

SUPPORTING INFORMATION

Lithium Ephedrate-Mediated Addition of a Lithium Acetylide to a Ketone: Solution Structures and Relative Reactivities of Mixed Aggregates Underlying the High Enantioselectivities

Andrew Thompson,* Edward G. Corley, Martha F. Huntington, and Edward J. J. Grabowski
Department of Process Research, Merck Research Laboratories
P.O. Box 2000, Rahway, New Jersey 07065
and
Julius F. Remenar and David B. Collum*
Department of Chemistry, Baker Laboratory
Cornell University
Ithaca, New York 14853-1301

Supporting Information

General Experimental Procedures (at the end)

- I. ^6Li NMR spectra of [^6Li]lithium cyclopropylacetylide
- II. ^6Li and ^{13}C NMR spectra of [$^6\text{Li},^{13}\text{C}$]lithium cyclopropylacetylide
- III. ^6Li and ^{15}N NMR spectra of *R,S*-LiOCH(Ph)CH(Me)N(CH₂)₄
- IV. ^6Li NMR spectra of 1:1 mixtures of [(CH₂)₂CHCCLi]:[*R,S*-LiOCH(Ph)CH(Me)N(CH₂)₄] showing aging effects.
- V. ^6Li , ^{13}C , and ^{15}N NMR spectra of 1:1 mixtures of [(CH₂)₂CHCCLi]:[*R,S*-LiOCH(Ph)CH(Me)N(CH₂)₄].
- VI. NMR spectra of 3:1 mixtures of [(CH₂)₂CHCCLi]:[*R,S*-LiOCH(Ph)CH(Me)N(CH₂)₄].
- VII. $^6\text{Li},^{13}\text{C}$ -HMQC spectrum of a 3:1 mixture of [(CH₂)₂CHCCLi]:[*R,S*-LiOCH(Ph)CH(Me)N(CH₂)₄].
- VIII. NMR spectra of samples containing the 1:3 [(CH₂)₂CHCCLi]:[*R,S*-LiOCH(Ph)CH(Me)N(CH₂)₄]mixed tetramer
- IX. Calculated 2:2 RLi:ROLi mixed tetramers
- X. Calculated 1:3 RLi:ROLi mixed tetramers
- XI. Calculated 3:1 RLi:ROLi mixed tetramers
- XII. Calculated 1:1 RLi:ROLi mixed dimers
- XIII. Calculated (ROLi)_n aggregates
- XIV. Calculated 2:2 RLi:ROLi mixed tetramer-based transition structures
- XV. Calculated 1:1 RLi:ROLi mixed dimer-based transition structures
- XVI. Calculated ligands and ketone heats of formation.

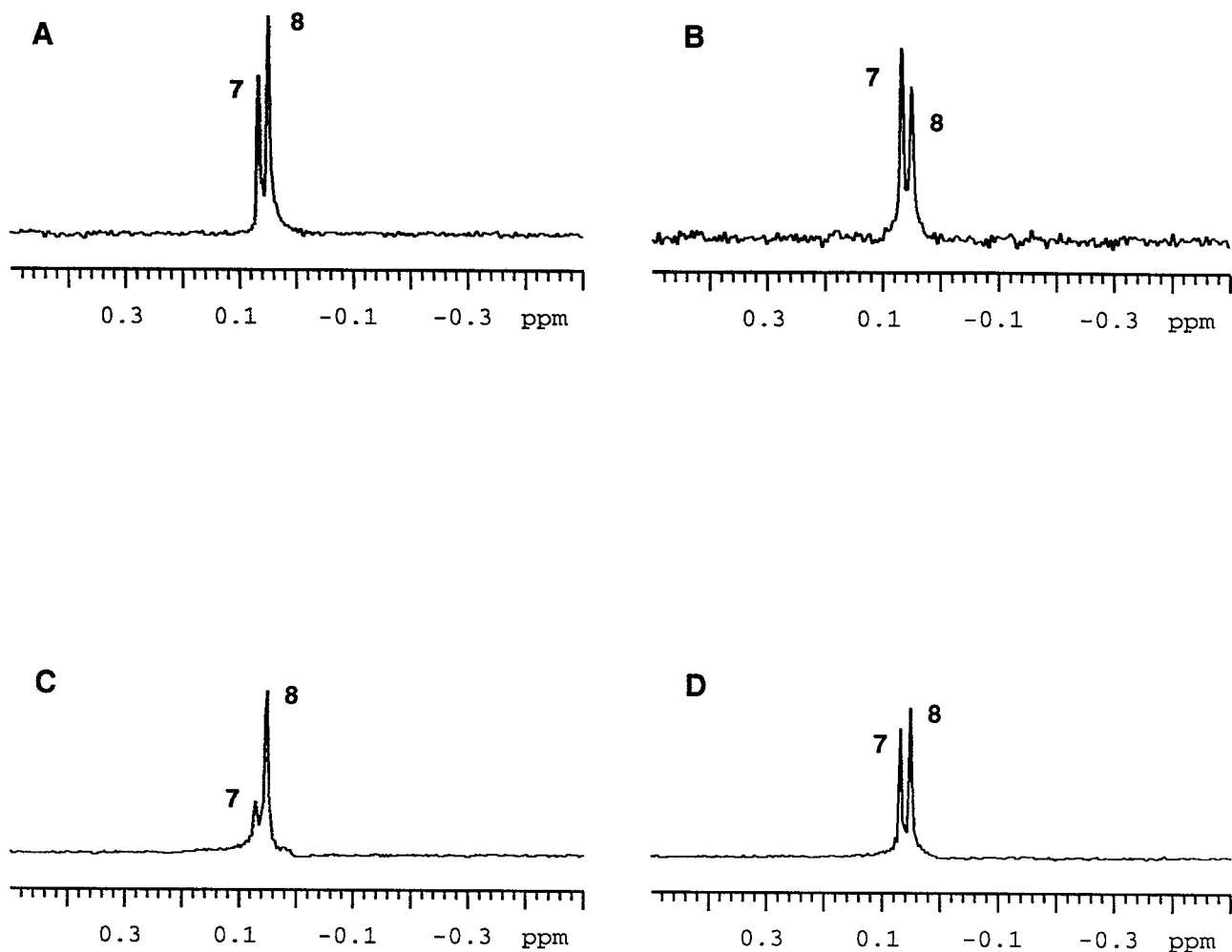


Figure 1. ${}^6\text{Li}$ NMR spectra of $[{}^6\text{Li}]$ lithium cyclopropylacetylide (**6**) in THF/pentane at $-125\text{ }^\circ\text{C}$ showing dimer (**7**) and tetramer (**8**). The samples contain: **A**. 0.05 M $[{}^6\text{Li}]\text{6}$ in 1:1 THF:pentane; **B**. 0.02 M $[{}^6\text{Li}]\text{6}$ in 1:1 THF:pentane; **C**. 0.1 M $[{}^6\text{Li}]\text{6}$ in 1:2 THF:pentane; **D**. 0.1 M $[{}^6\text{Li}]\text{6}$ in 3:1 THF:pentane.

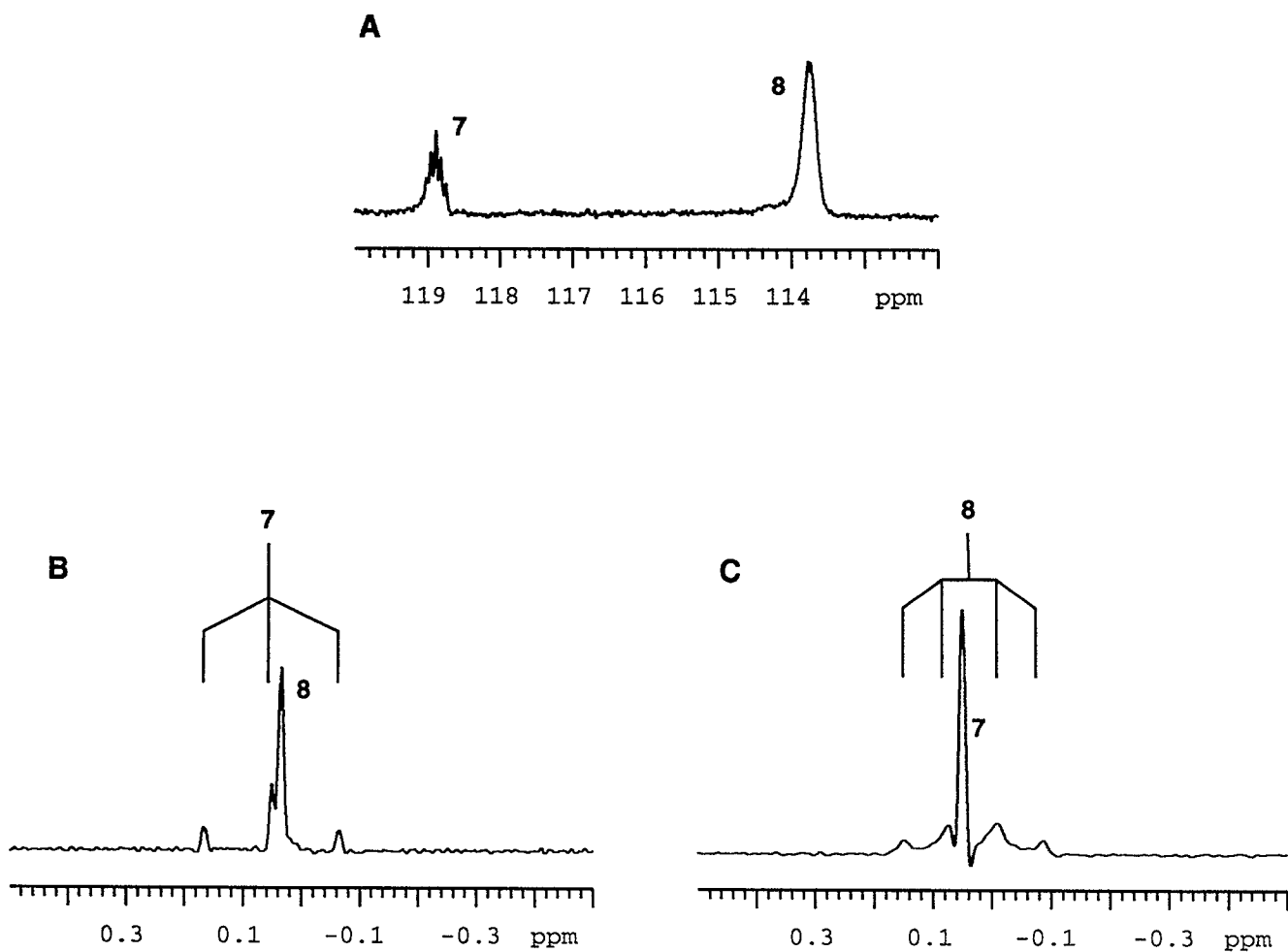


Figure II. ${}^6\text{Li}$ and ${}^{13}\text{C}$ NMR spectra of 0.10 M $[{}^6\text{Li}, {}^{13}\text{C}]$ lithium cyclopropylacetylide (**6**) in 1:1 THF:pentane at $-125\text{ }^\circ\text{C}$ showing dimer (**7**) and tetramer (**8**): **A**. ${}^{13}\text{C}$ NMR spectrum; **B**. ${}^6\text{Li}$ NMR spectrum with single-frequency ${}^{13}\text{C}$ decoupling at 113.7 ppm; **C**. ${}^6\text{Li}$ NMR spectrum with single-frequency ${}^{13}\text{C}$ decoupling at 118.9 ppm.

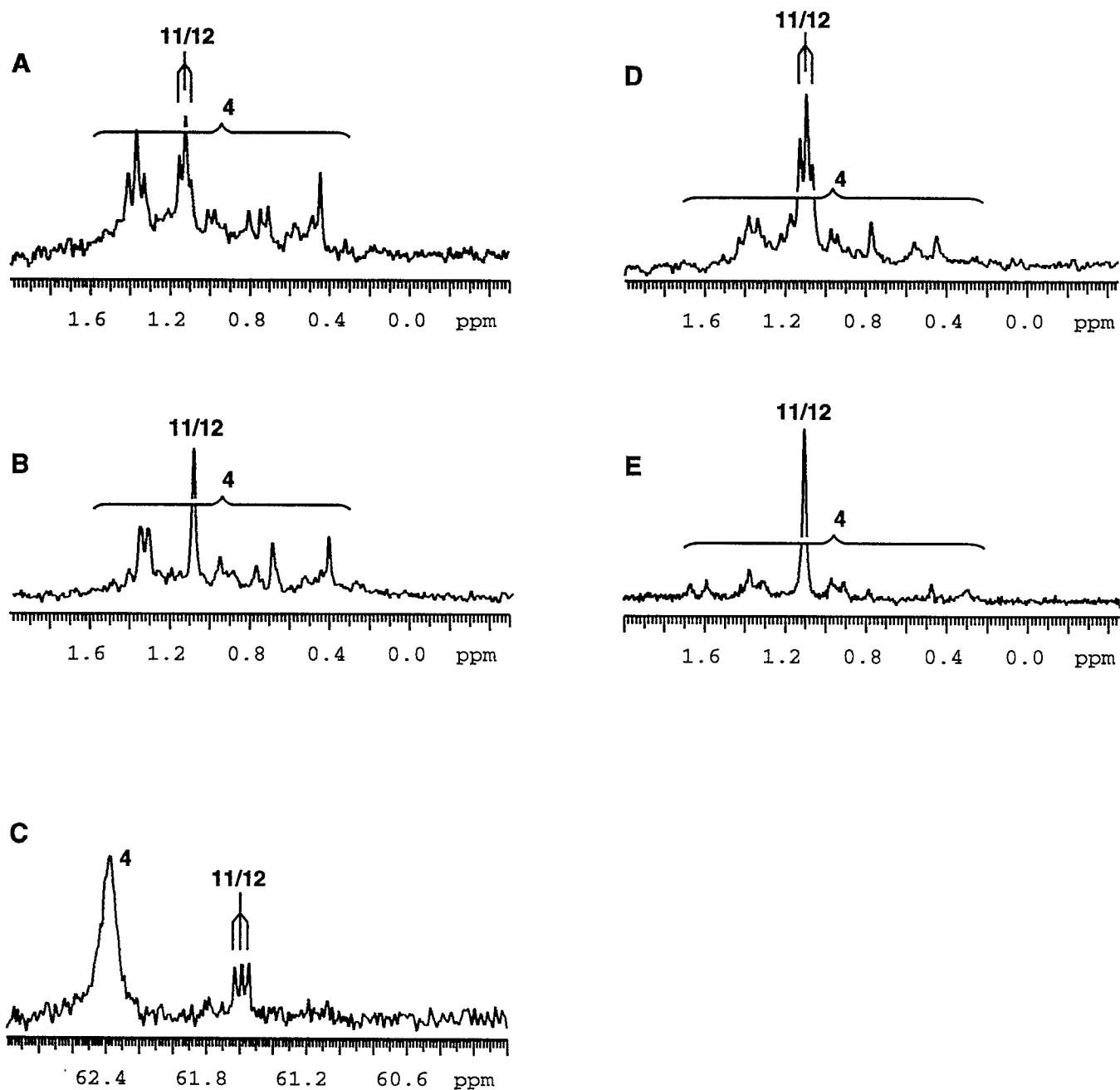


Figure III. NMR spectra of 0.10 M $[R,S\text{-LiOCH(Ph)CH(Me)N(CH}_2)_4]$ ($[^6\text{Li}]\mathbf{4}$) in 1:1 THF:pentane at $-125\text{ }^\circ\text{C}$ showing a mixture of oligomers ($\mathbf{4}$) and a 1:1 ROLi-ROH complex ($\mathbf{11/12}$). **A.** ^6Li NMR spectrum of $[^6\text{Li},^{15}\text{N}]\mathbf{4}$; **B.** $^6\text{Li}\{^{15}\text{N}\}$ NMR spectrum of $[^6\text{Li},^{15}\text{N}]\mathbf{4}$; **C.** ^{15}N NMR spectrum of $[^6\text{Li},^{15}\text{N}]\mathbf{4}$; **D.** ^6Li NMR spectrum of a 1:1 mixture of $[^6\text{Li},^{15}\text{N}]\mathbf{4}$ and $[^{15}\text{N}][R,S\text{-HOCH(Ph)CH(Me)N(CH}_2)_4]$ ($\mathbf{5}$); **E.** ^6Li NMR spectrum of 1:1 $[^6\text{Li}]\mathbf{4}:[^6\text{Li}]\mathbf{5}$.

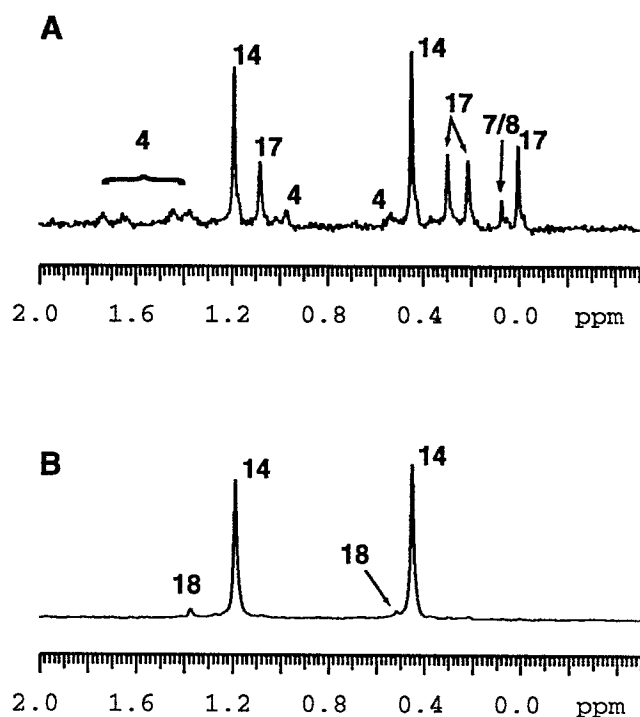


Figure IV. ^6Li NMR spectra of solutions containing a 1:1 mixture of $[\text{}^6\text{Li}]$ lithium cyclopropylacetylide (6) and $[\text{}^6\text{Li}][R,S\text{-LiOCH(Ph)CH(Me)N(CH}_2)_4]$ (4) (0.10 M total lithium titer) in 1:1 THF:pentane at $-125\text{ }^\circ\text{C}$ showing $(\text{ROLi})_n$ oligomers of 4, lithium cyclopropylacetylide dimer and tetramer (7 and 8), 2:2 RLi/ROLi mixed tetramer (14), 3:1 RLi/ROLi mixed tetramer (17), and 1:3 RLi/ROLi mixed tetramer (18). **A.** NMR spectrum taken without sample warming; **B.** NMR spectrum of the same sample after warming at $25\text{ }^\circ\text{C}$ for 30 minutes and cooling back to $-125\text{ }^\circ\text{C}$.

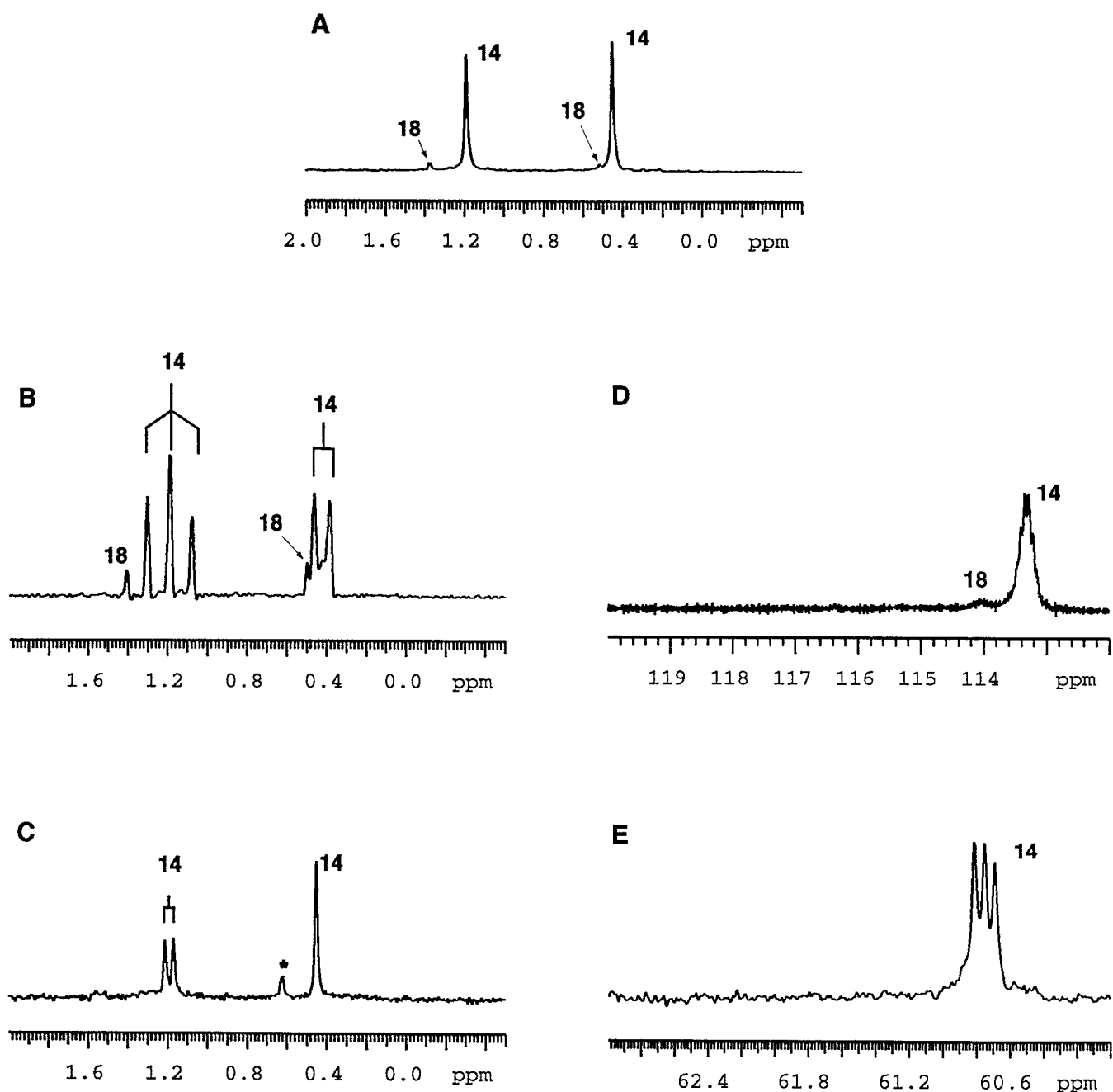


Figure V. ${}^6\text{Li}$ NMR spectra of lithium cyclopropylacetylide (**6**) and [*R,S*-LiOCH(Ph)CH(Me)N(CH₂)₄] (**4**) in 1:1 THF:pentane (0.10 M total lithium titer) at -125 °C showing 2:2 RLi/ROLi mixed tetramer (**14**) and 1:3 RLi/ROLi mixed tetramer (**18**). **A**. ${}^6\text{Li}$ NMR spectrum of 1:1 [${}^6\text{Li}$]**6**: [${}^6\text{Li}$]**4**; **B**. ${}^6\text{Li}$ NMR spectrum of 1:1 [${}^6\text{Li}, {}^{13}\text{C}$]**6**: [${}^6\text{Li}$]**4**; **C**. ${}^6\text{Li}$ NMR spectrum of 1:1 [${}^6\text{Li}$]**6**: [${}^6\text{Li}, {}^{15}\text{N}$]**4**, the "*" denotes an unknown species present in the ${}^{15}\text{N}$ labeled alkoxide; **D**. ${}^{13}\text{C}$ NMR spectrum of 3:1 [${}^6\text{Li}, {}^{13}\text{C}$]**6**: [${}^6\text{Li}$]**4**; **E**. ${}^{15}\text{N}$ NMR spectrum of 1:1 [${}^6\text{Li}$]**6**: [${}^6\text{Li}, {}^{15}\text{N}$]**4**.

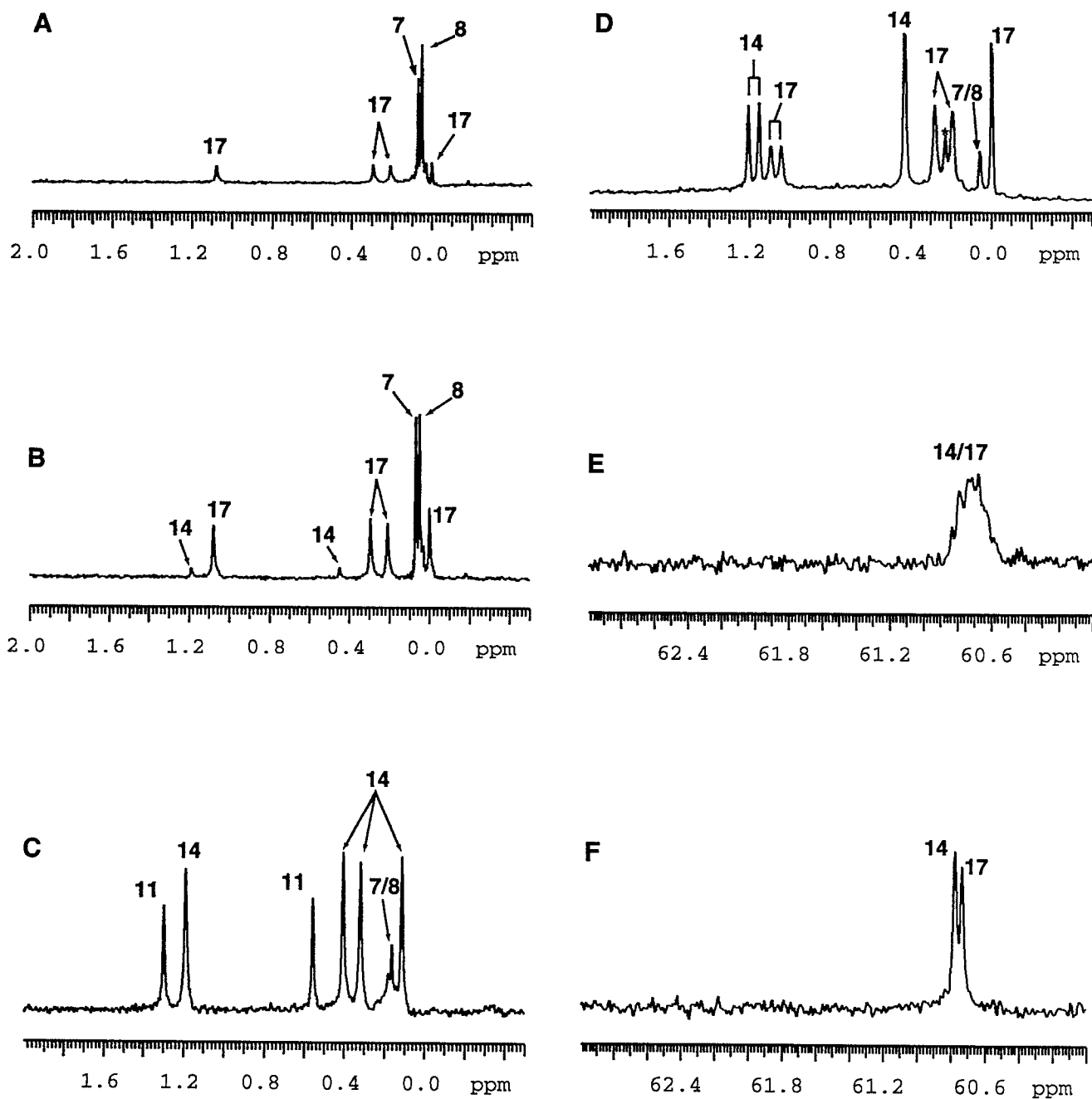


Figure VI. NMR spectra of solutions containing lithium cyclopropylacetylide (**6**) and [*R,S*-LiOCH(Ph)CH(Me)N(CH₂)₄] (**4**) in 1:1 THF:pentane (0.10 M total lithium titer) at -125 °C showing lithium cyclopropylacetylide dimer and tetramer (**7** and **8**), 2:2 RLi/ROLi mixed tetramer (**14**), and 3:1 RLi/ROLi mixed tetramer (**17**). **A**. ⁶Li NMR spectrum of 10:1 [⁶Li]**6**:⁶Li]**4**; **B**. ⁶Li NMR spectrum of 5:1 [⁶Li]**6**:⁶Li]**4**; **C**. ⁶Li NMR spectrum of 3:1 [⁶Li]**6**:⁶Li]**4**; **D**. ⁶Li NMR spectrum of 1:1 [⁶Li]**6**:⁶Li,¹⁵N]**4**. The "*" denotes an unknown species present only in the ¹⁵N-labelled alkoxide. **E**. ¹⁵N NMR spectrum; **F**. ¹⁵N NMR spectrum with single-frequency ⁶Li decoupling at 1.19 ppm. The "*" denotes an unknown impurity present only in the ¹⁵N-labelled **4**.

