 7533(1) | 35(1) |
| C(51) | 7799(2)  | 8057(1)  | 8605(1) | 37(1) |
| C(8)  | 12282(1) | 8031(1)  | 6103(1) | 32(1) |
| C(9)  | 13011(2) | 7621(1)  | 6128(1) | 41(1) |
| C(46) | 8224(2)  | 8654(1)  | 8764(1) | 43(1) |
| C(30) | 6985(2)  | 8306(1)  | 4937(1) | 38(1) |
| C(22) | 9597(2)  | 10677(1) | 5422(1) | 36(1) |
| C(42) | 5995(2)  | 6704(1)  | 6730(1) | 34(1) |
| C(35) | 6158(1)  | 7961(1)  | 5731(1) | 30(1) |
| C(45) | 8219(2)  | 7462(1)  | 7516(1) | 34(1) |
| C(15) | 9504(2)  | 8417(1)  | 5757(1) | 36(1) |
| C(44) | 8594(1)  | 7409(1)  | 6943(1) | 35(1) |
| C(26) | 12090(2) | 10335(1) | 7394(1) | 37(1) |
| C(13) | 12256(2) | 8526(1)  | 5709(1) | 37(1) |
| C(34) | 6110(2)  | 9116(1)  | 5410(1) | 40(1) |

|       |          |          |         |       |
|-------|----------|----------|---------|-------|
| C(55) | 4941(1)  | 9183(1)  | 7048(1) | 36(1) |
| C(38) | 5607(2)  | 6469(1)  | 5813(1) | 45(1) |
| C(21) | 8739(2)  | 10727(1) | 5553(1) | 43(1) |
| C(24) | 10586(2) | 10639(1) | 6207(1) | 32(1) |
| C(63) | 11452(2) | 8254(1)  | 8029(1) | 42(1) |
| C(5)  | 11271(2) | 7171(1)  | 7600(1) | 47(1) |
| C(32) | 6969(2)  | 9506(1)  | 4601(1) | 44(1) |
| C(27) | 12944(2) | 10342(1) | 7089(1) | 41(1) |
| C(16) | 9670(2)  | 9131(1)  | 5539(1) | 38(1) |
| C(50) | 7960(2)  | 7481(1)  | 8902(1) | 52(1) |
| C(57) | 4622(2)  | 7986(1)  | 7275(1) | 42(1) |
| C(20) | 8176(2)  | 11155(1) | 5275(1) | 50(1) |
| C(40) | 4907(2)  | 5877(1)  | 6541(1) | 48(1) |
| C(23) | 10213(2) | 10223(1) | 5741(1) | 33(1) |
| C(31) | 7488(2)  | 8863(1)  | 4651(1) | 45(1) |
| C(47) | 8788(2)  | 8666(2)  | 9205(1) | 51(1) |
| C(33) | 6604(2)  | 9698(1)  | 5151(1) | 44(1) |
| C(56) | 4219(2)  | 8665(1)  | 7139(1) | 39(1) |
| C(41) | 5405(2)  | 6223(1)  | 6914(1) | 43(1) |
| C(2)  | 10858(2) | 8054(1)  | 8495(1) | 53(1) |
| C(60) | 9345(2)  | 9902(1)  | 7700(1) | 38(1) |
| C(12) | 12932(2) | 8610(1)  | 5344(1) | 49(1) |
| C(64) | 7464(2)  | 10165(1) | 6869(1) | 50(1) |
| C(4)  | 10683(2) | 6937(1)  | 8054(1) | 56(1) |
| C(62) | 9673(2)  | 10823(1) | 8384(1) | 62(1) |
| C(65) | 6692(2)  | 10557(1) | 6642(1) | 54(1) |
| C(17) | 9888(2)  | 11084(2) | 5004(1) | 66(1) |
| C(49) | 8536(2)  | 7495(2)  | 9345(1) | 63(1) |
| C(19) | 8481(2)  | 11550(2) | 4869(1) | 65(1) |
| C(61) | 9859(2)  | 10115(1) | 8197(1) | 47(1) |
| C(48) | 8937(2)  | 8075(2)  | 9489(1) | 58(1) |
| C(11) | 13648(2) | 8200(1)  | 5382(1) | 52(1) |
| C(3)  | 10875(2) | 7293(2)  | 8592(1) | 57(1) |
| C(10) | 13696(2) | 7708(2)  | 5769(1) | 50(1) |
| C(39) | 5014(2)  | 5990(1)  | 5996(1) | 54(1) |
| C(66) | 6510(2)  | 11202(2) | 6934(2) | 87(1) |

|        |          |          |         |       |
|--------|----------|----------|---------|-------|
| C(18)  | 9341(2)  | 11533(2) | 4731(1) | 79(1) |
| Li(3A) | 9075(2)  | 9490(2)  | 6592(2) | 37(1) |
| Li(1A) | 10135(2) | 8285(2)  | 7108(2) | 36(1) |
| Li(2)  | 6838(2)  | 8130(2)  | 7032(2) | 34(1) |
| Li(1)  | 7619(3)  | 8553(2)  | 6085(2) | 37(1) |
| Li(3)  | 8286(3)  | 8854(2)  | 7290(2) | 36(1) |
| Li(2A) | 10754(2) | 9283(2)  | 6440(2) | 32(1) |
| N(4)   | 5945(1)  | 8539(1)  | 7629(1) | 32(1) |
| N(1A)  | 11227(1) | 7916(1)  | 7517(1) | 32(1) |
| N(1)   | 6671(1)  | 8514(1)  | 5478(1) | 28(1) |
| N(3)   | 7704(1)  | 8063(1)  | 7593(1) | 29(1) |
| N(2A)  | 10752(1) | 8296(1)  | 6400(1) | 30(1) |
| N(2)   | 7301(1)  | 7677(1)  | 6373(1) | 28(1) |
| N(3A)  | 9852(1)  | 9607(1)  | 5973(1) | 29(1) |

---

**Table 10.** Bond lengths [Å] and angles [°] for 5.

---

|              |          |
|--------------|----------|
| N(4A)-C(29)  | 1.479(3) |
| N(4A)-C(25)  | 1.485(3) |
| N(4A)-C(24)  | 1.490(3) |
| N(4A)-Li(2A) | 2.147(4) |
| C(1A)-C(60)  | 1.568(3) |
| C(1A)-Li(1A) | 2.158(5) |
| C(1A)-Li(3)  | 2.207(5) |
| C(1A)-Li(3A) | 2.267(5) |
| C(14)-N(2A)  | 1.464(3) |
| C(14)-C(15)  | 1.532(3) |
| C(29)-C(28)  | 1.531(3) |
| C(1)-C(64)   | 1.564(3) |
| C(1)-Li(1)   | 2.207(5) |
| C(1)-Li(3A)  | 2.238(4) |
| C(1)-Li(3)   | 2.248(5) |
| C(7)-N(2A)   | 1.449(3) |
| C(7)-C(6)    | 1.520(3) |
| C(7)-C(8)    | 1.544(3) |
| C(52)-N(3)   | 1.443(3) |
| C(52)-C(51)  | 1.523(3) |
| C(52)-C(53)  | 1.535(3) |
| C(36)-N(2)   | 1.452(3) |
| C(36)-C(37)  | 1.551(3) |
| C(36)-C(35)  | 1.536(3) |
| C(37)-C(42)  | 1.379(3) |
| C(37)-C(38)  | 1.383(3) |
| C(58)-N(4)   | 1.487(3) |
| C(58)-C(57)  | 1.524(3) |
| C(43)-N(2)   | 1.455(3) |
| C(43)-C(44)  | 1.518(3) |
| C(25)-C(26)  | 1.504(3) |
| C(6)-N(1A)   | 1.476(3) |
| C(53)-N(4)   | 1.483(3) |
| C(28)-C(27)  | 1.523(4) |

|              |          |
|--------------|----------|
| C(54)-N(4)   | 1.475(3) |
| C(54)-C(55)  | 1.507(3) |
| C(51)-C(50)  | 1.374(4) |
| C(51)-C(46)  | 1.407(4) |
| C(8)-C(13)   | 1.375(3) |
| C(8)-C(9)    | 1.392(3) |
| C(9)-C(10)   | 1.387(4) |
| C(46)-C(47)  | 1.388(4) |
| C(30)-N(1)   | 1.470(3) |
| C(30)-C(31)  | 1.520(3) |
| C(22)-C(17)  | 1.376(4) |
| C(22)-C(21)  | 1.371(3) |
| C(22)-C(23)  | 1.527(3) |
| C(42)-C(41)  | 1.393(3) |
| C(35)-N(1)   | 1.488(3) |
| C(45)-N(3)   | 1.444(3) |
| C(45)-C(44)  | 1.522(3) |
| C(45)-Li(2)  | 2.779(4) |
| C(15)-C(16)  | 1.532(3) |
| C(26)-C(27)  | 1.518(3) |
| C(13)-C(12)  | 1.386(4) |
| C(34)-N(1)   | 1.484(3) |
| C(34)-C(33)  | 1.521(4) |
| C(55)-C(56)  | 1.533(3) |
| C(38)-C(39)  | 1.394(4) |
| C(21)-C(20)  | 1.392(4) |
| C(24)-C(23)  | 1.520(3) |
| C(63)-N(1A)  | 1.461(3) |
| C(63)-C(2)   | 1.517(4) |
| C(5)-N(1A)   | 1.490(3) |
| C(5)-C(4)    | 1.510(4) |
| C(32)-C(33)  | 1.509(4) |
| C(32)-C(31)  | 1.510(4) |
| C(16)-N(3A)  | 1.446(3) |
| C(16)-Li(2A) | 2.786(5) |
| C(50)-C(49)  | 1.404(4) |

|                    |            |
|--------------------|------------|
| C(57)-C(56)        | 1.519(3)   |
| C(20)-C(19)        | 1.349(4)   |
| C(40)-C(39)        | 1.361(4)   |
| C(40)-C(41)        | 1.377(4)   |
| C(23)-N(3A)        | 1.456(3)   |
| C(47)-C(48)        | 1.379(4)   |
| C(2)-C(3)          | 1.526(4)   |
| C(60)-C(61)        | 1.512(4)   |
| C(12)-C(11)        | 1.378(4)   |
| C(64)-C(65)        | 1.529(4)   |
| C(4)-C(3)          | 1.519(4)   |
| C(62)-C(61)        | 1.502(4)   |
| C(65)-C(66)        | 1.490(4)   |
| C(17)-C(18)        | 1.397(4)   |
| C(49)-C(48)        | 1.352(4)   |
| C(19)-C(18)        | 1.375(5)   |
| C(11)-C(10)        | 1.361(4)   |
| Li(3A)-N(3A)       | 1.947(5)   |
| Li(1A)-N(2A)       | 1.977(5)   |
| Li(1A)-N(1A)       | 2.095(4)   |
| Li(2)-N(3)         | 1.923(4)   |
| Li(2)-N(2)         | 1.979(5)   |
| Li(2)-N(4)         | 2.167(4)   |
| Li(1)-N(2)         | 1.936(4)   |
| Li(1)-N(1)         | 2.089(4)   |
| Li(3)-N(3)         | 1.953(4)   |
| Li(2A)-N(3A)       | 1.916(4)   |
| Li(2A)-N(2A)       | 1.957(4)   |
|                    |            |
| C(29)-N(4A)-C(25)  | 109.02(17) |
| C(29)-N(4A)-C(24)  | 109.34(17) |
| C(25)-N(4A)-C(24)  | 107.86(17) |
| C(29)-N(4A)-Li(2A) | 109.02(17) |
| C(25)-N(4A)-Li(2A) | 123.59(18) |
| C(24)-N(4A)-Li(2A) | 96.86(16)  |
| C(60)-C(1A)-Li(1A) | 172.8(2)   |

|                     |            |
|---------------------|------------|
| C(60)-C(1A)-Li(3)   | 95.53(17)  |
| Li(1A)-C(1A)-Li(3)  | 90.84(17)  |
| C(60)-C(1A)-Li(3A)  | 94.65(17)  |
| Li(1A)-C(1A)-Li(3A) | 91.04(18)  |
| Li(3)-C(1A)-Li(3A)  | 66.31(16)  |
| N(2A)-C(14)-C(15)   | 113.33(19) |
| N(4A)-C(29)-C(28)   | 111.00(19) |
| C(64)-C(1)-Li(1)    | 162.9(2)   |
| C(64)-C(1)-Li(3A)   | 98.36(18)  |
| Li(1)-C(1)-Li(3A)   | 91.09(17)  |
| C(64)-C(1)-Li(3)    | 105.82(19) |
| Li(1)-C(1)-Li(3)    | 91.06(17)  |
| Li(3A)-C(1)-Li(3)   | 66.14(16)  |
| N(2A)-C(7)-C(6)     | 108.04(19) |
| N(2A)-C(7)-C(8)     | 115.69(19) |
| C(6)-C(7)-C(8)      | 108.90(17) |
| N(3)-C(52)-C(51)    | 113.37(18) |
| N(3)-C(52)-C(53)    | 108.32(19) |
| C(51)-C(52)-C(53)   | 111.8(2)   |
| N(2)-C(36)-C(37)    | 115.72(19) |
| N(2)-C(36)-C(35)    | 109.00(18) |
| C(37)-C(36)-C(35)   | 107.09(18) |
| C(42)-C(37)-C(38)   | 118.1(2)   |
| C(42)-C(37)-C(36)   | 122.1(2)   |
| C(38)-C(37)-C(36)   | 119.8(2)   |
| N(4)-C(58)-C(57)    | 110.9(2)   |
| N(2)-C(43)-C(44)    | 114.18(19) |
| N(4A)-C(25)-C(26)   | 112.39(19) |
| N(1A)-C(6)-C(7)     | 113.71(18) |
| N(4)-C(53)-C(52)    | 112.34(19) |
| C(27)-C(28)-C(29)   | 110.5(2)   |
| N(4)-C(54)-C(55)    | 111.37(19) |
| C(50)-C(51)-C(46)   | 117.7(2)   |
| C(50)-C(51)-C(52)   | 120.3(2)   |
| C(46)-C(51)-C(52)   | 122.0(2)   |
| C(13)-C(8)-C(9)     | 118.1(2)   |

