

Mechanism of Lithium Diisopropylamide-Mediated  
Substitution of 2,6-Difluoropyridine

Mihai S. Viciu, Lekha Gupta, and David B. Collum\*

Contribution from the Department of Chemistry and Chemical Biology  
Baker Laboratory, Cornell University  
Ithaca, New York 14853-1301

**Supporting Information**

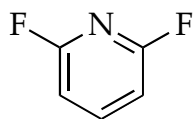
|  | Page  |
|--|---|
| <b>Part 1: NMR Spectroscopic Studies</b> |   |
| <b>I</b>                                 | <sup>6</sup> Li and <sup>15</sup> N NMR spectra of [ <sup>6</sup> Li, <sup>15</sup> N]LDA with 2,6-difluoropyridine ( <b>1</b> ) in THF/pentane at -90 °C S4                              |
| <b>II</b>                                | <sup>13</sup> C NMR spectrum of 2,6-difluoro-3-lithiopyridine ( <b>3</b> ) at -110 °C S5  |
| <b>III</b>                               | <sup>1</sup> H and <sup>13</sup> C NMR spectra of 2-fluoro-6-(diisopropylamino)pyridine ( <b>2</b> ) at 20 °C S6  |
| <b>Part 2: Rate Studies</b>              |   |
| <b>IV</b>                                | Plot of $k_{\text{obsd}}$ vs [THF] for the nucleophilic substitution of 2,6-difluoropyridine with LDA at 0 °C S7  |
| <b>V</b>                                 | Plot of $k_{\text{obsd}}$ vs [LDA] in 2.5 M THF for the nucleophilic substitution of 2,6-difluoropyridine at 0 °C S8  |
| <b>VI</b>                                | Plot of $k_{\text{obsd}}$ vs [ <i>i</i> -Pr <sub>2</sub> NH] in 2.5 M THF for the nucleophilic substitution of 2,6-difluoropyridine at 0 °C S9  |
| <b>VII</b>                               | Plot of $k_{\text{obsd}}$ vs [LDA] in 7.4 M THF for the nucleophilic substitution of 2,6-difluoropyridine at 0 °C S10   |
| <b>VIII</b>                              | Plot of $k_{\text{obsd}}$ vs [ <i>i</i> -Pr <sub>2</sub> NH] in 7.4 M THF for the nucleophilic substitution of 2,6-difluoropyridine at 0 °C S11   |
| <b>Part 3: DFT Computational Studies</b> |   |
| <b>IX</b>                                | Relative free energies for the solvation (! <i>G</i> , kcal/mol) of 2,6-difluoro-3-lithiopyridine ( <b>3</b> ) at 0 °C calculated using B3LYP level of theory with 6-31G(d) basis set S12 |

|                  |  |     |
|------------------|--|-----|
| <b>X</b>         | Relative free energies for the solvation ( $\Delta G$ , kcal/mol) of 2,6-difluoro-3-lithiopyridine ( <b>3</b> ) at -78 °C calculated using B3LYP level of theory with 6-31G(d) basis set   | S13 |
| <b>XI</b>        | Relative free energies for the solvation ( $\Delta G$ , kcal/mol) of 2,6-difluoro-3-lithiopyridine ( <b>3</b> ) at 0 °C calculated using single point MP2 corrections to B3LYP/6-31G(d) optimized structures   | S14 |
| <b>XII</b>       | Relative free energies for the solvation ( $\Delta G$ , kcal/mol) of 2,6-difluoro-3-lithiopyridine ( <b>3</b> ) at -78 °C calculated using single point MP2 corrections to B3LYP/6-31G(d) optimized structures   | S15 |
| <b>Table I</b>   | Optimized geometries at B3LYP level of theory with 6-31G(d) basis set for the serial solvation of 2,6-difluoro-3-lithiopyridine ( <b>3</b> ) with free energies (Hartrees), and cartesian coordinates (X,Y,Z)  | S16 |
| <b>Table II</b>  | Optimized geometries of reactants and monomer-based transition structures at B3LYP level of theory with 6-31G(d) basis set for the nucleophilic substitution of 2,6-difluoropyridine with free energies (Hartrees), and cartesian coordinates (X,Y,Z)        | S20 |
| <b>Table III</b> | Optimized geometries of reactants and monomer-based transition structures at B3LYP level of theory with 6-31+G(d) basis set for the nucleophilic substitution of 2,6-difluoropyridine with free energies (Hartrees), and cartesian coordinates (X,Y,Z)       | S27 |
| <b>Table IV</b>  | Optimized geometries at B3LYP level of theory with 6-31G(d) basis set for the solvation of LDA monomer with free energies (Hartrees), and cartesian coordinates (X,Y,Z)  | S35 |
| <b>Table V</b>   | Optimized geometries at B3LYP level of theory with 6-31G(d) basis set from the IRC calculations on monosolvated ( <b>10a</b> ) and trisolvated ( <b>8</b> ) monomeric transition structures with free energies (Hartrees), and cartesian coordinates (X,Y,Z) | S37 |

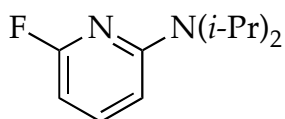
## Complete References:

(5c) Kuethe, J. T.; Zhong, Y.-L.; Alam, M.; Alorati, A. D.; Beutner, G. L.; Cai, D.; Fleitz, F. J.; Gibb, A. D.; Kassim, A.; Linn, K.; Mancheno, D.; Marcune, B.; Pye, P. J.; Scott, J. P.; Tellers, D. M.; Xiang, B.; Yasuda, N.; Yin, J.; Davies, I. W. *Tetrahedron* **2009**, *65*, 5013.

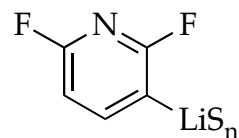
(17) Gaussian 03, Revision B.04, Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Montgomery, Jr., J. A.; Vreven, T.; Kudin, K. N.; Burant, J. C.; Millam, J. M.; Iyengar, S. S.; Tomasi, J.; Barone, V.; Mennucci, B.; Cossi, M.; Scalmani, G.; Rega, N.; Petersson, G. A.; Nakatsuji, H.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Klene, M.; Li, X.; Knox, J. E.; Hratchian, H. P.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Ayala, P. Y.; Morokuma, K.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Zakrzewski, V. G.; Dapprich, S.; Daniels, A. D.; Strain, M. C.; Farkas, O.; Malick, D. K.; Rabuck, A. D.; Raghavachari, K.; Foresman, J. B.; Ortiz, J. V.; Cui, Q.; Baboul, A. G.; Clifford, S.; Cioslowski, J.; Stefanov, B. B.; Liu, G.; Liashenko, A.; Piskorz, P.; Komaromi, I.; Martin, R. L.; Fox, D. J.; Keith, T.; Al-Laham, M. A.; Peng, C. Y.; Nanayakkara, A.; Challacombe, M.; Gill, P. M. W.; Johnson, B.; Chen, W.; Wong, M. W.; Gonzalez, C.; and Pople, J. A.; Gaussian, Inc., Wallingford CT, 2004.



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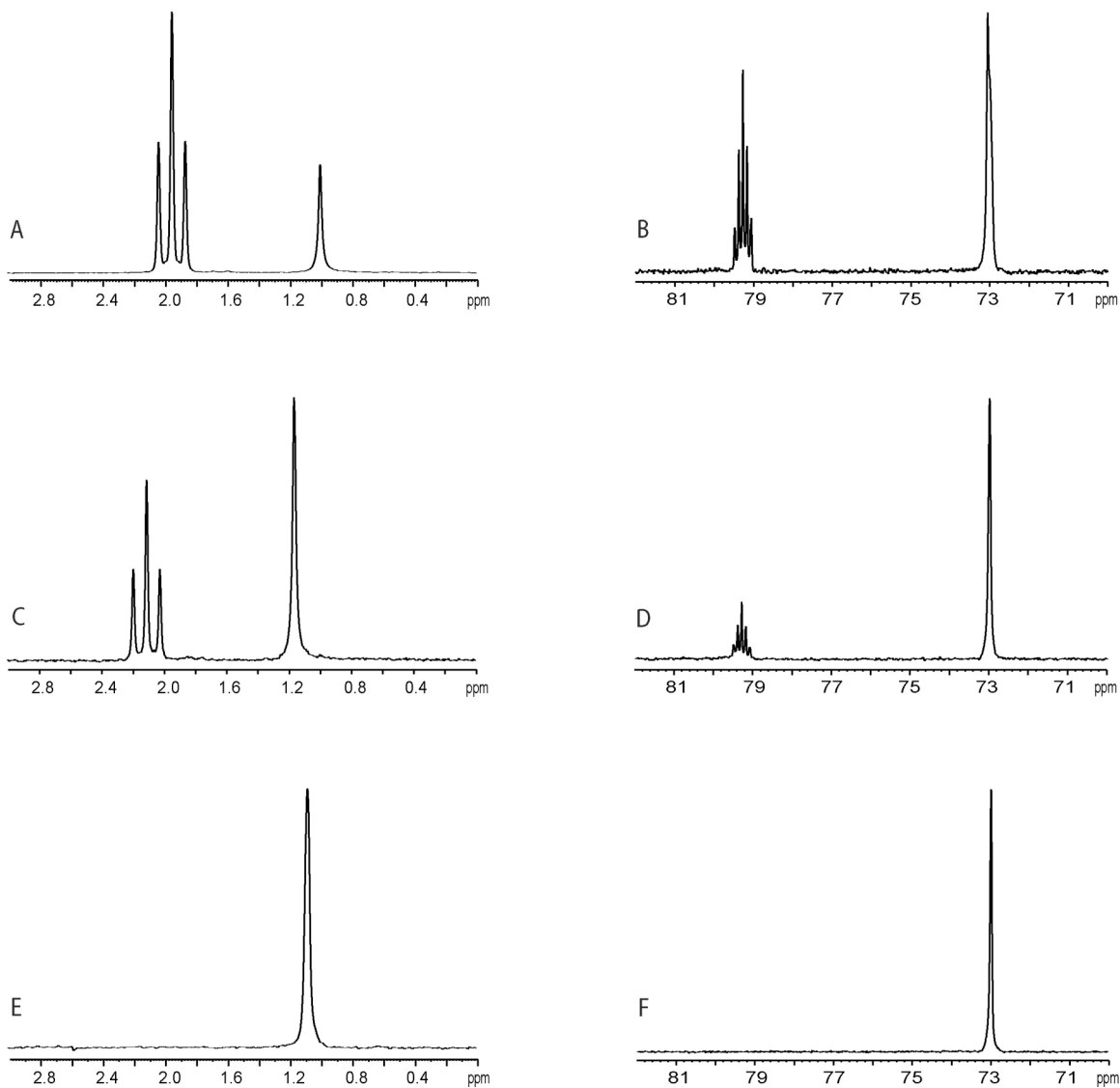


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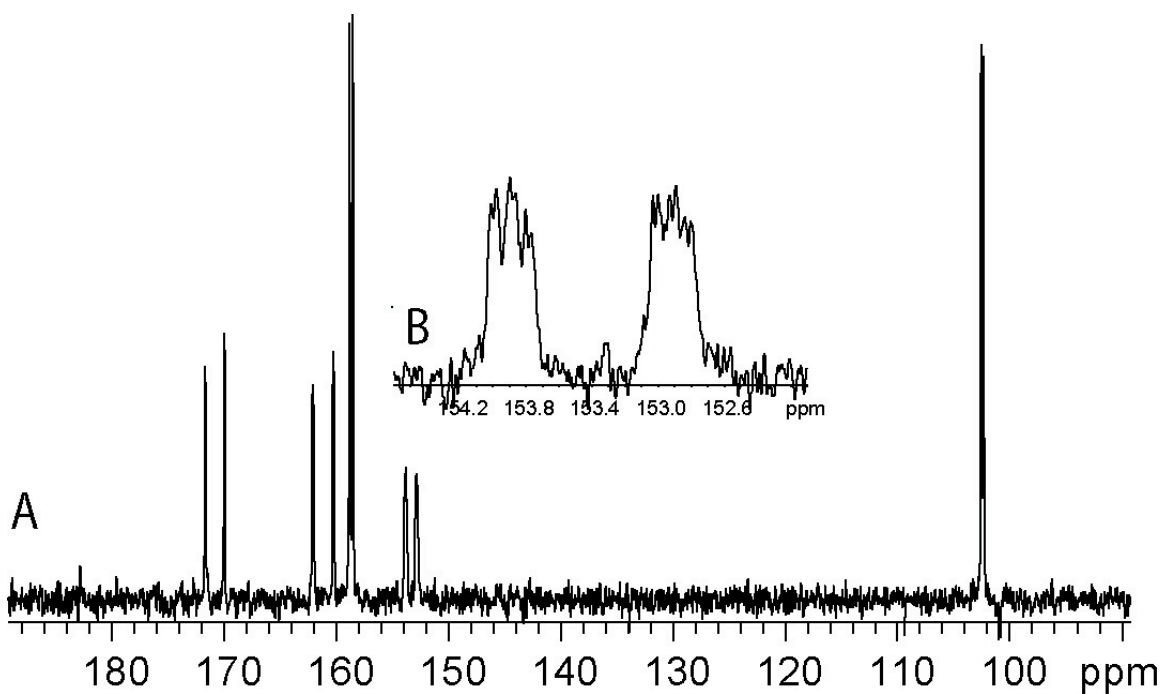


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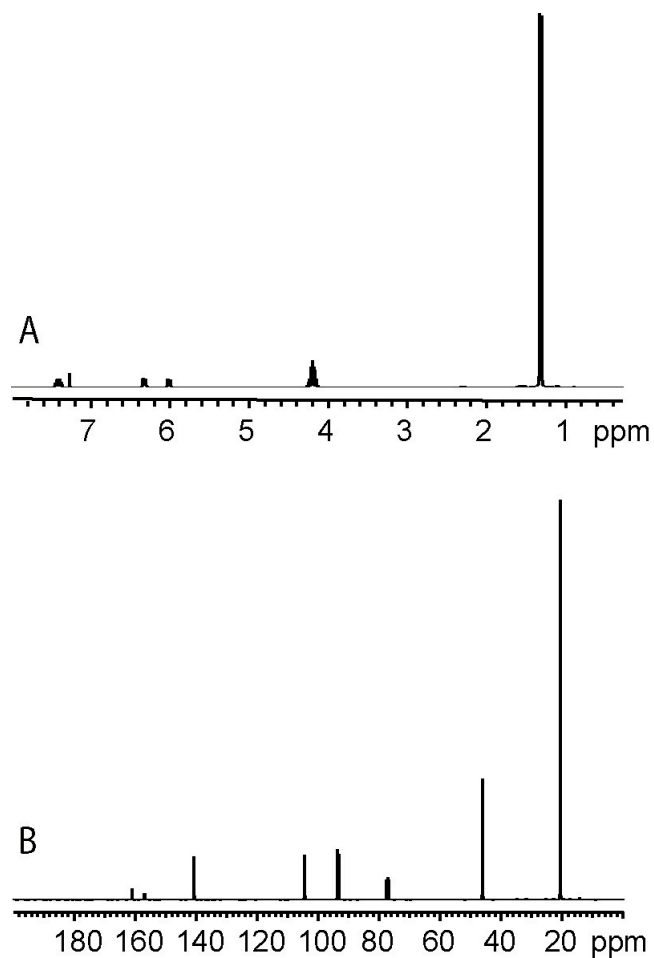
## Part 1: NMR Spectroscopic Studies



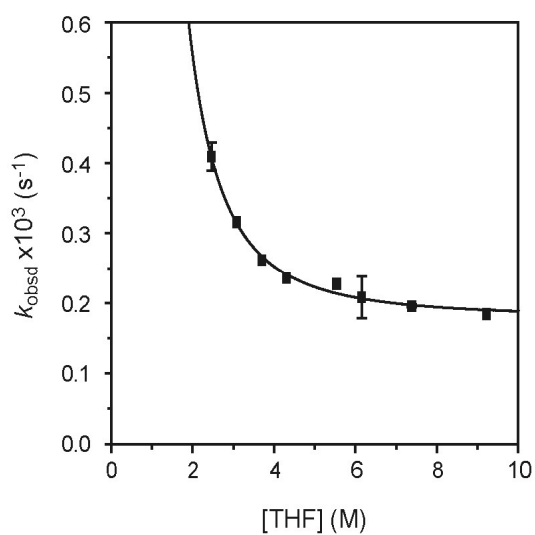
I.  $^6\text{Li}$  and  $^{15}\text{N}$  NMR spectra of 0.10 M [ $^6\text{Li}$ ,  $^{15}\text{N}$ ]LDA in 10.3 M THF / pentane recorded at  $-90\text{ }^\circ\text{C}$  in the presence of: (A) 0.025 M 2,6-difluoropyridine,  $^6\text{Li}$  spectrum; (B) 0.025 M 2,6-difluoropyridine,  $^{15}\text{N}$  spectrum; (C) 0.050 M 2,6-difluoropyridine,  $^6\text{Li}$  spectrum; (D) 0.050 M 2,6-difluoropyridine,  $^{15}\text{N}$  spectrum; (E) 0.10 M 2,6-difluoropyridine,  $^6\text{Li}$  spectrum; (F) 0.10 M 2,6-difluoropyridine,  $^{15}\text{N}$  spectrum.



