Reaction of Lithium Diethylamide
with an Alkyl Bromide and Alkyl Benzenesulfonate:
Origins of Alkylation, Elimination, and Sulfonation.

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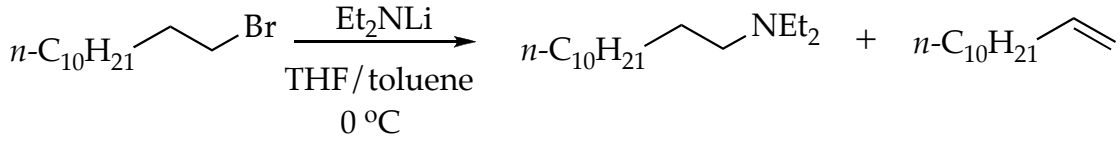
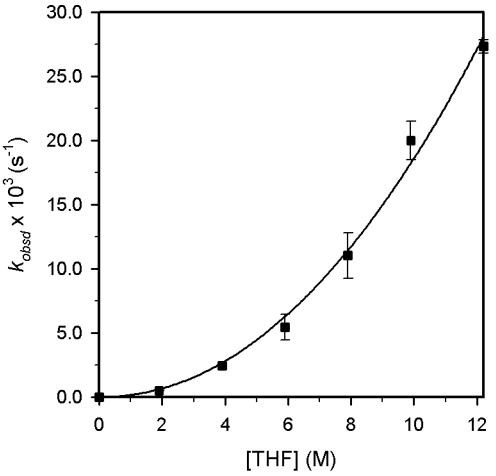
**Supporting Information**

**Complete Reference:**

(18) All calculations were performed with 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.

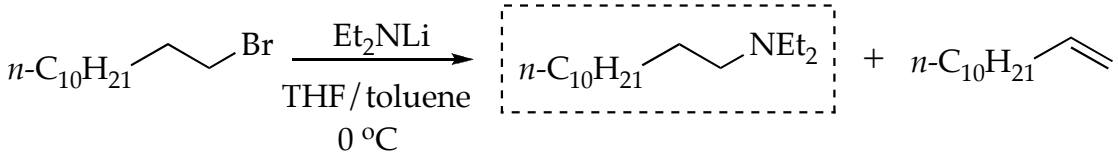
**Part 1: Rate Studies**

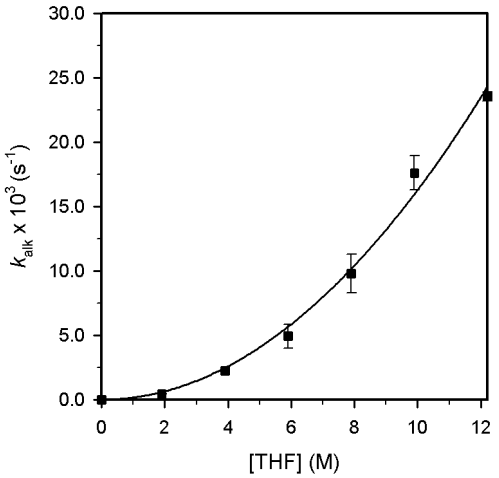



**I.** Plot of $k_{obsd}$ vs [THF] in toluene cosolvent for the reaction of **1** (0.004 M) with $Et_2NLi$ (0.10 M) at 0 °C. The curve depicts an unweighted least-squares fit to $k_{obsd} = k[THF]^n$ ($k = (1.6 \pm 0.4) \times 10^{-4}$, $n = 2.0 \pm 0.1$).

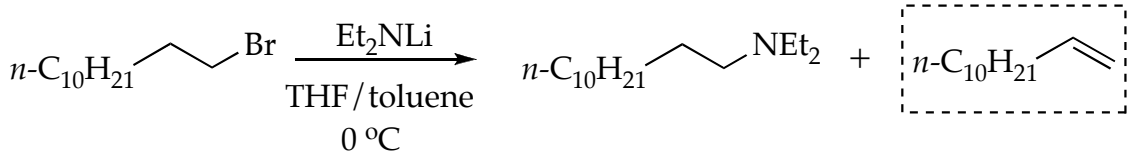
| [THF] (M) | $k_{obsd}1 \times 10^3$ ($s^{-1}$) | $k_{obsd}2 \times 10^3$ ($s^{-1}$) | $k_{obsd}avg \times 10^3$ ($s^{-1}$) |
|---|---|---|---|
| 1.9 | 0.466 ± 8E-3 | 0.47 ± 1E-2 | 0.468 ± 3E-3 |
| 3.9 | 2.24 ± 2E-2 | 2.61 ± 2E-2 | 2.4 ± 3E-1 |
| 5.9 | 4.7 ± 6E-1 | 6.1 ± 3E-1 | 5.4 ± 9E-1 |
| 7.9 | 9.77 ± 7E-2 | 12.3 ± 3E-1 | 11 ± 2 |
| 9.9 | 18.9 ± 9E-1 | 21.1 ± 3E-1 | 20 ± 2 |
| 12.2 | 26.9 ± 1E-1 | 27.7 ± 4E-1 | 27.3 ± 5E-1 |

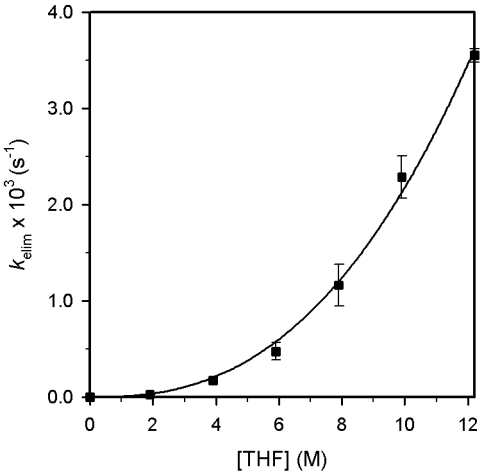



**II.** Plot of $k_{alk}$ vs [THF] in toluene cosolvent for the N-alkylation of **1** (0.004 M) with $Et_2NLi$ (0.10 M) at 0 °C. The curve depicts an unweighted least-squares fit to $k_{alk} = k[THF]^n$ ($k = (1.6 \pm 0.4) \times 10^{-4}$, $n = 2.0 \pm 0.1$).

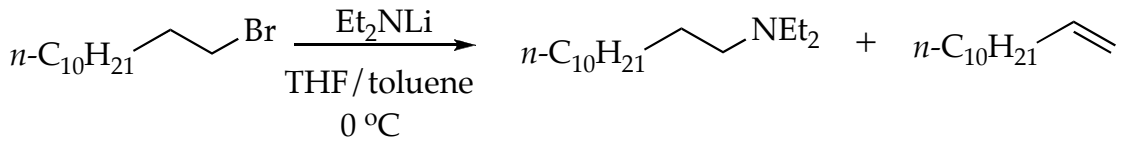
| [THF] (M) | $k_{alk}1 \times 10^3$ ($s^{-1}$) | $k_{alk}2 \times 10^3$ ($s^{-1}$) | $k_{alk}avg \times 10^3$ ($s^{-1}$) |
|---|---|---|---|
| 1.9 | 0.430 ± 4E-3 | 0.441 ± 4E-3 | 0.435 ± 8E-3 |
| 3.9 | 2.062 ± 4E-3 | 2.41 ± 2E-2 | 2.2 ± 2E-1 |
| 5.9 | 4.274 ± 9E-3 | 5.56 ± 4E-2 | 4.9 ± 9E-1 |
| 7.9 | 8.72 ± 1E-2 | 10.87 ± 5E-2 | 10 ± 2 |
| 9.9 | 16.67 ± 5E-2 | 18.54 ± 8E-2 | 18 ± 1 |
| 12.2 | 23.3 ± 4E-1 | 23.8 ± 8E-1 | 23.5 ± 4E-1 |

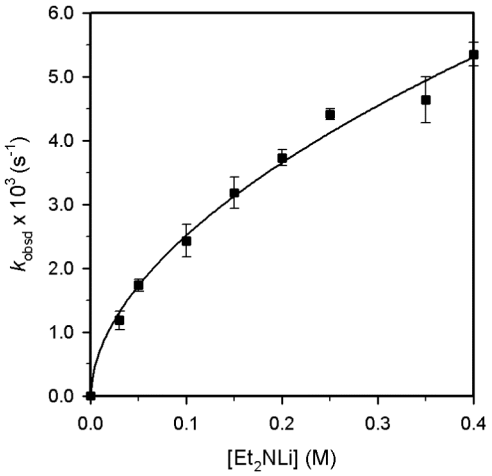



**III.** Plot of $k_{elim}$ vs [THF] in toluene cosolvent for the elimination of **1** (0.004 M) with $Et_2NLi$ (0.10 M) at 0 °C. The curve depicts an unweighted least-squares fit to $k_{elim} = k[THF]^n$ ($k = (6 \pm 2) \times 10^{-6}$, $n = 2.5 \pm 0.1$).

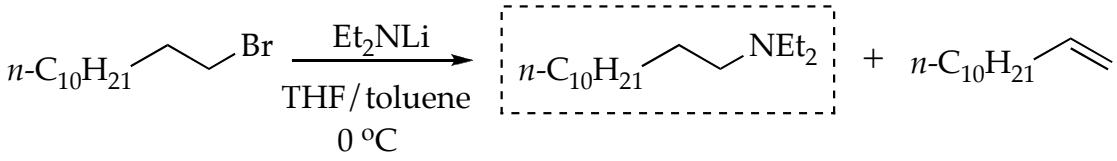
| [THF] (M) | $k_{elim}1 \times 10^3$ ($s^{-1}$) | $k_{elim}2 \times 10^3$ ($s^{-1}$) | $k_{elim}$avg $\times 10^3$ ($s^{-1}$) |
|---|---|---|---|
| 1.9 | 0.026 ± 1E-3 | 0.027 ± 1E-3 | 0.0265 ± 7E-4 |
| 3.9 | 0.162 ± 8E-3 | 0.184 ± 9E-3 | 0.17 ± 2E-2 |
| 5.9 | 0.41 ± 1E-2 | 0.54 ± 3E-2 | 0.47 ± 9E-2 |
| 7.9 | 1.01 ± 1E-2 | 1.313 ± 5E-3 | 1.2 ± 2E-1 |
| 9.9 | 2.13 ± 8E-2 | 2.44 ± 9E-2 | 2.3 ± 2E-1 |
| 12.2 | 3.6 ± 3E-1 | 3.5 ± 2E-1 | 3.55 ± 7E-2 |

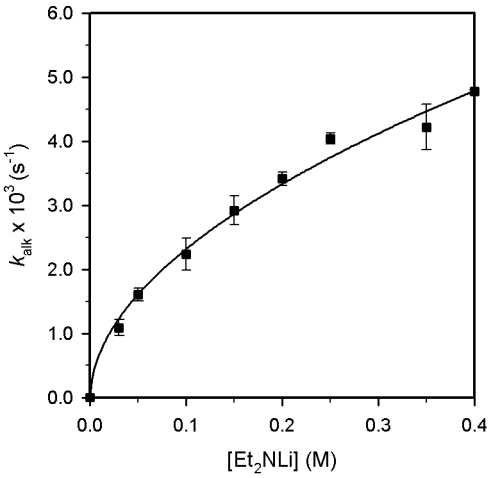



**IV.** Plot of $k_{obsd}$ vs [$Et_2NLi$] in THF (3.9 M) and toluene cosolvent for the reaction of **1** (0.004 M) with $Et_2NLi$ at 0 °C. The curve depicts an unweighted least-squares fit to $k_{obsd} = k[Et_2NLi]^n$ ($k = (8.7 \pm 0.4) \times 10^{-3}$, $n = 0.54 \pm 0.03$).

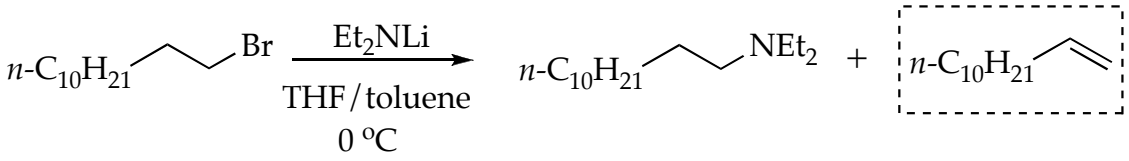
| [$Et_2NLi$] (M) | $k_{obsd}1 \times 10^3$ ($s^{-1}$) | $k_{obsd}2 \times 10^3$ ($s^{-1}$) | $k_{obsd}avg \times 10^3$ ($s^{-1}$) |
|---|---|---|---|
| 0.03 | 1.28 ± 6E-2 | 1.08 ± 5E-2 | 1.2 ± 1E-1 |
| 0.05 | 1.67 ± 3E-2 | 1.80 ± 1E-2 | 1.74 ± 9E-2 |
| 0.10 | 2.24 ± 2E-2 | 2.61 ± 2E-2 | 2.4 ± 3E-1 |
| 0.15 | 3.36 ± 6E-2 | 3.01 ± 7E-2 | 3.2 ± 2E-1 |
| 0.20 | 3.83 ± 8E-2 | 3.64 ± 8E-2 | 3.7 ± 1E-1 |
| 0.25 | 4.35 ± 7E-2 | 4.47 ± 8E-2 | 4.41 ± 8E-2 |
| 0.35 | 4.4 ± 3E-1 | 4.9 ± 1E-1 | 4.6 ± 3E-1 |
| 0.40 | 5.2 ± 1E-1 | 5.5 ± 2E-1 | 5.3 ± 2E-1 |

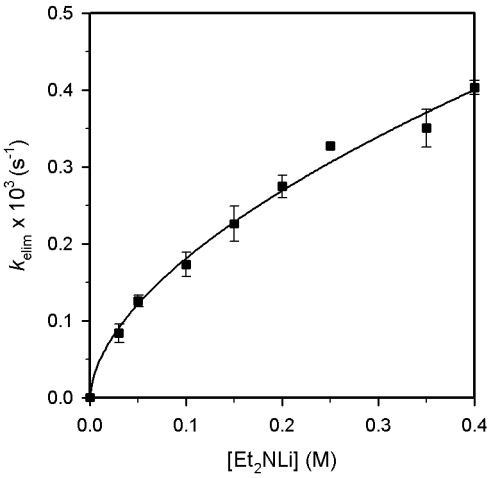



**V.** Plot of $k_{alk}$ vs [$Et_2NLi$] in THF (3.9 M) and toluene cosolvent for the N-alkylation of **1** (0.004 M) with $Et_2NLi$ at 0 °C. The curve depicts an unweighted least-squares fit to $k_{alk} = k[Et_2NLi]^n$ ($k = (7.7 \pm 0.3) \times 10^{-3}$, $n = 0.52 \pm 0.03$).