|                    |            |
|--------------------|------------|
| C(13)-C(8)-C(7)    | 122.2(2)   |
| C(9)-C(8)-C(7)     | 119.7(2)   |
| C(8)-C(9)-C(10)    | 121.4(3)   |
| C(51)-C(46)-C(47)  | 121.6(3)   |
| N(1)-C(30)-C(31)   | 112.3(2)   |
| C(17)-C(22)-C(21)  | 116.7(2)   |
| C(17)-C(22)-C(23)  | 121.3(2)   |
| C(21)-C(22)-C(23)  | 122.0(2)   |
| C(37)-C(42)-C(41)  | 121.3(2)   |
| N(1)-C(35)-C(36)   | 113.26(18) |
| N(3)-C(45)-C(44)   | 112.74(19) |
| N(3)-C(45)-Li(2)   | 40.40(13)  |
| C(44)-C(45)-Li(2)  | 86.22(15)  |
| C(16)-C(15)-C(14)  | 116.2(2)   |
| C(45)-C(44)-C(43)  | 116.29(19) |
| C(25)-C(26)-C(27)  | 111.2(2)   |
| C(12)-C(13)-C(8)   | 120.9(2)   |
| N(1)-C(34)-C(33)   | 111.1(2)   |
| C(54)-C(55)-C(56)  | 110.7(2)   |
| C(37)-C(38)-C(39)  | 120.6(3)   |
| C(22)-C(21)-C(20)  | 122.5(3)   |
| N(4A)-C(24)-C(23)  | 113.66(18) |
| N(1A)-C(63)-C(2)   | 112.3(2)   |
| N(1A)-C(5)-C(4)    | 112.1(2)   |
| C(33)-C(32)-C(31)  | 109.8(2)   |
| C(28)-C(27)-C(26)  | 109.6(2)   |
| N(3A)-C(16)-C(15)  | 112.2(2)   |
| N(3A)-C(16)-Li(2A) | 39.88(13)  |
| C(15)-C(16)-Li(2A) | 85.73(16)  |
| C(51)-C(50)-C(49)  | 120.5(3)   |
| C(56)-C(57)-C(58)  | 111.9(2)   |
| C(19)-C(20)-C(21)  | 119.5(3)   |
| C(39)-C(40)-C(41)  | 119.9(3)   |
| N(3A)-C(23)-C(24)  | 107.91(19) |
| N(3A)-C(23)-C(22)  | 116.80(19) |
| C(24)-C(23)-C(22)  | 107.64(19) |



|                    |            |
|--------------------|------------|
| C(32)-C(31)-C(30)  | 112.0(2)   |
| C(48)-C(47)-C(46)  | 118.8(3)   |
| C(32)-C(33)-C(34)  | 111.6(2)   |
| C(57)-C(56)-C(55)  | 108.93(19) |
| C(40)-C(41)-C(42)  | 119.6(3)   |
| C(3)-C(2)-C(63)    | 111.3(2)   |
| C(61)-C(60)-C(1A)  | 116.4(2)   |
| C(13)-C(12)-C(11)  | 119.7(3)   |
| C(65)-C(64)-C(1)   | 116.9(2)   |
| C(3)-C(4)-C(5)     | 112.1(2)   |
| C(66)-C(65)-C(64)  | 114.1(3)   |
| C(22)-C(17)-C(18)  | 121.9(3)   |
| C(48)-C(49)-C(50)  | 120.7(3)   |
| C(20)-C(19)-C(18)  | 120.4(3)   |
| C(62)-C(61)-C(60)  | 113.9(2)   |
| C(49)-C(48)-C(47)  | 120.7(3)   |
| C(10)-C(11)-C(12)  | 120.8(3)   |
| C(4)-C(3)-C(2)     | 108.7(2)   |
| C(11)-C(10)-C(9)   | 119.1(3)   |
| C(40)-C(39)-C(38)  | 120.5(3)   |
| C(19)-C(18)-C(17)  | 119.1(3)   |
| N(3A)-Li(3A)-C(1)  | 130.4(2)   |
| N(3A)-Li(3A)-C(1A) | 119.92(19) |
| C(1)-Li(3A)-C(1A)  | 109.18(19) |
| N(2A)-Li(1A)-N(1A) | 91.85(17)  |
| N(2A)-Li(1A)-C(1A) | 119.1(2)   |
| N(1A)-Li(1A)-C(1A) | 115.3(2)   |
| N(3)-Li(2)-N(2)    | 107.24(19) |
| N(3)-Li(2)-N(4)    | 89.46(18)  |
| N(2)-Li(2)-N(4)    | 161.6(2)   |
| N(3)-Li(2)-C(45)   | 29.13(9)   |
| N(2)-Li(2)-C(45)   | 81.50(14)  |
| N(4)-Li(2)-C(45)   | 112.43(18) |
| N(2)-Li(1)-N(1)    | 92.71(18)  |
| N(2)-Li(1)-C(1)    | 120.2(2)   |
| N(1)-Li(1)-C(1)    | 117.4(2)   |

|                    |            |
|--------------------|------------|
| N(3)-Li(3)-C(1A)   | 129.5(2)   |
| N(3)-Li(3)-C(1)    | 119.1(2)   |
| C(1A)-Li(3)-C(1)   | 110.99(19) |
| N(3A)-Li(2A)-N(2A) | 107.7(2)   |
| N(3A)-Li(2A)-N(4A) | 91.15(17)  |
| N(2A)-Li(2A)-N(4A) | 157.9(2)   |
| N(3A)-Li(2A)-C(16) | 28.95(10)  |
| N(2A)-Li(2A)-C(16) | 81.48(15)  |
| N(4A)-Li(2A)-C(16) | 113.48(17) |
| C(54)-N(4)-C(58)   | 108.74(17) |
| C(54)-N(4)-C(53)   | 109.14(18) |
| C(58)-N(4)-C(53)   | 110.29(19) |
| C(54)-N(4)-Li(2)   | 119.75(18) |
| C(58)-N(4)-Li(2)   | 109.98(17) |
| C(53)-N(4)-Li(2)   | 98.38(16)  |
| C(63)-N(1A)-C(6)   | 110.49(18) |
| C(63)-N(1A)-C(5)   | 109.0(2)   |
| C(6)-N(1A)-C(5)    | 108.29(19) |
| C(63)-N(1A)-Li(1A) | 116.24(19) |
| C(6)-N(1A)-Li(1A)  | 95.15(17)  |
| C(5)-N(1A)-Li(1A)  | 116.54(19) |
| C(30)-N(1)-C(35)   | 110.18(18) |
| C(30)-N(1)-C(34)   | 108.52(19) |
| C(35)-N(1)-C(34)   | 108.90(17) |
| C(30)-N(1)-Li(1)   | 114.70(18) |
| C(35)-N(1)-Li(1)   | 96.15(17)  |
| C(34)-N(1)-Li(1)   | 117.56(18) |
| C(52)-N(3)-C(45)   | 110.72(18) |
| C(52)-N(3)-Li(2)   | 104.93(18) |
| C(45)-N(3)-Li(2)   | 110.47(19) |
| C(52)-N(3)-Li(3)   | 126.93(19) |
| C(45)-N(3)-Li(3)   | 110.89(18) |
| Li(2)-N(3)-Li(3)   | 89.74(18)  |
| C(7)-N(2A)-C(14)   | 110.26(18) |
| C(7)-N(2A)-Li(2A)  | 120.25(18) |
| C(14)-N(2A)-Li(2A) | 115.03(19) |

|                     |            |
|---------------------|------------|
| C(7)-N(2A)-Li(1A)   | 103.66(18) |
| C(14)-N(2A)-Li(1A)  | 117.45(18) |
| Li(2A)-N(2A)-Li(1A) | 88.18(18)  |
| C(36)-N(2)-C(43)    | 109.21(17) |
| C(36)-N(2)-Li(1)    | 104.89(18) |
| C(43)-N(2)-Li(1)    | 119.10(19) |
| C(36)-N(2)-Li(2)    | 120.34(18) |
| C(43)-N(2)-Li(2)    | 113.26(18) |
| Li(1)-N(2)-Li(2)    | 89.01(18)  |
| C(16)-N(3A)-C(23)   | 109.53(18) |
| C(16)-N(3A)-Li(2A)  | 111.17(18) |
| C(23)-N(3A)-Li(2A)  | 103.38(18) |
| C(16)-N(3A)-Li(3A)  | 111.86(19) |
| C(23)-N(3A)-Li(3A)  | 129.80(19) |
| Li(2A)-N(3A)-Li(3A) | 86.99(18)  |

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Symmetry transformations used to generate equivalent atoms:

**Table 11.** Anisotropic displacement parameters ( $\text{\AA}^2 \times 10^3$ ) for 5. The anisotropic displacement factor exponent takes the form:  $-2p^2 [ h^2 a^{*2} U^{11} + \dots + 2 h k a^* b^* U^{12} ]$

|       | U <sup>11</sup> | U <sup>22</sup> | U <sup>33</sup> | U <sup>23</sup> | U <sup>13</sup> | U <sup>12</sup> |
|-------|-----------------|-----------------|-----------------|-----------------|-----------------|-----------------|
| N(4A) | 24(1)           | 26(1)           | 36(1)           | -3(1)           | -1(1)           | 3(1)            |
| C(1A) | 19(1)           | 26(1)           | 43(2)           | 0(1)            | -1(1)           | 3(1)            |
| C(14) | 26(1)           | 33(1)           | 43(2)           | -7(1)           | 1(1)            | -3(1)           |
| C(29) | 29(1)           | 34(1)           | 41(2)           | -2(1)           | 2(1)            | -1(1)           |
| C(1)  | 20(1)           | 29(1)           | 36(1)           | -7(1)           | 1(1)            | 0(1)            |
| C(7)  | 22(1)           | 24(1)           | 47(2)           | -4(1)           | 1(1)            | -5(1)           |
| C(52) | 25(1)           | 39(1)           | 36(1)           | -1(1)           | 0(1)            | 1(1)            |
| C(36) | 27(1)           | 28(1)           | 31(1)           | -4(1)           | 0(1)            | 2(1)            |
| C(37) | 30(1)           | 29(1)           | 37(2)           | 0(1)            | -2(1)           | 1(1)            |
| C(58) | 26(1)           | 35(1)           | 54(2)           | -1(1)           | 2(1)            | 2(1)            |
| C(43) | 27(1)           | 32(1)           | 39(2)           | -5(1)           | 2(1)            | 6(1)            |
| C(25) | 30(1)           | 30(1)           | 41(2)           | -6(1)           | -1(1)           | 0(1)            |
| C(6)  | 22(1)           | 30(1)           | 47(2)           | 3(1)            | 1(1)            | -2(1)           |
| C(53) | 27(1)           | 41(1)           | 36(2)           | -6(1)           | 4(1)            | 6(1)            |
| C(28) | 23(1)           | 38(1)           | 55(2)           | -2(1)           | 1(1)            | 3(1)            |
| C(54) | 24(1)           | 30(1)           | 51(2)           | -2(1)           | 5(1)            | 1(1)            |
| C(51) | 31(1)           | 48(2)           | 32(1)           | -2(1)           | 7(1)            | 9(1)            |
| C(8)  | 20(1)           | 31(1)           | 45(2)           | -15(1)          | -1(1)           | -5(1)           |
| C(9)  | 26(1)           | 49(2)           | 49(2)           | -12(1)          | -3(1)           | -4(1)           |
| C(46) | 36(1)           | 50(2)           | 43(2)           | 0(1)            | -2(1)           | -5(1)           |
| C(30) | 36(1)           | 37(1)           | 41(2)           | -3(1)           | -1(1)           | -3(1)           |
| C(22) | 38(1)           | 38(1)           | 31(1)           | 3(1)            | -5(1)           | -4(1)           |
| C(42) | 34(1)           | 31(1)           | 39(2)           | -1(1)           | 2(1)            | 3(1)            |
| C(35) | 23(1)           | 31(1)           | 34(1)           | -3(1)           | -5(1)           | -2(1)           |
| C(45) | 26(1)           | 37(1)           | 39(2)           | 2(1)            | -5(1)           | 9(1)            |
| C(15) | 26(1)           | 42(1)           | 39(2)           | -11(1)          | -7(1)           | -4(1)           |
| C(44) | 24(1)           | 36(1)           | 43(2)           | -7(1)           | -2(1)           | 13(1)           |
| C(26) | 34(1)           | 34(1)           | 42(2)           | -5(1)           | -6(1)           | 1(1)            |
| C(13) | 29(1)           | 33(1)           | 48(2)           | -11(1)          | 4(1)            | -8(1)           |
| C(34) | 39(1)           | 37(1)           | 44(2)           | 3(1)            | -8(1)           | 7(1)            |

