

Table S1. Summary of Calculated Energies, 195K.<sup>a</sup>

| Compound                          | ZPE <sup>b</sup> | Hcorr <sup>c</sup> | Gcorr <sup>d</sup> | S <sup>0</sup> | HF/3-21G    | B3P86/6-31G* |
|-----------------------------------|------------------|--------------------|--------------------|----------------|-------------|--------------|
| LiH                               | 1.87             | 1.36               | -6.04              | 37.9           | -7.92984    | -8.14395     |
| <i>i</i> -PrLi                    | 56.19            | 2.30               | -10.27             | 64.5           | -124.37754  | -126.51797   |
| propane                           | 63.84            | 1.93               | -9.38              | 58.0           | -117.61330  | -119.61915   |
| <i>t</i> -BuLi                    | 73.44            | 2.59               | -10.38             | 66.5           | -163.19589  | -165.97810   |
| isobutane                         | 81.28            | 2.19               | -9.87              | 61.8           | -156.43447  | -159.08074   |
| N-Boc-pyrrolidine (1)             | 158.78           | 4.31               | -14.03             | 91.4           | -551.85848  | -560.13881   |
| N-(MeOCO)pyrrolidine(7)           | 106.76           | 3.36               | -12.78             | 82.8           | -435.38465  | -441.74684   |
| (-)-sparteine                     | 246.90           | 4.24               | -14.21             | 94.7           | -688.22935  | -699.14618   |
| (-)-sparteine + LiH               | 251.72           | 4.67               | -14.33             | 97.5           | -696.24133  | -707.35139   |
| (-)-sparteine + <i>i</i> -PrLi    | 305.03           | 6.32               | -16.79             | 118.5          | -812.68743  | -825.72242   |
| (-)-sparteine + <i>t</i> -BuLi    | 322.48           | 6.56               | -17.08             | 121.3          | -851.50637  | -865.18368   |
| sparteine + <i>i</i> PrLi + 1 (3) | 464.76           | 10.82              | -22.13             | 169.0          | -1364.56160 | -1385.87123  |
| sparteine + <i>i</i> PrLi + 1 (4) | 464.99           | 10.62              | -21.72             | 165.9          | -1364.56792 | -1385.87621  |
| sparteine + <i>i</i> PrLi + 1 (5) | 464.94           | 10.77              | -21.94             | 167.7          | -1364.56280 | -1385.87202  |
| sparteine + <i>i</i> PrLi + 1 (6) | 464.82           | 10.76              | -21.85             | 167.3          | -1364.56330 | -1385.87117  |
| complex 3 TS (3-TS)               | 461.48           | 10.68              | -21.93             | 167.2          | -1364.52160 | -1385.84627  |
| complex 4 TS (4-TS)               | 461.79           | 10.47              | 21.24              | 162.6          | -1364.53232 | -1385.85355  |
| complex 5 TS (5-TS)               | 461.55           | 10.64              | -21.78             | 166.3          | -1364.52627 | -1385.84725  |

|                                       |        |       |        |       |             |             |
|---------------------------------------|--------|-------|--------|-------|-------------|-------------|
| complex 6 TS (6-TS)                   | 461.86 | 10.50 | -21.32 | 163.2 | -1364.52671 | -1385.84700 |
| complex 4 product                     | 400.23 | 8.74  | -19.97 | 142.7 | -1246.98643 | -1266.28471 |
| sparteine + <i>t</i> -BuLi + 1 (3')   | 482.15 | 10.78 | -21.61 | 166.1 | -1403.37764 | -1425.32885 |
| sparteine + <i>t</i> -BuLi + 1 (4')   | 482.36 | 11.09 | -22.36 | 171.6 | -1403.38102 | -1425.33196 |
| sparteine + <i>t</i> -BuLi + 1 (5')   | 482.16 | 11.05 | -22.43 | 171.7 | -1403.37741 | -1425.33082 |
| sparteine + <i>t</i> -BuLi + 1 (6')   | 482.22 | 11.05 | -22.22 | 170.7 | -1403.37906 | -1425.32866 |
| 3'-TS                                 | 479.03 | 10.86 | -21.59 | 166.4 | -1403.33227 | -1425.30005 |
| 4'-TS                                 | 479.00 | 10.99 | -22.34 | 170.9 | -1403.33549 | -1425.30150 |
| 5'-TS                                 | 478.18 | 11.09 | -22.81 | 173.9 | -1403.33627 | -1425.29516 |
| sparteine + <i>i</i> PrLi + 7 (3'')   | 412.96 | 9.69  | -20.96 | 157.1 | -1248.09589 | -1267.48449 |
| sparteine + <i>i</i> PrLi + 7 (4'')   | 413.15 | 9.55  | -21.31 | 153.2 | -1248.10008 | -1267.48830 |
| sparteine + <i>i</i> PrLi + 7 (5'')   | 413.05 | 9.72  | -20.83 | 156.6 | -1248.09648 | -1267.48530 |
| 3''-TS                                | 409.80 | 9.52  | -20.39 | 153.4 | -1248.05590 | -1267.45797 |
| 4''-TS                                | 409.98 | 9.37  | -20.02 | 150.7 | -1248.06336 | -1267.46467 |
| 5''-TS                                | 409.84 | 9.51  | -20.37 | 153.2 | -1248.05857 | -1267.45966 |
| diamine 8                             | 195.64 | 4.41  | -13.93 | 94.1  | -497.58160  | -505.54551  |
| diamine 8 + LiH                       | 200.17 | 4.91  | -14.13 | 97.6  | -505.59532  | -513.75163  |
| diamine 8 + <i>i</i> -PrLi            | 253.41 | 6.60  | -17.14 | 121.8 | -622.04083  | -632.12282  |
| diamine 8 + <i>i</i> -PrLi + 1 (3''') | 413.27 | 10.91 | -21.92 | 168.4 | -1173.91994 | -1192.27528 |
| diamine 8 + <i>i</i> -PrLi + 1 (4''') | 413.35 | 10.88 | -22.02 | 168.7 | -1173.92074 | -1192.27597 |
| 3'''-TS                               | 410.28 | 10.66 | -21.56 | 165.2 | -1173.88422 | -1192.25392 |
| 4'''-TS                               | 410.27 | 10.65 | -21.68 | 165.8 | -1173.88776 | -1192.25556 |

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- a. The total energies are given in Hartrees, and the other energies are given in kcal/mol. The entropies are given in cal/mol/degree.
- b. Zero point energies (kcal/mol) based on HF/3-21G frequencies scaled by 0.917.
- c. Correction to the enthalpy ( $H^\circ_{195} - H^\circ_0$ ) on going from 0 K to 195 K based on the scaled HF/3-21G frequencies. Energies are given to 0.01 and entropies are given to 0.1 to avoid round off errors. The relative energies are significant to a few tenths of a kcal/mol, and the relative entropies are significant to  $\sim 1$ -2 eu.
- d. Correction to the free energy ( $G^\circ_{195} - H^\circ_0$ ) on going from 0K to 195 K based on the scaled HF/3-21G frequencies and the calculated moments of inertia. The symmetry number was taken as 1 in all cases except isobutene and t-butyllithium ( $\sigma=3$ ) and propane ( $\sigma=2$ ).

Sparteine-iPrLi-N-bocpyrrolidine complex 3, B3P86/6-31G\* = -1385.8712

|    |   |           |           |           |
|----|---|-----------|-----------|-----------|
| O  | 1 |           |           |           |
| C  |   | 2.035951  | -2.227018 | 3.147282  |
| C  |   | 0.965253  | -1.568162 | 2.257333  |
| N  |   | 1.067522  | -0.097645 | 2.188647  |
| C  |   | 2.438330  | 0.332617  | 1.881513  |
| C  |   | 3.516030  | -0.247045 | 2.798435  |
| C  |   | 3.444036  | -1.771014 | 2.772583  |
| H  |   | 1.140158  | -1.923372 | 1.228928  |
| H  |   | 1.856767  | -1.983918 | 4.202377  |
| H  |   | 1.944835  | -3.317458 | 3.058668  |
| H  |   | 2.657305  | 0.011709  | 0.856706  |
| H  |   | 2.451814  | 1.426118  | 1.874088  |
| H  |   | 4.499163  | 0.107147  | 2.465108  |
| H  |   | 3.386568  | 0.114871  | 3.827253  |
| H  |   | 3.687946  | -2.127312 | 1.760520  |
| H  |   | 4.183943  | -2.215837 | 3.448691  |
| C  |   | 0.537070  | 0.607726  | 3.362183  |
| H  |   | 0.530148  | 1.674493  | 3.112061  |
| H  |   | 1.194459  | 0.492871  | 4.242513  |
| C  |   | -0.452295 | -1.994952 | 2.669887  |
| C  |   | -0.860559 | 0.140120  | 3.781645  |
| C  |   | -0.831728 | -1.367532 | 4.010310  |
| H  |   | -0.121886 | -1.634738 | 4.801057  |
| H  |   | -1.818272 | -1.726501 | 4.331220  |
| H  |   | -1.101409 | 0.659579  | 4.718793  |
| C  |   | -1.536760 | -1.642298 | 1.647546  |
| H  |   | -2.467271 | -2.158261 | 1.958932  |
| H  |   | -1.265150 | -2.028572 | 0.658093  |
| N  |   | -1.793136 | -0.203700 | 1.500202  |
| C  |   | -1.994964 | 0.463422  | 2.800057  |
| H  |   | -2.919394 | 0.050073  | 3.261231  |
| C  |   | -2.982903 | -0.021359 | 0.662051  |
| H  |   | -3.861895 | -0.484298 | 1.156160  |
| H  |   | -2.816522 | -0.566302 | -0.271842 |
| C  |   | -2.219111 | 1.959079  | 2.595567  |
| H  |   | -1.328739 | 2.399846  | 2.132181  |
| H  |   | -2.357799 | 2.432127  | 3.576363  |
| C  |   | -3.265184 | 1.448416  | 0.387155  |
| H  |   | -2.432506 | 1.876614  | -0.184867 |
| H  |   | -4.168626 | 1.531826  | -0.229336 |
| C  |   | -3.425253 | 2.216568  | 1.695910  |
| H  |   | -3.534597 | 3.289382  | 1.501617  |
| H  |   | -4.342685 | 1.887816  | 2.206444  |
| H  |   | -0.445665 | -3.090142 | 2.752237  |
| Li |   | -0.052477 | 0.642890  | 0.372906  |
| C  |   | 0.257480  | 2.698915  | -0.196051 |
| H  |   | -0.561726 | 3.220910  | 0.341801  |
| C  |   | -0.013195 | 2.967576  | -1.678671 |
| H  |   | 0.020067  | 4.041368  | -1.966015 |
| C  |   | 1.530231  | 3.448620  | 0.200574  |
| H  |   | 2.441510  | 2.990119  | -0.225198 |
| H  |   | 1.561535  | 4.509780  | -0.130462 |
| H  |   | 1.681622  | 3.467055  | 1.291576  |
| O  |   | -0.145100 | -0.684876 | -1.309457 |
| C  |   | 0.272303  | -0.635796 | -2.472910 |

|   |           |           |           |
|---|-----------|-----------|-----------|
| O | -0.415078 | -1.008009 | -3.569988 |
| C | -1.843483 | -1.296819 | -3.552575 |
| C | -2.607671 | -0.039591 | -3.158280 |
| H | -2.408563 | 0.765601  | -3.872392 |
| H | -3.684372 | -0.239867 | -3.158665 |
| H | -2.315375 | 0.305758  | -2.165570 |
| C | -2.140387 | -2.486902 | -2.647295 |
| H | -1.527670 | -3.345669 | -2.940871 |
| H | -1.933306 | -2.252864 | -1.603125 |
| H | -3.193600 | -2.770240 | -2.747334 |
| C | -2.127708 | -1.659894 | -5.005509 |
| H | -1.866119 | -0.829816 | -5.668600 |
| H | -1.548679 | -2.538854 | -5.304983 |
| H | -3.191175 | -1.883991 | -5.134348 |
| N | 1.510020  | -0.237224 | -2.812480 |
| C | 1.975835  | 0.001577  | -4.177478 |
| H | 2.318056  | -0.935348 | -4.638398 |
| H | 1.166130  | 0.401119  | -4.790748 |
| C | 2.476956  | 0.181149  | -1.800239 |
| C | 3.710301  | 0.564751  | -2.622259 |
| H | 4.366424  | -0.304528 | -2.750017 |
| C | 3.128007  | 0.984304  | -3.973819 |
| H | 3.856373  | 0.948921  | -4.788845 |
| H | 2.733386  | 2.004260  | -3.911461 |
| H | 4.290871  | 1.355952  | -2.141287 |
| H | 0.725585  | 2.472173  | -2.332880 |
| H | 2.066932  | 1.020091  | -1.222825 |
| H | 2.677620  | -0.646742 | -1.111415 |
| H | -0.997699 | 2.592695  | -2.000541 |