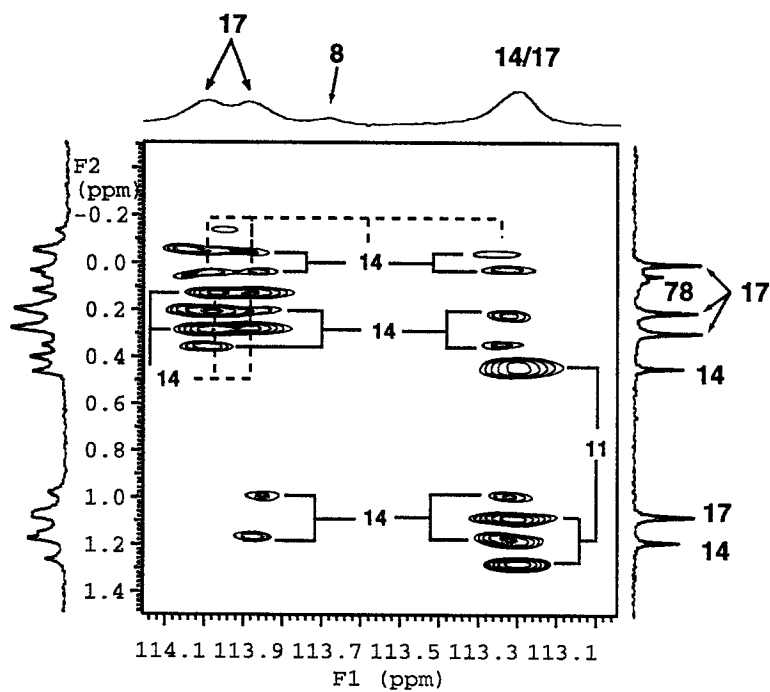


Figure VII. $^6\text{Li},^{13}\text{C}$ -HMQC spectrum recorded on a solution containing $[^6\text{Li},^{13}\text{C}]6$ and $[^6\text{Li}]4$ (3:1) in 1:1 THF:pentane (0.10 M total lithium titer) at $-125\text{ }^\circ\text{C}$ showing lithium cyclopropylacetylide dimer and tetramer (**7** and **8**), 2:2 RLi/ROLi mixed tetramer (**14**), and 3:1 RLi/ROLi mixed tetramer (**17**). The ^6Li NMR spectrum is on the left axis, the $^6\text{Li}\{^{13}\text{C}\}$ NMR spectrum is on the right axis, and the $^{13}\text{C}\{^6\text{Li}\}$ NMR spectrum is displayed on top.

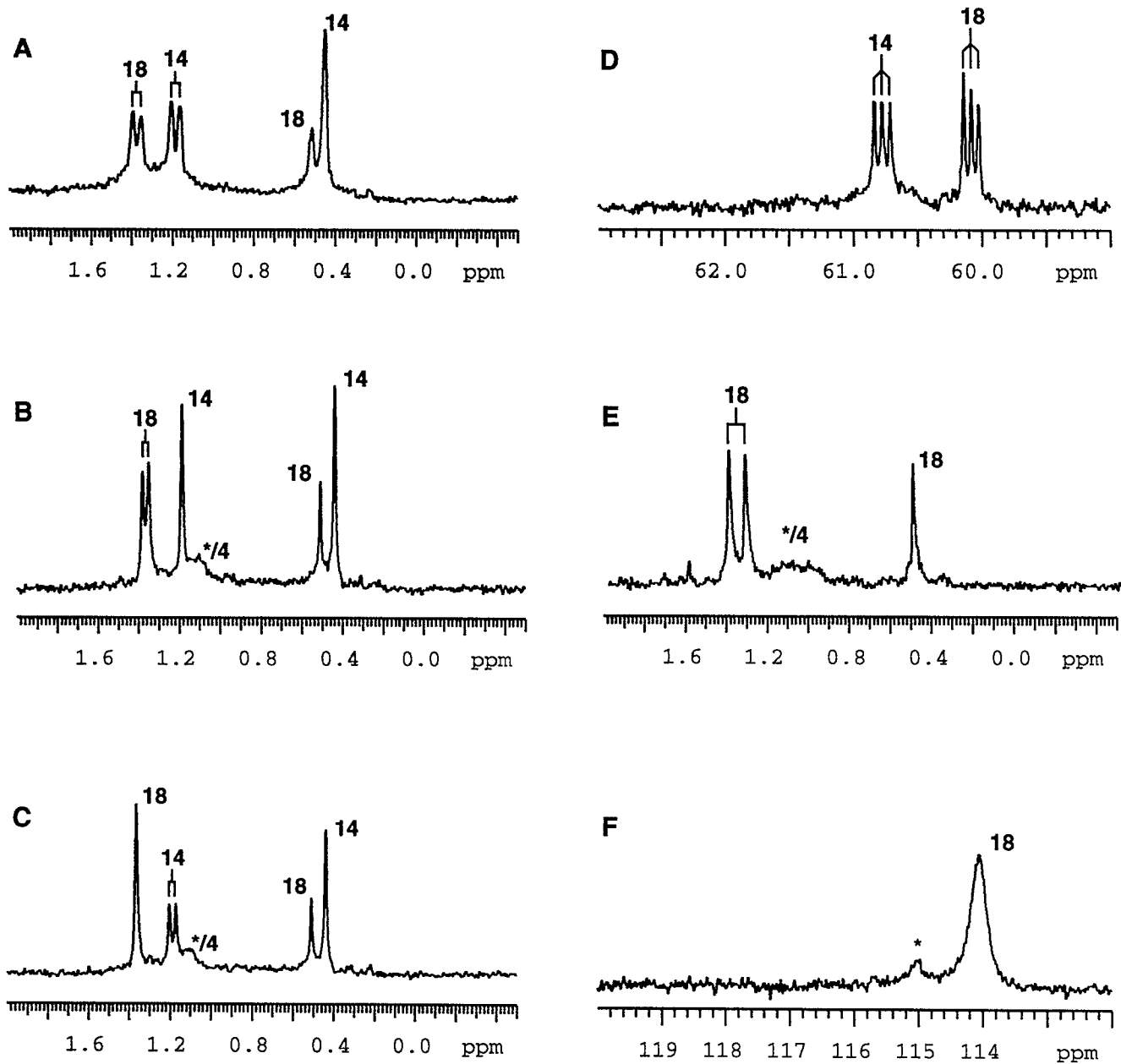


Figure VIII. ${}^6\text{Li}$, ${}^{13}\text{C}$, and ${}^{15}\text{N}$ NMR spectra of solutions containing the 1:3 mixed tetramer {lithium cyclopropylacetylide} $\{[R,S\text{-LiOCH(Ph)CH(Me)N(CH}_2)_4]\}_3$ (0.10 M total lithium titer) in 1:1 THF:pentane at $-125\text{ }^\circ\text{C}$. Spectra **A-D** were recorded on a sample containing 0.1 M $[{}^{15}\text{N}][R,S\text{-HOCH(Ph)CH(Me)N(CH}_2)_4]$ and 0.75 equiv. of $[{}^6\text{Li}]_6$ in 1:1 THF:pentane at $-125\text{ }^\circ\text{C}$. Spectra **E** and **F** were recorded on a sample containing $[{}^6\text{Li},{}^{13}\text{C}]_6$ and $[{}^6\text{Li}]_4$ in a 1:3 ratio (0.10 M total lithium titer) in 1:1 THF:pentane at $-125\text{ }^\circ\text{C}$. The "*" represents an unassigned species. **A**. ${}^6\text{Li}$ NMR spectrum; **B**. ${}^6\text{Li}$ NMR spectrum with ${}^{15}\text{N}$ single-frequency decoupling at 60.8 ppm; **C**. ${}^6\text{Li}$ NMR spectrum with single-frequency ${}^{15}\text{N}$ decoupling at 60.1 ppm; **D**. ${}^{15}\text{N}$ NMR spectrum; **E**. ${}^6\text{Li}$ NMR spectrum; **F**. ${}^{13}\text{C}$ NMR spectrum.

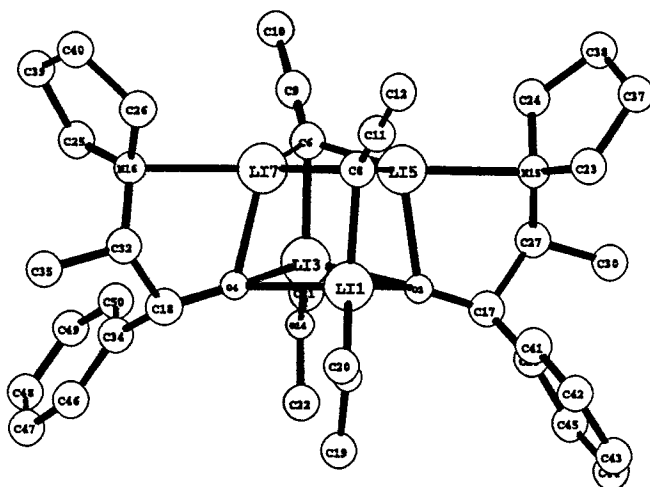


Figure IXA

$(\text{LiCCCH}_3)_2 \cdot [R,S\text{-LiOCH(Ph)CH(Me)N(CH}_2)_4]_2 \cdot (\text{Me}_2\text{O})_2$
 $\Delta H_f^\circ = -271.1 \text{ kcal/mol}$

| | | | | | | | |
|----|---------|---------|---------|---|---------|---------|---------|
| Li | .0000 | .0000 | .0000 | C | 3.8065 | -2.7782 | -4.1442 |
| O | 2.2238 | .0000 | .0000 | C | 4.3813 | -1.4549 | -4.6703 |
| Li | 1.8392 | 2.2493 | .0000 | C | -2.6861 | 5.6183 | -2.7354 |
| O | -.3344 | 2.2080 | .4616 | C | -3.3831 | 4.3942 | -3.3471 |
| Li | 1.7060 | .4631 | -2.0571 | C | 1.8193 | -2.9114 | .4642 |
| C | 1.7738 | 2.6126 | -2.1359 | C | 1.5384 | -4.1528 | 1.0700 |
| Li | -.2610 | 2.1095 | -1.7073 | C | 2.3642 | -4.6553 | 2.0870 |
| C | -.3826 | .0048 | -2.1350 | C | 3.4751 | -3.9018 | 2.5007 |
| C | 2.2523 | 3.4461 | -2.9047 | C | 3.7581 | -2.6685 | 1.8910 |
| C | 2.8243 | 4.4265 | -3.8028 | C | -1.3973 | 4.4888 | 3.0547 |
| C | -1.0231 | -.6981 | -2.9164 | C | -.9717 | 5.6053 | 3.7931 |
| C | -1.7842 | -1.5223 | -3.8310 | C | .0433 | 6.4372 | 3.2924 |
| O | -1.2987 | -1.1852 | 1.4514 | C | .6319 | 6.1292 | 2.0566 |
| O | 3.4331 | 3.1950 | 1.3308 | C | .2092 | 5.0040 | 1.3202 |
| N | 3.5562 | -1.0819 | -2.3721 | | | | |
| N | -2.1113 | 3.6511 | -1.3641 | | | | |
| C | 3.3099 | -.7762 | .2119 | | | | |
| C | -1.3394 | 2.9165 | 1.0229 | | | | |
| C | -.9414 | -1.0554 | 2.8056 | | | | |
| C | -2.4967 | -1.8358 | 1.1147 | | | | |
| C | 4.5353 | 3.9356 | .8741 | | | | |
| C | 3.3650 | 2.8241 | 2.6858 | | | | |
| C | 3.1938 | -2.4731 | -2.7563 | | | | |
| C | 4.1075 | -.3920 | -3.5793 | | | | |
| C | -1.8081 | 5.0927 | -1.5744 | | | | |
| C | -2.9149 | 3.1669 | -2.5288 | | | | |
| C | 4.2811 | -.8323 | -1.0876 | | | | |
| H | 3.9898 | -.2715 | .9795 | | | | |
| C | 2.9516 | -2.1498 | .8445 | | | | |
| C | 5.5558 | -1.6866 | -.8809 | | | | |
| H | 4.6649 | .2290 | -1.1535 | | | | |
| C | -2.5579 | 3.1754 | -.0180 | | | | |
| H | -1.8539 | 2.2769 | 1.8179 | | | | |
| C | -.8339 | 4.1692 | 1.7917 | | | | |
| C | -3.7456 | 3.9610 | .5900 | | | | |
| H | -2.9670 | 2.1343 | -1.1809 | | | | |

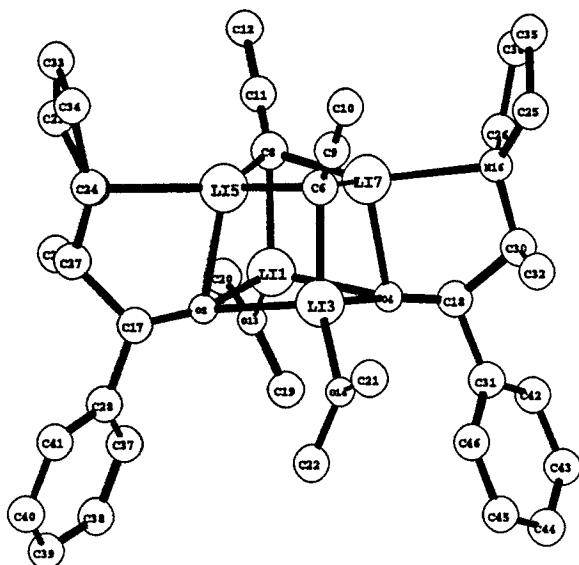


Figure IXB

$(\text{LiCCCH}_3)_2 \cdot [R,S\text{-LiOCH(Ph)CH(Me)N(CH}_2)_4]_2 \cdot (\text{Me}_2\text{O})_2$
 $\Delta H_f^\circ = -267.7 \text{ kcal/mol}$

| | | | | | | | |
|----|---------|---------|---------|---|---------|---------|---------|
| Li | .0000 | .0000 | .0000 | C | 3.5691 | -1.3678 | -4.9881 |
| O | 2.2711 | .0000 | .0000 | C | 4.6753 | -.4261 | -4.4900 |
| Li | 1.8332 | 2.2233 | .0000 | C | -2.8717 | 4.3710 | -3.6235 |
| O | -.3573 | 2.1791 | .5508 | C | -3.8576 | 3.3468 | -3.0410 |
| Li | 1.6451 | .4397 | -2.0724 | C | 2.8928 | -1.7124 | 2.3338 |
| C | 1.7458 | 2.5839 | -2.1379 | C | 3.3144 | -2.2785 | 3.5529 |
| Li | -.2934 | 2.1647 | -1.6485 | C | 4.6767 | -2.5013 | 3.8007 |
| C | -.4595 | .0736 | -2.1205 | C | 5.6179 | -2.1507 | 2.8176 |
| C | 2.2576 | 3.3205 | -2.9802 | C | 5.1946 | -1.5840 | 1.6047 |
| C | 2.8671 | 4.1869 | -3.9669 | C | -2.8137 | 3.2336 | 3.0847 |
| C | -1.1859 | -.4813 | -2.9452 | C | -2.9321 | 3.5278 | 4.4528 |
| C | -2.0397 | -1.1340 | -3.9152 | C | -1.7844 | 3.7738 | 5.2247 |
| O | -1.2485 | -1.4331 | 1.2795 | C | -.5236 | 3.7209 | 4.6111 |
| O | 3.3628 | 3.4318 | 1.1739 | C | -.4089 | 3.4282 | 3.2384 |
| N | 3.3530 | -1.1741 | -2.5562 | | | | |
| N | -2.0765 | 3.7450 | -1.3933 | | | | |
| C | 3.4184 | -.7155 | -.0331 | | | | |
| C | -1.4849 | 2.8249 | .9247 | | | | |
| C | -1.4331 | -1.0856 | 2.6298 | | | | |
| C | -2.0294 | -2.4630 | .7282 | | | | |
| C | 4.0449 | 4.5689 | .7106 | | | | |
| C | 3.7638 | 2.8383 | 2.3845 | | | | |
| C | 2.9440 | -2.0044 | -3.7261 | | | | |
| C | 4.5759 | -.4079 | -2.9468 | | | | |
| C | -1.9379 | 4.7781 | -2.4606 | | | | |
| C | -3.3800 | 3.0444 | -1.6019 | | | | |
| C | 3.4153 | -1.8378 | -1.2062 | | | | |
| C | 3.8205 | -1.3564 | 1.3280 | | | | |
| C | 2.3242 | -2.9202 | -1.0085 | | | | |
| C | -1.7899 | 4.1446 | .0295 | | | | |
| C | -1.5499 | 3.1805 | 2.4407 | | | | |
| C | -.6895 | 5.2297 | .1521 | | | | |

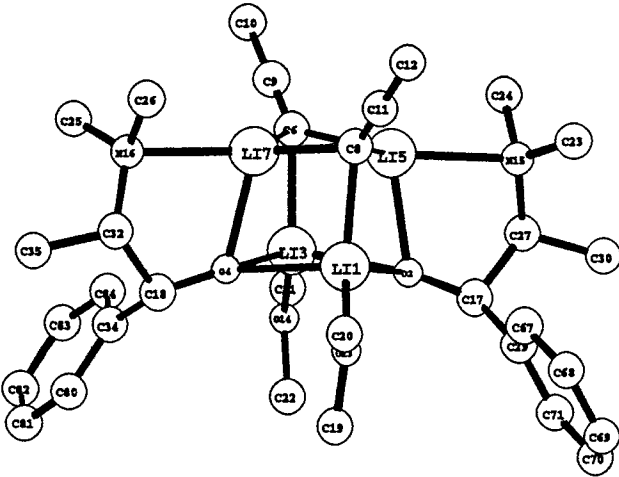


Figure IXC

$(\text{LiCCCH}_3)_2 \cdot [R,S\text{-LiOCH(Ph)CH(Me)N(CH}_2)_4]_2 \cdot (\text{Me}_2\text{O})_2$
 $\Delta H_f^\circ = -255.1 \text{ kcal/mol}$

| | | | | | | | | | | | |
|----|---------|---------|---------|---|---------|---------|---------|---|---------|---------|---------|
| Li | .0000 | .0000 | .0000 | H | -3.0851 | 2.3260 | .0520 | C | 3.5561 | -2.6913 | 1.9963 |
| O | 2.2261 | .0000 | .0000 | H | 2.4327 | 5.5145 | -3.4850 | H | 1.0403 | -2.5320 | -.3330 |
| Li | 1.8445 | 2.2561 | .0000 | H | 3.8205 | 4.4457 | -3.8648 | H | .4411 | -4.6518 | .7522 |
| O | -.3318 | 2.2138 | .4673 | H | 2.3230 | 4.3522 | -4.8455 | H | 1.7974 | -5.5576 | 2.6427 |
| Li | 1.7229 | .4827 | -2.0573 | H | -1.4539 | -2.6434 | -3.7008 | H | 3.7894 | -4.2782 | 3.4504 |
| C | 1.7527 | 2.6292 | -2.1365 | H | -2.7773 | -1.4369 | -3.7717 | H | 4.4291 | -2.1603 | 2.3818 |
| Li | -.2766 | 2.1013 | -1.7031 | H | -1.4086 | -1.3339 | -4.9245 | H | 5.0008 | -3.0722 | -.7614 |
| C | -.3619 | .0007 | -2.1410 | H | 2.7765 | -3.0138 | -2.0675 | H | 6.0995 | -2.0104 | -1.6847 |
| C | 2.1839 | 3.4831 | -2.9109 | H | 3.9912 | -2.8812 | -3.3785 | H | 5.9675 | -1.8257 | .0773 |
| C | 2.7096 | 4.4874 | -3.8112 | H | 2.3396 | -2.2086 | -3.6134 | C | -1.1668 | 4.4979 | 3.1282 |
| C | -.9577 | -.7216 | -2.9399 | H | 4.3903 | .8577 | -2.9994 | C | -.6627 | 5.5863 | 3.8589 |
| C | -1.6764 | -1.5664 | -3.8701 | H | 3.4150 | -.0412 | -4.2314 | C | .3532 | 6.3905 | 3.3162 |
| O | -1.3639 | -1.1416 | 1.4397 | H | 5.0852 | -.5776 | -3.8260 | C | .8647 | 6.0823 | 2.0465 |
| O | 3.4991 | 3.1570 | 1.2991 | H | -1.2470 | 5.5275 | -.8925 | C | .3649 | 4.9836 | 1.3178 |
| N | 3.5613 | -1.0235 | -2.3311 | H | -2.7083 | 5.5980 | -1.9276 | H | -1.9501 | 3.8929 | 3.5900 |
| N | -2.1043 | 3.5972 | -1.3240 | H | -1.1528 | 5.0057 | -2.6094 | H | -1.0620 | 5.8065 | 4.8496 |
| C | 3.2657 | -.8247 | .2541 | H | -3.0862 | 1.8428 | -2.1179 | H | .7405 | 7.2419 | 3.8759 |
| C | -1.2805 | 2.9639 | 1.0695 | H | -2.3765 | 2.9597 | -3.3531 | H | 1.6555 | 6.6992 | 1.6172 |
| C | -1.0486 | -.9957 | 2.8026 | H | -3.9152 | 3.3847 | -2.5203 | H | .8040 | 4.7869 | .3329 |
| C | -2.5682 | -1.7648 | 1.0750 | H | -.0643 | -.4712 | 2.8755 | H | -3.1469 | 5.3213 | .8376 |
| C | 4.6145 | 3.8504 | .8021 | H | -.9642 | -1.9870 | 3.3155 | H | -4.4337 | 4.4136 | -.0033 |
| C | 3.4720 | 2.7750 | 2.6524 | H | -1.8187 | -.3943 | 3.3478 | H | -3.9400 | 3.9327 | 1.6342 |
| C | 3.1572 | -2.3413 | -2.8645 | H | -2.6098 | -1.8065 | -.0398 | | | | |
| C | 4.1441 | -.1592 | -3.3894 | H | -3.4599 | -1.1997 | 1.4455 | | | | |
| C | -1.7957 | 4.9938 | -1.6965 | H | -2.6339 | -2.8091 | 1.4716 | | | | |
| C | -2.9105 | 2.9164 | -2.3695 | H | 4.4222 | 4.0860 | -.2720 | | | | |
| C | 4.2699 | -.9688 | -1.0126 | H | 5.5505 | 3.2415 | .8732 | | | | |
| H | 3.9521 | -.3412 | 1.0292 | H | 4.7866 | 4.8106 | 1.3504 | | | | |
| C | 2.8180 | -2.1645 | .9043 | H | 2.5133 | 2.2317 | 2.8392 | | | | |
| C | 5.3785 | -2.0341 | -.8401 | H | 3.5185 | 3.6623 | 3.3331 | | | | |
| H | 4.8294 | .0117 | -.9927 | H | 4.3255 | 2.1002 | 2.9135 | | | | |
| C | -2.5237 | 3.3051 | .0838 | C | 1.6717 | -2.8867 | .4897 | | | | |
| H | -1.7995 | 2.3424 | 1.8758 | C | 1.3152 | -4.1033 | 1.1067 | | | | |
| C | -.6827 | 4.1802 | 1.8322 | C | 2.0748 | -4.6158 | 2.1693 | | | | |
| C | -3.5519 | 4.3054 | .6634 | C | 3.1961 | -3.8983 | 2.6179 | | | | |