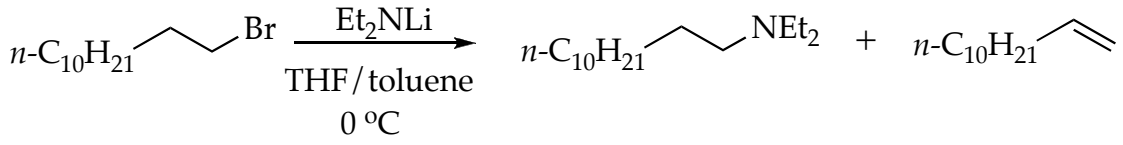
| [$Et_2NLi$] (M) | $k_{alk}1 \times 10^3$ ($s^{-1}$) | $k_{alk}2 \times 10^3$ ($s^{-1}$) | $k_{alk}avg \times 10^3$ ($s^{-1}$) |
|---|---|---|---|
| 0.03 | 1.177 ± 5E-3 | 0.999 ± 5E-3 | 1.1 ± 1E-1 |
| 0.05 | 1.536 ± 8E-3 | 1.680 ± 9E-3 | 1.6 ± 1E-1 |
| 0.10 | 2.062 ± 4E-3 | 2.41 ± 2E-2 | 2.2 ± 2E-1 |
| 0.15 | 3.08± 2E-2 | 2.76 ± 3E-2 | 2.9 ± 2E-1 |
| 0.20 | 3.49 ± 2E-2 | 3.34 ± 1E-2 | 3.4 ± 1E-1 |
| 0.25 | 3.98 ± 2E-2 | 4.10 ± 2E-2 | 4.04 ± 8E-2 |
| 0.35 | 3.97 ± 3E-2 | 4.47 ± 2E-2 | 4.2 ± 4E-1 |
| 0.40 | 4.75 ± 3E-2 | 4.8 ± 4E-1 | 4.77 ± 4E-2 |

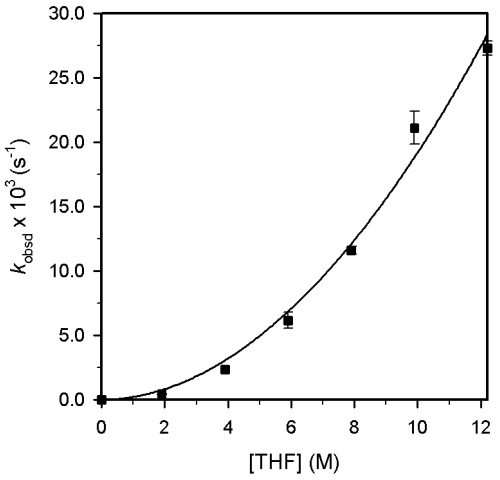



**VI.** Plot of $k_{elim}$ vs [$Et_2NLi$] in THF (3.9 M) and toluene cosolvent for the elimination of **1** with $Et_2NLi$ (0.004 M) at 0 °C. The curve depicts an unweighted least-squares fit to $k_{elim} = k[Et_2NLi]^n$ ($k = (6.8 \pm 0.3) \times 10^{-4}$, $n = 0.57 \pm 0.03$).

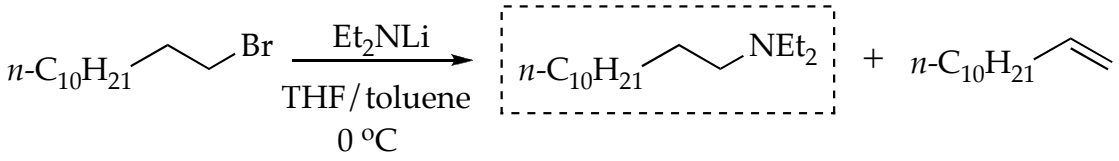
| [$Et_2NLi$] (M) | $k_{elim}1 \times 10^3$ ($s^{-1}$) | $k_{elim}2 \times 10^3$ ($s^{-1}$) | $k_{elim}avg \times 10^3$ ($s^{-1}$) |
|---|---|---|---|
| 0.03 | 0.092 ± 2E-3 | 0.075 ± 4E-3 | 0.08 ± 1E-2 |
| 0.05 | 0.120 ± 1E-3 | 0.131 ± 2E-3 | 0.125 ± 8E-3 |
| 0.10 | 0.162 ± 8E-3 | 0.184 ± 9E-3 | 0.17 ± 2E-2 |
| 0.15 | 0.242 ± 8E-3 | 0.21 ± 1E-2 | 0.23 ± 2E-2 |
| 0.20 | 0.285 ± 1E-3 | 0.264 ± 6E-3 | 0.27 ± 1E-2 |
| 0.25 | 0.325 ± 3E-3 | 0.33 ± 1E-2 | 0.327 ± 3E-3 |
| 0.35 | 0.333 ± 4E-3 | 0.368 ± 4E-3 | 0.35 ± 2E-2 |
| 0.40 | 0.397 ± 2E-3 | 0.41 ± 4E-2 | 0.403 ± 9E-3 |

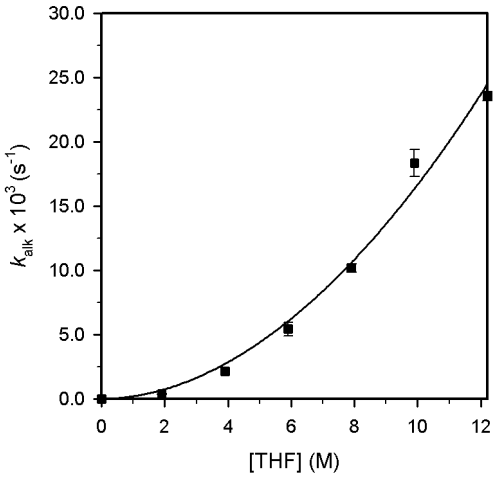



**VII.** Plot of $k_{obsd}$ vs [THF] in 2,2,5,5-$Me_4$THF cosolvent for the reaction of **1** (0.004 M) with $Et_2$NLi (0.10 M) at 0 °C. The curve depicts an unweighted least-squares fit to $k_{obsd} = k[THF]^n$ ($k = (2.1 \pm 0.6) \times 10^{-4}$, $n = 1.9 \pm 0.1$).

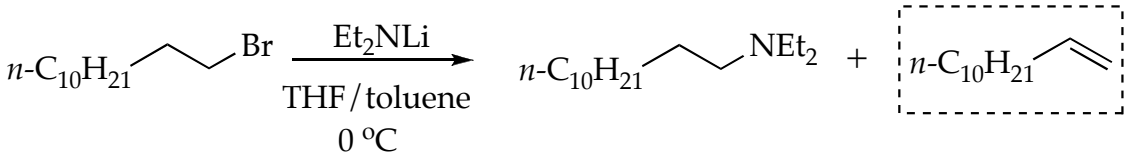
| [THF] (M) | $k_{obsd}1 \times 10^3$ ($s^{-1}$) | $k_{obsd}2 \times 10^3$ ($s^{-1}$) | $k_{obsd}$avg $\times 10^3$ ($s^{-1}$) |
|---|---|---|---|
| 1.9 | 0.39 ± 2E-2 | 0.44 ± 3E-2 | 0.41 ± 4E-2 |
| 3.9 | 2.4 ± 1E-1 | 2.3 ± 2E-1 | 2.35 ± 7E-2 |
| 5.9 | 5.7 ± 2E-1 | 6.6 ± 2E-1 | 6.1 ± 6E-1 |
| 7.9 | 11.8 ± 5E-1 | 11.4 ± 4E-1 | 11.6 ± 3E-1 |
| 9.9 | 22 ± 2 | 20.2 ± 4E-1 | 21 ± 1 |
| 12.2 | 26.9 ± 1E-1 | 27.7 ± 4E-1 | 27.3 ± 5E-1 |

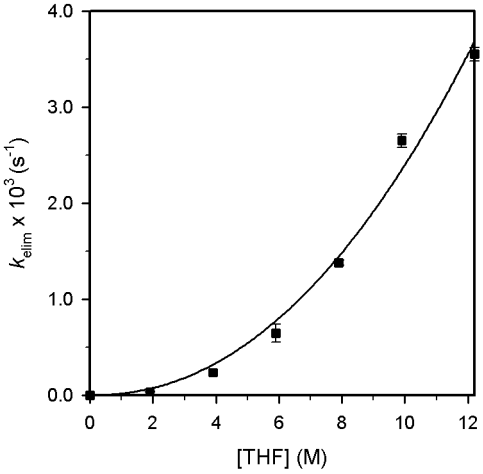



**VIII.** Plot of $k_{alk}$ vs [THF] in 2,2,5,5-tetramethyltetrahydrofuran cosolvent for the N-alkylation of **1** (0.004 M) with $Et_2NLi$ (0.10 M) at 0 °C. The curve depicts an unweighted least-squares fit to $k_{alk} = k[THF]^n$ ($k = (2.0 \pm 0.5) \times 10^{-4}$, $n = 1.9 \pm 0.1$).

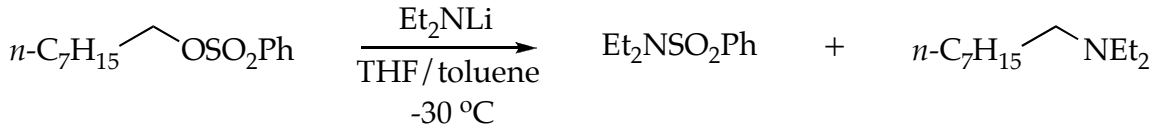
| [THF] (M) | $k_{alk}1 \times 10^3$ ($s^{-1}$) | $k_{alk}2 \times 10^3$ ($s^{-1}$) | $k_{alk}avg \times 10^3$ ($s^{-1}$) |
|---|---|---|---|
| 1.9 | 0.356 ± 6E-3 | 0.395 ± 5E-3 | 0.38 ± 3E-2 |
| 3.9 | 2.18 ± 5E-2 | 2.10 ± 1E-2 | 2.14 ± 6E-2 |
| 5.9 | 5.05 ± 8E-2 | 5.81 ± 5E-2 | 5.4 ± 5E-1 |
| 7.9 | 10.4 ± 1E-1 | 9.93 ± 4E-2 | 10.2 ± 3E-1 |
| 9.9 | 19.1 ± 3E-1 | 17.6 ± 1E-1 | 18 ± 1 |
| 12.2 | 23.3 ± 4E-1 | 23.8 ± 8E-1 | 23.5 ± 4E-1 |

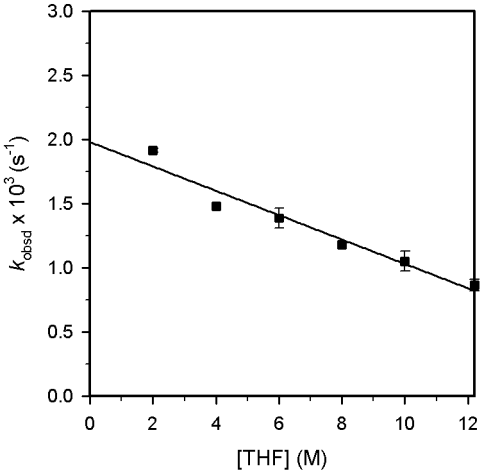



**IX.** Plot of $k_{elim}$ vs [THF] in 2,2,5,5-tetramethyltetrahydrofuran cosolvent for the elimination of **1** (0.004 M) with $Et_2NLi$ (0.10 M) at 0 °C. The curve depicts an unweighted least-squares fit to $k_{elim} = k[THF]^n$ ($k = (1.7 \pm 0.5) \times 10^{-5}$, $n = 2.1 \pm 0.1$).

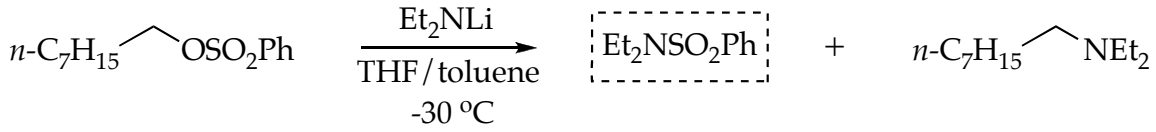
| [THF] (M) | $k_{elim}1 \times 10^3$ ($s^{-1}$) | $k_{elim}2 \times 10^3$ ($s^{-1}$) | $k_{elim}avg \times 10^3$ ($s^{-1}$) |
|---|---|---|---|
| 1.9 | 0.033 ± 4E-3 | 0.036 ± 4E-3 | 0.034 ± 2E-3 |
| 3.9 | 0.23 ± 3E-2 | 0.24 ± 1E-2 | 0.235 ± 7E-3 |
| 5.9 | 0.58 ± 8E-2 | 0.71 ± 5E-2 | 0.64 ± 9E-2 |
| 7.9 | 1.4 ± 1E-1 | 1.36 ± 5E-2 | 1.38 ± 3E-2 |
| 9.9 | 2.7 ± 3E-1 | 2.6 ± 1E-1 | 2.65 ± 7E-2 |
| 12.2 | 3.6 ± 3E-1 | 3.5 ± 2E-1 | 3.55 ± 7E-2 |

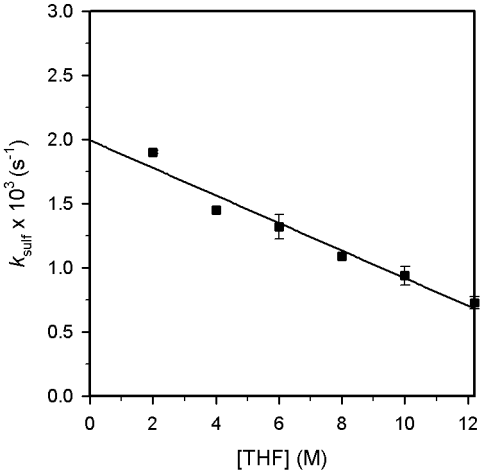



**X.** Plot of $k_{obsd}$ vs [THF] in toluene cosolvent for the reaction of **4** (0.004 M) with $Et_2NLi$ (0.10 M) at -30 °C. The curve depicts an unweighted least-squares fit to $k_{obsd} = c[THF] + k'$ ($c = (-9.5 \pm 0.8) \times 10^{-5}$, $k' = (1.98 \pm 0.06) \times 10^{-3}$).