|       |       |       |        |        |        |        |
|-------|-------|-------|--------|--------|--------|--------|
| C(55) | 21(1) | 34(1) | 53(2)  | 2(1)   | -3(1)  | 5(1)   |
| C(38) | 57(2) | 38(1) | 40(2)  | 4(1)   | -10(1) | -11(1) |
| C(21) | 42(2) | 35(1) | 53(2)  | 7(1)   | -6(1)  | 3(1)   |
| C(24) | 29(1) | 29(1) | 37(1)  | 1(1)   | -3(1)  | 3(1)   |
| C(63) | 35(1) | 49(2) | 42(2)  | 5(1)   | -3(1)  | -1(1)  |
| C(5)  | 37(2) | 35(1) | 70(2)  | 14(1)  | 6(2)   | 3(1)   |
| C(32) | 43(2) | 41(2) | 47(2)  | 11(1)  | -10(1) | -8(1)  |
| C(27) | 27(1) | 39(1) | 56(2)  | -4(1)  | -11(1) | 0(1)   |
| C(16) | 33(1) | 38(1) | 42(2)  | -2(1)  | -7(1)  | -1(1)  |
| C(50) | 63(2) | 43(2) | 48(2)  | -5(2)  | 0(2)   | 13(1)  |
| C(57) | 24(1) | 35(1) | 67(2)  | -7(1)  | -1(1)  | -4(1)  |
| C(20) | 48(2) | 42(2) | 61(2)  | 13(2)  | -18(2) | -4(1)  |
| C(40) | 41(2) | 39(2) | 64(2)  | 13(2)  | -7(2)  | -13(1) |
| C(23) | 26(1) | 39(1) | 33(1)  | -3(1)  | -1(1)  | 0(1)   |
| C(31) | 45(2) | 49(2) | 41(2)  | 5(1)   | 3(1)   | -4(1)  |
| C(47) | 42(2) | 66(2) | 45(2)  | -7(2)  | -4(2)  | 1(2)   |
| C(33) | 51(2) | 34(1) | 48(2)  | 8(1)   | -10(1) | 2(1)   |
| C(56) | 22(1) | 41(1) | 54(2)  | -1(1)  | 0(1)   | 2(1)   |
| C(41) | 42(2) | 42(2) | 44(2)  | 9(1)   | 7(1)   | 2(1)   |
| C(2)  | 50(2) | 61(2) | 48(2)  | 11(2)  | 4(2)   | 4(2)   |
| C(60) | 35(1) | 39(1) | 41(2)  | 2(1)   | 5(1)   | -2(1)  |
| C(12) | 41(2) | 48(2) | 57(2)  | -5(2)  | 9(2)   | -14(1) |
| C(64) | 34(2) | 51(2) | 65(2)  | -2(2)  | 0(2)   | -5(1)  |
| C(4)  | 43(2) | 45(2) | 80(2)  | 23(2)  | 15(2)  | 2(1)   |
| C(62) | 84(2) | 48(2) | 55(2)  | -10(2) | 8(2)   | -16(2) |
| C(65) | 48(2) | 46(2) | 69(2)  | 0(2)   | 5(2)   | 4(2)   |
| C(17) | 54(2) | 90(2) | 53(2)  | 21(2)  | -7(2)  | -1(2)  |
| C(49) | 79(2) | 56(2) | 56(2)  | -4(2)  | -23(2) | 26(2)  |
| C(19) | 55(2) | 74(2) | 68(2)  | 11(2)  | -26(2) | 4(2)   |
| C(61) | 56(2) | 42(2) | 43(2)  | -3(1)  | 4(2)   | -8(1)  |
| C(48) | 49(2) | 86(2) | 40(2)  | -12(2) | -8(2)  | 22(2)  |
| C(11) | 31(1) | 60(2) | 66(2)  | -19(2) | 14(2)  | -14(1) |
| C(3)  | 37(2) | 69(2) | 66(2)  | 31(2)  | 11(2)  | 4(1)   |
| C(10) | 24(1) | 59(2) | 68(2)  | -16(2) | -1(2)  | -2(1)  |
| C(39) | 62(2) | 46(2) | 53(2)  | 9(2)   | -23(2) | -24(2) |
| C(66) | 60(2) | 59(2) | 144(4) | -23(2) | -2(2)  | 11(2)  |

|        |       |        |       |       |        |       |
|--------|-------|--------|-------|-------|--------|-------|
| C(18)  | 76(2) | 101(3) | 59(2) | 40(2) | -12(2) | -3(2) |
| Li(3A) | 25(2) | 35(2)  | 50(3) | 2(2)  | -1(2)  | -3(2) |
| Li(1A) | 25(2) | 37(2)  | 46(3) | -4(2) | 2(2)   | 0(2)  |
| Li(2)  | 23(2) | 34(2)  | 45(3) | 1(2)  | -3(2)  | -1(2) |
| Li(1)  | 35(2) | 35(2)  | 40(2) | -4(2) | -8(2)  | -4(2) |
| Li(3)  | 30(2) | 36(2)  | 42(3) | -8(2) | 0(2)   | -3(2) |
| Li(2A) | 29(2) | 26(2)  | 42(2) | -6(2) | 0(2)   | -4(2) |
| N(4)   | 20(1) | 33(1)  | 42(1) | 1(1)  | 0(1)   | 4(1)  |
| N(1A)  | 26(1) | 28(1)  | 42(1) | 5(1)  | 1(1)   | 2(1)  |
| N(1)   | 24(1) | 28(1)  | 32(1) | 2(1)  | -4(1)  | 2(1)  |
| N(3)   | 22(1) | 33(1)  | 31(1) | -1(1) | 3(1)   | 5(1)  |
| N(2A)  | 19(1) | 29(1)  | 41(1) | -4(1) | -5(1)  | 1(1)  |
| N(2)   | 23(1) | 29(1)  | 33(1) | -1(1) | -5(1)  | 6(1)  |
| N(3A)  | 24(1) | 29(1)  | 34(1) | -2(1) | -3(1)  | -1(1) |

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**Table 12.** Hydrogen coordinates ( $\times 10^4$ ) and isotropic displacement parameters ( $\text{\AA}^2 \times 10^3$ ) for 5.

|        | x     | y     | z    | U(eq) |
|--------|-------|-------|------|-------|
| H(14A) | 10126 | 7543  | 6011 | 40    |
| H(14B) | 10709 | 7994  | 5613 | 40    |
| H(29A) | 12239 | 10802 | 6141 | 42    |
| H(29B) | 12032 | 10090 | 5858 | 42    |
| H(7)   | 11386 | 7426  | 6508 | 37    |
| H(52)  | 6913  | 7586  | 8105 | 40    |
| H(36)  | 7073  | 7197  | 5666 | 34    |
| H(58A) | 4944  | 8174  | 8085 | 46    |
| H(58B) | 5521  | 7590  | 7816 | 46    |
| H(43A) | 8312  | 7102  | 6158 | 39    |
| H(43B) | 7703  | 6757  | 6606 | 39    |
| H(25A) | 10829 | 10609 | 7258 | 40    |
| H(25B) | 11506 | 11118 | 6985 | 40    |
| H(6A)  | 12398 | 7871  | 7152 | 40    |
| H(6B)  | 11947 | 8594  | 7098 | 40    |
| H(53A) | 6215  | 8573  | 8443 | 42    |
| H(53B) | 6845  | 9035  | 8084 | 42    |
| H(28A) | 12708 | 9511  | 6593 | 46    |
| H(28B) | 13378 | 10032 | 6326 | 46    |
| H(54A) | 5996  | 9545  | 7468 | 42    |
| H(54B) | 5213  | 9340  | 7862 | 42    |
| H(9)   | 13041 | 7275  | 6396 | 49    |
| H(46)  | 8121  | 9058  | 8566 | 52    |
| H(30A) | 6486  | 8176  | 4706 | 46    |
| H(30B) | 7361  | 7905  | 4978 | 46    |
| H(42)  | 6335  | 6943  | 6989 | 41    |
| H(35A) | 5767  | 7768  | 5452 | 35    |
| H(35B) | 5796  | 8152  | 6026 | 35    |
| H(45A) | 7856  | 7059  | 7588 | 41    |
| H(45B) | 8696  | 7462  | 7785 | 41    |

|        |       |       |      |    |
|--------|-------|-------|------|----|
| H(15A) | 9192  | 8159  | 5472 | 43 |
| H(15B) | 9116  | 8452  | 6078 | 43 |
| H(44A) | 9082  | 7086  | 6953 | 41 |
| H(44B) | 8833  | 7856  | 6842 | 41 |
| H(26A) | 11940 | 9864  | 7491 | 44 |
| H(26B) | 12149 | 10596 | 7737 | 44 |
| H(13)  | 11767 | 8815  | 5686 | 44 |
| H(34A) | 5886  | 9258  | 5771 | 48 |
| H(34B) | 5610  | 8997  | 5176 | 48 |
| H(55A) | 5271  | 9062  | 6715 | 43 |
| H(55B) | 4685  | 9636  | 6991 | 43 |
| H(38)  | 5676  | 6543  | 5432 | 54 |
| H(21)  | 8520  | 10459 | 5844 | 52 |
| H(24A) | 10827 | 11063 | 6056 | 38 |
| H(24B) | 10114 | 10762 | 6461 | 38 |
| H(1A)  | 11421 | 8749  | 7975 | 50 |
| H(1B)  | 12054 | 8138  | 8127 | 50 |
| H(5A)  | 11872 | 7042  | 7687 | 57 |
| H(5B)  | 11106 | 6941  | 7256 | 57 |
| H(32A) | 7342  | 9875  | 4463 | 52 |
| H(32B) | 6492  | 9439  | 4336 | 52 |
| H(27A) | 13137 | 10814 | 7034 | 49 |
| H(27B) | 13389 | 10103 | 7306 | 49 |
| H(16A) | 10164 | 9120  | 5283 | 45 |
| H(16B) | 9156  | 9286  | 5333 | 45 |
| H(50)  | 7679  | 7071  | 8807 | 62 |
| H(57A) | 4926  | 7810  | 6949 | 50 |
| H(57B) | 4160  | 7661  | 7371 | 50 |
| H(20)  | 7581  | 11168 | 5370 | 60 |
| H(40)  | 4489  | 5560  | 6664 | 58 |
| H(23)  | 10698 | 10093 | 5493 | 39 |
| H(31A) | 8023  | 8958  | 4859 | 54 |
| H(31B) | 7657  | 8708  | 4281 | 54 |
| H(47)  | 9068  | 9073  | 9308 | 61 |
| H(33A) | 6213  | 10090 | 5108 | 53 |
| H(33B) | 7081  | 9835  | 5397 | 53 |



|        |       |       |      |     |
|--------|-------|-------|------|-----|
| H(56A) | 3842  | 8814  | 7443 | 47  |
| H(56B) | 3862  | 8626  | 6804 | 47  |
| H(41)  | 5346  | 6135  | 7294 | 51  |
| H(2A)  | 11040 | 8290  | 8833 | 63  |
| H(2B)  | 10261 | 8198  | 8408 | 63  |
| H(60A) | 9390  | 10264 | 7422 | 46  |
| H(60B) | 8730  | 9868  | 7807 | 46  |
| H(12)  | 12901 | 8949  | 5069 | 58  |
| H(64A) | 7384  | 10116 | 7268 | 60  |
| H(64B) | 7989  | 10441 | 6811 | 60  |
| H(4A)  | 10076 | 7025  | 7950 | 67  |
| H(4B)  | 10752 | 6444  | 8104 | 67  |
| H(62A) | 9051  | 10876 | 8442 | 94  |
| H(62B) | 9869  | 11144 | 8105 | 94  |
| H(62C) | 9980  | 10910 | 8728 | 94  |
| H(65A) | 6800  | 10658 | 6251 | 65  |
| H(65B) | 6173  | 10266 | 6662 | 65  |
| H(17)  | 10477 | 11058 | 4899 | 79  |
| H(49)  | 8646  | 7093  | 9545 | 76  |
| H(19)  | 8099  | 11841 | 4677 | 78  |
| H(61A) | 9733  | 9799  | 8500 | 56  |
| H(61B) | 10482 | 10077 | 8111 | 56  |
| H(48)  | 9326  | 8076  | 9789 | 69  |
| H(11)  | 14115 | 8262  | 5135 | 63  |
| H(3A)  | 11450 | 7154  | 8729 | 68  |
| H(3B)  | 10437 | 7168  | 8868 | 68  |
| H(10)  | 14192 | 7427  | 5793 | 60  |
| H(39)  | 4683  | 5740  | 5739 | 64  |
| H(66A) | 6969  | 11528 | 6855 | 131 |
| H(66B) | 6487  | 11118 | 7328 | 131 |
| H(66C) | 5955  | 11384 | 6811 | 131 |
| H(18)  | 9561  | 11822 | 4454 | 94  |

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## Crystallographic information for octalithio-aggregate (7)