II.  $^{13}\text{C}\{^1\text{H}\}$  NMR spectrum (125 MHz) of 0.050 M 2,6-difluoro-3-lithiopyridine (3) in 10.25 M THF/pentane at  $-110\text{ }^\circ\text{C}$ : (A)  $\delta$  170.78 (dd,  $^1J_{\text{C-F}} = 213.7$  Hz,  $^3J_{\text{C-F}} = 7.6$  Hz), 161.14 (dd,  $^1J_{\text{C-F}} = 228.8$  Hz,  $^3J_{\text{C-F}} = 15.1$  Hz), 158.62 (d,  $^2J_{\text{C-F}} = 37.6$  Hz), 153.41 (dtd,  $^2J_{\text{C-F}} = 122.5$  Hz,  $^1J_{\text{C-Li}} = 12.9$  Hz,  $^4J_{\text{C-F}} = 4.2$  Hz), 102.44 (dd,  $^3J_{\text{C-F}} = 26.0$  Hz,  $^3J_{\text{C-F}} = 4.6$  Hz). (B)  $\delta$  153.41 (dtd,  $^2J_{\text{C-F}} = 122.5$  Hz,  $^1J_{\text{C-Li}} = 12.9$  Hz,  $^4J_{\text{C-F}} = 4.2$  Hz).

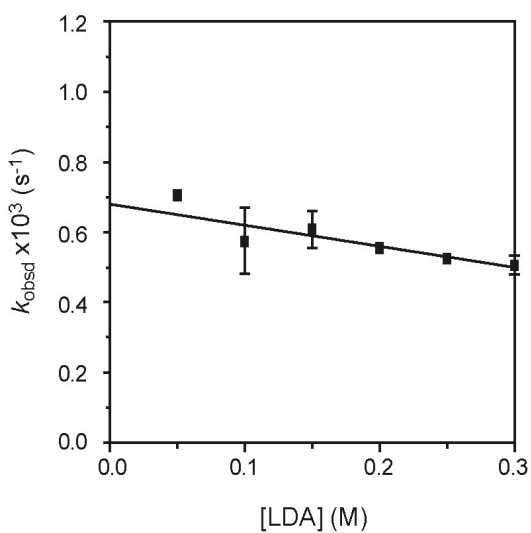


**III.**  $^1\text{H}$  and  $^{13}\text{C}$  NMR spectra of 2-fluoro-6-(diisopropylamino)pyridine (2): (A)  $^1\text{H}$  NMR (300 MHz,  $\text{CDCl}_3$ , 20 °C)  $\delta$  7.39 (q,  $J = 8.4$  Hz, 1H), 6.30 (dd,  $J = 8.3$  Hz, 2.9 Hz, 1H), 5.99 (dd,  $J = 7.6$  Hz, 3.2 Hz, 1H), 4.17 (sept,  $J = 6.8$  Hz, 2H), 1.29 (d,  $J = 6.5$  Hz, 12H) (B)  $^{13}\text{C}$  NMR (75 MHz,  $\text{CDCl}_3$ , 20 °C)  $\delta$  162.60 (d,  $J = 232.5$  Hz), 156.99 (d,  $J = 16.7$  Hz), 140.77 (d,  $J = 8.5$  Hz), 104.40 (d,  $J = 4.0$  Hz), 93.46 (d,  $J = 38.4$  Hz), 46.14 (s), 20.62 (s).



IV. Plot of  $k_{\text{obsd}}$  vs [THF] in hexane cosolvent for the nucleophilic substitution of 2,6-difluoropyridine (0.005 M) with LDA (0.10 M) and diisopropylamine (0.10 M) at 0 °C. The curve depicts an unweighted least-squares fit to  $k_{\text{obsd}} = k[\text{THF}]^n + k'$  ( $k = (1.9 \pm 0.7) \times 10^{-3}$ ,  $n = -2.4 \pm 0.4$ ,  $k' = (1.8 \pm 0.1) \times 10^{-4}$ ).

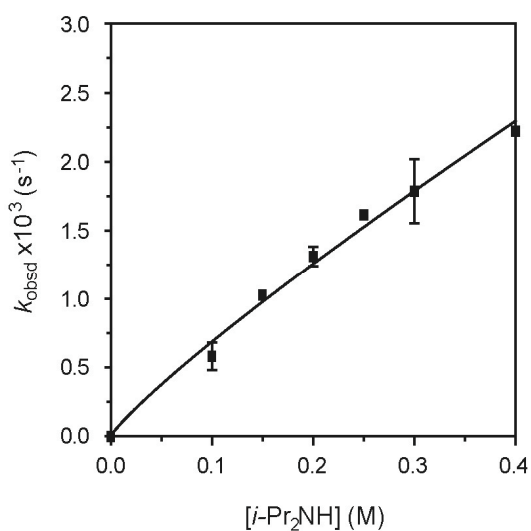
| [THF] (M) | $k_{\text{obsd}1} \times 10^3 \text{ (s}^{-1}\text{)}$ | $k_{\text{obsd}2} \times 10^3 \text{ (s}^{-1}\text{)}$ | $k_{\text{obsd} \text{avg}} \times 10^3 \text{ (s}^{-1}\text{)}$ |
|-----------|--|--|--|
| 2.460     | 0.395  | 0.423  | $0.41 \pm 2\text{E-}2$   |
| 3.075     | 0.316  | —  | —  |
| 3.700     | 0.262  | —  | —  |
| 4.300     | 0.236  | —  | —  |
| 5.535     | 0.227  | —  | —  |
| 6.150     | 0.187  | 0.229  | $0.21 \pm 3\text{E-}2$   |
| 7.380     | 0.197  | 0.194  | $0.195 \pm 2\text{E-}3$  |
| 9.220     | 0.184  | —  | —  |



V. Plot of  $k_{\text{obsd}}$  vs [LDA] in 2.5 M THF/hexane and 0.10 M diisopropylamine for the nucleophilic substitution of 2,6-difluoropyridine (0.005 M) at 0 °C. The curve depicts an unweighted least-squares fit to  $k_{\text{obsd}} = k[\text{LDA}] + k'$  ( $k = (-6 \pm 2) \times 10^{-4}$ ,  $k' = (6.8 \pm 0.4) \times 10^{-4}$ ).

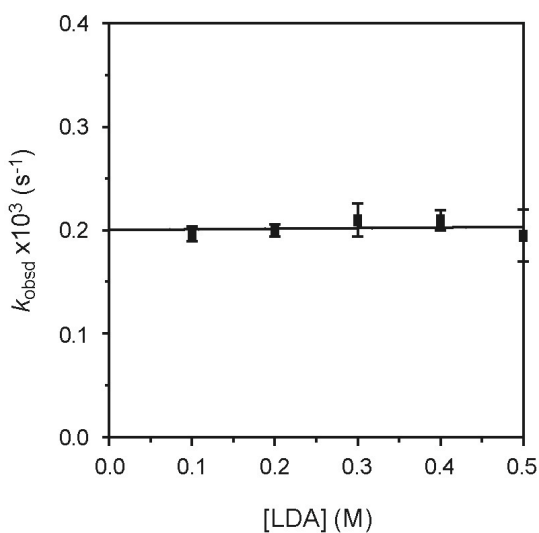
| [LDA] (M) | $k_{\text{obsd}1} \times 10^3$ (s <sup>-1</sup> ) | $k_{\text{obsd}2} \times 10^3$ (s <sup>-1</sup> ) | $k_{\text{obsd} \text{avg}} \times 10^3$ (s <sup>-1</sup> ) |
|-----------|---|---|---|
| 0.05      | 0.706   | —   | —   |
| 0.10      | 0.642   | 0.507   | $0.57 \pm 9\text{E-}2$                                      |
| 0.15      | 0.571   | 0.646   | $0.61 \pm 5\text{E-}2$                                      |
| 0.20      | 0.556   | —   | —   |
| 0.25      | 0.525   | —   | —   |
| 0.30      | 0.487   | 0.526   | $0.51 \pm 3\text{E-}2$                                      |





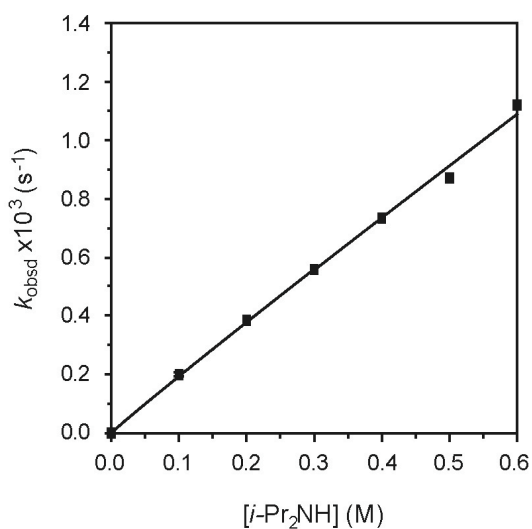
VI. Plot of  $k_{\text{obsd}}$  vs  $[i\text{-Pr}_2\text{NH}]$  in 2.5 M THF/hexane for the nucleophilic substitution of 2,6-difluoropyridine (0.005 M) with LDA (0.10 M) at 0 °C. The curve depicts an unweighted least-squares fit to  $k_{\text{obsd}} = k[i\text{-Pr}_2\text{NH}]^n$  ( $k = (5.1 \pm 0.5) \times 10^{-3}$ ,  $n = 0.87 \pm 0.07$ ).

| $[i\text{-Pr}_2\text{NH}]$ (M) | $k_{\text{obsd}1} \times 10^3$ (s <sup>-1</sup> ) | $k_{\text{obsd}2} \times 10^3$ (s <sup>-1</sup> ) | $k_{\text{obsd} \text{avg}} \times 10^3$ (s <sup>-1</sup> ) |
|--------------------------------|---|---|---|
| 0.10                           | 0.642   | 0.507   | $0.57 \pm 9\text{E-}2$                                      |
| 0.15                           | 1.025   | —   | —   |
| 0.20                           | 1.360   | 1.260   | $1.31 \pm 7\text{E-}2$                                      |
| 0.25                           | 1.615   | —   | —   |
| 0.30                           | 1.950   | 1.620   | $1.8 \pm 2\text{E-}1$                                       |
| 0.40                           | 2.220   | —   | —   |



**VII.** Plot of  $k_{\text{obsd}}$  vs [LDA] in 7.4 M THF/hexane and 0.10 M diisopropylamine for the nucleophilic substitution of 2,6-difluoropyridine (0.005 M) at 0 °C. The curve depicts an unweighted least-squares fit to  $k_{\text{obsd}} = k[\text{LDA}] + k'$  ( $k = (0.9 \pm 3.0) \times 10^{-5}$ ,  $k' = (1.9 \pm 0.1) \times 10^{-4}$ ).

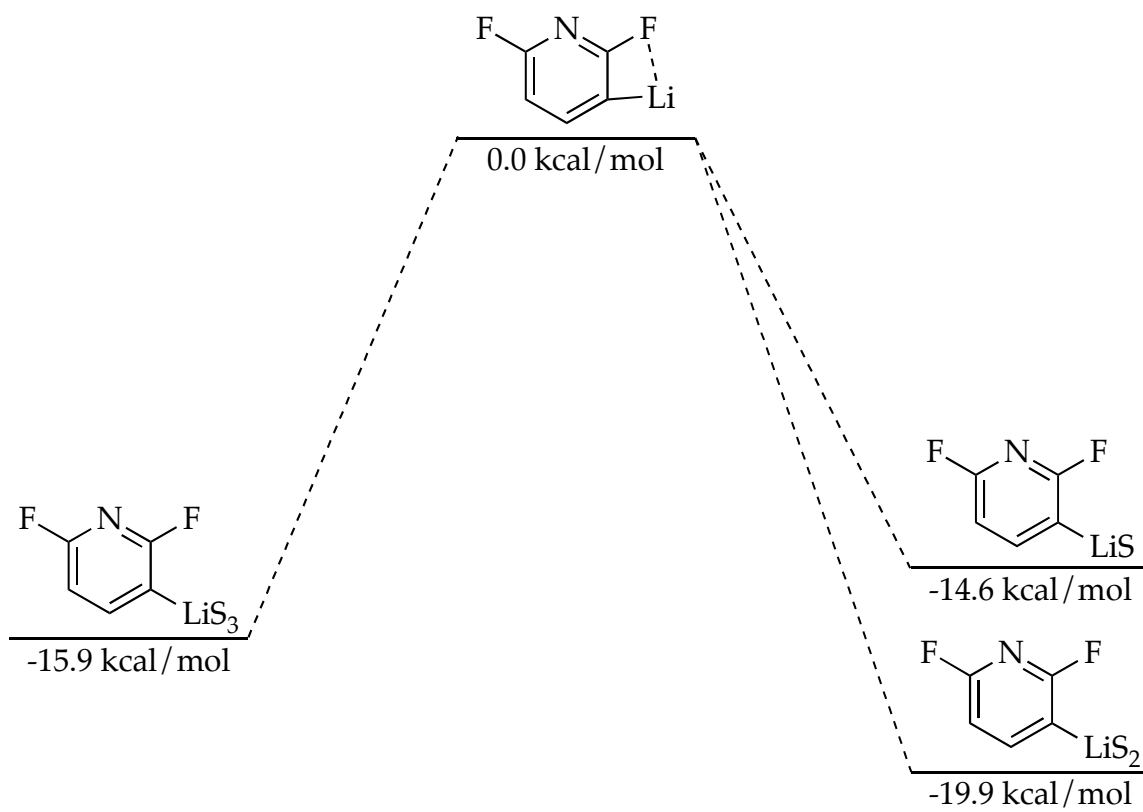
| [LDA] (M) | $k_{\text{obsd}1} \times 10^3 \text{ (s}^{-1}\text{)}$ | $k_{\text{obsd}2} \times 10^3 \text{ (s}^{-1}\text{)}$ | $k_{\text{obsd} \text{avg}} \times 10^3 \text{ (s}^{-1}\text{)}$ |
|-----------|--|--|--|
| 0.1       | 0.197  | 0.194  | $0.195 \pm 6\text{E-}3$  |
| 0.2       | 0.204  | 0.196  | $0.200 \pm 6\text{E-}3$  |
| 0.3       | 0.199  | 0.221  | $0.21 \pm 2\text{E-}2$   |
| 0.4       | 0.203  | 0.217  | $0.210 \pm 9\text{E-}3$  |
| 0.5       | 0.213  | 0.177  | $0.19 \pm 2\text{E-}2$   |



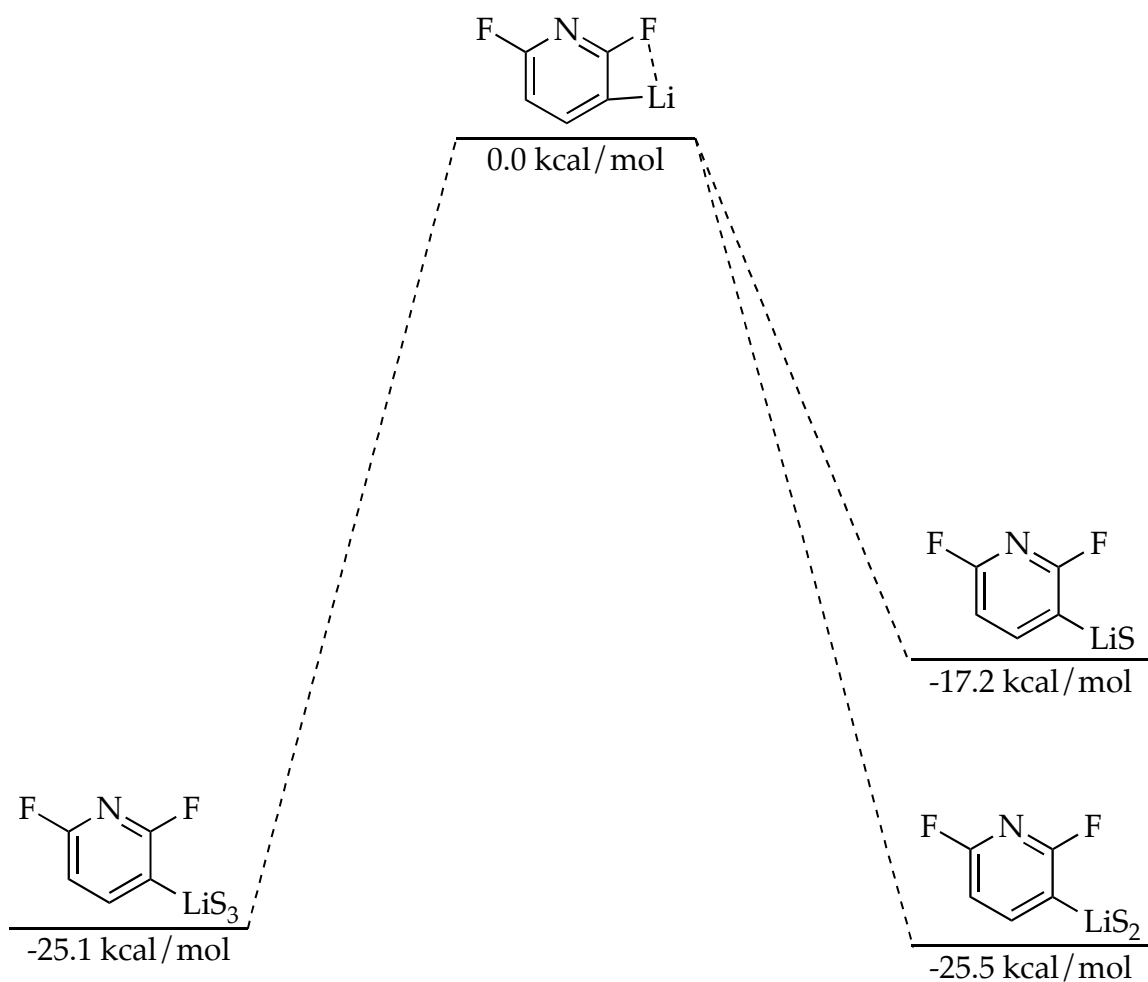
**VIII.** Plot of  $k_{\text{obsd}}$  vs  $[i\text{-Pr}_2\text{NH}]$  in 7.4 M THF/hexane for the nucleophilic substitution of 2,6-difluoropyridine (0.005 M) with LDA (0.10 M) at 0 °C. The curve depicts an unweighted least-squares fit to  $k_{\text{obsd}} = k[i\text{-Pr}_2\text{NH}]^n$  ( $k = (1.78 \pm 0.05) \times 10^{-3}$ ,  $n = 0.97 \pm 0.03$ ).