Sparteine-iPrLi-N-bocpyrrolidene complex 3TS, B3P86/6-31G\* = -1385.8463

|    |   |           |           |           |
|----|---|-----------|-----------|-----------|
| 0  | 1 |           |           |           |
| C  |   | 1.500435  | -2.252560 | 3.464445  |
| C  |   | 0.633859  | -1.564212 | 2.393524  |
| N  |   | 0.767712  | -0.089113 | 2.361915  |
| C  |   | 2.180008  | 0.333941  | 2.378217  |
| C  |   | 3.033661  | -0.289637 | 3.481462  |
| C  |   | 2.958810  | -1.809625 | 3.387808  |
| H  |   | 1.003097  | -1.915868 | 1.416208  |
| H  |   | 1.118630  | -2.026312 | 4.468087  |
| H  |   | 1.415423  | -3.339308 | 3.335235  |
| H  |   | 2.615334  | 0.071163  | 1.408982  |
| H  |   | 2.192115  | 1.426825  | 2.435373  |
| H  |   | 4.066324  | 0.061917  | 3.368921  |
| H  |   | 2.698580  | 0.039648  | 4.474468  |
| H  |   | 3.394466  | -2.135821 | 2.432192  |
| H  |   | 3.545630  | -2.286397 | 4.181876  |
| C  |   | 0.012553  | 0.608545  | 3.413835  |
| H  |   | 0.059907  | 1.679172  | 3.183171  |
| H  |   | 0.486230  | 0.483091  | 4.403468  |
| C  |   | -0.843019 | -1.977632 | 2.520337  |
| C  |   | -1.441643 | 0.150914  | 3.550845  |
| H  |   | -1.466899 | -1.358123 | 3.768626  |
| H  |   | -0.925563 | -1.636311 | 4.679692  |
| H  |   | -2.499039 | -1.711176 | 3.891438  |
| C  |   | -1.854929 | 0.665241  | 4.428811  |
| H  |   | -1.716469 | -1.612444 | 1.315576  |
| H  |   | -2.693979 | -2.115848 | 1.451608  |
| N  |   | -1.278010 | -1.997657 | 0.388184  |
| C  |   | -1.928694 | -0.168209 | 1.127913  |
| H  |   | -2.363719 | 0.491684  | 2.372464  |
| C  |   | -3.362731 | 0.087177  | 2.647972  |
| H  |   | -2.946926 | 0.022550  | 0.085555  |
| H  |   | -3.899234 | -0.444073 | 0.409232  |
| C  |   | -2.602270 | -0.505586 | -0.807204 |
| H  |   | -2.541005 | 1.990262  | 2.143605  |
| H  |   | -1.577857 | 2.438407  | 1.867663  |
| C  |   | -2.857202 | 2.455948  | 3.085919  |
| H  |   | -3.179873 | 1.494810  | -0.221231 |
| H  |   | -2.267614 | 1.923640  | -0.653677 |
| C  |   | -3.965159 | 1.581704  | -0.981864 |
| H  |   | -3.561427 | 2.261149  | 1.041322  |
| H  |   | -3.632187 | 3.335576  | 0.837332  |
| H  |   | -4.555494 | 1.935207  | 1.380204  |
| Li |   | -0.858456 | -3.073241 | 2.592708  |
| C  |   | 0.051586  | 0.396735  | 0.248694  |
| H  |   | 0.745890  | 2.480831  | -0.331268 |
| C  |   | -0.168812 | 2.544487  | 0.296186  |
| H  |   | 0.363998  | 2.915060  | -1.743089 |
| C  |   | 0.051359  | 3.972453  | -1.815835 |
| H  |   | 1.764614  | 3.448919  | 0.258406  |
| H  |   | 2.730456  | 3.367083  | -0.263120 |
| H  |   | 1.464078  | 4.509315  | 0.182876  |
| O  |   | 1.963942  | 3.251318  | 1.320831  |
| C  |   | -0.329549 | -0.650429 | -1.432041 |
|    |   | 0.446787  | -0.599079 | -2.413521 |

|   |           |           |           |
|---|-----------|-----------|-----------|
| O | 0.099943  | -0.927158 | -3.679498 |
| C | -1.271654 | -1.200130 | -4.068442 |
| C | -2.134954 | 0.037424  | -3.844783 |
| H | -1.724475 | 0.889321  | -4.396596 |
| H | -3.152858 | -0.146475 | -4.205219 |
| H | -2.179987 | 0.302047  | -2.785846 |
| H | -1.805483 | -2.428630 | -3.339050 |
| C | -1.129543 | -3.276918 | -3.489524 |
| H | -1.895612 | -2.242172 | -2.269642 |
| H | -2.788052 | -2.700337 | -3.740006 |
| H | -1.143232 | -1.492445 | -5.559842 |
| C | -0.714645 | -0.633077 | -6.084395 |
| H | -0.494542 | -2.357568 | -5.727829 |
| H | -2.127312 | -1.705936 | -5.988868 |
| H | 1.724025  | -0.257855 | -2.313156 |
| N | 2.648225  | -0.096341 | -3.427916 |
| C | 3.095386  | -1.064154 | -3.697561 |
| H | 2.131907  | 0.292081  | -4.308403 |
| H | 2.304994  | 0.114677  | -1.012929 |
| C | 3.756230  | 0.461121  | -1.369861 |
| C | 4.437314  | -0.396612 | -1.252275 |
| H | 3.692951  | 0.856200  | -2.849756 |
| C | 4.657457  | 0.778655  | -3.360994 |
| H | 3.349639  | 1.892645  | -2.943825 |
| H | 4.146682  | 1.274726  | -0.748452 |
| H | 1.218321  | 2.802262  | -2.428461 |
| H | 1.524680  | 1.239252  | -0.545172 |
| H | 2.269896  | -0.782628 | -0.369543 |
| H | -0.450764 | 2.306476  | -2.160827 |

Sparteine-iPrLi-N-bocpyrrolidne complex 4, B3P86 = -1385.8762

|    |   |           |           |           |
|----|---|-----------|-----------|-----------|
| O  | 1 |           |           |           |
| C  |   | 3.124795  | 0.063837  | 2.721706  |
| C  |   | 1.826154  | -0.287141 | 1.973505  |
| N  |   | 0.820214  | 0.791341  | 2.002020  |
| C  |   | 1.395336  | 2.074099  | 1.577049  |
| C  |   | 2.653617  | 2.492424  | 2.337296  |
| C  |   | 3.708193  | 1.392558  | 2.243311  |
| H  |   | 2.088814  | -0.411517 | 0.912280  |
| H  |   | 2.939096  | 0.126485  | 3.801646  |
| H  |   | 3.847859  | -0.750038 | 2.578181  |
| H  |   | 1.642379  | 1.982930  | 0.510260  |
| H  |   | 0.608408  | 2.831311  | 1.646235  |
| H  |   | 3.030393  | 3.434168  | 1.919974  |
| H  |   | 2.415732  | 2.692084  | 3.391000  |
| H  |   | 4.032101  | 1.293768  | 1.196674  |
| H  |   | 4.601590  | 1.650578  | 2.824762  |
| C  |   | 0.088985  | 0.906787  | 3.268466  |
| H  |   | -0.709578 | 1.639746  | 3.107679  |
| H  |   | 0.725389  | 1.303082  | 4.080352  |
| C  |   | 1.216107  | -1.609609 | 2.466827  |
| C  |   | -0.486847 | -0.427768 | 3.756347  |
| C  |   | 0.647019  | -1.441663 | 3.874028  |
| H  |   | 1.409495  | -1.101001 | 4.583671  |
| H  |   | 0.267913  | -2.401814 | 4.247597  |
| H  |   | -0.930897 | -0.241586 | 4.743374  |
| C  |   | 0.111270  | -2.166132 | 1.562619  |
| H  |   | -0.127864 | -3.188682 | 1.918416  |
| H  |   | 0.469574  | -2.255287 | 0.530751  |
| N  |   | -1.111591 | -1.353987 | 1.530006  |
| C  |   | -1.597662 | -1.034692 | 2.886390  |
| H  |   | -1.882637 | -1.987910 | 3.384873  |
| C  |   | -2.141892 | -2.079459 | 0.778048  |
| H  |   | -2.344669 | -3.054907 | 1.265830  |
| H  |   | -1.733374 | -2.296144 | -0.216469 |
| C  |   | -2.853961 | -0.171842 | 2.809748  |
| H  |   | -2.619376 | 0.771363  | 2.300873  |
| H  |   | -3.180381 | 0.067403  | 3.830114  |
| C  |   | -3.434831 | -1.283844 | 0.663130  |
| H  |   | -3.243400 | -0.371365 | 0.086648  |
| H  |   | -4.174560 | -1.880332 | 0.114642  |
| C  |   | -3.957650 | -0.890914 | 2.040707  |
| H  |   | -4.840943 | -0.249311 | 1.945979  |
| H  |   | -4.270271 | -1.789168 | 2.593693  |
| H  |   | 2.023175  | -2.354828 | 2.470541  |
| Li |   | -0.627603 | 0.467540  | 0.394593  |
| C  |   | -1.776484 | 2.262573  | 0.086121  |
| H  |   | -1.549217 | 2.710144  | 1.079989  |
| C  |   | -3.289015 | 2.405565  | -0.080425 |
| H  |   | -3.647852 | 3.456247  | -0.120326 |
| C  |   | -1.097219 | 3.170777  | -0.943149 |
| H  |   | -1.227202 | 2.792122  | -1.972577 |
| H  |   | -1.483162 | 4.213069  | -0.967532 |
| H  |   | -0.009746 | 3.247276  | -0.788896 |
| O  |   | 0.443743  | -0.353243 | -1.193342 |
| C  |   | 0.394178  | -0.355053 | -2.429894 |

|   |           |           |           |
|---|-----------|-----------|-----------|
| O | 1.455057  | -0.516097 | -3.246344 |
| C | 2.817092  | -0.670280 | -2.753962 |
| C | 3.618608  | -0.835079 | -4.040248 |
| H | 3.498951  | 0.041540  | -4.683953 |
| H | 4.681435  | -0.952282 | -3.807069 |
| H | -0.281861 | -1.055158 | -5.046391 |
| C | 2.935146  | -1.923546 | -1.894152 |
| H | 2.363321  | -1.824683 | -0.970569 |
| H | 2.568714  | -2.796821 | -2.443978 |
| H | 3.986235  | -2.098113 | -1.640847 |
| C | 3.249511  | 0.590031  | -2.015981 |
| H | 3.133690  | 1.467107  | -2.660756 |
| H | 2.652900  | 0.738382  | -1.114922 |
| H | 4.304381  | 0.510676  | -1.732096 |
| N | -0.728733 | -0.219255 | -3.151629 |
| C | -0.767967 | -0.175039 | -4.615581 |
| H | -0.232054 | 0.710738  | -4.978465 |
| H | 3.285527  | -1.718625 | -4.593514 |
| C | -2.039997 | 0.005903  | -2.541016 |
| C | -2.844510 | 0.603294  | -3.691570 |
| H | -2.664417 | 1.682813  | -3.744937 |
| C | -2.264909 | -0.098248 | -4.922911 |
| H | -2.465436 | 0.426828  | -5.861073 |
| H | -2.681132 | -1.109055 | -5.010332 |
| H | -3.919824 | 0.448682  | -3.570156 |
| H | -3.651530 | 1.946068  | -1.017734 |
| H | -2.469031 | -0.955247 | -2.221466 |
| H | -1.949127 | 0.659643  | -1.660464 |
| H | -3.852752 | 1.919798  | 0.730939  |

Sparteine-iPrLi-N-bocpyrrolidine complex 4 TS, B3P86/6-31G\* = -1385.8536

|    |   |           |           |           |
|----|---|-----------|-----------|-----------|
| O  | 1 |           |           |           |
| C  |   | -3.538241 | 0.035166  | -2.011812 |
| C  |   | -2.114508 | -0.316926 | -1.543886 |
| N  |   | -1.146650 | 0.790298  | -1.711126 |
| C  |   | -1.659368 | 2.034409  | -1.116717 |
| C  |   | -3.049070 | 2.451170  | -1.596740 |
| C  |   | -4.043426 | 1.319094  | -1.356875 |
| H  |   | -2.159666 | -0.494775 | -0.460900 |
| H  |   | -3.567423 | 0.158501  | -3.102001 |
| H  |   | -4.203456 | -0.805761 | -1.776567 |
| H  |   | -1.690820 | 1.879755  | -0.029993 |
| H  |   | -0.923072 | 2.823626  | -1.302236 |
| H  |   | -3.352675 | 3.361075  | -1.065194 |
| H  |   | -3.025503 | 2.706589  | -2.664768 |
| H  |   | -4.154616 | 1.159312  | -0.274843 |
| H  |   | -5.037282 | 1.579693  | -1.739936 |
| C  |   | -0.691992 | 0.984215  | -3.093346 |
| H  |   | 0.109262  | 1.732813  | -3.068329 |
| H  |   | -1.486879 | 1.400936  | -3.736846 |
| C  |   | -1.590247 | -1.597526 | -2.214658 |
| C  |   | -0.203431 | -0.310044 | -3.753870 |
| C  |   | -1.318779 | -1.349050 | -3.696431 |
| H  |   | -2.214148 | -0.997662 | -4.221052 |
| H  |   | -1.003883 | -2.278607 | -4.188090 |
| H  |   | 0.030456  | -0.065494 | -4.798697 |
| C  |   | -0.319096 | -2.168785 | -1.576207 |
| H  |   | -0.143940 | -3.167946 | -2.021079 |
| H  |   | -0.464149 | -2.309998 | -0.499015 |
| N  |   | 0.882179  | -1.335075 | -1.751181 |
| C  |   | 1.068833  | -0.928870 | -3.158661 |
| H  |   | 1.260589  | -1.846209 | -3.757468 |
| C  |   | 2.053993  | -2.098278 | -1.296780 |
| H  |   | 2.139900  | -3.029836 | -1.891513 |
| H  |   | 1.877217  | -2.394564 | -0.256756 |
| C  |   | 2.303932  | -0.043763 | -3.294264 |
| H  |   | 2.172993  | 0.865396  | -2.694909 |
| H  |   | 2.403189  | 0.266644  | -4.342346 |
| C  |   | 3.343414  | -1.297143 | -1.406754 |
| H  |   | 3.299241  | -0.451026 | -0.712220 |
| H  |   | 4.181164  | -1.930296 | -1.090418 |
| C  |   | 3.553446  | -0.784219 | -2.827375 |
| H  |   | 4.430542  | -0.128691 | -2.874120 |
| H  |   | 3.749946  | -1.628539 | -3.504036 |
| H  |   | -2.368448 | -2.363098 | -2.094426 |
| Li |   | 0.509511  | 0.303646  | -0.348995 |
| C  |   | 1.792717  | 2.156515  | -0.091841 |
| H  |   | 1.208049  | 2.237238  | -1.031322 |
| C  |   | 3.240235  | 2.495294  | -0.429005 |
| H  |   | 3.396495  | 3.554038  | -0.699008 |
| C  |   | 1.226025  | 3.163790  | 0.905253  |
| H  |   | 1.739550  | 3.076318  | 1.873390  |
| H  |   | 1.336281  | 4.216136  | 0.589205  |
| H  |   | 0.159195  | 2.996611  | 1.106457  |
| O  |   | -0.482756 | -0.307510 | 1.218664  |
| C  |   | -0.056330 | -0.300837 | 2.395578  |

