ELECTRONIC SUPPLEMENTARY INFORMATION

DFT investigation of hydrogen atom–abstraction reactions of NHC–boranes by various carbon–centered radicals: barriers and correlation analyses

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Table S10 List of Cartesian coordinates of located stationary points at the B3LYP/6-311++G(d,p) in BTF at 376 K.
Comparison and explanation of methods

The theoretical methods often used in the available computations of NHC-boranes (H-abstraction, addition, cyclization, complexation, etc.) are B3LYP\cite{1} and M06-2X\cite{2} with the 6-31+G(d) – 6-311++G(d,p) basis sets. Another example involved the B3PW91 method\cite{3}. Considering of the possible existence of weak interaction or other non-covalent interactions in transition states, we employed the two methods, B3LYP and M06-2X, combined with the 6-311++G(d,p) basis set to obtain the data and results in the original manuscript. Based on the referee’s review report, we further tested another two levels of theory, B3LYP-D3BJ/6-311++G(2d,2p) and ωB97DX/6-311++G(2d,2p). The results were analyzed along with the B3LYP- and M06-2X-computed results.

As shown in Fig. S19, the results at the B3LYP level have high linear correlations with those at the M06-2X ((a) and (b)), B3LYP-D3BJ ((c) and (d)), and ωB97DX ((e) and (f)) levels, R^2 varies in the ranges of 0.88–0.97 for kinetic barriers and 0.98–1.00 for thermodynamic reaction energies, reaction enthalpies, and reaction Gibbs free energies. Clearly, the transition states are more method-dependent than the minimum structures. A similar pattern was reflected in the correlation analysis among the B3LYP-D3BJ-, ωB97DX-, and M06-2X-computed results, as shown in Fig. S20.

The results indicate that the M06-2X, B3LYP-D3BJ, and ωB97DX methods gave a slightly different ordering of barriers to the H-atom abstractions by those reactant radicals with close nucleophilicity or electrophilicity index from the B3LYP method. Although this difference, we found that the results at the four levels of theory keep good consistence in predicting the statistical correlations of different physical quantities investigated in this study. Furthermore, the B3LYP-D3BJ and ωB97DX methods, the newly tested methods, did not improve those correlations relative to the B3LYP and M06-2X methods, but keep consistence with the B3LYP and M06-2X methods. It seems that such a result is closely related to the statistical nature of correlation analysis. Based on the assessment of different methods to the statistical correlations investigated in this study, we described the results using the B3LYP-computed data.
**Figure S1** Thermal contributions ($\Delta E_{\text{therm}}$) of the H-abstraction reactions by various radical reactants.

**Figure S2** Global nucleophilic (N) and electrophilic ($\omega$), and local nucleophilic ($N_C$) and electrophilic ($\omega_C$) indexes of radical reactants.
Figure S3 Plot of local nucleophilic index ($N_C$) vs spin density ($\rho_{s,C}$) for the attacking radicals.

$R^2 = 0.42$
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**Figure S5** Intrinsic barrier distribution of the H-abstraction reactions by various radical reactants.
**Figure S6** Change of percentages of intrinsic barrier ($\Delta E^*$) and thermal contribution ($\Delta E_{\text{therm}}^*$) in activation barrier ($\Delta E^*$) with increasing activation barrier for the H-abstraction reactions of NHC-BH$_3$ (a) and NHC-BH$_2$CN (b) by different radicals.
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Figure S8 Linear dependences of activation barrier ($\Delta E^*$) on intrinsic barrier ($\Delta E_0^*$) and thermal contribution ($\Delta E_{\text{therm}}^*$) (a) and plots of nucleophilic/electrophilic indexes vs activation barrier ($\Delta E^*$) for the H-abstraction reactions of NHC-BH$_3$ (b) and NHC-BH$_2$CN (c).
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**Figure S11** Bar chart of free energy barrier ($\Delta G^*$) and its three components, intrinsic barrier ($\Delta E^*_0$), thermal contribution ($\Delta E_{\text{therm}}^*$), and activation Gibbs free energy thermal correction ($\Delta G_{\text{corr}}^*$) for the H-abstraction reactions of NHC-BH$_3$ (a) and NHC-BH$_2$CN (b).
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Figure S14 Plots of global/local nucleophilic and electrophilic indexes of radical reactants vs free energy barriers ($\Delta G^*$) of H-abstraction reactions of NHC-BH$_3$ (a) and NHC-BH$_2$CN (b).
Figure S15 Analysis of linear dependences of thermal contribution ($\Delta E_{\text{therm}}^a$) on global nucleophilic ($N$), global electrophilic ($\omega$), local nucleophilic ($N_C$), and local electrophilic ($\omega_C$) indexes for the radicals of types I (a), II (b), III (c), and IV (d).
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**Figure S19** Correlation analysis of the kinetic and thermodynamic quantities of the H-abstraction reactions computed at the B3LYP/6-311++G(d,p) level with those computed at the B3LYP-D3BJ/6-311++G(2d,2p), ωB97DX/6-311++G(2d,2p), and M06-2X/6-311++G(d,p) levels of theory.
Figure S20 Correlation analysis of the kinetic and thermodynamic quantities of the H- abstraction reactions computed at the B3LYP-D3BJ/6-311++G(2d,2p), oB97X-D/6-311++G(2d,2p), and M06-2X/6-311++G(d,p).
Table S1: Total electronic energies (E, hartree), zero-point vibrational energies (ZPVE, hartree/particle), Gibbs free energies (G, hartree), enthalpies (H, hartree), thermal corrections to Gibbs free energy (G_corr, hartree), and thermal corrections to enthalpy (H_corr, hartree) of the structures of NHC-boranes, NHC-boryl radicals, and RH optimized at the B3LYP/6-31++G(d,p) in BTF at 376 K.

| Species      | E    | ZPVE  | G     | H     | G_corr | H_corr |
|--------------|------|-------|-------|-------|--------|--------|
| NHC-BH₃      | -331.598609 | 0.158913 | -331.484030 | -331.425269 | 0.114579 | 0.173340 |
| NHC-BH₂CN    | -423.905043 | 0.160229 | -423.795270 | -423.727771 | 0.109773 | 0.177272 |
| NHC-'BH₂     | -330.964966 | 0.148261 | -330.862962 | -330.802167 | 0.102004 | 0.162799 |
| NHC-B(')HCN  | -423.272422 | 0.149815 | -423.171992 | -423.106003 | 0.100429 | 0.166419 |
| CH₃NH₂       | -95.897929  | 0.063749  | -95.864445  | -95.828249  | 0.033484  | 0.069680 |
| CH₃CH=CF₂    | -316.484166 | 0.064019  | -316.457081 | -316.412112 | 0.027085  | 0.072054 |
| CH₃CH=CH₂    | -117.943653 | 0.078694  | -117.897366 | -117.858640 | 0.046287  | 0.085013 |
| CH(CH₃)₃     | -158.506768 | 0.130566  | -158.413172 | -158.366466 | 0.093596  | 0.140302 |
| CH₃N=CH₂     | -133.987655 | 0.067831  | -133.952565 | -133.913130 | 0.035090  | 0.074525 |
| CH₃Ph        | -271.641327 | 0.127177  | -271.555484 | -271.503397 | 0.085843  | 0.137930 |
| CH₃(CH₃)₂    | -119.181329 | 0.102610  | -119.112854 | -119.070887 | 0.068475  | 0.110441 |
| CH₃SH        | -438.746659 | 0.045838  | -438.732807 | -438.694630 | 0.013852  | 0.052029 |
| CH₃(CH₂)₂CH₃ | -158.505777 | 0.131047  | -158.412155 | -158.365013 | 0.093622  | 0.140764 |
| CH₃CH₂CH₂    | -119.181329 | 0.102610  | -119.112854 | -119.070887 | 0.068475  | 0.110441 |
| CH₃(CH₂)CN   | -172.127753 | 0.074022  | -172.089132 | -172.045820 | 0.038621  | 0.081933 |
| CH₃(CH₂)₃CN  | -250.777106 | 0.130729  | -250.688464 | -250.634495 | 0.088642  | 0.142611 |
| CH₃(CH₂)₄CN  | -211.452603 | 0.102318  | -211.389053 | -211.340395 | 0.063550  | 0.112208 |
| CH₃CH₃       | -79.856731  | 0.074104  | -79.813149  | -79.776540  | 0.043582  | 0.080192 |
| CH₃CH₂CN     | -172.127753 | 0.074022  | -172.089132 | -172.045820 | 0.038621  | 0.081933 |
| CH₃F         | -139.794816 | 0.038960  | -139.784071 | -139.750795 | 0.010745  | 0.044021 |
| CH₃OH        | -115.770082 | 0.051011  | -115.749106 | -115.713333 | 0.020976  | 0.056749 |
| CH₄          | -40.534131  | 0.044375  | -40.512734  | -40.484839  | 0.013297  | 0.049292 |
| CH₃CN        | -132.803769 | 0.045139  | -132.790282 | -132.752464 | 0.013486  | 0.051305 |
| CH₃CHO       | -153.886044 | 0.054893  | -153.863150 | -153.825413 | 0.022894  | 0.060631 |
| CH₃COOH      | -229.170954 | 0.061207  | -229.144045 | -229.103078 | 0.026909  | 0.067876 |
| CH₃F₂        | -239.070606 | 0.032416  | -239.070483 | -239.032706 | 0.000123  | 0.037900 |
| CH₃CF₃       | -377.690108 | 0.051636  | -377.675409 | -377.630156 | 0.014699  | 0.059952 |
| CH₃Cl        | -500.154807 | 0.037606  | -500.146974 | -500.111927 | 0.007833  | 0.042880 |
| CH₃OCH₃      | -155.080308 | 0.079196  | -155.034880 | -155.099376 | 0.045428  | 0.086552 |
| CH₃SCH₃      | -478.070995 | 0.075381  | -478.030670 | -478.096537 | 0.039425  | 0.083558 |
| CH₃NHMe      | -135.212683 | 0.091900  | -135.154595 | -135.113244 | 0.058088  | 0.099439 |
| CH₃NCOH      | -209.280668 | 0.073937  | -209.242695 | -209.198591 | 0.037973  | 0.082077 |
| CH₃COMe      | -193.223673 | 0.083020  | -193.176150 | -193.132895 | 0.047523  | 0.090778 |
| CH₃CONH₂     | -209.299005 | 0.073290  | -209.262444 | -209.217257 | 0.036561  | 0.081748 |
| CH₃CF₂H      | -278.407490 | 0.059916  | -278.382939 | -278.340122 | 0.024551  | 0.067368 |
| CH₃CFH₂      | -179.126891 | 0.067463  | -179.092678 | -179.052737 | 0.034213  | 0.074154 |
Table S2 Total electronic energies (E, hartree), zero-point vibrational energies (ZPVE, hartree/particle), Gibbs free energies (G, hartree), enthalpies (H, hartree), thermal corrections to Gibbs free energy (G$_{\text{corr}}$, hartree), and thermal corrections to enthalpy (H$_{\text{corr}}$, hartree) of the structures of the attacking radical R$^*$ optimized at the B3LYP/6-311++G(d,p) in BTF at 376 K.