| $[i\text{-Pr}_2\text{NH}]$ (M) | $k_{\text{obsd}1} \times 10^3$ (s <sup>-1</sup> ) | $k_{\text{obsd}2} \times 10^3$ (s <sup>-1</sup> ) | $k_{\text{obsd} \text{avg}} \times 10^3$ (s <sup>-1</sup> ) |
|--------------------------------|---|---|---|
| 0.1                            | 0.197   | 0.194   | $0.195 \pm 6\text{E-}3$                                     |
| 0.2                            | 0.383   | —   | —   |
| 0.3                            | 0.558   | —   | —   |
| 0.4                            | 0.735   | —   | —   |
| 0.5                            | 0.871   | —   | —   |
| 0.6                            | 1.120   | —   | —   |

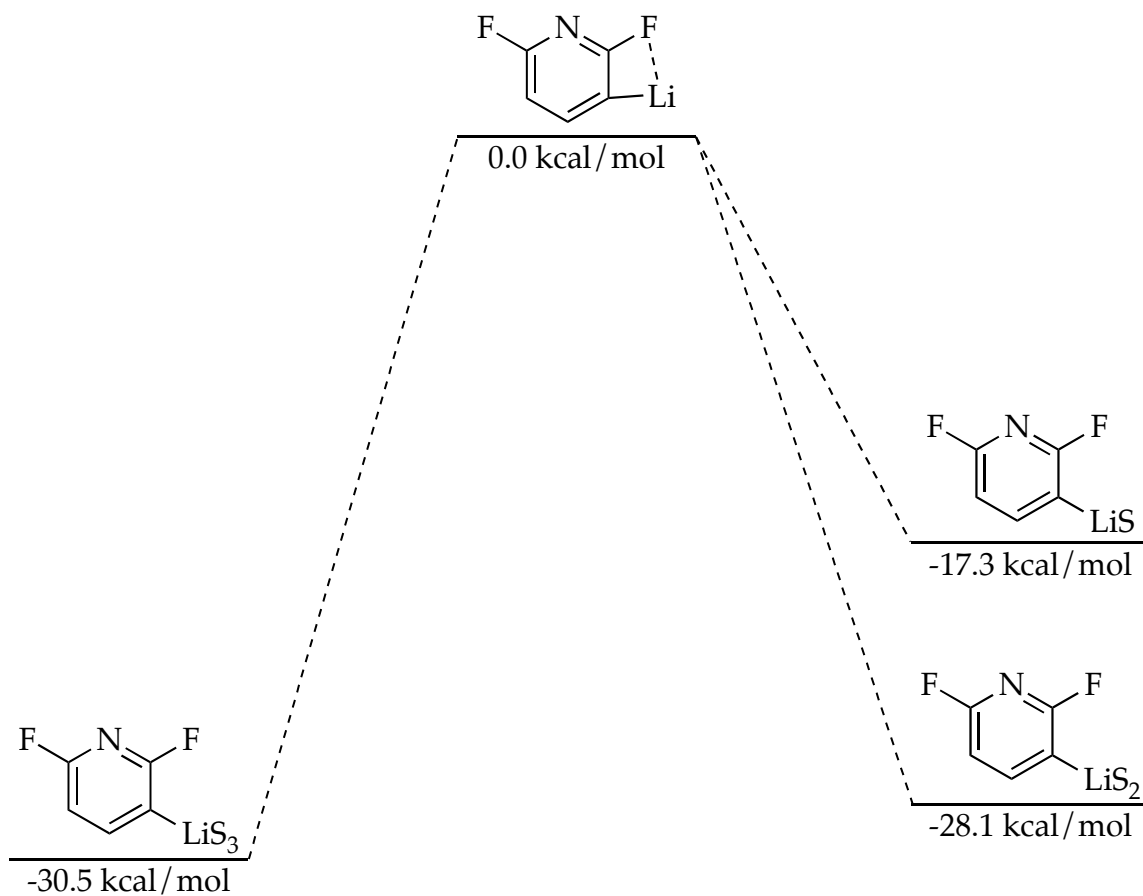
### Part 3: DFT Computational Studies



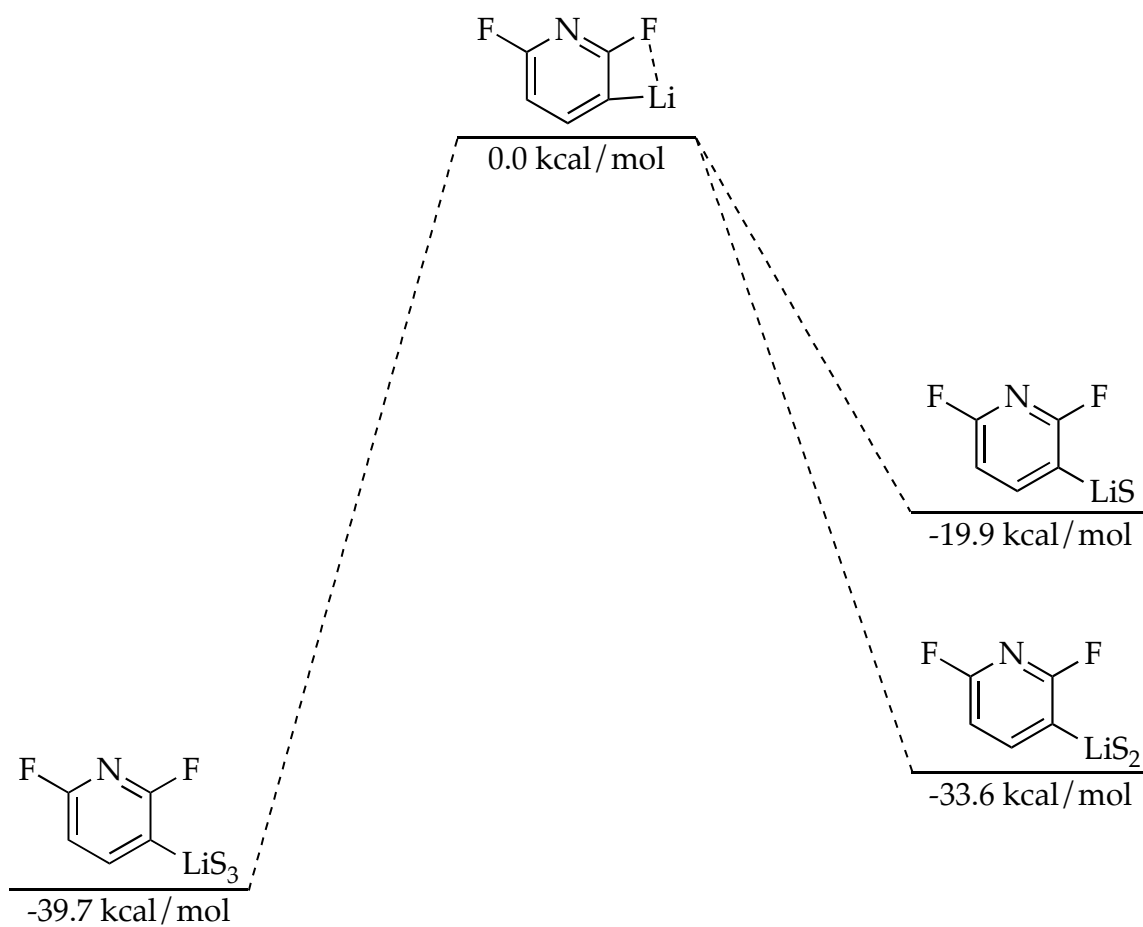
IX. Relative free energies for the solvation (!  $G$ , kcal/mol) of 2,6-difluoro-3-lithiopyridine (3) at 0 °C (S = THF) calculated using B3LYP level of theory with 6-31G(d) basis set.



X. Relative free energies for the solvation (!  $G$ , kcal/mol) of 2,6-difluoro-3-lithiopyridine (**3**) at  $-78 \text{ }^\circ\text{C}$  ( $S = \text{THF}$ ) calculated using B3LYP level of theory with 6-31G(d) basis set.



**XI.** Relative free energies for the solvation (!  $G$ , kcal/mol) of 2,6-difluoro-3-lithiopyridine (**3**) at 0 °C (S = THF) calculated using single point MP2 corrections to B3LYP/6-31G(d) optimized structures.



**XII.** Relative free energies for the solvation ( $\Delta G$ , kcal/mol) of 2,6-difluoro-3-lithiopyridine (**3**) at  $-78\text{ }^{\circ}\text{C}$  ( $S = \text{THF}$ ) calculated using calculated using single point MP2 corrections to B3LYP/6-31G(d) optimized structures.

**Table I.** Optimized geometries at B3LYP level of theory with 6-31G(d) basis set for the serial solvation of 2,6-difluoro-3-lithiopyridine (**3**) 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)


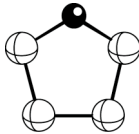
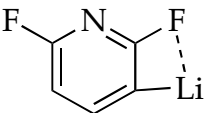
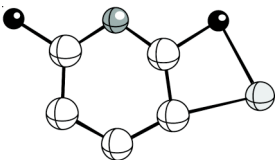
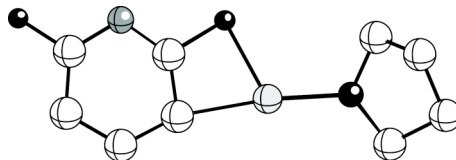
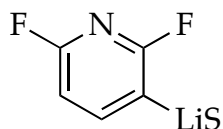
|   |   |   |          |
|---|---|---|----------|
|    |    | <p><math>G = -232.357835</math> (0 °C)<br/> <math>G = -232.349202</math> (-78 °C)<br/> <math>G_{\text{MP2}} = -231.577985</math> (0 °C)<br/> <math>G_{\text{MP2}} = -231.569352</math> (-78 °C)</p> |          |
| Atom  | X   | Y   | Z        |
| -----   |   |   |          |
| C   | -0.77676  | 0.78926   | -0.12614 |
| C   | -1.13241  | -0.69941  | 0.08086  |
| O   | -0.00028  | -1.43271  | -0.37154 |
| C   | 1.13192   | -0.69999  | 0.08156  |
| C   | 0.77743   | 0.78860   | -0.12707 |
| H   | -1.99954  | -1.03544  | -0.49441 |
| H   | -1.32099  | -0.90818  | 1.14790  |
| H   | 1.99943   | -1.03711  | -0.49250 |
| H   | 1.31917   | -0.90803  | 1.14900  |
| H   | 1.16400   | 1.14893   | -1.08517 |
| H   | 1.20108   | 1.42138   | 0.65905  |
| H   | -1.16426  | 1.15158   | -1.08311 |
| H   | -1.19880  | 1.42112   | 0.66158  |
| -----   |   |   |          |
|  |  | <p><math>G = -453.652840</math> (0 °C)<br/> <math>G = -453.643384</math> (-78 °C)<br/> <math>G_{\text{MP2}} = -452.375354</math> (0 °C)<br/> <math>G_{\text{MP2}} = -452.365898</math> (-78 °C)</p> |          |
| Atom  | X   | Y   | Z        |
| -----   |   |   |          |
| C   | 1.19546   | 0.56315   | -0.00003 |
| C   | 0.93012   | -0.79062  | -0.00002 |
| Li  | 3.09879   | 0.01350   | 0.00007  |
| F   | 2.12496   | -1.60980  | -0.00001 |
| N   | -0.17287  | -1.50168  | -0.00002 |
| C   | -1.26224  | -0.75016  | -0.00006 |
| C   | -1.26124  | 0.64286   | -0.00001 |
| C   | -0.01621  | 1.28382   | 0.00000  |
| F   | -2.43290  | -1.40856  | 0.00003  |
| H   | -2.20119  | 1.18413   | 0.00001  |
| H   | -0.00268  | 2.37335   | 0.00003  |



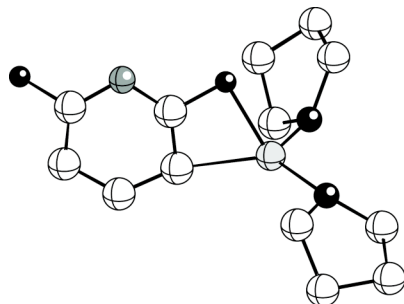
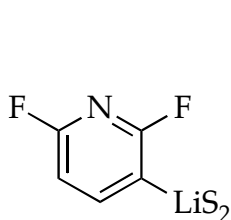
Table I (Continued).



$G = -686.033895$  (0 °C)  
 $G = -686.019972$  (-78 °C)  
 $G_{\text{MP2}} = -683.980860$  (0 °C)  
 $G_{\text{MP2}} = -683.966937$  (-78 °C)  
 S = THF

| Atom | X        | Y        | Z        |
|------|----------|----------|----------|
| C    | -2.55810 | 1.05916  | -0.12094 |
| O    | -1.56124 | 0.07902  | -0.52225 |
| C    | -2.07273 | -1.26826 | -0.32436 |
| C    | -3.23679 | -1.10522 | 0.64852  |
| C    | -3.81506 | 0.25494  | 0.22589  |
| Li   | 0.30151  | 0.35125  | -0.61216 |
| F    | 1.34844  | -1.32480 | -0.54288 |
| C    | 2.49653  | -0.50166 | -0.29878 |
| C    | 2.22141  | 0.85245  | -0.28049 |
| C    | 3.40837  | 1.57260  | -0.03647 |
| C    | 4.64473  | 0.93930  | 0.14954  |
| C    | 4.66062  | -0.45057 | 0.08512  |
| N    | 3.59752  | -1.20485 | -0.13846 |
| F    | 5.82357  | -1.10665 | 0.25855  |
| H    | 5.56391  | 1.48419  | 0.33704  |
| H    | 3.38499  | 2.66146  | 0.01320  |
| H    | -4.40660 | 0.73502  | 1.01025  |
| H    | -4.45296 | 0.13990  | -0.65761 |
| H    | -3.95949 | -1.92251 | 0.57319  |
| H    | -2.86886 | -1.06637 | 1.68014  |
| H    | -1.24994 | -1.88275 | 0.04903  |
| H    | -2.40253 | -1.66187 | -1.29371 |
| H    | -2.70154 | 1.76126  | -0.94719 |
| H    | -2.16575 | 1.60498  | 0.74481  |

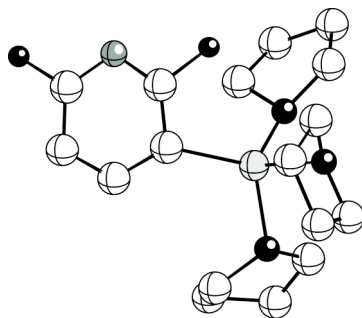
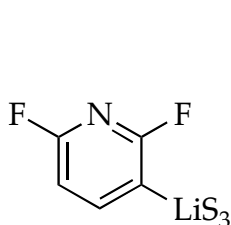
Table I (Continued).



$G = -918.400263$  (0 °C)  
 $G = -918.382414$  (-78 °C)  
 $G_{\text{MP2}} = -915.576090$  (0 °C)  
 $G_{\text{MP2}} = -915.558240$  (-78 °C)  
 S = THF

| Atom | X        | Y        | Z        | Atom | X        | Y        | Z        |
|------|----------|----------|----------|------|----------|----------|----------|
| C    | 0.39156  | 2.45585  | 1.20393  | H    | 2.25135  | -1.80815 | 2.44005  |
| O    | -0.41665 | 1.87910  | 0.14425  | H    | 4.54568  | -2.37239 | 1.63588  |
| C    | -0.33843 | 2.71035  | -1.04651 | H    | -0.61203 | -2.68247 | -0.38146 |
| C    | 0.48693  | 3.94063  | -0.65213 | H    | -1.76018 | -2.71761 | -1.75237 |
| C    | 1.35581  | 3.40345  | 0.49636  | H    | -2.99351 | -4.05097 | -0.10547 |
| Li   | -0.16844 | -0.04595 | -0.09555 | H    | -2.40014 | -3.04381 | 1.23084  |
| C    | 1.57137  | -0.96097 | 0.55969  | H    | -4.59985 | -2.02924 | 0.79634  |
| C    | 2.13337  | -0.76162 | -0.69084 | H    | -4.40161 | -2.23483 | -0.95124 |
| F    | 1.26886  | -0.15318 | -1.63642 | H    | -3.57799 | 0.01115  | -0.82692 |
| N    | 3.32570  | -1.02149 | -1.19408 | H    | -3.04139 | -0.18755 | 0.85816  |
| C    | 4.14428  | -1.59330 | -0.32806 | H    | 1.73203  | 4.18993  | 1.15726  |
| C    | 3.81463  | -1.90128 | 0.98698  | H    | 2.21115  | 2.84272  | 0.10328  |
| C    | 2.51763  | -1.57250 | 1.40829  | H    | 1.07224  | 4.32843  | -1.49074 |
| F    | 5.37933  | -1.88336 | -0.78569 | H    | -0.16606 | 4.74486  | -0.29327 |
| O    | -1.78513 | -1.00346 | -0.57018 | H    | 0.15222  | 2.12469  | -1.83120 |
| C    | -3.12283 | -0.68530 | -0.11554 | H    | -1.35716 | 2.95426  | -1.36398 |
| C    | -3.86863 | -2.02317 | -0.01720 | H    | 0.88018  | 1.62770  | 1.72308  |
| C    | -2.72500 | -3.03079 | 0.18397  | H    | -0.27008 | 2.99061  | 1.89870  |
| C    | -1.62920 | -2.44035 | -0.69820 |      |          |          |          |

Table I (Continued).