|   |           |           |           |
|---|-----------|-----------|-----------|
| O | -0.854236 | -0.441536 | 3.480488  |
| C | -2.279001 | -0.698142 | 3.380815  |
| C | -2.692899 | -0.852926 | 4.840477  |
| H | -2.459146 | 0.055736  | 5.403344  |
| H | -3.769282 | -1.038871 | 4.910561  |
| H | 1.274281  | -1.045619 | 4.675805  |
| C | -2.539855 | -1.994103 | 2.619273  |
| H | -2.236248 | -1.903974 | 1.575319  |
| H | -1.983883 | -2.819003 | 3.077299  |
| H | -3.606642 | -2.239075 | 2.659443  |
| C | -2.989078 | 0.496985  | 2.755178  |
| H | -2.760023 | 1.409257  | 3.315572  |
| H | -2.674747 | 0.634173  | 1.719687  |
| H | -4.073383 | 0.342755  | 2.780429  |
| N | 1.219868  | -0.179832 | 2.737602  |
| C | 1.682650  | -0.187067 | 4.134154  |
| H | 1.339402  | 0.720290  | 4.647322  |
| H | -2.163889 | -1.691231 | 5.304043  |
| C | 2.302529  | -0.013333 | 1.753209  |
| C | 3.443076  | 0.470674  | 2.643209  |
| H | 3.400705  | 1.560437  | 2.781029  |
| C | 3.204040  | -0.219891 | 3.994694  |
| H | 3.701548  | 0.261412  | 4.844226  |
| H | 3.550443  | -1.259479 | 3.946465  |
| H | 4.424477  | 0.237979  | 2.217194  |
| H | 3.899131  | 2.292151  | 0.428035  |
| H | 2.554488  | -1.021226 | 1.377359  |
| H | 1.961531  | 0.962938  | 0.717168  |
| H | 3.625354  | 1.894406  | -1.264266 |

Sparteine - iPrLi- N-bocpyrrolidine complex 5, B3P86 = -1385.8720

|    |   |           |           |           |
|----|---|-----------|-----------|-----------|
| O  | 1 |           |           |           |
| C  |   | -0.428244 | -2.112540 | -4.135574 |
| C  |   | 0.217528  | -1.133683 | -3.139690 |
| N  |   | -0.631640 | -0.846174 | -1.963807 |
| C  |   | -1.071442 | -2.093788 | -1.324195 |
| C  |   | -1.763445 | -3.085336 | -2.260302 |
| C  |   | -0.851906 | -3.405517 | -3.441452 |
| H  |   | 1.110499  | -1.627153 | -2.734986 |
| H  |   | -1.306581 | -1.660820 | -4.614991 |
| H  |   | 0.290697  | -2.322962 | -4.937675 |
| H  |   | -0.172689 | -2.565754 | -0.903802 |
| H  |   | -1.717710 | -1.832342 | -0.480746 |
| H  |   | -2.013767 | -3.994512 | -1.700072 |
| H  |   | -2.713278 | -2.670073 | -2.624722 |
| H  |   | 0.040862  | -3.931994 | -3.075493 |
| H  |   | -1.348594 | -4.078903 | -4.150081 |
| C  |   | -1.732599 | 0.082053  | -2.235715 |
| H  |   | -2.202343 | 0.320827  | -1.274472 |
| H  |   | -2.519444 | -0.374180 | -2.863481 |
| C  |   | 0.664817  | 0.172812  | -3.809816 |
| C  |   | -1.277434 | 1.366653  | -2.942342 |
| C  |   | -0.550483 | 0.994469  | -4.231168 |
| H  |   | -1.204862 | 0.433586  | -4.907480 |
| H  |   | -0.234907 | 1.899342  | -4.766179 |
| H  |   | -2.183876 | 1.942418  | -3.172517 |
| C  |   | 1.566942  | 1.044580  | -2.929287 |
| H  |   | 1.968508  | 1.858026  | -3.565986 |
| H  |   | 2.418891  | 0.461203  | -2.564279 |
| N  |   | 0.896375  | 1.628551  | -1.755894 |
| C  |   | -0.365217 | 2.294742  | -2.124694 |
| H  |   | -0.127547 | 3.148524  | -2.797771 |
| C  |   | 1.814470  | 2.579186  | -1.117832 |
| H  |   | 2.097388  | 3.370865  | -1.841449 |
| H  |   | 2.727579  | 2.032055  | -0.859128 |
| C  |   | -1.041035 | 2.881019  | -0.888864 |
| H  |   | -1.284398 | 2.073277  | -0.189402 |
| H  |   | -1.982644 | 3.355676  | -1.193738 |
| C  |   | 1.208249  | 3.220513  | 0.122841  |
| H  |   | 1.044247  | 2.446951  | 0.880900  |
| H  |   | 1.922189  | 3.942698  | 0.536716  |
| C  |   | -0.124833 | 3.887521  | -0.198877 |
| H  |   | -0.592475 | 4.278617  | 0.712459  |
| H  |   | 0.041106  | 4.746678  | -0.864781 |
| H  |   | 1.260885  | -0.103181 | -4.689426 |
| Li |   | 0.746860  | -0.123269 | -0.401853 |
| C  |   | 2.524655  | -1.390431 | -0.327305 |
| H  |   | 2.439846  | -1.771917 | -1.366894 |
| C  |   | 2.501039  | -2.645174 | 0.549101  |
| H  |   | 3.348254  | -3.342835 | 0.375349  |
| C  |   | 3.923391  | -0.773125 | -0.253553 |
| H  |   | 4.126904  | -0.304410 | 0.725103  |
| H  |   | 4.753491  | -1.496163 | -0.404765 |
| H  |   | 4.072092  | 0.022708  | -1.000737 |
| O  |   | -0.451651 | 0.340336  | 1.338292  |
| C  |   | -0.390132 | -0.040356 | 2.515619  |

|   |           |           |          |
|---|-----------|-----------|----------|
| O | -1.451425 | -0.393948 | 3.271048 |
| C | -2.821141 | -0.039939 | 2.924601 |
| C | -3.267039 | -0.750076 | 1.654210 |
| H | -3.076795 | -1.825257 | 1.732199 |
| H | -4.342231 | -0.602668 | 1.507076 |
| H | -2.735570 | -0.360209 | 0.786324 |
| C | -2.946267 | 1.474973  | 2.809440 |
| H | -2.605679 | 1.956355  | 3.731780 |
| H | -2.357174 | 1.856901  | 1.973201 |
| H | -3.994012 | 1.749045  | 2.648904 |
| C | -3.607886 | -0.553080 | 4.125165 |
| H | -3.485863 | -1.635197 | 4.231277 |
| H | -3.260884 | -0.074344 | 5.045580 |
| H | -4.672618 | -0.334587 | 3.998803 |
| N | 0.748333  | -0.149601 | 3.214380 |
| C | 0.870785  | -0.725288 | 4.550859 |
| H | 0.690666  | 0.038949  | 5.320434 |
| H | 0.140217  | -1.523221 | 4.691446 |
| C | 2.042933  | 0.233718  | 2.642388 |
| C | 3.049323  | -0.148885 | 3.735216 |
| H | 3.284664  | 0.721061  | 4.359868 |
| C | 2.319774  | -1.206587 | 4.568447 |
| H | 2.715744  | -1.307694 | 5.582836 |
| H | 2.384862  | -2.183251 | 4.076748 |
| H | 3.985857  | -0.515982 | 3.309206 |
| H | 2.544037  | -2.405619 | 1.625877 |
| H | 2.193954  | -0.288036 | 1.686934 |
| H | 2.055447  | 1.310350  | 2.438610 |
| H | 1.580778  | -3.234192 | 0.412181 |

Sparteine-iPrLi-N-bocpyrrolidine complex 5, TS, B3P86/6-31G\* = -1385.8473

|     |           |           |           |
|-----|-----------|-----------|-----------|
| 0,1 |           |           |           |
| C   | -3.903705 | -1.085202 | -2.092459 |
| C   | -3.026660 | -0.163471 | -1.228052 |
| N   | -1.769748 | -0.796354 | -0.778986 |
| C   | -1.036543 | -1.375888 | -1.915919 |
| C   | -1.851003 | -2.338331 | -2.779752 |
| C   | -3.118959 | -1.648008 | -3.276173 |
| H   | -2.722137 | 0.674577  | -1.872780 |
| H   | -4.293317 | -1.920526 | -1.497078 |
| H   | -4.775671 | -0.517076 | -2.441226 |
| H   | -0.706094 | -0.536303 | -2.543430 |
| H   | -0.134172 | -1.851258 | -1.520682 |
| H   | -1.232780 | -2.674129 | -3.621120 |
| H   | -2.115065 | -3.238379 | -2.207904 |
| H   | -2.842487 | -0.828822 | -3.955516 |
| H   | -3.742306 | -2.339956 | -3.854838 |
| C   | -1.945943 | -1.754419 | 0.322284  |
| H   | -0.943043 | -2.031699 | 0.663132  |
| H   | -2.438300 | -2.683284 | -0.014779 |
| C   | -3.784880 | 0.415413  | -0.025786 |
| C   | -2.770823 | -1.199224 | 1.491836  |
| C   | -4.112322 | -0.693504 | 0.970933  |
| H   | -4.690489 | -1.499460 | 0.506162  |
| H   | -4.718921 | -0.299916 | 1.796765  |
| H   | -2.926775 | -2.030401 | 2.192524  |
| C   | -3.034469 | 1.534182  | 0.708239  |
| H   | -3.748614 | 1.997653  | 1.416454  |
| H   | -2.731673 | 2.316115  | 0.002085  |
| N   | -1.830593 | 1.106733  | 1.445499  |
| C   | -2.114227 | -0.067706 | 2.296007  |
| H   | -2.867203 | 0.233859  | 3.056819  |
| C   | -1.381581 | 2.230876  | 2.282872  |
| H   | -2.204186 | 2.534599  | 2.960719  |
| H   | -1.176502 | 3.080411  | 1.622136  |
| C   | -0.862382 | -0.494100 | 3.057058  |
| H   | -0.074455 | -0.770889 | 2.346847  |
| H   | -1.101986 | -1.382559 | 3.655596  |
| C   | -0.147200 | 1.891623  | 3.106592  |
| H   | 0.703053  | 1.730570  | 2.434876  |
| H   | 0.102100  | 2.753416  | 3.737119  |
| C   | -0.367187 | 0.640232  | 3.949733  |
| H   | 0.559054  | 0.354505  | 4.461516  |
| H   | -1.112876 | 0.843651  | 4.732164  |
| H   | -4.708863 | 0.865399  | -0.412544 |
| Li  | -0.289015 | 0.649458  | -0.088531 |
| C   | -0.162698 | 2.310375  | -1.722874 |
| H   | -1.109986 | 1.741947  | -1.763009 |
| C   | 0.529040  | 2.160616  | -3.072210 |
| H   | -0.004288 | 2.649858  | -3.904603 |
| C   | -0.502841 | 3.770242  | -1.445945 |
| H   | 0.412663  | 4.353452  | -1.270963 |
| H   | -1.039982 | 4.267499  | -2.271545 |
| H   | -1.120792 | 3.891157  | -0.544685 |
| O   | 1.197794  | -0.515768 | 0.391606  |
| C   | 2.376175  | -0.360162 | -0.019789 |

|   |          |           |           |
|---|----------|-----------|-----------|
| O | 3.218365 | -1.396531 | -0.278106 |
| C | 3.114711 | -2.664920 | 0.419257  |
| C | 1.907144 | -3.456646 | -0.069442 |
| H | 1.924502 | -3.535582 | -1.161393 |
| H | 1.929224 | -4.469873 | 0.347211  |
| H | 0.979836 | -2.970211 | 0.233580  |
| C | 3.073456 | -2.437892 | 1.926776  |
| H | 3.944542 | -1.857506 | 2.248415  |
| H | 2.166875 | -1.902536 | 2.217107  |
| H | 3.091768 | -3.400054 | 2.449589  |
| C | 4.404573 | -3.374293 | 0.021025  |
| H | 4.455381 | -3.493759 | -1.065659 |
| H | 5.276070 | -2.797481 | 0.344867  |
| H | 4.450891 | -4.366073 | 0.481916  |
| N | 2.929259 | 0.819342  | -0.253758 |
| C | 4.283425 | 0.999944  | -0.775115 |
| H | 5.008222 | 0.982703  | 0.051732  |
| H | 4.545539 | 0.200514  | -1.470320 |
| C | 2.201412 | 2.088404  | -0.090680 |
| C | 3.242033 | 3.138372  | -0.499820 |
| H | 3.802576 | 3.540942  | 0.360363  |
| C | 4.210158 | 2.382167  | -1.414907 |
| H | 5.194105 | 2.854234  | -1.498297 |
| H | 3.788923 | 2.293838  | -2.422910 |
| H | 2.796611 | 3.997742  | -1.013070 |
| H | 1.533189 | 2.608809  | -3.037656 |
| H | 0.918648 | 2.078433  | -0.852034 |
| H | 1.951237 | 2.194596  | 0.974972  |
| H | 0.671069 | 1.107117  | -3.350442 |