| Species       | E       | ZPVE    | G       | H       | G$_{\text{corr}}$ | H$_{\text{corr}}$ |
|---------------|---------|---------|---------|---------|------------------|------------------|
| t-CH$_2$NH$_2$ | -95.241889 | 0.049797 | -95.222676 | -95.186061 | 0.019213 | 0.055828 |
| t-CH$_2$CH=CF$_2$ | -315.837554 | 0.050937 | -315.824789 | -315.777889 | 0.012765 | 0.072054 |
| t-CH$_2$=CH$_2$ | -117.299714 | 0.065741 | -117.267183 | -117.227178 | 0.032531 | 0.072536 |
| t-Bu        | -157.846072 | 0.115648 | -157.769752 | -157.720047 | 0.076321 | 0.126026 |
| t-CH$_2$N=CH$_2$ | -133.338363 | 0.053481 | -133.317900 | -133.278244 | 0.020463 | 0.060119 |
| t-CH$_2$Ph   | -270.989971 | 0.114088 | -270.915484 | -270.865727 | 0.074488 | 0.124245 |
| t-Pr        | -118.515994 | 0.087250 | -118.465036 | -118.420183 | 0.050958 | 0.095811 |
| t-CH$_3$SH   | -438.083398 | 0.031135 | -438.085822 | -438.045451 | -0.002420 | 0.037947 |
| t-^Bu       | -157.834182 | 0.116177 | -157.757574 | -157.707679 | 0.076608 | 0.126503 |
| t-^Pr       | -118.509910 | 0.087605 | -118.457793 | -118.414023 | 0.052118 | 0.095888 |
| (t-CH$_3$)CN | -171.473467 | 0.059786 | -171.450504 | -171.405552 | 0.022963 | 0.067915 |
| (t-CH$_3$)CN | -250.104950 | 0.115937 | -250.033139 | -249.976589 | 0.071811 | 0.128361 |
| (t-CH$_3$)CN | -210.779804 | 0.087401 | -210.733808 | -210.681898 | 0.045996 | 0.097906 |
| Et         | -79.185621 | 0.058826 | -79.158902 | -79.120105 | 0.026720 | 0.065516 |
| (t-CH$_3$)CN | -171.452840 | 0.058623 | -171.431393 | -171.385732 | 0.021447 | 0.067109 |
| t-CH$_2$F   | -139.121735 | 0.024305 | -139.127406 | -139.092110 | -0.005671 | 0.029625 |
| t-CH$_2$OH  | -115.099005 | 0.035103 | -115.094104 | -115.058418 | 0.049014 | 0.040587 |
| Me        | -39.855770 | 0.029550 | -39.852370 | -39.821029 | 0.003401 | 0.034741 |
| t-CH$_2$CN  | -132.139999 | 0.030847 | -132.141013 | -132.103102 | -0.001014 | 0.036897 |
| t-CH$_2$CHO | -153.228686 | 0.042493 | -153.218992 | -153.180050 | 0.009694 | 0.048636 |
| t-CH$_2$COOH | -228.505685 | 0.047944 | -228.493222 | -228.450361 | 0.012463 | 0.055324 |
| t-CH$_2$F   | -238.397362 | 0.018751 | -238.414131 | -238.373203 | -0.014069 | 0.024159 |
| t-CH$_2$CF$_3$ | -377.011042 | 0.036845 | -377.012725 | -376.965454 | -0.001683 | 0.045588 |
| t-CH$_2$Cl  | -499.483265 | 0.022436 | -499.493153 | -499.454860 | -0.009890 | 0.042880 |
| t-CH$_2$OCH$_3$ | -154.417897 | 0.065290 | -154.387158 | -154.345045 | 0.030739 | 0.072852 |
| t-CH$_2$SCH$_3$ | -477.409204 | 0.061023 | -477.385380 | -477.339551 | 0.023824 | 0.069653 |
| t-CH$_2$NHMe | -134.558203 | 0.078186 | -134.514558 | -134.472272 | 0.043645 | 0.085931 |
| t-CH$_2$NHCIGNH$_2$ | -208.621437 | 0.059738 | -208.597847 | -208.553471 | 0.023590 | 0.067966 |
| t-CH$_2$CONH$_2$ | -192.569282 | 0.070095 | -192.530397 | -192.484412 | 0.032585 | 0.078570 |
| t-CH$_2$CF$_2$H | -208.632887 | 0.059205 | -208.610732 | -208.565140 | 0.022155 | 0.067747 |
| t-CH$_2$CF$_2$H | -277.730770 | 0.045151 | -277.723055 | -277.676769 | 0.007715 | 0.053121 |
| t-CH$_2$CFH$_2$ | -179.126891 | 0.067463 | -179.092678 | -179.052737 | 0.034213 | 0.060035 |
Table S3 Spin densities ($\rho_{c}, e$) on the central C atoms, global nucleophilic ($N_{c}$, eV) and electrophilic indices ($\omega_{c}$, eV), and local nucleophilic ($\omega_{c}$, eV) and electrophilic indices ($\omega_{c}$, eV) of the attacking radical $R^\ast$ and NHC-boranes computed at the mpwpw91/6-311+G(d,p) in BTF.

| Species          | $\rho_{c}$ | $\omega$ | $\omega_{c}$ | N      | $N_{c}$ |
|------------------|------------|----------|--------------|--------|--------|
| $^\circ$CH$_2$NH$_2$ | 0.89       | 7.41     | 6.60         | 7.87   | 7.00   |
| $^\circ$CH$_3$CH=CF$_2$ | 0.71       | 21.50    | 15.27        | 6.58   | 4.67   |
| $^\circ$CH$_3$CH=CH$_2$ | 0.68       | 21.56    | 14.66        | 6.34   | 4.31   |
| $^\circ$Bu       | 0.95       | 8.50     | 8.08         | 7.33   | 6.97   |
| $^\circ$CH$_3$N=CH$_2$ | 0.66       | 23.38    | 15.43        | 5.91   | 3.90   |
| $^\circ$CH$_3$Ph  | 0.79       | 27.05    | 21.37        | 6.59   | 5.21   |
| $^\circ$Pr       | 1.03       | 9.57     | 9.85         | 7.01   | 7.22   |
| $^\circ$CH$_3$SH | 0.90       | 13.62    | 12.26        | 7.04   | 6.34   |
| $^\circ$Bu       | 1.13       | 12.01    | 13.57        | 6.47   | 7.31   |
| $^\circ$Pr       | 1.11       | 11.56    | 12.84        | 6.50   | 7.22   |
| $^\circ$CH(CH$_3$)CN | 0.82       | 31.72    | 26.01        | 5.44   | 4.46   |
| $^\circ$(CH$_3$)$_2$CN | 1.13       | 13.49    | 15.24        | 6.23   | 7.04   |
| $^\circ$(CH$_3$)$_3$CN | 1.12       | 14.88    | 16.66        | 5.99   | 6.71   |
| Et               | 1.10       | 11.31    | 12.44        | 6.49   | 7.14   |
| $^\circ$(CH$_2$)$_2$CN | 1.10       | 14.69    | 16.16        | 5.86   | 6.45   |
| $^\circ$CH$_3$F  | 1.04       | 13.10    | 13.62        | 6.11   | 6.35   |
| $^\circ$CH$_3$OH | 1.06       | 11.69    | 12.39        | 6.39   | 6.78   |
| Me               | 1.15       | 13.97    | 16.06        | 5.68   | 6.54   |
| $^\circ$CH$_2$CN | 0.87       | 34.90    | 30.37        | 4.78   | 4.16   |
| $^\circ$CH$_2$CHO | 0.84       | 43.45    | 36.50        | 4.77   | 4.00   |
| $^\circ$CH$_2$COOH | 0.96       | 33.13    | 31.81        | 4.69   | 4.51   |
| $^\circ$CH$_2$F  | 0.90       | 15.85    | 14.26        | 5.66   | 5.09   |
| $^\circ$CH$_2$CF$_3$ | 1.08       | 23.85    | 25.76        | 4.65   | 5.02   |
| $^\circ$CH$_2$Cl | 1.00       | 16.03    | 16.03        | 6.13   | 6.13   |
| $^\circ$CH$_2$OCH$_3$ | 0.95       | 10.42    | 9.90         | 7.25   | 6.88   |
| $^\circ$CH$_2$SCH$_3$ | 0.85       | 14.25    | 12.11        | 7.22   | 6.14   |
| $^\circ$CH$_2$NHMe | 0.87       | 8.04     | 7.00         | 8.01   | 6.97   |
| $^\circ$CH$_2$NCOH | 0.89       | 16.77    | 14.92        | 6.99   | 6.22   |
| $^\circ$CH$_2$COMe | 0.90       | 37.13    | 33.42        | 5.00   | 4.50   |
| $^\circ$CH$_2$CONH$_2$ | 0.98       | 27.83    | 27.27        | 5.15   | 5.05   |
| $^\circ$CH$_2$CF$_3$H | 1.07       | 22.38    | 23.95        | 4.98   | 5.33   |
| $^\circ$CH$_2$CFH$_2$ | 1.06       | 20.75    | 21.99        | 5.29   | 5.60   |
| NHC-BH$_1$       | /          | 4.61     | /            | 5.39   | /      |
| NHC-BH$_2$CN     | /          | 6.14     | /            | 4.84   | /      |
Table S4 Total electronic energies (E, hartree), zero-point vibrational energies (ZPVE, hartree/particle), Gibbs free energies (G, hartree), enthalpies (H, hartree), thermal corrections to Gibbs free energy (G\text{corr}, hartree), and thermal corrections to enthalpy (H\text{corr}, hartree) of the transition states (TS) of the H-atom abstraction reactions of NHC-BH\textsubscript{3} by R’ optimized at the B3LYP/6-311++G(d,p) in BTF at 376 K.