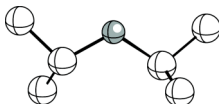


$G = -1150.751744$  (0 °C)  
 $G = -1150.731071$  (-78 °C)  
 $G_{\text{MP2}} = -1147.157941$  (0 °C)  
 $G_{\text{MP2}} = -915.137268$  (-78 °C)  
 S = THF

| Atom | X        | Y        | Z        | Atom | X        | Y        | Z        |
|------|----------|----------|----------|------|----------|----------|----------|
| Li   | 0.00251  | -0.13489 | -0.07830 | H    | 2.28500  | -1.33976 | 2.42167  |
| O    | -0.12535 | -1.17465 | -1.82404 | H    | -3.37145 | -1.36878 | 0.39383  |
| C    | 1.04265  | -1.14759 | -2.66928 | H    | -2.85748 | 0.32861  | 0.55163  |
| C    | 1.81355  | -2.41948 | -2.30127 | H    | -3.98140 | 0.18956  | 2.68463  |
| C    | 0.69701  | -3.41519 | -1.88657 | H    | -3.86211 | -1.57426 | 2.70354  |
| C    | -0.57551 | -2.54115 | -1.81156 | H    | -2.11081 | -1.01540 | 4.29762  |
| C    | 1.95005  | -0.01145 | 0.73439  | H    | -1.64557 | 0.43085  | 3.38053  |
| C    | 2.72903  | 0.89212  | 0.01664  | H    | -0.00537 | -1.16617 | 2.53120  |
| F    | 2.11403  | 1.54399  | -1.05225 | H    | -1.20672 | -2.49090 | 2.55429  |
| N    | 3.99414  | 1.26478  | 0.14880  | H    | -1.15819 | -2.67523 | -0.89876 |
| C    | 4.63569  | 0.67161  | 1.13732  | H    | -1.22546 | -2.70888 | -2.68251 |
| C    | 4.07584  | -0.27152 | 1.98738  | H    | 0.92242  | -3.87257 | -0.91910 |
| C    | 2.72948  | -0.59340 | 1.75847  | H    | 0.57182  | -4.22397 | -2.61335 |
| F    | 5.92779  | 1.02941  | 1.30387  | H    | 2.42368  | -2.78664 | -3.13189 |
| O    | -0.96233 | 1.61472  | -0.49142 | H    | 2.47193  | -2.20957 | -1.45457 |
| C    | -1.05864 | 2.04720  | -1.86325 | H    | 0.72122  | -1.15506 | -3.72201 |
| C    | -1.58136 | 3.50188  | -1.81366 | H    | 1.57686  | -0.22242 | -2.45457 |
| C    | -1.42379 | 3.90866  | -0.32403 | H    | -0.06314 | 1.99861  | -2.31890 |
| C    | -0.56771 | 2.78007  | 0.25937  | H    | -1.72148 | 1.34818  | -2.37671 |
| O    | -1.42454 | -1.05205 | 1.05957  | H    | -0.99427 | 4.14516  | -2.47564 |
| C    | -2.81907 | -0.65849 | 1.02017  | H    | -2.62557 | 3.56799  | -2.13283 |
| C    | -3.31386 | -0.65238 | 2.47880  | H    | -2.39989 | 3.93901  | 0.17107  |
| C    | -2.00795 | -0.59979 | 3.29075  | H    | -0.95299 | 4.88797  | -0.19869 |
| C    | -1.06168 | -1.41011 | 2.40948  | H    | 0.50324  | 2.95527  | 0.10841  |
| H    | 4.66851  | -0.72226 | 2.77680  | H    | -0.75278 | 2.56834  | 1.31492  |

**Table II.** Optimized geometries of reactants and monomer-based transition structures at B3LYP level of theory with 6-31G(d) basis set for the nucleophilic substitution of 2,6-difluoropyridine 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)

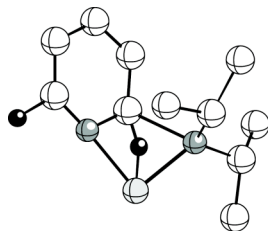
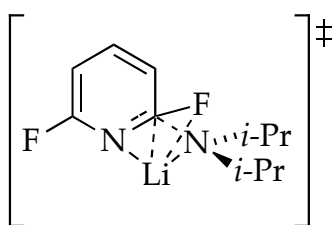
*i*-Pr<sub>2</sub>NH



$G = -292.249737$   
 $G_{\text{MP2}} = -291.164958$   
 (0 °C)

| Atom | X        | Y        | Z        |
|------|----------|----------|----------|
| C    | 1.24910  | -0.14802 | 0.16912  |
| N    | 0.01667  | -0.00296 | -0.62039 |
| C    | -1.23745 | 0.23551  | 0.11083  |
| C    | -1.71244 | -0.95470 | 0.96596  |
| C    | -2.31459 | 0.65098  | -0.89758 |
| C    | 1.71507  | 1.21758  | 0.69025  |
| C    | 2.32260  | -0.77825 | -0.72399 |
| H    | -0.95787 | -1.25730 | 1.70017  |
| H    | -2.62862 | -0.70690 | 1.51567  |
| H    | -1.93087 | -1.82281 | 0.32926  |
| H    | -2.52065 | -0.16487 | -1.60386 |
| H    | -3.25645 | 0.89733  | -0.39385 |
| H    | -1.98369 | 1.51946  | -1.47490 |
| H    | -1.05830 | 1.08725  | 0.77909  |
| H    | -0.10569 | -0.83728 | -1.19491 |
| H    | 0.97067  | 1.68300  | 1.34524  |
| H    | 2.64071  | 1.11215  | 1.26819  |
| H    | 1.89911  | 1.89793  | -0.14884 |
| H    | 2.48970  | -0.15821 | -1.61244 |
| H    | 3.27147  | -0.87689 | -0.18593 |
| H    | 2.02320  | -1.77972 | -1.05909 |
| H    | 1.10833  | -0.81327 | 1.04200  |

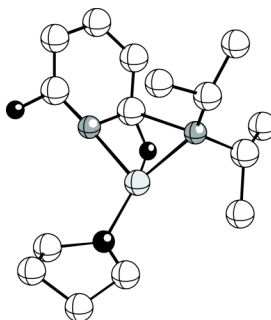
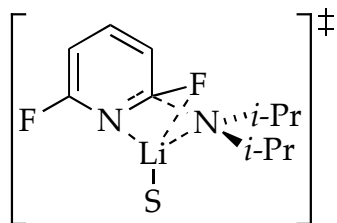
Table II (Continued).



**11a**  
 $G = -745.889359$   
 $G_{\text{MP2}} = -743.538202$   
 (0 °C)

| Atom | X        | Y        | Z        | Atom | X        | Y        | Z        |
|------|----------|----------|----------|------|----------|----------|----------|
| C    | -2.03362 | -0.42115 | -0.34145 | H    | -1.65051 | 1.95737  | 1.10780  |
| N    | -0.63571 | -0.04956 | -0.65930 | H    | -0.49959 | 3.19632  | 0.60452  |
| C    | -0.44812 | 1.41222  | -0.65262 | H    | 1.07600  | 1.36201  | -2.22665 |
| C    | -0.64302 | 2.11352  | 0.71017  | H    | 1.73930  | 1.59398  | -0.59614 |
| C    | 0.89883  | 1.83757  | -1.25293 | H    | 0.91002  | 2.92262  | -1.40916 |
| Li   | 0.22036  | -1.24685 | -1.87935 | H    | -1.22231 | 1.83060  | -1.32414 |
| C    | 0.92305  | -1.20159 | 0.25335  | H    | 4.48103  | 0.16488  | 0.78672  |
| F    | 0.08005  | -2.31654 | 0.14127  | H    | 2.86044  | 0.04707  | 2.73386  |
| N    | 1.82870  | -1.22305 | -0.75899 | H    | 0.56924  | -0.88200 | 2.37159  |
| C    | 3.02752  | -0.70707 | -0.53356 | H    | -1.95302 | -0.09591 | 1.82822  |
| C    | 3.47481  | -0.21787 | 0.67751  | H    | -3.39780 | -0.95618 | 1.27739  |
| C    | 2.55558  | -0.28984 | 1.74657  | H    | -1.84129 | -1.79786 | 1.35176  |
| C    | 1.28657  | -0.79886 | 1.56504  | H    | -1.97639 | -2.44991 | -1.17031 |
| F    | 3.84836  | -0.69890 | -1.59800 | H    | -3.59421 | -1.75377 | -1.13021 |
| C    | -2.31783 | -0.84248 | 1.11742  | H    | -2.44401 | -1.18473 | -2.34823 |
| C    | -2.53754 | -1.51547 | -1.30392 | H    | -2.66285 | 0.46370  | -0.53642 |
| H    | 0.07798  | 1.74775  | 1.44816  |      |          |          |          |

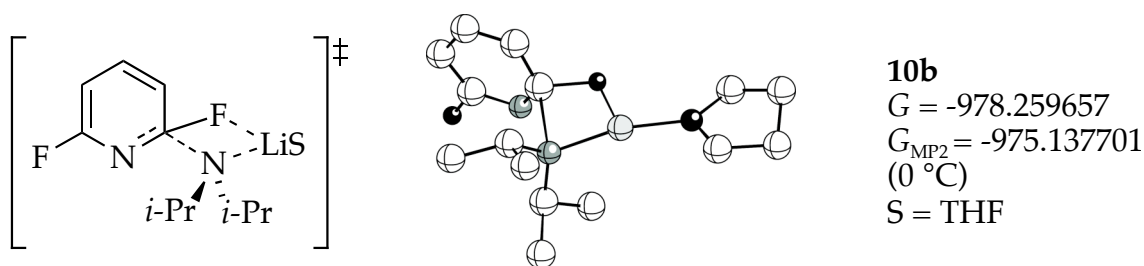
Table II (Continued).



**10a**  
 $G = -978.263965$   
 $G_{\text{MP2}} = -975.139814$   
 (0 °C)  
 S = THF

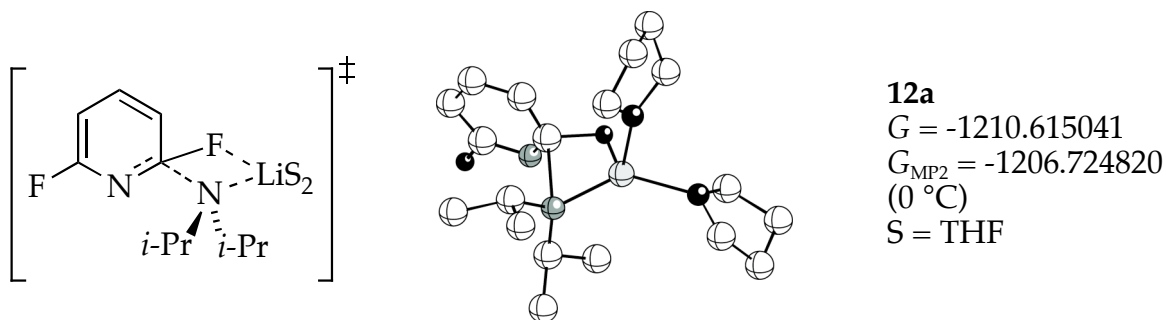
| Atom | X        | Y        | Z        | Atom | X        | Y        | Z        |
|------|----------|----------|----------|------|----------|----------|----------|
| C    | 1.52643  | -2.08614 | -0.33085 | H    | 3.10227  | -0.33951 | 2.96066  |
| N    | 1.06513  | -0.77224 | 0.16076  | H    | -0.36679 | 0.61180  | 2.00777  |
| C    | 1.42771  | -0.56846 | 1.57101  | H    | 1.09843  | 1.59173  | 1.79160  |
| C    | 2.93986  | -0.47956 | 1.88383  | H    | 0.86946  | 0.65955  | 3.27320  |
| C    | 0.71664  | 0.64544  | 2.18732  | H    | 1.05767  | -1.44965 | 2.13397  |
| Li   | -0.67222 | -0.15163 | -0.48301 | H    | 1.47238  | 4.52519  | 0.21448  |
| N    | 0.19256  | 1.62030  | -0.92395 | H    | 3.61626  | 3.33910  | -0.45320 |
| C    | 1.33506  | 0.94528  | -1.19632 | H    | 3.49274  | 1.03078  | -1.40387 |
| F    | 1.15242  | 0.06821  | -2.24642 | H    | -2.69885 | 1.80920  | -0.82275 |
| C    | 2.60638  | 1.56791  | -1.09078 | H    | -3.60741 | 0.79675  | -1.97856 |
| C    | 2.65635  | 2.84194  | -0.56542 | H    | -4.35084 | 1.42742  | 0.93008  |
| C    | 1.47619  | 3.52175  | -0.19073 | H    | -5.41947 | 1.47830  | -0.48571 |
| C    | 0.30064  | 2.83172  | -0.40749 | H    | -5.37056 | -0.96413 | -0.70346 |
| F    | -0.87927 | 3.41637  | -0.09461 | H    | -5.44256 | -0.77661 | 1.05660  |
| O    | -2.57984 | -0.22277 | -0.48239 | H    | -3.33651 | -2.13095 | -0.17624 |
| C    | -3.42987 | -1.13269 | 0.26159  | H    | -3.06811 | -1.16561 | 1.29612  |
| C    | -4.84608 | -0.55411 | 0.16721  | H    | 3.65763  | -1.59805 | -0.56590 |
| C    | -4.57959 | 0.94726  | -0.02847 | H    | 3.17989  | -3.13126 | -1.30926 |
| C    | -3.34275 | 0.93409  | -0.92228 | H    | 2.74862  | -1.59859 | -2.08491 |
| C    | 2.85793  | -2.09864 | -1.11901 | H    | 0.19493  | -2.18186 | -2.06444 |
| C    | 0.43170  | -2.77273 | -1.17109 | H    | 0.74738  | -3.76712 | -1.51237 |
| H    | 3.40106  | 0.36351  | 1.35894  | H    | -0.48585 | -2.90043 | -0.58081 |
| H    | 3.46622  | -1.39334 | 1.59188  | H    | 1.68663  | -2.73749 | 0.54729  |

Table II (Continued).



| Atom | X        | Y        | Z        | Atom | X        | Y        | Z        |
|------|----------|----------|----------|------|----------|----------|----------|
| C    | 3.28159  | -2.04667 | 0.43582  | H    | -0.97002 | -1.83964 | -2.07417 |
| O    | 2.72555  | -0.71514 | 0.27837  | H    | 0.60196  | 0.65774  | 2.48054  |
| C    | 3.76853  | 0.22785  | -0.08669 | H    | -0.83848 | 0.86587  | 3.47316  |
| C    | 5.08231  | -0.55551 | -0.00490 | H    | -0.67201 | -0.60511 | 2.51388  |
| C    | 4.62763  | -1.99791 | -0.28244 | H    | -1.48947 | 3.29960  | 0.77576  |
| Li   | 0.85908  | -0.37659 | 0.37312  | H    | -1.29499 | 3.01693  | 2.50585  |
| F    | -0.17256 | -1.89501 | 0.43575  | H    | 0.11344  | 2.93050  | 1.42837  |
| C    | -1.49079 | -1.43380 | 0.00713  | H    | -2.27729 | 0.99699  | 1.47844  |
| C    | -1.76745 | -1.78372 | -1.34193 | H    | 0.72692  | 1.98651  | -1.77012 |
| C    | -3.08876 | -2.02910 | -1.67005 | H    | -0.62268 | 2.63551  | -2.72403 |
| C    | -4.08732 | -1.99543 | -0.68271 | H    | -0.32060 | 3.23723  | -1.08640 |
| C    | -3.64282 | -1.75904 | 0.61239  | H    | -2.89818 | 2.52678  | -0.53425 |
| N    | -2.39614 | -1.54461 | 0.97698  | H    | -3.00347 | 1.93878  | -2.19431 |
| F    | -4.54144 | -1.79198 | 1.61598  | H    | -3.36041 | 0.84694  | -0.84978 |
| N    | -0.73114 | 0.61221  | 0.07022  | H    | -1.16590 | 0.42028  | -1.92064 |
| C    | -1.19548 | 1.17894  | 1.34286  | H    | 5.32721  | -2.75031 | 0.09239  |
| C    | -0.48597 | 0.47041  | 2.51380  | H    | 4.49280  | -2.16018 | -1.35807 |
| C    | -0.95592 | 2.69551  | 1.51239  | H    | 5.82463  | -0.19091 | -0.72035 |
| C    | -1.22589 | 1.22115  | -1.16687 | H    | 5.51333  | -0.47875 | 0.99973  |
| C    | -0.31044 | 2.34016  | -1.71276 | H    | 3.56303  | 0.58366  | -1.10280 |
| C    | -2.70564 | 1.66075  | -1.17568 | H    | 3.72092  | 1.07724  | 0.60076  |
| H    | -5.13145 | -2.19420 | -0.88816 | H    | 3.39947  | -2.25466 | 1.50670  |
| H    | -3.35302 | -2.27185 | -2.69633 | H    | 2.56733  | -2.75741 | 0.01311  |

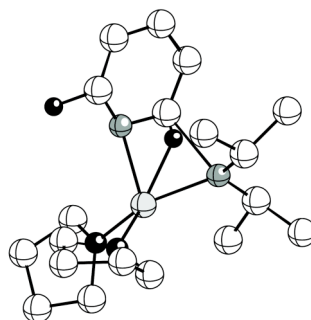
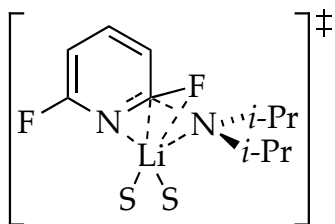
Table II (Continued).