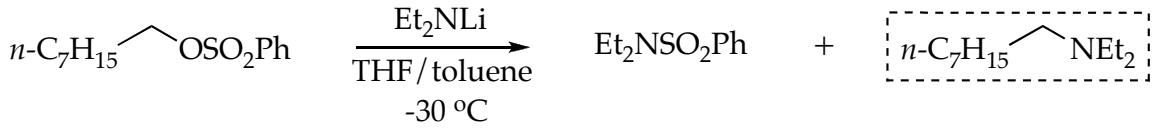
| [THF] (M) | $k_{obsd}1 \times 10^3$ ($s^{-1}$) | $k_{obsd}2 \times 10^3$ ($s^{-1}$) | $k_{obsd}$avg $\times 10^3$ ($s^{-1}$) |
|---|---|---|---|
| 2.0 | 1.90 ± 2E-2 | 1.93 ± 5E-2 | 1.92 ± 2E-2 |
| 4.0 | 1.5 ± 2E-1 | 1.47 ± 2E-2 | 1.49 ± 2E-2 |
| 6.0 | 1.44 ± 4E-2 | 1.31 ± 5E-2 | 1.38 ± 9E-2 |
| 8.0 | 1.17 ± 4E-2 | 1.18 ± 3E-2 | 1.175 ± 7E-3 |
| 10.0 | 1.10 ± 2E-2 | 0.99 ± 2E-2 | 1.05 ± 8E-2 |
| 12.2 | 0.90 ± 3E-2 | 0.83 ± 2E-2 | 0.87 ± 5E-2 |

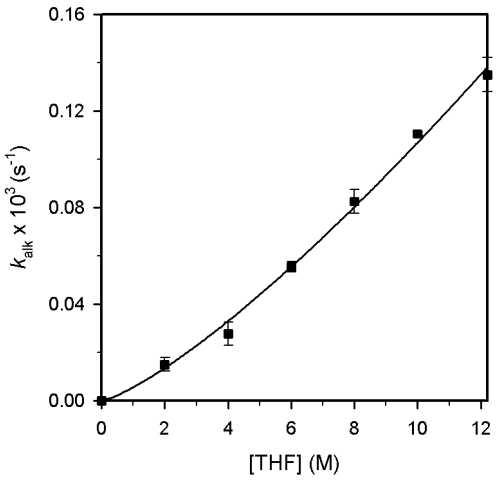



**XI.** Plot of $k_{sulf}$ vs [THF] in toluene cosolvent for the N-sulfonation of **4** (0.004 M) with $Et_2NLi$ (0.10 M) at -30 °C. The curve depicts an unweighted least-squares fit to $k_{obsd} = c[THF] + k'$ ($c = (-1.07 \pm 0.08) \times 10^{-4}$, $k' = (1.99 \pm 0.06) \times 10^{-3}$).

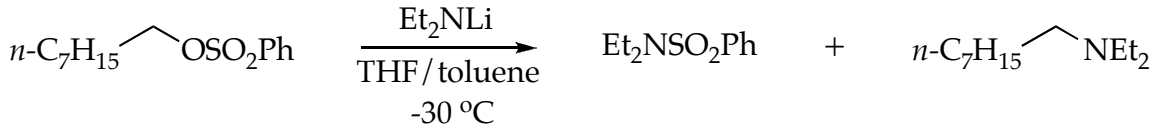
| [THF] (M) | $k_{sulf}1 \times 10^3$ ($s^{-1}$) | $k_{sulf}2 \times 10^3$ ($s^{-1}$) | $k_{sulf}avg \times 10^3$ ($s^{-1}$) |
|---|---|---|---|
| 2.0 | 1.892 ± 1E-3 | 1.9093 ± 8E-4 | 1.90 ± 1E-2 |
| 4.0 | 1.458 ± 1E-3 | 1.442 ± 2E-3 | 1.455 ± 4E-3 |
| 6.0 | 1.388 ± 4E-3 | 1.253 ± 3E-3 | 1.32 ± 9E-2 |
| 8.0 | 1.095 ± 8E-3 | 1.08 ± 4E-2 | 1.09 ± 1E-2 |
| 10.0 | 0.99 ± 1E-2 | 0.886 ± 8E-3 | 0.94 ± 7E-2 |
| 12.2 | 0.76 ± 1E-2 | 0.69 ± 1E-2 | 0.73 ± 5E-2 |

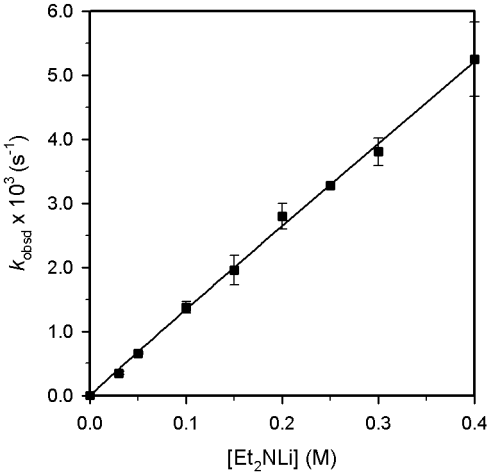



**XII.** Plot of $k_{alk}$ vs [THF] in toluene cosolvent for the N-alkylation of **4** (0.004 M) with $Et_2NLi$ (0.10 M) at -30 °C. The curve depicts an unweighted least-squares fit to $k_{alk} = k[THF]^n$ ($k = (5.5 \pm 0.7) \times 10^{-6}$, $n = 1.29 \pm 0.05$).

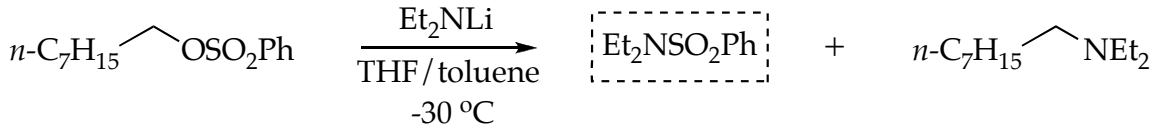
| [THF] (M) | $k_{alk}1 \times 10^3$ ($s^{-1}$) | $k_{alk}2 \times 10^3$ ($s^{-1}$) | $k_{alk}$avg $\times 10^3$ ($s^{-1}$) |
|---|---|---|---|
| 2.0 | 0.013 ± 1E-3 | 0.017 ± 1E-3 | 0.015 ± 3E-3 |
| 4.0 | 0.0243 ± 7E-4 | 0.031 ± 3E-3 | 0.028 ± 5E-3 |
| 6.0 | 0.054 ± 4E-3 | 0.057 ± 3E-3 | 0.055 ± 2E-3 |
| 8.0 | 0.079 ± 8E-3 | 0.086 ± 5E-3 | 0.083 ± 5E-3 |
| 10.0 | 0.11 ± 1E-2 | 0.111 ± 8E-3 | 0.1105 ± 7E-4 |
| 12.2 | 0.13 ± 1E-2 | 0.14 ± 1E-2 | 0.135 ± 7E-3 |

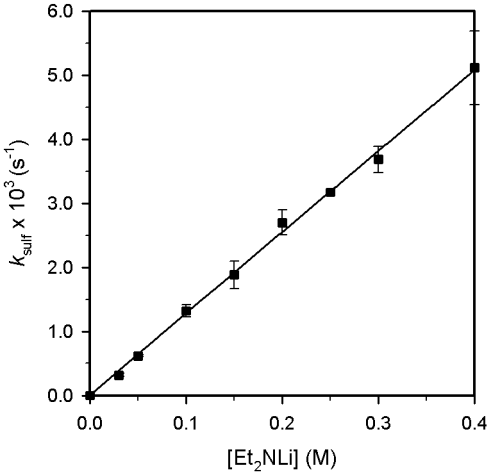



**XIII.** Plot of $k_{obsd}$ vs [$Et_2NLi$] in THF (6.0 M) and toluene cosolvent for the reaction of **4** (0.004 M) with $Et_2NLi$ at -30 °C. The curve depicts an unweighted least-squares fit to $k_{obsd} = k[Et_2NLi]^n$ ($k = (1.28 \pm 0.07) \times 10^{-2}$, $n = 0.98 \pm 0.04$).

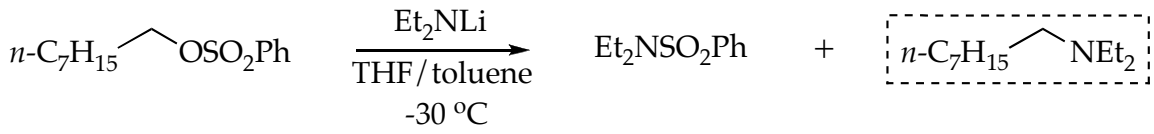
| [$Et_2NLi$] (M) | $k_{obsd}1 \times 10^3$ ($s^{-1}$) | $k_{obsd}2 \times 10^3$ ($s^{-1}$) | $k_{obsd}avg \times 10^3$ ($s^{-1}$) |
|---|---|---|---|
| 0.03 | 0.329 ± 6E-3 | 0.364 ± 7E-3 | 0.35 ± 2E-2 |
| 0.05 | 0.667 ± 9E-3 | 0.65 ± 2E-2 | 0.66 ± 1E-2 |
| 0.10 | 1.44 ± 4E-2 | 1.31 ± 5E-2 | 1.38 ± 9E-2 |
| 0.15 | 2.12 ± 6E-2 | 1.79 ± 7E-2 | 2.0 ± 2E-1 |
| 0.20 | 2.94 ± 6E-2 | 2.66 ± 3E-2 | 2.8 ± 2E-1 |
| 0.25 | 3.27 ± 6E-2 | 3.29 ± 7E-2 | 3.28 ± 1E-2 |
| 0.35 | 3.95 ± 5E-2 | 3.7 ± 1E-1 | 3.8 ± 2E-1 |
| 0.40 | 5.7 ± 1E-1 | 4.84 ± 9E-2 | 5.3 ± 6E-1 |

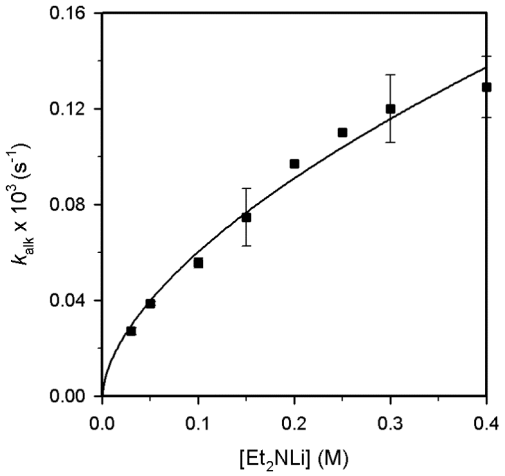



**XIV.** Plot of $k_{sulf}$ vs [$Et_2NLi$] in THF (6.0 M) and toluene cosolvent for the N-sulfonation of **4** (0.004 M) with $Et_2NLi$ at -30 °C. The curve depicts an unweighted least-squares fit to $k_{sulf} = k[Et_2NLi]^n$ ($k = (1.26 \pm 0.07) \times 10^{-2}$, $n = 0.99 \pm 0.04$).

| [$Et_2NLi$] (M) | $k_{sulf}1 \times 10^3$ ($s^{-1}$) | $k_{sulf}2 \times 10^3$ ($s^{-1}$) | $k_{sulf}avg \times 10^3$ ($s^{-1}$) |
|---|---|---|---|
| 0.03 | 0.303 ± 6E-3 | 0.336 ± 2E-3 | 0.32 ± 2E-2 |
| 0.05 | 0.628 ± 2E-3 | 0.610 ± 3E-3 | 0.62 ± 1E-2 |
| 0.10 | 1.388 ± 4E-3 | 1.253 ± 3E-3 | 1.3 ± 1E-1 |
| 0.15 | 1.728 ± 3E-3 | 2.036 ± 6E-3 | 1.9 ± 2E-1 |
| 0.20 | 2.838 ± 7E-3 | 2.561 ± 9E-3 | 2.7 ± 2E-1 |
| 0.25 | 3.163 ± 7E-3 | 3.18 ± 1E-2 | 3.17 ± 1E-2 |
| 0.35 | 3.83 ± 1E-2 | 3.54 ± 2E-2 | 3.7 ± 2E-1 |
| 0.40 | 5.521 ± 5E-3 | 4.71 ± 1E-2 | 5.1 ± 6E-1 |

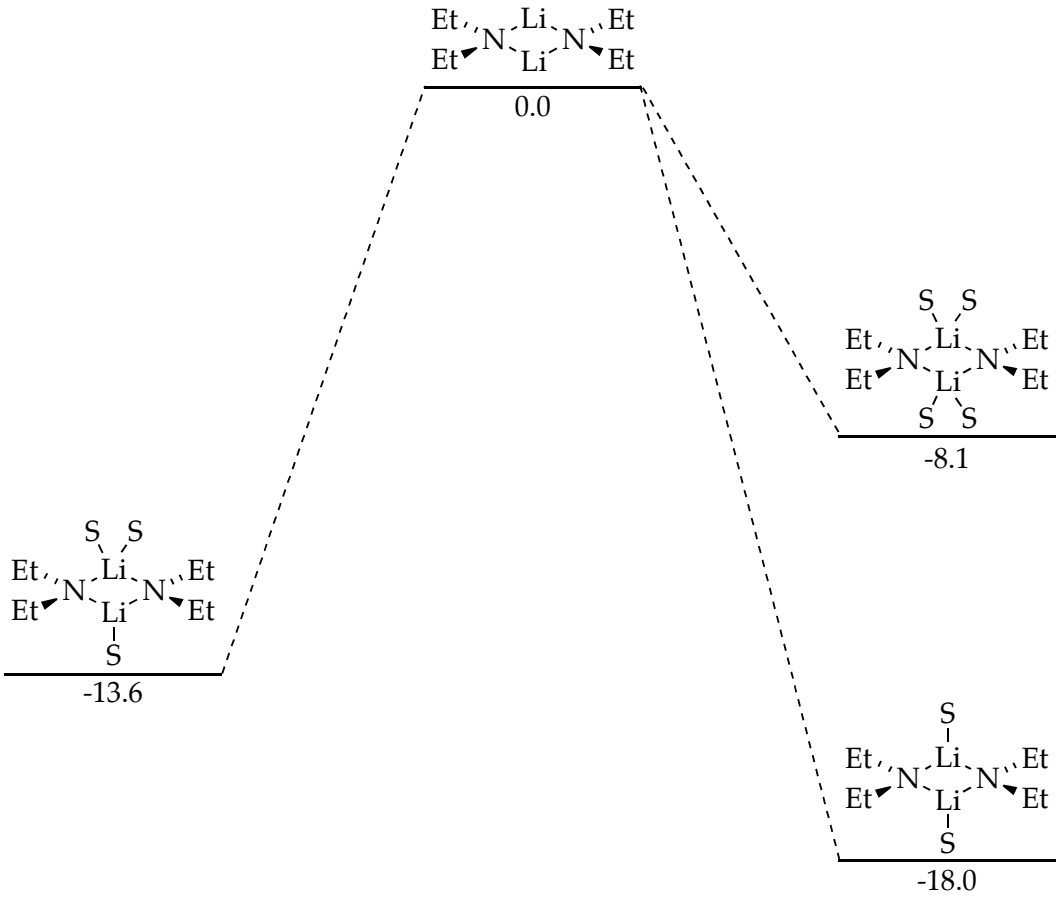



**XV.** Plot of $k_{alk}$ vs [$Et_2NLi$] in THF (6.0 M) and toluene cosolvent for the N-alkylation of **4** (0.004 M) with $Et_2NLi$ at -30 °C. The curve depicts an unweighted least-squares fit to $k_{alk} = k[Et_2NLi]^n$ ($k = (2.4 \pm 0.1) \times 10^{-4}$, $n = 0.59 \pm 0.04$).