Sparteine -iPrLi- N-bocpyrrolidine complex 6, B3P86 = -1385.8711

|    |   |           |           |           |
|----|---|-----------|-----------|-----------|
| O  | 1 |           |           |           |
| C  |   | 0.902691  | -1.214100 | 4.495753  |
| C  |   | 0.046174  | -0.790659 | 3.291067  |
| N  |   | 0.841058  | -0.299962 | 2.144740  |
| C  |   | 1.892882  | -1.258115 | 1.781922  |
| C  |   | 2.805637  | -1.673778 | 2.936218  |
| C  |   | 1.969099  | -2.229055 | 4.086282  |
| H  |   | -0.462845 | -1.689965 | 2.920580  |
| H  |   | 1.393676  | -0.345106 | 4.953059  |
| H  |   | 0.243526  | -1.638984 | 5.263611  |
| H  |   | 1.389506  | -2.151569 | 1.386334  |
| H  |   | 2.469501  | -0.823917 | 0.957634  |
| H  |   | 3.523101  | -2.421848 | 2.576877  |
| H  |   | 3.396389  | -0.815804 | 3.285759  |
| H  |   | 1.480845  | -3.158611 | 3.760571  |
| H  |   | 2.603216  | -2.488436 | 4.942599  |
| C  |   | 1.354042  | 1.062384  | 2.309647  |
| H  |   | 1.804833  | 1.358603  | 1.355089  |
| H  |   | 2.160656  | 1.117000  | 3.063479  |
| C  |   | -1.030794 | 0.237934  | 3.671993  |
| C  |   | 0.275761  | 2.069322  | 2.729357  |
| C  |   | -0.385850 | 1.578838  | 4.013831  |
| H  |   | 0.346402  | 1.484517  | 4.823662  |
| H  |   | -1.146620 | 2.295235  | 4.350698  |
| H  |   | 0.784982  | 3.026203  | 2.908004  |
| C  |   | -2.091910 | 0.464894  | 2.589385  |
| H  |   | -2.899726 | 1.075854  | 3.039862  |
| H  |   | -2.525425 | -0.490687 | 2.276899  |
| N  |   | -1.593475 | 1.132852  | 1.375071  |
| C  |   | -0.824120 | 2.346841  | 1.694334  |
| H  |   | -1.507779 | 3.079178  | 2.179293  |
| C  |   | -2.740005 | 1.461060  | 0.520457  |
| H  |   | -3.442330 | 2.119695  | 1.071565  |
| H  |   | -3.270989 | 0.526500  | 0.307554  |
| C  |   | -0.313810 | 3.002534  | 0.414333  |
| H  |   | 0.343342  | 2.303092  | -0.116088 |
| H  |   | 0.282652  | 3.885352  | 0.678085  |
| C  |   | -2.324746 | 2.149034  | -0.774089 |
| H  |   | -1.741901 | 1.451638  | -1.387340 |
| H  |   | -3.225294 | 2.407601  | -1.344317 |
| C  |   | -1.477680 | 3.385252  | -0.493843 |
| H  |   | -1.113937 | 3.826914  | -1.429335 |
| H  |   | -2.091428 | 4.151519  | 0.001141  |
| H  |   | -1.560748 | -0.162336 | 4.546310  |
| Li |   | -0.534661 | -0.622028 | 0.451855  |
| C  |   | -1.690904 | -2.447968 | 0.612072  |
| H  |   | -1.688941 | -2.632262 | 1.708916  |
| C  |   | -0.965610 | -3.654689 | 0.010013  |
| H  |   | -1.465702 | -4.631120 | 0.192778  |
| C  |   | -3.165443 | -2.532381 | 0.213903  |
| H  |   | -3.324251 | -2.339867 | -0.861327 |
| H  |   | -3.634813 | -3.523603 | 0.396535  |
| H  |   | -3.790415 | -1.798534 | 0.748610  |
| O  |   | 0.592863  | -0.211250 | -1.214243 |
| C  |   | 0.557683  | -0.140397 | -2.446935 |

|   |           |           |           |
|---|-----------|-----------|-----------|
| O | 1.569411  | 0.300565  | -3.222503 |
| C | 2.918885  | 0.501281  | -2.704985 |
| C | 2.939568  | 1.614207  | -1.665170 |
| H | 2.415830  | 1.309013  | -0.758853 |
| H | 3.976149  | 1.860378  | -1.411094 |
| H | 2.463015  | 2.516308  | -2.062335 |
| C | 3.692083  | 0.921584  | -3.949067 |
| H | 3.636687  | 0.145140  | -4.717953 |
| H | 3.284227  | 1.848729  | -4.363405 |
| H | 4.744383  | 1.086948  | -3.698355 |
| C | 3.455912  | -0.815395 | -2.156171 |
| H | 2.862715  | -1.155327 | -1.304996 |
| H | 3.434837  | -1.588733 | -2.930910 |
| H | 4.493712  | -0.686498 | -1.831569 |
| N | -0.500711 | -0.472261 | -3.206983 |
| C | -0.540782 | -0.341556 | -4.666444 |
| H | -0.512129 | 0.718434  | -4.946923 |
| H | 0.324633  | -0.826758 | -5.126664 |
| C | -1.714350 | -1.085625 | -2.667914 |
| C | -2.724777 | -0.852536 | -3.784224 |
| H | -3.133298 | 0.163152  | -3.716532 |
| C | -1.871083 | -1.000155 | -5.046753 |
| H | -2.318266 | -0.542009 | -5.933258 |
| H | -1.712769 | -2.062420 | -5.264708 |
| H | -3.558885 | -1.557319 | -3.740163 |
| H | -0.872194 | -3.581630 | -1.087014 |
| H | -1.550057 | -2.154826 | -2.490303 |
| H | -1.984918 | -0.653514 | -1.702822 |
| H | 0.063221  | -3.760676 | 0.389540  |

Sparteine-iPrLi-N-bocpyrrolidine complex 6 TS, B3P86/6-31G\* = -1385.8470

|    |   |           |           |           |
|----|---|-----------|-----------|-----------|
| O  | 1 |           |           |           |
| C  |   | 0.782041  | -1.034362 | 4.571097  |
| C  |   | -0.033999 | -0.547576 | 3.361086  |
| N  |   | 0.756209  | -0.467110 | 2.114624  |
| C  |   | 1.468816  | -1.727438 | 1.852773  |
| C  |   | 2.331734  | -2.227672 | 3.011138  |
| C  |   | 1.481063  | -2.359202 | 4.271779  |
| H  |   | -0.804993 | -1.310281 | 3.174812  |
| H  |   | 1.537208  | -0.289906 | 4.853935  |
| H  |   | 0.108921  | -1.138452 | 5.431695  |
| H  |   | 0.706970  | -2.487416 | 1.630845  |
| H  |   | 2.053772  | -1.591813 | 0.937835  |
| H  |   | 2.777290  | -3.191330 | 2.736201  |
| H  |   | 3.166734  | -1.537865 | 3.194574  |
| H  |   | 0.726256  | -3.143874 | 4.118043  |
| H  |   | 2.091164  | -2.672574 | 5.127205  |
| C  |   | 1.646490  | 0.700339  | 2.055861  |
| H  |   | 2.077502  | 0.722599  | 1.049618  |
| H  |   | 2.491909  | 0.610255  | 2.760277  |
| C  |   | -0.743967 | 0.787780  | 3.632020  |
| C  |   | 0.935949  | 2.024380  | 2.367903  |
| C  |   | 0.275173  | 1.919857  | 3.739012  |
| H  |   | 1.016836  | 1.727301  | 4.522186  |
| H  |   | -0.225980 | 2.861622  | 3.997498  |
| H  |   | 1.708722  | 2.804685  | 2.379522  |
| C  |   | -1.783822 | 1.172681  | 2.572378  |
| H  |   | -2.340265 | 2.049006  | 2.958599  |
| H  |   | -2.511775 | 0.364891  | 2.437514  |
| N  |   | -1.224789 | 1.494871  | 1.248526  |
| C  |   | -0.125077 | 2.474150  | 1.350805  |
| H  |   | -0.542925 | 3.422998  | 1.752912  |
| C  |   | -2.303598 | 2.030839  | 0.404950  |
| H  |   | -2.730274 | 2.937122  | 0.879794  |
| H  |   | -3.098654 | 1.279539  | 0.360803  |
| C  |   | 0.441132  | 2.784750  | -0.031839 |
| H  |   | 0.862519  | 1.871439  | -0.467663 |
| H  |   | 1.261505  | 3.505695  | 0.078019  |
| C  |   | -1.821279 | 2.368780  | -0.997664 |
| H  |   | -1.529812 | 1.444008  | -1.510298 |
| H  |   | -2.656650 | 2.795465  | -1.565527 |
| C  |   | -0.642469 | 3.335353  | -0.954082 |
| H  |   | -0.242666 | 3.504125  | -1.960621 |
| H  |   | -0.980462 | 4.312033  | -0.578272 |
| H  |   | -1.290242 | 0.676410  | 4.577968  |
| Li |   | -0.549270 | -0.406562 | 0.372960  |
| C  |   | -2.245681 | -1.877196 | 0.534299  |
| H  |   | -1.872878 | -1.573978 | 1.531394  |
| C  |   | -1.907704 | -3.352868 | 0.346848  |
| H  |   | -2.384472 | -4.015043 | 1.089763  |
| C  |   | -3.756176 | -1.678503 | 0.531158  |
| H  |   | -4.159353 | -1.831728 | -0.481647 |
| H  |   | -4.299973 | -2.373918 | 1.193083  |
| H  |   | -4.046631 | -0.661119 | 0.829561  |
| O  |   | 0.741821  | -0.559946 | -1.072937 |
| C  |   | 0.497103  | -0.387931 | -2.287359 |

|   |           |           |           |
|---|-----------|-----------|-----------|
| O | 1.415080  | 0.096111  | -3.164138 |
| C | 2.844799  | -0.059170 | -2.950751 |
| C | 3.334566  | 0.849035  | -1.829161 |
| H | 2.937604  | 0.521248  | -0.868018 |
| H | 4.429179  | 0.829001  | -1.786021 |
| H | 3.018191  | 1.881224  | -2.010292 |
| C | 3.432400  | 0.387825  | -4.284792 |
| H | 3.063773  | -0.243880 | -5.098423 |
| H | 3.151859  | 1.423715  | -4.499166 |
| H | 4.524685  | 0.322192  | -4.258596 |
| C | 3.176674  | -1.523079 | -2.681758 |
| H | 2.724596  | -1.860057 | -1.746478 |
| H | 2.808064  | -2.153468 | -3.497611 |
| H | 4.261953  | -1.652405 | -2.613219 |
| N | -0.671797 | -0.615658 | -2.876524 |
| C | -0.936399 | -0.254347 | -4.282517 |
| H | -0.763630 | 0.818383  | -4.428523 |
| H | -0.257798 | -0.788161 | -4.956000 |
| C | -1.825760 | -1.245570 | -2.215292 |
| C | -2.973411 | -0.698152 | -3.050783 |
| H | -3.264397 | 0.312028  | -2.725952 |
| C | -2.407146 | -0.638325 | -4.482038 |
| H | -2.921796 | 0.067821  | -5.143945 |
| H | -2.473333 | -1.630972 | -4.941975 |
| H | -3.866929 | -1.327312 | -2.984837 |
| H | -2.244372 | -3.702004 | -0.639679 |
| H | -1.739666 | -2.325684 | -2.429549 |
| H | -1.904885 | -1.319529 | -0.756395 |
| H | -0.825869 | -3.542661 | 0.385952  |

trans-1,2-Bis(dimethylamino)cyclohexane-iPrLi-N-Bocpyrrolidine complex  
 3"'"  
 B3P86/6-31G\* = -1192.2753