| Atom | X        | Y        | Z        | Atom | X        | Y        | Z        |
|------|----------|----------|----------|------|----------|----------|----------|
| Li   | 0.62316  | -0.03746 | -0.19172 | H    | -3.54524 | 0.92692  | 2.57567  |
| F    | -0.44404 | -0.02320 | -1.78568 | H    | -3.74041 | 0.01897  | 1.07021  |
| C    | -1.78168 | 0.14053  | -1.28704 | H    | -1.63404 | 1.32918  | 1.18581  |
| C    | -2.16585 | 1.50060  | -1.14645 | H    | 0.42462  | -2.79298 | -0.04877 |
| C    | -3.50961 | 1.79663  | -1.28883 | H    | -0.98146 | -3.85716 | -0.22715 |
| C    | -4.42862 | 0.78862  | -1.62347 | H    | -0.82481 | -2.44134 | -1.27366 |
| C    | -3.88414 | -0.47207 | -1.84026 | H    | -1.77445 | -2.20720 | 2.96025  |
| N    | -2.61288 | -0.79610 | -1.74231 | H    | -1.43981 | -3.71412 | 2.10735  |
| F    | -4.70611 | -1.46417 | -2.23724 | H    | -0.12081 | -2.57293 | 2.44547  |
| N    | -1.02509 | -0.56926 | 0.70495  | H    | -2.49054 | -2.09783 | 0.55005  |
| C    | -1.41571 | -1.97992 | 0.78431  | H    | -5.48692 | 0.97178  | -1.75965 |
| C    | -0.65345 | -2.81099 | -0.26197 | H    | -3.85466 | 2.81964  | -1.15958 |
| C    | -1.17816 | -2.64885 | 2.15865  | H    | -1.42487 | 2.25658  | -0.91568 |
| C    | -1.65564 | 0.33742  | 1.66837  | H    | 1.31914  | 1.95054  | -2.17922 |
| C    | -0.85021 | 0.52018  | 2.97780  | H    | 2.93348  | 2.05820  | -1.42961 |
| C    | -3.14725 | 0.09091  | 1.98639  | H    | 2.51555  | 4.42278  | -1.83570 |
| O    | 1.33405  | 1.85345  | -0.11842 | H    | 0.77446  | 4.22874  | -1.56265 |
| C    | 1.88668  | 2.37816  | -1.34853 | H    | 1.51959  | 5.06669  | 0.62688  |
| C    | 1.76693  | 3.89820  | -1.23471 | H    | 2.99637  | 4.08995  | 0.55059  |
| C    | 1.93506  | 4.11725  | 0.27683  | H    | 1.61768  | 2.55684  | 1.80805  |
| C    | 1.19820  | 2.90924  | 0.86162  | H    | 0.13086  | 3.11259  | 1.00894  |
| O    | 2.32190  | -0.95443 | -0.71683 | H    | 2.55931  | -0.89253 | -2.77176 |
| C    | 2.51624  | -1.64330 | -1.97738 | H    | 1.65235  | -2.29343 | -2.15292 |
| C    | 3.81168  | -2.44137 | -1.81389 | H    | 3.82942  | -3.33646 | -2.44233 |
| C    | 3.80896  | -2.75630 | -0.30948 | H    | 4.68047  | -1.82520 | -2.07438 |
| C    | 3.23008  | -1.47053 | 0.28333  | H    | 4.80129  | -2.98901 | 0.08784  |
| H    | 0.20163  | 0.73492  | 2.75331  | H    | 3.14767  | -3.60411 | -0.09838 |
| H    | -1.25095 | 1.35811  | 3.56631  | H    | 2.66475  | -1.62781 | 1.20688  |
| H    | -0.87353 | -0.37044 | 3.61298  | H    | 4.01081  | -0.72104 | 0.46871  |
| H    | -3.31152 | -0.82205 | 2.56811  |      |          |          |          |



Table II (Continued).



**12b**

$G = -1210.614205$

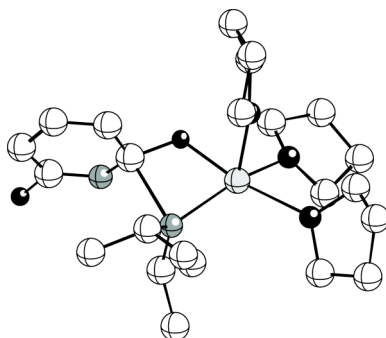
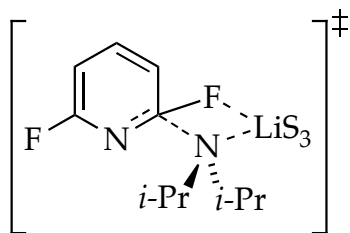
$G_{\text{MP2}} = -1206.723027$

(0 °C)

S = THF

| Atom | X        | Y        | Z        | Atom | X        | Y        | Z        |
|------|----------|----------|----------|------|----------|----------|----------|
| Li   | -0.54566 | 0.18282  | -0.31459 | H    | -1.25576 | 4.92817  | 0.46980  |
| N    | 0.58284  | -1.39503 | 0.19460  | H    | 0.38781  | 5.00524  | 1.13952  |
| C    | 0.24846  | -2.69567 | -0.41285 | H    | -1.18220 | 2.82565  | 1.72729  |
| C    | -0.31398 | -2.56755 | -1.83989 | H    | 0.53966  | 2.58437  | 1.29787  |
| C    | 1.36066  | -3.77448 | -0.41990 | H    | -2.36698 | -1.71420 | 1.01355  |
| C    | 0.96010  | -1.56029 | 1.60882  | H    | -3.26214 | -2.17012 | -0.45613 |
| C    | 0.37717  | -0.42600 | 2.47380  | H    | -5.11662 | -1.65696 | 1.07168  |
| C    | 2.47187  | -1.68681 | 1.91857  | H    | -4.21815 | -0.30201 | 1.78496  |
| F    | 0.78698  | 0.07318  | -1.85797 | H    | -5.56891 | 0.86991  | 0.10364  |
| C    | 1.91356  | -0.06880 | -1.01324 | H    | -5.39965 | -0.47002 | -1.03875 |
| N    | 2.07500  | 1.01825  | -0.24945 | H    | -3.56131 | 0.77712  | -1.88342 |
| C    | 3.29865  | 1.30760  | 0.14408  | H    | -3.33278 | 1.66347  | -0.35860 |
| C    | 4.45584  | 0.64549  | -0.22768 | H    | -0.71500 | -0.37130 | 2.36780  |
| C    | 4.27457  | -0.42046 | -1.13217 | H    | 0.60120  | -0.57604 | 3.53836  |
| C    | 3.01239  | -0.77407 | -1.56563 | H    | 0.80024  | 0.54037  | 2.18027  |
| F    | 3.39020  | 2.39057  | 0.95137  | H    | 3.00094  | -0.74823 | 1.73116  |
| O    | -2.51664 | -0.22384 | -0.38945 | H    | 2.62127  | -1.94426 | 2.97619  |
| C    | -3.09205 | -1.36787 | 0.27522  | H    | 2.95174  | -2.46023 | 1.31505  |
| C    | -4.40582 | -0.85360 | 0.85619  | H    | 0.49683  | -2.49487 | 1.97910  |
| C    | -4.88374 | 0.09618  | -0.25509 | H    | 0.45143  | -2.26369 | -2.56052 |
| C    | -3.56840 | 0.68762  | -0.79115 | H    | -0.70972 | -3.53689 | -2.16756 |
| O    | -0.83268 | 2.24020  | -0.22134 | H    | -1.12794 | -1.83691 | -1.89092 |
| C    | -0.42176 | 2.97956  | 0.95584  | H    | 1.67026  | -4.04758 | 0.59301  |
| C    | -0.27990 | 4.42755  | 0.49347  | H    | 0.99797  | -4.69005 | -0.90599 |
| C    | 0.27084  | 4.23313  | -0.92707 | H    | 2.24825  | -3.43287 | -0.96260 |
| C    | -0.50452 | 3.00517  | -1.41173 | H    | -0.57289 | -3.14203 | 0.18961  |
| H    | 0.07512  | 2.36665  | -2.08083 | H    | 2.84674  | -1.57355 | -2.27640 |
| H    | -1.44642 | 3.28489  | -1.90212 | H    | 5.14128  | -0.95986 | -1.50533 |
| H    | 1.34076  | 4.00643  | -0.88225 | H    | 5.42755  | 0.96508  | 0.12622  |
| H    | 0.12345  | 5.10147  | -1.57640 |      |          |          |          |

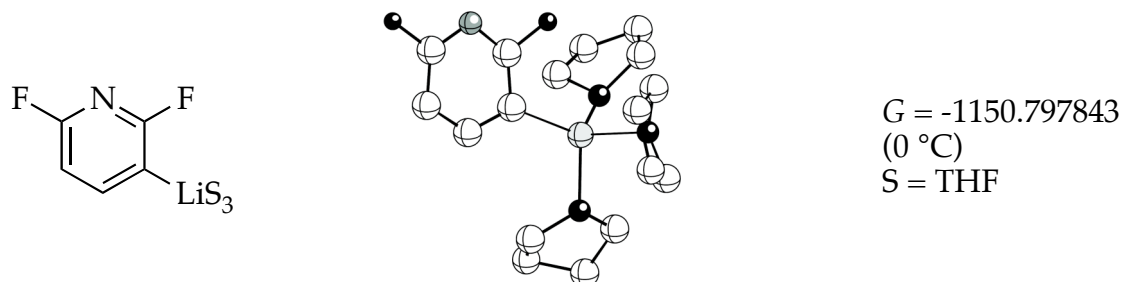
Table II (Continued).



**8a**  
 $G = -1442.960433$   
 $G_{\text{MP2}} = -1438.301908$   
 (0 °C)  
 S = THF

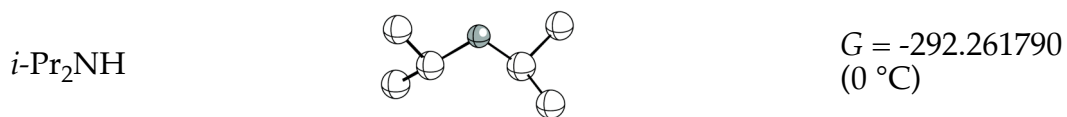
| Atom | X        | Y        | Z        | Atom | X        | Y        | Z        |
|------|----------|----------|----------|------|----------|----------|----------|
| Li   | 0.25361  | 0.29434  | 0.00257  | H    | 3.47318  | -2.77878 | 0.02420  |
| N    | -1.34269 | -0.52402 | -0.93382 | H    | 3.61030  | -2.89682 | -2.39688 |
| C    | -1.75625 | 0.01882  | -2.22791 | H    | 4.51535  | -1.38282 | -2.48681 |
| C    | -1.15416 | 1.42090  | -2.42093 | H    | 2.45154  | -0.29888 | -2.81460 |
| C    | -1.36961 | -0.81552 | -3.47447 | H    | 1.51958  | -1.71153 | -2.27944 |
| C    | -1.79820 | -1.87847 | -0.61952 | H    | 0.20400  | -2.75372 | -0.61284 |
| C    | -0.79158 | -2.99073 | -1.00551 | H    | -1.09927 | -3.96144 | -0.58917 |
| C    | -3.22085 | -2.27178 | -1.08128 | H    | -0.70299 | -3.11155 | -2.09045 |
| F    | -1.27872 | 1.42974  | 0.83273  | H    | -3.29548 | -2.40531 | -2.16540 |
| C    | -2.50359 | 0.77143  | 0.60512  | H    | -3.51316 | -3.22312 | -0.61790 |
| C    | -2.91237 | -0.08697 | 1.65676  | H    | -3.95636 | -1.51935 | -0.78425 |
| C    | -4.26970 | -0.31258 | 1.80166  | H    | -1.84636 | -1.92220 | 0.48267  |
| C    | -5.19015 | 0.33912  | 0.96547  | H    | -0.05881 | 1.35653  | -2.49284 |
| C    | -4.64356 | 1.22968  | 0.04782  | H    | -1.52067 | 1.87404  | -3.35062 |
| N    | -3.36533 | 1.49897  | -0.10626 | H    | -1.41835 | 2.08468  | -1.59677 |
| F    | -5.48421 | 1.93559  | -0.73538 | H    | -1.81246 | -1.81421 | -3.47928 |
| O    | 2.16719  | -0.49895 | -0.75999 | H    | -1.70787 | -0.30509 | -4.38658 |
| O    | 0.74612  | -0.44455 | 1.96516  | H    | -0.28026 | -0.93107 | -3.54102 |
| O    | 1.32217  | 2.28365  | 0.04511  | H    | -2.85583 | 0.14770  | -2.26729 |
| C    | 2.14315  | 2.74203  | -1.03669 | H    | -0.04266 | 1.16639  | 2.98765  |
| C    | 2.91188  | 3.94125  | -0.46471 | H    | 1.70486  | 0.90107  | 3.21931  |
| C    | 1.93220  | 4.51592  | 0.59458  | H    | 0.89732  | -0.14181 | 5.25388  |
| C    | 0.78794  | 3.47919  | 0.64079  | H    | -0.62069 | -0.63212 | 4.48327  |
| C    | 0.72809  | 0.40672  | 3.13419  | H    | 0.66865  | -2.71951 | 4.36790  |
| C    | 0.45806  | -0.51765 | 4.32499  | H    | 2.15948  | -1.83529 | 3.99380  |
| C    | 1.07209  | -1.84380 | 3.85084  | H    | 1.44092  | -2.37550 | 1.73628  |
| C    | 0.72526  | -1.83355 | 2.36119  | H    | -0.27516 | -2.24189 | 2.17386  |
| C    | 2.39036  | -1.09246 | -2.05964 | H    | -6.26173 | 0.20637  | 1.04524  |
| C    | 3.70492  | -1.89864 | -1.95996 | H    | -4.62750 | -0.98530 | 2.57733  |
| C    | 3.98959  | -1.93430 | -0.44672 | H    | -2.17551 | -0.55341 | 2.29850  |
| C    | 3.36684  | -0.61848 | 0.01506  | H    | 2.76764  | 1.90612  | -1.35201 |
| H    | 3.07450  | -0.58651 | 1.06553  | H    | 1.50355  | 3.04673  | -1.87838 |
| H    | 4.04089  | 0.22885  | -0.19082 | H    | 3.84076  | 3.60772  | 0.00908  |
| H    | 5.05568  | -2.00998 | -0.21087 | H    | 3.17488  | 4.66735  | -1.23982 |
| H    | 1.55461  | 5.50453  | 0.31680  | H    | -0.08188 | 3.81338  | 0.06101  |
| H    | 2.42148  | 4.61374  | 1.56831  | H    | 0.45534  | 3.22711  | 1.64815  |

**Table III.** Optimized geometries of reactants and monomer-based transition structures at B3LYP level of theory with 6-31+G(d) basis set for the nucleophilic substitution of 2,6-difluoropyridine with free energies (Hartrees), and cartesian coordinates (X,Y,Z).

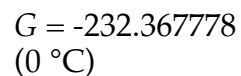
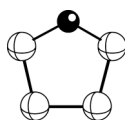


| Atom | X        | Y        | Z        | Atom | X        | Y        | Z        |
|------|----------|----------|----------|------|----------|----------|----------|
| Li   | 0.02911  | -0.14039 | -0.05877 | H    | 2.18286  | -1.17073 | 2.47038  |
| O    | -1.37324 | -0.92242 | 1.18009  | H    | -3.16104 | -1.56802 | 0.34096  |
| C    | -1.08929 | -1.05151 | 2.59156  | H    | -2.94016 | 0.19625  | 0.44643  |
| C    | -2.26573 | -0.37706 | 3.29362  | H    | -4.28145 | -0.05666 | 2.44237  |
| C    | -3.44055 | -0.75404 | 2.37376  | H    | -3.81386 | -1.75374 | 2.62619  |
| C    | -2.79855 | -0.75144 | 0.97608  | H    | -2.39745 | -0.72466 | 4.32330  |
| C    | 1.98202  | 0.09146  | 0.71235  | H    | -2.12177 | 0.70998  | 3.31556  |
| C    | 2.68876  | -0.47173 | 1.79989  | H    | -0.12024 | -0.58131 | 2.77040  |
| C    | 4.03629  | -0.19205 | 2.08423  | H    | -1.02606 | -2.11901 | 2.84884  |
| C    | 4.66799  | 0.69170  | 1.22160  | H    | -0.92949 | -2.84696 | -0.62284 |
| N    | 4.10064  | 1.26291  | 0.17995  | H    | -1.15336 | -2.96866 | -2.39018 |
| C    | 2.82844  | 0.93326  | -0.00485 | H    | 1.23687  | -3.87019 | -0.77786 |
| F    | 2.30015  | 1.56322  | -1.13175 | H    | 0.74333  | -4.37090 | -2.39908 |
| F    | 5.97389  | 1.01381  | 1.43678  | H    | 2.39147  | -2.84030 | -3.22941 |
| O    | -0.91366 | 1.59082  | -0.60303 | H    | 2.62050  | -2.18045 | -1.59994 |
| C    | -0.60223 | 2.77977  | 0.14966  | H    | 0.55124  | -1.33178 | -3.67948 |
| C    | -1.47611 | 3.87022  | -0.48187 | H    | 1.47381  | -0.29571 | -2.54718 |
| C    | -1.58823 | 3.42821  | -1.96701 | H    | 0.02181  | 1.99991  | -2.40786 |
| C    | -0.98944 | 2.00280  | -1.98241 | H    | -1.60160 | 1.26371  | -2.50424 |
| O    | -0.09341 | -1.32455 | -1.70609 | H    | -1.02695 | 4.09071  | -2.63337 |
| C    | -0.44080 | -2.71664 | -1.59060 | H    | -2.63029 | 3.43057  | -2.30196 |
| C    | 0.87997  | -3.50346 | -1.74478 | H    | -2.46431 | 3.88767  | -0.00939 |
| C    | 1.87052  | -2.46639 | -2.34213 | H    | -1.03323 | 4.86469  | -0.36857 |
| C    | 0.98017  | -1.26075 | -2.66780 | H    | 0.46777  | 2.99967  | 0.04851  |
| H    | 4.57085  | -0.62979 | 2.92155  | H    | -0.82598 | 2.56996  | 1.19840  |

Table III (Continued).