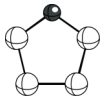
| [$Et_2NLi$] (M) | $k_{alk}1 \times 10^3$ ($s^{-1}$) | $k_{alk}2 \times 10^3$ ($s^{-1}$) | $k_{alk}avg \times 10^3$ ($s^{-1}$) |
|---|---|---|---|
| 0.03 | 0.026 ± 2E-3 | 0.028 ± 2E-3 | 0.027 ± 1E-3 |
| 0.05 | 0.039 ± 2E-3 | 0.038 ± 3E-3 | 0.0385 ± 7E-4 |
| 0.10 | 0.054 ± 4E-3 | 0.057 ± 3E-3 | 0.055 ± 2E-3 |
| 0.15 | 0.083 ± 6E-3 | 0.066 ± 3E-3 | 0.07 ± 1E-2 |
| 0.20 | 0.098 ± 7E-3 | 0.096 ± 8E-3 | 0.097 ± 1E-3 |
| 0.25 | 0.110 ± 7E-3 | 0.11 ± 1E-2 | 0.11 ± 0 |
| 0.35 | 0.13 ± 1E-2 | 0.11 ± 2E-2 | 0.12 ± 1E-2 |
| 0.40 | 0.138 ± 5E-3 | 0.12 ± 1E-2 | 0.13 ± 1E-20.40 |

**Part 2: DFT Computational Studies**



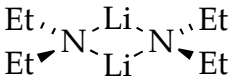

**XVI.** Relative free energies for the solvation ($\Delta G$, kcal/mol) of $Et_2NLi$ with THF (S = THF) calculated using B3LYP level of theory with 6-31G(d) basis set at -90 °C.

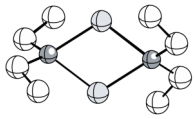
**Table I.** Optimized geometries at B3LYP level of theory with 6-31G(d) basis set for the serial solvation of $Et_2NLi$ with THF with free energies (*G*, Hartrees) and cartesian coordinates (X, Y, Z) at -90 °C.

*G* = -232.347930
(-90 °C)

| Atom | X | Y | Z | Atom | X | Y | Z |
|---|---|---|---|---|---|---|---|
| C | 1.13237 | -0.69946 | 0.08092 | | | | |
| O | 0.00023 | -1.43271 | -0.37154 | H | -1.16402 | 1.14915 | -1.08500 |
| C | -1.13196 | -0.69994 | 0.08150 | H | -1.20089 | 1.42136 | 0.65927 |
| C | -0.77738 | 0.78865 | -0.12699 | H | -1.99944 | -1.03696 | -0.49266 |
| C | 0.77682 | 0.78920 | -0.12622 | H | -1.31932 | -0.90804 | 1.14890 |
| H | 1.19899 | 1.42114 | 0.66137 | H | 1.32083 | -0.90816 | 1.14799 |
| H | 1.16423 | 1.15136 | -1.08328 | H | 1.99953 | -1.03559 | -0.49425 |

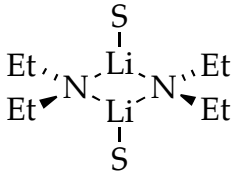


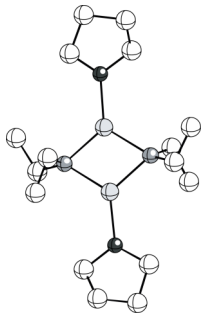



*G* = -441.267084
(-90 °C)
S = THF

| Atom | X | Y | Z | Atom | X | Y | Z |
|---|---|---|---|---|---|---|---|
| N | -1.61287 | 0.00001 | -0.00000 | H | 3.02647 | 1.56976 | 0.33251 |
| C | -2.46755 | 1.07535 | 0.48941 | H | 0.90588 | -2.60145 | 0.63673 |
| C | -1.69571 | 2.15553 | 1.25365 | H | 2.35926 | -2.96537 | 1.57759 |
| Li | 0.00000 | 0.00004 | 1.12061 | H | 1.22889 | -1.75324 | 2.16919 |
| Li | -0.00000 | -0.00005 | -1.12062 | H | 3.02634 | -1.56989 | -0.33256 |
| N | 1.61287 | -0.00001 | -0.00000 | H | 3.25304 | -0.68494 | 1.16895 |
| C | 2.46753 | -1.07538 | 0.48941 | H | -0.90596 | 2.60150 | 0.63662 |
| C | 1.69568 | -2.15550 | 1.25371 | H | -2.35931 | 2.96537 | 1.57755 |
| C | 2.46757 | 1.07532 | -0.48944 | H | -1.22885 | 1.75331 | 2.16911 |
| C | 1.69574 | 2.15552 | -1.25364 | H | -3.25302 | 0.68491 | 1.16900 |
| C | -2.46754 | -1.07536 | -0.48940 | H | -3.02641 | 1.56983 | -0.33255 |
| C | -1.69571 | -2.15549 | -1.25370 | H | -0.90591 | -2.60145 | -0.63672 |
| H | 0.90603 | 2.60152 | -0.63657 | H | -2.35930 | -2.96536 | -1.57756 |
| H | 2.35936 | 2.96534 | -1.57756 | H | -1.22893 | -1.75325 | -2.16919 |
| H | 1.22882 | 1.75333 | -2.16909 | H | -3.02635 | -1.56986 | 0.33258 |
| H | 3.25301 | 0.68486 | -1.16906 | H | -3.25306 | -0.68492 | -1.16894 |

**Table I (Continued).**

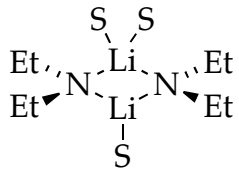


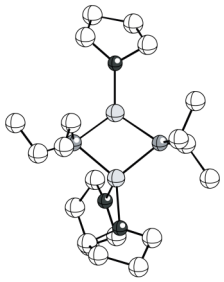



*G* = -905.991622
(-90 °C)
S = THF

| Atom | X | Y | Z | Atom | X | Y | Z |
|---|---|---|---|---|---|---|---|
| Li | -1.18777 | 0.06068 | 0.28533 | H | -4.31804 | -1.26059 | 1.37174 |
| O | -3.13515 | 0.09835 | 0.32686 | H | 1.63650 | -2.33786 | 2.35094 |
| C | -3.93036 | -1.10699 | 0.35496 | H | 0.70633 | -3.78915 | 2.78884 |
| C | -5.05997 | -0.85054 | -0.63873 | H | 1.52137 | -3.69860 | 1.21942 |
| C | -5.33666 | 0.64549 | -0.41423 | H | -0.79856 | -1.90558 | 2.14451 |
| C | -3.93586 | 1.21372 | -0.14016 | H | -0.99553 | -3.29638 | 1.09158 |
| N | -0.05931 | -1.57116 | 0.21754 | H | -1.71750 | -2.10320 | -2.01764 |
| C | -0.29581 | -2.47179 | 1.34046 | H | -0.72328 | -3.43569 | -2.64814 |
| C | 0.96399 | -3.11338 | 1.96112 | H | -1.54100 | -3.60366 | -1.08680 |
| Li | 1.18894 | -0.02177 | 0.30402 | H | 0.95375 | -3.11012 | -0.88752 |
| N | 0.06100 | 1.60870 | 0.21578 | H | 0.69058 | -1.59355 | -1.73619 |
| C | -0.18840 | 2.34544 | -1.01760 | H | 1.75857 | 2.14874 | -1.98835 |
| C | 1.05745 | 2.94511 | -1.70510 | H | 0.79061 | 3.50229 | -2.61432 |
| C | 0.27921 | 2.49471 | 1.35429 | H | 1.58572 | 3.63743 | -1.03801 |
| C | -0.99155 | 3.12866 | 1.96027 | H | -0.91802 | 3.17120 | -0.88589 |
| O | 3.13588 | -0.09082 | 0.36686 | H | -0.65885 | 1.66261 | -1.74909 |
| C | 3.89889 | -1.24096 | -0.08044 | H | -1.67167 | 2.34810 | 2.32621 |
| C | 5.30425 | -0.71593 | -0.41239 | H | -0.74959 | 3.79271 | 2.80212 |
| C | 5.05788 | 0.77933 | -0.67445 | H | -1.53460 | 3.72410 | 1.21608 |
| C | 3.96288 | 1.09306 | 0.34106 | H | 0.76763 | 1.91822 | 2.16005 |
| C | 0.21684 | -2.29063 | -1.02016 | H | 0.98351 | 3.32171 | 1.12792 |
| C | -1.01112 | -2.89521 | -1.73530 | H | 4.38168 | 1.26361 | 1.34272 |
| H | -3.92719 | 1.99626 | 0.62396 | H | 3.31840 | 1.93291 | 0.07409 |
| H | -3.46236 | 1.60756 | -1.04637 | H | 4.68567 | 0.93890 | -1.69333 |
| H | -5.98500 | 0.78352 | 0.45872 | H | 5.95164 | 1.39484 | -0.53534 |
| H | -5.81829 | 1.12910 | -1.26910 | H | 5.97518 | -0.84401 | 0.44487 |
| H | -4.71156 | -1.03135 | -1.66249 | H | 5.74816 | -1.23679 | -1.26577 |
| H | -5.93376 | -1.48331 | -0.45681 | H | 3.39120 | -1.65621 | -0.95786 |
| H | -3.27104 | -1.93688 | 0.09340 | H | 3.89409 | -1.99491 | 0.71188 |

**Table I (Continued).**

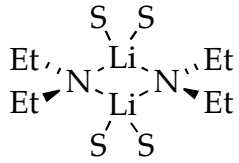


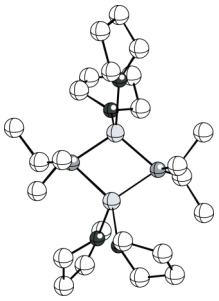



*G* = -1138.332641
(-90 °C)
S = THF

| Atom | X | Y | Z | Atom | X | Y | Z |
|---|---|---|---|---|---|---|---|
| Li | -0.94920 | -0.00381 | -0.07959 | H | -0.78821 | -2.61715 | -2.30553 |
| N | 0.27495 | -0.98090 | -1.39758 | H | 1.87701 | 1.88838 | 2.49866 |
| Li | 1.37298 | -0.54130 | 0.18531 | H | 1.00022 | 2.24242 | 4.00533 |
| N | 0.12940 | -0.18560 | 1.66686 | H | 1.79118 | 0.67317 | 3.78720 |
| C | 0.37453 | -1.46238 | 2.33171 | H | -0.73663 | 0.60003 | 3.46325 |
| C | -0.86781 | -2.18048 | 2.90219 | H | -0.57707 | 1.72279 | 2.12749 |
| C | -0.06307 | 0.88775 | 2.62904 | H | -1.56954 | -2.42586 | 2.09554 |
| C | 1.22354 | 1.45633 | 3.26931 | H | -0.59457 | -3.11439 | 3.41367 |
| O | 3.32654 | -0.45501 | 0.14205 | H | -1.39329 | -1.54797 | 3.62800 |
| C | 4.12112 | -0.69095 | -1.03189 | H | 0.83139 | -2.16738 | 1.60961 |
| C | 5.28241 | 0.30647 | -0.91374 | H | 1.11435 | -1.38508 | 3.15656 |
| C | 5.44457 | 0.50359 | 0.61987 | H | 4.56691 | -1.25458 | 1.59989 |
| C | 4.25315 | -0.27002 | 1.22485 | H | 3.72304 | 0.25949 | 2.01769 |
| C | -0.02991 | -2.40140 | -1.52332 | H | 5.40131 | 1.56407 | 0.88408 |
| C | 1.16969 | -3.33821 | -1.79342 | H | 6.39626 | 0.11091 | 0.99003 |
| C | 0.62749 | -0.37252 | -2.67061 | H | 6.19210 | -0.06949 | -1.39113 |
| C | -0.52171 | -0.19770 | -3.68871 | H | 5.01933 | 1.25232 | -1.39716 |
| O | -1.07618 | 2.03525 | -0.49963 | H | 3.47540 | -0.54530 | -1.89872 |
| C | 0.03218 | 2.94259 | -0.49555 | H | 4.47962 | -1.73070 | -1.02373 |
| C | -0.58786 | 4.34308 | -0.31080 | H | -3.04801 | 2.17224 | -1.00884 |
| C | -2.06273 | 4.15787 | -0.76749 | H | -1.91147 | 2.60964 | -2.31116 |
| C | -2.11547 | 2.69192 | -1.23268 | H | -2.34729 | 4.84723 | -1.56822 |
| O | -2.97519 | -0.32433 | -0.08058 | H | -2.74807 | 4.32028 | 0.06991 |
| C | -3.59671 | -1.33301 | -0.91264 | H | -0.54249 | 4.65395 | 0.73685 |
| C | -4.92108 | -1.68235 | -0.22649 | H | -0.05752 | 5.09514 | -0.90288 |
| C | -4.59822 | -1.42133 | 1.25322 | H | 0.56719 | 2.86732 | -1.45403 |
| C | -3.69310 | -0.19216 | 1.16746 | H | 0.70060 | 2.63599 | 0.31095 |
| H | -0.16985 | 0.29024 | -4.60898 | H | -2.92457 | -2.19602 | -0.97161 |
| H | -0.95794 | -1.16142 | -3.97658 | H | -3.71961 | -0.92119 | -1.91870 |
| H | -1.32388 | 0.41500 | -3.25814 | H | -5.72054 | -1.01286 | -0.56648 |
| H | 1.03444 | 0.63333 | -2.46775 | H | -5.23404 | -2.71138 | -0.42743 |
| H | 1.44391 | -0.90812 | -3.20473 | H | -4.04804 | -2.26728 | 1.68076 |
| H | 1.90804 | -3.26430 | -0.98321 | H | -5.48654 | -1.24580 | 1.86771 |
| H | 0.84968 | -4.38728 | -1.86544 | H | -4.28077 | 0.73645 | 1.14157 |
| H | 1.67899 | -3.08610 | -2.73139 | H | -2.95372 | -0.12612 | 1.96877 |
| H | -0.49163 | -2.73601 | -0.57884 | | | | |