| TS   | R’        | E       | ZPVE   | G      | H      | G\text{corr} | H\text{corr} |
|------|-----------|---------|--------|--------|--------|--------------|--------------|
| TS1  | ‘CH\textsubscript{2}NH\textsubscript{2} | -426.816451 | 0.206641 | -426.666498 | -426.588998 | 0.149953 | 0.227453 |
| TS2  | ‘CH\textsubscript{2}CH=CF\textsubscript{2} | -647.414469 | 0.208130 | -647.269559 | -647.182587 | 0.144910 | 0.231882 |
| TS3  | ‘CH\textsubscript{2}CH=CH\textsubscript{2} | -448.857976 | 0.223163 | -448.712458 | -448.631106 | 0.163518 | 0.244870 |
| TS4  | ‘Bu       | -489.427749 | 0.273155 | -489.216453 | -489.129628 | 0.211296 | 0.298120 |
| TS5  | ‘CH\textsubscript{2}N=CH\textsubscript{2} | -464.919843 | 0.211902 | -464.765727 | -464.686783 | 0.154116 | 0.233060 |
| TS6  | ‘CH\textsubscript{2}Ph  | -602.570213 | 0.271349 | -602.363553 | -602.273572 | 0.206660 | 0.296641 |
| TS7  | ‘Pr       | -450.098514 | 0.245329 | -449.913550 | -449.830261 | 0.184964 | 0.268253 |
| TS8  | ‘CH\textsubscript{2}SH  | -769.666686 | 0.189545 | -769.535709 | -769.456322 | 0.130977 | 0.210364 |
| TS9  | ‘Bu       | -489.418979 | 0.274016 | -489.209102 | -489.120144 | 0.209877 | 0.298835 |
| TS10 | ‘Pr       | -450.094485 | 0.245685 | -449.910453 | -449.825982 | 0.184032 | 0.268503 |
| TS11 | ‘CH(CH\textsubscript{3})CN | -503.060776 | 0.217839 | -502.903934 | -502.820144 | 0.156842 | 0.240632 |
| TS12 | ‘(CH\textsubscript{2})\textsubscript{4}CN | -581.691095 | 0.273669 | -581.486598 | -581.390428 | 0.204497 | 0.300667 |
| TS13 | ‘(CH\textsubscript{2})\textsubscript{2}CN | -542.366977 | 0.245301 | -542.187677 | -542.096651 | 0.179300 | 0.270326 |
| TS14 | ‘Et       | -410.770134 | 0.216844 | -410.612824 | -410.532177 | 0.157310 | 0.237957 |
| TS15 | ‘(CH\textsubscript{2})\textsubscript{2}CN | -503.043135 | 0.217095 | -502.885557 | -502.804212 | 0.157577 | 0.238922 |
| TS16 | ‘CH\textsubscript{2}F  | -470.710394 | 0.182348 | -470.585206 | -470.508367 | 0.125188 | 0.202027 |
| TS17 | ‘CH\textsubscript{2}OH  | -446.895131 | 0.194601 | -446.715776 | -446.647432 | 0.137737 | 0.214781 |
| TS18 | ‘Me       | -371.443995 | 0.188197 | -371.312926 | -371.236539 | 0.131069 | 0.207456 |
| TS19 | ‘CH\textsubscript{2}CN | -463.734286 | 0.189598 | -463.602989 | -463.520424 | 0.131297 | 0.210262 |
| TS20 | ‘CH\textsubscript{2}CHO | -484.825349 | 0.201410 | -484.681719 | -484.603283 | 0.143630 | 0.220666 |
| TS21 | ‘CH\textsubscript{2}COOH | -560.102537 | 0.206555 | -559.956590 | -559.873860 | 0.145947 | 0.228677 |
| TS22 | ‘CH\textsubscript{2}F\textsubscript{3} | -569.899294 | 0.175505 | -569.875130 | -569.793906 | 0.114794 | 0.196018 |
| TS23 | ‘CH\textsubscript{2}CF\textsubscript{3} | -708.608259 | 0.195327 | -708.478465 | -708.389448 | 0.129794 | 0.218811 |
| TS24 | ‘CH\textsubscript{2}Cl  | -831.072538 | 0.181262 | -830.950469 | -830.871258 | 0.122069 | 0.201280 |
| TS25 | ‘CH\textsubscript{2}OCH\textsubscript{3} | -485.999459 | 0.222603 | -485.837356 | -485.754702 | 0.162103 | 0.244757 |
| TS26 | ‘CH\textsubscript{2}SCH\textsubscript{3} | -808.990728 | 0.218940 | -808.837374 | -808.748789 | 0.156954 | 0.241939 |
| TS27 | ‘CH\textsubscript{2}NHMe | -466.131480 | 0.234713 | -465.957303 | -465.874083 | 0.174177 | 0.257397 |
| TS28 | ‘CH\textsubscript{2}NCOH | -540.203977 | 0.217536 | -540.048413 | -539.963665 | 0.155564 | 0.240312 |
| TS29 | ‘CH\textsubscript{2}COMe | -524.158408 | 0.228758 | -523.991320 | -523.906571 | 0.167088 | 0.251837 |
| TS30 | ‘CH\textsubscript{2}CONH\textsubscript{2} | -540.226637 | 0.218068 | -540.068869 | -539.985794 | 0.157768 | 0.240843 |
| TS31 | ‘CH\textsubscript{2}CF\textsubscript{3}H | -609.324635 | 0.203358 | -609.183038 | -609.098829 | 0.141597 | 0.225806 |
| TS32 | ‘CH\textsubscript{2}CF\textsubscript{2}H | -510.044323 | 0.210797 | -509.894053 | -509.811809 | 0.150270 | 0.232514 |
Table S5 Total electronic energies (E, hartree), zero-point vibrational energies (ZPVE, hartree/particle), Gibbs free energies (G, hartree), enthalpies (H, hartree), thermal corrections to Gibbs free energy (G_{corr}, hartree), and thermal corrections to enthalpy (H_{corr}, hartree) of the transition states (TS) of the H-atom abstraction reactions of NHCH2CN by R' optimized at the B3LYP/6-311++G(d,p) in BTF at 376 K.

| TS   | R'       | E       | ZPVE   | G       | H       | G_{corr} | H_{corr} |
|------|----------|---------|--------|---------|---------|----------|----------|
| TS33 | ‘CH2NH2  | -519.125015 | 0.207962 | -518.977746 | -518.893853 | 0.147269 | 0.231162 |
| TS34 | ‘CH2CH=CF2 | -739.719650 | 0.209222 | -739.578081 | -739.484207 | 0.141569 | 0.235443 |
| TS35 | ‘CH2CH=CH2 | -541.180978 | 0.224435 | -541.018726 | -540.932483 | 0.162252 | 0.248495 |
| TS36 | ‘Bu        | -581.734877 | 0.274458 | -581.526187 | -581.432960 | 0.208690 | 0.301917 |
| TS37 | ‘CH3N=CH2 | -557.223429 | 0.212907 | -557.072909 | -556.986858 | 0.150520 | 0.236571 |
| TS38 | ‘CH2Ph     | -694.875263 | 0.272455 | -694.671260 | -694.570575 | 0.204003 | 0.300187 |
| TS39 | ‘Pr        | -542.405651 | 0.246565 | -542.232707 | -542.133730 | 0.181944 | 0.271922 |
| TS40 | ‘CH2SH     | -861.972673 | 0.190635 | -861.845716 | -861.758754 | 0.126957 | 0.213919 |
| TS41 | ‘Bu        | -581.725623 | 0.275282 | -581.518726 | -581.423130 | 0.206897 | 0.302493 |
| TS42 | ‘Pr        | -542.401037 | 0.247025 | -542.219205 | -542.128820 | 0.181833 | 0.272217 |
| TS43 | ‘CH(CH3)CN | -595.363769 | 0.218935 | -595.209157 | -595.119649 | 0.154612 | 0.244120 |
| TS44 | (CH2)3CN   | -673.997262 | 0.275096 | -673.847787 | -673.759273 | 0.203487 | 0.304389 |
| TS45 | (CH2)2CN   | -634.672876 | 0.246742 | -634.495149 | -634.398858 | 0.177727 | 0.274018 |
| TS46 | Et         | -503.076804 | 0.218388 | -502.920661 | -502.835111 | 0.156142 | 0.241693 |
| TS47 | (CH2)2CN   | -595.347909 | 0.218434 | -595.195599 | -595.104170 | 0.152309 | 0.243738 |
| TS48 | ‘CH3F      | -563.015949 | 0.183576 | -562.894630 | -562.810329 | 0.121319 | 0.205620 |
| TS49 | ‘CH3OH     | -538.966589 | 0.195951 | -538.861122 | -538.778919 | 0.153467 | 0.218570 |
| TS50 | Me         | -463.749830 | 0.189518 | -463.619946 | -463.538794 | 0.129884 | 0.211036 |
| TS51 | ‘CH2CN     | -556.036572 | 0.190610 | -555.907333 | -555.823012 | 0.129239 | 0.213560 |
| TS52 | ‘CH2CHO    | -577.126905 | 0.201845 | -576.986001 | -576.901966 | 0.140904 | 0.224939 |
| TS53 | ‘CH2COOH   | -652.404420 | 0.207333 | -652.261248 | -652.172624 | 0.143172 | 0.231796 |
| TS54 | ‘CHF2      | -662.294432 | 0.176776 | -662.180464 | -662.094908 | 0.113968 | 0.199524 |
| TS55 | ‘CH3CF3    | -800.911570 | 0.196397 | -800.781436 | -800.689513 | 0.130134 | 0.225057 |
| TS56 | ‘CH3Cl     | -923.377425 | 0.182407 | -923.253767 | -923.172672 | 0.120058 | 0.204753 |
| TS57 | ‘CH3OCH3   | -578.306064 | 0.223870 | -578.147563 | -578.058139 | 0.159041 | 0.248465 |
| TS58 | ‘CH3SCH3   | -901.297163 | 0.220172 | -901.142345 | -901.051595 | 0.154818 | 0.245568 |
| TS59 | ‘CH2NHMe   | -558.440044 | 0.235952 | -558.268637 | -558.178875 | 0.171407 | 0.261169 |
| TS60 | ‘CH2NCOH   | -632.590691 | 0.218903 | -632.355387 | -632.265700 | 0.154304 | 0.243991 |
| TS61 | ‘CH2COME   | -616.460429 | 0.229441 | -616.295831 | -616.205469 | 0.164598 | 0.254960 |
| TS62 | ‘CH2CONH2  | -632.529673 | 0.218396 | -632.377556 | -632.285622 | 0.152117 | 0.244051 |
| TS63 | ‘CH2CF2H   | -701.628736 | 0.204503 | -701.488902 | -701.394956 | 0.139834 | 0.229280 |
| TS64 | ‘CH2CFH2   | -602.348647 | 0.211989 | -602.209958 | -602.112573 | 0.147689 | 0.236074 |
Table S6  Activation barrier ($\Delta E^*$), activation zero-point vibrational energy correction ($\Delta E_{ZPV}^*$), intrinsic barrier ($\Delta E_i^*$), thermal contribution ($\Delta E_{therm}^*$), activation Gibbs free energy correction ($\Delta G_{corr}^*$), and Gibbs free energy barrier ($\Delta G^*$) of the H-atom abstraction reactions of NHC-BH$_3$ by R’ computed at the B3LYP/6-311++G(d,p) in BTF at 376 K. All units are in kcal mol$^{-1}$.