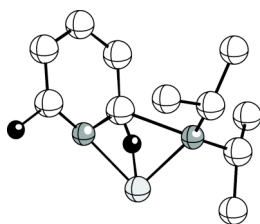
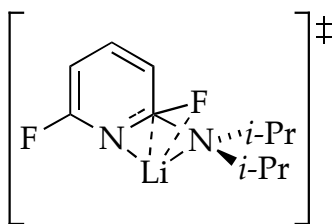


| Atom | X        | Y        | Z        | Atom | X        | Y        | Z        |
|------|----------|----------|----------|------|----------|----------|----------|
| C    | 1.25205  | -0.10825 | 0.19533  | H    | -3.26961 | 0.73254  | -0.61409 |
| N    | 0.01598  | -0.15608 | -0.60098 | H    | -2.00776 | 1.06652  | -1.82798 |
| C    | -1.24103 | 0.26150  | 0.04114  | H    | -1.06959 | 1.26476  | 0.45157  |
| C    | -1.70735 | -0.65538 | 1.18950  | H    | -0.10634 | -1.09537 | -0.97955 |
| C    | -2.32344 | 0.37624  | -1.03901 | H    | 0.96873  | 1.94424  | 0.92274  |
| C    | 1.71423  | 1.34213  | 0.39131  | H    | 2.63924  | 1.37196  | 0.98027  |
| C    | 2.32837  | -0.92485 | -0.52887 | H    | 1.90110  | 1.81419  | -0.58069 |
| H    | -0.94806 | -0.74952 | 1.97402  | H    | 2.50240  | -0.52193 | -1.53419 |
| H    | -2.61983 | -0.26482 | 1.65780  | H    | 3.27451  | -0.89820 | 0.02353  |
| H    | -1.93021 | -1.66321 | 0.81217  | H    | 2.03132  | -1.97740 | -0.62896 |
| H    | -2.51569 | -0.60203 | -1.50187 | H    | 1.11099  | -0.55702 | 1.19680  |



| Atom | X        | Y        | Z        | Atom | X        | Y        | Z        |
|------|----------|----------|----------|------|----------|----------|----------|
| C    | -0.77749 | 0.78984  | -0.12470 | H    | 1.99931  | -1.03598 | -0.49993 |
| C    | -1.13763 | -0.69731 | 0.08036  | H    | 1.32321  | -0.91394 | 1.14655  |
| O    | -0.00025 | -1.43373 | -0.36726 | H    | 1.16584  | 1.15203  | -1.08284 |
| C    | 1.13720  | -0.69784 | 0.08098  | H    | 1.19941  | 1.42106  | 0.66359  |
| C    | 0.77808  | 0.78927  | -0.12552 | H    | -1.16605 | 1.15436  | -1.08102 |
| H    | -1.99940 | -1.03451 | -0.50161 | H    | -1.19740 | 1.42083  | 0.66581  |
| H    | -1.32482 | -0.91407 | 1.14559  |      |          |          |          |

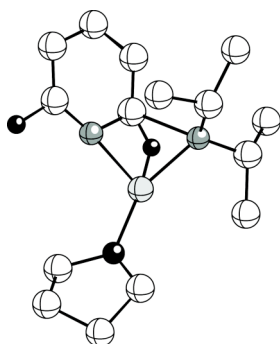
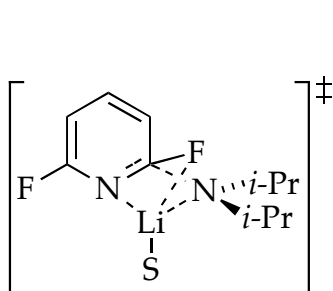
Table III (Continued).



**11a**  
 $G = -745.919026$   
 (0 °C)

| Atom | X        | Y        | Z        | Atom | X        | Y        | Z        |
|------|----------|----------|----------|------|----------|----------|----------|
| C    | -2.03433 | -0.46884 | -0.35232 | H    | -1.72686 | 1.97619  | 1.02016  |
| N    | -0.63697 | -0.08375 | -0.65702 | H    | -0.56998 | 3.20636  | 0.50819  |
| C    | -0.47008 | 1.38220  | -0.68582 | H    | 1.08749  | 1.32035  | -2.23283 |
| C    | -0.70860 | 2.12613  | 0.64803  | H    | 1.71722  | 1.58041  | -0.59242 |
| C    | 0.88670  | 1.80695  | -1.26795 | H    | 0.89385  | 2.88932  | -1.44375 |
| Li   | 0.29894  | -1.18252 | -1.89023 | H    | -1.23337 | 1.76869  | -1.38960 |
| C    | 0.93722  | -1.18088 | 0.32901  | H    | 4.51611  | 0.19769  | 0.73450  |
| F    | 0.10614  | -2.30237 | 0.32925  | H    | 2.91219  | 0.22198  | 2.70332  |
| N    | 1.82866  | -1.25674 | -0.69637 | H    | 0.60940  | -0.70841 | 2.42311  |
| C    | 3.03185  | -0.73811 | -0.50959 | H    | -1.98507 | -0.05570 | 1.80679  |
| C    | 3.50525  | -0.18267 | 0.66106  | H    | -3.43766 | -0.90654 | 1.26060  |
| C    | 2.59419  | -0.17526 | 1.74260  | H    | -1.90244 | -1.77886 | 1.40611  |
| C    | 1.31774  | -0.68016 | 1.60416  | H    | -1.90696 | -2.52846 | -1.09457 |
| F    | 3.83919  | -0.78860 | -1.59762 | H    | -3.54626 | -1.87608 | -1.09910 |
| C    | -2.35149 | -0.82369 | 1.11963  | H    | -2.39916 | -1.32957 | -2.32971 |
| C    | -2.49366 | -1.61752 | -1.27241 | H    | -2.67245 | 0.39596  | -0.60491 |
| H    | -0.00679 | 1.79250  | 1.41971  |      |          |          |          |

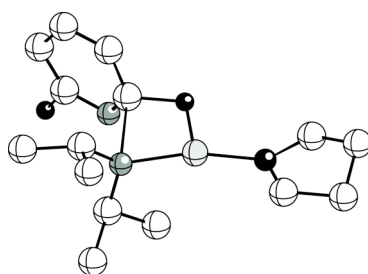
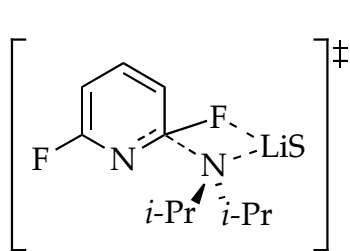
Table III (Continued).



**10a**  
 $G = -978.299402$   
 (0 °C)  
 S = THF

| Atom | X        | Y        | Z        | Atom | X        | Y        | Z        |
|------|----------|----------|----------|------|----------|----------|----------|
| C    | 1.36379  | -2.13000 | -0.36441 | H    | 3.06652  | -0.56641 | 2.96193  |
| N    | 1.01228  | -0.78889 | 0.14485  | H    | -0.28422 | 0.71669  | 2.00344  |
| C    | 1.38959  | -0.63426 | 1.55894  | H    | 1.27345  | 1.54684  | 1.80400  |
| C    | 2.90196  | -0.69663 | 1.88348  | H    | 0.94360  | 0.62402  | 3.27253  |
| C    | 0.79675  | 0.63823  | 2.18552  | H    | 0.93056  | -1.48168 | 2.11042  |
| Li   | -0.66992 | 0.00986  | -0.42002 | H    | 1.81980  | 4.48582  | 0.25590  |
| N    | 0.34861  | 1.68215  | -0.91678 | H    | 3.88535  | 3.14968  | -0.38346 |
| C    | 1.44627  | 0.93486  | -1.18803 | H    | 3.60875  | 0.85889  | -1.35065 |
| F    | 1.23033  | 0.09420  | -2.26428 | H    | -2.79159 | 2.02056  | -0.70953 |
| C    | 2.75870  | 1.45772  | -1.04691 | H    | -3.50434 | 0.95089  | -1.94721 |
| C    | 2.89359  | 2.72438  | -0.51557 | H    | -4.60235 | 1.55473  | 0.85394  |
| C    | 1.75815  | 3.48667  | -0.15651 | H    | -5.50955 | 1.49827  | -0.67019 |
| C    | 0.54144  | 2.87924  | -0.39290 | H    | -5.26632 | -0.93776 | -0.81490 |
| F    | -0.60364 | 3.54731  | -0.08118 | H    | -5.53728 | -0.72126 | 0.92371  |
| O    | -2.57702 | -0.00349 | -0.34907 | H    | -3.22329 | -1.94756 | -0.03104 |
| C    | -3.43243 | -0.94454 | 0.35254  | H    | -3.17272 | -0.90926 | 1.41748  |
| C    | -4.86700 | -0.47360 | 0.09483  | H    | 3.53175  | -1.80649 | -0.56733 |
| C    | -4.68790 | 1.04027  | -0.11079 | H    | 2.94941  | -3.30907 | -1.30090 |
| C    | -3.36412 | 1.10456  | -0.86950 | H    | 2.65398  | -1.75748 | -2.10409 |
| C    | 2.70545  | -2.25134 | -1.12915 | H    | 0.05987  | -2.08525 | -2.12484 |
| C    | 0.22903  | -2.70506 | -1.23556 | H    | 0.46623  | -3.71934 | -1.58375 |
| H    | 3.45111  | 0.09293  | 1.35869  | H    | -0.70788 | -2.76234 | -0.66455 |
| H    | 3.33684  | -1.66137 | 1.60381  | H    | 1.44840  | -2.80565 | 0.50710  |

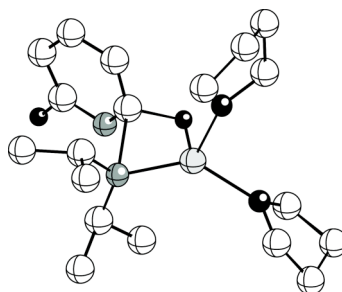
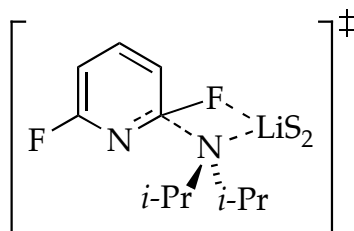
Table III (Continued).



**10b**  
 $G = -978.296603$   
 (0 °C)  
 S = THF

| Atom | X        | Y        | Z        | Atom | X        | Y        | Z        |
|------|----------|----------|----------|------|----------|----------|----------|
| C    | -1.05833 | 1.02392  | 1.38255  | H    | -1.30664 | -1.63332 | -2.33582 |
| N    | -0.72859 | 0.57733  | 0.02178  | H    | 3.52868  | 1.05857  | 0.43294  |
| C    | -1.30377 | 1.32751  | -1.09865 | H    | 3.76755  | 0.53343  | -1.25456 |
| C    | -2.76111 | 1.81147  | -0.93419 | H    | 5.93500  | -0.08535 | -0.34576 |
| C    | -0.39447 | 2.47001  | -1.60939 | H    | 5.24396  | -0.44142 | 1.24828  |
| Li   | 0.84723  | -0.46368 | 0.05909  | H    | 5.40454  | -2.69127 | 0.27498  |
| F    | -0.23540 | -1.97284 | 0.04975  | H    | 4.90630  | -2.09409 | -1.31935 |
| C    | -1.57645 | -1.43559 | -0.17683 | H    | 2.74026  | -2.80932 | -0.49153 |
| C    | -2.01512 | -1.62651 | -1.51514 | H    | 3.16910  | -2.39751 | 1.18940  |
| C    | -3.37423 | -1.80049 | -1.71418 | H    | 0.62156  | 2.09553  | -1.78993 |
| C    | -4.25766 | -1.84501 | -0.62041 | H    | -0.77911 | 2.87069  | -2.55830 |
| C    | -3.65839 | -1.76387 | 0.62997  | H    | -0.32194 | 3.30187  | -0.90166 |
| N    | -2.37446 | -1.62564 | 0.87318  | H    | -2.86496 | 2.61915  | -0.20195 |
| F    | -4.44604 | -1.87993 | 1.73132  | H    | -3.13388 | 2.19329  | -1.89349 |
| O    | 2.71845  | -0.78721 | -0.04450 | H    | -3.41852 | 0.99167  | -0.62792 |
| C    | 3.76798  | 0.20528  | -0.20788 | H    | -1.33949 | 0.60852  | -1.93228 |
| C    | 5.06692  | -0.50909 | 0.16831  | H    | 0.81233  | 0.35553  | 2.30554  |
| C    | 4.77089  | -1.96227 | -0.23917 | H    | -0.53937 | 0.48029  | 3.43083  |
| C    | 3.29702  | -2.11079 | 0.13857  | H    | -0.48488 | -0.88414 | 2.31675  |
| C    | -0.74745 | 2.50927  | 1.68190  | H    | -1.32695 | 3.20412  | 1.07055  |
| C    | -0.27325 | 0.18305  | 2.40949  | H    | -0.97859 | 2.72871  | 2.73296  |
| H    | -5.32578 | -1.98959 | -0.72569 | H    | 0.31775  | 2.72257  | 1.51874  |
| H    | -3.75965 | -1.92387 | -2.72353 | H    | -2.13105 | 0.86104  | 1.59525  |

Table III (Continued).

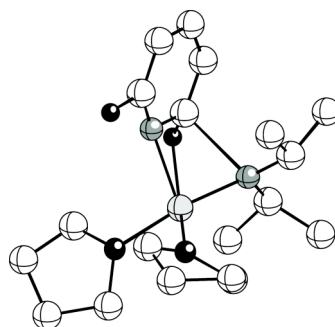
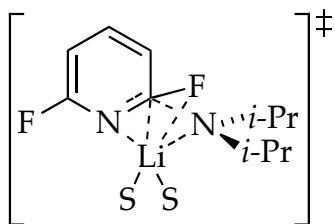


**12a**  
 $G = -1210.657993$   
 (0 °C)  
 S = THF

| Atom | X        | Y        | Z        | Atom | X        | Y        | Z        |
|------|----------|----------|----------|------|----------|----------|----------|
| Li   | 0.58190  | -0.09018 | -0.18342 | H    | -3.53273 | 1.23383  | 2.49902  |
| F    | -0.50087 | -0.09001 | -1.79335 | H    | -3.77902 | 0.24277  | 1.05486  |
| C    | -1.83432 | 0.13674  | -1.30898 | H    | -1.59642 | 1.45182  | 1.10675  |
| C    | -2.18335 | 1.51222  | -1.24011 | H    | 0.26265  | -2.84578 | 0.13939  |
| C    | -3.51897 | 1.83692  | -1.40533 | H    | -1.20257 | -3.83122 | -0.02480 |
| C    | -4.46651 | 0.83639  | -1.68766 | H    | -0.93326 | -2.48641 | -1.13709 |
| C    | -3.95048 | -0.44563 | -1.83408 | H    | -1.93858 | -1.98443 | 3.06627  |
| N    | -2.69189 | -0.80079 | -1.71511 | H    | -1.63468 | -3.54164 | 2.29651  |
| F    | -4.80404 | -1.44543 | -2.18096 | H    | -0.28739 | -2.42038 | 2.59323  |
| N    | -1.09346 | -0.49813 | 0.72305  | H    | -2.62344 | -1.96842 | 0.64695  |
| C    | -1.54522 | -1.88421 | 0.88276  | H    | -5.51977 | 1.04078  | -1.83562 |
| C    | -0.80928 | -2.80960 | -0.10233 | H    | -3.83615 | 2.87473  | -1.33311 |
| C    | -1.34355 | -2.48229 | 2.29721  | H    | -1.42338 | 2.26277  | -1.05602 |
| C    | -1.67591 | 0.48860  | 1.63810  | H    | 1.37146  | 1.85916  | -2.24283 |
| C    | -0.86762 | 0.69435  | 2.94499  | H    | 2.99644  | 1.79324  | -1.50926 |
| C    | -3.17984 | 0.34156  | 1.96481  | H    | 2.82860  | 4.19023  | -1.91728 |
| O    | 1.40016  | 1.76119  | -0.18044 | H    | 1.07998  | 4.18529  | -1.61942 |
| C    | 1.99055  | 2.22504  | -1.41918 | H    | 1.93732  | 4.93640  | 0.55934  |
| C    | 2.03575  | 3.74908  | -1.30491 | H    | 3.30874  | 3.81756  | 0.46067  |
| C    | 2.25035  | 3.94955  | 0.20432  | H    | 1.81345  | 2.42007  | 1.73895  |
| C    | 1.40619  | 2.82230  | 0.80669  | H    | 0.36945  | 3.13275  | 0.98445  |
| O    | 2.21869  | -1.11900 | -0.69234 | H    | 2.27054  | -1.19425 | -2.75651 |
| C    | 2.37457  | -1.88439 | -1.91453 | H    | 1.56979  | -2.62677 | -1.96554 |
| C    | 3.75288  | -2.53847 | -1.80952 | H    | 3.81900  | -3.46215 | -2.39281 |
| C    | 3.88451  | -2.76892 | -0.29450 | H    | 4.53390  | -1.85446 | -2.16410 |
| C    | 3.20811  | -1.52258 | 0.28449  | H    | 4.92172  | -2.87160 | 0.03982  |
| H    | 0.20178  | 0.79676  | 2.72423  | H    | 3.33997  | -3.67280 | 0.00273  |
| H    | -1.19845 | 1.60814  | 3.46090  | H    | 2.69707  | -1.70427 | 1.23544  |
| H    | -0.97974 | -0.13891 | 3.64594  | H    | 3.91736  | -0.69445 | 0.41578  |
| H    | -3.39201 | -0.52268 | 2.60350  |      |          |          |          |



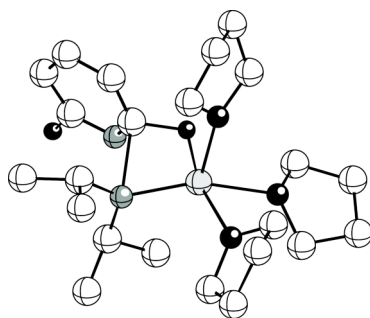
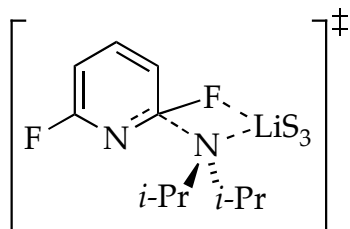
Table III (Continued).