|    |   |           |           |           |
|----|---|-----------|-----------|-----------|
| O  | 1 |           |           |           |
| C  |   | -0.181084 | -0.875508 | -3.123514 |
| C  |   | 0.513164  | 0.500566  | -3.121148 |
| C  |   | 1.447978  | 0.629125  | -4.337621 |
| C  |   | 0.735407  | 0.366537  | -5.661401 |
| C  |   | 0.090172  | -1.014788 | -5.651659 |
| C  |   | -0.871259 | -1.136700 | -4.472713 |
| C  |   | 1.907594  | 1.624093  | -4.345617 |
| H  |   | -0.270244 | 1.267135  | -3.208948 |
| H  |   | 0.604558  | -1.635824 | -3.015419 |
| H  |   | -0.039652 | 1.129034  | -5.823915 |
| H  |   | 1.444157  | 0.459355  | -6.493126 |
| H  |   | -0.443648 | -1.201587 | -6.591225 |
| H  |   | 0.872609  | -1.783885 | -5.577215 |
| H  |   | -1.682736 | -0.411037 | -4.612470 |
| H  |   | -1.337719 | -2.129590 | -4.458678 |
| H  |   | 2.268507  | -0.094492 | -4.238019 |
| H  |   | -1.063941 | -1.045245 | -1.950116 |
| N  |   | 1.172670  | 0.771198  | -1.827294 |
| N  |   | -2.400867 | -0.478384 | -2.122647 |
| C  |   | -2.332173 | 0.566275  | -2.433404 |
| H  |   | -3.014220 | -1.038449 | -2.849057 |
| H  |   | -2.911641 | -0.479612 | -1.156983 |
| H  |   | -1.161382 | -2.441646 | -1.549000 |
| C  |   | -1.622119 | -3.086303 | -2.318700 |
| H  |   | -0.167615 | -2.833741 | -1.312487 |
| H  |   | -1.774383 | -2.513971 | -0.645713 |
| H  |   | 2.347045  | -0.052255 | -1.566512 |
| C  |   | 3.195918  | 0.171090  | -2.234281 |
| H  |   | 2.673945  | 0.119903  | -0.538408 |
| H  |   | 2.102678  | -1.113879 | -1.654943 |
| H  |   | 1.508988  | 2.181915  | -1.666696 |
| C  |   | 1.850525  | 2.354210  | -0.641469 |
| H  |   | 2.306777  | 2.520166  | -2.350196 |
| H  |   | 0.617012  | 2.793559  | -1.822109 |
| H  |   | -0.385460 | 0.341364  | -0.343987 |
| Li |   | -1.594308 | 2.062419  | 0.080336  |
| C  |   | -1.320536 | 2.641983  | -0.829491 |
| H  |   | -0.970170 | 2.812193  | 1.258865  |
| C  |   | -1.346871 | 3.848078  | 1.409200  |
| H  |   | -3.112721 | 2.190419  | 0.187458  |
| C  |   | -3.517534 | 1.639487  | 1.056065  |
| H  |   | -3.477673 | 3.231847  | 0.318517  |
| H  |   | -3.635936 | 1.791333  | -0.695022 |
| H  |   | 0.529242  | -0.634660 | 1.187717  |
| O  |   | 0.286217  | -0.599501 | 2.401284  |
| C  |   | 1.213323  | -0.496420 | 3.372223  |
| O  |   | 2.622903  | -0.263090 | 3.080673  |
| C  |   | 3.246959  | -0.215768 | 4.470455  |
| C  |   | 3.091798  | -1.163010 | 4.995973  |
| H  |   | 4.323325  | -0.034430 | 4.391995  |
| H  |   | -0.618568 | 0.267304  | 4.765679  |
| H  |   | 2.787781  | 1.078053  | 2.376727  |
| C  |   |           |           |           |

|   |           |           |          |
|---|-----------|-----------|----------|
| H | 2.273194  | 1.079531  | 1.414598 |
| H | 2.373001  | 1.884379  | 2.989581 |
| H | 3.850734  | 1.283456  | 2.211303 |
| C | 3.199890  | -1.426184 | 2.280937 |
| H | 3.017528  | -2.370521 | 2.804428 |
| H | 2.751351  | -1.484281 | 1.288846 |
| H | 4.282853  | -1.298949 | 2.177526 |
| N | -0.946307 | -0.697940 | 2.922240 |
| C | -1.292156 | -0.468863 | 4.323806 |
| H | -1.202640 | -1.400074 | 4.900413 |
| H | 2.802266  | 0.587282  | 5.065876 |
| C | -2.125669 | -0.818239 | 2.059945 |
| C | -3.293507 | -0.792171 | 3.050001 |
| H | -3.551552 | -1.810406 | 3.366126 |
| C | -2.743016 | 0.000862  | 4.237221 |
| H | -3.294644 | -0.168446 | 5.166314 |
| H | -2.767512 | 1.072818  | 4.012433 |
| H | -4.186310 | -0.339848 | 2.610964 |
| H | -1.163967 | 2.293437  | 2.214957 |
| H | -2.137939 | 0.022122  | 1.348120 |
| H | -2.081566 | -1.754577 | 1.491672 |
| H | 0.125775  | 2.893515  | 1.176143 |

trans-1,2-Bis(dimethylamine)cyclohexane-iPrLi-N-Bocpyrrolidine complex  
 3"Ts  
 B3P86/6-31G\* = -1192.2539

|    |           |           |           |
|----|-----------|-----------|-----------|
| 0  | 1         |           |           |
| C  | -0.027733 | -0.872186 | 3.127402  |
| C  | -0.692851 | 0.513130  | 3.017297  |
| C  | -1.694010 | 0.709178  | 4.169555  |
| C  | -1.055345 | 0.509381  | 5.541769  |
| C  | -0.414631 | -0.871114 | 5.639646  |
| C  | 0.601388  | -1.063065 | 4.516748  |
| H  | -2.142108 | 1.707295  | 4.104285  |
| H  | 0.096341  | 1.273046  | 3.120671  |
| H  | -0.826521 | -1.620467 | 3.035914  |
| H  | -0.287660 | 1.278724  | 5.707253  |
| H  | -1.807583 | 0.645377  | 6.327970  |
| H  | 0.072647  | -1.004458 | 6.612845  |
| H  | -1.194694 | -1.643042 | 5.571425  |
| H  | 1.413557  | -0.337222 | 4.653269  |
| H  | 1.057363  | -2.058952 | 4.579116  |
| H  | -2.515448 | -0.011521 | 4.057142  |
| N  | 0.892992  | -1.137073 | 1.999540  |
| N  | -1.265083 | 0.730094  | 1.672842  |
| C  | 2.238783  | -0.593290 | 2.189499  |
| H  | 2.186530  | 0.464597  | 2.457591  |
| H  | 2.812677  | -1.130068 | 2.962413  |
| H  | 2.780014  | -0.661895 | 1.242165  |
| C  | 0.974930  | -2.565995 | 1.713511  |
| H  | 1.374624  | -3.152094 | 2.559156  |
| H  | -0.015635 | -2.953481 | 1.456165  |
| H  | 1.632378  | -2.724981 | 0.854511  |
| C  | -2.417338 | -0.112500 | 1.361880  |
| H  | -3.313406 | 0.144762  | 1.950062  |
| H  | -2.650580 | 0.000368  | 0.300996  |
| H  | -2.180356 | -1.166293 | 1.527244  |
| C  | -1.609519 | 2.129258  | 1.440866  |
| H  | -1.883959 | 2.259293  | 0.389734  |
| H  | -2.456777 | 2.475849  | 2.056244  |
| H  | -0.742770 | 2.765450  | 1.641422  |
| Li | 0.288305  | 0.098379  | 0.267616  |
| C  | 1.699753  | 1.855943  | -0.090316 |
| H  | 1.206039  | 2.027276  | 0.888594  |
| C  | 1.026377  | 2.739043  | -1.135195 |
| H  | 1.134884  | 3.823618  | -0.951201 |
| C  | 3.163479  | 2.251041  | 0.063447  |
| H  | 3.711047  | 2.073630  | -0.874378 |
| H  | 3.315253  | 3.316794  | 0.309743  |
| H  | 3.675856  | 1.666992  | 0.840711  |
| O  | -0.750204 | -0.470243 | -1.268982 |
| C  | -0.220016 | -0.492455 | -2.403854 |
| O  | -0.917394 | -0.427487 | -3.561809 |
| C  | -2.359899 | -0.259216 | -3.582742 |
| C  | -2.672374 | -0.240316 | -5.075194 |
| H  | -2.357105 | -1.176634 | -5.545717 |
| H  | -3.748156 | -0.115537 | -5.233715 |
| H  | 1.219509  | 0.132732  | -4.568053 |
| C  | -2.749596 | 1.070523  | -2.945186 |

|   |           |           |           |
|---|-----------|-----------|-----------|
| H | -2.498143 | 1.080091  | -1.883559 |
| H | -2.223736 | 1.895304  | -3.437002 |
| H | -3.826702 | 1.236001  | -3.056823 |
| C | -3.045987 | -1.447012 | -2.914456 |
| H | -2.713227 | -2.382448 | -3.376382 |
| H | -2.815893 | -1.481915 | -1.848889 |
| H | -4.130913 | -1.369727 | -3.045176 |
| N | 1.086054  | -0.616675 | -2.600207 |
| C | 1.749557  | -0.546464 | -3.897163 |
| H | 1.771897  | -1.539718 | -4.368657 |
| H | -2.150113 | 0.585893  | -5.567320 |
| C | 2.030709  | -0.688262 | -1.469635 |
| C | 3.393845  | -0.756483 | -2.167409 |
| H | 3.734118  | -1.790789 | -2.336728 |
| C | 3.154369  | -0.080965 | -3.521707 |
| H | 3.898133  | -0.343583 | -4.280414 |
| H | 3.157422  | 1.008957  | -3.403998 |
| H | 4.181364  | -0.251639 | -1.597121 |
| H | 1.462811  | 2.552584  | -2.128454 |
| H | 1.844249  | 0.511679  | -0.687650 |
| H | 1.827553  | -1.622652 | -0.922529 |
| H | -0.050006 | 2.536051  | -1.227191 |

trans-1,2-Bis(dimethylamino)cyclohexane-iPrLi-N-bocpyrrolidine complex 4'''  
 B3P86/6-31G\* = -1192.2760

|    |   |           |           |           |
|----|---|-----------|-----------|-----------|
| O  | 1 |           |           |           |
| C  |   | 0.779351  | 0.099608  | 3.021537  |
| C  |   | -0.614181 | -0.551716 | 3.114380  |
| C  |   | -0.613592 | -1.699943 | 4.139247  |
| C  |   | -0.112334 | -1.265685 | 5.513194  |
| C  |   | 1.288838  | -0.675311 | 5.398788  |
| C  |   | 1.289206  | 0.494310  | 4.418357  |
| H  |   | -1.622897 | -2.122215 | 4.215443  |
| H  |   | -1.309977 | 0.216955  | 3.478502  |
| H  |   | 1.467964  | -0.658003 | 2.620047  |
| H  |   | -0.791726 | -0.513035 | 5.938211  |
| H  |   | -0.120711 | -2.119018 | 6.202006  |
| H  |   | 1.652665  | -0.342823 | 6.378429  |
| H  |   | 1.985400  | -1.452964 | 5.053300  |
| H  |   | 0.646184  | 1.285329  | 4.826326  |
| H  |   | 2.295378  | 0.923029  | 4.335118  |
| H  |   | 0.036038  | -2.507760 | 3.776155  |
| N  |   | 0.794718  | 1.204883  | 2.041334  |
| N  |   | -1.120715 | -0.939209 | 1.782315  |
| C  |   | 0.206733  | 2.449892  | 2.532536  |
| H  |   | -0.792837 | 2.268239  | 2.934686  |
| H  |   | 0.820945  | 2.939590  | 3.306650  |
| H  |   | 0.089444  | 3.138331  | 1.692480  |
| C  |   | 2.136105  | 1.463537  | 1.537742  |
| H  |   | 2.836326  | 1.814689  | 2.316374  |
| H  |   | 2.544509  | 0.556942  | 1.082272  |
| H  |   | 2.083709  | 2.237393  | 0.766050  |
| C  |   | -0.544987 | -2.173644 | 1.260545  |
| H  |   | -0.890184 | -3.074688 | 1.794212  |
| H  |   | -0.820665 | -2.274164 | 0.207656  |
| H  |   | 0.546542  | -2.135682 | 1.304863  |
| C  |   | -2.577534 | -1.011174 | 1.753501  |
| H  |   | -2.907919 | -1.203994 | 0.729136  |
| H  |   | -2.985752 | -1.807754 | 2.400735  |
| H  |   | -3.000181 | -0.049283 | 2.053300  |
| Li |   | -0.587744 | 0.660647  | 0.375934  |
| C  |   | -1.979557 | 2.173099  | -0.247358 |
| H  |   | -1.803894 | 2.908454  | 0.564217  |
| C  |   | -3.498501 | 2.020665  | -0.320219 |
| H  |   | -4.036796 | 2.943400  | -0.628431 |
| C  |   | -1.489916 | 2.853531  | -1.527929 |
| H  |   | -1.565108 | 2.190095  | -2.408067 |
| H  |   | -2.051223 | 3.771701  | -1.809572 |
| H  |   | -0.429530 | 3.146096  | -1.464837 |
| O  |   | 0.564164  | -0.202980 | -1.067303 |
| C  |   | 0.448500  | -0.440461 | -2.274974 |
| O  |   | 1.466810  | -0.464540 | -3.156650 |
| C  |   | 2.830426  | -0.111891 | -2.779151 |
| C  |   | 3.594625  | -0.293339 | -4.085095 |
| H  |   | 3.189037  | 0.361088  | -4.862437 |
| H  |   | 4.650712  | -0.046009 | -3.939380 |
| H  |   | -0.179551 | -1.759834 | -4.667322 |
| C  |   | 3.354447  | -1.075244 | -1.719594 |
| H  |   | 2.807890  | -0.962579 | -0.782533 |

|   |           |           |           |
|---|-----------|-----------|-----------|
| H | 3.252023  | -2.109465 | -2.064837 |
| H | 4.417044  | -0.880551 | -1.539530 |
| C | 2.878911  | 1.342094  | -2.326991 |
| H | 2.495580  | 1.997870  | -3.115095 |
| H | 2.278131  | 1.488388  | -1.428764 |
| H | 3.913688  | 1.630646  | -2.113637 |
| N | -0.708671 | -0.740618 | -2.887479 |
| C | -0.844619 | -0.959839 | -4.329461 |
| H | -0.572741 | -0.047926 | -4.875202 |
| H | 3.525512  | -1.328620 | -4.433212 |
| C | -1.997230 | -0.704979 | -2.193420 |
| C | -2.990645 | -0.536286 | -3.339825 |
| H | -3.086652 | 0.526598  | -3.586798 |
| C | -2.328133 | -1.295890 | -4.492341 |
| H | -2.707907 | -1.012016 | -5.477795 |
| H | -2.483473 | -2.374765 | -4.372114 |
| H | -3.985280 | -0.912891 | -3.086887 |
| H | -3.815947 | 1.250673  | -1.046417 |
| H | -2.164586 | -1.658491 | -1.669539 |
| H | -2.013330 | 0.114564  | -1.458972 |
| H | -3.933216 | 1.719296  | 0.645040  |

trans-1,2-Bis(dimethylamino)cyclohexane-iPrLi-N-bocpyrrolidine complex  
 4''Ts  
 B3P86/6-31G\* = -1192.2556.