**Table I (Continued).**

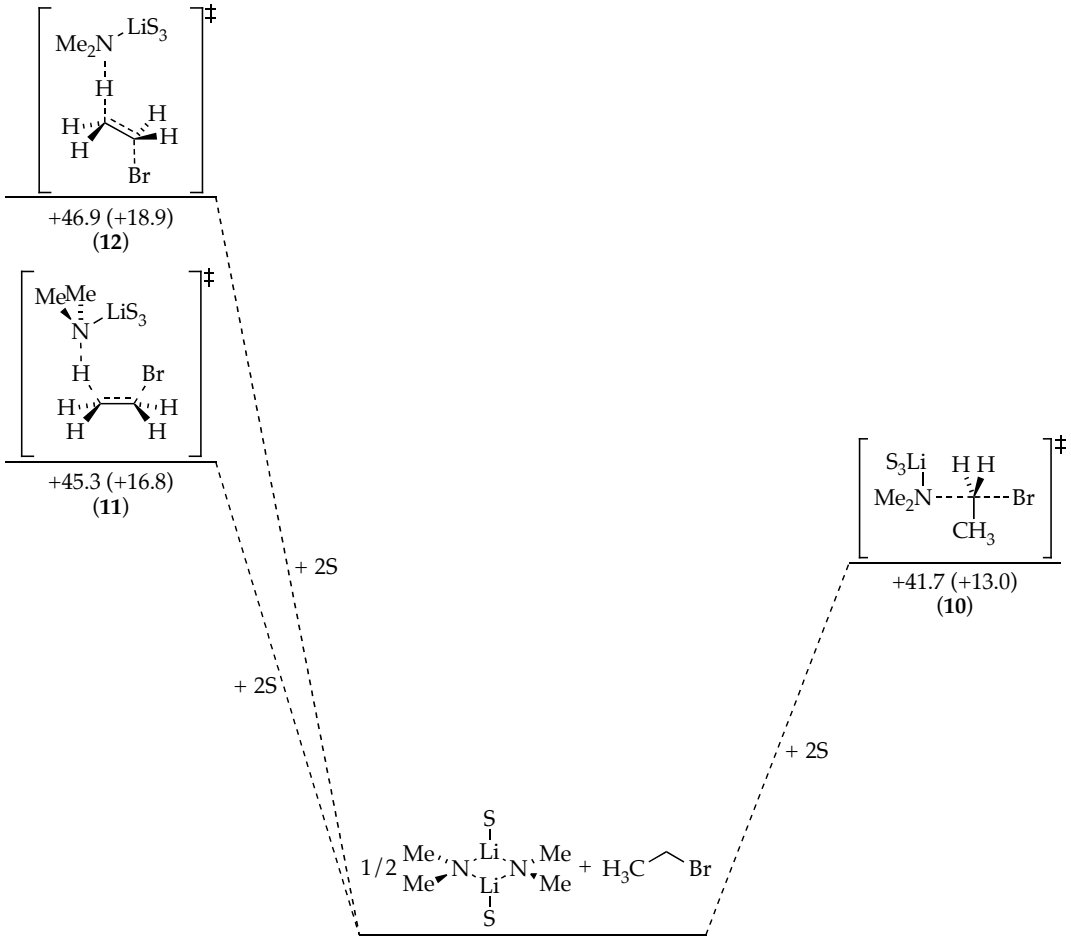


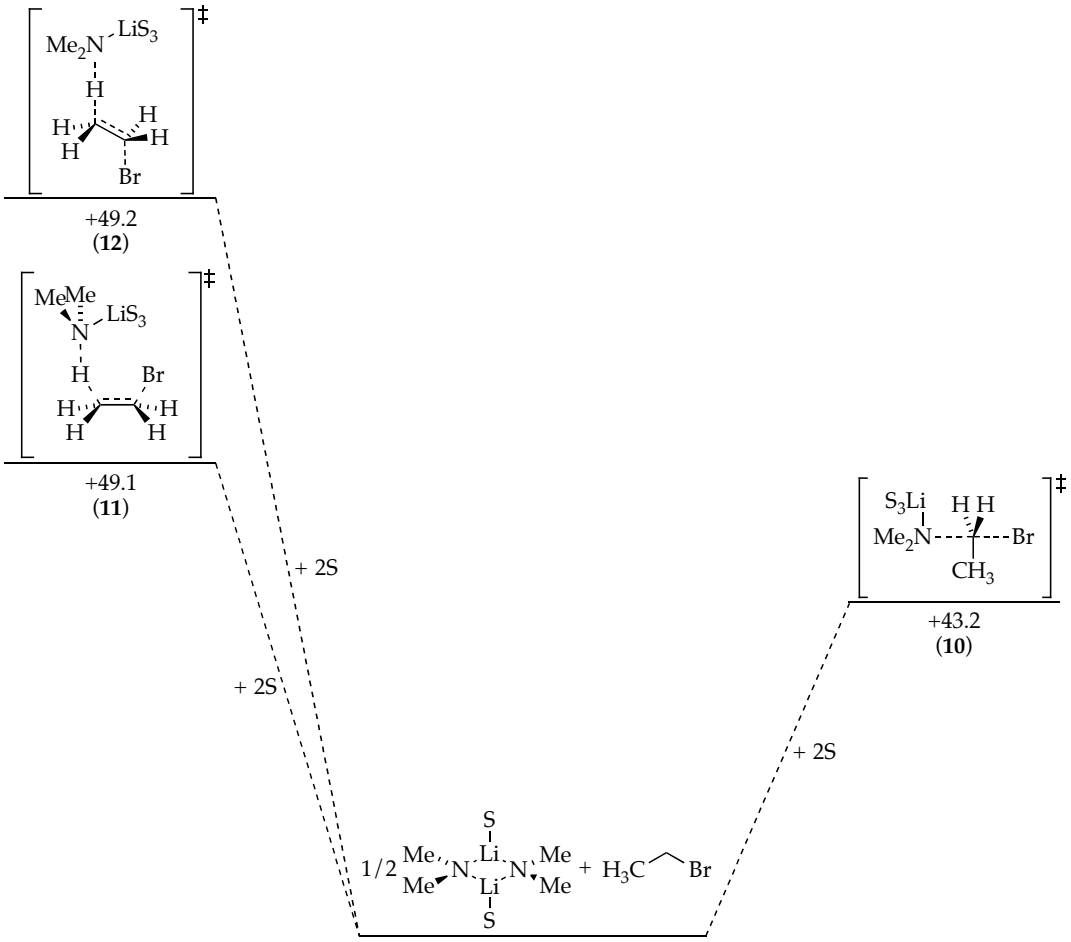
*G* = -1370.6717
(-90 °C)
S = THF

| Atom | X | Y | Z | Atom | X | Y | Z |
|---|---|---|---|---|---|---|---|
| Li | -1.359791 | -0.098372 | 0.191622 | H | -1.321498 | -2.293238 | -2.256459 |
| O | -3.217047 | -1.210572 | 0.397360 | C | -0.377995 | 0.232500 | -2.676346 |
| C | -4.337971 | -0.927040 | -0.450352 | C | -1.725832 | 0.196124 | -3.434224 |
| C | -4.434289 | -2.127537 | -1.401245 | H | -2.550328 | 0.491711 | -2.772104 |
| C | -3.845975 | -3.297413 | -0.567524 | H | -1.715138 | 0.878509 | -4.296330 |
| C | -3.301297 | -2.611138 | 0.704314 | H | -1.952085 | -0.805765 | -3.818208 |
| H | -3.983589 | -2.752383 | 1.555471 | H | 0.408233 | 0.008787 | -3.432593 |
| H | -2.304016 | -2.940680 | 0.998088 | H | -0.200494 | 1.281030 | -2.390470 |
| H | -3.044598 | -3.797741 | -1.116797 | Li | 1.138431 | -0.194024 | -0.042566 |
| H | -4.600503 | -4.049148 | -0.315258 | N | 0.037107 | -0.170738 | 1.688633 |
| H | -3.823416 | -1.947162 | -2.289408 | C | -0.088212 | -1.387553 | 2.476318 |
| H | -5.463073 | -2.311336 | -1.726521 | C | -1.246273 | -1.439331 | 3.499506 |
| H | -4.139309 | 0.026560 | -0.940928 | H | -2.204576 | -1.220749 | 3.012929 |
| H | -5.246707 | -0.833579 | 0.166461 | H | -1.312779 | -2.429280 | 3.972422 |
| O | -2.434710 | 1.706636 | 0.182689 | H | -1.109531 | -0.704846 | 4.302132 |
| C | -3.114418 | 2.082125 | 1.390392 | H | -0.225856 | -2.228521 | 1.774791 |
| C | -3.922970 | 3.324036 | 0.997058 | H | 0.833746 | -1.646670 | 3.045906 |
| C | -3.034344 | 3.998238 | -0.082291 | C | 0.255029 | 0.999827 | 2.523543 |
| C | -1.963875 | 2.927875 | -0.406336 | C | 1.504786 | 0.983202 | 3.434584 |
| H | -0.992205 | 3.191025 | 0.034471 | H | 2.410430 | 0.763711 | 2.855003 |
| H | -1.826840 | 2.741067 | -1.472752 | H | 1.640298 | 1.950404 | 3.939317 |
| H | -2.567482 | 4.916054 | 0.288465 | H | 1.425212 | 0.219102 | 4.216693 |
| H | -3.619406 | 4.263335 | -0.967757 | H | -0.603112 | 1.236852 | 3.192893 |
| H | -4.887028 | 3.027767 | 0.570869 | H | 0.339906 | 1.875191 | 1.856919 |
| H | -4.121705 | 3.976694 | 1.852548 | O | 2.290044 | 1.575799 | -0.527879 |
| H | -3.712401 | 1.225919 | 1.706508 | C | 2.469544 | 2.110300 | -1.854368 |
| H | -2.377138 | 2.309426 | 2.172402 | C | 3.810777 | 2.841882 | -1.819539 |
| N | -0.275394 | -0.576863 | -1.474904 | C | 3.815250 | 3.405044 | -0.390124 |
| C | -0.370517 | -2.002519 | -1.756768 | C | 3.133601 | 2.284795 | 0.407258 |
| C | 0.767824 | -2.623767 | -2.598026 | H | 2.514708 | 2.654083 | 1.228943 |
| H | 1.736406 | -2.444717 | -2.116599 | H | 3.861345 | 1.573815 | 0.817222 |
| H | 0.630858 | -3.708692 | -2.711096 | H | 3.221214 | 4.325566 | -0.345579 |
| H | 0.812280 | -2.194049 | -3.605935 | H | 4.816952 | 3.634131 | -0.014057 |
| H | -0.384637 | -2.535881 | -0.790636 | H | 4.638886 | 2.135838 | -1.959276 |

| | | | |
|---|---|---|---|
| H | 3.889903 | 3.613324 | -2.591678 |
| H | 2.423642 | 1.279050 | -2.561099 |
| H | 1.648435 | 2.803244 | -2.083596 |
| O | 2.914938 | -1.363211 | 0.099491 |
| C | 2.995366 | -2.591651 | 0.836347 |
| C | 4.479383 | -2.730050 | 1.225181 |
| C | 5.221562 | -1.871666 | 0.162513 |
| C | 4.084236 | -1.327604 | -0.723580 |
| H | 4.221114 | -0.296003 | -1.051552 |
| H | 3.931947 | -1.964057 | -1.608263 |
| H | 5.767863 | -1.052265 | 0.639909 |
| H | 5.942054 | -2.452686 | -0.421341 |
| H | 4.652969 | -2.335304 | 2.230564 |
| H | 4.800894 | -3.775956 | 1.219784 |
| H | 2.674566 | -3.422808 | 0.190486 |
| H | 2.311550 | -2.509559 | 1.680801 |

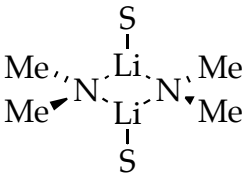


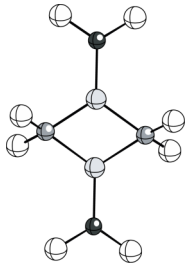

**XVII.** Free energies of activation ($\Delta G^{\ddagger}$, kcal/mol) for the reaction of EtBr with $Me_2NLi$ calculated using B3LYP level of theory with SVP basis set for Br and 6-31G(d) basis set for the rest of atoms at 25 °C (S = $Me_2O$). Values in parentheses correspond to the enthalpies of activation ($\Delta H^{\ddagger}$, kcal/mol).




**XVIII.** Free energies of activation ($\Delta G^{\ddagger}$, kcal/mol) for the reaction of EtBr with $Me_2NLi$ calculated using single point MP2 corrections to B3LYP/6-31G(d)-SVP optimized structures at 25 °C (S = $Me_2O$).