**Table 13.** Crystal data and structure refinement for 7.

|                                   |  |          |
|-----------------------------------|--|----------|
| Identification code               | 7  |          |
| Empirical formula                 | C <sub>90</sub> H <sub>128</sub> Li <sub>8</sub> N <sub>8</sub> O <sub>8</sub> |          |
| Formula weight                    | 1505.52  |          |
| Temperature                       | 100(2) K   |          |
| Wavelength                        | 0.71073 Å  |          |
| Crystal system                    | Orthorhombic   |          |
| Space group                       | P2(1)2(1)2(1)  |          |
| Unit cell dimensions              | a = 21.1765(15) Å  | a = 90°. |
|                                   | b = 23.7194(17) Å  | b = 90°. |
|                                   | c = 24.744(2) Å  | g = 90°. |
| Volume                            | 12428.9(16) Å <sup>3</sup>   |          |
| Z                                 | 4  |          |
| Density (calculated)              | 0.805 Mg/m <sup>3</sup>  |          |
| Absorption coefficient            | 0.050 mm <sup>-1</sup>   |          |
| F(000)                            | 3248   |          |
| Crystal size                      | 0.15 x 0.15 x 0.10 mm <sup>3</sup>   |          |
| Theta range for data collection   | 1.53 to 23.82°.  |          |
| Index ranges                      | -24<=h<=17, -26<=k<=20, -20<=l<=28   |          |
| Reflections collected             | 28869  |          |
| Independent reflections           | 9929 [R(int) = 0.0625]   |          |
| Completeness to theta = 23.82°    | 96.1 %   |          |
| Absorption correction             | Semi-empirical from equivalents  |          |
| Max. and min. transmission        | 0.9950 and 0.9926  |          |
| Refinement method                 | Full-matrix least-squares on F <sup>2</sup>                                    |          |
| Data / restraints / parameters    | 9929 / 291 / 1138  |          |
| Goodness-of-fit on F <sup>2</sup> | 0.893  |          |
| Final R indices [I>2sigma(I)]     | R1 = 0.0689, wR2 = 0.1657  |          |
| R indices (all data)              | R1 = 0.1206, wR2 = 0.1836  |          |
| Absolute structure parameter      | 1(10)  |          |
| Largest diff. peak and hole       | 0.199 and -0.180 e.Å <sup>-3</sup>   |          |

**Table 14.** Atomic coordinates ( $\times 10^4$ ) and equivalent isotropic displacement parameters ( $\text{\AA}^2 \times 10^3$ ) for 7.  $U(\text{eq})$  is defined as one third of the trace of the orthogonalized  $U^{\text{ij}}$  tensor.

|        | x       | y       | z       | U(eq)  |
|--------|---------|---------|---------|--------|
| Li(1A) | 6161(5) | 5959(5) | 2822(5) | 70(3)  |
| Li(1)  | 3794(5) | 7844(4) | 1251(4) | 60(3)  |
| Li(2A) | 6657(4) | 5908(4) | 1943(4) | 53(3)  |
| Li(2)  | 4740(5) | 8068(4) | 686(4)  | 52(3)  |
| Li(3)  | 6206(6) | 8044(5) | 1681(5) | 78(4)  |
| Li(3A) | 5294(5) | 5909(4) | 812(4)  | 60(3)  |
| Li(4)  | 5301(4) | 7477(4) | 1366(4) | 48(2)  |
| Li(4A) | 5762(4) | 6456(4) | 1574(4) | 50(3)  |
| O(1)   | 6181(2) | 6517(2) | 2254(2) | 55(1)  |
| O(2)   | 5879(2) | 7349(2) | 1926(2) | 51(1)  |
| O(3)   | 5031(2) | 6583(2) | 1178(2) | 48(1)  |
| O(4)   | 4500(2) | 7385(2) | 1058(2) | 49(1)  |
| O(6)   | 3688(2) | 7820(2) | 2038(2) | 63(1)  |
| O(7)   | 4905(2) | 5473(2) | 242(2)  | 61(1)  |
| N(1A)  | 6872(3) | 5877(2) | 3455(2) | 68(2)  |
| N(1)   | 2916(2) | 7953(2) | 809(2)  | 55(1)  |
| N(2A)  | 6557(2) | 5301(2) | 2456(2) | 52(1)  |
| N(2)   | 4081(2) | 8594(2) | 952(2)  | 56(1)  |
| N(3A)  | 6155(2) | 5766(2) | 1229(2) | 51(1)  |
| N(3)   | 5603(2) | 8244(2) | 1051(2) | 47(1)  |
| N(4A)  | 7399(2) | 6298(2) | 1455(2) | 54(1)  |
| N(4)   | 5203(2) | 7834(2) | -42(2)  | 46(1)  |
| C(1)   | 7009(3) | 5057(3) | 2826(3) | 57(2)  |
| C(2)   | 7311(3) | 5518(3) | 3148(3) | 68(2)  |
| C(3)   | 6586(4) | 5531(3) | 3871(3) | 80(2)  |
| C(4)   | 6162(5) | 5869(5) | 4225(4) | 120(3) |
| C(5)   | 6524(5) | 6362(5) | 4506(4) | 122(3) |
| C(6)   | 6863(5) | 6688(4) | 4081(4) | 114(3) |
| C(7)   | 7246(4) | 6327(3) | 3718(3) | 87(2)  |
| C(8)   | 7527(3) | 4693(3) | 2574(3) | 63(2)  |

|       |          |          |         |        |
|-------|----------|----------|---------|--------|
| C(9)  | 7612(3)  | 4664(3)  | 2057(4) | 69(2)  |
| C(10) | 8084(4)  | 4348(3)  | 1823(4) | 96(3)  |
| C(11) | 8478(4)  | 4042(4)  | 2169(5) | 104(3) |
| C(12) | 8381(4)  | 4084(3)  | 2714(5) | 97(3)  |
| C(13) | 7909(3)  | 4400(3)  | 2921(3) | 72(2)  |
| C(14) | 3553(3)  | 8847(3)  | 674(3)  | 63(2)  |
| C(15) | 3148(3)  | 8379(3)  | 413(3)  | 57(2)  |
| C(16) | 2487(3)  | 8231(3)  | 1199(3) | 61(2)  |
| C(17) | 2197(3)  | 7800(3)  | 1567(3) | 67(2)  |
| C(18) | 1831(3)  | 7353(3)  | 1256(3) | 71(2)  |
| C(19) | 2267(3)  | 7071(3)  | 853(3)  | 58(2)  |
| C(20) | 2573(3)  | 7526(2)  | 495(3)  | 55(2)  |
| C(21) | 3716(3)  | 9284(3)  | 241(3)  | 55(2)  |
| C(22) | 4311(4)  | 9367(3)  | 74(3)   | 68(2)  |
| C(23) | 4454(4)  | 9759(3)  | -328(3) | 82(2)  |
| C(24) | 3984(5)  | 10077(3) | -546(3) | 90(3)  |
| C(25) | 3368(4)  | 10005(3) | -362(3) | 78(2)  |
| C(26) | 3231(3)  | 9613(3)  | 30(3)   | 62(2)  |
| C(27) | 6682(3)  | 5769(2)  | 845(3)  | 53(2)  |
| C(28) | 7038(3)  | 6329(2)  | 937(3)  | 57(2)  |
| C(29) | 8004(3)  | 6010(2)  | 1362(3) | 53(2)  |
| C(30) | 8375(3)  | 5956(3)  | 1860(3) | 65(2)  |
| C(31) | 8508(3)  | 6550(3)  | 2106(3) | 73(2)  |
| C(32) | 7888(3)  | 6867(3)  | 2171(3) | 65(2)  |
| C(33) | 7520(3)  | 6879(3)  | 1642(3) | 57(2)  |
| C(34) | 6491(3)  | 5699(3)  | 272(3)  | 52(2)  |
| C(35) | 6266(3)  | 6132(3)  | -52(3)  | 55(2)  |
| C(36) | 6088(3)  | 6046(3)  | -577(3) | 66(2)  |
| C(37) | 6161(3)  | 5515(3)  | -808(3) | 65(2)  |
| C(38) | 6384(3)  | 5078(3)  | -495(3) | 74(2)  |
| C(39) | 6558(3)  | 5159(3)  | 42(3)   | 66(2)  |
| C(40) | 6000(3)  | 7035(3)  | 2357(3) | 48(2)  |
| C(41) | 5856(6)  | 7176(5)  | 2873(6) | 45(4)  |
| C(42) | 5590(5)  | 7680(5)  | 3095(4) | 45(3)  |
| C(43) | 5460(8)  | 8179(7)  | 2830(5) | 45(5)  |
| C(44) | 5175(10) | 8629(8)  | 3078(7) | 62(6)  |

|        |          |          |          |        |
|--------|----------|----------|----------|--------|
| C(45)  | 5021(7)  | 8612(5)  | 3624(6)  | 65(4)  |
| C(46)  | 5179(7)  | 8141(6)  | 3903(5)  | 90(5)  |
| C(47)  | 5472(5)  | 7674(4)  | 3635(5)  | 67(4)  |
| C(41') | 6148(10) | 7294(8)  | 2842(10) | 58(6)  |
| C(42') | 5881(8)  | 7803(7)  | 3059(7)  | 64(6)  |
| C(43') | 5384(15) | 8111(12) | 2834(10) | 85(11) |
| C(44') | 5160(20) | 8584(15) | 3087(11) | 87(12) |
| C(45') | 5391(12) | 8771(9)  | 3579(10) | 97(8)  |
| C(46') | 5915(11) | 8506(8)  | 3782(7)  | 104(7) |
| C(47') | 6131(9)  | 8011(7)  | 3520(8)  | 87(6)  |
| C(48)  | 4502(3)  | 6828(3)  | 1087(2)  | 53(2)  |
| C(49)  | 3933(3)  | 6547(2)  | 968(2)   | 52(2)  |
| C(50)  | 3792(3)  | 5957(3)  | 1055(3)  | 56(2)  |
| C(51)  | 3258(3)  | 5741(3)  | 794(3)   | 77(2)  |
| C(52)  | 3070(4)  | 5173(3)  | 852(4)   | 89(2)  |
| C(53)  | 3419(4)  | 4839(4)  | 1183(4)  | 106(3) |
| C(54)  | 3945(4)  | 5036(3)  | 1449(4)  | 93(3)  |
| C(55)  | 4121(3)  | 5593(3)  | 1373(3)  | 71(2)  |
| O(5)   | 5266(2)  | 5882(2)  | 3058(2)  | 72(1)  |
| C(56)  | 4990(4)  | 5392(3)  | 3293(4)  | 100(3) |
| C(57)  | 4400(4)  | 5307(4)  | 3015(5)  | 121(3) |
| C(58)  | 4183(4)  | 5900(4)  | 2922(4)  | 117(3) |
| C(59)  | 4771(3)  | 6237(3)  | 2874(3)  | 84(2)  |
| C(60)  | 5841(3)  | 7836(2)  | 186(2)   | 50(2)  |
| C(61)  | 5947(3)  | 8332(2)  | 547(2)   | 49(2)  |
| C(62)  | 5014(3)  | 7259(2)  | -198(2)  | 49(2)  |
| C(63)  | 4351(3)  | 7252(2)  | -419(3)  | 57(2)  |
| C(64)  | 4286(3)  | 7642(3)  | -892(3)  | 70(2)  |
| C(65)  | 4533(3)  | 8227(2)  | -739(3)  | 57(2)  |
| C(66)  | 5180(3)  | 8202(2)  | -511(2)  | 53(2)  |
| C(67)  | 6639(3)  | 8472(3)  | 615(2)   | 49(2)  |
| C(68)  | 6844(4)  | 9022(3)  | 501(3)   | 79(2)  |
| C(69)  | 7484(4)  | 9156(3)  | 575(3)   | 91(2)  |
| C(70)  | 7907(3)  | 8768(3)  | 742(3)   | 75(2)  |
| C(71)  | 7692(3)  | 8227(3)  | 849(3)   | 68(2)  |
| C(72)  | 7064(3)  | 8099(3)  | 782(3)   | 56(2)  |

|        |          |         |          |        |
|--------|----------|---------|----------|--------|
| C(73)  | 3965(4)  | 7370(3) | 2336(3)  | 77(2)  |
| C(74)  | 3769(5)  | 7465(4) | 2913(4)  | 110(3) |
| C(75)  | 3364(5)  | 7993(4) | 2895(4)  | 118(3) |
| C(76)  | 3524(4)  | 8274(3) | 2386(3)  | 76(2)  |
| C(77)  | 4528(3)  | 5739(3) | -179(3)  | 61(2)  |
| C(78)  | 4232(4)  | 5272(3) | -480(4)  | 109(3) |
| C(79)  | 4483(6)  | 4755(4) | -293(4)  | 139(4) |
| C(80)  | 4847(4)  | 4864(3) | 210(3)   | 75(2)  |
| O(8)   | 6786(12) | 8483(8) | 2087(9)  | 71(5)  |
| C(81)  | 7217(11) | 8179(7) | 2396(11) | 115(7) |
| C(82)  | 7596(10) | 8550(8) | 2706(10) | 151(7) |
| C(83)  | 7523(12) | 9098(8) | 2432(11) | 168(8) |
| C(84)  | 6911(11) | 9058(8) | 2148(10) | 116(7) |
| O(8')  | 6896(13) | 8367(8) | 2087(10) | 65(5)  |
| C(81') | 7033(9)  | 8227(7) | 2632(7)  | 78(5)  |
| C(82') | 7019(14) | 8730(9) | 2927(7)  | 147(7) |
| C(83') | 6910(16) | 9188(8) | 2519(9)  | 152(8) |
| C(84') | 7129(13) | 8918(9) | 2015(8)  | 107(7) |
| C(85)  | 6131(3)  | 4868(2) | 2280(3)  | 59(2)  |
| C(86)  | 5658(3)  | 5079(3) | 1856(3)  | 63(2)  |
| C(87)  | 5935(3)  | 5176(3) | 1311(3)  | 64(2)  |
| C(88)  | 4318(3)  | 9014(3) | 1326(3)  | 64(2)  |
| C(89)  | 4900(3)  | 8807(2) | 1644(3)  | 56(2)  |
| C(90)  | 5495(3)  | 8793(2) | 1322(3)  | 56(2)  |

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**Table 15.** Bond lengths [Å] and angles [°] for 7.