| R’  | $\Delta E^*$ | $\Delta E_{ZPV}^*$ | $\Delta E_i^*$ | $\Delta E_{therm}^*$ | $\Delta G_{corr}^*$ | $\Delta G^*$ |
|-----|--------------|-------------------|---------------|-----------------|------------------|---------|
| ‘CH$_2$NH$_2$ | 13.79 | -1.30 | 19.32 | -5.53 | 10.14 | 25.23 |
| ‘CH$_2$CH=CF$_2$ | 12.53 | -1.08 | 15.67 | -3.13 | 11.02 | 24.64 |
| ‘CH$_2$CH=CH$_2$ | 13.09 | -0.94 | 15.49 | -2.41 | 10.30 | 24.32 |
| tBu | 9.74 | -0.88 | 16.10 | -6.36 | 12.80 | 23.42 |
| ‘CH$_2$N=CH$_2$ | 10.44 | -0.31 | 13.94 | -3.50 | 11.97 | 22.72 |
| ‘CH$_2$Ph | 10.49 | -1.04 | 14.90 | -4.41 | 11.04 | 22.57 |
| tPr | 9.57 | -0.52 | 16.98 | -7.41 | 12.19 | 22.29 |
| ‘CH$_3$SH | 9.30 | -0.32 | 16.34 | -7.04 | 11.81 | 21.43 |
| ‘Bu | 7.99 | -0.67 | 16.92 | -8.93 | 11.73 | 20.40 |
| nPr | 8.28 | -0.52 | 17.17 | -8.89 | 10.88 | 19.68 |
| ‘CH(CH$_3$)CN | 6.55 | -0.54 | 11.27 | -4.72 | 12.11 | 19.20 |
| t(CH$_3$)CN | 7.08 | -0.74 | 16.05 | -8.97 | 11.36 | 19.18 |
| ‘CH$_3$OH | 6.54 | -0.64 | 15.56 | -9.02 | 11.75 | 18.93 |
| Et | 8.28 | -0.56 | 17.03 | -8.75 | 10.05 | 18.89 |
| t(CH$_3$)CN | 4.94 | -0.28 | 14.07 | -9.13 | 13.52 | 18.74 |
| ‘CH$_3$F | 5.70 | -0.55 | 14.72 | -9.02 | 10.22 | 16.46 |
| ‘CH$_3$OH | 5.39 | 0.30 | 13.61 | -8.22 | 11.46 | 16.54 |
| Me | 6.35 | -0.17 | 16.64 | -10.29 | 8.21 | 14.73 |
| ‘CH$_3$CN | 2.61 | -0.10 | 9.00 | -6.39 | 11.13 | 13.84 |
| ‘CH$_3$CHO | 1.22 | 0.00 | 6.20 | -4.98 | 12.15 | 13.37 |
| ‘CH$_3$COOH | 0.91 | -0.19 | 7.10 | -6.18 | 11.86 | 12.97 |
| ‘CHF$_2$ | 2.44 | -1.35 | 10.90 | -8.46 | 8.96 | 12.76 |
| ‘CH$_3$CF$_3$ | 0.60 | -0.27 | 8.78 | -8.17 | 10.60 | 11.48 |
| ‘CH$_3$Cl | 5.80 | -0.05 | 14.37 | -8.56 | 10.91 | 16.76 |
| ‘CH$_3$OCH$_3$ | 9.69 | -1.00 | 16.74 | -7.05 | 10.53 | 21.23 |
| ‘CH$_3$SCH$_3$ | 10.10 | -0.62 | 16.66 | -6.57 | 11.64 | 22.36 |
| ‘CH$_3$NHMe | 14.40 | -1.50 | 19.58 | -5.18 | 10.01 | 25.91 |
| ‘CH$_3$NHOH | 9.38 | -0.70 | 15.53 | -6.15 | 10.92 | 21.00 |
| ‘CH$_3$COMe | 1.84 | -0.16 | 7.64 | -5.79 | 12.50 | 14.50 |
| ‘CH$_3$CONH$_2$ | 3.02 | -0.03 | 10.07 | -7.05 | 13.20 | 16.25 |
| ‘CH$_3$CF$_3$H | 2.53 | -0.44 | 11.51 | -8.98 | 12.11 | 15.09 |
| ‘CH$_3$CFH$_2$ | 4.05 | -0.53 | 12.90 | -8.85 | 12.27 | 16.85 |
Table S7 Reaction energies ($\Delta E$, kcal mol$^{-1}$), reaction Gibbs free energies ($\Delta G$, kcal mol$^{-1}$), reaction enthalpies ($\Delta H$, kcal mol$^{-1}$), rate constants ($k_H$, L mol$^{-1}$ s$^{-1}$) and activation energies (Ea, kcal mol$^{-1}$) of the H-atom abstraction reactions of NHC-BH$_3$ by R$^\bullet$ computed at the B3LYP/6-311++G(d,p) in BTF at 376 K.

| R$^\bullet$ | $\Delta E$ | $\Delta G$ | $\Delta H$ | $k_H$ | Ea |
|------------|------------|------------|------------|-------|----|
| *CH$_3$NH$_2$ | -11.98 | -12.99 | -11.98 | 9.716×10$^5$ | 14.47 |
| *CH$_2$CH=CF$_2$ | -6.61 | -7.04 | -6.98 | 2.283×10$^2$ | 13.30 |
| *CH$_2$CH=CH$_2$ | -5.02 | -5.72 | -5.25 | 3.447×10$^2$ | 13.83 |
| tBu | -14.30 | -14.03 | -14.63 | 9.821×10$^2$ | 10.39 |
| *CH$_2$N=CH$_2$ | -7.50 | -8.53 | -7.39 | 2.613×10$^3$ | 11.04 |
| *CH$_3$Ph | -9.59 | -11.88 | -9.14 | 3.232×10$^3$ | 11.44 |
| iPr | -16.93 | -16.79 | -17.32 | 4.319×10$^3$ | 10.14 |
| *CH$_2$SH | -16.04 | -16.26 | -16.36 | 1.292×10$^4$ | 9.71 |
| $^\alpha$Bu | -21.17 | -21.03 | -21.48 | 5.006×10$^4$ | 8.72 |
| $^\alpha$Pr | -20.97 | -21.33 | -21.19 | 1.300×10$^5$ | 9.04 |
| *CH(CH$_3$)$_2$CN | -10.70 | -11.02 | -10.77 | 2.455×10$^5$ | 7.38 |
| *(CH$_2$)$_2$CN | -21.57 | -21.50 | -21.84 | 2.475×10$^5$ | 7.90 |
| *(CH$_2$)$_3$CN | -21.89 | -21.45 | -22.21 | 3.364×10$^5$ | 7.35 |
| Et | -20.61 | -20.82 | -20.92 | 3.831×10$^5$ | 8.97 |
| *(CH$_2$)$_2$CN | -22.92 | -23.01 | -23.21 | 3.840×10$^5$ | 5.26 |
| *CH$_2$F | -22.24 | -22.34 | -22.33 | 9.002×10$^6$ | 6.41 |
| *CH$_2$OH | -20.19 | -21.29 | -19.96 | 9.906×10$^6$ | 6.13 |
| Me | -25.44 | -24.66 | -25.54 | 8.676×10$^7$ | 6.96 |
| *CH$_2$NCN | -16.62 | -17.70 | -16.48 | 2.597×10$^8$ | 3.64 |
| *CH$_2$CHO | -13.78 | -14.49 | -13.97 | 4.411×10$^8$ | 2.37 |
| *CH$_2$COOH | -18.21 | -18.67 | -18.58 | 7.545×10$^8$ | 2.18 |
| *CHF$_2$ | -22.96 | -23.84 | -22.84 | 1.117×10$^9$ | 3.73 |
| *CH$_2$CF$_3$ | -25.91 | -26.11 | -26.10 | 5.428×10$^9$ | 1.94 |
| *CH$_2$Cl | -20.95 | -20.55 | -21.31 | 5.513×10$^6$ | 6.49 |
| *CH$_2$OCH$_3$ | -16.01 | -16.73 | -16.07 | 1.924×10$^4$ | 10.34 |
| *CH$_2$SCH$_3$ | -14.77 | -15.20 | -14.99 | 4.087×10$^3$ | 10.66 |
| *CH$_2$NHMe | -11.15 | -11.90 | -11.21 | 3.976×10 | 15.16 |
| *CH$_2$NCOH | -13.83 | -14.92 | -13.82 | 2.564×10$^4$ | 10.03 |
| *CH$_2$COMe | -15.55 | -15.49 | -15.93 | 1.005×10$^8$ | 2.98 |
| *CH$_2$CONH$_2$ | -18.22 | -19.23 | -18.21 | 1.029×10$^7$ | 3.86 |
| *CH$_2$CF$_2$H | -24.45 | -24.36 | -24.71 | 4.698×10$^7$ | 3.56 |
| *CH$_2$CFH$_2$ | -22.69 | -21.80 | -23.01 | 4.987×10$^6$ | 4.88 |
Table S8 Activation barrier ($\Delta E^*$), activation zero-point vibrational energy correction ($\Delta E_{ZPVE}^*$), intrinsic barrier ($\Delta E^*_0$), thermal contribution ($\Delta E_{\text{therm}}^*$), activation Gibbs free energy correction ($\Delta G_{\text{corr}}^*$), and Gibbs free energy barrier ($\Delta G^*$) of the H-atom abstraction reactions of NHC-BH$_2$CN by $R^*$ computed at the B3LYP/6-311++G(d,p) in BTF at 376 K. All units are in kcal mol$^{-1}$.

| $R^*$          | $\Delta E^*$ | $\Delta E_{ZPVE}^*$ | $\Delta E^*_0$ | $\Delta E_{\text{therm}}^*$ | $\Delta G_{\text{corr}}^*$ | $\Delta G^*$ |
|----------------|--------------|---------------------|----------------|-----------------------------|-----------------------------|-------------|
| CH$_2$NH$_2$   | 12.46        | -1.30               | 18.16          | -5.70                       | 11.47                       | 25.22       |
| CH$_2$CH=CF$_2$| 13.18        | -1.22               | 16.54          | -3.36                       | 11.94                       | 26.34       |
| CH$_2$CH=CH$_2$| 13.96        | -0.96               | 16.60          | -2.64                       | 12.52                       | 27.44       |
| tBu            | 9.30         | -0.89               | 15.83          | -6.53                       | 14.18                       | 24.37       |
| CH$_3$N=CH$_2$ | 12.03        | -0.50               | 15.77          | -3.74                       | 12.73                       | 25.26       |
| CH$_2$Ph       | 11.23        | -1.17               | 15.86          | -4.64                       | 12.39                       | 24.78       |
| tPr            | 9.08         | -0.57               | 16.65          | -7.57                       | 13.31                       | 22.97       |
| CH$_3$SH       | 9.44         | -0.46               | 16.68          | -7.24                       | 12.30                       | 22.20       |
| tBu            | 7.83         | -0.71               | 16.93          | -9.10                       | 12.87                       | 21.41       |
| tPr            | 8.22         | -0.51               | 17.29          | -9.07                       | 12.51                       | 21.25       |
| (CH$_3$)CN     | 8.57         | -0.68               | 13.59          | -5.02                       | 13.73                       | 22.98       |
| (CH$_2$)$_2$CN | 7.32         | -0.67               | 16.51          | -9.19                       | 13.74                       | 21.73       |
| (CH$_2$)$_2$CN | 6.96         | -0.56               | 16.22          | -9.26                       | 13.78                       | 21.29       |
| Et             | 8.28         | -0.42               | 17.21          | -8.93                       | 12.33                       | 21.03       |
| (CH$_2$)$_2$CN | 6.00         | -0.26               | 15.49          | -9.49                       | 13.23                       | 19.49       |
| CH$_2$F        | 6.19         | -0.60               | 15.47          | -9.28                       | 10.80                       | 17.60       |
| CH$_3$OH       | 5.07         | 0.39                | 13.42          | -8.35                       | 13.05                       | 17.73       |
| Me             | 6.73         | -0.16               | 17.26          | -10.53                      | 10.49                       | 17.38       |
| CH$_3$CN       | 5.02         | -0.29               | 12.06          | -7.04                       | 12.85                       | 18.17       |
| CH$_3$CHO      | 3.73         | -0.55               | 9.53           | -5.80                       | 13.45                       | 17.73       |
| CH$_3$COOH     | 3.43         | -0.53               | 10.75          | -7.32                       | 13.14                       | 17.10       |
| CHF$_3$        | 3.62         | -1.38               | 12.62          | -9.00                       | 11.46                       | 16.46       |
| CH$_2$CF$_3$   | 2.41         | -0.42               | 11.97          | -9.56                       | 13.83                       | 16.67       |
| CH$_3$Cl       | 6.67         | -0.16               | 15.54          | -8.87                       | 12.66                       | 19.49       |
| CH$_3$OCH$_3$  | 9.22         | -1.03               | 16.43          | -7.22                       | 11.63                       | 21.88       |
| CH$_3$SCH$_3$  | 10.04        | -0.68               | 16.81          | -6.77                       | 13.32                       | 24.04       |
| CH$_3$NHMe     | 13.01        | -1.55               | 18.38          | -5.36                       | 11.29                       | 25.85       |
| CH$_3$NCOH     | 9.87         | -0.67               | 16.24          | -6.37                       | 13.14                       | 23.68       |
| CH$_3$COMe     | 4.21         | -0.55               | 10.73          | -6.52                       | 13.96                       | 18.72       |
| CH$_3$CONH$_2$ | 4.53         | -0.65               | 12.07          | -7.54                       | 12.67                       | 17.85       |
| CH$_3$CF$_2$H  | 3.89         | -0.55               | 13.48          | -9.59                       | 14.02                       | 18.46       |
| CH$_3$CFH$_2$  | 5.29         | -0.61               | 14.58          | -9.29                       | 13.67                       | 19.57       |
**Table S9** Reaction energies (Δ_E, kcal mol⁻¹), reaction Gibbs free energies (Δ_G, kcal mol⁻¹), reaction enthalpies (Δ_H, kcal mol⁻¹), rate constants (k_H, L mol⁻¹ s⁻¹) and activation energies (E_a, kcal mol⁻¹) of the H-atom abstraction reactions of NHC-BH₂CN by R’ computed at the B3LYP/6-311++G(d,p) in BTF at 376 K.