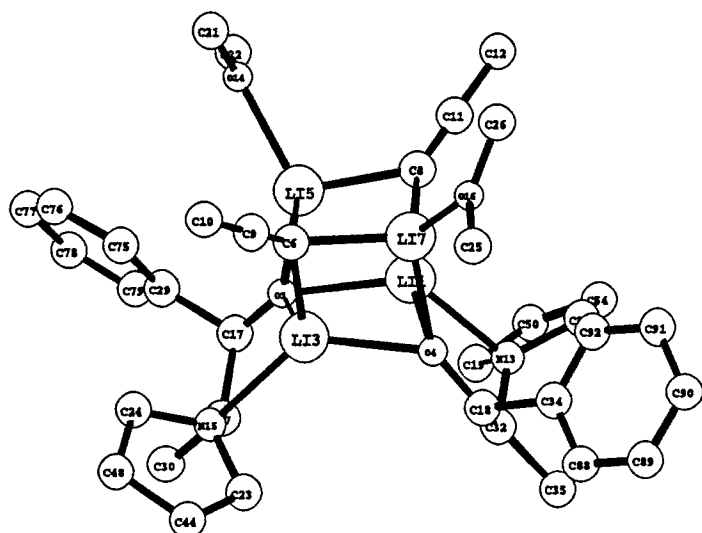


Figure IXD

$(\text{LiCCCH}_3)_2 \cdot [R,S\text{-LiOCH(Ph)CH(Me)N(CH}_2)_4]_2 \cdot (\text{Me}_2\text{O})_2$

$\Delta H_f^\circ = -270.2 \text{ kcal/mol}$

| | | | | | | | | | | | |
|----|---------|---------|---------|---|---------|---------|---------|---|---------|---------|---------|
| Li | .0000 | .0000 | .0000 | H | -.1921 | .8157 | 3.0450 | H | -1.2135 | 5.6116 | -3.2954 |
| O | 2.2759 | .0000 | .0000 | H | 3.6311 | 5.1653 | -2.7888 | H | -2.0034 | 2.1384 | -4.3545 |
| Li | 1.8280 | 2.1155 | .0000 | H | 3.7715 | 4.0299 | -4.1679 | H | -1.9187 | 3.8250 | -5.0152 |
| O | -.3773 | 2.0271 | .5800 | H | 2.3481 | 5.1111 | -4.0394 | H | -3.3530 | 3.3115 | -4.0395 |
| Li | 1.6769 | .4220 | -2.1249 | H | -2.5224 | -2.4167 | -2.8297 | C | 5.0217 | -.4505 | -1.0978 |
| C | 1.7445 | 2.6127 | -2.0471 | H | -2.8222 | -1.1016 | -4.0092 | C | 6.1374 | -1.0229 | -1.7414 |
| Li | -.3113 | 2.1053 | -1.6865 | H | -1.4518 | -2.2294 | -4.2547 | C | 6.7106 | -2.2085 | -1.2572 |
| C | -.4248 | -.0419 | -2.0742 | H | 2.1687 | 3.3823 | 2.1455 | C | 6.1534 | -2.8248 | -.1244 |
| C | 2.3511 | 3.4712 | -2.6878 | C | 4.1582 | 4.3323 | 2.3180 | C | 5.0479 | -2.2474 | .5215 |
| C | 3.0523 | 4.4828 | -3.4496 | H | 3.1816 | 2.7619 | 3.4848 | H | 4.6034 | .4643 | -1.5286 |
| C | -1.1611 | -.7878 | -2.7200 | H | 4.8193 | 2.5783 | -.2598 | H | 6.5575 | -.5389 | -2.6242 |
| C | -2.0219 | -1.6672 | -3.4820 | H | 5.8398 | 1.8318 | 1.0030 | H | 7.5747 | -2.6482 | -1.7551 |
| N | -1.4757 | -.3502 | 1.8605 | C | 5.3230 | 3.9207 | 1.4061 | H | 6.5796 | -3.7539 | .2558 |
| O | 2.5208 | -.7032 | -3.9652 | H | .1615 | -1.7357 | 1.8472 | H | 4.6400 | -2.7641 | 1.3928 |
| N | 3.7216 | 2.0533 | 1.4876 | C | -1.7516 | -2.7695 | 2.2471 | H | 5.7357 | .0562 | 2.4130 |
| O | -1.5783 | 3.5731 | -2.9595 | H | -.5120 | -1.4576 | 3.4822 | H | 4.9278 | .9277 | 3.7410 |
| C | 3.2492 | -.4384 | .8281 | H | -2.9533 | -.5134 | .3364 | H | 4.4999 | -.7641 | 3.4064 |
| C | -1.1155 | 2.2407 | 1.6913 | H | -3.6459 | -.1046 | 1.9320 | C | -2.8670 | 4.0415 | 2.2252 |
| C | -.7962 | -1.5643 | 2.4063 | C | -3.0843 | -2.2109 | 1.7277 | C | -4.0755 | 4.7240 | 2.0090 |
| C | -2.8546 | -.7104 | 1.4327 | H | 3.6190 | 5.2135 | 1.9087 | C | -4.9143 | 4.3540 | .9446 |
| C | 2.8212 | -.0655 | -5.1796 | H | 4.5217 | 4.6369 | 3.3228 | C | -4.5195 | 3.3099 | .0949 |
| C | 2.6803 | -2.0964 | -3.8630 | H | 6.2802 | 3.8940 | 1.9707 | C | -3.3017 | 2.6334 | .3080 |
| C | 3.2211 | 3.1067 | 2.4219 | H | 5.4736 | 4.6527 | .5848 | H | -2.2408 | 4.3660 | 3.0590 |
| C | 4.9789 | 2.5221 | .8455 | H | -1.3309 | -3.5213 | 1.5452 | H | -4.3620 | 5.5429 | 2.6698 |
| C | -1.6282 | 4.9104 | -2.5281 | H | -1.8861 | -3.2978 | 3.2152 | H | -5.8577 | 4.8743 | .7796 |
| C | -2.2435 | 3.2073 | -4.1406 | H | -3.8937 | -2.3466 | 2.4773 | H | -5.1597 | 3.0177 | -.7387 |
| C | 3.6139 | .6451 | 1.9809 | H | -3.4198 | -2.7491 | .8160 | H | -3.0334 | 1.8396 | -.3954 |
| H | 2.8498 | -1.3055 | 1.4560 | H | 2.5494 | 1.0127 | -5.0795 | H | -3.1939 | 1.3311 | 3.6343 |
| C | 4.4662 | -1.0342 | .0663 | H | 2.2452 | -.4976 | -6.0360 | H | -2.1318 | .2057 | 4.5184 |
| C | 4.7618 | .1987 | 2.9198 | H | 3.9103 | -.1385 | -5.4262 | H | -1.7495 | 1.9407 | 4.4881 |
| H | 2.6942 | .6268 | 2.6370 | H | 2.3256 | -2.4107 | -2.8512 | | | | |
| C | -1.2349 | .9156 | 2.6216 | H | 3.7510 | -2.3994 | -3.9798 | | | | |
| H | -.5500 | 2.9507 | 2.3859 | H | 2.0846 | -2.6441 | -4.6358 | | | | |
| C | -2.4596 | 2.9633 | 1.3960 | H | -1.0145 | 4.9959 | -1.5982 | | | | |
| C | -2.1353 | 1.1052 | 3.8671 | H | -2.6743 | 5.2347 | -2.2998 | | | | |

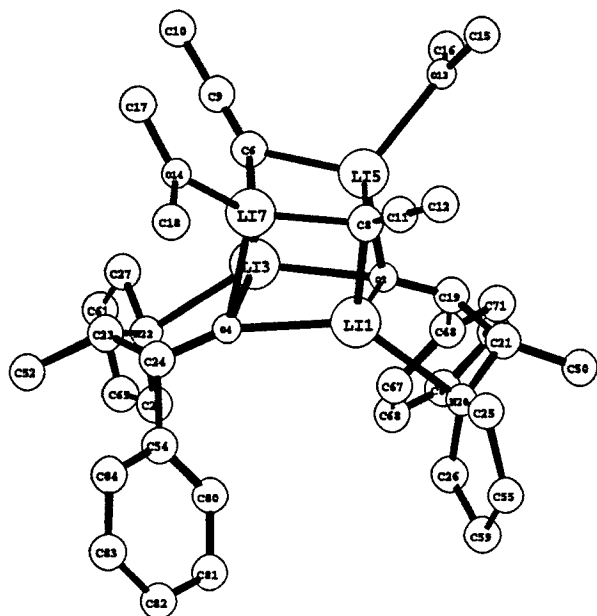
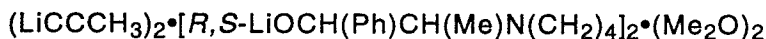


Figure IXE



$\Delta H_f^\circ = -266.5 \text{ kcal/mol}$

| | | | | | | | | | | | |
|----|---------|---------|---------|---|---------|---------|---------|---|---------|---------|--------|
| Li | .0000 | .0000 | .0000 | H | -3.3031 | -1.4658 | -2.8727 | C | 3.8096 | 4.7195 | 1.9513 |
| O | 2.1753 | .0000 | .0000 | H | -2.4529 | -1.1702 | -4.4227 | H | 2.9801 | 2.7325 | 2.4858 |
| Li | 1.7127 | 2.2359 | .0000 | H | 1.2927 | -1.4395 | -4.6344 | C | 4.9492 | .1312 | .9382 |
| O | -4.160 | 2.2041 | .4294 | H | 2.8053 | -2.4412 | -4.6843 | C | 6.3444 | .1624 | 1.1284 |
| Li | 1.6342 | .4533 | -2.1454 | H | 2.6334 | -1.0101 | -5.7785 | C | 7.1052 | -1.0111 | 1.0143 |
| C | 1.7806 | 2.5730 | -2.1298 | H | 4.5136 | .3317 | -2.8285 | C | 6.4585 | -2.2189 | .7032 |
| Li | -.3077 | 2.0835 | -1.8291 | H | 4.6776 | .1573 | -4.6290 | C | 5.0672 | -2.2465 | .5133 |
| C | -.4799 | -.0184 | -2.1059 | H | 4.8801 | -1.2896 | -3.5621 | H | 4.4028 | 1.0725 | 1.0356 |
| C | 2.4964 | 3.3717 | -2.7341 | H | -.4397 | 4.3237 | -4.0357 | H | 6.8358 | 1.1066 | 1.3666 |
| C | 3.3186 | 4.3131 | -3.4644 | H | -1.9196 | 5.2978 | -3.6420 | H | 8.1845 | -.9862 | 1.1637 |
| C | -1.3296 | -.6978 | -2.6821 | H | -1.9845 | 4.0430 | -4.9444 | H | 7.0375 | -3.1381 | .6077 |
| C | -2.3099 | -1.5088 | -3.3724 | H | -3.2664 | 2.2585 | -1.9100 | H | 4.6047 | -3.2040 | .2646 |
| O | 2.9192 | -.5689 | -3.7489 | H | -3.7787 | 2.6905 | -3.5984 | H | 1.7919 | -.1060 | 3.0514 |
| O | -1.8719 | 3.3086 | -2.9838 | H | -3.7480 | 3.9632 | -2.3131 | H | 1.8916 | -1.7027 | 3.8641 |
| C | 2.4014 | -1.4002 | -4.7556 | H | 2.6508 | -1.9425 | -.4420 | H | 3.3408 | -.9883 | 3.1606 |
| C | 4.3056 | -.3389 | -3.6973 | C | 4.2750 | -1.0750 | .6329 | C | -2.9536 | 1.8749 | 1.8492 |
| C | -1.5511 | 4.2846 | -3.9414 | H | 2.4587 | -2.8559 | 1.7889 | C | -4.2838 | 1.7860 | 2.3036 |
| C | -3.2241 | 3.0514 | -2.6957 | C | 2.2505 | -1.1118 | 2.9942 | C | -5.0350 | 2.9473 | 2.5393 |
| C | 2.7388 | -1.1646 | .3905 | H | -.2996 | 4.7575 | 2.6409 | C | -4.4457 | 4.2022 | 2.3118 |
| N | .5381 | -2.0341 | 1.3201 | C | .1086 | 2.8596 | 3.5175 | C | -3.1195 | 4.2876 | 1.8574 |
| C | 1.9897 | -1.8399 | 1.6565 | H | -.9505 | 4.1802 | .3902 | H | -2.4125 | .9408 | 1.6786 |
| N | 1.4768 | 4.0347 | 1.6903 | C | -2.3359 | 3.1277 | 1.6223 | H | -4.7321 | .8060 | 2.4725 |
| C | .1166 | 3.7766 | 2.2741 | C | -1.1981 | -3.6861 | .7818 | H | -6.0635 | 2.8776 | 2.8931 |
| C | -.8780 | 3.2848 | 1.0964 | H | .9523 | -4.0788 | .6749 | H | -5.0190 | 5.1132 | 2.4871 |
| C | .2480 | -3.2320 | .4778 | H | .3676 | -2.9696 | -.6012 | H | -2.7024 | 5.2818 | 1.6838 |
| C | -.4848 | -1.9680 | 2.4002 | H | -.1255 | -2.3852 | 3.3739 | H | .5503 | 1.8608 | 3.3378 |
| C | 1.6188 | 5.3510 | .9999 | C | -1.7024 | -2.8003 | 1.9321 | H | .6424 | 3.3217 | 4.3756 |
| C | 2.6925 | 3.8123 | 2.5204 | H | -.7621 | -.9021 | 2.5913 | H | -.9301 | 2.7026 | 3.8752 |
| H | 3.0071 | 5.3640 | -3.2725 | C | 3.1061 | 5.7669 | 1.0738 | H | -1.8476 | -3.5955 | -.1142 |
| H | 4.3908 | 4.2281 | -3.1801 | H | .9869 | 6.1503 | 1.4627 | H | -1.2201 | -4.7604 | 1.0668 |
| H | 3.2530 | 4.1445 | -4.5625 | H | 1.2799 | 5.2586 | -.0601 | H | -2.5395 | -2.1480 | 1.6023 |
| H | -2.0036 | -2.5780 | -3.4090 | H | 2.5435 | 4.0693 | 3.5989 | H | -2.1043 | -3.4120 | 2.7681 |

| | | | |
|---|--------|--------|--------|
| H | 3.5623 | 5.8206 | .0629 |
| H | 3.2075 | 6.7849 | 1.5084 |
| H | 4.5502 | 4.1343 | 1.3645 |
| H | 4.3828 | 5.1984 | 2.7738 |

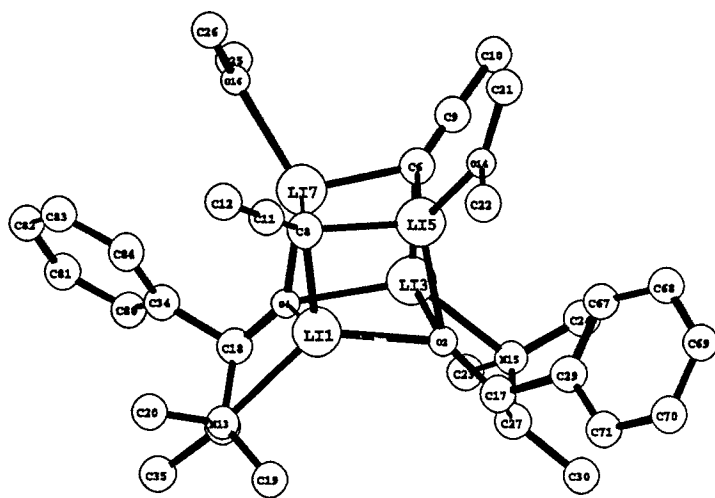
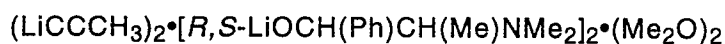


Figure IXF



$\Delta H_f^\circ = -254.5 \text{ kcal/mol}$

| | | | | | | | | | | | |
|----|---------|---------|---------|---|---------|---------|---------|---|---------|---------|---------|
| Li | .0000 | .0000 | .0000 | C | 5.0415 | .2170 | 2.6573 | H | 3.3862 | -2.5403 | -4.2838 |
| O | 2.2709 | .0000 | .0000 | H | 2.9460 | .5484 | 2.6477 | H | 1.6253 | -2.4730 | -4.6871 |
| Li | 1.8304 | 2.1130 | .0000 | C | -1.3415 | .9782 | 2.5960 | H | -9.9564 | 5.0344 | -1.6693 |
| O | -3.586 | 2.0467 | .5872 | H | -5.953 | 2.9945 | 2.3752 | H | -2.4693 | 5.4377 | -2.5889 |
| Li | 1.6492 | .4250 | -2.1355 | C | -2.4514 | 3.0406 | 1.2880 | H | -8.650 | 5.5233 | -3.4180 |
| C | 1.7335 | 2.6124 | -2.0498 | C | -2.3532 | 1.1579 | 3.7525 | H | -2.1765 | 2.1062 | -4.2570 |
| Li | -3.277 | 2.1230 | -1.6791 | H | -3.451 | .8955 | 3.1203 | H | -1.6538 | 3.6342 | -5.0859 |
| C | -4.530 | -.0305 | -2.0607 | H | 3.0653 | 5.4691 | -2.8687 | H | -3.2487 | 3.5687 | -4.2344 |
| C | 2.3640 | 3.4736 | -2.6633 | H | 4.1636 | 4.2120 | -3.5217 | C | 4.9201 | -.4878 | -1.2914 |
| C | 3.0935 | 4.4884 | -3.3935 | H | 2.6685 | 4.6449 | -4.4101 | C | 5.9734 | -1.0777 | -2.0191 |
| C | -1.2388 | -.7545 | -2.6721 | H | -2.1074 | -2.6603 | -3.0315 | C | 6.5538 | -2.2802 | -1.5876 |
| C | -2.1550 | -1.6101 | -3.3959 | H | -3.2082 | -1.2688 | -3.2851 | C | 6.0680 | -2.8961 | -.4223 |
| N | -1.5158 | -.2866 | 1.8131 | H | -1.9258 | -1.6264 | -4.4848 | C | 5.0254 | -2.3017 | .3076 |
| O | 2.4702 | -.6728 | -4.0177 | H | 2.1530 | 2.6174 | 2.6966 | H | 4.4973 | .4463 | -1.6765 |
| N | 3.7659 | 2.0299 | 1.3789 | H | 2.8767 | 3.9542 | 1.7097 | H | 6.3410 | -.5936 | -2.9249 |
| O | -1.5619 | 3.5907 | -2.9908 | H | 3.7491 | 3.3060 | 3.1462 | H | 7.3693 | -2.7334 | -2.1512 |
| C | 3.2928 | -.4579 | .7559 | H | 5.5224 | 1.8251 | .1481 | H | 6.5013 | -3.8373 | -.0821 |
| C | -1.1421 | 2.2903 | 1.6608 | H | 5.7389 | 2.9285 | 1.5447 | H | 4.6715 | -2.8173 | 1.2029 |
| C | -.6788 | -1.4283 | 2.2636 | H | 4.7535 | 3.4483 | .1326 | H | 5.9554 | .1573 | 2.0348 |
| C | -2.8825 | -.7182 | 1.4549 | H | .3664 | -1.1082 | 2.4945 | H | 5.2518 | .9306 | 3.4822 |
| C | 2.7909 | -.0225 | -5.2201 | H | -.6350 | -2.2108 | 1.4617 | H | 4.8999 | -.7759 | 3.1328 |
| C | 2.4095 | -2.0776 | -3.9938 | H | -1.0769 | -1.9240 | 3.1842 | C | -2.8836 | 4.1299 | 2.0888 |
| C | 3.1087 | 3.0147 | 2.2762 | H | -3.5237 | .1378 | 1.1576 | C | -4.0621 | 4.8373 | 1.7994 |
| C | 5.0023 | 2.5742 | .7811 | H | -3.4074 | -1.2491 | 2.2878 | C | -4.8445 | 4.4802 | .6887 |
| C | -1.4626 | 4.9545 | -2.6622 | H | -2.8397 | -1.4229 | .5901 | C | -4.4248 | 3.4224 | -.1321 |
| C | -2.1860 | 3.2205 | -4.1930 | H | 2.8056 | 1.0762 | -5.0239 | C | -3.2370 | 2.7194 | .1542 |
| C | 3.7673 | .6170 | 1.8763 | H | 2.0397 | -.2320 | -6.0223 | H | -2.3000 | 4.4450 | 2.9565 |
| H | 2.9233 | -1.3173 | 1.4118 | H | 3.7970 | -.3273 | -5.6034 | H | -4.3681 | 5.6662 | 2.4387 |
| C | 4.4391 | -1.0734 | -.0948 | H | 2.1612 | -2.3949 | -2.9517 | H | -5.7647 | 5.0203 | .4660 |

| | | | |
|---|---------|--------|---------|
| H | -5.0233 | 3.1396 | -9.9993 |
| H | -2.9521 | 1.9074 | -5.235 |
| H | -3.3966 | 1.3250 | 3.4211 |
| H | -2.3599 | .2745 | 4.4260 |
| H | -2.0630 | 2.0260 | 4.3803 |

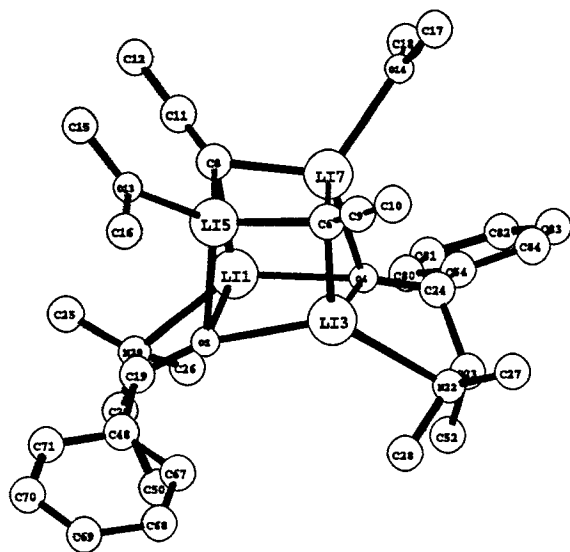


Figure IXG

$(\text{LiC}(\text{C}\text{H}_3)_2)_2 \cdot [R,S\text{-LiOCH}(\text{Ph})\text{CH}(\text{Me})\text{NMe}_2]_2 \cdot (\text{Me}_2\text{O})_2$
 $\Delta H_f^\circ = -251.6 \text{ kcal/mol}$

| | | | | | | | | | | | |
|----|---------|---------|---------|---|---------|---------|---------|---|---------|---------|--------|
| Li | .0000 | .0000 | .0000 | C | 2.6653 | 3.3331 | 2.2704 | H | -1.0022 | -3.2084 | .2624 |
| O | 2.1811 | .0000 | .0000 | H | 2.8058 | 5.5281 | -3.0927 | H | .0673 | -4.1500 | 1.3618 |
| Li | 1.6910 | 2.2442 | .0000 | H | 4.2361 | 4.4477 | -3.0716 | H | .6762 | -3.5971 | -.2403 |
| O | -.4306 | 2.2005 | .5071 | H | 3.0920 | 4.3933 | -4.4503 | H | -.5602 | -2.1405 | 3.1107 |
| Li | 1.5965 | .5090 | -2.1512 | H | -1.8728 | -2.7065 | -3.2961 | H | -1.4636 | -1.4015 | 1.7471 |
| C | 1.7046 | 2.6291 | -2.1015 | H | -3.2353 | -1.6855 | -2.7349 | H | -.1379 | -.4732 | 2.5678 |
| Li | -.3744 | 2.0813 | -1.7780 | H | -2.4569 | -1.3522 | -4.3147 | H | 2.7954 | 5.3797 | .5811 |
| C | -.5117 | -.0169 | -2.0734 | H | 1.2449 | -1.2778 | -4.7125 | H | 2.0237 | 6.0929 | 2.0421 |
| C | 2.3825 | 3.4895 | -2.6635 | H | 2.7666 | -2.2618 | -4.8162 | H | 1.0541 | 5.8134 | .5504 |
| C | 3.1591 | 4.5036 | -3.3450 | H | 2.5690 | -.7917 | -5.8530 | H | 3.0020 | 3.8222 | 3.2188 |
| C | -1.3204 | -.7697 | -2.6165 | H | 4.4670 | .4618 | -2.8779 | H | 3.5475 | 3.3481 | 1.5757 |
| C | -2.2573 | -1.6628 | -3.2649 | H | 4.5947 | .3853 | -4.6884 | H | 2.4286 | 2.2664 | 2.5090 |
| O | 2.8729 | -.4268 | -3.8104 | H | 4.8531 | -1.1099 | -3.7033 | C | 4.9775 | -.0621 | .9469 |
| O | -1.9838 | 3.2615 | -2.9071 | H | -.5939 | 4.2786 | -4.0125 | C | 6.3772 | -.0925 | 1.1007 |
| C | 2.3518 | -1.2229 | -4.8435 | H | -2.0748 | 5.2400 | -3.5910 | C | 7.1012 | -1.2535 | .7910 |
| C | 4.2547 | -.1673 | -3.7764 | H | -2.1593 | 3.9666 | -4.8743 | C | 6.4124 | -2.3846 | .3218 |
| C | -1.7017 | 4.2274 | -3.8869 | H | -3.3343 | 2.2009 | -1.7885 | C | 5.0168 | -2.3486 | .1685 |
| C | -3.3246 | 2.9769 | -2.5920 | H | -3.8832 | 2.5818 | -3.4777 | H | 4.4597 | .8639 | 1.2027 |
| C | 2.7181 | -1.2095 | .2739 | H | -3.8658 | 3.8834 | -2.2214 | H | 6.8995 | .7938 | 1.4633 |
| N | .5101 | -2.0276 | 1.2146 | H | 2.5764 | -1.9096 | -.6196 | H | 8.1842 | -1.2780 | .9115 |
| C | 1.9865 | -1.9899 | 1.4909 | C | 4.2617 | -1.1899 | .4822 | H | 6.9621 | -3.2936 | .0748 |
| N | 1.5184 | 4.0193 | 1.6334 | H | 2.3696 | -3.0479 | 1.4293 | H | 4.5210 | -3.2468 | -.2059 |
| C | .1460 | 3.9045 | 2.2345 | C | 2.3859 | -1.5355 | 2.9120 | H | 2.2115 | -.4596 | 3.1077 |
| C | -.8646 | 3.3330 | 1.1028 | H | -.2184 | 4.9492 | 2.4484 | H | 1.8542 | -2.1159 | 3.6962 |
| C | .0463 | -3.3049 | .6298 | C | .0779 | 3.2021 | 3.6084 | H | 3.4662 | -1.7277 | 3.0807 |
| C | -.4440 | -1.4875 | 2.2096 | H | -.9196 | 4.1800 | .3358 | C | -2.9297 | 2.0405 | 2.0717 |
| C | 1.8607 | 5.3883 | 1.1893 | C | -2.3179 | 3.2463 | 1.6568 | C | -4.2545 | 2.0152 | 2.5491 |

| | | | | | | | | | | | |
|---|---------|--------|--------|---|---------|--------|--------|---|--------|--------|--------|
| C | -5.0067 | 3.1971 | 2.6228 | H | -4.6966 | 1.0689 | 2.8634 | H | .2687 | 2.1119 | 3.5681 |
| C | -4.4229 | 4.4069 | 2.2105 | H | -6.0313 | 3.1780 | 2.9940 | H | .7903 | 3.6468 | 4.3358 |
| C | -3.1022 | 4.4276 | 1.7335 | H | -4.9964 | 5.3333 | 2.2599 | H | -.9289 | 3.3417 | 4.0548 |
| H | -2.3859 | 1.0950 | 2.0352 | H | -2.6888 | 5.3874 | 1.4164 | | | | |