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|               |           |
|---------------|-----------|
| Li(1A)-O(1)   | 1.931(12) |
| Li(1A)-O(5)   | 1.991(12) |
| Li(1A)-N(2A)  | 1.989(12) |
| Li(1A)-N(1A)  | 2.183(13) |
| Li(1A)-Li(2A) | 2.418(16) |
| Li(1A)-Li(4A) | 3.412(15) |
| Li(1)-O(4)    | 1.912(10) |
| Li(1)-O(6)    | 1.962(12) |
| Li(1)-N(2)    | 2.019(12) |
| Li(1)-N(1)    | 2.172(11) |
| Li(1)-Li(4)   | 3.322(13) |
| Li(2A)-O(1)   | 1.922(11) |
| Li(2A)-N(2A)  | 1.930(11) |
| Li(2A)-N(3A)  | 2.089(11) |
| Li(2A)-N(4A)  | 2.187(11) |
| Li(2)-O(4)    | 1.932(11) |
| Li(2)-N(2)    | 1.984(11) |
| Li(2)-N(3)    | 2.081(11) |
| Li(2)-N(4)    | 2.123(11) |
| Li(3)-O(2)    | 1.888(12) |
| Li(3)-O(8)    | 1.90(2)   |
| Li(3)-O(8')   | 1.93(2)   |
| Li(3)-N(3)    | 2.068(13) |
| Li(3A)-O(3)   | 1.920(11) |
| Li(3A)-O(7)   | 1.931(11) |
| Li(3A)-N(3A)  | 2.123(12) |
| Li(4)-O(4)    | 1.873(10) |
| Li(4)-O(2)    | 1.873(11) |
| Li(4)-N(3)    | 2.079(10) |
| Li(4)-O(3)    | 2.245(10) |
| Li(4A)-O(3)   | 1.857(10) |
| Li(4A)-O(1)   | 1.909(11) |
| Li(4A)-N(3A)  | 2.025(11) |
| Li(4A)-O(2)   | 2.303(10) |

|             |           |
|-------------|-----------|
| O(1)-C(40)  | 1.312(7)  |
| O(2)-C(40)  | 1.326(7)  |
| O(3)-C(48)  | 1.283(7)  |
| O(4)-C(48)  | 1.322(6)  |
| O(6)-C(76)  | 1.421(7)  |
| O(6)-C(73)  | 1.425(7)  |
| O(7)-C(80)  | 1.453(7)  |
| O(7)-C(77)  | 1.455(7)  |
| N(1A)-C(3)  | 1.449(8)  |
| N(1A)-C(2)  | 1.471(8)  |
| N(1A)-C(7)  | 1.479(9)  |
| N(1)-C(20)  | 1.470(7)  |
| N(1)-C(16)  | 1.480(7)  |
| N(1)-C(15)  | 1.489(8)  |
| N(2A)-C(85) | 1.434(7)  |
| N(2A)-C(1)  | 1.446(7)  |
| N(2)-C(14)  | 1.444(7)  |
| N(2)-C(88)  | 1.450(7)  |
| N(3A)-C(27) | 1.464(7)  |
| N(3A)-C(87) | 1.488(7)  |
| N(3)-C(61)  | 1.459(7)  |
| N(3)-C(90)  | 1.484(7)  |
| N(4A)-C(29) | 1.470(7)  |
| N(4A)-C(33) | 1.477(7)  |
| N(4A)-C(28) | 1.495(7)  |
| N(4)-C(66)  | 1.453(7)  |
| N(4)-C(60)  | 1.466(7)  |
| N(4)-C(62)  | 1.473(6)  |
| C(1)-C(2)   | 1.497(8)  |
| C(1)-C(8)   | 1.528(9)  |
| C(3)-C(4)   | 1.489(11) |
| C(4)-C(5)   | 1.563(12) |
| C(5)-C(6)   | 1.490(12) |
| C(6)-C(7)   | 1.483(11) |
| C(8)-C(9)   | 1.295(9)  |
| C(8)-C(13)  | 1.370(9)  |



|              |           |
|--------------|-----------|
| C(9)-C(10)   | 1.376(10) |
| C(10)-C(11)  | 1.400(11) |
| C(11)-C(12)  | 1.368(12) |
| C(12)-C(13)  | 1.349(10) |
| C(14)-C(21)  | 1.530(9)  |
| C(14)-C(15)  | 1.544(8)  |
| C(16)-C(17)  | 1.500(8)  |
| C(17)-C(18)  | 1.521(9)  |
| C(18)-C(19)  | 1.514(9)  |
| C(19)-C(20)  | 1.538(8)  |
| C(21)-C(22)  | 1.342(9)  |
| C(21)-C(26)  | 1.392(8)  |
| C(22)-C(23)  | 1.395(9)  |
| C(23)-C(24)  | 1.360(10) |
| C(24)-C(25)  | 1.392(10) |
| C(25)-C(26)  | 1.373(9)  |
| C(27)-C(34)  | 1.483(8)  |
| C(27)-C(28)  | 1.544(8)  |
| C(29)-C(30)  | 1.466(8)  |
| C(30)-C(31)  | 1.561(9)  |
| C(31)-C(32)  | 1.522(9)  |
| C(32)-C(33)  | 1.523(9)  |
| C(34)-C(35)  | 1.388(8)  |
| C(34)-C(39)  | 1.409(8)  |
| C(35)-C(36)  | 1.366(9)  |
| C(36)-C(37)  | 1.393(9)  |
| C(37)-C(38)  | 1.379(9)  |
| C(38)-C(39)  | 1.394(9)  |
| C(40)-C(41)  | 1.356(15) |
| C(40)-C(41') | 1.38(2)   |
| C(41)-C(42)  | 1.429(12) |
| C(42)-C(43)  | 1.380(14) |
| C(42)-C(47)  | 1.361(13) |
| C(43)-C(44)  | 1.372(11) |
| C(44)-C(45)  | 1.391(17) |
| C(45)-C(46)  | 1.356(14) |

|               |           |
|---------------|-----------|
| C(46)-C(47)   | 1.432(14) |
| C(41')-C(42') | 1.437(16) |
| C(42')-C(47') | 1.350(16) |
| C(42')-C(43') | 1.396(18) |
| C(43')-C(44') | 1.374(15) |
| C(44')-C(45') | 1.39(2)   |
| C(45')-C(46') | 1.369(18) |
| C(46')-C(47') | 1.416(18) |
| C(48)-C(49)   | 1.408(8)  |
| C(49)-C(50)   | 1.448(8)  |
| C(50)-C(55)   | 1.359(8)  |
| C(50)-C(51)   | 1.398(9)  |
| C(51)-C(52)   | 1.414(9)  |
| C(52)-C(53)   | 1.358(10) |
| C(53)-C(54)   | 1.376(11) |
| C(54)-C(55)   | 1.385(9)  |
| O(5)-C(59)    | 1.419(7)  |
| O(5)-C(56)    | 1.426(7)  |
| C(56)-C(57)   | 1.442(10) |
| C(57)-C(58)   | 1.498(10) |
| C(58)-C(59)   | 1.486(9)  |
| C(60)-C(61)   | 1.495(8)  |
| C(61)-C(67)   | 1.512(8)  |
| C(62)-C(63)   | 1.507(8)  |
| C(63)-C(64)   | 1.500(8)  |
| C(64)-C(65)   | 1.530(8)  |
| C(65)-C(66)   | 1.481(8)  |
| C(67)-C(72)   | 1.328(8)  |
| C(67)-C(68)   | 1.404(8)  |
| C(68)-C(69)   | 1.403(10) |
| C(69)-C(70)   | 1.349(9)  |
| C(70)-C(71)   | 1.388(9)  |
| C(71)-C(72)   | 1.373(8)  |
| C(73)-C(74)   | 1.504(10) |
| C(74)-C(75)   | 1.517(11) |
| C(75)-C(76)   | 1.466(10) |

|               |           |
|---------------|-----------|
| C(77)-C(78)   | 1.474(9)  |
| C(78)-C(79)   | 1.416(10) |
| C(79)-C(80)   | 1.488(10) |
| O(8)-C(81)    | 1.394(16) |
| O(8)-C(84)    | 1.397(14) |
| C(81)-C(82)   | 1.416(16) |
| C(82)-C(83)   | 1.474(16) |
| C(83)-C(84)   | 1.476(17) |
| O(8')-C(81')  | 1.417(16) |
| O(8')-C(84')  | 1.409(14) |
| C(81')-C(82') | 1.400(16) |
| C(82')-C(83') | 1.501(17) |
| C(83')-C(84') | 1.476(17) |
| C(85)-C(86)   | 1.534(8)  |
| C(86)-C(87)   | 1.488(9)  |
| C(88)-C(89)   | 1.543(8)  |
| C(89)-C(90)   | 1.489(8)  |

|                      |          |
|----------------------|----------|
| O(1)-Li(1A)-O(5)     | 107.3(5) |
| O(1)-Li(1A)-N(2A)    | 101.4(6) |
| O(5)-Li(1A)-N(2A)    | 117.6(6) |
| O(1)-Li(1A)-N(1A)    | 124.6(6) |
| O(5)-Li(1A)-N(1A)    | 116.0(6) |
| N(2A)-Li(1A)-N(1A)   | 88.0(4)  |
| O(1)-Li(1A)-Li(2A)   | 51.0(4)  |
| O(5)-Li(1A)-Li(2A)   | 132.3(6) |
| N(2A)-Li(1A)-Li(2A)  | 50.8(4)  |
| N(1A)-Li(1A)-Li(2A)  | 110.0(5) |
| O(1)-Li(1A)-Li(4A)   | 27.1(3)  |
| O(5)-Li(1A)-Li(4A)   | 93.6(4)  |
| N(2A)-Li(1A)-Li(4A)  | 87.9(5)  |
| N(1A)-Li(1A)-Li(4A)  | 148.4(5) |
| Li(2A)-Li(1A)-Li(4A) | 46.4(3)  |
| O(4)-Li(1)-O(6)      | 108.7(5) |
| O(4)-Li(1)-N(2)      | 100.1(5) |
| O(6)-Li(1)-N(2)      | 115.0(5) |

|                     |          |
|---------------------|----------|
| O(4)-Li(1)-N(1)     | 127.8(5) |
| O(6)-Li(1)-N(1)     | 113.9(5) |
| N(2)-Li(1)-N(1)     | 88.2(5)  |
| O(4)-Li(1)-Li(4)    | 28.3(3)  |
| O(6)-Li(1)-Li(4)    | 90.9(4)  |
| N(2)-Li(1)-Li(4)    | 88.4(4)  |
| N(1)-Li(1)-Li(4)    | 153.8(5) |
| O(1)-Li(2A)-N(2A)   | 103.9(5) |
| O(1)-Li(2A)-N(3A)   | 101.2(5) |
| N(2A)-Li(2A)-N(3A)  | 112.4(5) |
| O(1)-Li(2A)-N(4A)   | 106.2(5) |
| N(2A)-Li(2A)-N(4A)  | 139.2(5) |
| N(3A)-Li(2A)-N(4A)  | 88.1(4)  |
| O(1)-Li(2A)-Li(1A)  | 51.3(4)  |
| N(2A)-Li(2A)-Li(1A) | 53.0(4)  |
| N(3A)-Li(2A)-Li(1A) | 123.2(5) |
| N(4A)-Li(2A)-Li(1A) | 142.0(5) |
| O(4)-Li(2)-N(2)     | 100.6(5) |
| O(4)-Li(2)-N(3)     | 101.1(5) |
| N(2)-Li(2)-N(3)     | 110.4(5) |
| O(4)-Li(2)-N(4)     | 107.8(5) |
| N(2)-Li(2)-N(4)     | 140.3(5) |
| N(3)-Li(2)-N(4)     | 90.9(4)  |
| O(2)-Li(3)-O(8)     | 123.1(9) |
| O(2)-Li(3)-O(8')    | 117.1(9) |
| O(8)-Li(3)-O(8')    | 10.8(12) |
| O(2)-Li(3)-N(3)     | 102.4(6) |
| O(8)-Li(3)-N(3)     | 132.3(8) |
| O(8')-Li(3)-N(3)    | 140.2(9) |
| O(3)-Li(3A)-O(7)    | 131.7(6) |
| O(3)-Li(3A)-N(3A)   | 98.8(5)  |
| O(7)-Li(3A)-N(3A)   | 129.5(6) |
| O(4)-Li(4)-O(2)     | 150.9(6) |
| O(4)-Li(4)-N(3)     | 103.2(5) |
| O(2)-Li(4)-N(3)     | 102.6(5) |
| O(4)-Li(4)-O(3)     | 64.8(3)  |