**Table II.** Optimized geometries of reactants and transition structures calculated at B3LYP level of theory using SVP basis set for Br and 6-31G(d) basis set for the rest of atoms, for the reaction of EtBr with $Me_2NLi$, with free energies (*G*, Hartrees), enthalpies (*H*, Hartrees), and cartesian coordinates (X,Y,Z) at 25 °C. (Note: $G_{MP2}$ includes single point MP2 corrections to B3LYP/6-31G(d)-SVP optimized structures)

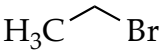


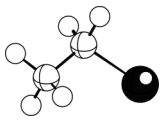



*G* = -594.095723
*H* = -594.012498
$G_{MP2}$ = -591.9718824
S = $Me_2O$

| Atom | X | Y | Z | Atom | X | Y | Z |
|---|---|---|---|---|---|---|---|
| N | -0.00029 | 1.58912 | 0.00241 | H | 0.24405 | -1.82190 | 2.08420 |
| C | -0.13735 | 2.43163 | -1.16832 | H | -1.02167 | 3.10935 | -1.13224 |
| C | 0.13657 | 2.43144 | 1.17332 | H | 0.73155 | 3.10793 | -1.33862 |
| Li | 1.17676 | 0.00019 | -0.09846 | H | -0.24444 | 1.82175 | -2.07925 |
| Li | -1.17703 | -0.00005 | 0.10335 | H | -0.73258 | 3.10736 | 1.34387 |
| N | 0.00008 | -1.58897 | 0.00255 | H | 0.24401 | 1.82140 | 2.08410 |
| C | 0.13711 | -2.43165 | 1.17317 | H | 1.02063 | 3.10949 | 1.13727 |
| C | -0.13646 | -2.43113 | -1.16851 | H | -3.18143 | -2.02649 | 0.06426 |
| O | -3.11150 | -0.00013 | 0.08916 | H | -4.59271 | -1.25114 | 0.85061 |
| C | -3.88399 | -1.19293 | 0.01302 | H | -4.44014 | -1.23550 | -0.93378 |
| C | -3.88449 | 1.19232 | 0.01288 | H | -4.44076 | 1.23448 | -0.93387 |
| O | 3.11106 | 0.00022 | -0.08852 | H | -4.59315 | 1.25039 | 0.85053 |
| C | 3.88437 | 1.19281 | -0.01786 | H | -3.18228 | 2.02618 | 0.06390 |
| C | 3.88421 | -1.19250 | -0.01816 | H | 3.18163 | 2.02652 | -0.06389 |
| H | -0.24374 | -1.82097 | -2.07923 | H | 4.44743 | 1.23510 | 0.92485 |
| H | 0.73278 | -3.10696 | -1.33897 | H | 4.58697 | 1.25099 | -0.86060 |
| H | -1.02046 | -3.10927 | -1.13278 | H | 4.58696 | -1.25046 | -0.86079 |
| H | -0.73173 | -3.10807 | 1.34328 | H | 4.44710 | -1.23520 | 0.92464 |
| H | 1.02152 | -3.10925 | 1.13707 | H | 3.18138 | -2.02610 | -0.06461 |

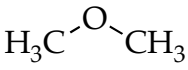
**Table II (Continued).**

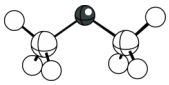




$G$ = -2653.059326
$H$ = -2653.026798
$G_{MP2}$ = -2651.202161

| Atom | X | Y | Z |
|---|---|---|---|
| C | -0.55881 | -0.59674 | 0.00000 |
| C | 0.61513 | 0.36648 | 0.00000 |
| Br | 0.01565 | 2.25184 | 0.00000 |
| H | 1.23836 | 0.26391 | 0.88902 |
| H | 1.23836 | 0.26391 | -0.88902 |
| H | -0.18075 | -1.62781 | 0.00000 |
| H | -1.18397 | -0.46079 | 0.88731 |
| H | -1.18397 | -0.46079 | -0.88731 |

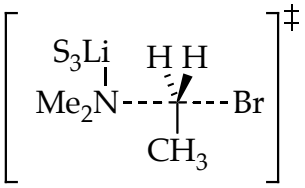


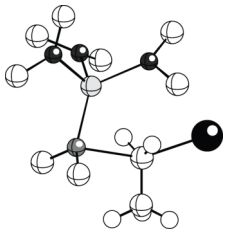


$G$ = -154.970104
$H$ = -154.939502
$G_{MP2}$ = -154.4483767

| Atom | X | Y | Z |
|---|---|---|---|
| C | -1.17099 | 0.04651 | 0.00000 |
| O | -0.00000 | 0.83197 | 0.00000 |
| C | 1.17099 | 0.04651 | 0.00000 |
| H | 1.23209 | -0.59788 | -0.89294 |
| H | 2.02183 | 0.73315 | -0.00008 |
| H | 1.23216 | -0.59777 | 0.89301 |
| H | -1.23215 | -0.59779 | -0.89300 |
| H | -1.23211 | -0.59786 | 0.89295 |
| H | -2.02183 | 0.73315 | 0.00005 |

**Table II (Continued).**

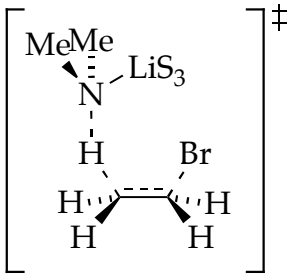


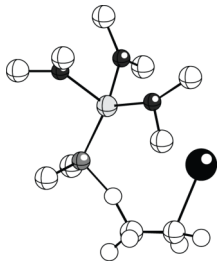



$G$ = -3259.980987
$H$ = -3259.891266
$G_{MP2}$ = -3256.016051
S = $Me_2O$

| Atom | X | Y | Z | Atom | X | Y | Z |
|---|---|---|---|---|---|---|---|
| C | 2.36876 | 0.93362 | -0.08970 | H | 0.06630 | 1.91528 | 1.97005 |
| C | 3.11661 | 2.23184 | -0.13929 | H | -3.91919 | -1.88989 | -0.48309 |
| Br | 4.11544 | -0.69227 | -0.03162 | H | -3.33549 | -1.39662 | -2.09959 |
| N | 0.07956 | 1.67173 | -0.11763 | H | -2.29683 | -2.40264 | -1.05203 |
| C | -0.07895 | 2.48106 | -1.30253 | H | -2.61720 | 1.51845 | -0.11374 |
| C | -0.08496 | 2.50281 | 1.05215 | H | -3.51823 | 0.95023 | -1.54906 |
| Li | -0.42315 | -0.22576 | -0.04232 | H | -4.12813 | 0.56266 | 0.08832 |
| O | 0.33446 | -1.71090 | -1.23875 | H | 1.76881 | -1.39813 | 1.84265 |
| C | 0.88406 | -1.40245 | -2.51957 | H | 1.13690 | -0.46555 | 3.23118 |
| C | 0.90109 | -2.90925 | -0.70089 | H | 0.88764 | -2.23494 | 3.15622 |
| O | -0.26279 | -1.11766 | 1.82804 | H | -1.51445 | -1.92292 | 3.28426 |
| C | 0.94932 | -1.31424 | 2.55943 | H | -1.29100 | -0.14929 | 3.36289 |
| C | -1.39282 | -1.00885 | 2.68581 | H | -2.26535 | -0.87035 | 2.04601 |
| O | -2.40459 | -0.45764 | -0.49115 | H | 1.97330 | -1.28731 | -2.45445 |
| C | -3.22300 | 0.70812 | -0.51888 | H | 0.64399 | -2.19752 | -3.23983 |
| C | -3.03166 | -1.59674 | -1.06231 | H | 0.42940 | -0.46606 | -2.85085 |
| H | 1.98180 | 0.57889 | 0.84609 | H | 0.40301 | -3.09194 | 0.25242 |
| H | 1.98123 | 0.50149 | -0.99117 | H | 0.71570 | -3.75321 | -1.38053 |
| H | 0.07991 | 1.88079 | -2.21132 | H | 1.97931 | -2.78408 | -0.54372 |
| H | -1.08914 | 2.93864 | -1.39372 | H | 2.41784 | 3.07872 | -0.15478 |
| H | 0.62844 | 3.33736 | -1.35610 | H | 3.76491 | 2.34149 | 0.73427 |
| H | 0.62320 | 3.35931 | 1.09560 | H | 3.74131 | 2.28873 | -1.03477 |
| H | -1.09537 | 2.96498 | 1.12800 | | | | |

**Table II (Continued).**

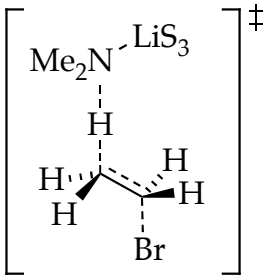


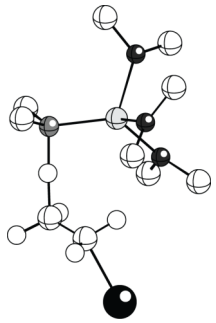



$G$ = -3259.975168
$H$ = -3259.885193
$G_{MP2}$ = -3256.006667
S = $Me_2O$

| Atom | X | Y | Z | Atom | X | Y | Z |
|---|---|---|---|---|---|---|---|
| C | -2.95558 | 2.03235 | 0.19069 | H | -1.25948 | -2.01674 | -1.76822 |
| C | -4.00431 | 1.05187 | 0.19925 | H | 2.65677 | -2.06682 | -0.69371 |
| Br | -3.27444 | -1.18026 | -0.11134 | H | 1.93255 | -3.61514 | -1.23390 |
| N | -0.44847 | 1.38780 | -0.74507 | H | 2.30156 | -2.33738 | -2.42651 |
| C | -0.78096 | 1.38058 | -2.16137 | H | 3.27830 | 1.92910 | -0.22501 |
| C | 0.12528 | 2.67551 | -0.39460 | H | 4.11371 | 0.43916 | -0.76105 |
| Li | 0.35318 | -0.26904 | -0.00833 | H | 2.54272 | 0.90922 | -1.48887 |
| O | -0.06512 | -0.93827 | 1.86341 | H | 2.36389 | -0.45574 | 2.31711 |
| C | -0.89388 | -0.07796 | 2.64621 | H | 4.00849 | -0.38225 | 1.60178 |
| C | -0.37827 | -2.31498 | 2.07312 | H | 0.27135 | -2.89246 | 1.41287 |
| O | 0.68779 | -1.94847 | -1.16670 | H | 3.16075 | 1.12495 | 2.05560 |
| C | -0.30914 | -2.47610 | -2.04415 | H | -0.18557 | -2.59414 | 3.11922 |
| C | 1.96325 | -2.52796 | -1.39731 | H | -1.42597 | -2.51014 | 1.81880 |
| O | 2.39890 | 0.14157 | 0.38459 | H | -1.94764 | -0.23325 | 2.39132 |
| C | 3.13174 | 0.89713 | -0.57048 | H | -0.73044 | -0.26520 | 3.71749 |
| C | 3.02538 | 0.10831 | 1.65917 | H | -0.60880 | 0.94772 | 2.40457 |
| H | -1.82828 | 1.57418 | -0.16745 | H | -1.25507 | 0.42996 | -2.43218 |
| H | -4.47862 | 0.77653 | 1.13459 | H | -1.48879 | 2.18789 | -2.44342 |
| H | -4.67055 | 0.98889 | -0.65433 | H | 0.10760 | 1.51738 | -2.80938 |
| H | -3.10218 | 2.80663 | -0.57109 | H | 1.01909 | 2.92763 | -0.99681 |
| H | -2.75667 | 2.47215 | 1.17312 | H | -0.58208 | 3.51905 | -0.53901 |
| H | -0.06111 | -2.24476 | -3.08957 | H | 0.42951 | 2.68794 | 0.66209 |
| H | -0.38044 | -3.56643 | -1.92513 | | | | |