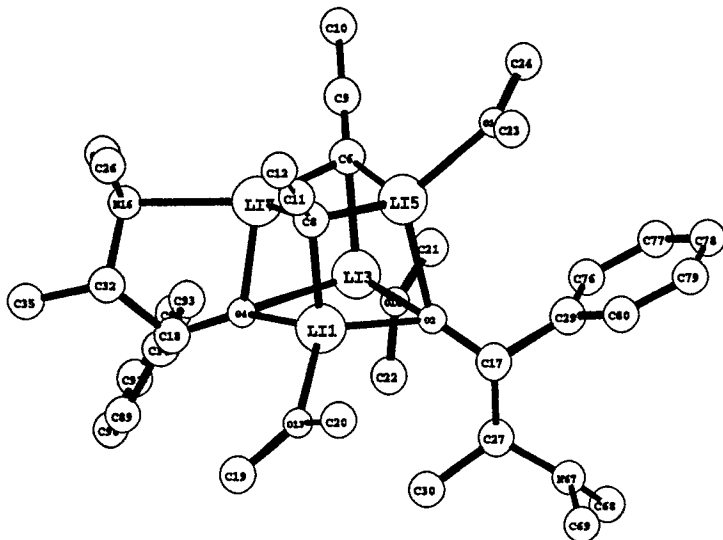
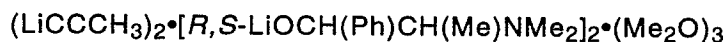


Figure IXH



$\Delta H_f^\circ = -302.5 \text{ kcal/mol}$

| | | | | | | | | | | | |
|----|---------|---------|---------|---|---------|---------|---------|---|---------|---------|---------|
| Li | .0000 | .0000 | .0000 | C | 2.1123 | -.7459 | 2.9503 | H | -2.0566 | -3.2636 | -.0299 |
| O | 2.2199 | .0000 | .0000 | H | 3.8425 | .2141 | 2.1262 | H | -.8978 | -3.7506 | 1.2708 |
| Li | 1.8428 | 2.2179 | .0000 | C | -2.6631 | 3.1291 | .2125 | H | 4.2678 | 4.0853 | -.6093 |
| O | -.3908 | 2.1805 | .5365 | H | -1.8464 | 2.1630 | 1.9616 | H | 5.4423 | 3.8987 | .7601 |
| Li | 1.6452 | .5249 | -2.1299 | C | -.8754 | 4.0795 | 1.9676 | H | 4.3296 | 5.3238 | .7158 |
| C | 1.6244 | 2.6717 | -2.0990 | C | -3.7423 | 4.0464 | .8358 | H | 2.5381 | 2.8891 | 2.9046 |
| Li | -.3891 | 2.1201 | -1.6164 | H | -3.1594 | 2.1158 | .1659 | H | 3.4019 | 4.4818 | 3.0067 |
| C | -.4539 | .0248 | -2.1034 | H | 1.9680 | 5.6637 | -3.3298 | H | 4.3541 | 2.9482 | 2.9556 |
| C | 1.9042 | 3.5887 | -2.8721 | H | 3.3515 | 4.7095 | -3.9520 | N | 4.3699 | -1.7922 | 2.4814 |
| C | 2.2559 | 4.6781 | -3.7585 | H | 1.7489 | 4.5845 | -4.7444 | C | 5.4877 | -1.2843 | 3.2770 |
| C | -1.1708 | -.6353 | -2.8555 | H | -3.0721 | -1.4199 | -3.3915 | C | 3.9667 | -3.1585 | 2.8084 |
| C | -2.0161 | -1.4062 | -3.7421 | H | -2.0150 | -.9896 | -4.7738 | H | 5.9345 | -.3801 | 2.8049 |
| O | -1.1902 | -1.6851 | 1.0438 | H | -1.6785 | -2.4643 | -3.8124 | H | 6.2961 | -2.0487 | 3.3445 |
| O | 3.4226 | 3.4876 | 1.1575 | H | 3.3101 | -2.3603 | -4.5290 | H | 5.2044 | -1.0095 | 4.3236 |
| O | 2.7525 | -.4272 | -3.9249 | H | 1.7935 | -1.7125 | -5.2712 | H | 3.1478 | -3.5194 | 2.1488 |
| N | -2.2967 | 3.4810 | -1.1973 | H | 1.8135 | -2.2015 | -3.5196 | H | 3.6199 | -3.2811 | 3.8652 |
| C | 3.0173 | -.9945 | .4755 | H | 4.6046 | -.2208 | -4.8921 | H | 4.8298 | -3.8511 | 2.6653 |
| C | -1.3813 | 2.8444 | 1.1705 | H | 3.8711 | 1.2701 | -4.1697 | C | 5.2024 | -.0865 | -.6254 |
| C | -2.1217 | -1.4396 | 2.0661 | H | 3.2000 | .5745 | -5.7089 | C | 6.3971 | -.2812 | -1.3449 |
| C | -1.1094 | -2.9758 | .4916 | H | -1.5152 | 5.4369 | -.7294 | C | 6.7322 | -1.5525 | -1.8364 |
| C | 4.4092 | 4.2311 | .4879 | H | -3.0016 | 5.4706 | -1.7270 | C | 5.8570 | -2.6275 | -1.6094 |
| C | 3.4374 | 3.4557 | 2.5628 | H | -1.4393 | 4.9661 | -2.4620 | C | 4.6646 | -2.4303 | -.8918 |
| C | 2.4086 | -1.7263 | -4.3364 | H | -3.2708 | 1.7293 | -2.0070 | H | 4.9888 | .9186 | -.2553 |
| C | 3.6430 | .3220 | -4.7126 | H | -2.6089 | 2.8844 | -3.2318 | H | 7.0679 | .5614 | -1.5177 |
| C | -2.0584 | 4.9008 | -1.5349 | H | -4.1339 | 3.2646 | -2.3535 | H | 7.6607 | -1.7042 | -2.3867 |
| C | -3.1184 | 2.8101 | -2.2377 | H | -1.9655 | -.3970 | 2.4319 | H | 6.1051 | -3.6197 | -1.9881 |
| C | 3.3628 | -.7982 | 2.0354 | H | -1.9909 | -2.1385 | 2.9300 | H | 4.0124 | -3.2925 | -.7381 |
| H | 2.4617 | -1.9854 | .4039 | H | -3.1744 | -1.5393 | 1.6998 | H | 1.4939 | -1.6654 | 2.8988 |
| C | 4.3136 | -1.1593 | -.3695 | H | -.2739 | -2.9835 | -.2496 | H | 2.4028 | -.6089 | 4.0147 |

| | | | | | | | | | | | |
|---|---------|--------|--------|---|---------|--------|--------|---|---------|--------|--------|
| H | 1.4576 | .1141 | 2.6926 | C | .0653 | 5.0072 | 1.4596 | H | .5031 | 4.8821 | .4644 |
| C | -1.3504 | 4.2975 | 3.2878 | H | -2.0488 | 3.5951 | 3.7480 | H | -3.4014 | 5.0829 | 1.0246 |
| C | -.9460 | 5.4094 | 4.0447 | H | -1.3356 | 5.5499 | 5.0536 | H | -4.6437 | 4.1107 | .1899 |
| C | -.0428 | 6.3400 | 3.5044 | H | .2637 | 7.2110 | 4.0835 | H | -4.0844 | 3.6281 | 1.8053 |
| C | .4621 | 6.1313 | 2.2123 | H | 1.1677 | 6.8448 | 1.7844 | | | | |

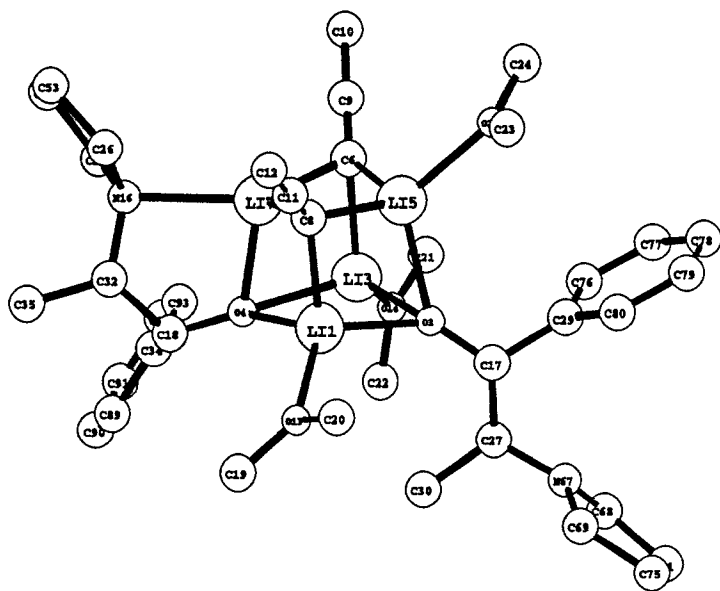


Figure IXi

$(\text{LiCCCH}_3)_2 \cdot [R,S\text{-LiOCH(Ph)CH(Me)NMe}_2]_2 \cdot (\text{Me}_2\text{O})_3$
 $\Delta H_f^\circ = -321.2 \text{ kcal/mol}$

| | | | | | | | | | | | |
|----|---------|---------|---------|---|---------|---------|---------|---|---------|---------|---------|
| Li | .0000 | .0000 | .0000 | H | 2.4999 | -1.9791 | .4122 | H | -1.8911 | -.4285 | 2.4860 |
| O | 2.2118 | .0000 | .0000 | C | 4.3254 | -1.1104 | -.3825 | H | -1.9531 | -2.1815 | 2.9376 |
| Li | 1.8382 | 2.2135 | .0000 | C | 2.1303 | -.6965 | 2.9421 | H | -3.1415 | -1.5200 | 1.7447 |
| O | -.3931 | 2.1888 | .5283 | H | 3.8772 | .2398 | 2.1158 | H | -.3095 | -2.9771 | -.2962 |
| Li | 1.6229 | .5209 | -2.1293 | C | -2.6854 | 3.0183 | .0985 | H | -2.0630 | -3.3111 | .0460 |
| C | 1.6353 | 2.6705 | -2.1023 | H | -1.9014 | 2.1059 | 1.8941 | H | -.8044 | -3.7485 | 1.2695 |
| Li | -.3787 | 2.1453 | -1.6241 | C | -1.0275 | 4.0677 | 1.9303 | H | 4.2736 | 4.0745 | -.5620 |
| C | -.4791 | .0439 | -2.0947 | C | -3.9204 | 3.6864 | .7514 | H | 5.3737 | 4.0214 | .8785 |
| C | 1.9421 | 3.5841 | -2.8689 | H | -3.0187 | 1.9574 | -.1066 | H | 4.1902 | 5.3774 | .6995 |
| C | 2.3270 | 4.6669 | -3.7494 | H | 2.0725 | 5.6585 | -3.3134 | H | 2.4207 | 2.9385 | 2.9093 |
| C | -1.2560 | -.5893 | -2.8095 | H | 3.4225 | 4.6641 | -3.9458 | H | 3.2354 | 4.5573 | 3.0037 |
| C | -2.1719 | -1.3365 | -3.6445 | H | 1.8145 | 4.5962 | -4.7344 | H | 4.2309 | 3.0502 | 3.0300 |
| O | -1.1753 | -1.6965 | 1.0482 | H | -3.2110 | -1.2991 | -3.2480 | N | 4.3794 | -1.7594 | 2.4849 |
| O | 3.3588 | 3.5169 | 1.1835 | H | -2.1989 | -.9366 | -4.6824 | C | 5.5086 | -1.2996 | 3.3045 |
| O | 2.7045 | -.4454 | -3.9349 | H | -1.8828 | -2.4092 | -3.7111 | C | 4.0337 | -3.1502 | 2.8011 |
| N | -2.2926 | 3.5825 | -1.2309 | H | 3.2010 | -2.3861 | -4.5642 | H | 6.2240 | -.7200 | 2.6726 |
| C | 3.0332 | -.9756 | .4744 | H | 1.6976 | -1.6883 | -5.2877 | C | 6.1774 | -2.5646 | 3.8859 |
| C | -1.4387 | 2.8078 | 1.1193 | H | 1.7172 | -2.1958 | -3.5414 | H | 5.1991 | -.6110 | 4.1314 |
| C | -2.0806 | -1.4564 | 2.0950 | H | 4.5081 | -.2766 | -4.9986 | H | 3.8142 | -3.7165 | 1.8653 |
| C | -1.0926 | -2.9885 | .5001 | H | 3.8915 | 1.2070 | -4.1623 | H | 3.1211 | -3.2514 | 3.4404 |
| C | 4.3418 | 4.2814 | .5325 | H | 3.0997 | .6225 | -5.6914 | C | 5.2547 | -3.7457 | 3.5386 |
| C | 3.3170 | 3.5218 | 2.5885 | H | -1.0311 | 5.2387 | -1.6522 | C | 5.2124 | -.0280 | -.6037 |
| C | 2.3192 | -1.7289 | -4.3580 | H | -2.2926 | 5.6197 | -.4452 | C | 6.4033 | -.1942 | -1.3360 |
| C | 3.5859 | .2999 | -4.7364 | C | -3.0284 | 5.5598 | -2.5103 | C | 6.7361 | -1.4460 | -1.8770 |
| C | -2.1002 | 5.0502 | -1.3820 | H | -2.3925 | 2.5141 | -3.0835 | C | 5.8618 | -2.5286 | -1.6875 |
| C | -3.0779 | 3.0929 | -2.4065 | C | -3.6543 | 4.3166 | -3.1585 | C | 4.6729 | -2.3598 | -.9565 |
| C | 3.3832 | -.7667 | 2.0314 | H | -3.9020 | 2.3958 | -2.1227 | H | 4.9985 | .9621 | -.1949 |

| | | | | | | | | | | | |
|---|---------|---------|---------|---|---------|--------|--------|---|---------|---------|---------|
| H | 7.0728 | .6549 | -1.4800 | C | .2249 | 6.1652 | 2.2339 | H | -3.8107 | 6.2374 | -2.1059 |
| H | 7.6618 | -1.5763 | -2.4374 | C | -.0973 | 5.0283 | 1.4659 | H | -2.4587 | 6.1597 | -3.2512 |
| H | 6.1063 | -3.5055 | -2.1063 | H | -2.2712 | 3.5477 | 3.6518 | H | -3.4203 | 4.2623 | -4.2428 |
| H | 4.0201 | -3.2266 | -.8348 | H | -1.6967 | 5.5312 | 4.9810 | H | -4.7630 | 4.3404 | -3.0868 |
| H | 1.4809 | -1.5919 | 2.8574 | H | -.1036 | 7.2413 | 4.0891 | H | 7.1927 | -2.7101 | 3.4604 |
| H | 2.4149 | -.6005 | 4.0125 | H | .9288 | 6.8998 | 1.8400 | H | 6.3144 | -2.4707 | 4.9844 |
| H | 1.5087 | .1936 | 2.7049 | H | .3921 | 4.9167 | .4941 | H | 4.9373 | -4.2920 | 4.4523 |
| C | -1.5761 | 4.2730 | 3.2235 | H | -3.7481 | 4.7250 | 1.0943 | H | 5.7798 | -4.4896 | 2.9024 |
| C | -1.2502 | 5.4009 | 3.9946 | H | -4.7869 | 3.7130 | .0574 | | | | |
| C | -.3518 | 6.3599 | 3.4979 | H | -4.2481 | 3.0992 | 1.6347 | | | | |

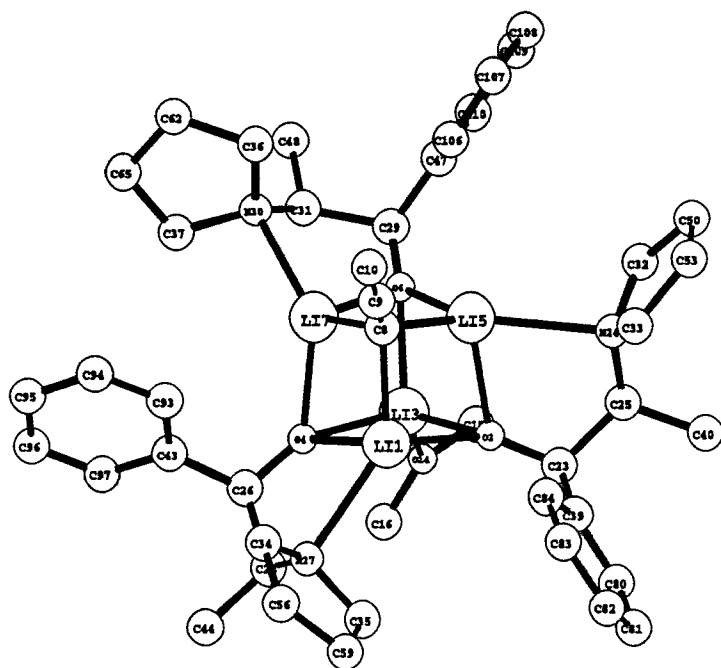


Figure XA

(LiCCCH₃)₃·[*R,S*-LiOCH(Ph)CH(Me)N(CH₂)₄]₃·(Me₂O)

$\Delta H_f^\circ = -223.0$ kcal/mol

| | | | | | | | | | | | |
|----|---------|---------|---------|---|---------|---------|---------|---|---------|---------|---------|
| Li | .0000 | .0000 | .0000 | C | 1.0666 | 4.5960 | -3.2549 | H | -.0570 | -1.4587 | 2.4408 |
| O | 2.2376 | .0000 | .0000 | C | 4.7610 | -.6778 | -3.1596 | C | -2.0523 | 4.3448 | -5.1687 |
| Li | 1.8677 | 2.1978 | .0000 | C | 3.4219 | -2.5760 | -2.4846 | H | -1.0094 | 2.4827 | -4.6400 |
| O | -.3472 | 2.1226 | .3415 | C | -2.8446 | -.4601 | 1.5386 | H | -.0045 | 3.6602 | -5.5387 |
| Li | 1.8331 | .2488 | -2.1254 | C | -.9450 | -.9959 | 2.9369 | C | -2.4407 | 5.2391 | -3.9826 |
| O | 1.8005 | 2.4852 | -2.2162 | C | -.7795 | 3.5744 | -4.7437 | H | -.9880 | 5.9641 | -2.5094 |
| Li | -.3133 | 2.0705 | -1.8895 | C | -1.3874 | 4.9896 | -2.8789 | H | -1.8504 | 4.4959 | -1.9899 |
| C | -.3021 | -.0892 | -2.1454 | H | 3.7840 | -.3401 | 1.2829 | H | 4.7884 | -1.4796 | -5.2123 |
| C | -.9931 | -.8318 | -2.8440 | C | 2.6792 | -2.1677 | .9986 | H | 6.1268 | -2.0553 | -4.2023 |
| C | -1.8074 | -1.7039 | -3.6638 | C | 5.5448 | -1.9216 | -.2566 | H | 4.8454 | -3.8916 | -3.5338 |
| H | -2.8930 | -1.5305 | -3.4918 | H | 4.8492 | .0430 | -.7099 | H | 3.5071 | -3.3298 | -4.5529 |
| H | -1.6050 | -2.7762 | -3.4464 | H | -.8297 | 3.4323 | 1.8262 | H | -4.1388 | -1.5197 | 2.9741 |
| H | -1.6145 | -1.5439 | -4.7479 | C | -2.5905 | 2.9924 | .6686 | H | -3.5022 | -2.5576 | 1.6844 |
| O | 3.2421 | 3.4862 | 1.2196 | C | -2.3485 | 1.8637 | 3.5995 | H | -1.6500 | -3.0822 | 3.0234 |
| C | 4.5251 | 3.7438 | .7053 | H | -.3484 | 1.4876 | 2.9605 | H | -2.2998 | -2.0544 | 4.3134 |
| C | 2.8712 | 4.0416 | 2.4555 | H | 3.0666 | 4.0156 | -2.6732 | H | -1.8644 | 4.9494 | -6.0818 |
| H | 4.6315 | 3.1839 | -.2557 | C | 2.7068 | 2.8393 | -4.4398 | H | -2.8713 | 3.6422 | -5.4316 |
| H | 5.3299 | 3.4059 | 1.4058 | C | 1.4679 | 5.7221 | -4.2403 | H | -3.4634 | 5.0067 | -3.6183 |
| H | 4.6789 | 4.8342 | .5054 | H | 1.0859 | 5.0888 | -2.2383 | H | -2.4594 | 6.3103 | -4.2779 |
| H | 1.8433 | 3.6817 | 2.7004 | C | 5.0448 | -1.8027 | -4.1814 | C | 3.2996 | -2.7344 | 2.1430 |
| H | 2.8607 | 5.1600 | 2.4200 | H | 4.2329 | .1786 | -3.6461 | C | 2.8725 | -3.9568 | 2.6872 |
| H | 3.5626 | 3.7289 | 3.2779 | H | 5.7238 | -.2623 | -2.7773 | C | 1.7963 | -4.6495 | 2.1081 |
| C | 3.2206 | -.8291 | .4178 | C | 4.2025 | -3.0109 | -3.7478 | C | 1.1424 | -4.0921 | .9988 |
| N | 3.8831 | -1.2195 | -2.0799 | H | 2.3261 | -2.5230 | -2.7112 | C | 1.5638 | -2.8583 | .4606 |
| C | 4.3877 | -.9881 | -.6918 | H | 3.5429 | -3.3414 | -1.6849 | H | 4.1314 | -2.2230 | 2.6322 |
| C | -1.2391 | 2.5175 | 1.2778 | C | -3.2360 | -1.7141 | 2.3562 | H | 3.3785 | -4.3679 | 3.5614 |
| N | -1.5198 | .0267 | 2.0126 | H | -2.7557 | -.7232 | .4534 | H | 1.4706 | -5.6053 | 2.5186 |
| C | -1.3686 | 1.4395 | 2.4771 | H | -3.6500 | .3052 | 1.6134 | H | .2998 | -4.6173 | .5462 |
| C | 2.1807 | 3.4342 | -3.1011 | C | -2.0263 | -2.0595 | 3.2363 | H | 1.0078 | -2.4696 | -.4013 |
| N | -.3288 | 4.0860 | -3.4203 | H | -.5661 | -.5620 | 3.8928 | H | 5.2495 | -2.9817 | -1.1337 |

| | | | | | | | | | | | |
|---|---------|---------|---------|---|---------|--------|---------|---|--------|--------|---------|
| H | 6.3849 | -1.9036 | -.9825 | H | -6.0685 | 4.2485 | -.7159 | C | 4.3170 | 2.9628 | -6.3061 |
| H | 5.9669 | -1.5803 | .7116 | H | -4.9860 | 5.4136 | 1.2154 | C | 3.8211 | 3.4410 | -5.0821 |
| C | -3.1959 | 2.3842 | -.4606 | H | -2.8168 | 4.6505 | 2.0760 | H | 1.3073 | 1.1488 | -4.6093 |
| C | -4.4440 | 2.8286 | -.9451 | H | -3.4069 | 1.9204 | 3.2793 | H | 2.1732 | .3479 | -6.7585 |
| C | -5.1020 | 3.9111 | -.3416 | H | -2.3105 | 1.1686 | 4.4645 | H | 4.0926 | 1.4857 | -7.8805 |
| C | -4.4959 | 4.5590 | .7475 | H | -2.0675 | 2.8623 | 3.9943 | H | 5.1683 | 3.4561 | -6.7765 |
| C | -3.2586 | 4.1090 | 1.2369 | C | 2.1493 | 1.6909 | -5.0570 | H | 4.3243 | 4.2983 | -4.6301 |
| H | -2.7305 | 1.5351 | -.9769 | C | 2.6397 | 1.2168 | -6.2917 | H | 1.5474 | 5.3938 | -5.2948 |
| H | -4.9015 | 2.3236 | -1.7974 | C | 3.7192 | 1.8519 | -6.9242 | H | .7461 | 6.5655 | -4.2194 |
| | | | | | | | | H | 2.4501 | 6.1506 | -3.9511 |

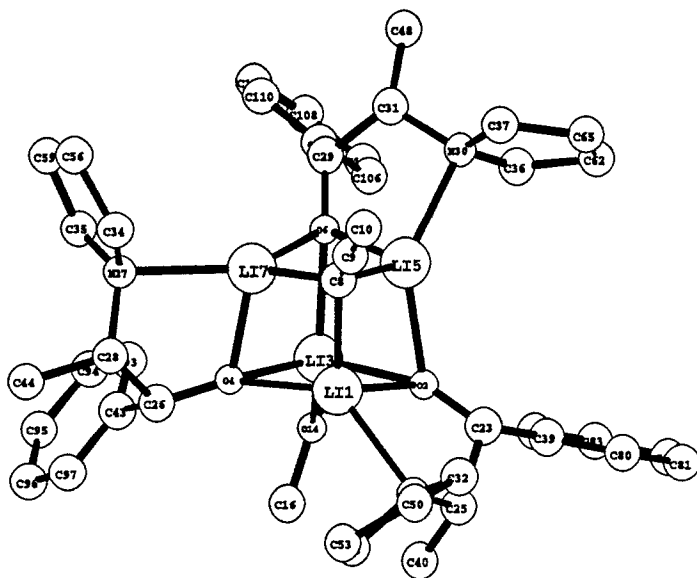


Figure XB

(LiCCCH₃)₃·[R,S-LiOCH(Ph)CH(Me)N(CH₂)₄]₃·(Me₂O)