|                     |          |
|---------------------|----------|
| O(2)-Li(4)-O(3)     | 99.6(4)  |
| N(3)-Li(4)-O(3)     | 145.7(5) |
| O(4)-Li(4)-Li(1)    | 29.0(3)  |
| O(2)-Li(4)-Li(1)    | 137.2(5) |
| N(3)-Li(4)-Li(1)    | 92.0(4)  |
| O(3)-Li(4)-Li(1)    | 89.1(3)  |
| O(3)-Li(4A)-O(1)    | 147.3(6) |
| O(3)-Li(4A)-N(3A)   | 104.5(5) |
| O(1)-Li(4A)-N(3A)   | 104.0(5) |
| O(3)-Li(4A)-O(2)    | 98.1(4)  |
| O(1)-Li(4A)-O(2)    | 63.1(3)  |
| N(3A)-Li(4A)-O(2)   | 149.2(5) |
| O(3)-Li(4A)-Li(1A)  | 137.7(5) |
| O(1)-Li(4A)-Li(1A)  | 27.5(3)  |
| N(3A)-Li(4A)-Li(1A) | 90.0(4)  |
| O(2)-Li(4A)-Li(1A)  | 87.1(4)  |
| C(40)-O(1)-Li(4A)   | 96.1(5)  |
| C(40)-O(1)-Li(2A)   | 159.2(5) |
| Li(4A)-O(1)-Li(2A)  | 80.4(4)  |
| C(40)-O(1)-Li(1A)   | 119.7(5) |
| Li(4A)-O(1)-Li(1A)  | 125.4(5) |
| Li(2A)-O(1)-Li(1A)  | 77.7(5)  |
| C(40)-O(2)-Li(4)    | 144.3(4) |
| C(40)-O(2)-Li(3)    | 132.7(5) |
| Li(4)-O(2)-Li(3)    | 82.0(5)  |
| C(40)-O(2)-Li(4A)   | 79.0(4)  |
| Li(4)-O(2)-Li(4A)   | 78.4(4)  |
| Li(3)-O(2)-Li(4A)   | 136.2(5) |
| C(48)-O(3)-Li(4A)   | 153.4(5) |
| C(48)-O(3)-Li(3A)   | 123.3(5) |
| Li(4A)-O(3)-Li(3A)  | 82.7(5)  |
| C(48)-O(3)-Li(4)    | 80.3(4)  |
| Li(4A)-O(3)-Li(4)   | 80.3(4)  |
| Li(3A)-O(3)-Li(4)   | 144.2(4) |
| C(48)-O(4)-Li(4)    | 95.3(5)  |
| C(48)-O(4)-Li(1)    | 123.9(5) |

|                     |          |
|---------------------|----------|
| Li(4)-O(4)-Li(1)    | 122.7(5) |
| C(48)-O(4)-Li(2)    | 149.7(5) |
| Li(4)-O(4)-Li(2)    | 81.8(4)  |
| Li(1)-O(4)-Li(2)    | 81.2(5)  |
| C(76)-O(6)-C(73)    | 110.8(5) |
| C(76)-O(6)-Li(1)    | 127.4(5) |
| C(73)-O(6)-Li(1)    | 119.3(5) |
| C(80)-O(7)-C(77)    | 110.2(5) |
| C(80)-O(7)-Li(3A)   | 127.4(5) |
| C(77)-O(7)-Li(3A)   | 121.7(5) |
| C(3)-N(1A)-C(2)     | 107.7(6) |
| C(3)-N(1A)-C(7)     | 108.7(6) |
| C(2)-N(1A)-C(7)     | 107.9(6) |
| C(3)-N(1A)-Li(1A)   | 105.8(5) |
| C(2)-N(1A)-Li(1A)   | 96.7(5)  |
| C(7)-N(1A)-Li(1A)   | 128.3(5) |
| C(20)-N(1)-C(16)    | 110.4(5) |
| C(20)-N(1)-C(15)    | 106.4(5) |
| C(16)-N(1)-C(15)    | 109.3(5) |
| C(20)-N(1)-Li(1)    | 127.3(5) |
| C(16)-N(1)-Li(1)    | 104.5(4) |
| C(15)-N(1)-Li(1)    | 97.4(5)  |
| C(85)-N(2A)-C(1)    | 108.7(4) |
| C(85)-N(2A)-Li(2A)  | 113.8(5) |
| C(1)-N(2A)-Li(2A)   | 130.0(5) |
| C(85)-N(2A)-Li(1A)  | 115.8(5) |
| C(1)-N(2A)-Li(1A)   | 107.8(5) |
| Li(2A)-N(2A)-Li(1A) | 76.2(5)  |
| C(14)-N(2)-C(88)    | 106.6(5) |
| C(14)-N(2)-Li(2)    | 130.5(5) |
| C(88)-N(2)-Li(2)    | 113.6(5) |
| C(14)-N(2)-Li(1)    | 107.9(5) |
| C(88)-N(2)-Li(1)    | 118.5(5) |
| Li(2)-N(2)-Li(1)    | 77.3(4)  |
| C(27)-N(3A)-C(87)   | 109.3(5) |
| C(27)-N(3A)-Li(4A)  | 125.6(4) |

|                     |          |
|---------------------|----------|
| C(87)-N(3A)-Li(4A)  | 125.0(5) |
| C(27)-N(3A)-Li(2A)  | 99.2(4)  |
| C(87)-N(3A)-Li(2A)  | 101.2(4) |
| Li(4A)-N(3A)-Li(2A) | 73.9(4)  |
| C(27)-N(3A)-Li(3A)  | 109.8(4) |
| C(87)-N(3A)-Li(3A)  | 87.0(4)  |
| Li(4A)-N(3A)-Li(3A) | 73.9(4)  |
| Li(2A)-N(3A)-Li(3A) | 145.3(5) |
| C(61)-N(3)-C(90)    | 109.7(4) |
| C(61)-N(3)-Li(3)    | 111.7(5) |
| C(90)-N(3)-Li(3)    | 87.5(5)  |
| C(61)-N(3)-Li(2)    | 95.5(4)  |
| C(90)-N(3)-Li(2)    | 103.6(4) |
| Li(3)-N(3)-Li(2)    | 145.4(5) |
| C(61)-N(3)-Li(4)    | 126.9(4) |
| C(90)-N(3)-Li(4)    | 123.5(5) |
| Li(3)-N(3)-Li(4)    | 73.0(5)  |
| Li(2)-N(3)-Li(4)    | 73.6(4)  |
| C(29)-N(4A)-C(33)   | 109.3(5) |
| C(29)-N(4A)-C(28)   | 109.6(5) |
| C(33)-N(4A)-C(28)   | 108.2(5) |
| C(29)-N(4A)-Li(2A)  | 121.1(4) |
| C(33)-N(4A)-Li(2A)  | 110.3(4) |
| C(28)-N(4A)-Li(2A)  | 97.3(4)  |
| C(66)-N(4)-C(60)    | 109.7(4) |
| C(66)-N(4)-C(62)    | 109.7(4) |
| C(60)-N(4)-C(62)    | 110.7(4) |
| C(66)-N(4)-Li(2)    | 120.3(4) |
| C(60)-N(4)-Li(2)    | 95.7(4)  |
| C(62)-N(4)-Li(2)    | 109.9(5) |
| N(2A)-C(1)-C(2)     | 109.1(5) |
| N(2A)-C(1)-C(8)     | 116.3(5) |
| C(2)-C(1)-C(8)      | 108.8(5) |
| N(1A)-C(2)-C(1)     | 115.3(5) |
| N(1A)-C(3)-C(4)     | 111.4(7) |
| C(3)-C(4)-C(5)      | 111.6(8) |

|                   |          |
|-------------------|----------|
| C(6)-C(5)-C(4)    | 108.1(8) |
| C(5)-C(6)-C(7)    | 113.1(8) |
| N(1A)-C(7)-C(6)   | 113.0(7) |
| C(9)-C(8)-C(13)   | 120.7(7) |
| C(9)-C(8)-C(1)    | 122.2(7) |
| C(13)-C(8)-C(1)   | 117.1(7) |
| C(8)-C(9)-C(10)   | 123.1(8) |
| C(9)-C(10)-C(11)  | 117.2(8) |
| C(12)-C(11)-C(10) | 118.5(9) |
| C(13)-C(12)-C(11) | 121.7(9) |
| C(12)-C(13)-C(8)  | 118.8(8) |
| N(2)-C(14)-C(21)  | 116.1(5) |
| N(2)-C(14)-C(15)  | 109.2(5) |
| C(21)-C(14)-C(15) | 108.6(5) |
| N(1)-C(15)-C(14)  | 113.3(5) |
| N(1)-C(16)-C(17)  | 110.1(5) |
| C(16)-C(17)-C(18) | 112.1(6) |
| C(19)-C(18)-C(17) | 109.2(5) |
| C(18)-C(19)-C(20) | 109.1(5) |
| N(1)-C(20)-C(19)  | 112.8(5) |
| C(22)-C(21)-C(26) | 119.6(6) |
| C(22)-C(21)-C(14) | 121.9(6) |
| C(26)-C(21)-C(14) | 118.5(6) |
| C(21)-C(22)-C(23) | 121.5(7) |
| C(24)-C(23)-C(22) | 119.6(8) |
| C(23)-C(24)-C(25) | 119.2(8) |
| C(26)-C(25)-C(24) | 120.7(7) |
| C(25)-C(26)-C(21) | 119.4(7) |
| N(3A)-C(27)-C(34) | 114.3(5) |
| N(3A)-C(27)-C(28) | 106.3(5) |
| C(34)-C(27)-C(28) | 111.6(5) |
| N(4A)-C(28)-C(27) | 109.5(5) |
| C(30)-C(29)-N(4A) | 112.1(5) |
| C(29)-C(30)-C(31) | 110.2(5) |
| C(32)-C(31)-C(30) | 109.4(5) |
| C(31)-C(32)-C(33) | 111.1(6) |



|                      |           |
|----------------------|-----------|
| N(4A)-C(33)-C(32)    | 109.9(5)  |
| C(35)-C(34)-C(39)    | 118.3(6)  |
| C(35)-C(34)-C(27)    | 124.4(6)  |
| C(39)-C(34)-C(27)    | 117.4(6)  |
| C(36)-C(35)-C(34)    | 122.3(6)  |
| C(35)-C(36)-C(37)    | 119.7(7)  |
| C(38)-C(37)-C(36)    | 119.1(7)  |
| C(37)-C(38)-C(39)    | 121.5(7)  |
| C(38)-C(39)-C(34)    | 119.0(7)  |
| O(1)-C(40)-O(2)      | 115.2(5)  |
| O(1)-C(40)-C(41)     | 118.7(8)  |
| O(2)-C(40)-C(41)     | 125.2(8)  |
| O(1)-C(40)-C(41')    | 121.1(11) |
| O(2)-C(40)-C(41')    | 119.5(11) |
| C(41)-C(40)-C(41')   | 28.8(7)   |
| C(40)-C(41)-C(42)    | 131.0(12) |
| C(43)-C(42)-C(47)    | 116.0(10) |
| C(43)-C(42)-C(41)    | 127.8(10) |
| C(47)-C(42)-C(41)    | 116.1(11) |
| C(42)-C(43)-C(44)    | 122.9(12) |
| C(43)-C(44)-C(45)    | 121.0(14) |
| C(46)-C(45)-C(44)    | 117.5(12) |
| C(45)-C(46)-C(47)    | 120.6(11) |
| C(42)-C(47)-C(46)    | 121.8(10) |
| C(40)-C(41')-C(42')  | 127.4(19) |
| C(47')-C(42')-C(41') | 117.9(16) |
| C(47')-C(42')-C(43') | 116.2(16) |
| C(41')-C(42')-C(43') | 125.9(17) |
| C(44')-C(43')-C(42') | 120.7(19) |
| C(43')-C(44')-C(45') | 122.3(19) |
| C(46')-C(45')-C(44') | 117.7(18) |
| C(47')-C(46')-C(45') | 118.3(16) |
| C(42')-C(47')-C(46') | 124.2(16) |
| O(3)-C(48)-O(4)      | 117.7(5)  |
| O(3)-C(48)-C(49)     | 124.8(5)  |
| O(4)-C(48)-C(49)     | 117.3(6)  |

|                   |          |
|-------------------|----------|
| C(48)-C(49)-C(50) | 127.0(6) |
| C(55)-C(50)-C(51) | 116.6(6) |
| C(55)-C(50)-C(49) | 126.5(6) |
| C(51)-C(50)-C(49) | 116.8(6) |
| C(50)-C(51)-C(52) | 122.0(7) |
| C(53)-C(52)-C(51) | 117.6(8) |
| C(52)-C(53)-C(54) | 122.2(8) |
| C(53)-C(54)-C(55) | 118.3(8) |
| C(50)-C(55)-C(54) | 123.2(7) |
| C(59)-O(5)-C(56)  | 108.2(5) |
| C(59)-O(5)-Li(1A) | 123.7(5) |
| C(56)-O(5)-Li(1A) | 125.7(5) |
| O(5)-C(56)-C(57)  | 105.9(7) |
| C(56)-C(57)-C(58) | 102.0(7) |
| C(59)-C(58)-C(57) | 105.1(6) |
| O(5)-C(59)-C(58)  | 105.9(6) |
| N(4)-C(60)-C(61)  | 111.7(5) |
| N(3)-C(61)-C(60)  | 108.9(5) |
| N(3)-C(61)-C(67)  | 114.8(5) |
| C(60)-C(61)-C(67) | 112.5(5) |
| N(4)-C(62)-C(63)  | 111.0(4) |
| C(64)-C(63)-C(62) | 111.2(5) |
| C(63)-C(64)-C(65) | 109.6(5) |
| C(66)-C(65)-C(64) | 112.0(5) |
| N(4)-C(66)-C(65)  | 111.1(5) |
| C(72)-C(67)-C(68) | 118.2(6) |
| C(72)-C(67)-C(61) | 123.1(5) |
| C(68)-C(67)-C(61) | 118.7(6) |
| C(69)-C(68)-C(67) | 118.8(7) |
| C(70)-C(69)-C(68) | 121.8(7) |
| C(69)-C(70)-C(71) | 118.1(7) |
| C(72)-C(71)-C(70) | 119.9(7) |
| C(67)-C(72)-C(71) | 123.1(6) |
| O(6)-C(73)-C(74)  | 105.3(6) |
| C(73)-C(74)-C(75) | 104.7(7) |
| C(76)-C(75)-C(74) | 105.6(7) |

|                      |           |
|----------------------|-----------|
| O(6)-C(76)-C(75)     | 103.5(6)  |
| O(7)-C(77)-C(78)     | 105.7(5)  |
| C(79)-C(78)-C(77)    | 109.0(7)  |
| C(78)-C(79)-C(80)    | 108.4(7)  |
| O(7)-C(80)-C(79)     | 105.3(6)  |
| C(81)-O(8)-C(84)     | 108.7(12) |
| C(81)-O(8)-Li(3)     | 115.5(14) |
| C(84)-O(8)-Li(3)     | 135.7(14) |
| O(8)-C(81)-C(82)     | 110.2(13) |
| C(81)-C(82)-C(83)    | 103.9(13) |
| C(82)-C(83)-C(84)    | 104.7(13) |
| O(8)-C(84)-C(83)     | 106.4(14) |
| C(81')-O(8')-C(84')  | 105.4(13) |
| C(81')-O(8')-Li(3)   | 124(2)    |
| C(84')-O(8')-Li(3)   | 124.5(15) |
| O(8')-C(81')-C(82')  | 107.0(13) |
| C(81')-C(82')-C(83') | 105.5(13) |
| C(82')-C(83')-C(84') | 102.0(14) |
| O(8')-C(84')-C(83')  | 100.6(16) |
| N(2A)-C(85)-C(86)    | 112.6(5)  |
| C(87)-C(86)-C(85)    | 114.4(6)  |
| N(3A)-C(87)-C(86)    | 113.2(5)  |
| N(2)-C(88)-C(89)     | 112.5(5)  |
| C(90)-C(89)-C(88)    | 114.2(5)  |
| N(3)-C(90)-C(89)     | 113.1(5)  |