| R’      | Δ_E  | Δ_G  | Δ_H  | k_H  | E_a  |
|---------|------|------|------|------|------|
| ‘CH₃NH₂ | -12.48 | -11.60 | -12.81 | 9.478×10⁴ | 13.02 |
| ‘CH₂CH=CF₂ | -7.11 | -5.66 | -7.82 | 2.502×10³ | 13.87 |
| ‘CH₂CH=CH₂ | -5.51 | -4.33 | -6.08 | 5.752 | 14.50 |
| ‘Bu     | -14.79 | -12.64 | -15.47 | 2.707×10² | 9.90  |
| ‘CH₂N=CH₂ | -7.99 | -7.15 | -8.23 | 9.858×10⁴ | 12.50 |
| ‘CH₃Ph  | -10.08 | -10.49 | -9.98  | 1.793×10³ | 12.05 |
| ‘iPr    | -17.42 | -15.40 | -18.16 | 1.719×10³ | 9.55  |
| ‘CH₂SH  | -16.54 | -14.88 | -17.20 | 4.892×10³ | 9.70  |
| ‘nBu    | -21.46 | -19.94 | -22.02 | 1.592×10⁴ | 8.85  |
| ‘CH(CH₃)CN | -11.20 | -9.63  | -11.61 | 1.789×10³ | 9.12  |
| ‘(CH₂)₄CN | -22.06 | -20.11 | -22.68 | 8.322×10³ | 7.93  |
| ‘(CH₂)₂CN | -22.39 | -20.06 | -23.05 | 1.460×10⁴ | 7.53  |
| Et      | -21.10 | -19.43 | -21.75 | 2.181×10⁴ | 8.70  |
| ‘(CH₂)₂CN | -23.41 | -21.62 | -24.05 | 1.499×10⁵ | 6.70  |
| ‘CH₂F   | -22.73 | -20.95 | -23.17 | 2.050×10⁶ | 6.67  |
| ‘CH₂OH  | -20.68 | -19.91 | -20.80 | 2.006×10⁶ | 5.65  |
| Me      | -25.93 | -23.27 | -26.38 | 2.541×10⁶ | 7.13  |
| ‘CH₂CN  | -17.11 | -16.31 | -17.32 | 9.200×10⁵ | 5.68  |
| ‘CH₂CHO | -14.28 | -13.10 | -14.81 | 1.496×10⁶ | 4.54  |
| ‘CH₂COOH| -18.70 | -17.28 | -19.42 | 3.262×10⁶ | 4.41  |
| ‘CHF₂   | -23.45 | -22.45 | -23.68 | 8.511×10⁶ | 4.61  |
| ‘CH₂CF₃ | -26.40 | -24.73 | -26.94 | 5.506×10⁶ | 3.36  |
| ‘CH₂Cl  | -21.44 | -19.17 | -22.15 | 1.548×10⁵ | 7.04  |
| ‘CH₂OCH₃| -16.50 | -15.34 | -16.91 | 7.991×10³ | 9.77  |
| ‘CH₂SCH₃| -15.26 | -13.81 | -15.82 | 4.455×10² | 10.43 |
| ‘CH₂NHMe| -11.65 | -10.52 | -12.05 | 4.168×10⁴ | 13.77 |
| ‘CH₂NCOH| -14.32 | -13.54 | -14.65 | 7.399×10² | 10.31 |
| ‘CH₂COMe| -16.04 | -14.10 | -16.76 | 4.189×10⁵ | 5.05  |
| ‘CH₂CONH₂| -18.72 | -17.84 | -19.04 | 1.314×10⁶ | 5.42  |
| ‘CH₂CF₂H | -24.94 | -22.97 | -25.54 | 5.462×10⁵ | 4.67  |
| ‘CH₂CFH₂ | -23.18 | -20.41 | -23.84 | 1.386×10⁵ | 5.93  |
**Table S10** List of Cartesian coordinates of located stationary points at the B3LYP/6-311++G(d,p) in BTF at 376 K.

|          | C        | H        | N          | C        | H        | N          | C        | H        | N          | C        | H        | N          | C        | H        | N          | C        | H        | N          | C        | H        | N          | C        | H        | N          | C        | H        | N          |
|----------|----------|----------|------------|----------|----------|------------|----------|----------|------------|----------|----------|------------|----------|----------|------------|----------|----------|------------|----------|----------|------------|----------|----------|------------|----------|----------|------------|----------|----------|------------|----------|----------|------------|
| NHC-BH₃  | C -0.01195714 | 0.59840928 | 0.00036495 | C 0.73707899 | -1.53072526 | 0.00011759 | C -0.61881869 | -1.57624954 | 0.00042152 | H 1.47209526 | -2.32046818 | -0.00000226 | H -1.29830022 | -2.41421970 | 0.00051089 | N -1.05797167 | -0.26736399 | 0.00054185 | N 1.09067807 | -0.19342460 | 0.00003154 | C -2.45575981 | 0.13090918 | -0.00001993 | H -2.84203125 | 0.14052088 | 1.02242385 | H -2.52405257 | 1.13131172 | -0.42381889 | H -3.04262714 | -0.56361400 | -0.60659156 | C 2.46988939 | 0.26781691 | -0.00018273 | H 2.98413017 | -0.09760485 | -0.89279452 | H 2.46515966 | 1.35601416 | -0.00036653 | H 2.98430299 | -0.09728658 | 0.89246058 | H -0.75242955 | 2.53027330 | 0.99719241 | H 0.97620839 | 2.71293274 | 0.00121087 | H -0.75026207 | 2.52988543 | -0.99859987 | B -0.12474699 | 2.19536235 | 0.00003058 |
| NHC-BH₂CN | C -2.18891000 | 0.10316100 | -0.44796100 | H -3.16413200 | -0.22345100 | -0.76400600 | C -1.64983200 | 1.34538000 | -0.37200500 | H -2.06288100 | 2.30928500 | -0.61321700 | N -0.36361400 | 1.19231200 | 0.11182200 | C 0.58360200 | 2.29060000 | 0.30667900 | H 1.24384900 | 2.04762000 | 1.13593900 | H 1.17605500 | 2.44451000 | -0.59611200 | H 0.02694600 | 3.19718400 | 0.53710900 | N -1.21834800 | -0.78307000 | -0.01512000 | C -1.40775200 | -2.23458200 | 0.06338800 | H -2.37653300 | -2.47287500 | -0.37059800 | H -0.62577800 | -2.74422300 | -0.49598200 | H -1.38470600 | -2.56290900 | 1.10156300 | C -0.09321800 | -0.11569000 | 0.33054800 | H 1.60289300 | -0.11062300 | 1.89804900 | H 1.11531700 | -1.89769200 | 1.19181000 | B 1.27503600 | -0.73559300 | 0.91207100 | C 2.43621600 | -0.61991100 | -0.16311600 | N 3.29527000 | -0.54104200 | -0.93814700 |
| NHC-·BH₂   | C 0.67933135 | -1.50803756 | -0.00001675 | H 1.37528748 | -2.32932407 | -0.00008529 |
|   | C     |   | H     |   | N     |   |
|---|-------|---|-------|---|-------|---|
|   | -0.67934825 | -1.50804538 | 0.00016982 |
| H | -1.37531925 | -2.32931900 | 0.00024863 |
| N | -1.09459266 | -0.19302203 | 0.0007515  |
| C | -2.47794991 | 0.25000429  | 0.00003513 |
| H | -2.68613661 | 0.85154082  | 0.88732044 |
| H | -2.68600282 | 0.85210227  | -0.88703497|
| H | -3.12638188 | -0.62469493 | -0.00036498|
| N | 1.09458972  | -0.19302400 | -0.00017431|
| C | 2.47795222  | 0.24998040  | 0.00004520 |
| H | 3.12636629  | -0.62473117 | -0.00101163|
| H | 2.68589571  | 0.85270947  | -0.88654576|
| H | 2.68628550  | 0.85088166  | 0.88780404 |
| C | -0.00001074 | 0.66097157  | -0.00002694|
| B | 0.00001983  | 2.16353766  | 0.00006256 |
| H | 1.03675603  | 2.75808017  | 0.00012678 |
| H | -1.03667703 | 2.75814872  | 0.00015898 |

|   | C     |   | H     |   | N     |   |
|---|-------|---|-------|---|-------|---|
|   | -2.24247489 | 0.54701648  | -0.0003643 |
| H | -3.31780369 | 0.50501618  | -0.00006248|
| C | -1.40195708 | 1.61455324  | -0.0001640 |
| H | -1.61311999 | 2.66980752  | -0.00003119|
| N | -0.11324127 | 1.12509943  | 0.00001660 |
| C | 1.08359139  | 1.95959081  | 0.00003099 |
| H | 1.68378147  | 1.76257506  | 0.88837966 |
| H | 1.68375510  | 1.76265221  | -0.88835317|
| H | 0.77420617  | 3.00281185  | 0.00008206 |
| N | -1.46285303 | -0.58868237 | -0.0001699 |
| C | -1.98160341 | -1.95187280 | 0.00000390 |
| H | -3.06877883 | -1.90583526 | -0.00006615|
| H | -1.64301017 | -2.48621627 | -0.88838518|
| H | -1.64311914 | -2.48614928 | 0.88847549 |
| C | -0.12706772 | -0.25168886 | 0.00002274 |
| H | 0.76938919  | -2.41009137 | 0.00006640 |
| B | 1.01747705  | -1.24646575 | 0.00005393 |
| C | 2.48773786  | -0.85242498 | 0.00002088 |
| N | 3.63008826  | -0.61831558 | -0.00007520|

|   | C     |   | H     |   | N     |   |
|---|-------|---|-------|---|-------|---|
|   | -0.71057100 | -0.00000100 | 0.01716100|
| H | -1.12162800 | 0.88097900  | -0.48157700|
| H | -1.06828800 | -0.00007300 | 1.05616300|
| H | -1.12164600 | -0.88089900 | -0.48170800|
| N | 0.75339700  | -0.00000100 | -0.12456100|
| H | 1.15060400  | 0.81209800  | 0.33804100 |
| H | 1.15060800  | -0.81209800 | 0.33804100 |

|   | C     |   | H     |   |
|---|-------|---|-------|---|
|   | -2.00947700 | 0.02868600 | 0.00000700 |
| H | -2.82210900 | -0.69764300 | -0.00005200 |
|   | X    | Y    | Z    |
|---|------|------|------|
| H | -2.12947100 | 0.66423700 | -0.88173700 |
| H | -2.12952300 | 0.66415000 | 0.88180700 |
| C | -0.68108100 | -0.68195900 | 0.00001200 |
| H | -0.64341100 | -1.76371700 | 0.00002800 |
| F | 1.67857300 | -0.65667200 | 0.00000500 |
| F | 1.65133600 | 1.26054000 | 0.00002200 |