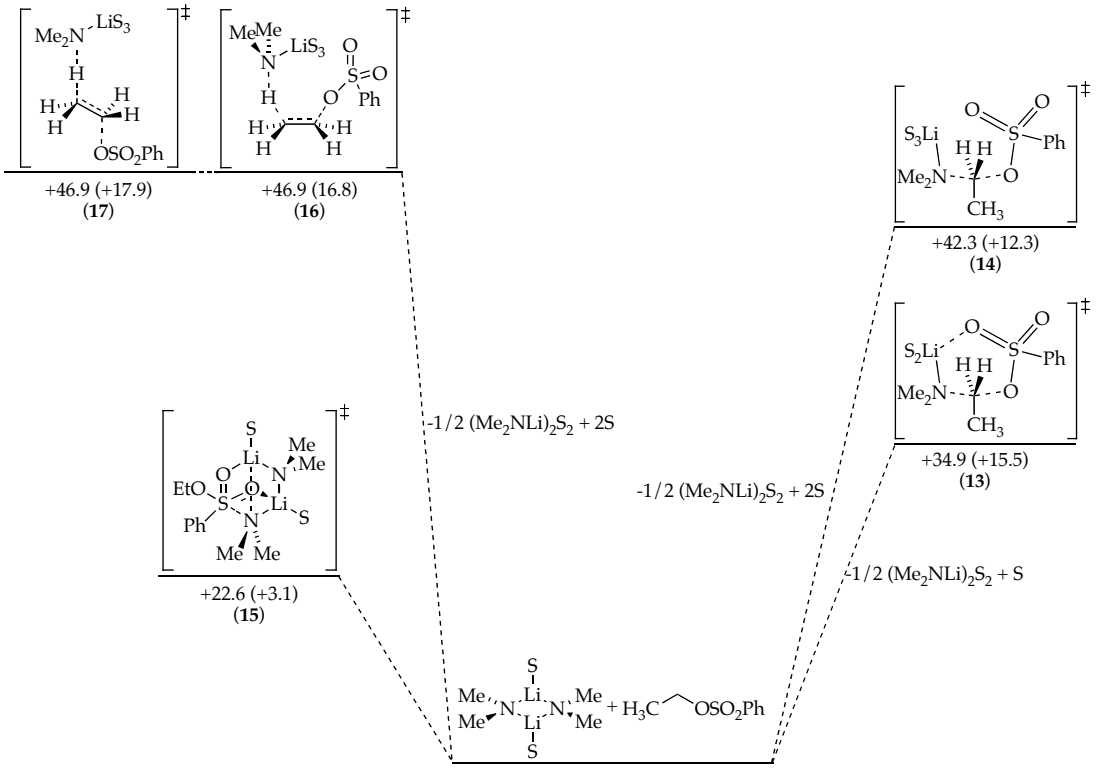
**Table II (Continued).**



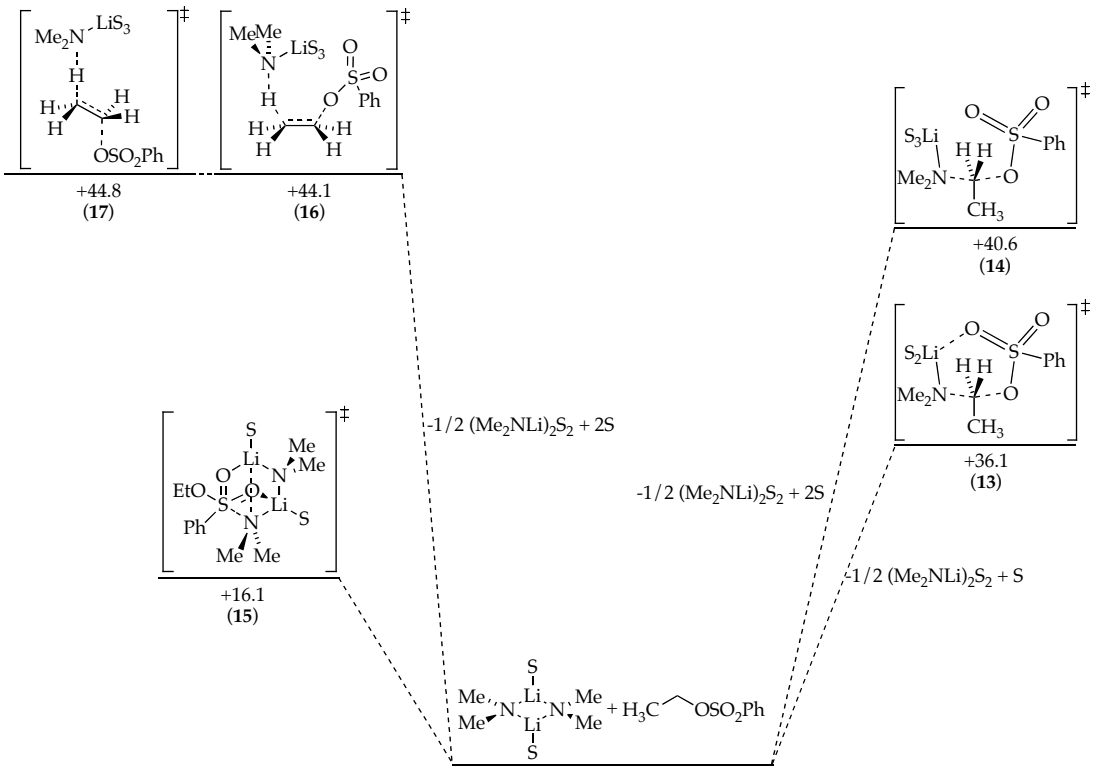



$G$ = -3259.972702
$H$ = -3259.881948
$G_{MP2}$ = -3256.006477
S = $Me_2O$

| Atom | X | Y | Z | Atom | X | Y | Z |
|---|---|---|---|---|---|---|---|
| H | -1.26487 | 1.86225 | -0.08054 | H | -0.00248 | 3.70262 | 1.06152 |
| N | 0.10572 | 1.87050 | -0.04567 | H | 0.00029 | 3.56407 | -1.35695 |
| C | 0.48195 | 2.57114 | -1.26613 | H | 1.57091 | 2.74635 | -1.34445 |
| C | 0.44206 | 2.68945 | 1.11005 | H | 0.18224 | 1.98667 | -2.14753 |
| Li | 0.40905 | -0.10492 | -0.01562 | H | 4.19514 | -0.19097 | -0.34097 |
| O | -0.80100 | -1.43187 | -1.01668 | H | 3.49074 | 0.81418 | -1.64453 |
| C | -1.44360 | -1.07031 | -2.24375 | H | 2.97201 | 1.06510 | 0.04426 |
| C | -1.42090 | -2.57258 | -0.41746 | H | 2.24645 | -1.95260 | 1.39492 |
| O | 0.52940 | -0.96860 | 1.83991 | H | 2.22615 | -1.21510 | 3.02407 |
| C | -0.33956 | -0.60979 | 2.91229 | H | 1.28748 | -2.70408 | 2.70927 |
| C | 1.63166 | -1.75530 | 2.27382 | H | -2.48735 | -2.38389 | -0.23957 |
| O | 2.21007 | -0.60747 | -0.81841 | H | -1.31131 | -3.45206 | -1.06765 |
| C | 3.28440 | 0.31840 | -0.68684 | H | -0.90923 | -2.74989 | 0.52976 |
| C | 2.45405 | -1.60603 | -1.80128 | H | -2.50841 | -0.87106 | -2.07577 |
| C | -2.62478 | 1.77557 | -0.31555 | H | -0.95329 | -0.16670 | -2.61058 |
| C | -3.09561 | 0.71813 | 0.53670 | H | -1.33114 | -1.87641 | -2.98263 |
| Br | -5.00135 | -0.35372 | -0.06897 | H | 1.56129 | -2.23101 | -1.84286 |
| H | -3.14353 | 2.72983 | -0.19116 | H | 2.62979 | -1.15030 | -2.78567 |
| H | -2.57929 | 1.51081 | -1.37732 | H | 3.32763 | -2.21632 | -1.53100 |
| H | -3.40384 | 0.99994 | 1.54215 | H | -0.76613 | -1.50754 | 3.38034 |
| H | -2.51534 | -0.19939 | 0.53030 | H | 0.20151 | -0.02899 | 3.67127 |
| H | 0.07145 | 2.21876 | 2.03040 | H | -1.14086 | -0.00227 | 2.49114 |
| H | 1.53244 | 2.83540 | 1.23337 | | | | |

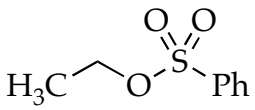


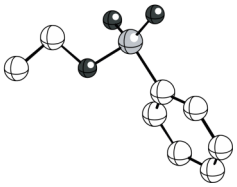

**XIX.** Free energies of activation ($\Delta G^{\ddagger}$, kcal/mol) for the reaction of $EtOSO_2Ph$ with $Me_2NLi$ calculated using B3LYP level of theory with SVP basis set for S and 6-31G(d) basis set for the rest of atoms at 25 °C (S = $Me_2O$). Values in parentheses correspond to the enthalpies of activation ($\Delta H^{\ddagger}$, kcal/mol).




**XX.** Free energies of activation ($\Delta G^{\ddagger}$, kcal/mol) for the reaction of $EtOSO_2Ph$ with $Me_2NLi$ calculated using single point MP2 corrections to B3LYP/6-31G(d)-SVP optimized structures at 25 °C (S = $Me_2O$).

**Table III.** Optimized geometries of reactant and transition structure calculated at B3LYP level of theory using SVP basis set for S and 6-31G(d) basis set for the rest of atoms, for the reaction of $EtOSO_2Ph$ with $Me_2NLi$, with free energies (*G*, Hartrees), enthalpies (*H*, Hartrees) and cartesian coordinates (X,Y,Z) at 25 °C. (Note: $G_{MP2}$ includes single point MP2 corrections to B3LYP/6-31G(d)-SVP optimized structures)

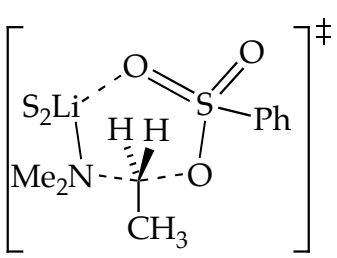


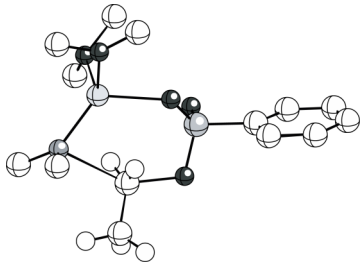



*G* = -934.410892
H = -934.357927
$G_{MP2}$ = -932.2256042

| Atom | X | Y | Z | Atom | X | Y | Z |
|---|---|---|---|---|---|---|---|
| S | 0.65338 | -1.30081 | 0.00085 | C | -1.63851 | -0.40605 | 1.22145 |
| O | 0.92232 | -1.97919 | -1.27244 | H | -1.12143 | -0.62872 | -2.14838 |
| O | 0.92252 | -1.97701 | 1.27525 | H | -3.44530 | 0.29557 | -2.15334 |
| O | 1.44650 | 0.14611 | -0.00044 | H | -4.59316 | 0.75574 | -0.00047 |
| C | 2.89826 | 0.04184 | -0.00085 | H | -3.44525 | 0.29847 | 2.15299 |
| C | 3.44324 | 1.45792 | -0.00027 | H | -1.12137 | -0.62581 | 2.14922 |
| C | -1.00885 | -0.64928 | 0.00043 | H | 3.11006 | 2.00240 | 0.88867 |
| C | -1.63854 | -0.40770 | -1.22089 | H | 4.53859 | 1.43018 | -0.00069 |
| C | -2.93651 | 0.10295 | -1.21331 | H | 3.10941 | 2.00338 | -0.88838 |
| C | -3.58126 | 0.36004 | -0.00022 | H | 3.21094 | -0.51189 | -0.89257 |
| C | -2.93648 | 0.10458 | 1.21320 | H | 3.21141 | -0.51273 | 0.89019 |

**Table III (Continued).**

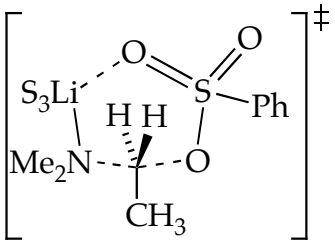


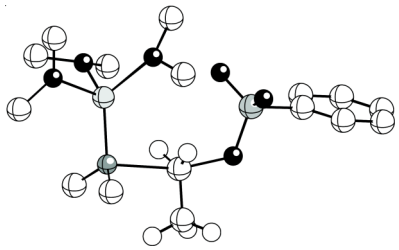



(**13**)
*G* = -1386.373193
*H* = -1386.279001
$G_{MP2}$ = -1382.602451
S = $Me_2O$

| Atom | X | Y | Z | Atom | X | Y | Z |
|---|---|---|---|---|---|---|---|
| C | -0.23702 | 2.12260 | -0.05938 | H | -0.73343 | -2.74064 | -2.74818 |
| C | -0.34392 | 3.59030 | -0.32214 | H | 0.27067 | -2.56286 | -1.27636 |
| N | -2.44877 | 1.12868 | -0.47219 | H | -3.62733 | -1.52759 | -0.96871 |
| C | -3.45228 | 1.86994 | 0.24830 | H | -3.08567 | -2.16522 | -2.54728 |
| C | -2.66987 | 1.29736 | -1.88885 | H | -3.32216 | -3.28740 | -1.17090 |
| Li | -1.36632 | -0.43346 | 0.12635 | H | -0.78385 | -2.92473 | 1.44865 |
| O | 0.78601 | -0.47341 | 0.05847 | H | 0.28082 | -1.99011 | 2.54400 |
| S | 1.74760 | 0.42521 | 0.78606 | H | -1.17780 | -2.81753 | 3.18895 |
| O | 1.50878 | 1.90469 | 0.35870 | H | -2.01960 | -0.70729 | 4.00905 |
| O | 1.79224 | 0.25216 | 2.25157 | H | -0.58333 | 0.14925 | 3.35720 |
| C | 3.38180 | 0.08626 | 0.13273 | H | -2.23398 | 0.60805 | 2.82218 |
| C | 3.58338 | 0.09402 | -1.24992 | H | -3.46795 | 2.95735 | -0.00137 |
| C | 4.85757 | -0.17277 | -1.74677 | H | -4.49065 | 1.51899 | 0.05759 |
| C | 5.91220 | -0.44133 | -0.86773 | H | -3.29315 | 1.79903 | 1.33478 |
| C | 5.69506 | -0.44411 | 0.51117 | H | -1.89492 | 0.77272 | -2.47037 |
| C | 4.42237 | -0.17846 | 1.02164 | H | -3.64970 | 0.90296 | -2.23908 |
| O | -1.54535 | -1.13284 | 2.02728 | H | -2.65552 | 2.36235 | -2.21817 |
| C | -1.58932 | -0.22001 | 3.12260 | H | -1.37091 | 3.82014 | -0.63330 |
| C | -0.75385 | -2.28025 | 2.32858 | H | -0.11592 | 4.17359 | 0.57446 |
| O | -1.66685 | -2.03063 | -1.02910 | H | 0.33428 | 3.89601 | -1.12422 |
| C | -3.00107 | -2.27563 | -1.45742 | H | 4.22668 | -0.17563 | 2.08832 |
| C | -0.70545 | -2.86683 | -1.65627 | H | 2.75669 | 0.30445 | -1.92074 |
| H | -0.62952 | 1.75379 | 0.87127 | H | 6.51507 | -0.65268 | 1.19253 |
| H | -0.19867 | 1.45445 | -0.89668 | H | 5.02927 | -0.17065 | -2.81952 |
| H | -0.89028 | -3.92445 | -1.41707 | H | 6.90395 | -0.64782 | -1.26073 |

**Table III (Continued).**

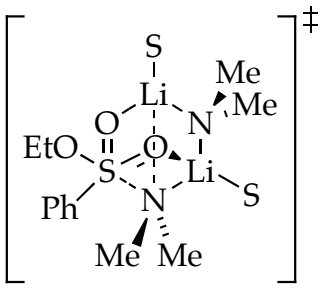


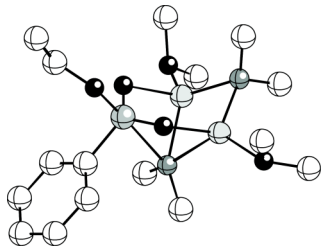



(**14**)
*G* = -1541.331460
*H* = -1541.223547
$G_{MP2}$ = -1537.043616
S = $Me_2O$

| Atom | X | Y | Z | Atom | X | Y | Z |
|---|---|---|---|---|---|---|---|
| Li | -1.96456 | -0.24647 | -0.03571 | H | -1.62490 | 3.48323 | -1.28006 |
| N | -1.67834 | 1.70847 | -0.06715 | H | -0.60811 | -0.12361 | 3.19618 |
| C | -2.10733 | 2.43630 | 1.10484 | H | -0.52871 | -1.90858 | 3.26677 |
| C | -2.05115 | 2.45610 | -1.24693 | H | 0.24388 | -1.03950 | 1.90968 |
| C | 0.73524 | 1.70806 | -0.00705 | H | -3.82321 | -1.26472 | 1.95797 |
| C | 0.97286 | 3.18879 | -0.03956 | H | -2.93540 | -2.08626 | 3.27845 |
| O | 2.51299 | 1.24192 | 0.06705 | H | -3.05992 | -0.30159 | 3.25861 |
| S | 2.78967 | -0.25459 | -0.25062 | H | -4.51318 | 1.13484 | -0.00295 |
| O | 2.20104 | -1.14563 | 0.78369 | H | -5.28071 | 0.52169 | -1.49457 |
| O | 2.47087 | -0.58218 | -1.66179 | H | -5.80350 | -0.10864 | 0.09613 |
| C | 4.57604 | -0.32649 | -0.06875 | H | -5.13630 | -2.41774 | -0.60828 |
| C | 5.12486 | -0.61721 | 1.18071 | H | -4.69155 | -1.72302 | -2.19473 |
| C | 6.51287 | -0.65051 | 1.31910 | H | -3.45819 | -2.57761 | -1.22502 |
| C | 7.33402 | -0.39616 | 0.21729 | H | 0.38820 | -0.97790 | -2.61863 |
| C | 6.77003 | -0.11200 | -1.02932 | H | -0.93586 | -1.99133 | -3.28846 |
| C | 5.38323 | -0.07638 | -1.17911 | H | -1.25643 | -0.29415 | -2.82874 |
| O | -1.80351 | -1.13213 | 1.81635 | H | -0.56671 | -3.57937 | -1.47414 |
| C | -0.60656 | -1.04300 | 2.59390 | H | 0.71424 | -2.53834 | -0.76082 |
| C | -2.96681 | -1.19886 | 2.63025 | H | -0.73422 | -2.95709 | 0.19664 |
| O | -3.91671 | -0.72862 | -0.53721 | H | 0.47350 | 1.22799 | 0.91973 |
| C | -4.94242 | 0.25573 | -0.48350 | H | 0.51259 | 1.17863 | -0.91752 |
| C | -4.33195 | -1.92748 | -1.17611 | H | 0.03125 | 3.74338 | 0.00384 |
| O | -1.06718 | -1.57110 | -1.25258 | H | 1.58779 | 3.48954 | 0.81368 |
| C | -0.68488 | -1.19070 | -2.57714 | H | 1.49939 | 3.47014 | -0.95559 |
| C | -0.36128 | -2.73178 | -0.80385 | H | 4.92307 | 0.12733 | -2.14017 |
| H | -1.66933 | 3.45660 | 1.18708 | H | 7.41015 | 0.07753 | -1.88672 |
| H | -3.20840 | 2.60262 | 1.15183 | H | 8.41469 | -0.42476 | 0.32908 |
| H | -1.82886 | 1.89586 | 2.02196 | H | 6.95339 | -0.87940 | 2.28575 |
| H | -1.70881 | 1.94355 | -2.15848 | H | 4.46820 | -0.82632 | 2.01852 |
| H | -3.14905 | 2.60298 | -1.35375 | | | | |