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Symmetry transformations used to generate equivalent atoms

**Table 16.** Anisotropic displacement parameters ( $\text{\AA}^2 \times 10^3$ ) for 7. The anisotropic displacement factor exponent takes the form:  $-2p^2 [ h^2 a^{*2} U^{11} + \dots + 2 h k a^* b^* U^{12} ]$

|        | U <sup>11</sup> | U <sup>22</sup> | U <sup>33</sup> | U <sup>23</sup> | U <sup>13</sup> | U <sup>12</sup> |
|--------|-----------------|-----------------|-----------------|-----------------|-----------------|-----------------|
| Li(1A) | 66(7)           | 67(7)           | 78(8)           | 11(6)           | -2(6)           | 15(6)           |
| Li(1)  | 62(6)           | 46(6)           | 71(7)           | -18(6)          | 2(6)            | 13(5)           |
| Li(2A) | 59(6)           | 41(6)           | 58(7)           | -2(5)           | -3(5)           | 1(5)            |
| Li(2)  | 55(6)           | 56(7)           | 46(6)           | 4(5)            | 2(5)            | 8(5)            |
| Li(3)  | 103(9)          | 54(7)           | 76(8)           | 1(6)            | -19(7)          | 1(6)            |
| Li(3A) | 70(7)           | 44(6)           | 66(7)           | 0(6)            | -1(6)           | -3(5)           |
| Li(4)  | 53(6)           | 39(6)           | 53(6)           | 5(5)            | 7(5)            | 0(5)            |
| Li(4A) | 45(5)           | 48(6)           | 57(6)           | 0(5)            | -3(5)           | -7(5)           |
| O(1)   | 66(3)           | 37(3)           | 61(3)           | 3(2)            | -3(2)           | 0(2)            |
| O(2)   | 61(2)           | 36(2)           | 56(3)           | 4(2)            | -6(2)           | 0(2)            |
| O(3)   | 50(2)           | 38(2)           | 56(3)           | 4(2)            | -8(2)           | 5(2)            |
| O(4)   | 52(2)           | 34(2)           | 61(3)           | -4(2)           | -3(2)           | 2(2)            |
| O(6)   | 81(3)           | 51(3)           | 56(3)           | -5(3)           | -3(2)           | 7(2)            |
| O(7)   | 70(3)           | 46(3)           | 68(3)           | 2(2)            | -10(2)          | -13(2)          |
| N(1A)  | 78(4)           | 64(4)           | 63(4)           | 8(3)            | -12(3)          | -12(3)          |
| N(1)   | 67(3)           | 49(3)           | 49(3)           | -17(3)          | -5(3)           | 5(3)            |
| N(2A)  | 55(3)           | 42(3)           | 59(3)           | 6(3)            | -7(3)           | -3(3)           |
| N(2)   | 69(3)           | 39(3)           | 60(3)           | -7(3)           | -14(3)          | 4(3)            |
| N(3A)  | 60(3)           | 31(3)           | 63(3)           | 7(3)            | -5(3)           | -6(2)           |
| N(3)   | 59(3)           | 31(3)           | 50(3)           | -3(2)           | 1(3)            | 5(2)            |
| N(4A)  | 56(3)           | 57(4)           | 49(3)           | 2(3)            | 0(3)            | -1(3)           |
| N(4)   | 49(3)           | 36(3)           | 53(3)           | -2(3)           | -8(2)           | 2(2)            |
| C(1)   | 68(4)           | 50(4)           | 53(4)           | 10(4)           | -1(4)           | -9(4)           |
| C(2)   | 64(4)           | 66(5)           | 74(5)           | 15(4)           | -15(4)          | 5(4)            |
| C(3)   | 83(5)           | 82(5)           | 75(5)           | 9(5)            | 13(5)           | 8(4)            |
| C(4)   | 125(7)          | 140(9)          | 96(7)           | 30(7)           | -18(7)          | 10(7)           |
| C(5)   | 115(7)          | 157(10)         | 92(7)           | -21(8)          | -9(6)           | 34(7)           |
| C(6)   | 124(8)          | 107(7)          | 112(8)          | -7(7)           | -39(7)          | 7(6)            |
| C(7)   | 107(6)          | 82(6)           | 73(5)           | 1(5)            | -8(5)           | 12(5)           |
| C(8)   | 65(5)           | 47(4)           | 76(5)           | 13(4)           | -5(4)           | 1(4)            |

|       |        |        |        |        |        |        |
|-------|--------|--------|--------|--------|--------|--------|
| C(9)  | 74(5)  | 53(5)  | 80(6)  | 16(4)  | 5(5)   | 11(4)  |
| C(10) | 125(7) | 63(5)  | 99(7)  | 13(5)  | 11(6)  | 9(5)   |
| C(11) | 116(7) | 77(6)  | 119(8) | 19(6)  | 3(7)   | 19(5)  |
| C(12) | 104(7) | 65(6)  | 122(9) | 24(6)  | -21(7) | -6(5)  |
| C(13) | 59(4)  | 61(5)  | 95(6)  | 21(5)  | 5(4)   | 4(4)   |
| C(14) | 68(5)  | 51(4)  | 70(5)  | -20(4) | -12(4) | 5(4)   |
| C(15) | 75(4)  | 41(4)  | 55(4)  | -4(4)  | -3(4)  | 9(3)   |
| C(16) | 69(4)  | 55(4)  | 58(4)  | -2(4)  | -5(4)  | 9(4)   |
| C(17) | 59(4)  | 76(5)  | 67(5)  | -6(4)  | 5(4)   | 6(4)   |
| C(18) | 67(4)  | 62(5)  | 85(5)  | 1(4)   | -10(4) | 6(4)   |
| C(19) | 53(4)  | 50(4)  | 72(5)  | 4(4)   | -1(4)  | 5(3)   |
| C(20) | 57(4)  | 49(4)  | 60(4)  | -7(4)  | 0(3)   | 9(3)   |
| C(21) | 71(5)  | 40(4)  | 53(4)  | -1(3)  | -2(4)  | 2(4)   |
| C(22) | 85(6)  | 52(5)  | 66(5)  | -4(4)  | -7(4)  | -1(4)  |
| C(23) | 109(6) | 49(5)  | 86(6)  | -1(5)  | 2(5)   | 4(5)   |
| C(24) | 133(8) | 54(5)  | 82(6)  | 13(4)  | -13(6) | -2(5)  |
| C(25) | 101(7) | 47(5)  | 86(6)  | 3(4)   | -20(5) | 10(4)  |
| C(26) | 84(5)  | 46(4)  | 57(5)  | -4(4)  | -15(4) | 10(4)  |
| C(27) | 61(4)  | 38(4)  | 61(4)  | 2(3)   | -1(4)  | -1(3)  |
| C(28) | 65(4)  | 43(4)  | 62(4)  | -6(3)  | 5(4)   | -2(3)  |
| C(29) | 50(4)  | 40(4)  | 68(5)  | -7(3)  | 3(3)   | 2(3)   |
| C(30) | 66(4)  | 63(5)  | 65(5)  | 1(4)   | -5(4)  | 5(4)   |
| C(31) | 72(5)  | 82(5)  | 66(5)  | 15(4)  | -15(4) | -8(4)  |
| C(32) | 75(5)  | 45(4)  | 74(5)  | -1(4)  | -6(4)  | -15(4) |
| C(33) | 64(4)  | 52(4)  | 56(4)  | 4(3)   | 3(4)   | -5(3)  |
| C(34) | 55(4)  | 46(4)  | 54(4)  | -15(4) | 3(3)   | -3(3)  |
| C(35) | 56(4)  | 45(4)  | 63(5)  | -2(4)  | 2(3)   | 0(3)   |
| C(36) | 67(4)  | 64(5)  | 66(5)  | -5(4)  | 3(4)   | 3(4)   |
| C(37) | 66(4)  | 71(5)  | 59(4)  | -15(5) | 4(4)   | -1(4)  |
| C(38) | 80(5)  | 64(5)  | 78(6)  | -17(5) | -16(4) | 9(4)   |
| C(39) | 65(4)  | 57(5)  | 76(5)  | -3(4)  | -6(4)  | -1(4)  |
| C(40) | 60(4)  | 37(4)  | 47(4)  | 4(4)   | 0(4)   | -8(3)  |
| C(41) | 62(10) | 28(7)  | 45(8)  | 4(6)   | 0(8)   | -5(7)  |
| C(42) | 64(9)  | 44(8)  | 27(6)  | 1(6)   | 5(6)   | -14(7) |
| C(43) | 57(9)  | 48(11) | 29(8)  | 7(8)   | 10(6)  | -12(7) |
| C(44) | 68(12) | 41(12) | 76(16) | -2(11) | 24(10) | 2(9)   |

|        |         |        |         |         |         |        |
|--------|---------|--------|---------|---------|---------|--------|
| C(45)  | 82(10)  | 57(9)  | 56(9)   | -12(7)  | -3(9)   | 4(7)   |
| C(46)  | 126(12) | 82(10) | 63(8)   | 15(8)   | 3(8)    | 8(9)   |
| C(47)  | 89(9)   | 46(7)  | 67(9)   | 9(6)    | 12(7)   | 19(6)  |
| C(41') | 56(15)  | 43(10) | 75(14)  | 13(9)   | -12(13) | -21(9) |
| C(42') | 92(15)  | 25(10) | 75(12)  | 17(8)   | -14(10) | -5(9)  |
| C(43') | 120(20) | 38(17) | 90(20)  | -12(14) | -47(15) | 6(12)  |
| C(44') | 120(30) | 60(20) | 80(20)  | -5(18)  | -21(18) | 28(17) |
| C(45') | 150(20) | 66(14) | 76(16)  | -16(11) | -16(15) | 13(12) |
| C(46') | 157(18) | 93(14) | 61(12)  | -9(10)  | -26(12) | 14(12) |
| C(47') | 103(14) | 54(11) | 102(13) | 1(8)    | -38(11) | -2(9)  |
| C(48)  | 70(5)   | 37(4)  | 50(4)   | -4(3)   | 1(4)    | -4(4)  |
| C(49)  | 56(4)   | 37(4)  | 62(4)   | 1(3)    | -4(3)   | 5(3)   |
| C(50)  | 50(4)   | 43(4)  | 74(5)   | -13(4)  | -1(4)   | -16(3) |
| C(51)  | 67(5)   | 51(5)  | 114(6)  | 0(5)    | 11(5)   | -14(4) |
| C(52)  | 77(5)   | 75(6)  | 115(7)  | -1(5)   | 2(5)    | -13(5) |
| C(53)  | 102(7)  | 73(6)  | 141(8)  | 27(6)   | -7(7)   | -17(6) |
| C(54)  | 79(5)   | 71(6)  | 129(7)  | 1(5)    | -12(5)  | -13(5) |
| C(55)  | 68(4)   | 48(5)  | 97(6)   | 16(4)   | -10(4)  | -15(4) |
| O(5)   | 64(3)   | 56(3)  | 96(4)   | 18(3)   | 1(3)    | 1(2)   |
| C(56)  | 80(6)   | 67(5)  | 154(8)  | 36(6)   | 24(6)   | -2(4)  |
| C(57)  | 82(6)   | 95(7)  | 185(10) | 16(7)   | -21(7)  | -15(5) |
| C(58)  | 82(6)   | 106(7) | 164(9)  | 39(7)   | -4(6)   | -4(6)  |
| C(59)  | 70(5)   | 69(5)  | 112(6)  | 1(5)    | 2(5)    | 19(5)  |
| C(60)  | 53(4)   | 52(4)  | 46(4)   | -3(3)   | 9(3)    | -2(3)  |
| C(61)  | 54(4)   | 40(4)  | 52(4)   | 9(3)    | -7(3)   | 7(3)   |
| C(62)  | 52(4)   | 41(4)  | 53(4)   | 1(3)    | -2(3)   | 4(3)   |
| C(63)  | 65(4)   | 37(4)  | 67(5)   | -8(4)   | -2(4)   | -7(3)  |
| C(64)  | 79(5)   | 62(5)  | 70(5)   | 11(4)   | -4(4)   | -3(4)  |
| C(65)  | 68(4)   | 39(4)  | 62(4)   | 3(3)    | -3(4)   | -10(3) |
| C(66)  | 56(4)   | 47(4)  | 55(4)   | -9(4)   | -5(3)   | -4(3)  |
| C(67)  | 57(4)   | 33(4)  | 58(4)   | 0(3)    | 1(3)    | -10(3) |
| C(68)  | 77(5)   | 63(5)  | 97(6)   | 17(4)   | -4(4)   | -4(4)  |
| C(69)  | 86(6)   | 58(5)  | 128(7)  | 1(5)    | -6(5)   | -27(5) |
| C(70)  | 60(4)   | 59(5)  | 107(6)  | 2(5)    | 2(4)    | 0(4)   |
| C(71)  | 56(4)   | 50(5)  | 97(6)   | 3(4)    | 7(4)    | -2(3)  |
| C(72)  | 56(4)   | 42(4)  | 68(5)   | 1(3)    | -3(4)   | -2(3)  |