| CH₃CH=CH₂ | C | 1.24070900 | -0.15748500 | 0.00000000 |
| H | 2.01938300 | 0.60749200 | -0.00002800 |
| H | 1.39555600 | -0.78804600 | -0.88103300 |
| H | 1.39558600 | -0.78800000 | 0.88106300 |
| C | -0.13860100 | 0.45854000 | 0.00000000 |
| H | -0.18492100 | 1.54571100 | 0.00000000 |
| C | -1.28251800 | -0.22498000 | 0.00000000 |
| H | -1.29987200 | -1.31189900 | -0.00001000 |
| H | -2.24328100 | 0.27829500 | 0.00001000 |

| CH(CH₃)₂ | C | -1.45656600 | -0.11922700 | 0.09590200 |
| H | -2.06067400 | 0.71811300 | -0.26656700 |
| H | -1.91546400 | -1.04502100 | -0.26437600 |
| H | -1.51344800 | -0.12249600 | 1.19039300 |
| C | 0.83153100 | -1.20178400 | 0.09589800 |
| H | 1.86232300 | -1.13693000 | -0.26562300 |
| H | 0.86428200 | -1.24882000 | 1.19040300 |
| H | 0.40749800 | -2.14362800 | -0.26547800 |
| C | 0.62502400 | 1.32103500 | 0.09587900 |
| H | 0.64894700 | 1.37285300 | 1.19036100 |
| H | 1.65287200 | 1.42454400 | -0.26508400 |
| H | 0.05375700 | 2.18141100 | -0.26590300 |
| C | -0.00000800 | -0.00002300 | -0.37232400 |
| H | 0.00002400 | -0.00002900 | -1.47026000 |

| CH₃N=CH₂ | C | -1.18290100 | 0.18280400 | -0.00000100 |
| H | -2.16331800 | -0.29172700 | 0.00009100 |
| H | -1.15626900 | 1.28066600 | -0.00002000 |
| N | -0.14182200 | -0.53643000 | 0.00002900 |
| C | 1.15041000 | 0.13477700 | 0.00007000 |
| H | 1.71772900 | -0.18567400 | -0.87825200 |
| H | 1.07250400 | 1.23070000 | -0.00079400 |
| H | 1.71705100 | -0.18444300 | 0.87914500 |

| CH₃Ph | C | 1.20023500 | -1.20429900 | 0.00207700 |
| C | -0.19455000 | -1.20145700 | -0.00906000 |
| C | -0.19453300 | 0.00000100 | -0.01132300 |
| C | -0.19454900 | 1.20145700 | -0.00906000 |
| C | 1.20023600 | 1.20429900 | 0.00207700 |
| C | 1.90405500 | 0.00000000 | 0.00849300 |
| Chemical | X1           | Y1           | Z1           | X2           | Y2           | Z2           | X3           | Y3           | Z3           |
|----------|--------------|--------------|--------------|--------------|--------------|--------------|--------------|--------------|--------------|
| H        | 1.73672400   | -2.14698000  | 0.00174500   | H            | -0.73234000  | -2.14435700  | -0.01812000  | H            | -0.73233900  | 2.14435800   | 0.00174500   |
| H        | 2.98825100   | 0.00000100   | 0.01413800   | C            | -2.42414600  | 0.00000000   | 0.00899800   | H            | -2.82932500  | -0.88525100  | -0.48644700  |
| C        | 3.29882500   | -0.00003200  | 1.03758100   | H            | -0.81258000  | -0.00003200  | 1.03758100   | C            | 1.27709900   | -0.25992100  | 0.00000000   |
| C        | 1.27709900   | -0.25992100  | 0.00000000   | H            | -1.32103700  | -0.90522400  | 0.88338500   | H            | -1.32103700  | -0.90522400  | 0.88338500   |
| H        | 0.00000000   | 0.58620200   | 0.00000000   | H            | 0.00000000   | -0.08751300  | 0.00000000   | C            | 0.00000000   | 1.24454400   | -0.87611300  |
| CH₂CH₃   | C            | -1.16695200  | 0.01961400   | H            | -1.53228100  | -1.00668100  | -0.00005800  | H            | -1.52643300  | 0.52617200   | -0.89409800  |
| H        | 1.27709900   | -0.25992100  | 0.00000000   | C            | 0.66684400   | -0.08751300  | 0.00000000   | H            | 0.91736600   | 1.23694900   | -0.00000100  |
| CH₂SH    | C            | -1.16695200  | 0.01961400   | H            | -1.53228100  | -1.00668100  | -0.00005800  | H            | -1.52643300  | 0.52617200   | -0.89409800  |
| H        | 1.27709900   | -0.25992100  | 0.00000000   | C            | 0.66684400   | -0.08751300  | 0.00000000   | H            | 0.91736600   | 1.23694900   | -0.00000100  |
| CH₃(CH₂)₂C | C           | 1.96230300   | -0.12104800  | H            | 2.10908000   | -0.75092900  | -0.88356900  | H            | 2.10912800   | -0.75082100  | 0.88363200   |
| H        | 2.74833900   | 0.63982300   | -0.00007300  | C            | 0.56849100   | 0.51391100   | 0.00000300   | H            | 0.46396400   | 1.16514400   | -0.87688500  |
| H        | -0.56849100  | -0.51391100  | 0.00000000   | H            | 0.46396400   | 1.16514400   | -0.87688500  | C            | -0.46396400  | -1.16514400  | 0.87689300   |
| H        | -0.46396500  | -1.16515200  | -0.87687900  | C            | -1.96230300  | 0.12104800   | -0.00003000  | H            | -2.10909700  | 0.75088600   | -0.88359700  |
| H        | -2.74833900  | -0.63982300  | -0.00002000  | H            | -2.10911200  | 0.75086400   | 0.88360400   | C            | -1.27709900  | -0.25992100  | 0.00000000   |
| CH₃CH₂CH₃ | C           | -1.27709900  | -0.25992100  | H            | -1.32103700  | -0.90522400  | 0.88338500   | H            | -1.73672600  | 2.14697900   | 0.00174500   |
| CH₂(CH₃)CN | C   | 1.65044300 | 0.48407200 | 0.00000000 |
|            | H   | 1.69682600 | 1.13921300 | -0.87766700 |
|            | H   | 1.69682600 | 1.13921300 | 0.87766700  |
|            | C   | 0.31500700 | -0.26621600 | 0.00000000  |
|            | H   | 0.25290000 | -0.91514800 | -0.87916200 |
|            | H   | 0.25290000 | -0.91514800 | 0.87916200  |
|            | C   | -0.88660100 | 0.70132200 | 0.00000000  |
|            | H   | -0.85471600 | 1.35226500 | -0.87928500 |
|            | H   | -0.85471600 | 1.35226500 | 0.87928500  |
|            | C   | -2.17212700 | 0.00984100 | 0.00000000  |
|            | N   | -3.18081400 | -0.55133900 | 0.00000000  |
|            | C   | 2.85597200 | -0.45970800 | 0.00000000  |
|            | H   | 2.85256800 | -1.10501200 | -0.88378100 |
|            | H   | 3.79437300 | 0.10087200 | 0.00000000  |
|            | H   | 2.85256800 | -1.10501200 | 0.88378100  |
| CH₃(CH₂)₂CN | C   | -0.88031000 | -0.52757400 | 0.00000000  |
|            | H   | -0.71884600 | -1.15822500 | 0.87853300  |
|            | H   | -0.71884600 | -1.15822500 | -0.87853300 |
|            | C   | 0.16253700 | 0.61015400 | 0.00000000  |
|            | H   | 0.03232900 | 1.24858800 | 0.87942400  |
|            | H   | 0.03233000 | 1.24858800 | -0.87942400 |
|            | C   | 1.53753700 | 0.11988600 | 0.00000000  |
|            | N   | 2.61884000 | -0.28392600 | 0.00000000  |
|            | C   | -2.30829700 | 0.01991500 | 0.00000000  |
|            | H   | -3.03290900 | -0.79761700 | 0.00000000  |
|            | H   | -2.49737000 | 0.63504300 | 0.88467200  |
|            | H   | -2.49737000 | 0.63504300 | -0.88467200 |
| CH₄CH₃    | C   | 0.76569900 | -0.00003000 | 0.00000000  |