**12b**  
 $G = -1210.655548$   
 (0 °C)  
 S = THF

| Atom | X        | Y        | Z        | Atom | X        | Y        | Z        |
|------|----------|----------|----------|------|----------|----------|----------|
| C    | 1.56317  | -0.38561 | 2.28872  | H    | 2.68721  | 2.62667  | -1.01032 |
| N    | 1.45858  | 0.03059  | 0.87228  | H    | 2.51241  | 0.98590  | -1.63369 |
| C    | 2.34820  | 1.15950  | 0.55365  | H    | 2.07481  | 2.00876  | 1.20771  |
| C    | 3.86350  | 0.91988  | 0.78193  | H    | 2.51192  | -0.89100 | -4.31773 |
| C    | 2.14193  | 1.68284  | -0.87748 | H    | 4.38521  | -1.67226 | -2.78347 |
| Li   | -0.33984 | -0.22385 | -0.02844 | H    | 3.85892  | -2.19694 | -0.39292 |
| N    | 0.76446  | -1.32206 | -1.45781 | H    | -2.93749 | -1.43709 | 2.02651  |
| C    | 1.76985  | -1.66231 | -0.61472 | H    | -3.35186 | -0.11180 | 0.90777  |
| F    | 1.38625  | -2.55730 | 0.36018  | H    | -4.83501 | -2.55946 | 1.18110  |
| C    | 3.10251  | -1.83266 | -1.07813 | H    | -4.94364 | -1.51309 | -0.23561 |
| C    | 3.37442  | -1.55006 | -2.40186 | H    | -3.64751 | -2.96622 | -1.53272 |
| C    | 2.34863  | -1.12095 | -3.27236 | H    | -3.74541 | -4.15914 | -0.23092 |
| C    | 1.09150  | -1.03698 | -2.70265 | H    | -1.66305 | -3.41514 | 0.74923  |
| F    | 0.04712  | -0.63200 | -3.48168 | H    | -1.29410 | -2.99744 | -0.94473 |
| O    | -1.96946 | -1.43724 | 0.19263  | H    | -1.43463 | 1.45339  | -2.50397 |
| C    | -1.99732 | -2.83993 | -0.12707 | H    | -2.93096 | 0.85301  | -1.75460 |
| C    | -3.46682 | -3.12661 | -0.46486 | H    | -2.74865 | 3.48850  | -2.64805 |
| C    | -4.24908 | -2.08711 | 0.38593  | H    | -3.67209 | 3.08339  | -1.19007 |
| C    | -3.14395 | -1.18206 | 0.97674  | H    | -2.03444 | 4.67121  | -0.28658 |
| O    | -1.44188 | 1.41815  | -0.43055 | H    | -0.74822 | 4.01290  | -1.31757 |
| C    | -1.33452 | 2.67181  | 0.28409  | H    | -0.32891 | 2.72821  | 0.70770  |
| C    | -1.64870 | 3.75596  | -0.74701 | H    | -2.06629 | 2.67193  | 1.10456  |
| C    | -2.67572 | 3.04927  | -1.64812 | H    | 0.85961  | 1.47618  | 3.21219  |
| C    | -2.14549 | 1.61195  | -1.68515 | H    | 1.67394  | 0.36592  | 4.32913  |
| C    | 1.69923  | 0.77360  | 3.31039  | H    | 2.62799  | 1.34233  | 3.21156  |
| C    | 0.32608  | -1.19244 | 2.72863  | H    | 0.11943  | -2.03372 | 2.06722  |
| H    | 4.27444  | 0.23594  | 0.03371  | H    | 0.47157  | -1.58981 | 3.74207  |
| H    | 4.41372  | 1.86823  | 0.70598  | H    | -0.56126 | -0.54302 | 2.75465  |
| H    | 4.07207  | 0.49589  | 1.76970  | H    | 2.44491  | -1.04030 | 2.43874  |
| H    | 1.08267  | 1.87374  | -1.08393 |      |          |          |          |

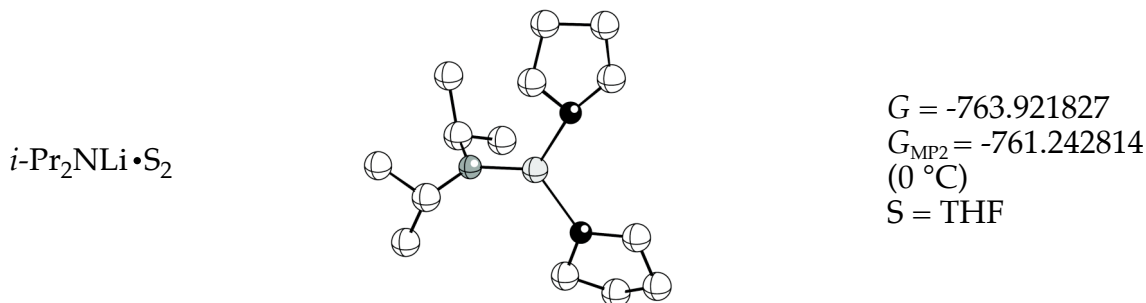
Table III (Continued).



**8a**  
 $G = -1443.002678$   
 (0 °C)  
 S = THF

| Atom | X        | Y        | Z        | Atom | X        | Y        | Z        |
|------|----------|----------|----------|------|----------|----------|----------|
| Li   | 0.25361  | 0.29434  | 0.00257  | H    | 4.51535  | -1.38282 | -2.48681 |
| N    | -1.34269 | -0.52402 | -0.93382 | H    | 2.45154  | -0.29888 | -2.81460 |
| C    | -1.75625 | 0.01882  | -2.22791 | H    | 1.51958  | -1.71153 | -2.27944 |
| C    | -1.15416 | 1.42090  | -2.42093 | H    | 0.20400  | -2.75372 | -0.61284 |
| C    | -1.36961 | -0.81552 | -3.47447 | H    | -1.09927 | -3.96144 | -0.58917 |
| C    | -1.79820 | -1.87847 | -0.61952 | H    | -0.70299 | -3.11155 | -2.09045 |
| C    | -0.79158 | -2.99073 | -1.00551 | H    | -3.29548 | -2.40531 | -2.16540 |
| C    | -3.22085 | -2.27178 | -1.08128 | H    | -3.51316 | -3.22312 | -0.61790 |
| F    | -1.27872 | 1.42974  | 0.83273  | H    | -3.95636 | -1.51935 | -0.78425 |
| C    | -2.50359 | 0.77143  | 0.60512  | H    | -1.84636 | -1.92220 | 0.48267  |
| C    | -2.91237 | -0.08697 | 1.65676  | H    | -0.05881 | 1.35653  | -2.49284 |
| C    | -4.26970 | -0.31258 | 1.80166  | H    | -1.52067 | 1.87404  | -3.35062 |
| C    | -5.19015 | 0.33912  | 0.96547  | H    | -1.41835 | 2.08468  | -1.59677 |
| C    | -4.64356 | 1.22968  | 0.04782  | H    | -1.81246 | -1.81421 | -3.47928 |
| N    | -3.36533 | 1.49897  | -0.10626 | H    | -1.70787 | -0.30509 | -4.38658 |
| F    | -5.48421 | 1.93559  | -0.73538 | H    | -0.28026 | -0.93107 | -3.54102 |
| O    | 2.16719  | -0.49895 | -0.75999 | H    | -2.85583 | 0.14770  | -2.26729 |
| O    | 0.74612  | -0.44455 | 1.96516  | H    | -0.04266 | 1.16639  | 2.98765  |
| O    | 1.32217  | 2.28365  | 0.04511  | H    | 1.70486  | 0.90107  | 3.21931  |
| C    | 2.14315  | 2.74203  | -1.03669 | H    | 0.89732  | -0.14181 | 5.25388  |
| C    | 2.91188  | 3.94125  | -0.46471 | H    | -0.62069 | -0.63212 | 4.48327  |
| C    | 1.93220  | 4.51592  | 0.59458  | H    | 0.66865  | -2.71952 | 4.36790  |
| C    | 0.78794  | 3.47919  | 0.64079  | H    | 2.15948  | -1.83529 | 3.99380  |
| C    | 0.72809  | 0.40672  | 3.13419  | H    | 1.44092  | -2.37550 | 1.73628  |
| C    | 0.45806  | -0.51766 | 4.32499  | H    | -0.27516 | -2.24189 | 2.17386  |
| C    | 1.07209  | -1.84381 | 3.85084  | H    | -6.26173 | 0.20637  | 1.04524  |
| C    | 0.72526  | -1.83355 | 2.36119  | H    | -4.62750 | -0.98530 | 2.57733  |
| C    | 2.39036  | -1.09246 | -2.05964 | H    | -2.17551 | -0.55341 | 2.29850  |
| C    | 3.70492  | -1.89864 | -1.95996 | H    | 2.76764  | 1.90612  | -1.35201 |
| C    | 3.98959  | -1.93430 | -0.44672 | H    | 1.50355  | 3.04673  | -1.87838 |
| C    | 3.36684  | -0.61848 | 0.01506  | H    | 3.84076  | 3.60772  | 0.00908  |
| H    | 3.07450  | -0.58651 | 1.06553  | H    | 3.17488  | 4.66735  | -1.23982 |
| H    | 4.04089  | 0.22885  | -0.19082 | H    | 1.55461  | 5.50453  | 0.31680  |
| H    | 5.05568  | -2.00998 | -0.21087 | H    | 2.42148  | 4.61374  | 1.56831  |
| H    | 3.47318  | -2.77878 | 0.02420  | H    | -0.08188 | 3.81338  | 0.06101  |
| H    | 3.61030  | -2.89682 | -2.39688 | H    | 0.45534  | 3.22711  | 1.64815  |

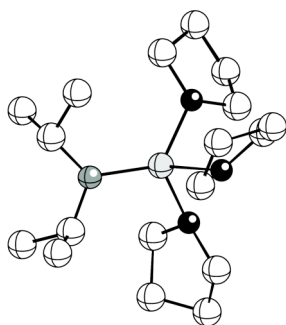
**Table IV.** Optimized geometries at B3LYP level of theory with 6-31G(d) basis set for the solvation of LDA monomer with free energies (Hartrees), and cartesian coordinates (X,Y,Z). (Note:  $G_{\text{MP2}}$  includes single point MP2 corrections to B3LYP/6-31G(d) optimized structures)



| Atom | X        | Y        | Z        | Atom | X        | Y        | Z        |
|------|----------|----------|----------|------|----------|----------|----------|
| C    | 0.53584  | -2.31846 | -1.11557 | H    | -2.34804 | -1.31446 | 0.22222  |
| N    | 0.54228  | -1.32502 | -0.04871 | H    | -3.40247 | -1.03144 | -1.19260 |
| C    | 1.23590  | -1.71823 | 1.16664  | H    | -0.18239 | 3.68916  | 0.46720  |
| C    | 2.65946  | -1.11706 | 1.29862  | H    | 0.75791  | 2.52348  | 1.43574  |
| C    | 0.41645  | -1.31502 | 2.40970  | H    | 1.82060  | 4.64663  | -0.49727 |
| Li   | -0.28135 | 0.31461  | -0.36284 | H    | 2.45225  | 4.22679  | 1.10609  |
| O    | -2.20978 | 0.56437  | -0.57645 | H    | 3.31466  | 2.07890  | 0.28078  |
| C    | -3.01619 | -0.59767 | -0.25994 | H    | 3.67824  | 3.14913  | -1.08653 |
| C    | -4.14305 | -0.05168 | 0.61037  | H    | 2.06743  | 0.89858  | -1.39927 |
| C    | -4.41849 | 1.30833  | -0.05429 | H    | 1.71145  | 2.40651  | -2.30325 |
| C    | -3.01785 | 1.76028  | -0.50223 | H    | 2.59834  | -0.01980 | 1.34288  |
| O    | 0.58515  | 2.08541  | -0.58902 | H    | 3.17692  | -1.46017 | 2.20752  |
| C    | 1.84656  | 1.96591  | -1.30764 | H    | 3.27774  | -1.37958 | 0.43458  |
| C    | 2.87076  | 2.73693  | -0.47431 | H    | -0.55856 | -1.81522 | 2.40479  |
| C    | 2.00615  | 3.81693  | 0.19501  | H    | 0.92795  | -1.55505 | 3.35263  |
| C    | 0.70989  | 3.05516  | 0.47581  | H    | 0.23397  | -0.22827 | 2.40357  |
| C    | 1.92773  | -2.71287 | -1.67360 | H    | 1.36333  | -2.81540 | 1.22780  |
| C    | -0.25703 | -3.61264 | -0.79002 | H    | -1.28169 | -3.36672 | -0.48788 |
| H    | -3.01951 | 2.25151  | -1.48109 | H    | -0.30743 | -4.28879 | -1.65526 |
| H    | -2.55232 | 2.43651  | 0.22440  | H    | 0.20519  | -4.17195 | 0.03271  |
| H    | -4.89142 | 2.03155  | 0.61671  | H    | 2.52640  | -3.23743 | -0.91803 |
| H    | -5.07438 | 1.17812  | -0.92251 | H    | 1.84331  | -3.37850 | -2.54454 |
| H    | -5.01925 | -0.70655 | 0.62649  | H    | 2.48421  | -1.81790 | -1.97729 |
| H    | -3.79498 | 0.08189  | 1.64150  | H    | 0.00011  | -1.85081 | -1.96365 |

Table IV (Continued).

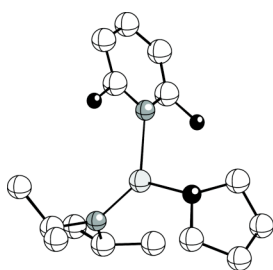
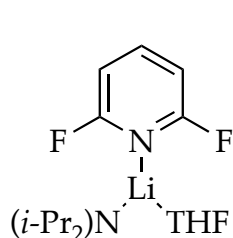
*i*-Pr<sub>2</sub>NLi•S<sub>3</sub>



G = -996.270707  
G<sub>MP2</sub> = -992.824425  
(0 °C)  
S = THF

| Atom | X        | Y        | Z        | Atom | X        | Y        | Z        |
|------|----------|----------|----------|------|----------|----------|----------|
| Li   | 0.19850  | 0.00829  | -0.10075 |      |          |          |          |
| N    | -1.35509 | -0.69168 | 0.79093  | H    | -0.28373 | -3.24415 | 2.81719  |
| C    | -2.66311 | -0.29169 | 0.28843  | H    | -0.53892 | -3.30828 | 1.05717  |
| C    | -3.52636 | -1.45068 | -0.28560 | H    | -1.95141 | 0.03676  | 3.42365  |
| C    | -3.55264 | 0.53438  | 1.25753  | H    | -1.26053 | -1.40749 | 4.19145  |
| C    | -1.39567 | -1.52589 | 1.98122  | H    | -0.21480 | -0.26283 | 3.32163  |
| C    | -0.33161 | -2.63946 | 1.90048  | H    | -2.36776 | -2.04681 | 2.08229  |
| C    | -1.19919 | -0.74928 | 3.31083  | H    | -1.22387 | 1.08943  | -2.63241 |
| O    | -0.09301 | 1.83406  | -1.05923 | H    | 0.33930  | 1.81160  | -3.08011 |
| C    | -0.73055 | 2.86302  | -0.26371 | H    | -0.50845 | 4.06479  | -2.77778 |
| C    | -1.82521 | 3.45978  | -1.15078 | H    | -1.99215 | 3.27950  | -3.34924 |
| C    | -1.23608 | 3.27393  | -2.55827 | H    | -2.75184 | 2.88566  | -1.04501 |
| C    | -0.53529 | 1.91926  | -2.43190 | H    | -2.03934 | 4.50423  | -0.90461 |
| O    | 0.89142  | -1.08095 | -1.74852 | H    | 0.02651  | 3.61459  | 0.00098  |
| C    | 0.01344  | -2.19728 | -2.04284 | H    | -1.10640 | 2.39148  | 0.64756  |
| C    | 0.90948  | -3.43222 | -1.99998 | H    | 2.29032  | 2.07277  | -0.60030 |
| C    | 2.23425  | -2.88226 | -2.55212 | H    | 3.68297  | 0.95952  | -0.54752 |
| C    | 2.26555  | -1.46149 | -1.97278 | H    | 4.51968  | 2.73575  | 0.89431  |
| O    | 2.08314  | 0.49953  | 0.70192  | H    | 2.90228  | 3.04721  | 1.55631  |
| C    | 2.47985  | 0.34053  | 2.08602  | H    | 3.85735  | 1.56613  | 3.27624  |
| C    | 3.75563  | 1.17172  | 2.26090  | H    | 4.64485  | 0.56870  | 2.04168  |
| C    | 3.57903  | 2.26393  | 1.19451  | H    | 2.62215  | -0.72532 | 2.28773  |
| C    | 2.92585  | 1.47827  | 0.05854  | H    | 1.66435  | 0.70531  | 2.71896  |
| H    | -2.99748 | 1.38957  | 1.66150  | H    | 2.72795  | -0.73446 | -2.65067 |
| H    | -4.45465 | 0.91410  | 0.75511  | H    | 2.78922  | -1.42250 | -1.01080 |
| H    | -3.88833 | -0.07204 | 2.10816  | H    | 2.20554  | -2.85085 | -3.64786 |
| H    | -3.77502 | -2.18785 | 0.48794  | H    | 3.10841  | -3.47046 | -2.25560 |
| H    | -4.47612 | -1.08559 | -0.70283 | H    | 1.03286  | -3.77096 | -0.96478 |
| H    | -2.98767 | -1.97653 | -1.08213 | H    | 0.50915  | -4.26376 | -2.58806 |
| H    | -2.46686 | 0.37551  | -0.57075 | H    | -0.77103 | -2.17368 | -1.28142 |
| H    | 0.66375  | -2.20011 | 1.73936  | H    | -0.42257 | -2.05276 | -3.04213 |

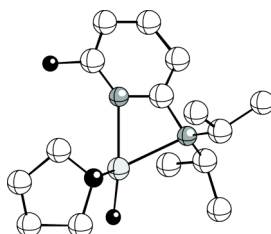
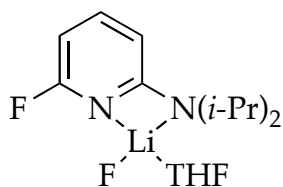
**Table V.** Optimized geometries at B3LYP level of theory with 6-31G(d) basis set from the IRC calculations on monosolvated (**10a**) and trisolvated (**8**) monomeric transition structures with free energies (Hartrees), and cartesian coordinates (X,Y,Z).