|        |         |         |         |         |         |         |
|--------|---------|---------|---------|---------|---------|---------|
| C(73)  | 103(6)  | 59(5)   | 70(5)   | 3(4)    | -2(5)   | 13(4)   |
| C(74)  | 141(8)  | 95(7)   | 95(7)   | 13(5)   | 15(6)   | 31(6)   |
| C(75)  | 157(8)  | 132(8)  | 66(6)   | -7(6)   | 9(6)    | 30(7)   |
| C(76)  | 93(5)   | 66(5)   | 67(5)   | -17(5)  | -1(4)   | 18(4)   |
| C(77)  | 68(4)   | 53(4)   | 62(4)   | -1(4)   | -14(4)  | 7(3)    |
| C(78)  | 127(7)  | 81(5)   | 120(7)  | -26(5)  | -42(6)  | 15(5)   |
| C(79)  | 203(10) | 72(5)   | 142(8)  | 3(6)    | -79(7)  | -20(6)  |
| C(80)  | 101(5)  | 40(4)   | 84(5)   | 0(4)    | -10(4)  | -14(4)  |
| O(8)   | 91(12)  | 48(8)   | 73(8)   | -10(7)  | -1(6)   | -13(8)  |
| C(81)  | 110(15) | 83(9)   | 152(16) | -23(11) | -40(12) | 20(9)   |
| C(82)  | 132(14) | 136(12) | 184(16) | -38(11) | -70(11) | 15(11)  |
| C(83)  | 173(15) | 122(11) | 209(17) | -21(12) | -69(14) | -59(12) |
| C(84)  | 156(15) | 60(9)   | 133(14) | -37(11) | -35(12) | 8(10)   |
| O(8')  | 58(9)   | 43(8)   | 92(8)   | 4(7)    | -18(8)  | 9(7)    |
| C(81') | 45(9)   | 101(9)  | 87(10)  | -7(8)   | -3(9)   | 5(9)    |
| C(82') | 163(16) | 153(13) | 125(10) | -52(9)  | -26(13) | 62(14)  |
| C(83') | 195(18) | 93(9)   | 168(15) | -54(9)  | -22(16) | 28(14)  |
| C(84') | 131(16) | 48(11)  | 142(11) | -19(9)  | -15(12) | -7(11)  |
| C(85)  | 63(4)   | 40(4)   | 75(5)   | 11(4)   | -9(4)   | -10(3)  |
| C(86)  | 82(5)   | 34(4)   | 73(5)   | 12(4)   | -12(4)  | -14(3)  |
| C(87)  | 74(4)   | 45(4)   | 74(5)   | 7(4)    | -25(4)  | -3(3)   |
| C(88)  | 76(4)   | 57(4)   | 58(4)   | -5(4)   | -14(4)  | 10(4)   |
| C(89)  | 72(4)   | 35(4)   | 61(4)   | -7(3)   | -13(4)  | 1(3)    |
| C(90)  | 66(4)   | 44(4)   | 57(4)   | -9(3)   | -6(4)   | 1(3)    |

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**Table 17.** Hydrogen coordinates ( $\times 10^4$ ) and isotropic displacement parameters ( $\text{\AA}^2 \times 10^3$ ) for 7.

|        | x    | y    | z    | U(eq) |
|--------|------|------|------|-------|
| H(1A)  | 6769 | 4814 | 3084 | 68    |
| H(2A)  | 7614 | 5346 | 3404 | 81    |
| H(2B)  | 7555 | 5761 | 2898 | 81    |
| H(3A)  | 6922 | 5357 | 4094 | 96    |
| H(3B)  | 6341 | 5224 | 3700 | 96    |
| H(4A)  | 5976 | 5620 | 4504 | 144   |
| H(4B)  | 5813 | 6025 | 4005 | 144   |
| H(5A)  | 6223 | 6610 | 4699 | 146   |
| H(5B)  | 6829 | 6210 | 4772 | 146   |
| H(6A)  | 7144 | 6967 | 4258 | 137   |
| H(6B)  | 6551 | 6899 | 3863 | 137   |
| H(7A)  | 7440 | 6566 | 3435 | 105   |
| H(7B)  | 7592 | 6153 | 3929 | 105   |
| H(9A)  | 7336 | 4871 | 1828 | 83    |
| H(10A) | 8139 | 4338 | 1442 | 115   |
| H(11A) | 8804 | 3809 | 2029 | 125   |
| H(12A) | 8653 | 3887 | 2954 | 117   |
| H(13A) | 7843 | 4418 | 3301 | 86    |
| H(14A) | 3285 | 9039 | 952  | 75    |
| H(15A) | 2780 | 8554 | 231  | 68    |
| H(15B) | 3402 | 8185 | 134  | 68    |
| H(16A) | 2150 | 8433 | 1001 | 73    |
| H(16B) | 2725 | 8510 | 1415 | 73    |
| H(17A) | 1909 | 7991 | 1823 | 81    |
| H(17B) | 2535 | 7615 | 1779 | 81    |
| H(18A) | 1661 | 7068 | 1510 | 86    |
| H(18B) | 1472 | 7529 | 1064 | 86    |
| H(19A) | 2025 | 6804 | 626  | 70    |
| H(19B) | 2599 | 6858 | 1047 | 70    |
| H(20A) | 2869 | 7342 | 240  | 66    |



|        |      |       |       |     |
|--------|------|-------|-------|-----|
| H(20B) | 2240 | 7713  | 279   | 66  |
| H(22A) | 4643 | 9154  | 232   | 81  |
| H(23A) | 4877 | 9803  | -450  | 98  |
| H(24A) | 4075 | 10346 | -819  | 108 |
| H(25A) | 3039 | 10230 | -509  | 93  |
| H(26A) | 2810 | 9568  | 155   | 75  |
| H(27A) | 6972 | 5452  | 941   | 64  |
| H(28A) | 7332 | 6398  | 633   | 68  |
| H(28B) | 6733 | 6645  | 952   | 68  |
| H(29A) | 7922 | 5630  | 1213  | 64  |
| H(29B) | 8252 | 6224  | 1092  | 64  |
| H(30A) | 8780 | 5764  | 1780  | 78  |
| H(30B) | 8140 | 5723  | 2125  | 78  |
| H(31A) | 8716 | 6509  | 2462  | 88  |
| H(31B) | 8795 | 6764  | 1865  | 88  |
| H(32A) | 7976 | 7258  | 2289  | 78  |
| H(32B) | 7630 | 6682  | 2454  | 78  |
| H(33A) | 7114 | 7078  | 1697  | 69  |
| H(33B) | 7765 | 7086  | 1365  | 69  |
| H(35A) | 6235 | 6501  | 95    | 65  |
| H(36A) | 5915 | 6347  | -782  | 79  |
| H(37A) | 6058 | 5455  | -1178 | 78  |
| H(38A) | 6419 | 4712  | -649  | 89  |
| H(39A) | 6719 | 4855  | 251   | 79  |
| H(41A) | 5946 | 6892  | 3132  | 54  |
| H(43A) | 5573 | 8211  | 2460  | 54  |
| H(44A) | 5082 | 8958  | 2873  | 74  |
| H(45A) | 4812 | 8918  | 3794  | 78  |
| H(46A) | 5096 | 8121  | 4279  | 108 |
| H(47A) | 5586 | 7351  | 3840  | 81  |
| H(41B) | 6461 | 7115  | 3056  | 69  |
| H(43B) | 5202 | 7991  | 2502  | 102 |
| H(44B) | 4826 | 8791  | 2920  | 104 |
| H(45B) | 5195 | 9071  | 3769  | 116 |
| H(46B) | 6128 | 8650  | 4090  | 124 |
| H(47B) | 6474 | 7814  | 3678  | 104 |

|        |      |      |       |     |
|--------|------|------|-------|-----|
| H(49A) | 3606 | 6769 | 813   | 62  |
| H(51A) | 3015 | 5984 | 571   | 93  |
| H(52A) | 2712 | 5029 | 666   | 107 |
| H(53A) | 3296 | 4457 | 1232  | 127 |
| H(54A) | 4182 | 4795 | 1680  | 111 |
| H(55A) | 4489 | 5727 | 1551  | 85  |
| H(56A) | 4917 | 5449 | 3685  | 120 |
| H(56B) | 5270 | 5061 | 3245  | 120 |
| H(57A) | 4096 | 5095 | 3241  | 145 |
| H(57B) | 4463 | 5104 | 2669  | 145 |
| H(58A) | 3930 | 5926 | 2586  | 141 |
| H(58B) | 3923 | 6034 | 3228  | 141 |
| H(59A) | 4844 | 6351 | 2494  | 101 |
| H(59B) | 4744 | 6581 | 3100  | 101 |
| H(60A) | 6154 | 7844 | -112  | 61  |
| H(60B) | 5908 | 7485 | 394   | 61  |
| H(61A) | 5747 | 8664 | 365   | 59  |
| H(62A) | 5040 | 7008 | 121   | 59  |
| H(62B) | 5309 | 7114 | -476  | 59  |
| H(63A) | 4242 | 6863 | -532  | 68  |
| H(63B) | 4053 | 7366 | -131  | 68  |
| H(64A) | 3837 | 7669 | -1000 | 84  |
| H(64B) | 4528 | 7493 | -1203 | 84  |
| H(65A) | 4535 | 8471 | -1064 | 68  |
| H(65B) | 4246 | 8399 | -470  | 68  |
| H(66A) | 5476 | 8061 | -790  | 63  |
| H(66B) | 5316 | 8586 | -405  | 63  |
| H(68A) | 6554 | 9299 | 376   | 95  |
| H(69A) | 7623 | 9530 | 504   | 109 |
| H(70A) | 8339 | 8863 | 786   | 90  |
| H(71A) | 7978 | 7945 | 968   | 81  |
| H(72A) | 6928 | 7726 | 859   | 67  |
| H(73A) | 4431 | 7377 | 2302  | 93  |
| H(73B) | 3808 | 7001 | 2204  | 93  |
| H(74A) | 4142 | 7522 | 3147  | 132 |
| H(74B) | 3523 | 7140 | 3051  | 132 |

|        |      |      |      |     |
|--------|------|------|------|-----|
| H(75A) | 2910 | 7894 | 2905 | 142 |
| H(75B) | 3460 | 8240 | 3207 | 142 |
| H(76A) | 3158 | 8486 | 2242 | 91  |
| H(76B) | 3883 | 8536 | 2434 | 91  |
| H(77A) | 4800 | 5966 | -421 | 73  |
| H(77B) | 4203 | 5987 | -19  | 73  |
| H(78A) | 3769 | 5279 | -424 | 131 |
| H(78B) | 4316 | 5315 | -871 | 131 |
| H(79A) | 4763 | 4589 | -572 | 167 |
| H(79B) | 4137 | 4485 | -220 | 167 |
| H(80A) | 4620 | 4715 | 529  | 90  |
| H(80B) | 5269 | 4685 | 191  | 90  |
| H(81A) | 7490 | 7950 | 2156 | 138 |
| H(81B) | 6988 | 7919 | 2640 | 138 |
| H(82A) | 8043 | 8428 | 2705 | 181 |
| H(82B) | 7444 | 8571 | 3084 | 181 |
| H(83A) | 7871 | 9162 | 2172 | 202 |
| H(83B) | 7518 | 9410 | 2697 | 202 |
| H(84A) | 6574 | 9242 | 2362 | 139 |
| H(84B) | 6936 | 9244 | 1791 | 139 |
| H(81C) | 7455 | 8050 | 2658 | 93  |
| H(81D) | 6715 | 7959 | 2773 | 93  |
| H(82C) | 7424 | 8790 | 3119 | 176 |
| H(82D) | 6673 | 8723 | 3196 | 176 |
| H(83C) | 7161 | 9528 | 2604 | 182 |
| H(83D) | 6458 | 9291 | 2496 | 182 |
| H(84C) | 6943 | 9100 | 1691 | 129 |
| H(84D) | 7595 | 8923 | 1986 | 129 |
| H(85A) | 5897 | 4722 | 2596 | 71  |
| H(85B) | 6378 | 4553 | 2125 | 71  |
| H(86A) | 5313 | 4800 | 1823 | 76  |
| H(86B) | 5470 | 5436 | 1986 | 76  |
| H(87A) | 6296 | 4917 | 1260 | 77  |
| H(87B) | 5615 | 5085 | 1033 | 77  |
| H(88A) | 3979 | 9115 | 1584 | 76  |
| H(88B) | 4432 | 9359 | 1122 | 76  |

|        |      |      |      |    |
|--------|------|------|------|----|
| H(89A) | 4964 | 9057 | 1959 | 67 |
| H(89B) | 4814 | 8423 | 1782 | 67 |
| H(90B) | 5478 | 9094 | 1045 | 67 |
| H(90A) | 5856 | 8875 | 1564 | 67 |

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