$\Delta H_f^\circ = -219.3$ kcal/mol

| | | | | | | | | | | | |
|----|---------|---------|---------|---|---------|---------|---------|---|---------|---------|---------|
| Li | .0000 | .0000 | .0000 | H | 2.4274 | 4.5287 | 3.2990 | H | 2.2106 | -2.5585 | 2.2265 |
| O | 2.1670 | .0000 | .0000 | H | 3.3952 | 3.0288 | 3.5810 | H | -1.8125 | 2.4806 | 1.7425 |
| Li | 1.7782 | 2.3009 | .0000 | C | 2.5816 | -1.1736 | .5323 | C | -9.678 | 4.4021 | 1.2619 |
| O | -.4233 | 2.2523 | .2712 | N | .3221 | -1.8563 | 1.5034 | C | -3.9390 | 3.7857 | .4457 |
| Li | 1.6532 | .2927 | -2.1661 | C | 1.7572 | -1.5925 | 1.8673 | H | -3.0893 | 1.8991 | -.0777 |
| O | 1.6834 | 2.4152 | -2.3394 | C | -1.4285 | 2.9922 | .7957 | C | 3.0192 | 4.0913 | -3.4802 |
| Li | -.5220 | 1.9182 | -1.8349 | N | -2.4837 | 3.2253 | -1.5909 | H | 1.0678 | 3.3832 | -4.0259 |
| C | -.4647 | -.1970 | -2.0688 | C | -2.7535 | 2.9772 | -.1389 | C | 3.0558 | 2.3388 | -5.9271 |
| C | -1.0970 | -1.0360 | -2.7113 | C | 2.0013 | 2.9171 | -3.5526 | H | 1.3243 | 1.4744 | -5.0279 |
| C | -1.8466 | -2.0206 | -3.4628 | N | 2.9547 | .5271 | -4.1160 | C | -1.3944 | -3.5892 | 1.2139 |
| H | -2.8497 | -2.1992 | -3.0155 | C | 2.3505 | 1.7812 | -4.6652 | H | .2300 | -3.1414 | -.2089 |
| H | -1.3193 | -2.9998 | -3.4950 | C | .0649 | -3.1937 | .8941 | H | .7592 | -3.9811 | 1.2806 |
| H | -2.0066 | -1.6962 | -4.5151 | C | -.7653 | -1.5653 | 2.4797 | C | -1.9538 | -2.4935 | 2.1347 |
| O | 3.0046 | 3.4822 | 1.5731 | C | -3.4142 | 2.5340 | -2.5361 | H | -1.0575 | -.4859 | 2.4115 |
| C | 4.1310 | 4.2331 | 1.1964 | C | -2.2385 | 4.6123 | -2.0745 | H | -.4668 | -1.7519 | 3.5413 |
| C | 2.6159 | 3.4917 | 2.9244 | C | 4.3929 | .4983 | -3.7355 | C | -3.6950 | 3.4810 | -3.7245 |
| H | 4.3479 | 4.0093 | .1260 | C | 2.6092 | -.7289 | -4.8476 | H | -4.3812 | 2.2394 | -2.0597 |
| H | 5.0345 | 3.9720 | 1.8025 | H | 2.4011 | -2.0236 | -.2093 | H | -2.9406 | 1.5812 | -2.8864 |
| H | 3.9506 | 5.3318 | 1.3057 | C | 4.1153 | -1.2557 | .7944 | C | -3.0236 | 4.8207 | -3.3904 |
| H | 1.6725 | 2.9036 | 3.0188 | C | 1.9427 | -.6061 | 3.0440 | H | -1.1421 | 4.7403 | -2.2567 |

| | | | | | | | | | | | |
|---|---------|---------|---------|---|---------|---------|--------|---|---------|--------|---------|
| H | -2.5306 | 5.3953 | -1.3368 | C | 4.7440 | -2.5279 | .8408 | H | 1.0451 | 7.0693 | .4274 |
| C | 4.9743 | -.8768 | -4.1404 | C | 6.1249 | -2.6623 | 1.0577 | H | .0524 | 8.0017 | 2.5216 |
| H | 4.4805 | .6511 | -2.6307 | C | 6.9273 | -1.5218 | 1.2296 | H | -1.5489 | 6.6102 | 3.8468 |
| H | 4.9908 | 1.3075 | -4.2176 | C | 6.3307 | -.2532 | 1.1782 | H | -2.1783 | 4.3634 | 3.0828 |
| C | 3.8349 | -1.6686 | -4.7980 | C | 4.9446 | -.1227 | .9644 | H | -3.7444 | 4.8721 | .5350 |
| H | 2.3201 | -.5497 | -5.9124 | H | 4.1587 | -3.4394 | .7018 | H | -4.8592 | 3.6731 | -1.650 |
| H | 1.7175 | -1.2044 | -4.3627 | H | 6.5747 | -3.6552 | 1.0918 | H | -4.1917 | 3.4097 | 1.4591 |
| H | -1.9975 | -3.6901 | .2872 | H | 7.9994 | -1.6220 | 1.3984 | C | 4.2729 | 4.0132 | -2.8326 |
| H | -1.4300 | -4.5826 | 1.7115 | H | 6.9436 | .6403 | 1.3039 | C | 5.1678 | 5.1013 | -2.8263 |
| H | -2.3940 | -2.9253 | 3.0589 | H | 4.5295 | .8862 | .9302 | C | 4.8226 | 6.3103 | -3.4480 |
| H | -2.7744 | -1.9316 | 1.6387 | H | 1.3990 | .3520 | 2.9179 | C | 3.5701 | 6.4227 | -4.0750 |
| H | -3.2985 | 3.0584 | -4.6727 | H | 1.6172 | -1.0582 | 4.0063 | C | 2.6860 | 5.3315 | -4.0884 |
| H | -4.7880 | 3.6062 | -3.8800 | H | 3.0163 | -.3640 | 3.1840 | H | 4.5798 | 3.1017 | -2.3174 |
| H | -3.7768 | 5.6300 | -3.2772 | C | -.0213 | 5.1869 | .5571 | H | 6.1357 | 5.0010 | -2.3334 |
| H | -2.3469 | 5.1466 | -4.2088 | C | .3333 | 6.4765 | 1.0038 | H | 5.5147 | 7.1522 | -3.4436 |
| H | 5.8297 | -.7519 | -4.8391 | C | -.2196 | 7.0025 | 2.1814 | H | 3.2835 | 7.3592 | -4.5548 |
| H | 5.3789 | -1.4140 | -3.2565 | C | -1.1238 | 6.2221 | 2.9205 | H | 1.7232 | 5.4629 | -4.5869 |
| H | 3.6059 | -2.5935 | -4.2262 | C | -1.4830 | 4.9411 | 2.4701 | H | 4.0563 | 2.7713 | -5.7324 |
| H | 4.1157 | -2.0036 | -5.8197 | H | .4559 | 4.8198 | -.3583 | H | 3.1889 | 1.5598 | -6.7069 |
| | | | | | | | | H | 2.4347 | 3.1352 | -6.3876 |

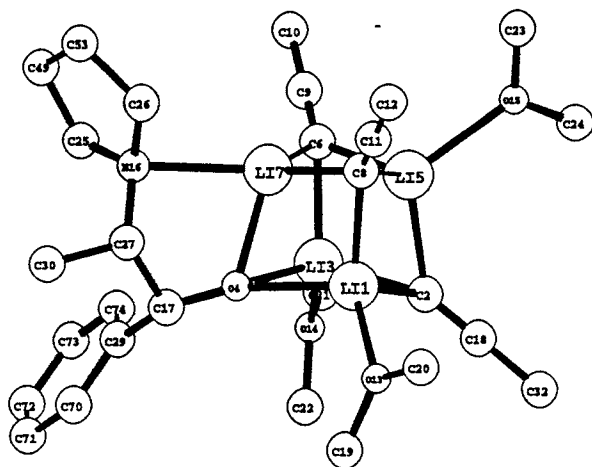


Figure XIA

$(\text{LiCCCH}_3)_3 \cdot [R,S\text{-LiOCH(Ph)CH(Me)N(CH}_2)_4]_2 \cdot (\text{Me}_2\text{O})_3$
 $\Delta H_f^\circ = -317.4 \text{ kcal/mol}$

| | | | | | | | | | | | |
|----|---------|---------|---------|---|---------|---------|---------|---|---------|---------|---------|
| Li | .0000 | .0000 | .0000 | C | -1.5317 | 2.7472 | 1.1914 | H | 4.8384 | -1.1006 | 1.4275 |
| C | 2.1266 | .0000 | .0000 | C | 2.9337 | -.7457 | .5535 | H | 3.4863 | -2.0181 | 2.1638 |
| Li | 1.6981 | 2.1140 | .0000 | C | -.9430 | -1.3620 | 2.7332 | H | 4.1305 | -2.5017 | .5627 |
| O | -.4946 | 2.1318 | .5826 | C | -1.3510 | -2.8611 | .8715 | H | 2.6628 | 5.5079 | -3.2185 |
| Li | 1.5163 | .5203 | -2.0187 | C | 4.3643 | 3.9013 | .7840 | H | 3.4900 | 4.2363 | -4.1734 |
| C | 1.5450 | 2.6674 | -2.0907 | C | 3.2819 | 2.8521 | 2.6818 | H | 1.8198 | 4.7309 | -4.5964 |
| Li | -.4457 | 2.0982 | -1.5700 | C | 2.2262 | -.5180 | -5.0140 | H | -3.2000 | -1.6647 | -3.0437 |
| C | -.5794 | .0041 | -2.0718 | C | 4.1010 | -.8539 | -3.5171 | H | -2.4916 | -.9497 | -4.5269 |
| C | 1.9840 | 3.5275 | -2.8528 | C | -2.0815 | 5.0606 | -1.2537 | H | -1.7944 | -2.4482 | -3.8334 |
| C | 2.5089 | 4.5393 | -3.7442 | C | -3.1275 | 3.1680 | -2.3362 | H | 2.0974 | -1.5892 | -5.3112 |
| C | -1.3434 | -.6701 | -2.7609 | C | -2.7613 | 3.0191 | .1684 | H | 2.8529 | -.0179 | -5.7946 |
| C | -2.2416 | -1.4633 | -3.5720 | H | -2.0131 | 2.0249 | 1.9356 | H | 1.2237 | -.0264 | -4.9984 |
| O | -.8798 | -1.6292 | 1.3548 | C | -1.0897 | 3.9620 | 2.0535 | H | 4.1746 | -1.9658 | -3.6200 |
| O | 3.2969 | 3.1548 | 1.3090 | C | -3.9824 | 3.7079 | .8254 | H | 4.4001 | -.5689 | -2.4800 |
| O | 2.7892 | -.4003 | -3.7317 | H | -3.1243 | 1.9736 | -.0637 | H | 4.8281 | -.3937 | -4.2324 |
| N | -2.3371 | 3.5996 | -1.1429 | C | 3.8831 | -1.6248 | 1.2014 | H | -2.2716 | 5.6151 | -.3072 |

| | | | | | | | | | | | |
|---|---------|---------|---------|---|---------|---------|---------|---|---------|--------|--------|
| C | -2.9638 | 5.6330 | -2.3886 | H | -1.1279 | -2.9106 | -2.2212 | C | .2768 | 5.9672 | 2.4696 |
| H | -1.0001 | 5.2130 | -1.4960 | H | -2.4553 | -2.9666 | 1.0182 | C | -.0931 | 4.8831 | 1.6489 |
| H | -3.9936 | 2.5144 | -2.0745 | H | -.8525 | -3.7277 | 1.3737 | H | -2.4131 | 3.4578 | 3.7191 |
| H | -2.4653 | 2.5580 | -3.0089 | H | 4.1913 | 4.0268 | -.3115 | H | -1.7579 | 5.3510 | 5.1386 |
| C | -3.6233 | 4.4308 | -3.0805 | H | 5.3473 | 3.3880 | .9334 | H | -.0350 | 6.9884 | 4.3584 |
| H | -3.7280 | 6.3316 | -1.9853 | H | 4.4317 | 4.9157 | 1.2515 | H | 1.0357 | 6.6704 | 2.1238 |
| H | -2.3546 | 6.2265 | -3.1027 | H | 2.3521 | 2.2712 | 2.8976 | H | .4137 | 4.7812 | .6845 |
| H | -3.3564 | 4.3869 | -4.1577 | H | 3.2784 | 3.7771 | 3.3115 | H | -4.3435 | 3.1036 | 1.6838 |
| H | -4.7314 | 4.5041 | -3.0433 | H | 4.1673 | 2.2374 | 2.9826 | H | -3.7784 | 4.7279 | 1.2050 |
| H | -4.609 | -.3711 | 2.9167 | C | -1.6635 | 4.1543 | 3.3371 | H | -4.8373 | 3.7893 | .1215 |
| H | -4.023 | -2.1360 | 3.3343 | C | -1.2918 | 5.2304 | 4.1602 | | | | |
| H | -2.0003 | -1.3217 | 3.0979 | C | -.3214 | 6.1483 | 3.7259 | | | | |

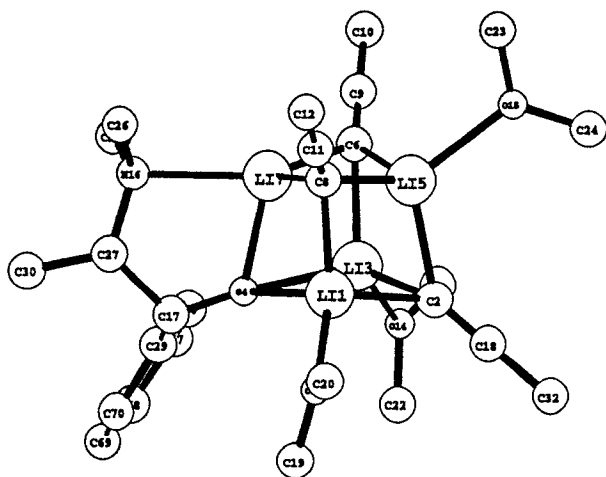


Figure XIB

$(\text{LiCCCH}_3)_3 \cdot [R, S\text{-LiOCH(Ph)CH(Me)NMe}_2]_2 \cdot (\text{Me}_2\text{O})_3$

$\Delta H_f^\circ = -309.3 \text{ kcal/mol}$

| | | | | | | | | | | | |
|----|---------|---------|---------|---|---------|---------|---------|---|---------|---------|---------|
| Li | .0000 | .0000 | .0000 | C | 2.3066 | -.2155 | -5.0644 | H | 3.9041 | -2.1530 | -3.8986 |
| C | 2.1295 | .0000 | .0000 | C | 3.9846 | -1.0914 | -3.5540 | H | 4.2090 | -1.0876 | -2.4610 |
| Li | 1.7024 | 2.1130 | .0000 | C | -2.0374 | 4.9153 | -1.4245 | H | 4.8435 | -.6189 | -4.0937 |
| O | -.4924 | 2.1286 | .5872 | C | -3.1634 | 2.8676 | -2.1679 | H | -1.4699 | 5.4113 | -.6096 |
| Li | 1.5274 | .5226 | -2.0208 | C | -2.7315 | 3.1486 | .2910 | H | -2.9548 | 5.5291 | -1.6062 |
| C | 1.5265 | 2.6687 | -2.0874 | H | -1.9558 | 2.0853 | 2.0031 | H | -1.4162 | 4.9704 | -2.3510 |
| Li | -.4651 | 2.0719 | -1.5648 | C | -.9223 | 3.9686 | 2.0981 | H | -3.3340 | 1.7845 | -1.9595 |
| C | -.5572 | -.0188 | -2.0816 | C | -3.7676 | 4.1076 | .9234 | H | -2.6475 | 2.9529 | -3.1580 |
| C | 1.9438 | 3.5519 | -2.8353 | H | -3.2759 | 2.1615 | .2280 | H | -4.1704 | 3.3416 | -2.2802 |
| C | 2.4464 | 4.5909 | -3.7082 | C | 3.8629 | -1.6323 | 1.2247 | H | -.3508 | -.3889 | 2.9070 |
| C | -1.2416 | -.7220 | -2.8234 | H | 4.9085 | -1.2625 | 1.1330 | H | -.3574 | -2.1582 | 3.3114 |
| C | -2.0527 | -1.5474 | -3.6921 | H | 3.6404 | -1.7278 | 2.3109 | H | -1.9238 | -1.2677 | 3.1509 |
| O | -.8967 | -1.6143 | 1.3578 | H | 3.8348 | -2.6563 | .7901 | H | -1.2941 | -2.8618 | -.2148 |
| O | 3.3648 | 3.1169 | 1.2799 | H | 2.4076 | 5.5899 | -3.2198 | H | -2.5512 | -2.8713 | 1.0964 |
| O | 2.7871 | -.3859 | -3.7544 | H | 3.5047 | 4.4046 | -3.9974 | H | -.9690 | -3.7112 | 1.3538 |
| N | -2.3376 | 3.5028 | -1.1099 | H | 1.8536 | 4.6581 | -4.6474 | H | 4.1956 | 4.0149 | -.3599 |
| C | -1.4687 | 2.7891 | 1.2454 | H | -3.0607 | -1.7313 | -3.2582 | H | 5.3971 | 3.2901 | .7920 |
| C | 2.9260 | -.7489 | .5646 | H | -2.2025 | -1.0703 | -4.6862 | H | 4.5604 | 4.8374 | 1.2149 |
| C | -.8867 | -1.3549 | 2.7393 | H | -1.5823 | -2.5402 | -3.8689 | H | 2.4606 | 2.2528 | 2.9019 |
| C | -1.4530 | -2.8158 | .8890 | H | 2.0556 | -1.1951 | -5.5438 | H | 3.4930 | 3.6938 | 3.2927 |
| C | 4.4274 | 3.8435 | .7184 | H | 3.0507 | .3058 | -5.7177 | H | 4.2730 | 2.1151 | 2.8830 |
| C | 3.4088 | 2.7850 | 2.6453 | H | 1.3803 | .4069 | -5.0160 | C | .0823 | 4.8579 | 1.6455 |

| | | | | | | | | | | | |
|---|-------|--------|--------|---|---------|--------|--------|---|---------|--------|--------|
| C | .5391 | 5.9165 | 2.4563 | C | -.9496 | 5.2092 | 4.2300 | H | -1.3504 | 5.3316 | 5.2369 |
| C | .0246 | 6.0995 | 3.7487 | C | -1.4101 | 4.1603 | 3.4173 | H | -2.1618 | 3.4858 | 3.8329 |
| | | | | H | .5259 | 4.7536 | .6501 | H | -3.3743 | 5.1195 | 1.1423 |
| | | | | H | 1.2988 | 6.5996 | 2.0736 | H | -4.6560 | 4.2366 | .2692 |
| | | | | H | .3780 | 6.9200 | 4.3730 | H | -4.1440 | 3.6845 | 1.8780 |

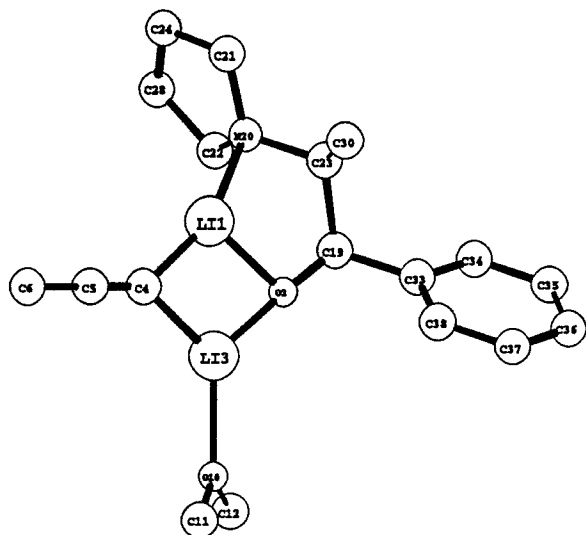


Figure X11A

(LiCCCH₃)•[R,S-LiOCH(Ph)CH(Me)N(CH₂)₄]•(Me₂O)

$\Delta H_f^\circ = -129.1$ kcal/mol

| | | | | | | | |
|----|---------|---------|---------|---|---------|---------|---------|
| Li | .0000 | .0000 | .0000 | C | -.3735 | -2.8239 | -3.0354 |
| O | 2.0569 | .0000 | .0000 | H | 1.6650 | -2.9129 | -2.2494 |
| Li | 1.4312 | 1.8941 | .0000 | C | .5744 | -2.1311 | 1.7408 |
| C | -.5816 | 1.8789 | .0001 | H | 1.7201 | -3.3307 | .3357 |
| C | -1.5570 | 2.6186 | -.0080 | H | 3.0622 | -1.5915 | -.7802 |
| C | -2.7083 | 3.4928 | -.0192 | C | 3.5763 | -1.4105 | 1.2792 |
| H | -3.6576 | 2.9152 | .0315 | C | 4.4839 | -2.4995 | 1.2306 |
| H | -2.6982 | 4.1922 | .8462 | C | 5.4903 | -2.6603 | 2.1974 |
| H | -2.7433 | 4.1099 | -.9444 | C | 5.6235 | -1.7293 | 3.2407 |
| O | 2.7282 | 3.6188 | -.0906 | C | 4.7410 | -.6399 | 3.3038 |
| C | 2.4802 | 4.8146 | .6061 | C | 3.7313 | -.4822 | 2.3352 |
| C | 3.8971 | 3.4773 | -.8620 | H | 4.4197 | -3.2381 | .4290 |
| H | 1.5240 | 4.6884 | 1.1708 | H | 6.1701 | -3.5109 | 2.1355 |
| H | 2.3749 | 5.6833 | -.0906 | H | 6.4039 | -1.8516 | 3.9919 |
| H | 3.2980 | 5.0484 | 1.3329 | H | 4.8357 | .0907 | 4.1082 |
| H | 3.8651 | 2.4732 | -1.3543 | H | 3.0678 | .3816 | 2.4299 |
| H | 4.8178 | 3.5413 | -.2295 | H | 1.3262 | -2.1566 | 2.5578 |
| H | 3.9660 | 4.2637 | -1.6551 | H | -.0190 | -1.1870 | 1.8676 |
| C | 2.5112 | -1.2549 | .1590 | H | -.1095 | -2.9809 | 1.9594 |
| N | .2617 | -2.1720 | -.7548 | H | -2.4295 | -2.7459 | -2.2611 |
| C | -.9574 | -3.0253 | -.6460 | H | -1.7098 | -4.3674 | -2.2160 |
| C | .7651 | -2.2556 | -2.1577 | H | -.0035 | -3.6641 | -3.6615 |
| C | 1.2751 | -2.2998 | .3573 | H | -.7526 | -2.0576 | -3.7446 |
| C | -1.4788 | -3.2898 | -2.0755 | | | | |
| H | -1.7296 | -2.4931 | -.0365 | | | | |
| H | -.7578 | -4.0017 | -.1385 | | | | |
| H | 1.0625 | -1.2383 | -2.5119 | | | | |

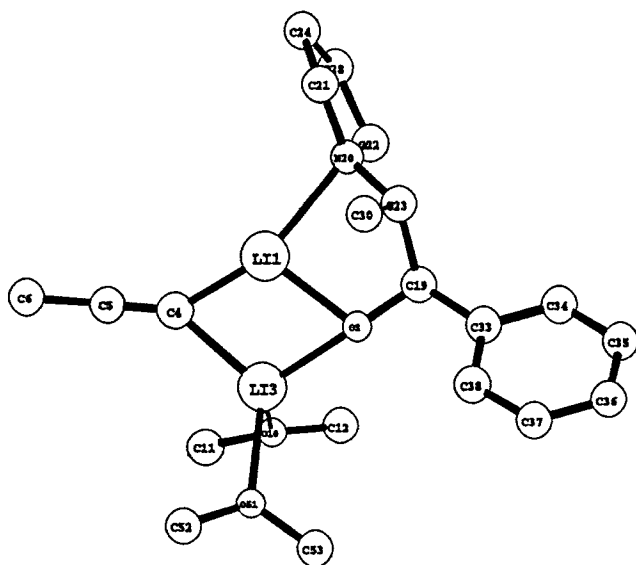


Figure XIIB

(LiCCCH₃)•[*R,S*-LiOCH(Ph)CH(Me)N(CH₂)₄]•(Me₂O)₂

$\Delta H_f^\circ = -178.9$ kcal/mol

| | | | | | | | |
|----|---------|---------|---------|---|---------|---------|---------|
| Li | .0000 | .0000 | .0000 | C | 3.7402 | -1.6896 | .4579 |
| O | 2.0454 | .0000 | .0000 | C | 4.6005 | -2.6390 | -.1508 |
| Li | 1.4231 | 2.0085 | .0000 | C | 5.7957 | -3.0498 | .4622 |
| C | -.6342 | 1.8468 | .0689 | C | 6.1702 | -2.5173 | 1.7071 |
| C | -1.6474 | 2.5336 | .1095 | C | 5.3367 | -1.5735 | 2.3266 |
| C | -2.8422 | 3.3446 | .1561 | C | 4.1384 | -1.1657 | 1.7102 |
| H | -3.7587 | 2.7168 | .2179 | H | 4.3484 | -3.0709 | -1.1217 |
| H | -2.8444 | 4.0214 | 1.0397 | H | 6.4346 | -3.7830 | -.0313 |
| H | -2.9395 | 3.9842 | -.7497 | H | 7.0972 | -2.8336 | 2.1853 |
| O | 2.2054 | 3.2844 | -1.7313 | H | 5.6166 | -1.1529 | 3.2933 |
| C | 1.4953 | 4.4291 | -2.1311 | H | 3.5209 | -.4329 | 2.2332 |
| C | 3.1477 | 2.7191 | -2.6073 | H | 1.6271 | -2.4668 | 2.1173 |
| H | .8293 | 4.7335 | -1.2878 | H | .1865 | -1.4562 | 1.7581 |
| H | .8661 | 4.2378 | -3.0359 | H | .1254 | -3.2486 | 1.6330 |
| H | 2.1820 | 5.2823 | -2.3632 | H | -2.8177 | -2.4438 | -2.1159 |
| H | 3.6265 | 1.8535 | -2.0891 | H | -2.1228 | -4.0517 | -2.4012 |
| H | 3.9480 | 3.4519 | -2.8835 | H | -.6548 | -3.1426 | -3.9861 |
| H | 2.6739 | 2.3569 | -3.5540 | H | -1.3697 | -1.5407 | -3.7186 |
| C | 2.4477 | -1.2474 | -.2862 | O | 2.4404 | 3.2945 | 1.5757 |
| N | .0808 | -2.0692 | -.9721 | C | 1.7020 | 4.0471 | 2.5046 |
| C | -1.1229 | -2.9323 | -.7951 | C | 3.8267 | 3.1527 | 1.7561 |
| C | .3697 | -1.9696 | -2.4328 | H | 2.0735 | 5.1009 | 2.5738 |
| C | 1.2482 | -2.3303 | -.0513 | H | 1.7426 | 3.6005 | 3.5295 |
| C | -1.8579 | -3.0019 | -2.1519 | H | .6389 | 4.0687 | 2.1646 |
| H | -1.7851 | -2.4911 | -.0096 | H | 4.0773 | 2.6950 | 2.7457 |
| H | -.8650 | -3.9678 | -.4604 | H | 4.3529 | 4.1391 | 1.6924 |
| H | .6438 | -.9171 | -2.6924 | H | 4.2167 | 2.4900 | .9461 |
| C | -.9036 | -2.4027 | -3.1954 | | | | |
| H | 1.2250 | -2.6198 | -2.7438 | | | | |
| C | .7626 | -2.3596 | 1.4292 | | | | |
| H | 1.6753 | -3.3434 | -.2807 | | | | |
| H | 2.7356 | -1.3339 | -1.3862 | | | | |