|    |   |           |           |           |
|----|---|-----------|-----------|-----------|
| 0  | 1 |           |           |           |
| C  |   | 0.774674  | 0.254036  | 2.824707  |
| C  |   | -0.425194 | -0.697802 | 3.002651  |
| C  |   | -0.078623 | -1.848085 | 3.962802  |
| C  |   | 0.448331  | -1.356092 | 5.307941  |
| C  |   | 1.671589  | -0.469131 | 5.100286  |
| C  |   | 1.321449  | 0.703899  | 4.190031  |
| H  |   | -0.961842 | -2.483138 | 4.103716  |
| H  |   | -1.235285 | -0.117165 | 3.465088  |
| H  |   | 1.568070  | -0.312053 | 2.316222  |
| H  |   | -0.331998 | -0.783984 | 5.830113  |
| H  |   | 0.690982  | -2.211686 | 5.949415  |
| H  |   | 2.050547  | -0.097984 | 6.059986  |
| H  |   | 2.481428  | -1.062299 | 4.651569  |
| H  |   | 0.564866  | 1.317404  | 4.697010  |
| H  |   | 2.197252  | 1.347066  | 4.042423  |
| H  |   | 0.692036  | -2.482004 | 3.504842  |
| N  |   | 0.446504  | 1.372610  | 1.913232  |
| N  |   | -0.957426 | -1.145786 | 1.696560  |
| C  |   | -0.363076 | 2.423450  | 2.527582  |
| H  |   | -1.248853 | 1.998754  | 3.006881  |
| H  |   | 0.192696  | 3.012470  | 3.275312  |
| H  |   | -0.708138 | 3.105265  | 1.745841  |
| C  |   | 1.646101  | 1.968200  | 1.333982  |
| H  |   | 2.286591  | 2.465667  | 2.082376  |
| H  |   | 2.225949  | 1.201024  | 0.816412  |
| H  |   | 1.348205  | 2.719124  | 0.595771  |
| C  |   | -0.215840 | -2.254474 | 1.097328  |
| H  |   | -0.358343 | -3.207148 | 1.632651  |
| H  |   | -0.555501 | -2.387080 | 0.066816  |
| H  |   | 0.852133  | -2.024476 | 1.061050  |
| C  |   | -2.377261 | -1.478871 | 1.769890  |
| H  |   | -2.742688 | -1.703683 | 0.764253  |
| H  |   | -2.582649 | -2.348672 | 2.417490  |
| H  |   | -2.940677 | -0.618884 | 2.142709  |
| Li |   | -0.691931 | 0.427980  | 0.260373  |
| C  |   | -2.507837 | 1.594122  | -0.218732 |
| H  |   | -2.312754 | 1.689271  | 0.867832  |
| C  |   | -4.016171 | 1.447808  | -0.374845 |
| H  |   | -4.588959 | 2.319457  | -0.013018 |
| C  |   | -2.007922 | 2.856270  | -0.913216 |
| H  |   | -2.132423 | 2.771139  | -2.002982 |
| H  |   | -2.533568 | 3.781576  | -0.613116 |
| H  |   | -0.933884 | 3.032753  | -0.744497 |
| O  |   | 0.711736  | 0.066599  | -1.011950 |
| C  |   | 0.524904  | -0.286617 | -2.194703 |
| O  |   | 1.515583  | -0.356555 | -3.114438 |
| C  |   | 2.878109  | 0.051780  | -2.819416 |
| C  |   | 3.598254  | -0.210541 | -4.137668 |
| H  |   | 3.145913  | 0.373186  | -4.945073 |
| H  |   | 4.652887  | 0.070098  | -4.053965 |
| H  |   | -0.147040 | -1.835408 | -4.408971 |
| C  |   | 3.472492  | -0.815752 | -1.713839 |

|   |           |           |           |
|---|-----------|-----------|-----------|
| H | 2.961047  | -0.645361 | -0.765711 |
| H | 3.381448  | -1.874981 | -1.976749 |
| H | 4.536548  | -0.584893 | -1.593564 |
| C | 2.919020  | 1.537672  | -2.479812 |
| H | 2.483007  | 2.123279  | -3.295772 |
| H | 2.361016  | 1.741682  | -1.565295 |
| H | 3.956622  | 1.861491  | -2.343658 |
| N | -0.643918 | -0.665187 | -2.703826 |
| C | -0.813509 | -1.014698 | -4.124469 |
| H | -0.559432 | -0.152104 | -4.752984 |
| H | 3.540012  | -1.270330 | -4.404221 |
| C | -1.904945 | -0.657704 | -1.941489 |
| C | -2.925241 | -0.573210 | -3.071840 |
| H | -3.066061 | 0.470329  | -3.389169 |
| C | -2.296329 | -1.373953 | -4.221706 |
| H | -2.705808 | -1.143450 | -5.211729 |
| H | -2.433399 | -2.447367 | -4.043433 |
| H | -3.906197 | -0.957154 | -2.774713 |
| H | -4.292115 | 1.313098  | -1.430180 |
| H | -2.007197 | -1.648729 | -1.458769 |
| H | -2.083492 | 0.421183  | -1.013979 |
| H | -4.397683 | 0.567125  | 0.161207  |

Sparteine-iPrLi-N-Mebocpyrrolidine complex 3", B3P86/6-31G\* = -1267.4845

|    |   |           |           |           |
|----|---|-----------|-----------|-----------|
| O  | 1 |           |           |           |
| C  |   | 3.179902  | -1.264381 | 2.099401  |
| C  |   | 1.734661  | -1.060372 | 1.609400  |
| N  |   | 1.374205  | 0.356125  | 1.398686  |
| C  |   | 2.372451  | 1.048896  | 0.573492  |
| C  |   | 3.812595  | 0.924813  | 1.071838  |
| C  |   | 4.186680  | -0.549075 | 1.201176  |
| H  |   | 1.659739  | -1.531499 | 0.617319  |
| H  |   | 3.293011  | -0.891325 | 3.125219  |
| H  |   | 3.390905  | -2.340970 | 2.135005  |
| H  |   | 2.316501  | 0.616063  | -0.432600 |
| H  |   | 2.062273  | 2.093468  | 0.478448  |
| H  |   | 4.480992  | 1.440456  | 0.371657  |
| H  |   | 3.929774  | 1.426636  | 2.041672  |
| H  |   | 4.178605  | -1.011762 | 0.203025  |
| H  |   | 5.203515  | -0.667125 | 1.593959  |
| C  |   | 1.068419  | 1.100933  | 2.625600  |
| H  |   | 0.677379  | 2.076453  | 2.315638  |
| H  |   | 1.974967  | 1.298232  | 3.225540  |
| C  |   | 0.718625  | -1.747511 | 2.536404  |
| C  |   | 0.071191  | 0.381925  | 3.541822  |
| C  |   | 0.617629  | -1.004961 | 3.866728  |
| H  |   | 1.588745  | -0.937751 | 4.369908  |
| H  |   | -0.060096 | -1.536988 | 4.546755  |
| H  |   | -0.007614 | 0.980296  | 4.459064  |
| C  |   | -0.686529 | -1.867616 | 1.940163  |
| H  |   | -1.278813 | -2.523837 | 2.609078  |
| H  |   | -0.642234 | -2.349564 | 0.957608  |
| N  |   | -1.379415 | -0.584548 | 1.764179  |
| C  |   | -1.355474 | 0.230414  | 2.993749  |
| H  |   | -1.923732 | -0.312314 | 3.781348  |
| C  |   | -2.765095 | -0.848430 | 1.358934  |
| H  |   | -3.277466 | -1.442388 | 2.143472  |
| H  |   | -2.729380 | -1.468140 | 0.457241  |
| C  |   | -2.065870 | 1.561716  | 2.763366  |
| H  |   | -1.538636 | 2.128748  | 1.987704  |
| H  |   | -2.028283 | 2.146248  | 3.691478  |
| C  |   | -3.539411 | 0.434965  | 1.095878  |
| H  |   | -3.086720 | 0.957679  | 0.245562  |
| H  |   | -4.570481 | 0.181432  | 0.820787  |
| C  |   | -3.509967 | 1.341967  | 2.321771  |
| H  |   | -3.991968 | 2.300764  | 2.100893  |
| H  |   | -4.079608 | 0.878127  | 3.140552  |
| H  |   | 1.077492  | -2.772356 | 2.700846  |
| Li |   | -0.366180 | 0.430335  | 0.060585  |
| C  |   | -0.948121 | 2.301617  | -0.841612 |
| H  |   | -1.641289 | 2.712414  | -0.077847 |
| C  |   | -1.800214 | 2.144928  | -2.104575 |
| H  |   | -2.211059 | 3.097488  | -2.504853 |
| C  |   | 0.070622  | 3.416952  | -1.084615 |
| H  |   | 0.874485  | 3.115819  | -1.780328 |
| H  |   | -0.359221 | 4.342904  | -1.524798 |
| H  |   | 0.576185  | 3.727095  | -0.156738 |
| O  |   | -0.327641 | -1.222431 | -1.227956 |
| C  |   | -0.472145 | -1.337104 | -2.449475 |

|   |           |           |           |
|---|-----------|-----------|-----------|
| O | -1.382383 | -2.161579 | -3.010109 |
| C | -2.240317 | -2.851903 | -2.109908 |
| N | 0.260783  | -0.707164 | -3.375037 |
| C | -0.014727 | -0.706701 | -4.812031 |
| H | 0.476530  | -1.561590 | -5.296159 |
| H | -1.087978 | -0.786089 | -4.992952 |
| C | 1.293492  | 0.257260  | -2.991882 |
| C | 1.787277  | 0.802011  | -4.335205 |
| H | 2.636263  | 0.209456  | -4.695837 |
| C | 0.587218  | 0.621254  | -5.268966 |
| H | 0.861206  | 0.612523  | -6.327457 |
| H | -0.137370 | 1.426231  | -5.107926 |
| H | 2.113203  | 1.841816  | -4.255462 |
| H | -1.229393 | 1.703796  | -2.940054 |
| H | 0.850462  | 1.027363  | -2.348270 |
| H | 2.087965  | -0.246825 | -2.431283 |
| H | -2.663995 | 1.478692  | -1.950184 |
| H | -1.665189 | -3.366595 | -1.337116 |
| H | -2.943475 | -2.159797 | -1.639366 |
| H | -2.783825 | -3.572698 | -2.721290 |

Sparteine-iPrLi-N-Mebocpyrrolideine Complex 3<sup>TS</sup>, B3P86/6-31G\* = -1267.4580

|    |   |           |           |           |
|----|---|-----------|-----------|-----------|
| O  | 1 |           |           |           |
| C  |   | -0.895109 | -0.829392 | -3.860722 |
| C  |   | -0.898515 | -0.830358 | -2.314916 |
| N  |   | 0.473299  | -0.835217 | -1.734374 |
| C  |   | 1.321000  | 0.246846  | -2.308714 |
| C  |   | 1.376829  | 0.236069  | -3.844885 |
| C  |   | -0.049982 | 0.333492  | -4.409177 |
| H  |   | -1.352759 | 0.098138  | -1.988042 |
| H  |   | -0.495180 | -1.760370 | -4.243573 |
| H  |   | -1.920643 | -0.744591 | -4.206913 |
| H  |   | 0.910706  | 1.189138  | -1.978491 |
| H  |   | 2.307895  | 0.158168  | -1.879477 |
| H  |   | 1.977253  | 1.076353  | -4.177145 |
| H  |   | 1.852147  | -0.669189 | -4.207529 |
| H  |   | -0.491604 | 1.278699  | -4.105690 |
| H  |   | -0.037561 | 0.308629  | -5.493382 |
| C  |   | 1.159850  | -2.150096 | -1.741575 |
| H  |   | 2.055021  | -2.046571 | -1.143595 |
| H  |   | 1.473373  | -2.418202 | -2.748155 |
| C  |   | -1.727510 | -1.998861 | -1.749642 |
| C  |   | 0.288053  | -3.303813 | -1.213761 |
| C  |   | -1.024725 | -3.337485 | -2.004305 |
| H  |   | -0.835897 | -3.492777 | -3.058701 |
| H  |   | -1.648237 | -4.156860 | -1.660463 |
| H  |   | 0.841447  | -4.223699 | -1.379839 |
| C  |   | -2.015551 | -1.867531 | -0.243268 |
| H  |   | -2.738933 | -2.639668 | 0.026217  |
| H  |   | -2.441694 | -0.900709 | -0.028825 |
| N  |   | -0.806874 | -2.014280 | 0.619675  |
| C  |   | -0.046359 | -3.248556 | 0.287434  |
| H  |   | -0.690555 | -4.109901 | 0.489356  |
| C  |   | -1.237526 | -2.015294 | 2.045770  |
| H  |   | -1.947320 | -2.828275 | 2.208886  |
| H  |   | -1.742795 | -1.077593 | 2.226926  |
| C  |   | 1.183163  | -3.384067 | 1.194515  |
| H  |   | 1.844354  | -2.541541 | 1.048537  |
| H  |   | 1.718023  | -4.289138 | 0.923973  |
| C  |   | -0.053504 | -2.172960 | 3.006400  |
| H  |   | 0.588483  | -1.307242 | 2.932428  |
| H  |   | -0.432593 | -2.221406 | 4.021976  |
| C  |   | 0.754462  | -3.435995 | 2.670398  |
| H  |   | 1.625373  | -3.504898 | 3.312099  |
| H  |   | 0.145234  | -4.319503 | 2.841131  |
| H  |   | -2.689878 | -1.981899 | -2.253071 |
| Li |   | 0.115286  | -0.163082 | 0.189977  |
| C  |   | 2.150126  | 0.662212  | 1.333676  |
| H  |   | 1.896168  | -0.403026 | 1.278556  |
| C  |   | 2.035425  | 1.101418  | 2.811980  |
| H  |   | 2.686009  | 0.538279  | 3.483949  |
| C  |   | 3.616672  | 0.804829  | 0.868054  |
| H  |   | 3.898258  | 1.854692  | 0.838168  |
| H  |   | 4.326014  | 0.296991  | 1.524884  |
| H  |   | 3.757401  | 0.406430  | -0.134219 |
| O  |   | -1.238951 | 1.069071  | 0.469763  |
| C  |   | -1.347460 | 2.234259  | 0.931071  |