**Table III (Continued).**

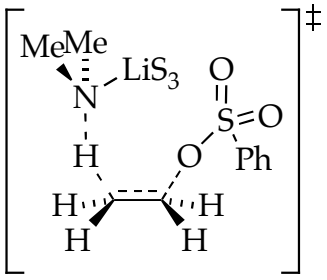


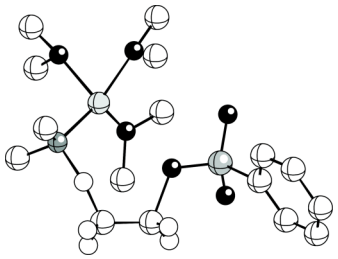



(**15**)
$G$ = -1528.470612
$H$ = -1528.365538
$G_{MP2}$ = -1524.171891
S = $Me_2O$

| Atom | X | Y | Z | Atom | X | Y | Z |
|---|---|---|---|---|---|---|---|
| S | 1.25159 | 0.09864 | 0.72457 | H | 2.07021 | -1.86879 | 2.69432 |
| O | 0.49808 | 1.35929 | 0.92243 | H | -2.80902 | -3.35349 | 1.01822 |
| Li | -1.24846 | 1.26416 | -0.06143 | H | -1.88138 | -4.80975 | 0.52167 |
| Li | -1.10902 | -1.14041 | -0.27174 | H | -1.04977 | -3.44299 | 1.32286 |
| O | 0.63322 | -1.25395 | 0.75897 | H | -2.17015 | -2.91220 | -2.54233 |
| N | 0.07709 | 0.18212 | -1.47781 | H | -2.53553 | -4.49586 | -1.80149 |
| C | 0.26320 | 1.42787 | -2.20156 | H | -3.49521 | -3.04995 | -1.34766 |
| C | 0.38727 | -0.90439 | -2.38975 | H | 0.08420 | 2.29942 | -1.55847 |
| N | -2.57207 | -0.07541 | 0.50761 | H | 1.28890 | 1.54249 | -2.60898 |
| C | -2.85450 | -0.14968 | 1.92515 | H | -0.41979 | 1.51681 | -3.06985 |
| C | -3.81872 | -0.13909 | -0.22134 | H | -0.29404 | -0.92969 | -3.26445 |
| O | -1.54089 | -3.10195 | -0.61910 | H | 1.41248 | -0.84029 | -2.80960 |
| C | -1.84829 | -3.71676 | 0.63107 | H | 0.31405 | -1.88040 | -1.89119 |
| C | -2.49692 | -3.41137 | -1.62746 | H | -1.92469 | -0.10187 | 2.50969 |
| O | -1.79258 | 3.21948 | -0.02319 | H | -3.51055 | 0.67320 | 2.29303 |
| C | -1.56989 | 3.85648 | 1.23321 | H | -3.37839 | -1.08652 | 2.22829 |
| C | -3.06138 | 3.54338 | -0.58105 | H | -3.64268 | -0.08279 | -1.30811 |
| C | 2.65327 | 0.23560 | -0.35634 | H | -4.39973 | -1.07496 | -0.03994 |
| C | 3.19530 | 1.50426 | -0.59374 | H | -4.53097 | 0.68201 | 0.02816 |
| C | 4.34982 | 1.60886 | -1.36699 | H | -1.58145 | 4.94898 | 1.11521 |
| C | 4.96274 | 0.46534 | -1.88671 | H | -2.33829 | 3.56117 | 1.96091 |
| C | 4.41088 | -0.79290 | -1.63850 | H | -0.59010 | 3.53092 | 1.58417 |
| C | 3.25282 | -0.91973 | -0.87017 | H | -3.13400 | 3.02813 | -1.54108 |
| O | 2.07740 | 0.14588 | 2.18604 | H | -3.87565 | 3.20614 | 0.07358 |
| C | 2.77620 | -1.03587 | 2.62120 | H | -3.14488 | 4.62715 | -0.74373 |
| C | 3.39568 | -0.71066 | 3.97039 | H | 2.81598 | -1.89273 | -0.67549 |
| H | 2.62124 | -0.43789 | 4.69395 | H | 4.88138 | -1.68509 | -2.04237 |
| H | 3.93716 | -1.58385 | 4.35183 | H | 5.86465 | 0.55571 | -2.48522 |
| H | 4.09831 | 0.12412 | 3.88487 | H | 4.77445 | 2.59032 | -1.55903 |
| H | 3.55280 | -1.30085 | 1.89090 | H | 2.71863 | 2.38420 | -0.17644 |

**Table III (Continued).**

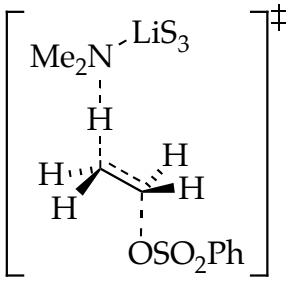


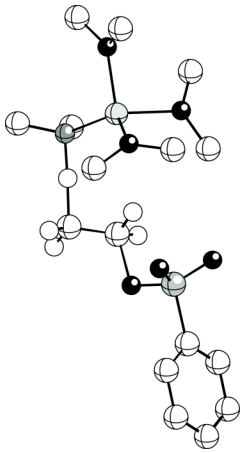



(**16**)
*G* = -1541.324155
*H* = -1541.216364
$G_{MP2}$ = -1537.038062
S = $Me_2O$

| Atom | X | Y | Z | Atom | X | Y | Z |
|---|---|---|---|---|---|---|---|
| S | 2.27268 | -0.37844 | 0.95502 | H | 0.21254 | 3.61978 | 0.23807 |
| O | 1.75804 | -1.76051 | 0.86493 | H | 0.69235 | 3.40532 | -1.48434 |
| O | 2.35911 | 0.25025 | 2.29209 | H | 2.08666 | 2.33248 | 0.93983 |
| O | 1.43862 | 0.50772 | -0.04656 | H | 2.59969 | 2.15547 | -0.78322 |
| C | 1.76128 | 2.20307 | -0.09016 | H | 0.92653 | -2.32306 | -1.35634 |
| C | 0.57564 | 2.91335 | -0.51460 | H | -0.23823 | -2.71564 | -2.67088 |
| N | -1.69901 | 1.47515 | -1.04182 | H | 0.12698 | -1.01007 | -2.25912 |
| Li | -1.63075 | -0.22177 | 0.00658 | H | -2.11896 | -3.10411 | 0.39195 |
| O | -1.29750 | -0.04489 | 2.02602 | H | -1.43383 | -4.01311 | -0.98364 |
| C | -0.86700 | 1.21045 | 2.55937 | H | -0.35829 | -3.45786 | 0.33938 |
| C | -0.97717 | -1.12640 | 2.89894 | H | -4.91804 | 0.52761 | 0.91335 |
| O | -1.07107 | -1.96432 | -0.92054 | H | -5.26356 | -1.12681 | 1.50329 |
| C | 0.00385 | -2.01540 | -1.85786 | H | -3.84345 | -0.22595 | 2.12659 |
| C | -1.24626 | -3.21057 | -0.25501 | H | -3.55497 | -1.58721 | -1.67413 |
| O | -3.60935 | -0.95317 | 0.25059 | H | -5.10474 | -1.91370 | -0.83565 |
| C | -4.29116 | -1.18695 | -0.97615 | H | -4.70800 | -0.25302 | -1.37702 |
| C | -4.46427 | -0.41479 | 1.25043 | H | -0.79012 | 0.81598 | -2.82298 |
| C | -1.63502 | 1.43460 | -2.49434 | H | -2.55014 | 1.01507 | -2.95393 |
| C | -2.74429 | 2.40627 | -0.64752 | H | -1.49214 | 2.43711 | -2.94782 |
| C | 3.94152 | -0.37547 | 0.27283 | H | -2.55944 | 3.44158 | -1.00210 |
| C | 4.17270 | -0.95853 | -0.97602 | H | -3.74042 | 2.12366 | -1.04055 |
| C | 5.46542 | -0.95655 | -1.49719 | H | -2.83204 | 2.45149 | 0.44701 |
| C | 6.51415 | -0.38146 | -0.77213 | H | -1.36230 | -2.03814 | 2.43945 |
| C | 6.27116 | 0.19336 | 0.47630 | H | 0.10648 | -1.21220 | 3.02721 |
| C | 4.97861 | 0.19975 | 1.00639 | H | -1.45802 | -0.98251 | 3.87780 |
| H | 4.76616 | 0.63648 | 1.97606 | H | -1.07196 | 1.96645 | 1.80147 |
| H | 7.08647 | 0.63685 | 1.04113 | H | -1.42658 | 1.44186 | 3.47782 |
| H | 7.52058 | -0.38435 | -1.18185 | H | 0.20587 | 1.18531 | 2.77328 |
| H | 5.65645 | -1.40588 | -2.46783 | H | -0.49434 | 2.12304 | -0.71393 |
| H | 3.35291 | -1.40669 | -1.52793 | | | | |

**Table III (Continued).**



(**17**)
*G* = -1541.324279
*H* = -1541.214592
$G_{MP2}$ = -1541.214592
S = $Me_2O$

| Atom | X | Y | Z | Atom | X | Y | Z |
|---|---|---|---|---|---|---|---|
| C | 1.12543 | 1.30889 | 0.22198 | H | 0.80325 | 3.37801 | -0.23926 |
| C | 0.50188 | 2.36758 | -0.52937 | H | 0.57014 | 2.23802 | -1.61509 |
| O | 2.75403 | 1.08227 | -0.09701 | H | 0.73796 | 0.31798 | -0.01120 |
| S | 3.20034 | -0.43287 | -0.05207 | H | 1.17980 | 1.46457 | 1.29897 |
| O | 2.75802 | -1.07127 | 1.20998 | H | -5.50932 | 0.13686 | -1.46262 |
| O | 2.84313 | -1.12563 | -1.31321 | H | -5.96782 | -0.61363 | 0.09611 |
| C | -0.43866 | -0.75375 | -2.43653 | H | -4.88367 | 0.81644 | 0.06530 |
| O | -0.94453 | -1.25296 | -1.19289 | H | -3.24872 | -2.67119 | -1.19147 |
| C | -0.33046 | -2.49316 | -0.82652 | H | -4.95116 | -2.76141 | -0.63949 |
| Li | -2.14398 | -0.14481 | -0.02432 | H | -4.55148 | -1.97992 | -2.19832 |
| N | -2.17961 | 1.86532 | -0.12011 | H | -0.51008 | -0.06636 | 3.16017 |
| C | -2.79672 | 2.53358 | -1.25960 | H | -0.52570 | -1.85349 | 3.22898 |
| C | -2.51607 | 2.57661 | 1.10753 | H | 0.24309 | -1.02228 | 1.85119 |
| O | -3.99312 | -0.91647 | -0.49633 | H | -3.82867 | -1.09921 | 2.06497 |
| C | -4.20614 | -2.15041 | -1.16892 | H | -2.89991 | -1.92772 | 3.34864 |
| C | -5.16031 | -0.10390 | -0.44928 | H | -2.98631 | -0.14070 | 3.32167 |
| O | -1.81361 | -1.00891 | 1.82984 | H | -2.52684 | 2.01927 | -2.19234 |
| C | -0.58348 | -0.98365 | 2.56061 | H | -3.89978 | 2.55235 | -1.20373 |
| C | -2.94146 | -1.04366 | 2.69694 | H | -2.47114 | 3.58678 | -1.36252 |
| C | 4.98358 | -0.25378 | -0.00860 | H | -2.22756 | 3.64522 | 1.07649 |
| C | 5.69281 | -0.19847 | -1.20900 | H | -3.59788 | 2.55219 | 1.33683 |
| C | 7.07749 | -0.03241 | -1.16721 | H | -1.99010 | 2.12372 | 1.95921 |
| C | 7.73483 | 0.07310 | 0.06146 | H | -0.71134 | -1.43448 | -3.25568 |
| C | 7.01078 | 0.00924 | 1.25522 | H | -0.89923 | 0.22198 | -2.60073 |
| C | 5.62576 | -0.15500 | 1.22637 | H | 0.65065 | -0.65122 | -2.39043 |
| H | 5.04436 | -0.21998 | 2.13994 | H | -0.54920 | -3.26286 | -1.58104 |
| H | 7.52520 | 0.08393 | 2.20939 | H | 0.75387 | -2.37122 | -0.73431 |
| H | 8.81369 | 0.20091 | 0.08898 | H | -0.76185 | -2.78788 | 0.13183 |
| H | 7.64338 | 0.01052 | -2.09377 | H | -0.89021 | 2.11572 | -0.27532 |
| H | 5.16267 | -0.29642 | -2.15028 | | | | |