**13**  
 $G = -978.284647$   
 (0 °C)  
 S = THF

| Atom | X        | Y        | Z        | Atom | X        | Y        | Z        |
|------|----------|----------|----------|------|----------|----------|----------|
| C    | 0.46810  | 2.65236  | -0.65972 | H    | 0.12577  | 2.71721  | 3.40233  |
| N    | 0.50805  | 1.46642  | 0.18083  | H    | 1.98400  | -0.11029 | 1.79790  |
| C    | 0.85628  | 1.74230  | 1.55917  | H    | 0.28299  | -0.22472 | 2.31387  |
| C    | -0.20750 | 2.52448  | 2.37165  | H    | 1.46259  | 0.60425  | 3.33854  |
| C    | 1.16824  | 0.42939  | 2.29603  | H    | 1.78245  | 2.35995  | 1.61554  |
| Li   | 0.01022  | -0.24489 | -0.35959 | H    | -4.24142 | -2.24612 | 1.87631  |
| O    | 1.14670  | -1.71325 | -0.98863 | H    | -5.80638 | -1.36277 | 0.09788  |
| C    | 2.52199  | -1.32654 | -1.27226 | H    | -4.81273 | -0.27914 | -1.95871 |
| C    | 3.41720  | -2.41814 | -0.65169 | H    | 0.24864  | -3.13951 | 0.18013  |
| C    | 2.45941  | -3.18842 | 0.27621  | H    | 1.04730  | -3.77378 | -1.28529 |
| C    | 1.12939  | -3.05116 | -0.46006 | H    | 2.39306  | -2.70075 | 1.25482  |
| N    | -1.97522 | -1.04553 | -0.31005 | H    | 2.75473  | -4.23104 | 0.42853  |
| C    | -2.81414 | -0.59985 | -1.23435 | H    | 3.81060  | -3.08243 | -1.42915 |
| F    | -2.23298 | -0.03636 | -2.29815 | H    | 4.27008  | -1.99221 | -0.11570 |
| C    | -4.19780 | -0.67534 | -1.16023 | H    | 2.64547  | -1.25069 | -2.35794 |
| C    | -4.73066 | -1.27645 | -0.01822 | H    | 2.65743  | -0.33694 | -0.82766 |
| C    | -3.87984 | -1.76951 | 0.97361  | H    | -1.53709 | 3.32194  | -0.07182 |
| C    | -2.51867 | -1.61813 | 0.75320  | H    | -0.96579 | 4.06678  | -1.58212 |
| F    | -1.64277 | -2.07090 | 1.66198  | H    | -1.49822 | 2.37260  | -1.56472 |
| C    | -0.96561 | 3.14063  | -0.98765 | H    | 0.78308  | 1.55663  | -2.52056 |
| C    | 1.22318  | 2.41034  | -1.98335 | H    | 1.18262  | 3.27878  | -2.65607 |
| H    | -1.14756 | 1.95646  | 2.41098  | H    | 2.27523  | 2.17423  | -1.78650 |
| H    | -0.42302 | 3.49352  | 1.90910  | H    | 0.98263  | 3.49657  | -0.15839 |

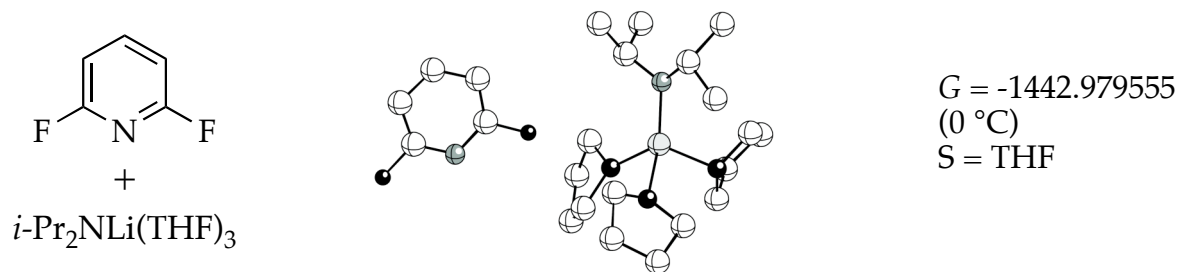
Table V (Continued).



**14**  
 $G = -978.347810$   
 (0 °C)  
 S = THF

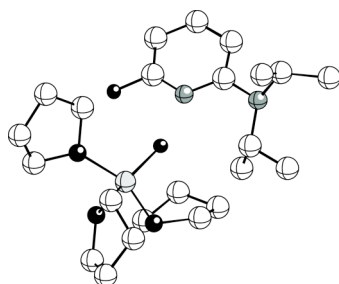
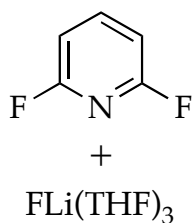
| Atom | X        | Y        | Z        | Atom | X        | Y        | Z        |
|------|----------|----------|----------|------|----------|----------|----------|
| C    | 2.05838  | -1.42304 | -0.97928 | H    | 2.88826  | -1.42516 | 3.01965  |
| N    | 1.34502  | -0.55233 | 0.01931  | H    | -0.52710 | -0.25149 | 2.00402  |
| C    | 1.51205  | 0.85160  | -0.17817 | H    | 0.79129  | 0.85859  | 2.43656  |
| C    | 2.74014  | 1.52080  | -0.22599 | H    | 0.54307  | -0.62107 | 3.36891  |
| C    | 2.74933  | 2.90176  | -0.43259 | H    | 1.10420  | -2.02073 | 1.44983  |
| C    | 1.54784  | 3.58964  | -0.58363 | H    | 1.49474  | 4.65957  | -0.74583 |
| C    | 0.38995  | 2.82127  | -0.52858 | H    | 3.69115  | 3.44160  | -0.47365 |
| N    | 0.35003  | 1.51869  | -0.34286 | H    | 3.66566  | 0.96804  | -0.11767 |
| Li   | -0.87265 | -0.26451 | -0.63487 | H    | -3.16487 | 1.27493  | 1.86596  |
| O    | -2.53464 | -0.13639 | 0.47321  | H    | -2.68617 | 1.90952  | 0.27641  |
| C    | -3.21864 | 1.09945  | 0.78468  | H    | -5.33262 | 0.68043  | 1.11823  |
| C    | -4.66723 | 0.93733  | 0.28578  | H    | -5.04883 | 1.85373  | -0.17469 |
| C    | -4.56654 | -0.24025 | -0.70010 | H    | -4.23194 | 0.10211  | -1.68595 |
| C    | -3.47965 | -1.10051 | -0.06565 | H    | -5.51313 | -0.77544 | -0.82435 |
| F    | -1.15600 | -1.35321 | -1.86031 | H    | -2.90948 | -1.70350 | -0.77659 |
| F    | -0.79914 | 3.42764  | -0.68059 | H    | -3.87454 | -1.71247 | 0.75841  |
| C    | 1.45688  | -0.98675 | 1.45069  | H    | 2.22700  | 0.12324  | -2.54918 |
| C    | 2.88721  | -0.97584 | 2.01999  | H    | 2.40294  | -1.54178 | -3.10170 |
| C    | 0.50626  | -0.19695 | 2.35917  | H    | 0.78397  | -0.94433 | -2.64771 |
| C    | 1.85295  | -0.89602 | -2.40805 | H    | 0.43078  | -2.80954 | -1.16025 |
| C    | 1.50039  | -2.85258 | -0.92524 | H    | 2.00443  | -3.45595 | -1.68873 |
| H    | 3.27511  | 0.04463  | 2.11909  | H    | 1.66253  | -3.35319 | 0.03469  |
| H    | 3.58315  | -1.55114 | 1.40076  | H    | 3.13844  | -1.44039 | -0.75312 |

**Table V (Continued).**



| Atom | X        | Y        | Z        | Atom | X        | Y        | Z        |
|------|----------|----------|----------|------|----------|----------|----------|
| Li   | 0.98827  | -0.15210 | 0.28350  | H    | 5.56399  | -0.78653 | -1.58133 |
| N    | 0.86880  | 1.75616  | 0.14832  | H    | 4.62032  | 0.12802  | 0.36129  |
| C    | -0.04269 | 2.23205  | -0.88527 | H    | 3.32162  | 0.94952  | -0.55272 |
| C    | 0.62320  | 2.68457  | -2.21731 | H    | 1.33536  | 1.92080  | -2.55338 |
| C    | -1.06699 | 3.30911  | -0.44901 | H    | -0.12229 | 2.83368  | -3.01483 |
| C    | 1.38608  | 2.75770  | 1.06057  | H    | 1.17915  | 3.62256  | -2.10810 |
| C    | 2.02201  | 2.06652  | 2.27943  | H    | -0.59614 | 4.27851  | -0.24507 |
| C    | 2.42220  | 3.75980  | 0.47776  | H    | -1.81624 | 3.47520  | -1.23640 |
| O    | -0.05536 | -1.43804 | -1.06549 | H    | -1.58415 | 2.99493  | 0.46703  |
| C    | -0.44498 | -1.12038 | -2.40989 | H    | -0.66159 | 1.36260  | -1.17015 |
| C    | -0.53962 | -2.47829 | -3.12844 | H    | 2.85175  | 1.41534  | 1.97217  |
| C    | -0.83121 | -3.48190 | -1.97765 | H    | 2.41801  | 2.79426  | 2.99996  |
| C    | -0.82300 | -2.60065 | -0.71253 | H    | 1.28046  | 1.44492  | 2.79429  |
| F    | -2.88646 | -0.08080 | -0.15633 | H    | 1.98886  | 4.36260  | -0.32636 |
| C    | -4.20168 | 0.20950  | -0.17070 | H    | 2.78832  | 4.45573  | 1.24778  |
| N    | -5.01056 | -0.83202 | -0.15339 | H    | 3.28708  | 3.22580  | 0.06178  |
| C    | -6.30324 | -0.56136 | -0.16663 | H    | 0.57782  | 3.39628  | 1.47860  |
| C    | -6.85791 | 0.71475  | -0.19637 | H    | -1.84002 | -2.29096 | -0.44151 |
| C    | -5.96274 | 1.78477  | -0.21393 | H    | -0.34458 | -3.05301 | 0.15696  |
| C    | -4.58837 | 1.54463  | -0.20118 | H    | -0.05501 | -4.25191 | -1.92730 |
| F    | -7.12139 | -1.62116 | -0.14938 | H    | -1.79182 | -3.99115 | -2.09928 |
| O    | 2.89641  | -0.97459 | -0.03480 | H    | -1.32188 | -2.47443 | -3.89331 |
| C    | 3.87809  | 0.01603  | -0.43887 | H    | 0.40522  | -2.72160 | -3.62444 |
| C    | 4.51843  | -0.50428 | -1.74649 | H    | 0.30207  | -0.43814 | -2.81922 |
| C    | 3.67440  | -1.74453 | -2.10304 | H    | -1.41724 | -0.61007 | -2.39278 |
| C    | 3.17039  | -2.19306 | -0.73227 | H    | -7.93296 | 0.84776  | -0.20516 |
| O    | 0.42363  | -1.25241 | 1.95134  | H    | -6.33469 | 2.80463  | -0.23751 |
| C    | -0.78178 | -0.84715 | 2.62443  | H    | -3.84692 | 2.33419  | -0.21436 |
| C    | -0.97523 | -1.87181 | 3.76074  | H    | 2.11543  | -2.26148 | 2.51163  |
| C    | 0.44300  | -2.47492 | 3.96688  | H    | 1.76769  | -0.80070 | 3.46833  |
| C    | 1.32164  | -1.68094 | 2.98499  | H    | 0.44917  | -3.54014 | 3.71537  |
| H    | 2.24294  | -2.76799 | -0.76386 | H    | 0.79897  | -2.37628 | 4.99677  |
| H    | 3.93862  | -2.77295 | -0.19563 | H    | -1.35938 | -1.39117 | 4.66545  |
| H    | 4.24561  | -2.51915 | -2.62466 | H    | -1.68976 | -2.64868 | 3.47281  |
| H    | 2.82159  | -1.46351 | -2.73069 | H    | -0.64939 | 0.17033  | 3.01501  |
| H    | 4.50141  | 0.25041  | -2.53816 | H    | -1.58074 | -0.83334 | 1.88200  |

**Table V (Continued).**



$G = -1443.053274$   
(0 °C)  
S = THF

| Atom | X        | Y        | Z        | Atom | X        | Y        | Z        |
|------|----------|----------|----------|------|----------|----------|----------|
| Li   | -2.35889 | -0.06713 | -0.12736 | H    | -2.69127 | -3.33174 | -3.58417 |
| F    | -0.80181 | 0.29945  | -0.66020 | H    | -1.79969 | -3.28989 | -1.37860 |
| C    | 1.21955  | 2.35597  | 0.27413  | H    | -1.10445 | -1.64522 | -1.59204 |
| F    | 0.30994  | 2.56378  | 1.25428  | H    | 5.73511  | -0.89053 | -2.00082 |
| N    | 2.01103  | 1.32484  | 0.44851  | H    | 7.11769  | -0.19555 | -1.12920 |
| C    | 2.92906  | 1.06499  | -0.49953 | H    | 6.30158  | -1.62205 | -0.49016 |
| C    | 3.06486  | 1.89821  | -1.62830 | H    | 5.68382  | -0.32478 | 1.81751  |
| C    | 2.23810  | 3.00865  | -1.74730 | H    | 6.68533  | 0.98219  | 1.17692  |
| C    | 1.27277  | 3.26596  | -0.77281 | H    | 5.01013  | 1.30571  | 1.66501  |
| N    | 3.75426  | -0.06944 | -0.34863 | H    | 5.27401  | 1.23496  | -0.78025 |
| C    | 3.15420  | -1.16263 | 0.46665  | H    | 2.08120  | -2.04323 | -1.19943 |
| C    | 1.85249  | -1.63785 | -0.20523 | H    | 1.41668  | -2.44830 | 0.39362  |
| C    | 4.06987  | -2.38259 | 0.63387  | H    | 1.09393  | -0.85712 | -0.31188 |
| C    | 5.20060  | 0.28155  | -0.25005 | H    | 4.99444  | -2.17285 | 1.17607  |
| C    | 5.66859  | 0.57091  | 1.18942  | H    | 3.52395  | -3.13884 | 1.20878  |
| C    | 6.13810  | -0.67376 | -1.00614 | H    | 4.32630  | -2.82550 | -0.33464 |
| O    | -2.49058 | -0.43364 | 1.84740  | H    | 2.90952  | -0.77948 | 1.46781  |
| C    | -1.17413 | -0.27508 | 2.44296  | H    | -4.94329 | 1.09538  | 1.04958  |
| C    | -0.82253 | -1.66243 | 2.97063  | H    | -5.41528 | 2.45301  | -0.01182 |
| C    | -2.18936 | -2.17903 | 3.45017  | H    | -4.41433 | 3.67635  | 1.86443  |
| C    | -3.15639 | -1.58405 | 2.41377  | H    | -3.20296 | 2.39993  | 2.10043  |
| O    | -3.63036 | 1.48780  | -0.47175 | H    | -1.82327 | 3.73841  | 0.73136  |
| C    | -2.81292 | 2.61853  | -0.87380 | H    | -3.19616 | 4.59002  | 0.00496  |
| C    | -2.82513 | 3.60802  | 0.31719  | H    | -3.25269 | 3.06435  | -1.77612 |
| C    | -3.77527 | 2.95223  | 1.34906  | H    | -1.82852 | 2.20013  | -1.09415 |
| C    | -4.57096 | 1.96253  | 0.49818  | H    | 0.58789  | 4.10363  | -0.82619 |
| O    | -3.10058 | -1.67878 | -1.12962 | H    | 2.32443  | 3.66062  | -2.61257 |
| C    | -1.95889 | -2.29307 | -1.80541 | H    | 3.78058  | 1.64867  | -2.40389 |
| C    | -2.31570 | -2.34114 | -3.30089 | H    | -4.10643 | -1.26217 | 2.85694  |
| C    | -3.43420 | -1.29284 | -3.42565 | H    | -3.37158 | -2.28165 | 1.59646  |
| C    | -4.14999 | -1.44314 | -2.08562 | H    | -2.41120 | -1.78933 | 4.45065  |
| H    | -4.68792 | -0.54706 | -1.76746 | H    | -2.25117 | -3.27078 | 3.49479  |
| H    | -4.84202 | -2.29906 | -2.09397 | H    | -0.43583 | -2.28560 | 2.15622  |
| H    | -4.09410 | -1.46355 | -4.28225 | H    | -0.07086 | -1.63284 | 3.76540  |
| H    | -3.00901 | -0.28631 | -3.50646 | H    | -0.51944 | 0.10005  | 1.65539  |
| H    | -1.45115 | -2.11629 | -3.93222 | H    | -1.23965 | 0.45948  | 3.25802  |