|   |           |          |           |
|---|-----------|----------|-----------|
| O | -2.495666 | 2.595203 | 1.563622  |
| C | -3.581037 | 1.647975 | 1.653383  |
| N | -0.464953 | 3.181468 | 0.856612  |
| C | -0.613454 | 4.511938 | 1.469134  |
| H | -1.023050 | 5.205746 | 0.743084  |
| H | -1.260547 | 4.470054 | 2.328816  |
| C | 0.885865  | 2.985606 | 0.193932  |
| C | 1.643541  | 4.281522 | 0.614426  |
| H | 1.666702  | 5.011647 | -0.190883 |
| C | 0.843144  | 4.867206 | 1.803669  |
| H | 0.986753  | 5.933222 | 1.924890  |
| H | 1.126909  | 4.364385 | 2.719501  |
| H | 2.665552  | 4.070737 | 0.901337  |
| H | 2.308030  | 2.149778 | 2.902782  |
| H | 1.457721  | 1.730084 | 0.663768  |
| H | 0.699883  | 3.012271 | -0.879375 |
| H | 1.014694  | 1.006865 | 3.178367  |
| H | -3.907568 | 1.345262 | 0.670063  |
| H | -3.286375 | 0.775863 | 2.214800  |
| H | -4.369822 | 2.173092 | 2.165203  |

Sparteine-iPrLi-N-Mebocpyrrolidine Complex 4", B3P86/6-31G\* = -1267.4883

|    |   |           |           |           |
|----|---|-----------|-----------|-----------|
| O  | 1 |           |           |           |
| C  |   | -0.735773 | -0.805931 | -4.031195 |
| C  |   | -0.759417 | -0.805487 | -2.492756 |
| N  |   | 0.583751  | -0.765879 | -1.883965 |
| C  |   | 1.392009  | 0.325692  | -2.441588 |
| C  |   | 1.494677  | 0.326483  | -3.966960 |
| C  |   | 0.097409  | 0.350653  | -4.581105 |
| H  |   | -1.248228 | 0.126094  | -2.171560 |
| H  |   | -0.321732 | -1.750226 | -4.407450 |
| H  |   | -1.767782 | -0.749651 | -4.401895 |
| H  |   | 0.928313  | 1.268327  | -2.118045 |
| H  |   | 2.378318  | 0.286794  | -1.968790 |
| H  |   | 2.081227  | 1.195395  | -4.289420 |
| H  |   | 2.037938  | -0.562872 | -4.314025 |
| H  |   | -0.390015 | 1.304653  | -4.328759 |
| H  |   | 0.145148  | 0.304342  | -5.675735 |
| C  |   | 1.298777  | -2.046368 | -1.886432 |
| H  |   | 2.203789  | -1.905003 | -1.285086 |
| H  |   | 1.632196  | -2.335059 | -2.899627 |
| C  |   | -1.573881 | -1.982989 | -1.932443 |
| C  |   | 0.456001  | -3.204479 | -1.339993 |
| C  |   | -0.831900 | -3.299506 | -2.152582 |
| H  |   | -0.616950 | -3.471946 | -3.213320 |
| H  |   | -1.444338 | -4.142735 | -1.807688 |
| H  |   | 1.050224  | -4.119244 | -1.466752 |
| C  |   | -1.908122 | -1.855480 | -0.443073 |
| H  |   | -2.634232 | -2.655232 | -0.193209 |
| H  |   | -2.396851 | -0.895135 | -0.244095 |
| N  |   | -0.744891 | -1.946569 | 0.447834  |
| C  |   | 0.090251  | -3.127165 | 0.150508  |
| H  |   | -0.510923 | -4.039783 | 0.359622  |
| C  |   | -1.214563 | -1.989385 | 1.837890  |
| H  |   | -1.871832 | -2.871149 | 1.982296  |
| H  |   | -1.831200 | -1.098101 | 2.005194  |
| C  |   | 1.300642  | -3.159554 | 1.079422  |
| H  |   | 1.904586  | -2.256848 | 0.923286  |
| H  |   | 1.919420  | -4.029621 | 0.824744  |
| C  |   | -0.064148 | -2.038630 | 2.833576  |
| H  |   | 0.512836  | -1.109067 | 2.762543  |
| H  |   | -0.473688 | -2.103526 | 3.849295  |
| C  |   | 0.858967  | -3.216377 | 2.538536  |
| H  |   | 1.728630  | -3.197469 | 3.204888  |
| H  |   | 0.329251  | -4.161979 | 2.727579  |
| H  |   | -2.532691 | -1.994633 | -2.468341 |
| Li |   | 0.429297  | -0.114526 | 0.177181  |
| C  |   | 2.344411  | 0.458938  | 0.962228  |
| H  |   | 2.946301  | -0.113784 | 0.220328  |
| C  |   | 2.958722  | 0.120431  | 2.320140  |
| H  |   | 4.014404  | 0.445614  | 2.439032  |
| C  |   | 2.628536  | 1.935172  | 0.670033  |
| H  |   | 2.056044  | 2.601678  | 1.338688  |
| H  |   | 3.690262  | 2.237197  | 0.801074  |
| H  |   | 2.348761  | 2.226694  | -0.354327 |
| O  |   | -1.043326 | 1.283314  | 0.091256  |
| C  |   | -1.173027 | 2.416888  | 0.566069  |

|   |           |           |           |
|---|-----------|-----------|-----------|
| O | -1.629662 | 3.462370  | -0.156406 |
| C | -1.961039 | 3.177227  | -1.509954 |
| H | -2.034518 | 4.532378  | 2.144313  |
| N | -0.916921 | 2.763302  | 1.830914  |
| C | -1.045913 | 4.120441  | 2.364702  |
| H | -0.296517 | 4.778139  | 1.906814  |
| C | -0.337503 | 1.819751  | 2.790747  |
| C | 0.182362  | 2.738690  | 3.894600  |
| H | 1.197681  | 3.069144  | 3.649868  |
| C | -0.786547 | 3.924261  | 3.858701  |
| H | -0.387959 | 4.827283  | 4.329134  |
| H | -1.721860 | 3.664452  | 4.368676  |
| H | 0.217719  | 2.239381  | 4.866387  |
| H | 2.416939  | 0.601028  | 3.154395  |
| H | -1.121091 | 1.146521  | 3.166492  |
| H | 0.442463  | 1.220531  | 2.299132  |
| H | 2.944559  | -0.959209 | 2.533993  |
| H | -2.744719 | 2.417092  | -1.569274 |
| H | -2.319051 | 4.119779  | -1.925055 |
| H | -1.083978 | 2.832232  | -2.063572 |

Sparteine-iPrLi-N-Mebocpyrrolidene Complex 4"TS, B3P86/6-31G\* = -1267.4647

|    |   |           |           |           |
|----|---|-----------|-----------|-----------|
| O  | 1 |           |           |           |
| C  |   | -0.861439 | -0.749813 | -3.999206 |
| C  |   | -0.861509 | -0.752074 | -2.453389 |
| N  |   | 0.514508  | -0.750112 | -1.883003 |
| C  |   | 1.330053  | 0.361474  | -2.441210 |
| C  |   | 1.385395  | 0.373892  | -3.977933 |
| C  |   | -0.042528 | 0.433518  | -4.545077 |
| H  |   | -1.310610 | 0.172166  | -2.117345 |
| H  |   | -0.442881 | -1.671164 | -4.385542 |
| H  |   | -1.888652 | -0.685677 | -4.345250 |
| H  |   | 0.881324  | 1.283155  | -2.094764 |
| H  |   | 2.321828  | 0.298001  | -2.016901 |
| H  |   | 1.961349  | 1.234861  | -4.300821 |
| H  |   | 1.888223  | -0.513037 | -4.348364 |
| H  |   | -0.509245 | 1.367044  | -4.241902 |
| H  |   | -0.026439 | 0.411749  | -5.629309 |
| C  |   | 1.210400  | -2.056744 | -1.918126 |
| H  |   | 2.123246  | -1.952761 | -1.347685 |
| H  |   | 1.492526  | -2.326473 | -2.933813 |
| C  |   | -1.682668 | -1.923772 | -1.885642 |
| C  |   | 0.351534  | -3.205004 | -1.359194 |
| C  |   | -0.970829 | -3.259030 | -2.132662 |
| H  |   | -0.793071 | -3.423803 | -3.187862 |
| H  |   | -1.582919 | -4.080089 | -1.772601 |
| H  |   | 0.906925  | -4.125451 | -1.515281 |
| C  |   | -1.972734 | -1.786551 | -0.380654 |
| H  |   | -2.692833 | -2.559847 | -0.107621 |
| H  |   | -2.412412 | -0.821454 | -0.173103 |
| N  |   | -0.764535 | -1.918958 | 0.481817  |
| C  |   | 0.035978  | -3.128781 | 0.146132  |
| H  |   | -0.571269 | -4.010211 | 0.372603  |
| C  |   | -1.193309 | -1.953569 | 1.909205  |
| H  |   | -1.851708 | -2.809779 | 2.065628  |
| H  |   | -1.756464 | -1.051512 | 2.105180  |
| C  |   | 1.283398  | -3.194196 | 1.036324  |
| H  |   | 1.894970  | -2.317063 | 0.875818  |
| H  |   | 1.863575  | -4.070482 | 0.763329  |
| C  |   | 0.005306  | -2.042857 | 2.859109  |
| H  |   | 0.590244  | -1.138916 | 2.774539  |
| H  |   | -0.361594 | -2.110062 | 3.878153  |
| C  |   | 0.878719  | -3.259798 | 2.518411  |
| H  |   | 1.761663  | -3.273938 | 3.147093  |
| H  |   | 0.324862  | -4.176413 | 2.703074  |
| H  |   | -2.644777 | -1.916355 | -2.389938 |
| Li |   | 0.196838  | -0.119988 | 0.086402  |
| C  |   | 2.252565  | 0.685007  | 1.099063  |
| H  |   | 2.362312  | -0.042797 | 0.285230  |
| C  |   | 3.187250  | 0.236246  | 2.246115  |
| H  |   | 4.244085  | 0.289861  | 1.978414  |
| C  |   | 2.720849  | 2.063508  | 0.571953  |
| H  |   | 2.643611  | 2.805835  | 1.361694  |
| H  |   | 3.757511  | 2.061847  | 0.229669  |
| H  |   | 2.100316  | 2.408716  | -0.251591 |
| O  |   | -0.953254 | 1.329173  | -0.070405 |
| C  |   | -1.111359 | 2.399058  | 0.566516  |

|   |           |           |           |
|---|-----------|-----------|-----------|
| O | -1.723357 | 3.450672  | -0.034454 |
| C | -2.194105 | 3.306160  | -1.392701 |
| H | -2.054759 | 4.198258  | 2.406722  |
| N | -0.766125 | 2.629082  | 1.797647  |
| C | -1.015056 | 3.917243  | 2.484669  |
| H | -0.410359 | 4.694494  | 2.035910  |
| C | 0.000794  | 1.625135  | 2.632485  |
| C | 0.531449  | 2.548219  | 3.748322  |
| H | 1.452527  | 3.029226  | 3.438659  |
| C | -0.568035 | 3.625002  | 3.929746  |
| H | -0.221611 | 4.521543  | 4.428851  |
| H | -1.395011 | 3.205822  | 4.491111  |
| H | 0.722169  | 1.999308  | 4.662123  |
| H | 3.041013  | 0.871158  | 3.117241  |
| H | -0.745400 | 0.955508  | 3.065825  |
| H | 1.033489  | 1.020000  | 1.809798  |
| H | 2.980048  | -0.785803 | 2.553760  |
| H | -2.931669 | 2.520910  | -1.459712 |
| H | -2.633294 | 4.257630  | -1.640575 |
| H | -1.376086 | 3.083472  | -2.059554 |