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|        | C          | H           |         |        |
|--------|------------|-------------|---------|--------|
| H      | 1.16238000 | 0.50966700  | -0.88261800 |
| H      | 1.16238000 | 0.50966500  | 0.88261900  |
| H      | 1.16240700 | -1.01920200 | -0.0000100  |
| C      | -0.76570300| 0.00000500  | 0.00000000  |
| H      | -1.16239900| -0.50960300 | 0.88264400  |
| H      | -1.16234700| 1.01922000  | 0.0000100   |
| H      | -1.16239900| -0.50960200 | -0.88264500 |
|        | CH\textsubscript{3}CH\textsubscript{2}CN | C          | 0.00000000 | 0.80707100 |
|        | H          | 0.29921600  | 1.38570300 | 0.87851800 |
|        | H          | 0.29921600  | 1.38570300 | -0.87851800 |
|        | C          | 0.77075500  | -0.43407200 | 0.00000000 |
|        | N          | 1.36961100  | -1.42065400 | 0.00000000 |
|        | C          | -1.51974500 | 0.56543900 | 0.00000000 |
|        | H          | -2.03617500 | 1.52659000 | 0.00000000 |
|        | H          | -1.82779500 | 0.00798000 | -0.88604300 |
|        | H          | -1.82779500 | 0.00798000 | 0.88604300  |
|        | CH\textsubscript{3}F | C          | 0.00000000 | 0.00000000 |
|        | H          | 0.00000000  | 1.03539900 | -0.98842700 |
|        | H          | -0.89668200 | -0.51769900 | -0.98842700 |
|        | H          | 0.89668200  | -0.51769900 | -0.98842700 |
|        | F          | 0.00000000  | 0.00000000 | 0.76112300  |
|        | CH\textsubscript{3}OH | C          | 0.67140000 | -0.01982600 |
|        | H          | 1.08981700  | 0.98679100 | -0.00119400 |
|        | H          | 1.02440500  | -0.54858900 | -0.89178300 |
|        | H          | 1.02459200  | -0.54656400 | 0.89292000  |
|        | O          | -0.75260800 | 0.12286600 | 0.00000400  |
|        | H          | -1.14635000 | -0.75560400 | 0.00013000  |
|        | CH\textsubscript{4} | C          | 0.00000000 | 0.00000000 |
|        | H          | 0.62993900  | 0.62993900 | 0.62993900  |
|        | H          | -0.62993900 | -0.62993900 | 0.62993900  |
|        | H          | -0.62993900 | 0.62993900 | -0.62993900 |
|        | H          | 0.62993900  | -0.62993900 | -0.62993900 |
|        | CH\textsubscript{3}CN | C          | 0.00014200 | -1.17539600 |
|        | H          | 0.51303100  | -1.54879700 | 0.88806100  |
|        | H          | 0.51303100  | -1.54879700 | -0.88806100 |
|        | C          | 0.00000000  | 0.27879300 | 0.00000000  |
|        | N          | -0.00023800 | 1.43232000 | 0.00000000  |
|        | H          | -1.02525200 | -1.54902600 | 0.00000000  |
|        | CH\textsubscript{3}CHO | C          | -1.16891100 | -0.13639100 |
|        | H          | -1.31116400 | -0.76926000 | 0.88103200  |
|        | H          | -1.91354900 | 0.65978300  | 0.00001800  |
|        | H          | -1.31119700 | -0.76926000 | -0.88102200 |
|        | C          | 0.23337500  | 0.41041900  | -0.00002300 |
|        | H          | 0.33646200  | 1.51344000  | 0.00004600  |
|                | O    | 1.22658300 | -0.28485900 | 0.00000600 |
|----------------|------|------------|-------------|------------|
| **CH₃COOH**   | C    | 1.38959900 | -0.17233000 | 0.00000900 |
|                | H    | 1.59792900 | -1.24006500 | 0.00002600 |
|                | H    | 1.83776600 | 0.29197800  | 0.88079200 |
|                | H    | 1.83783400 | 0.29196400  | -0.88074600|
|                | C    | -0.08581100| 0.11622300  | -0.00005400|
|                | O    | -0.83771600| -1.00584200 | 0.00000700 |
|                | H    | -1.77220000| -0.74270900 | 0.00003500 |
|                | O    | -0.57779200| 1.22277600  | 0.00001400 |
| **CH₂F₂**     | C    | 0.00000000 | 0.51617100  | 0.00000000 |
|                | H    | -0.00008400| 1.10623400  | 0.91518000 |
|                | H    | -0.00008400| 1.10623400  | -0.91518000|
|                | F    | -1.10814400| -0.29492800 | 0.00000000 |
|                | F    | 1.10816200 | -0.29501600 | 0.00000000 |
| **CH₂CF₃**    | C    | 1.48437100 | -0.00056000 | -0.00059300|
|                | H    | 1.84466100 | 0.11871100  | -1.02202200|
|                | H    | 1.84468500 | -0.94485200 | 0.40674000 |
|                | H    | 1.84499400 | 0.82425700  | 0.61346100 |
|                | C    | -0.01414000| -0.00002500 | -0.00021900|
|                | F    | -0.53264000| -1.00789500 | -0.74819300|
|                | F    | -0.53106700| -0.14418200 | 1.24715400 |
|                | F    | -0.53137400| 1.15267700  | -0.49821800|
| **CH₃Cl**     | C    | 0.00000000 | 0.00000000  | -1.14883400|
|                | H    | 0.00000000 | 1.03433700  | -1.48178400|
|                | H    | -0.89576200| -0.51716800 | -1.48178400|
|                | H    | 0.89576200 | -0.51716800 | -1.48178400|
|                | Cl   | 0.00000000 | 0.00000000  | 0.66696200 |
| **CH₃OCH₃**   | O    | 0.00000000 | 0.59143100  | 0.00000400 |
|                | C    | -1.17949800| -0.19698100 | 0.00000100 |
|                | H    | -1.23180100| -0.83465900 | 0.89262500 |
|                | H    | -2.02859100| 0.48675200  | -0.00090300|
|                | H    | -1.23095600| -0.83592700 | -0.89176100|
|                | C    | 1.17949500 | -0.19698400 | -0.00000200|
|                | H    | 1.23168500 | -0.83481800 | -0.89251600|
|                | H    | 2.02857800 | 0.48676200  | 0.00065900 |
|                | H    | 1.23108300 | -0.83576900 | 0.89187300 |
| **CH₃SCH₃**   | C    | -1.39902600| -0.51353100 | 0.00000000 |
|                | H    | -2.31384200| 0.07971800  | 0.00000000 |
|                | H    | -1.37977100| -1.13929500 | 0.89368300 |
|                | H    | -1.37977100| -1.13929500 | -0.89368300|
|                | S    | 0.00000000 | 0.66000700  | 0.00000000 |
|                | C    | 1.39902600 | -0.51353100 | 0.00000000 |
|                | H    | 1.37977100 | -1.13929500 | -0.89368300|
|                | H    | 2.31384200 | 0.07971800  | 0.00000000 |
|                | H     | C (X) | C (Y) | C (Z) |
|----------------|-------|-------|-------|-------|
| **CH₃NHMe**    |       |       |       |       |
| C              | 1.21769000 | -0.22380700 | 0.02016200 |
| H              | 1.28393700 | -0.97021200 | -0.77713900 |
| H              | 2.09292900 | 0.42525300  | -0.05488500 |
| H              | 1.26342400 | -0.75877500 | 0.98373400  |
| N              | 0.000000000 | 0.56627300  | -0.15178400 |
| H              | 0.000000000 | 1.32923500  | 0.51712100  |
| C              | -1.21769100 | -0.22380700 | 0.02016200  |
| H              | -2.09292900 | 0.42525300  | -0.05488500 |
| H              | -1.28393700 | -0.97021200 | -0.77713900 |
| H              | -1.26342400 | -0.75877500 | 0.98373400  |
| **CH₃NHOH**    |       |       |       |       |
| N              | -0.392373000 | -0.40735500  | -0.00004300 |
| H              | -0.262404000 | -1.41117900 | 0.00000700  |
| C              | 0.723548000 | 0.34508900  | -0.00007000 |
| H              | 0.511166000 | 1.427520000 | -0.00004100 |
| O              | 1.870610000 | -0.091584000 | 0.00002800 |
| C              | -1.751185000 | 0.117952000 | 0.00003000 |
| H              | -1.711229000 | 1.207612000 | -0.000889000 |
| H              | -2.295285000 | -0.209728000 | 0.88859000 |
| H              | -2.294692000 | -0.208314000 | 0.88953200 |
| **CH₃COMe**    |       |       |       |       |
| C              | -1.280818000 | -0.62908300 | 0.00000000 |
| H              | -1.108405000 | -1.70535800 | -0.00007000 |
| H              | -1.869023000 | -0.35773000 | 0.88074600 |
| H              | -1.869031000 | -0.35771900 | -0.88073700 |
| C              | 0.005692000 | 0.173917000 | 0.000000000 |
| O              | -0.021115000 | 1.392087000 | 0.00000000 |
| C              | 1.303548000 | -0.595064000 | 0.00000000 |
| H              | 1.344014000 | -1.248237000 | 0.877901000 |
| H              | 1.344015000 | -1.248236000 | -0.877902000 |
| H              | 2.156825000 | 0.081977000 | 0.00000100 |
| **CH₃CONH₂**   |       |       |       |       |
| C              | 1.360824000 | -0.34156500 | -0.000010000 |
| H              | 1.457094000 | -1.42766600 | -0.00027900 |
| H              | 1.863535000 | 0.061921000 | 0.88135900 |
| H              | 1.863724000 | 0.062427000 | -0.88101300 |
| C              | -0.076615000 | 0.137419000 | -0.00010000 |
| O              | -0.358599000 | 1.334354000 | 0.00000200 |
| N              | -1.030424000 | -0.826022000 | 0.00001800 |
| H              | -2.003278000 | -0.557320000 | 0.00008900 |
| H              | -0.804567000 | -1.807161000 | 0.00002400 |
| **CH₃CF₂H**    |       |       |       |       |
| C              | 0.050629000 | 0.000724000 | 0.36315100 |
| H              | 0.190871000 | 0.000303000 | 1.444385000 |
| F              | 0.720741000 | -1.104083000 | -0.13588200 |
| F              | 0.719627000 | 1.104338000 | -0.13609600 |
| C              | -1.377917000 | -0.000675000 | -0.09442700 |

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|        |        |        |        |
|--------|--------|--------|--------|
|        | H      | -1.88455000 | -0.88808100 | 0.28859400 |
|        | H      | -1.88612500 | 0.88625300  | 0.28781500  |
|        | H      | -1.41977700 | -0.00106400 | -1.18533800 |
| CH₃CF₂| C      | 0.09449500  | 0.55421300  | -0.00003500 |
|        | H      | 0.20096500  | 1.17574200  | 0.89108600  |
|        | F      | 1.19941500  | -0.33926200 | 0.00001500  |
|        | C      | -1.19631200 | -0.22873400 | -0.00001700 |
|        | H      | -1.27234000 | -0.85816000 | 0.88927200  |
|        | H      | -2.04081700 | 0.46664400  | 0.00005600  |
|        | H      | -1.27291100 | -0.85891800 | -0.88899000 |
|        | H      | 0.20126900  | 1.17553000  | -0.89124900 |
| •CH₂NH₂| C      | 0.72866700  | 0.00001100  | 0.07718200  |
|        | H      | 1.24332700  | -0.93220900 | -0.11624400 |
|        | H      | 1.24285400  | 0.93242600  | -0.11652100 |
|        | N      | -0.65439100 | -0.00000500 | -0.09154600 |
|        | H      | -1.13861300 | -0.83668900 | 0.20505200  |
|        | H      | -1.13882800 | 0.83644000  | 0.20544200  |
| •CH₂CH=CF₂| C     | -0.43087500 | -0.04969900 | -0.00000600 |
|        | C      | 0.80388700  | -0.63610900 | 0.00008400  |
|        | H      | 0.79127500  | -1.72014600 | 0.00018500  |
|        | C      | 2.00790100  | 0.05066500  | 0.00005300  |
|        | H      | 2.94214700  | -0.49274000 | 0.00013000  |
|        | H      | 2.04534200  | 1.13218600  | -0.00004900 |
|        | F      | -0.64941900 | 1.26007800  | 0.00000000  |
|        | F      | -1.57994100 | -0.71657200 | 0.00002000  |
| •CH₂CH=CH₂| C     | -1.22867500 | -0.19644100 | -0.00007800 |
|        | H      | -2.15537600 | 0.36337100  | -0.00013300 |
|        | H      | -1.29629500 | -1.27933200 | 0.00012500  |
|        | C      | 0.00003200  | 0.44303900  | 0.00018900  |
|        | H      | 0.00007100  | 1.53126200  | -0.00026500 |
|        | C      | 1.22864800  | -0.19650900 | -0.00013000 |
|        | H      | 2.15527300  | 0.36354200  | -0.00023900 |
|        | H      | 1.29629600  | -1.27937400 | -0.00007100 |
| tBu    | C      | 1.47985300  | -0.12886800 | 0.01565300  |
|        | H      | 1.86371300  | -1.05302300 | -0.42816900 |
|        | H      | 2.01737200  | 0.71545300  | -0.42773500 |
|        | H      | 1.76157600  | -0.15364800 | 1.08421400  |
|        | C      | 0.00014400  | -0.00004900 | -0.16108100 |
|        | C      | -0.62829500 | 1.34575500  | 0.01564300  |
|        | H      | -1.62746800 | 1.38963600  | -0.42961700 |
|        | H      | -0.74979600 | 1.60125900  | 1.08418800  |
|        | H      | -0.01878700 | 2.14047800  | -0.42627300 |
|        | C      | -0.85157000 | -1.21691000 | 0.01564000  |
|        | H      | -1.01572400 | -1.44737300 | 1.08417300  |
|        | H      | -1.84305500 | -1.08719300 | -0.42989600 |
|        | H      | -0.38862200 | -2.10515500 | -0.42604000 |
| •CH₂N=CH₂| C     | 1.14180000  | 0.15634300  | -0.00008600 |
|        | H      | 2.07309100  | -0.39842300 | 0.00020000  |
|    | H     | N    | C     |
|----|-------|------|-------|
| 1.17809700 | 1.24931800 | -0.0009200 |
| 0.00011800 | -0.51110100 | 0.00005800 |
| -1.14156100 | 0.15622200 | 0.00009900 |
| -2.07329200 | -0.39794200 | -0.00032400 |
| -1.17850300 | 1.24936000 | 0.00027700 |