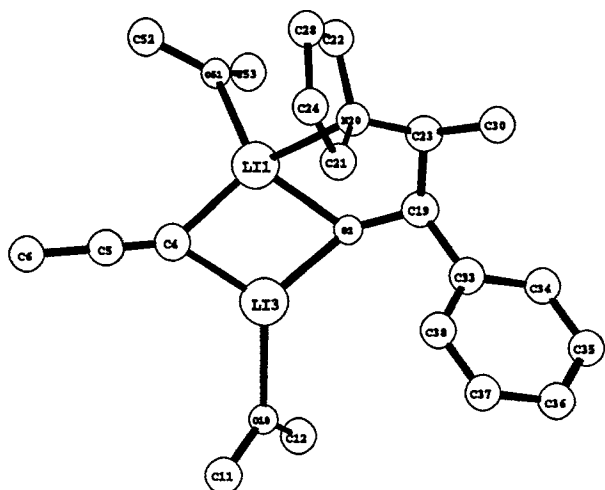


Figure XIIC

(LiCCCH₃)•[*R,S*-LiOCH(Ph)CH(Me)N(CH₂)₄]•(Me₂O)₂
 $\Delta H_f^\circ = -177.8$ kcal/mol

| | | | | | | | |
|----|---------|---------|---------|---|---------|---------|---------|
| Li | .0000 | .0000 | .0000 | C | 5.3368 | -1.0891 | .9673 |
| O | 2.0522 | .0000 | .0000 | C | 6.5067 | -.6140 | 1.5835 |
| Li | 1.5436 | 1.9244 | .0000 | C | 6.4531 | .5045 | 2.4314 |
| C | -.4483 | 1.9874 | .0601 | C | 5.2218 | 1.1429 | 2.6473 |
| C | -1.3997 | 2.7545 | .1399 | C | 4.0502 | .6671 | 2.0268 |
| C | -2.5206 | 3.6610 | .2304 | H | 5.4209 | -1.9543 | .3063 |
| H | -3.4746 | 3.1156 | .4067 | H | 7.4584 | -1.1141 | 1.4003 |
| H | -2.3954 | 4.3855 | 1.0660 | H | 7.3580 | .8736 | 2.9142 |
| H | -2.6463 | 4.2528 | -.7039 | H | 5.1710 | 2.0142 | 3.3018 |
| O | 2.8027 | 3.6408 | -.4468 | H | 3.1166 | 1.2036 | 2.2288 |
| C | 2.6709 | 4.8836 | .1962 | H | 3.5745 | -3.5222 | 1.7192 |
| C | 3.7119 | 3.4849 | -1.5091 | H | 3.2380 | -2.3882 | 3.0596 |
| H | 1.9312 | 4.7611 | 1.0251 | H | 2.1423 | -3.7545 | 2.7409 |
| H | 2.3009 | 5.6744 | -.5030 | H | -1.2147 | -.4382 | 4.1424 |
| H | 3.6414 | 5.2307 | .6313 | H | -.1185 | -1.6170 | 4.8873 |
| H | 3.6330 | 2.4313 | -1.8769 | H | -1.2330 | -3.3358 | 3.7647 |
| H | 4.7648 | 3.6747 | -1.1818 | H | -2.2856 | -2.1535 | 2.9646 |
| H | 3.4824 | 4.1798 | -2.3559 | O | -1.2451 | -1.0100 | -1.6108 |
| C | 2.8159 | -1.0068 | .4505 | C | -2.6379 | -.8312 | -1.6578 |
| N | .6501 | -1.6131 | 1.7656 | C | -.5577 | -1.4054 | -2.7714 |
| C | .6380 | -.7755 | 2.9970 | H | -3.1662 | -1.7788 | -1.9336 |
| C | -.4505 | -2.6151 | 1.8381 | H | -2.9376 | -.0430 | -2.3922 |
| C | 1.9532 | -2.1290 | 1.2430 | H | -2.9777 | -.5218 | -.6394 |
| C | -.5119 | -1.2661 | 3.9090 | H | -.6847 | -.6706 | -3.6057 |
| H | .4787 | .2963 | 2.7113 | H | -.9091 | -2.4036 | -3.1373 |
| H | 1.6001 | -.8091 | 3.5608 | H | .5284 | -1.4824 | -2.5208 |
| H | -1.1272 | -2.4746 | .9582 | | | | |
| C | -1.2209 | -2.4033 | 3.1606 | | | | |
| H | -.0916 | -3.6711 | 1.7755 | | | | |
| C | 2.7658 | -2.9779 | 2.2499 | | | | |
| H | 1.6727 | -2.8509 | .4213 | | | | |
| H | 3.2181 | -1.6111 | -.4319 | | | | |
| C | 4.0792 | -.4711 | 1.1836 | | | | |

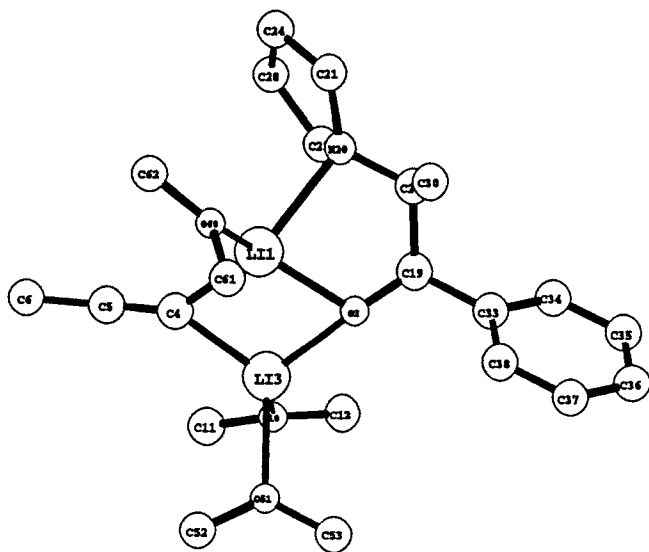


Figure XIID

(LiCCCH₃)•[*R,S*-LiOCH(Ph)CH(Me)N(CH₂)₄]•(Me₂O)₃

$\Delta H_f^\circ = -226.4$ kcal/mol

| | | | | | | | | | | | |
|----|---------|---------|---------|---|---------|---------|---------|---|---------|---------|--------|
| Li | .0000 | .0000 | .0000 | C | 5.0903 | -1.8025 | -1.0745 | H | -3.3019 | -1.8405 | 1.7395 |
| O | 2.0805 | .0000 | .0000 | C | 6.3671 | -2.1718 | -.6190 | H | -3.0629 | -.8413 | .2439 |
| Li | 1.5723 | 2.0407 | .0000 | C | 6.6739 | -2.1098 | .7503 | | | | |
| C | -.4559 | 1.9702 | -.1416 | C | 5.6906 | -1.6765 | 1.6531 | | | | |
| C | -1.4512 | 2.6676 | -.2997 | C | 4.4117 | -1.3097 | 1.1936 | | | | |
| C | -2.6219 | 3.4910 | -.4894 | H | 4.8934 | -1.8591 | -2.1472 | | | | |
| H | -3.5517 | 2.8802 | -.5278 | H | 7.1215 | -2.5064 | -1.3319 | | | | |
| H | -2.7461 | 4.2269 | .3369 | H | 7.6638 | -2.3945 | 1.1067 | | | | |
| H | -2.5692 | 4.0693 | -1.4392 | H | 5.9167 | -1.6245 | 2.7190 | | | | |
| O | 2.6036 | 3.4225 | -1.5220 | H | 3.6780 | -.9849 | 1.9340 | | | | |
| C | 1.9097 | 4.5442 | -2.0062 | H | 2.5526 | -3.4368 | .6118 | | | | |
| C | 3.7560 | 2.9879 | -2.1976 | H | 1.0159 | -2.6262 | 1.0432 | | | | |
| H | 1.0653 | 4.7568 | -1.3074 | H | 1.0364 | -4.0680 | -.0195 | | | | |
| H | 1.4950 | 4.3692 | -3.0304 | H | -2.5230 | -2.1816 | -2.5827 | | | | |
| H | 2.5655 | 5.4505 | -2.0514 | H | -1.6763 | -3.3055 | -3.6622 | | | | |
| H | 4.1995 | 2.1440 | -1.6170 | H | -.6149 | -1.5031 | -4.7209 | | | | |
| H | 4.5227 | 3.7997 | -2.2787 | H | -1.4871 | -.3780 | -3.6619 | | | | |
| H | 3.5233 | 2.6321 | -3.2325 | O | 2.4470 | 3.2187 | 1.7554 | | | | |
| C | 2.6920 | -.9330 | -.7445 | C | 1.6441 | 4.0603 | 2.5426 | | | | |
| N | .4262 | -1.8012 | -1.6118 | C | 3.7257 | 2.8638 | 2.2166 | | | | |
| C | -.5823 | -2.8815 | -1.8028 | H | 2.1406 | 5.0445 | 2.7381 | | | | |
| C | .4792 | -1.0075 | -2.8776 | H | 1.3981 | 3.5986 | 3.5317 | | | | |
| C | 1.7495 | -2.2194 | -1.0313 | H | .6935 | 4.2491 | 1.9886 | | | | |
| C | -1.5156 | -2.4602 | -2.9591 | H | 3.6816 | 2.3058 | 3.1854 | | | | |
| H | -1.1595 | -3.0255 | -.8587 | H | 4.3752 | 3.7633 | 2.3691 | | | | |
| H | -.1203 | -3.8699 | -2.0511 | H | 4.2027 | 2.2109 | 1.4467 | | | | |
| H | .5856 | .0820 | -2.6469 | O | -1.5014 | -.7919 | 1.5628 | | | | |
| C | -.8313 | -1.2747 | -3.6551 | C | -1.0135 | -.6900 | 2.8769 | | | | |
| H | 1.3494 | -1.2887 | -3.5234 | C | -2.8853 | -.8788 | 1.3456 | | | | |
| C | 1.5656 | -3.1196 | .2157 | H | -1.2353 | -1.6143 | 3.4692 | | | | |
| H | 2.2964 | -2.8433 | -1.7928 | H | -1.4530 | .1797 | 3.4270 | | | | |
| H | 2.9482 | -.5270 | -1.7813 | H | .0958 | -.5582 | 2.8261 | | | | |
| C | 4.0796 | -1.3647 | -.1812 | H | -3.4475 | -.0394 | 1.8248 | | | | |

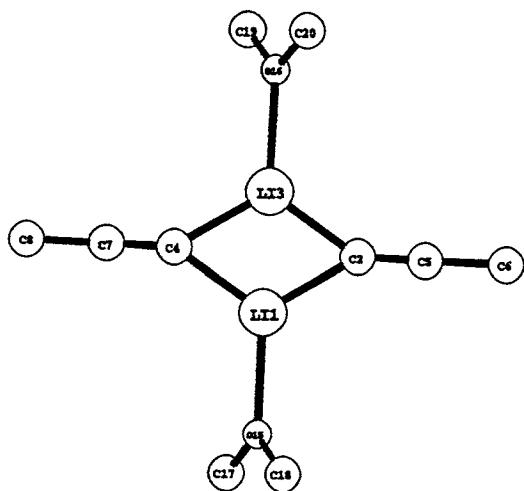
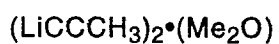


Figure XIII A



$\Delta H_f^\circ = -159.6 \text{ kcal/mol}$

| | | | |
|----|---------|---------|---------|
| Li | .0000 | .0000 | .0000 |
| C | 1.9931 | .0000 | .0000 |
| Li | 1.1812 | 1.8203 | .0000 |
| C | -.8120 | 1.8202 | .0007 |
| C | 3.0202 | -.6652 | -.0047 |
| C | 4.2330 | -1.4508 | -.0103 |
| C | -1.8375 | 2.4877 | .0065 |
| C | -3.0486 | 3.2760 | .0134 |
| H | 4.0119 | -2.5412 | -.0021 |
| H | 4.8495 | -1.2437 | -.9131 |
| H | 4.8642 | -1.2334 | .8799 |
| H | -3.9548 | 2.6304 | .0036 |
| H | -3.1105 | 3.9214 | .9176 |
| H | -3.1066 | 3.9429 | -.8754 |
| O | -1.1867 | -1.8259 | -.0026 |
| O | 2.3664 | 3.6470 | -.0004 |
| C | -1.8234 | -2.2475 | -1.1829 |
| C | -1.3110 | -2.5729 | 1.1818 |
| C | 2.4630 | 4.4137 | -1.1747 |
| C | 3.0302 | 4.0495 | 1.1716 |
| H | -1.5741 | -1.5092 | -1.9856 |
| H | -2.9348 | -2.2868 | -1.0626 |
| H | -1.4721 | -3.2598 | -1.5045 |
| H | -.7297 | -2.0451 | 1.9789 |
| H | -.9024 | -3.6075 | 1.0640 |
| H | -2.3774 | -2.6552 | 1.5098 |
| H | 1.8671 | 3.8968 | -1.9681 |
| H | 3.5220 | 4.5057 | -1.5237 |
| H | 2.0532 | 5.4446 | -1.0311 |
| H | 2.7983 | 3.2993 | 1.9684 |
| H | 2.6878 | 5.0572 | 1.5166 |
| H | 4.1387 | 4.0895 | 1.0267 |

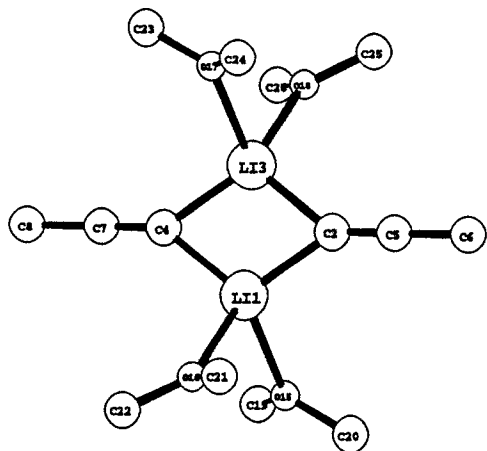
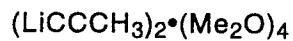


Figure XIII B



$\Delta H_f^\circ = -256.1 \text{ kcal/mol}$

| | | | | | | | | | | | |
|----|---------|---------|---------|---|---------|---------|---------|---|---------|---------|---------|
| Li | .0000 | .0000 | .0000 | C | -1.6871 | -.8644 | -2.6547 | H | -2.6012 | -.4136 | 2.7830 |
| C | 2.0342 | .0000 | .0000 | C | -.2078 | -2.6234 | -1.8933 | H | -2.9405 | -2.0340 | 2.0539 |
| Li | 1.3639 | 1.9208 | .0000 | C | -.2608 | -1.8793 | 2.6532 | H | .9635 | 4.7969 | .9826 |
| C | -.6705 | 1.9206 | .0008 | C | -2.4089 | -1.0618 | 1.8919 | H | 2.3148 | 5.3713 | 2.0456 |
| C | 3.0338 | -.7074 | -.0252 | C | 1.5708 | 4.5496 | 1.8861 | H | .8948 | 4.5220 | 2.7770 |
| C | 4.2120 | -1.5405 | -.0548 | C | 3.0451 | 2.7902 | 2.6562 | H | 3.4780 | 1.8351 | 2.2737 |
| C | -1.6678 | 2.6312 | .0275 | C | 3.7768 | 2.9816 | -1.8883 | H | 2.4934 | 2.5803 | 3.6068 |
| C | -2.8425 | 3.4692 | .0571 | C | 1.6292 | 3.7931 | -2.6576 | H | 3.8874 | 3.4877 | 2.8966 |
| H | 3.9496 | -2.6222 | -.0736 | H | -2.1218 | .0882 | -2.2678 | H | 4.2109 | 2.4900 | -.9848 |
| H | 4.8370 | -1.3384 | -.9536 | H | -2.5280 | -1.5632 | -2.8960 | H | 4.3071 | 3.9549 | -2.0481 |
| H | 4.8565 | -1.3744 | .8378 | H | -1.1378 | -.6495 | -3.6056 | H | 3.9732 | 2.3341 | -2.7791 |
| H | -3.7776 | 2.8653 | .0711 | H | .3999 | -2.8735 | -.9908 | H | .5850 | 3.8869 | -2.2745 |
| H | -2.8599 | 4.1227 | .9583 | H | .4681 | -2.5911 | -2.7841 | H | 1.6125 | 3.2026 | -3.6079 |
| H | -2.8954 | 4.1358 | -.8332 | H | -.9505 | -3.4455 | -2.0561 | H | 2.0099 | 4.8181 | -2.8985 |
| O | -.8402 | -1.3900 | -1.6652 | H | .7819 | -1.9755 | 2.2665 | | | | |
| O | -1.0359 | -1.2524 | 1.6638 | H | -.6434 | -2.9037 | 2.8939 | | | | |
| O | 2.2016 | 3.3144 | 1.6631 | H | -.2392 | -1.2904 | 3.6044 | | | | |
| O | 2.4028 | 3.1698 | -1.6646 | H | -2.8450 | -.5698 | .9896 | | | | |

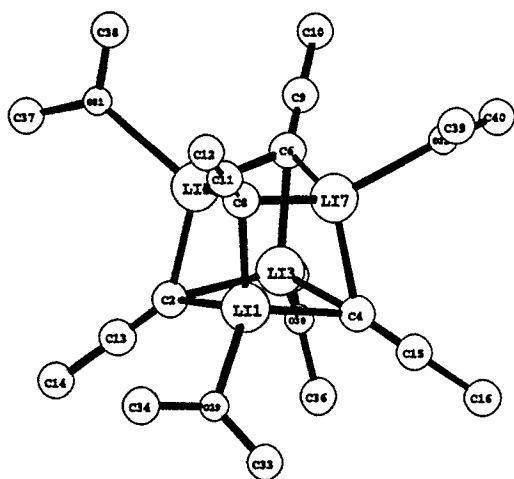
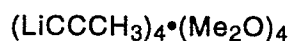


Figure XIII C



$\Delta H_f^\circ = -364.5 \text{ kcal/mol}$

| | | | | | | | |
|----|---------|---------|---------|---|---------|---------|---------|
| Li | .0000 | .0000 | .0000 | C | 2.2703 | -.1976 | -5.0590 |
| C | 2.1532 | .0000 | .0000 | C | -3.4541 | 2.6963 | -2.8722 |
| Li | 1.4989 | 2.0420 | .0000 | C | -2.1180 | 4.6588 | -2.3967 |
| C | -.5641 | 1.9913 | .6275 | H | -2.0206 | -.4931 | 2.3927 |
| Li | 1.4800 | .4936 | -1.9945 | H | -2.7782 | -2.1126 | 2.0874 |
| C | 1.4314 | 2.6388 | -2.0750 | H | -1.4186 | -1.9617 | 3.2717 |
| Li | -.5352 | 1.9541 | -1.5144 | H | .2485 | -2.9908 | .0727 |
| C | -.5793 | -.1331 | -2.0660 | H | .0344 | -3.5688 | 1.7808 |
| C | 1.9029 | 3.4910 | -2.8257 | H | -1.3340 | -3.7037 | .6053 |
| C | 2.4554 | 4.4975 | -3.7057 | H | 3.9604 | 3.9551 | -.2444 |
| C | -1.2394 | -.9177 | -2.7448 | H | 3.7213 | 5.2179 | 1.0391 |
| C | -2.0186 | -1.8400 | -3.5417 | H | 4.9033 | 3.8736 | 1.3016 |
| C | 3.0320 | -.6221 | .5940 | H | 1.8678 | 2.5569 | 2.9816 |
| C | 4.0696 | -1.3515 | 1.2897 | H | 3.5970 | 2.9877 | 3.3179 |
| C | -1.2726 | 2.5700 | 1.4495 | H | 2.3587 | 4.2972 | 3.1616 |
| C | -2.1012 | 3.2510 | 2.4202 | H | 4.1636 | -1.1116 | -2.4637 |
| H | 2.3527 | 5.5184 | -3.2747 | H | 3.8998 | -2.1302 | -3.9420 |
| H | 3.5384 | 4.3259 | -3.8949 | H | 4.8084 | -.5709 | -4.0704 |
| H | 1.9436 | 4.5026 | -4.6938 | H | 1.3183 | .3836 | -5.0005 |
| H | -3.0191 | -2.0254 | -3.0913 | H | 2.9994 | .3757 | -5.6851 |
| H | -2.1860 | -1.4510 | -4.5709 | H | 2.0647 | -1.1691 | -5.5752 |
| H | -1.5117 | -2.8257 | -3.6391 | H | -3.4178 | 1.5966 | -2.6855 |
| H | 5.0780 | -.9324 | 1.0757 | H | -4.3618 | 3.1104 | -2.3653 |
| H | 3.9244 | -1.3180 | 2.3923 | H | -3.5656 | 2.8702 | -3.9721 |
| H | 4.0870 | -2.4234 | .9909 | H | -1.1516 | 4.9112 | -1.8975 |
| H | -1.8430 | 2.9512 | 3.4604 | H | -2.0967 | 5.0563 | -3.4427 |
| H | -1.9832 | 4.3556 | 2.3554 | H | -2.9448 | 5.1777 | -1.8494 |
| H | -3.1799 | 3.0237 | 2.2687 | | | | |
| O | -.8863 | -1.7601 | 1.2546 | | | | |
| O | 2.8771 | 3.3314 | 1.3764 | | | | |
| O | 2.7435 | -.3930 | -3.7500 | | | | |
| O | -2.2682 | 3.2617 | -2.3757 | | | | |
| C | -1.8133 | -1.5850 | 2.2947 | | | | |
| C | -.4736 | -3.0619 | .9220 | | | | |
| C | 3.9090 | 4.1299 | .8567 | | | | |
| C | 2.6742 | 3.2987 | 2.7665 | | | | |
| C | 3.9531 | -1.0801 | -3.5590 | | | | |

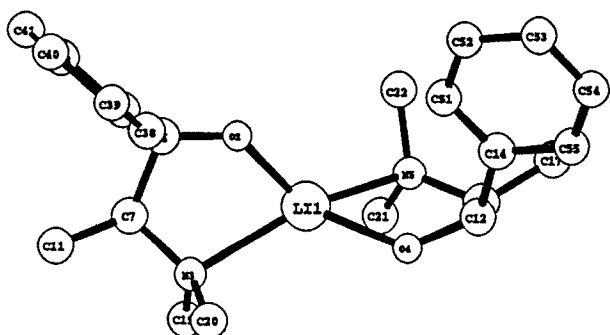


Figure XIID

$[R,S\text{-LiOCH(Ph)CH(Me)N(CH}_2)_4] \cdot [R,S\text{-HOCH(Ph)CH(Me)N(CH}_2)_4]$

$\Delta H_f^\circ = -44.7 \text{ kcal/mol}$

| | | | | | | | |
|----|---------|---------|---------|---|---------|---------|---------|
| Li | .0000 | .0000 | .0000 | H | 2.0627 | 4.6154 | -.0146 |
| O | 1.8789 | .0000 | .0000 | H | 3.6112 | 3.8139 | .3125 |
| N | .4607 | 2.3370 | .0000 | H | 2.8179 | 3.6061 | -1.2768 |
| O | -1.2519 | -1.0082 | -1.5359 | C | 3.8796 | .7860 | -2.0240 |
| N | -1.2815 | -1.5666 | 1.1736 | C | 5.0438 | .7652 | -2.8142 |
| C | 2.6804 | 1.0191 | .2857 | C | 6.3008 | .9944 | -2.2334 |
| C | 1.9041 | 2.4481 | .4044 | C | 6.3830 | 1.2408 | -.8531 |
| C | 3.9364 | 1.0419 | -.6336 | C | 5.2179 | 1.2604 | -.0678 |
| H | 3.1017 | .9110 | 1.3446 | H | 2.9266 | .5897 | -2.5179 |
| H | 1.8962 | 2.6341 | 1.5158 | H | 4.9676 | .5662 | -3.8839 |
| C | 2.6303 | 3.6757 | -.1874 | H | 7.2026 | .9783 | -2.8453 |
| C | -1.8080 | -2.2686 | -1.2338 | H | 7.3538 | 1.4146 | -.3876 |
| C | -2.2592 | -2.2673 | .2946 | H | 5.3241 | 1.4458 | 1.0030 |
| C | -.9186 | -3.4188 | -1.7301 | H | -3.1366 | -3.5758 | 1.8338 |
| H | -2.7858 | -2.3490 | -1.8017 | H | -3.5634 | -4.0224 | .1649 |
| H | -3.2009 | -1.6442 | .2831 | H | -1.9446 | -4.4266 | .8058 |
| C | -2.7342 | -3.6511 | .8023 | C | .4948 | -3.3996 | -1.6485 |
| H | -1.1367 | -.8981 | -2.4707 | C | 1.2610 | -4.4724 | -2.1461 |
| C | -.4698 | 3.1003 | .8586 | C | .6374 | -5.5817 | -2.7381 |
| C | .1345 | 2.4632 | -1.4382 | C | -.7645 | -5.6121 | -2.8365 |
| C | -1.8791 | -.5212 | 2.0426 | C | -1.5290 | -4.5430 | -2.3434 |
| C | -.2362 | -2.3604 | 1.8647 | H | 1.0332 | -2.5567 | -1.2052 |
| H | -1.5278 | 2.8494 | .6047 | H | 2.3488 | -4.4347 | -2.0715 |
| H | -.3654 | 4.2081 | .7608 | H | 1.2350 | -6.4092 | -3.1212 |
| H | -.3158 | 2.8431 | 1.9321 | H | -1.2622 | -6.4650 | -3.2992 |
| H | .1705 | 3.5180 | -1.8096 | H | -2.6146 | -4.5965 | -2.4490 |
| H | -.9087 | 2.0992 | -1.6264 | | | | |
| H | .8269 | 1.8655 | -2.0743 | | | | |
| H | -1.0787 | .0470 | 2.5783 | | | | |
| H | -2.5624 | -.9440 | 2.8200 | | | | |
| H | -2.4746 | .2044 | 1.4353 | | | | |
| H | -.6343 | -2.9112 | 2.7531 | | | | |
| H | .5780 | -1.6864 | 2.2255 | | | | |
| H | .2193 | -3.1126 | 1.1846 | | | | |