Sparteine-iPrLi-N-Mebocpyrrolidine complex 5", B3P86/6-31G\* = -1267.4853

|    |   |           |           |           |
|----|---|-----------|-----------|-----------|
| O  | 1 |           |           |           |
| C  |   | -2.256469 | 0.422900  | 3.699632  |
| C  |   | -1.151986 | 0.708571  | 2.667643  |
| N  |   | -0.966819 | -0.383444 | 1.690491  |
| C  |   | -2.242492 | -0.751869 | 1.065040  |
| C  |   | -3.363619 | -1.092617 | 2.048236  |
| C  |   | -3.574738 | 0.070593  | 3.013349  |
| H  |   | -1.479487 | 1.573223  | 2.073999  |
| H  |   | -1.967427 | -0.405025 | 4.360279  |
| H  |   | -2.379001 | 1.306055  | 4.339650  |
| H  |   | -2.552981 | 0.102844  | 0.447844  |
| H  |   | -2.047048 | -1.583771 | 0.379858  |
| H  |   | -4.281558 | -1.310358 | 1.488492  |
| H  |   | -3.115288 | -2.002323 | 2.612398  |
| H  |   | -3.939886 | 0.943268  | 2.453279  |
| H  |   | -4.343133 | -0.171924 | 3.757199  |
| C  |   | -0.228266 | -1.540784 | 2.203340  |
| H  |   | -0.032727 | -2.198094 | 1.348109  |
| H  |   | -0.822458 | -2.128801 | 2.926472  |
| C  |   | 0.187532  | 1.068354  | 3.325336  |
| C  |   | 1.085342  | -1.160931 | 2.901875  |
| C  |   | 0.786541  | -0.157237 | 4.011533  |
| H  |   | 0.102306  | -0.580752 | 4.755447  |
| H  |   | 1.709333  | 0.112941  | 4.541237  |
| H  |   | 1.497853  | -2.084743 | 3.329726  |
| C  |   | 1.222913  | 1.644159  | 2.351396  |
| H  |   | 2.066556  | 2.035319  | 2.954205  |
| H  |   | 0.795419  | 2.487199  | 1.797041  |
| N  |   | 1.732673  | 0.681349  | 1.361513  |
| C  |   | 2.178364  | -0.570639 | 1.997241  |
| H  |   | 3.032158  | -0.335664 | 2.671168  |
| C  |   | 2.837653  | 1.307287  | 0.625607  |
| H  |   | 3.644322  | 1.592027  | 1.331780  |
| H  |   | 2.455225  | 2.229260  | 0.175073  |
| C  |   | 2.697504  | -1.551418 | 0.949402  |
| H  |   | 1.886660  | -1.815923 | 0.261966  |
| H  |   | 3.021230  | -2.468879 | 1.458224  |
| C  |   | 3.406399  | 0.388903  | -0.446654 |
| H  |   | 2.636460  | 0.206577  | -1.205415 |
| H  |   | 4.242828  | 0.895100  | -0.943590 |
| C  |   | 3.848804  | -0.941811 | 0.153790  |
| H  |   | 4.183480  | -1.630008 | -0.631576 |
| H  |   | 4.709176  | -0.777304 | 0.818971  |
| H  |   | -0.017125 | 1.854900  | 4.063578  |
| Li |   | 0.026787  | 0.518073  | -0.021980 |
| C  |   | -0.872990 | 2.409013  | -0.595570 |
| H  |   | -1.207628 | 2.682784  | 0.428549  |
| C  |   | -2.146175 | 2.443160  | -1.444902 |
| H  |   | -2.625378 | 3.443606  | -1.511175 |
| C  |   | 0.026306  | 3.567042  | -1.035935 |
| H  |   | 0.473324  | 3.396272  | -2.031152 |
| H  |   | -0.492174 | 4.546800  | -1.116581 |
| H  |   | 0.873584  | 3.725374  | -0.349848 |
| O  |   | 0.238220  | -1.131400 | -1.263006 |
| C  |   | -0.160212 | -1.400963 | -2.402286 |

|   |           |           |           |
|---|-----------|-----------|-----------|
| O | -0.680867 | -2.605437 | -2.726885 |
| C | -0.726531 | -3.565272 | -1.678363 |
| N | -0.111026 | -0.576079 | -3.451626 |
| C | -0.748777 | -0.812922 | -4.744339 |
| H | -0.061348 | -1.334206 | -5.425340 |
| H | -1.638228 | -1.433332 | -4.621204 |
| C | 0.467979  | 0.769015  | -3.341688 |
| C | 0.152159  | 1.406167  | -4.701040 |
| H | 1.003403  | 1.293251  | -5.382959 |
| C | -1.044217 | 0.606215  | -5.224200 |
| H | -1.163237 | 0.665826  | -6.309741 |
| H | -1.968311 | 0.963979  | -4.756857 |
| H | -0.059555 | 2.473654  | -4.604791 |
| H | -1.959488 | 2.146560  | -2.492354 |
| H | 0.019318  | 1.291243  | -2.484256 |
| H | 1.547004  | 0.697984  | -3.163160 |
| H | -2.920749 | 1.754287  | -1.073243 |
| H | -1.063644 | -4.490022 | -2.147665 |
| H | 0.261404  | -3.705249 | -1.232796 |
| H | -1.432303 | -3.265755 | -0.899081 |

Sparteine-iPrLi-N-mebocpyrrolidine, complex 5<sup>TS</sup>, B3P86 = -1267.4597

|    |   |           |           |           |
|----|---|-----------|-----------|-----------|
| O  | 1 |           |           |           |
| C  |   | -2.218727 | -0.387698 | -3.685034 |
| C  |   | -1.146094 | -0.702653 | -2.628501 |
| N  |   | -0.946919 | 0.382274  | -1.646912 |
| C  |   | -2.225123 | 0.806718  | -1.056038 |
| C  |   | -3.308985 | 1.176505  | -2.069198 |
| C  |   | -3.538705 | 0.013048  | -3.029628 |
| H  |   | -1.520712 | -1.560566 | -2.049499 |
| H  |   | -1.889338 | 0.426325  | -4.343472 |
| H  |   | -2.355456 | -1.270283 | -4.322941 |
| H  |   | -2.589294 | -0.028982 | -0.442428 |
| H  |   | -2.010147 | 1.632750  | -0.370891 |
| H  |   | -4.230762 | 1.430613  | -1.532017 |
| H  |   | -3.017701 | 2.072612  | -2.633975 |
| H  |   | -3.945841 | -0.842373 | -2.471387 |
| H  |   | -4.281814 | 0.274364  | -3.792249 |
| C  |   | -0.164059 | 1.518419  | -2.154393 |
| H  |   | 0.036798  | 2.168021  | -1.295437 |
| H  |   | -0.735169 | 2.117264  | -2.885642 |
| C  |   | 0.196461  | -1.106711 | -3.252287 |
| C  |   | 1.146142  | 1.099972  | -2.837592 |
| C  |   | 0.838340  | 0.094226  | -3.942574 |
| H  |   | 0.176477  | 0.525088  | -4.701857 |
| H  |   | 1.761410  | -0.205994 | -4.454916 |
| H  |   | 1.584692  | 2.010374  | -3.267532 |
| C  |   | 1.198383  | -1.695310 | -2.249754 |
| H  |   | 2.039258  | -2.118144 | -2.833038 |
| H  |   | 0.741611  | -2.525052 | -1.697531 |
| N  |   | 1.726857  | -0.737694 | -1.260708 |
| C  |   | 2.217497  | 0.490734  | -1.920473 |
| H  |   | 3.058430  | 0.205031  | -2.589798 |
| C  |   | 2.825644  | -1.387271 | -0.528048 |
| H  |   | 3.604628  | -1.714973 | -1.245251 |
| H  |   | 2.423810  | -2.289135 | -0.052855 |
| C  |   | 2.781111  | 1.470869  | -0.895963 |
| H  |   | 1.991355  | 1.776515  | -0.200496 |
| H  |   | 3.126423  | 2.367306  | -1.427322 |
| C  |   | 3.449315  | -0.470370 | 0.514970  |
| H  |   | 2.707210  | -0.249779 | 1.289960  |
| H  |   | 4.275949  | -1.000664 | 1.002634  |
| C  |   | 3.926708  | 0.834360  | -0.113761 |
| H  |   | 4.296090  | 1.520084  | 0.657486  |
| H  |   | 4.769573  | 0.633384  | -0.791119 |
| H  |   | -0.012662 | -1.899161 | -3.982907 |
| Li |   | 0.088846  | -0.321139 | 0.127578  |
| C  |   | -1.003972 | -2.217175 | 0.877586  |
| H  |   | -1.167965 | -2.013167 | -0.197117 |
| C  |   | -2.367747 | -2.246559 | 1.557610  |
| H  |   | -3.002747 | -3.092974 | 1.246825  |
| C  |   | -0.307805 | -3.568082 | 0.997579  |
| H  |   | 0.024803  | -3.739214 | 2.031552  |
| H  |   | -0.947876 | -4.424198 | 0.725084  |
| H  |   | 0.592604  | -3.629988 | 0.369993  |
| O  |   | 0.164170  | 1.311117  | 1.135665  |
| C  |   | -0.178041 | 1.459168  | 2.333803  |

|   |           |           |          |
|---|-----------|-----------|----------|
| O | -0.626637 | 2.659255  | 2.791962 |
| C | -0.684870 | 3.701001  | 1.833004 |
| N | -0.114648 | 0.527066  | 3.266589 |
| C | -0.601801 | 0.704024  | 4.632275 |
| H | 0.191543  | 1.128889  | 5.264170 |
| H | -1.455695 | 1.384401  | 4.657745 |
| C | 0.378177  | -0.837724 | 2.999418 |
| C | 0.156295  | -1.549029 | 4.342341 |
| H | 1.060923  | -1.561327 | 4.972821 |
| C | -0.929488 | -0.726879 | 5.045904 |
| H | -0.940344 | -0.854813 | 6.132843 |
| H | -1.920096 | -0.996303 | 4.661436 |
| H | -0.152650 | -2.593632 | 4.222872 |
| H | -2.247691 | -2.327400 | 2.647863 |
| H | -0.290249 | -1.429650 | 1.786695 |
| H | 1.454984  | -0.766060 | 2.784880 |
| H | -2.940518 | -1.326031 | 1.378670 |
| H | -1.002407 | 4.586994  | 2.385211 |
| H | 0.293056  | 3.876284  | 1.375826 |
| H | -1.410259 | 3.480977  | 1.043098 |

Sparteine - tBuLi -N-bocpyrrolidine complex 3, B3P86/6-31G\* = -1425.3289

|    |   |           |           |           |
|----|---|-----------|-----------|-----------|
| O  | 1 |           |           |           |
| C  |   | 2.994223  | -1.853970 | 2.225210  |
| C  |   | 1.623779  | -1.374074 | 1.712148  |
| N  |   | 1.352976  | 0.054075  | 1.977417  |
| C  |   | 2.474087  | 0.907207  | 1.560843  |
| C  |   | 3.838887  | 0.493092  | 2.111690  |
| C  |   | 4.129703  | -0.957247 | 1.738011  |
| H  |   | 1.635813  | -1.470070 | 0.615013  |
| H  |   | 3.005102  | -1.872284 | 3.322542  |
| H  |   | 3.149849  | -2.889522 | 1.895359  |
| H  |   | 2.516634  | 0.886289  | 0.465524  |
| H  |   | 2.225062  | 1.936039  | 1.835220  |
| H  |   | 4.606223  | 1.165757  | 1.709428  |
| H  |   | 3.865861  | 0.607373  | 3.203860  |
| H  |   | 4.219010  | -1.038622 | 0.644309  |
| H  |   | 5.087532  | -1.289993 | 2.155724  |
| C  |   | 0.943914  | 0.353229  | 3.355303  |
| H  |   | 0.627955  | 1.402464  | 3.371803  |
| H  |   | 1.787635  | 0.266402  | 4.063279  |
| C  |   | 0.483071  | -2.255995 | 2.247349  |
| C  |   | -0.174316 | -0.555906 | 3.869883  |
| C  |   | 0.270893  | -2.008496 | 3.739088  |
| H  |   | 1.182561  | -2.194944 | 4.317881  |
| H  |   | -0.500766 | -2.684918 | 4.129148  |
| H  |   | -0.329428 | -0.303524 | 4.927474  |
| C  |   | -0.854755 | -2.057603 | 1.529480  |
| H  |   | -1.541276 | -2.855336 | 1.877522  |
| H  |   | -0.725055 | -2.182522 | 0.449135  |
| N  |   | -1.469896 | -0.741650 | 1.746226  |
| C  |   | -1.534435 | -0.392073 | 3.179116  |
| H  |   | -2.213872 | -1.116985 | 3.679637  |
| C  |   | -2.825979 | -0.753726 | 1.184056  |
| H  |   | -3.436784 | -1.521785 | 1.701279  |
| H  |   | -2.749981 | -1.057986 | 0.135584  |
| C  |   | -2.142528 | 0.995492  | 3.356041  |
| H  |   | -1.507494 | 1.741652  | 2.864764  |
| H  |   | -2.168740 | 1.235761  | 4.426871  |
| C  |   | -3.500882 | 0.604986  | 1.300386  |
| H  |   | -2.938898 | 1.334737  | 0.704106  |
| H  |   | -4.511525 | 0.542234  | 0.878629  |
| C  |   | -3.543247 | 1.062662  | 2.755286  |
| H  |   | -3.941354 | 2.081060  | 2.826751  |
| H  |   | -4.221038 | 0.411997  | 3.327576  |
| H  |   | 0.778506  | -3.299675 | 2.074053  |
| Li |   | -0.236232 | 0.713603  | 0.532241  |
| C  |   | -0.450744 | 2.825095  | 0.030858  |
| C  |   | -1.301886 | 2.920462  | -1.233888 |
| H  |   | -1.408364 | 3.968927  | -1.602593 |
| C  |   | 0.883785  | 3.482136  | -0.312784 |
| H  |   | 1.436868  | 2.940541  | -1.098143 |
| H  |   | 0.759840  | 4.522675  | -0.697449 |
| H  |   | 1.557094  | 3.562951  | 0.554264  |
| O  |   | -0.173172 | -0.528622 | -1.321576 |
| C  |   | 0.065187  | -0.471711 | -2.532331 |
| O  |   | -0.784714 | -0.791006 | -3.525738 |