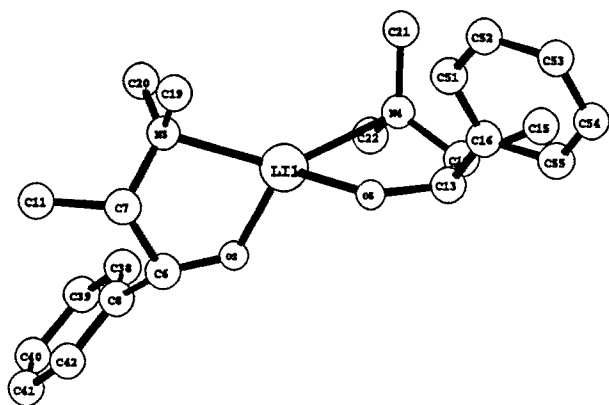


Figure XIII E

$[R,S\text{-LiOCH(Ph)CH(Me)N(CH}_2)_4] \cdot [R,S\text{-HOCH(Ph)CH(Me)N(CH}_2)_4]$

$\Delta H_f^\circ = -44.5 \text{ kcal/mol}$

| | | | | | | | |
|----|---------|---------|---------|---|---------|---------|---------|
| Li | .0000 | .0000 | .0000 | H | -.9859 | -2.4916 | -2.6589 |
| O | 1.8898 | .0000 | .0000 | H | .3774 | -2.0492 | -1.5644 |
| N | .3550 | 2.2859 | .0000 | H | 1.8092 | 4.6300 | .4158 |
| N | -1.5860 | -1.5898 | -.7703 | H | 3.3882 | 3.8718 | .7055 |
| O | -.7476 | -1.0666 | 1.7814 | H | 2.6846 | 3.8644 | -.9377 |
| C | 2.6422 | 1.0707 | .2270 | C | 3.5884 | .9713 | -2.2072 |
| C | 1.7660 | 2.4201 | .5018 | C | 4.6499 | 1.0785 | -3.1250 |
| C | 3.7753 | 1.2280 | -.8285 | C | 5.9343 | 1.4367 | -2.6872 |
| H | 3.1935 | .9663 | 1.2249 | C | 6.1484 | 1.6801 | -1.3207 |
| H | 1.6926 | 2.4389 | 1.6269 | C | 5.0853 | 1.5723 | -4.083 |
| C | 2.4414 | 3.7591 | .1378 | H | 2.6132 | .6701 | -2.5934 |
| C | -1.5809 | -2.7336 | .1855 | H | 4.4726 | .8774 | -4.1822 |
| C | -1.4824 | -2.2647 | 1.7082 | H | 6.7565 | 1.5203 | -3.3977 |
| H | -.6070 | -3.2836 | .0303 | H | 7.1434 | 1.9499 | -.9649 |
| C | -2.6671 | -3.8069 | -.0724 | H | 5.2962 | 1.7562 | .6473 |
| C | -2.7834 | -2.1585 | 2.5225 | H | -2.6345 | -4.1614 | -1.1235 |
| H | -.8725 | -3.0847 | 2.1966 | H | -2.4816 | -4.6955 | .5658 |
| H | -.2563 | -1.0118 | 2.5916 | H | -3.6994 | -3.4615 | .1297 |
| C | -.6814 | 2.7756 | .9368 | C | -3.5795 | -.9904 | 2.5722 |
| C | .0776 | 2.6604 | -1.4025 | C | -4.7476 | -.9370 | 3.3561 |
| C | -2.8824 | -1.0067 | -1.1716 | C | -5.1453 | -2.0482 | 4.1157 |
| C | -.6385 | -1.7338 | -1.9130 | C | -4.3609 | -3.2144 | 4.0910 |
| H | -1.6994 | 2.4859 | .5768 | C | -3.1951 | -3.2648 | 3.3096 |
| H | -.6821 | 3.8867 | 1.0579 | H | -3.3047 | -.0958 | 2.0104 |
| H | -.5445 | 2.3292 | 1.9503 | H | -5.3434 | -.0236 | 3.3730 |
| H | -.0143 | 3.7644 | -1.5557 | H | -6.0506 | -2.0068 | 4.7217 |
| H | -.8923 | 2.2096 | -1.7325 | H | -4.6545 | -4.0823 | 4.6825 |
| H | .8697 | 2.2936 | -2.0910 | H | -2.6050 | -4.1836 | 3.3271 |
| H | -3.3964 | -1.5888 | -1.9751 | | | | |
| H | -2.7231 | .0280 | -1.5591 | | | | |
| H | -3.5847 | -.9353 | -.3137 | | | | |
| H | -.5436 | -.7584 | -2.4571 | | | | |

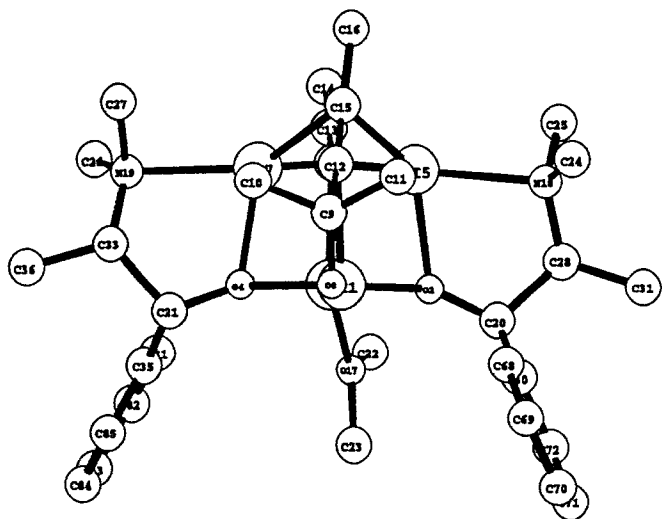


Figure XIVA

(LiCCCH₃)₂[*R,S*-LiOCH(Ph)CH(CH₃)NMe₂]₂·(Me₂O)·(CH₃COCH₃)
 $\Delta H_f^\circ = -198.8$ KCAL/MOL

| | | | | | | | | | | | |
|----|---------|---------|---------|---|---------|---------|---------|---|---------|---------|--------|
| Li | .0000 | .0000 | .0000 | H | -2.9360 | 2.6735 | -.7806 | H | 1.0503 | -2.5236 | .3779 |
| O | 2.2237 | .0000 | .0000 | H | 3.4513 | 4.2426 | -4.6086 | H | .3236 | -4.1629 | 2.0571 |
| Li | 1.9393 | 2.2442 | .0000 | H | 4.7625 | 4.0479 | -3.4015 | H | 1.5809 | -4.4481 | 4.1980 |
| O | -.2655 | 2.2802 | .0656 | H | 3.5101 | 5.3098 | -3.1689 | H | 3.5875 | -3.0235 | 4.6445 |
| Li | 2.1246 | .3832 | -2.0981 | H | .1721 | 1.4443 | -4.8882 | H | 4.3267 | -1.3574 | 2.9977 |
| C | 2.1674 | 2.5128 | -2.1710 | H | -.0987 | -.2885 | -5.2508 | H | 4.6026 | -3.3425 | .0054 |
| Li | .0618 | 2.2789 | -2.0323 | H | 1.5220 | .2631 | -4.7210 | H | 5.9555 | -2.6543 | -.9346 |
| O | -1.5716 | -1.3286 | -.0073 | H | 4.5739 | 4.0460 | .0689 | H | 5.7435 | -2.1951 | .7664 |
| C | -1.7621 | -1.3836 | -1.2763 | H | 5.5265 | 3.2102 | 1.3683 | C | .3607 | 4.9263 | 1.3245 |
| C | -3.1179 | -.7921 | -1.7805 | H | 4.7024 | 4.7821 | 1.7208 | C | .7513 | 5.9215 | 2.2437 |
| C | -1.4349 | -2.7542 | -1.9568 | H | 2.2454 | 2.2068 | 2.8921 | C | .0412 | 6.1078 | 3.4394 |
| C | -.5315 | -.2894 | -2.1411 | H | 3.1624 | 3.6501 | 3.5096 | C | -1.0636 | 5.2849 | 3.7153 |
| C | 2.8616 | 3.3216 | -2.7871 | H | 4.0304 | 2.0915 | 3.2250 | C | -1.4607 | 4.3033 | 2.7923 |
| C | 3.6784 | 4.2678 | -3.5198 | H | 2.5265 | -3.0007 | -1.5767 | H | .9581 | 4.8167 | .4122 |
| C | .0007 | .1346 | -3.1760 | H | 3.9038 | -3.3354 | -2.6815 | H | 1.6126 | 6.5531 | 2.0215 |
| C | .4261 | .4095 | -4.5576 | H | 2.4925 | -2.3937 | -3.2711 | H | .3446 | 6.8791 | 4.1473 |
| O | 3.4356 | 3.1264 | 1.4979 | H | 4.9435 | .3379 | -2.7551 | H | -1.6157 | 5.4078 | 4.6478 |
| N | 3.7656 | -1.2840 | -1.9652 | H | 4.0964 | -.6663 | -3.9945 | H | -2.3201 | 3.6797 | 3.0478 |
| N | -1.6144 | 3.9022 | -1.8797 | H | 5.5743 | -1.2927 | -3.1873 | H | -2.8146 | 5.6027 | .2196 |
| C | 3.2507 | -.7077 | .5325 | H | -.6158 | 5.6712 | -1.1501 | H | -4.0301 | 4.9033 | -.8839 |
| C | -1.2779 | 3.0290 | .5705 | H | -1.8621 | 6.0031 | -2.3934 | H | -3.8722 | 4.2704 | .7682 |
| C | 4.6103 | 3.8178 | 1.1610 | H | -.2963 | 5.2552 | -2.8690 | | | | |
| C | 3.2175 | 2.7561 | 2.8388 | H | -2.6179 | 2.3553 | -3.0024 | | | | |
| C | 3.1515 | -2.5635 | -2.3846 | H | -1.7072 | 3.5581 | -3.9953 | | | | |
| C | 4.6394 | -.7046 | -3.0174 | H | -3.2930 | 3.9996 | -3.2728 | | | | |
| C | -1.0811 | 5.2695 | -2.0740 | H | -3.3400 | .1978 | -1.3372 | | | | |
| C | -2.3470 | 3.4349 | -3.0856 | H | -3.9445 | -1.4756 | -1.4906 | | | | |
| C | 4.3300 | -1.1974 | -.5775 | H | -3.1497 | -.6872 | -2.8835 | | | | |
| H | 3.9018 | -.0130 | 1.1641 | H | -.4115 | -3.1125 | -1.7321 | | | | |
| C | 2.7656 | -1.7938 | 1.5297 | H | -1.5397 | -2.7105 | -3.0595 | | | | |
| C | 5.1874 | -2.4183 | -.1676 | H | -2.1445 | -3.5249 | -1.5875 | | | | |
| H | 5.0649 | -.3405 | -.5965 | C | 1.6251 | -2.6015 | 1.3052 | | | | |
| C | -2.2893 | 3.5752 | -.5780 | C | 1.2048 | -3.5521 | 2.2583 | | | | |
| H | -1.9695 | 2.3609 | 1.1823 | C | 1.9075 | -3.7134 | 3.4619 | | | | |
| C | -.7751 | 4.1147 | 1.5633 | C | 3.0354 | -2.9131 | 3.7105 | | | | |
| C | -3.2893 | 4.6529 | -.0951 | C | 3.4519 | -1.9668 | 2.7606 | | | | |

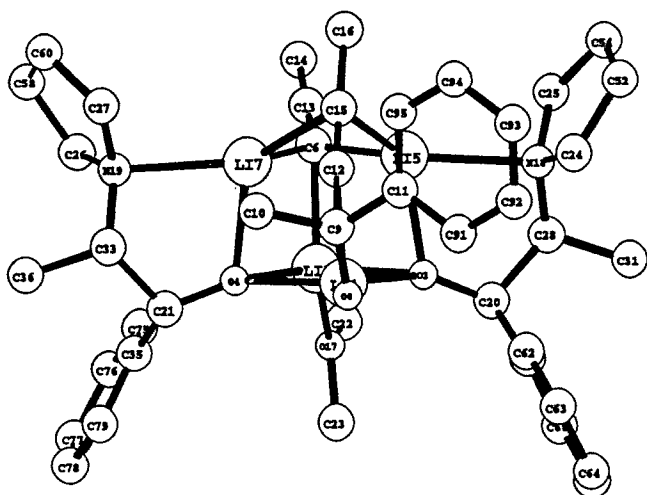


Figure XIVB

$(\text{LiCCCH}_3)_2 \cdot [R,S\text{-LiOCH(Ph)CH(CH}_3\text{)N(CH}_2\text{)}_4]_2 \cdot (\text{Me}_2\text{O}) \cdot (\text{PhCOCH}_3)$

$\Delta H_f^\circ = -175.9 \text{ kcal/mol}$

| | | | | | | | | | | | |
|----|---------|---------|---------|---|---------|---------|---------|---|---------|---------|---------|
| Li | .0000 | .0000 | .0000 | H | -1.9163 | 2.4352 | 1.2480 | H | 1.2274 | -2.6245 | .2697 |
| O | 2.2234 | .0000 | .0000 | C | -.7273 | 4.2210 | 1.4632 | H | .6519 | -4.4062 | 1.8651 |
| Li | 1.9356 | 2.2475 | .0000 | C | -3.3865 | 4.5167 | -.0819 | H | 1.9353 | -4.6906 | 3.9869 |
| O | -.2570 | 2.2896 | .0743 | H | -2.8811 | 2.5684 | -.7752 | H | 3.8184 | -3.1271 | 4.5041 |
| Li | 2.1366 | .3692 | -2.1003 | H | 3.5553 | 4.1548 | -4.6022 | H | 4.4137 | -1.3316 | 2.9386 |
| C | 2.1704 | 2.4999 | -2.1670 | H | 4.8387 | 3.9271 | -3.3711 | H | 5.0834 | -3.0252 | .0942 |
| Li | .0557 | 2.2650 | -2.0238 | H | 3.6283 | 5.2352 | -3.1732 | H | 6.2517 | -2.1898 | -.9601 |
| O | -1.5255 | -1.3908 | .0485 | H | .2934 | 1.4148 | -4.7989 | H | 6.0152 | -1.6288 | .7071 |
| C | -1.8556 | -1.3994 | -1.1895 | H | -.0639 | -.2929 | -5.1947 | C | .3882 | 5.0262 | 1.1263 |
| C | -3.2012 | -.6777 | -1.5259 | H | 1.5675 | .1519 | -4.6075 | C | .8014 | 6.0849 | 1.9609 |
| C | -1.7302 | -2.7540 | -1.9372 | H | 4.5790 | 4.0431 | .1237 | C | .1347 | 6.3455 | 3.1675 |
| C | -.5903 | -.3320 | -2.1005 | H | 5.4825 | 3.2309 | 1.4722 | C | -.9490 | 5.5328 | 3.5405 |
| C | 2.9032 | 3.2757 | -2.7812 | H | 4.6439 | 4.8070 | 1.7669 | C | -1.3682 | 4.4866 | 2.7022 |
| C | 3.7652 | 4.1838 | -3.5100 | H | 2.1500 | 2.2386 | 2.8839 | H | .9519 | 4.8619 | .2013 |
| C | -.0092 | .0929 | -3.1081 | H | 3.0337 | 3.6971 | 3.5147 | H | 1.6466 | 6.7075 | 1.6637 |
| C | .4767 | .3628 | -4.4728 | H | 3.9210 | 2.1397 | 3.2875 | H | .4551 | 7.1660 | 3.8096 |
| O | 3.3882 | 3.1457 | 1.5234 | H | 2.1103 | -2.5299 | -2.3627 | H | -1.4673 | 5.7138 | 4.4828 |
| N | 3.8132 | -1.3055 | -1.9886 | H | 3.3804 | -3.3721 | -1.4305 | H | -2.2096 | 3.8737 | 3.0326 |
| N | -1.6811 | 3.8817 | -1.8929 | C | 3.8277 | -3.1965 | -3.5696 | H | -2.9845 | 5.4942 | .2479 |
| C | 3.2947 | -.6646 | .5008 | H | 4.2196 | .0022 | -3.6336 | H | -4.1459 | 4.7264 | -.8645 |
| C | -1.2549 | 3.0658 | .5665 | C | 4.7205 | -2.0880 | -4.1470 | H | -3.9375 | 4.0796 | .7767 |
| C | 4.5742 | 3.8334 | 1.2200 | H | 5.7022 | -.6144 | -2.8534 | H | -3.3675 | .2128 | -.8883 |
| C | 3.1201 | 2.7936 | 2.8601 | H | -.0024 | 5.1524 | -2.2134 | H | -4.0436 | -1.3777 | -1.3381 |
| C | 3.2188 | -2.6449 | -2.2587 | H | -1.2730 | 5.9189 | -1.2162 | H | -3.2703 | -.3523 | -2.5821 |
| C | 4.6665 | -.9074 | -3.1502 | C | -1.7379 | 5.8681 | -3.3577 | C | -1.5347 | -3.9568 | -1.2112 |
| C | -1.1113 | 5.2451 | -2.0878 | H | -1.9819 | 2.6794 | -3.6366 | C | -1.4799 | -5.2055 | -1.8577 |
| C | -2.4873 | 3.5265 | -3.1019 | C | -2.5796 | 4.7676 | -4.0197 | C | -1.6263 | -5.2925 | -3.2507 |
| C | 4.3955 | -1.0216 | -.6382 | H | -3.5128 | 3.1632 | -2.8530 | C | -1.8353 | -4.1171 | -3.9895 |
| H | 3.9026 | .0419 | 1.1623 | C | 1.8173 | -2.7087 | 1.1865 | C | -1.8910 | -2.8714 | -3.3403 |
| C | 2.8920 | -1.8261 | 1.4472 | C | 1.4807 | -3.7349 | 2.0932 | H | -1.4332 | -3.9479 | -.1243 |
| C | 5.4792 | -2.0279 | -.1790 | C | 2.1983 | -3.8969 | 3.2876 | H | -1.3263 | -6.1107 | -1.2690 |
| H | 4.9493 | -.0429 | -.7574 | C | 3.2571 | -3.0193 | 3.5753 | H | -1.5832 | -6.2594 | -3.7521 |
| C | -2.3097 | 3.5214 | -.5797 | C | 3.5921 | -1.9993 | 2.6706 | H | -1.9595 | -4.1682 | -5.0718 |

| | | | | | | | | | | | |
|---|---------|---------|---------|---|---------|---------|---------|---|---------|--------|---------|
| H | -2.0712 | -1.9922 | -3.9611 | H | 4.3739 | -1.7738 | -5.1546 | H | -0.9502 | 6.2436 | -4.0447 |
| H | 4.4140 | -4.1202 | -3.3753 | H | 5.7647 | -2.4434 | -4.2814 | H | -2.2092 | 4.5347 | -5.0407 |
| H | 3.0301 | -3.4867 | -4.2859 | H | -2.3636 | 6.7494 | -3.0998 | H | -3.6356 | 5.0898 | -4.1444 |

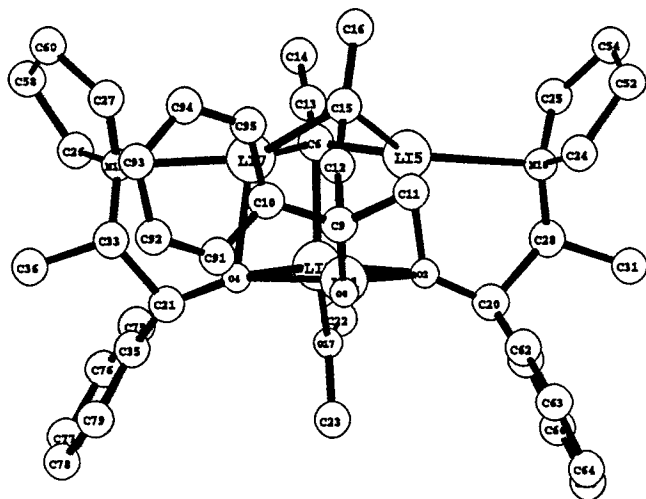


Figure XIVC



$\Delta H_f^\circ = -175.4 \text{ kcal/mol}$

| | | | | | | | | | | | |
|----|---------|---------|---------|---|---------|---------|---------|---|---------|---------|---------|
| Li | .0000 | .0000 | .0000 | H | 4.9545 | -.0112 | -.6745 | C | 1.3758 | -3.7711 | 1.9661 |
| O | 2.2210 | .0000 | .0000 | C | -2.3390 | 3.4231 | -.5971 | C | 2.0586 | -3.9824 | 3.1733 |
| Li | 1.9292 | 2.2472 | .0000 | H | -1.9426 | 2.3443 | 1.2359 | C | 3.1232 | -3.1319 | 3.5165 |
| O | -.2575 | 2.2685 | .0911 | C | -.8244 | 4.1693 | 1.4860 | C | 3.4985 | -2.0885 | 2.6553 |
| Li | 2.1526 | .3762 | -2.0992 | C | -3.4875 | 4.3392 | -.1077 | H | 1.1936 | -2.6019 | .1727 |
| C | 2.1536 | 2.5044 | -2.1697 | H | -2.8432 | 2.4415 | -.8359 | H | .5414 | -4.4186 | 1.6932 |
| Li | .0455 | 2.2468 | -2.0132 | H | 3.4738 | 4.1906 | -4.6174 | H | 1.7644 | -4.7929 | 3.8400 |
| O | -1.5787 | -1.3222 | .0544 | H | 4.7723 | 4.0088 | -3.3947 | H | 3.6574 | -3.2786 | 4.4559 |
| C | -1.8454 | -1.4101 | -1.1956 | H | 3.5221 | 5.2781 | -3.1928 | H | 4.3216 | -1.4421 | 2.9675 |
| C | -3.2276 | -.8748 | -1.6515 | H | .2853 | 1.2864 | -4.8766 | H | 5.1094 | -3.0052 | .1303 |
| C | -1.5216 | -2.7939 | -1.8526 | H | .0402 | -.4627 | -5.1664 | H | 6.2957 | -2.1327 | -.8731 |
| C | -.6051 | -.3104 | -2.1027 | H | 1.6249 | .1196 | -4.5686 | H | 5.9997 | -1.6059 | .7958 |
| C | 2.8627 | 3.2980 | -2.7890 | H | 4.5415 | 4.0856 | .1069 | C | .2841 | 4.9999 | 1.1905 |
| C | 3.6902 | 4.2305 | -3.5269 | H | 5.4624 | 3.3092 | 1.4647 | C | .6494 | 6.0604 | 2.0446 |
| C | .0041 | .0661 | -3.1130 | H | 4.5826 | 4.8658 | 1.7434 | C | -.0613 | 6.2998 | 3.2303 |
| C | .5195 | .2714 | -4.4772 | H | 2.1493 | 2.2498 | 2.8787 | C | -1.1405 | 5.4637 | 3.5622 |
| O | 3.3711 | 3.1704 | 1.5123 | H | 3.0098 | 3.7255 | 3.5016 | C | -1.5107 | 4.4147 | 2.7047 |
| N | 3.8725 | -1.2694 | -1.9587 | H | 3.9226 | 2.1818 | 3.2799 | H | .8808 | 4.8526 | .2837 |
| N | -1.6927 | 3.8586 | -1.8787 | H | 2.2165 | -2.5202 | -2.4342 | H | 1.4917 | 6.7009 | 1.7792 |
| C | 3.2736 | -.6776 | .5227 | H | 3.4489 | -3.3488 | -1.4421 | H | .2220 | 7.1216 | 3.8878 |
| C | -1.2928 | 3.0037 | .5706 | C | 4.0055 | -3.1439 | -3.5542 | H | -1.6932 | 5.6284 | 4.4879 |
| C | 4.5394 | 3.8859 | 1.2052 | H | 4.2808 | .0629 | -3.5830 | H | -2.3493 | 3.7826 | 3.0045 |
| C | 3.1102 | 2.8206 | 2.8511 | C | 4.8821 | -2.0018 | -4.0899 | H | -3.1542 | 5.3312 | .2544 |
| C | 3.3198 | -2.6168 | -2.2714 | H | 5.7602 | -.4985 | -2.7560 | H | -4.2373 | 4.5216 | -.9061 |
| C | 4.7478 | -.8307 | -3.0891 | H | -.0673 | 5.2131 | -2.1090 | H | -4.0335 | 3.8499 | .7256 |
| C | -1.1816 | 5.2520 | -2.0096 | H | -1.3961 | 5.8852 | -1.1192 | H | -.5312 | -3.1863 | -1.5493 |
| C | -2.4443 | 3.5106 | -3.1245 | C | -1.8034 | 5.8930 | -3.2728 | H | -1.5377 | -2.7656 | -2.9594 |
| C | 4.4125 | -.9996 | -.5878 | H | -1.8776 | 2.7150 | -3.6780 | H | -2.2858 | -3.5322 | -1.5283 |
| H | 3.8549 | .0099 | 1.2264 | C | -2.5773 | 4.7813 | -3.9957 | C | -4.2386 | -.6094 | -.6913 |
| C | 2.8349 | -1.8650 | 1.4199 | H | -3.4551 | 3.0842 | -2.9206 | C | -5.5329 | -.2156 | -1.0785 |
| C | 5.4974 | -1.9972 | -.1133 | C | 1.7549 | -2.7226 | 1.1030 | C | -5.8574 | -.0736 | -2.4367 |

| | | | | | | | | | | | |
|---|---------|--------|--------|---|---------|---------|---------|---|---------|---------|---------|
| C | -1.4452 | 4.3449 | 2.7708 | H | -4.0928 | 4.7720 | -.8757 | C | -5.8016 | -.1739 | -2.6435 |
| H | .9629 | 4.8057 | .3685 | H | -3.9142 | 4.1347 | .7730 | C | -4.8030 | -.5220 | -3.5669 |
| H | 1.6229 | 6.5784 | 1.9351 | H | -.4657 | -3.1887 | -1.4425 | C | -3.5216 | -.8911 | -3.1211 |
| H | .3628 | 6.9536 | 4.0575 | H | -1.3788 | -2.8169 | -2.9270 | H | -4.0406 | -.5725 | .2490 |
| H | -1.5947 | 5.4935 | 4.5997 | H | -2.2134 | -3.5587 | -1.5306 | H | -6.2676 | .0698 | -.5434 |
| H | -2.3027 | 3.7266 | 3.0447 | C | -4.2180 | -.5658 | -.8287 | H | -6.7969 | .1083 | -2.9870 |
| H | -2.9164 | 5.5180 | .2397 | C | -5.5015 | -.1968 | -1.2726 | H | -5.0206 | -.5105 | -4.6355 |
| | | | | | | | | H | -2.7855 | -1.1563 | -3.8819 |

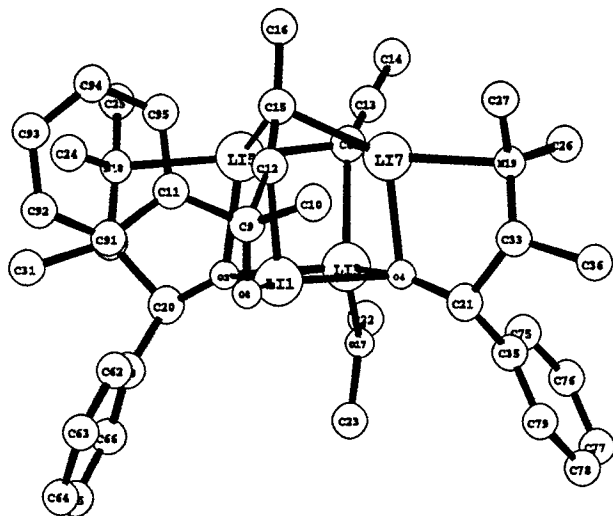


Figure XIVE

$(\text{LiCCCH}_3)_2 \cdot [R,S\text{-LiOCH(Ph)CH(CH}_3\text{)NMe}_2]_2 \cdot (\text{Me}_2\text{O}) \cdot (\text{PhCOCH}_3)$
 $\Delta H_f^\circ = -159.2 \text{ kcal/mol}$

| | | | | | | | | | | | |
|----|---------|---------|---------|---|---------|---------|---------|---|---------|---------|---------|
| Li | .0000 | .0000 | .0000 | C | -1.0462 | 5.2676 | -2.0985 | H | 3.6875 | -3.4147 | -2.6177 |
| O | 2.2274 | .0000 | .0000 | C | -2.3527 | 3.4482 | -3.0872 | H | 2.3497 | -2.3960 | -3.2466 |
| Li | 1.9481 | 2.2445 | .0000 | C | 4.2995 | -1.2549 | -.6034 | H | 4.9509 | .1966 | -2.8297 |
| O | -.2598 | 2.2857 | .0564 | H | 3.9595 | .0363 | 1.0809 | H | 4.0283 | -.7899 | -4.0272 |
| Li | 2.1169 | .3756 | -2.0989 | C | 2.8299 | -1.7098 | 1.6008 | H | 5.4826 | -1.4779 | -3.2279 |
| C | 2.1890 | 2.5077 | -2.1662 | C | 5.0992 | -2.5144 | -.1933 | H | -.5672 | 5.6673 | -1.1807 |
| Li | .0800 | 2.2946 | -2.0400 | H | 5.0792 | -.4400 | -.6547 | H | -1.8173 | 6.0122 | -2.4167 |
| O | -1.5529 | -1.3608 | .0440 | C | -2.2721 | 3.6027 | -.5831 | H | -.2679 | 5.2349 | -2.8996 |
| C | -1.8421 | -1.4137 | -1.2030 | H | -1.9614 | 2.3835 | 1.1750 | H | -2.6316 | 2.3712 | -2.9979 |
| C | -3.1914 | -.7315 | -1.6006 | C | -.7497 | 4.1256 | 1.5549 | H | -1.7239 | 3.5637 | -4.0053 |
| C | -1.6632 | -2.7866 | -1.9049 | C | -3.2506 | 4.7001 | -.1002 | H | -3.2958 | 4.0211 | -3.2635 |
| C | -.5795 | -.3362 | -2.1066 | H | -2.9357 | 2.7116 | -.7770 | C | 1.6762 | -2.5199 | 1.4751 |
| C | 2.9151 | 3.2918 | -2.7777 | H | 3.5572 | 4.1775 | -4.5987 | C | 1.2965 | -3.4099 | 2.5009 |
| C | 3.7640 | 4.2125 | -3.5062 | H | 4.8412 | 3.9736 | -3.3644 | C | 2.0532 | -3.5073 | 3.6784 |
| C | -.0331 | .1361 | -3.1127 | H | 3.6090 | 5.2620 | -3.1718 | C | 3.1961 | -2.7038 | 3.8278 |
| C | .4068 | .4667 | -4.4800 | H | -.1503 | -.1649 | -5.2109 | C | 3.5729 | -1.8177 | 2.8060 |
| O | 3.4417 | 3.1266 | 1.5047 | H | 1.4944 | .2728 | -4.6559 | H | 1.0604 | -2.4896 | .5714 |
| N | 3.6998 | -1.3337 | -1.9764 | H | .2045 | 1.5294 | -4.7585 | H | .4044 | -4.0255 | 2.3781 |
| N | -1.6009 | 3.9105 | -1.8913 | H | 4.5854 | 4.0448 | .0791 | H | 1.7569 | -4.1956 | 4.4699 |
| C | 3.2741 | -.6867 | .5213 | H | 5.5331 | 3.1988 | 1.3755 | H | 3.7909 | -2.7652 | 4.7398 |
| C | -1.2636 | 3.0448 | .5625 | H | 4.7182 | 4.7742 | 1.7335 | H | 4.4624 | -1.2044 | 2.9652 |
| C | 4.6205 | 3.8124 | 1.1702 | H | 2.2478 | 2.2074 | 2.8958 | H | 4.4688 | -3.4007 | .0148 |
| C | 3.2199 | 2.7568 | 2.8450 | H | 3.1628 | 3.6510 | 3.5153 | H | 5.8300 | -2.8081 | -.9767 |
| C | 2.9932 | -2.5799 | -2.3515 | H | 4.0317 | 2.0926 | 3.2341 | H | 5.6950 | -2.3059 | .7193 |
| C | 4.5853 | -.8338 | -3.0586 | H | 2.3369 | -2.9389 | -1.5294 | C | .3883 | 4.9327 | 1.3112 |

| | | | | | | | | | | | |
|---|---------|--------|--------|---|---------|---------|---------|---|---------|---------|---------|
| C | .7866 | 5.9264 | 2.2288 | H | -2.7578 | 5.6434 | .2062 | C | -1.6574 | -4.2107 | -3.9180 |
| C | .0830 | 6.1148 | 3.4279 | H | -3.9919 | 4.9589 | -.8858 | C | -1.7602 | -2.9476 | -3.3094 |
| C | -1.0232 | 5.2954 | 3.7090 | H | -3.8348 | 4.3325 | .7686 | H | -1.4255 | -3.9225 | -.0459 |
| C | -1.4284 | 4.3158 | 2.7875 | H | -3.3685 | .2048 | -1.0356 | H | -1.2366 | -6.1152 | -1.1196 |
| H | .9813 | 4.8210 | .3962 | H | -4.0281 | -1.4233 | -1.3639 | H | -1.3837 | -6.3409 | -3.6060 |
| H | 1.6489 | 6.5552 | 2.0025 | H | -3.2575 | -.4902 | -2.6793 | H | -1.7334 | -4.2955 | -5.0026 |
| H | .3923 | 6.8849 | 4.1345 | C | -1.4804 | -3.9643 | -1.1355 | H | -1.9259 | -2.0903 | -3.9638 |
| H | -1.5701 | 5.4197 | 4.6444 | C | -1.3786 | -5.2303 | -1.7413 | | | | |
| H | -2.2890 | 3.6953 | 3.0467 | C | -1.4631 | -5.3605 | -3.1361 | | | | |

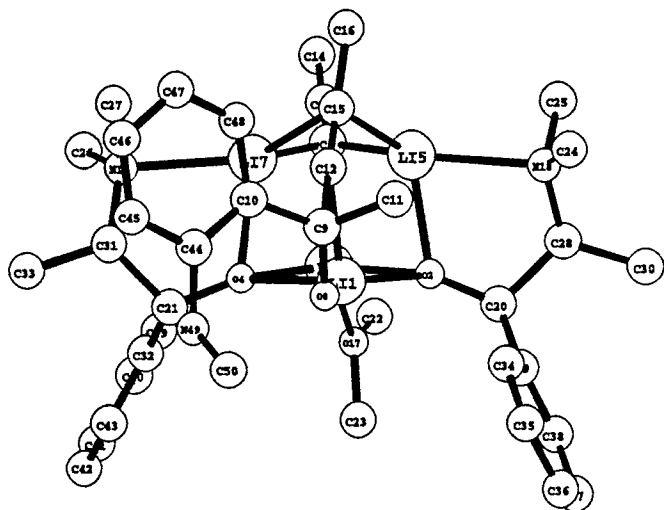


Figure XIVF

$(\text{LiCCCH}_3)_2 \cdot [R,S\text{-LiOCH(Ph)CH(CH}_3\text{)NMe}_2]_2 \cdot (\text{Me}_2\text{O}) \cdot (\text{ortho-MeNH-PhCOCH}_3)$
 $\Delta H_f^\circ = -150.7 \text{ kcal/mol}$

| | | | | | | | | | | | |
|----|---------|---------|---------|---|---------|---------|---------|---|---------|---------|---------|
| Li | .0000 | .0000 | .0000 | C | 3.2208 | 2.7858 | 2.8414 | C | -5.6901 | -.4409 | -1.5046 |
| O | 2.2211 | .0000 | .0000 | C | 3.1031 | -2.5882 | -2.3402 | C | -5.8244 | -.3317 | -2.8927 |
| Li | 1.9506 | 2.2524 | .0000 | C | 4.6418 | -.7761 | -2.9941 | C | -4.7016 | -.5434 | -3.7069 |
| O | -.2467 | 2.2662 | .0807 | C | -1.1768 | 5.2813 | -2.0432 | C | -3.4676 | -.8564 | -3.1209 |
| Li | 2.1392 | .3843 | -2.0984 | C | -2.3322 | 3.3847 | -3.0698 | N | -4.5035 | -.8014 | .5302 |
| C | 2.1727 | 2.5129 | -2.1700 | C | 4.3150 | -1.2316 | -.5504 | C | -4.8726 | -2.0696 | 1.1644 |
| Li | .0655 | 2.2782 | -2.0243 | C | 2.7561 | -1.7486 | 1.5820 | H | -3.6747 | -.4225 | .9585 |
| O | -1.6575 | -1.2505 | .0696 | C | 5.1386 | -2.4701 | -.1245 | | | | |
| C | -1.8947 | -1.4219 | -1.1758 | C | -2.2940 | 3.5133 | -.5607 | | | | |
| C | -3.2818 | -.9752 | -1.7172 | C | -.7379 | 4.1466 | 1.5273 | | | | |
| C | -1.4923 | -2.8240 | -1.7480 | C | -3.3526 | 4.5310 | -.0729 | | | | |
| C | -.6397 | -.3249 | -2.0895 | C | 1.5932 | -2.5345 | 1.3977 | | | | |
| C | 2.8603 | 3.3271 | -2.7867 | C | 1.1684 | -3.4511 | 2.3814 | | | | |
| C | 3.6681 | 4.2797 | -3.5211 | C | 1.8883 | -3.5986 | 3.5768 | | | | |
| C | -.0280 | .0961 | -3.0804 | C | 3.0380 | -2.8184 | 3.7859 | | | | |
| C | .4748 | .3558 | -4.4417 | C | 3.4593 | -1.9060 | 2.8053 | | | | |
| O | 3.4526 | 3.1298 | 1.4960 | C | .3995 | 4.9420 | 1.2433 | | | | |
| N | 3.7507 | -1.3199 | -1.9378 | C | .8057 | 5.9704 | 2.1182 | | | | |
| N | -1.6329 | 3.8858 | -1.8573 | C | .1101 | 6.2084 | 3.3132 | | | | |
| C | 3.2457 | -.6982 | .5489 | C | -.9962 | 5.4039 | 3.6336 | | | | |
| C | -1.2549 | 3.0228 | .5857 | C | -1.4087 | 4.3885 | 2.7551 | | | | |
| C | 4.6357 | 3.8054 | 1.1560 | C | -4.4403 | -.7667 | -.9017 | | | | |

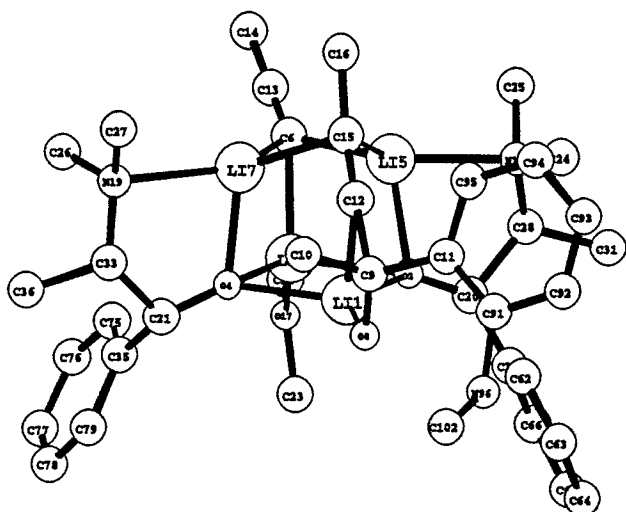


Figure XIVG

$(\text{LiCCCH}_3)_2 \cdot [R,S\text{-LiOCH(Ph)CH(CH}_3\text{)NMe}_2]_2 \cdot (\text{Me}_2\text{O}) \cdot (\text{ortho-MeNH-PhCOCH}_3)$

$\Delta H_f^\circ = -149.4 \text{ kcal/mol}$

| | | | | | | | | | | | |
|----|---------|---------|---------|---|---------|---------|---------|---|---------|---------|---------|
| Li | .0000 | .0000 | .0000 | C | -3.3364 | 4.6135 | -.1296 | H | 4.4722 | -1.1501 | 2.9556 |
| O | 2.2248 | .0000 | .0000 | H | -2.9755 | 2.6291 | -.7976 | H | 4.6791 | -3.2749 | -.0446 |
| Li | 1.9158 | 2.2495 | .0000 | H | 3.5074 | 4.2547 | -4.5674 | H | 5.9987 | -2.5693 | -1.0176 |
| O | -.2927 | 2.2674 | .0316 | H | 4.7818 | 4.0750 | -3.3193 | H | 5.8187 | -2.1055 | .6853 |
| Li | 2.1156 | .3889 | -2.0955 | H | 3.5131 | 5.3282 | -3.1313 | C | .3101 | 4.9304 | 1.2699 |
| C | 2.1637 | 2.5228 | -2.1634 | H | -.2398 | -.0925 | -5.1518 | C | .6917 | 5.9384 | 2.1790 |
| Li | .0575 | 2.2891 | -2.0632 | H | 1.4333 | .2611 | -4.6247 | C | -.0157 | 6.1259 | 3.3760 |
| O | -1.5921 | -1.3177 | .1166 | H | .1831 | 1.5643 | -4.6277 | C | -1.1086 | 5.2911 | 3.6638 |
| C | -1.8484 | -1.5196 | -1.1202 | H | 4.5298 | 4.0827 | .1166 | C | -1.4971 | 4.2969 | 2.7508 |
| C | -3.1694 | -.8882 | -1.6698 | H | 5.4671 | 3.2549 | 1.4322 | H | .9056 | 4.8207 | .3563 |
| C | -1.6767 | -2.9728 | -1.6511 | H | 4.6206 | 4.8178 | 1.7714 | H | 1.5439 | 6.5790 | 1.9477 |
| C | -.5815 | -.4578 | -2.0657 | H | 2.1732 | 2.2090 | 2.8935 | H | .2805 | 6.9071 | 4.0760 |
| C | 2.8683 | 3.3365 | -2.7614 | H | 3.0533 | 3.6673 | 3.5293 | H | -1.6581 | 5.4146 | 4.5977 |
| C | 3.7003 | 4.2861 | -3.4722 | H | 3.9527 | 2.1236 | 3.2619 | H | -2.3473 | 3.6645 | 3.0153 |
| C | -.0535 | .0861 | -3.0448 | H | 2.4890 | -2.9230 | -1.5697 | H | -2.8651 | 5.5695 | .1712 |
| C | .3582 | .4819 | -4.4057 | H | 3.8667 | -3.3190 | -2.6553 | H | -4.0851 | 4.8512 | -.9148 |
| O | 3.3750 | 3.1497 | 1.5235 | H | 2.4774 | -2.3704 | -3.2831 | H | -3.9101 | 4.2365 | .7422 |
| N | 3.7645 | -1.2434 | -2.0045 | H | 4.9535 | .3442 | -2.8454 | H | -3.3443 | .1315 | -1.2747 |
| N | -1.6719 | 3.8544 | -1.9203 | H | 4.0610 | -.6618 | -4.0494 | H | -4.0333 | -1.5129 | -1.3591 |
| C | 3.2989 | -.6553 | .5056 | H | 5.5452 | -1.3037 | -3.2665 | H | -3.1889 | -.8325 | -2.7759 |
| C | -1.3104 | 3.0090 | .5372 | H | -.6742 | 5.6348 | -1.2161 | C | -1.9274 | -4.1386 | -.8556 |
| C | 4.5487 | 3.8534 | 1.2089 | H | -1.9303 | 5.9495 | -2.4538 | C | -1.7737 | -5.4364 | -1.4215 |
| C | 3.1367 | 2.7747 | 2.8597 | H | -.3654 | 5.2015 | -2.9333 | C | -1.4169 | -5.6089 | -2.7640 |
| C | 3.1275 | -2.5245 | -2.3871 | H | -2.6670 | 2.2908 | -3.0240 | C | -1.2132 | -4.4780 | -3.5671 |
| C | 4.6253 | -.6962 | -3.0845 | H | -1.8057 | 3.5139 | -4.0349 | C | -1.3487 | -3.1969 | -3.0124 |
| C | -1.1446 | 5.2219 | -2.1325 | H | -3.3825 | 3.9215 | -3.2762 | N | -2.2999 | -4.1696 | .5284 |
| C | -2.4214 | 3.3759 | -3.1113 | C | 1.8200 | -2.6280 | 1.3768 | H | -1.9312 | -6.3263 | -.8081 |
| C | 4.3577 | -1.1372 | -.6302 | C | 1.5087 | -3.5909 | 2.3590 | H | -1.3026 | -6.6105 | -3.1791 |
| H | 3.9474 | .0806 | 1.0921 | C | 2.2571 | -3.6718 | 3.5429 | H | -.9534 | -4.5906 | -4.6200 |
| C | 2.9054 | -1.7365 | 1.5468 | C | 3.3240 | -2.7796 | 3.7424 | H | -1.2041 | -2.3582 | -3.6950 |
| C | 5.2445 | -2.3419 | -.2343 | C | 3.6383 | -1.8277 | 2.7598 | H | -1.8659 | -3.4375 | 1.0647 |
| H | 5.0777 | -.2685 | -.6735 | H | 1.2040 | -2.6032 | .4736 | C | -3.7249 | -4.2566 | .8533 |
| C | -2.3333 | 3.5371 | -.6091 | H | .6788 | -4.2795 | 2.1969 | H | -3.8281 | -4.3797 | 1.9559 |
| H | -1.9918 | 2.3377 | 1.1570 | H | 2.0125 | -4.4160 | 4.3009 | H | -4.3205 | -3.3607 | .5580 |
| C | -.8147 | 4.1070 | 1.5200 | H | 3.9089 | -2.8249 | 4.6617 | H | -4.1874 | -5.1425 | .3631 |

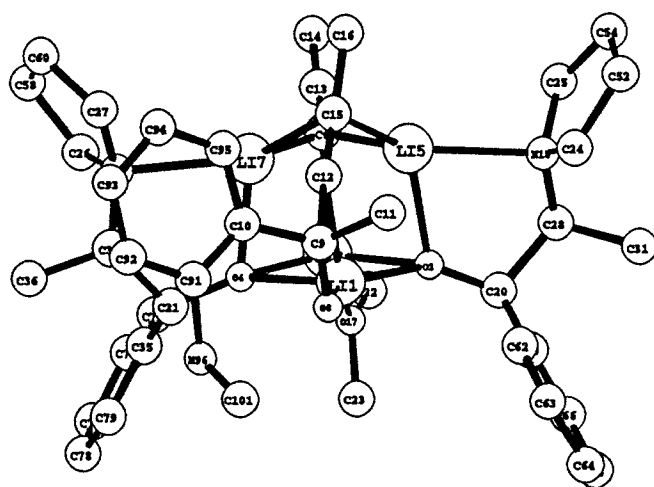
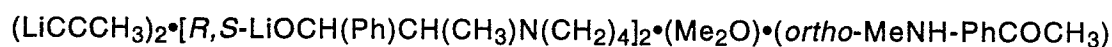


Figure XIVH



$\Delta H_f^\circ = -167.0 \text{ kcal/mol}$

| | | | | | | | | | | | |
|----|---------|---------|---------|---|---------|---------|---------|---|---------|---------|---------|
| Li | .0000 | .0000 | .0000 | C | -.8157 | 4.1776 | 1.4781 | H | 1.7099 | -4.7890 | 3.8374 |
| O | 2.2142 | .0000 | .0000 | C | -3.5006 | 4.3139 | -.0964 | H | 3.6103 | -3.2881 | 4.4635 |
| Li | 1.9278 | 2.2532 | .0000 | H | -2.8382 | 2.4227 | -.8255 | H | 4.2934 | -1.4544 | 2.9799 |
| O | -.2563 | 2.2652 | .0959 | H | 3.4414 | 4.2089 | -4.6215 | H | 5.0897 | -3.0149 | .1520 |
| Li | 2.1584 | .3815 | -2.0977 | H | 4.7505 | 4.0272 | -3.4101 | H | 6.2858 | -2.1486 | -.8451 |
| C | 2.1485 | 2.5072 | -2.1698 | H | 3.4971 | 5.2909 | -3.1928 | H | 5.9824 | -1.6192 | .8217 |
| Li | .0385 | 2.2485 | -2.0100 | H | .3063 | 1.2519 | -4.8389 | C | .2952 | 5.0010 | 1.1713 |
| O | -1.6258 | -1.2834 | .0871 | H | .0682 | -.5003 | -5.1133 | C | .6661 | 6.0690 | 2.0136 |
| C | -1.9178 | -1.4056 | -1.1524 | H | 1.6405 | .0883 | -4.4909 | C | -.0411 | 6.3234 | 3.1983 |
| C | -3.3160 | -.9123 | -1.6204 | H | 4.5512 | 4.0725 | .0980 | C | -1.1227 | 5.4949 | 3.5411 |
| C | -1.5771 | -2.7951 | -1.7915 | H | 5.4685 | 3.3055 | 1.4635 | C | -1.4985 | 4.4382 | 2.6955 |
| C | -.6618 | -.3177 | -2.0776 | H | 4.5910 | 4.8658 | 1.7283 | H | .8890 | 4.8431 | .2642 |
| C | 2.8487 | 3.3066 | -2.7918 | H | 2.1516 | 2.2630 | 2.8807 | H | 1.5101 | 6.7039 | 1.7396 |
| C | 3.6665 | 4.2454 | -3.5326 | H | 3.0172 | 3.7394 | 3.4948 | H | .2466 | 7.1511 | 3.8464 |
| C | -.0157 | .0518 | -3.0671 | H | 3.9245 | 2.1911 | 3.2826 | H | -1.6729 | 5.6714 | 4.4661 |
| C | .5326 | .2418 | -4.4219 | H | 2.2139 | -2.5182 | -2.4252 | H | -2.3389 | 3.8124 | 3.0037 |
| O | 3.3769 | 3.1707 | 1.5089 | H | 3.4426 | -3.3530 | -1.4339 | H | -3.1767 | 5.3103 | .2623 |
| N | 3.8739 | -1.2739 | -1.9456 | C | 4.0023 | -3.1453 | -3.5449 | H | -4.2549 | 4.4862 | -.8927 |
| N | -1.7042 | 3.8520 | -1.8716 | H | 4.3025 | .0618 | -3.5619 | H | -4.0379 | 3.8202 | .7398 |
| C | 3.2610 | -.6804 | .5310 | C | 4.8867 | -2.0066 | -4.0749 | H | -.5761 | -3.1648 | -1.4946 |
| C | -1.2897 | 3.0035 | .5764 | H | 5.7725 | -.5174 | -2.7307 | H | -1.6078 | -2.7855 | -2.8982 |
| C | 4.5470 | 3.8817 | 1.1979 | H | -.0955 | 5.2235 | -2.1156 | H | -2.3229 | -3.5428 | -1.4471 |
| C | 3.1144 | 2.8303 | 2.8497 | H | -1.4198 | 5.8791 | -1.1088 | C | -4.4500 | -.7683 | -.7577 |
| C | 3.3168 | -2.6187 | -2.2618 | C | -1.8508 | 5.8897 | -3.2580 | C | -5.7168 | -.4012 | -1.2974 |
| C | 4.7585 | -.8385 | -3.0700 | H | -1.8741 | 2.7181 | -3.6784 | C | -5.8911 | -.1867 | -2.6689 |
| C | -1.2090 | 5.2510 | -2.0036 | C | -2.6172 | 4.7712 | -3.9784 | C | -4.7919 | -.3307 | -3.5285 |
| C | -2.4549 | 3.4975 | -3.1162 | H | -3.4556 | 3.0491 | -2.9105 | C | -3.5409 | -.6844 | -3.0043 |
| C | 4.4061 | -1.0067 | -.5713 | C | 1.7259 | -2.7152 | 1.1031 | N | -4.4697 | -.9093 | .6691 |
| H | 3.8390 | .0055 | 1.2388 | C | 1.3362 | -3.7622 | 1.9633 | H | -6.5792 | -.2759 | -.6389 |
| C | 2.8108 | -1.8657 | 1.4254 | C | 2.0124 | -3.9796 | 3.1731 | H | -6.8690 | .0902 | -3.0635 |
| C | 5.4837 | -2.0089 | -.0900 | C | 3.0812 | -3.1367 | 3.5219 | H | -4.9085 | -.1725 | -4.6010 |
| H | 4.9527 | -.0205 | -.6542 | C | 3.4675 | -2.0949 | 2.6634 | H | -2.7277 | -.7937 | -3.7246 |
| C | -2.3438 | 3.4098 | -.5883 | H | 1.1698 | -2.5899 | .1701 | C | -4.8170 | -2.2214 | 1.2201 |
| H | -1.9327 | 2.3492 | 1.2527 | H | .4990 | -4.4042 | 1.6859 | H | -3.6297 | -.5584 | 1.0993 |