| `CH2Ph | C     | N    | C     |
|-------|-------|------|-------|
| -1.13265600 | -1.21123300 | -0.0000400 |
| 0.25193100 | -1.21814800 | -0.0000200 |
| 0.99453800 | 0.00000000 | 0.0000100 |
| 0.25193100 | 1.21814800 | -0.0000100 |
| -1.13265600 | 1.21123300 | 0.0000400 |
| -1.83803900 | 0.00000000 | 0.0000100 |
| -1.67507200 | -2.15038300 | -0.0001500 |
| 0.79111900 | -2.15951000 | -0.0000400 |
| 0.79111900 | 2.15951000 | 0.0000200 |
| -1.67507200 | 2.15038300 | 0.0000200 |
| -2.92176600 | 0.00000000 | 0.0000100 |
| 2.40026100 | 0.00000000 | 0.00000000 |
| 2.95890700 | 0.92791800 | -0.00007800 |
| 2.95890700 | -0.92791800 | 0.00008100 |

| `Pr | C     | N    | C     |
|     | 0.00000000 | 0.53528000 | -0.04531000 |
|     | 1.61041700 | 1.01137200 | 0.00000000 |
|     | 1.29718300 | -0.19806800 | 0.00257000 |
|     | 1.31632600 | -1.03096600 | -0.71213700 |
|     | 2.14632100 | 0.45528000 | -0.21239200 |
|     | 1.47790900 | -0.64695900 | 0.99434700 |
|     | -1.29718400 | -0.19806600 | 0.00257000 |
|     | -2.14633800 | 0.45532300 | -0.21220000 |
|     | -1.31640300 | -1.03084400 | -0.71227600 |
|     | -1.47781300 | -0.64713000 | 0.99428800 |

| `CH2SH | C     | N    | C     |
|-------|-------|------|-------|
| 1.14623600 | 0.02202900 | -0.00038600 |
| 1.64496300 | 0.97837600 | 0.00145900 |
| 1.69352100 | -0.90811200 | 0.00022900 |
| -0.58460600 | -0.08950100 | 0.00009200 |
| -0.86220500 | 1.22958300 | -0.00084300 |

| `Bu | C     | N    | C     |
|-----|-------|------|-------|
| 1.88995700 | 0.11630600 | 0.00000700 |
| 2.03105400 | 0.74655300 | 0.88369700 |
| 2.03104700 | 0.74662800 | -0.88363300 |
| 2.68062100 | -0.63922500 | -0.00033000 |
| 0.50409600 | -0.53389300 | -0.00010000 |
| 0.39638800 | -1.18057500 | -0.87757800 |
| 0.39638100 | -1.18059500 | 0.87754500 |
| -0.64411000 | 0.50979000 | -0.00005000 |
| -0.51796200 | 1.15105600 | -0.88115500 |
| -0.51794900 | 1.15106400 | 0.88113800 |
| -2.00540900 | -0.09509100 | 0.00007000 |
| -2.48337600 | -0.38879700 | 0.92758900 |
| -2.48340800 | -0.38877800 | -0.92756500 |

| `Pr | C     | N    | C     |
|-----|-------|------|-------|
| -0.08095800 | 0.55132500 | 0.05107600 |
| -0.10807300 | 1.32014300 | -0.73115000 |
| -0.08502900 | 1.11650600 | 0.99995900 |

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|   | C          | H          | N          |
|---|------------|------------|------------|
| 1 | -1.30514100 | -0.29365400 | -0.03056800 |
| 2 | -2.26185700 | 0.13531600  | -0.30510500 |
| 3 | -1.29306400 | -1.31992200 | 0.32085400  |
| 4 | 1.22919100  | -0.76306400 | -0.99678800 |
| 5 | 1.30810200  | 0.41539300  | 0.06196000  |
| 6 | 1.28500400  | -0.99398100 | 0.75560000  |

CH(CH₃)CN

|   | C          | H          | N          |
|---|------------|------------|------------|
| 1 | -0.44502300 | 0.56625800  | 0.000001100|
| 2 | -0.58833800 | 1.64120000  | 0.000111000|
| 3 | -1.63110700 | -0.33792300 | 0.000006000|
| 4 | -2.25696900 | -0.14014900 | 0.878283000|
| 5 | -2.25750400 | -0.14032100 | -0.87772700|
| 6 | -1.34810000 | -1.39004200 | -0.00050900|
| 7 | 0.86100900  | 0.10713600  | -0.00011500|
| 8 | 1.96309100  | -0.28323100 | 0.000062000|

(CH₂)₄CN

|   | C          | H          | N          |
|---|------------|------------|------------|
| 1 | -1.43145200 | 2.56908100  | 0.000000000|
| 2 | -1.36632500 | 3.12461200  | 0.928192000|
| 3 | -1.36632500 | 3.12461200  | -0.92819200|
| 4 | -1.42811600 | 1.07921600  | 0.000000000|
| 5 | -1.95860000 | 0.70137200  | 0.881880000|
| 6 | -1.95860000 | 0.70137200  | -0.88188000|
| 7 | 0.00000000  | 0.47991200  | 0.000000000|
| 8 | 0.54628200  | 0.82877200  | -0.88098900|
| 9 | 0.54628200  | 0.82877200  | 0.880989000|
| 10| -0.04337500 | -1.06287700 | 0.000000000|
| 11| -0.58048800 | -1.43076600 | -0.87974000|
| 12| -0.58048800 | -1.43076600 | 0.879740000|
| 13| 1.28644300  | -1.66330700 | 0.000000000|
| 14| 2.34532200  | -2.12287500 | 0.000000000|

(CH₂)₃CN

|   | C          | H          | N          |
|---|------------|------------|------------|
| 1 | -0.09513800 | 0.63057200  | -0.00000100|
| 2 | 0.04158600  | 1.26346500  | 0.880551000|
| 3 | 0.04158700  | 1.26346400  | -0.88055300|
| 4 | 0.95414600  | -0.52791700 | 0.000001000|
| 5 | 0.77096000  | -1.14726700 | 0.882557000|
| 6 | 0.77096100  | -1.14726800 | -0.88255400|
| 7 | -1.46646200 | 0.13223700  | -0.00001000|
| 8 | -2.54171000 | -0.28731200 | -0.00001000|
| 9 | 2.35121900  | -0.01468000 | 0.00001000  |
| 10| 2.85213900  | 0.22875700  | -0.92915000|
| 11| 2.85214000  | 0.22875600  | 0.92915300  |

Et

|   | C          | H          | N          |
|---|------------|------------|------------|
| 1 | -0.00982900 | -0.69350900 | 0.000000000|
| 2 | -0.50460200 | -1.10064700 | 0.887174000|
| 3 | -0.50460200 | -1.10064700 | -0.88717400|
| 4 | 1.01369200  | -1.10298600 | 0.000000000|
| 5 | -0.00982900 | 0.79405900  | 0.000000000|
| 6 | 0.05673200  | 1.35048900  | -0.92723000|
| 7 | 0.05673200  | 1.35048900  | 0.92723000  |

(CH₂)₂CN

|   | C          | H          | N          |
|---|------------|------------|------------|
| 1 | 0.55731000 | 0.59935800  | 0.030637000|
| 2 | 0.66330700 | 1.20470200  | 0.944581000|
| 3 | 0.68123500 | 1.30527500  | -0.79918600|

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|     |   X      |   Y      |   Z      |
|-----|----------|----------|----------|
| C   | 1.5888290 | -0.4830940 | -0.0269400 |
| H   | 1.3524640 | -1.4988300 | 0.2568190 |
| H   | 2.6140430 | -0.2113390 | -0.2373680 |
| C   | -0.8166210 | 0.0996750 | -0.0017820 |
| N   | -1.8985930 | -0.2993490 | -0.0251910 |
| CH   | 0.0241290 | 0.6637270 | 0.0000000 |
| H   | -0.1809690 | 1.1109180 | 0.9622360 |
| H   | -0.1809690 | 1.1109180 | -0.9622360 |
| F   | 0.0241290 | -0.6893550 | 0.0000000 |
| CH   | 0.0355530 | 0.6895600 | 0.0000000 |
| H   | 0.1825750 | 1.1925190 | -0.9491480 |
| H   | 0.1825750 | 1.1925190 | 0.9491480 |
| O   | 0.0355530 | -0.6849700 | 0.0000000 |
| Me   | 0.0000010 | 0.0000120 | 0.0000000 |
| CH   | -0.0078160 | -1.1985740 | 0.0000000 |
| H   | -0.0116650 | -1.7502330 | 0.9329090 |
| H   | -0.0116650 | -1.7502330 | -0.9329090 |
| C   | 0.0000000 | 0.1822660 | 0.0000000 |
| O   | -0.8628900 | -1.0390140 | 0.0000000 |
| CH   | 0.0299020 | 0.5162970 | 0.0000000 |
| H   | -0.7176560 | 1.3066400 | 0.0000000 |
| F   | 0.0299020 | -0.2446900 | -1.0989990 |
| F   | 0.0299020 | -0.2446900 | 1.0989990 |
| CH   | 1.1295360 | 0.0000140 | -0.0014400 |
| H   | 1.6232890 | 0.9580560 | 0.0033560 |
| H   | 1.6232750 | -0.9581280 | 0.0033550 |
|       | Cl     | -0.58963400 | -0.00000100 | 0.00011300 |
|-------|--------|-------------|-------------|------------|
| 'CH₂OCH₃ | O      | -0.09456000 | -0.54175400 | -0.03332000 |
|        | C      | 1.14645600  | 0.16876200  | 0.01088300  |
|        | H      | 1.26595000  | 0.66739600  | 0.97715300  |
|        | H      | 1.93622800  | -0.56784500 | -0.12407600 |
|        | H      | 1.19148700  | 0.90996000  | -0.79335500 |
|        | C      | -1.20795800 | 0.22667400  | -0.19814800 |
|        | H      | -1.13645100 | 1.27780800  | -0.19814800 |
|        | H      | -2.13172300 | -0.32590100 | -0.03634300 |
| 'CH₂SCH₃ | C      | -1.36137500 | 0.57671500  | 0.02831800  |
|        | H      | -1.14349700 | 1.61976300  | -0.15461500 |
|        | H      | -2.37855700 | 0.21265500  | 0.04480300  |
|        | S      | -0.11006500 | -0.60674900 | -0.01023800 |
|        | C      | 1.39347100  | 0.42814500  | 0.01054600  |
|        | H      | 1.43400600  | 1.01448000  | 0.92822200  |
|        | H      | 2.24443800  | -0.25098300 | -0.02712500 |
|        | H      | 1.41207000  | 1.08291300  | -0.86066800 |
| 'CH₂NHMe | C      | 1.25874200  | -0.25181200 | 0.08389300  |
|         | H      | 1.25282200  | -1.28903700 | -0.22986600 |
|         | H      | 2.18816400  | 0.30203600  | 0.05041400  |
|         | N      | 0.09524600  | 0.46832000  | -0.12797700 |
|         | H      | 0.11805200  | 1.42270200  | 0.20513900  |
|         | C      | -1.19530600 | -0.18650400 | 0.03120400  |
|         | H      | -1.98896500 | 0.48292300  | -0.30335000 |
|         | H      | -1.22264000 | -1.08629500 | -0.58839500 |
|         | H      | -1.39477200 | -0.48067200 | 1.07118400  |
| 'CH₂NCOH | C      | -1.76683900 | 0.12322000  | -0.00010500 |
|         | H      | -1.91145300 | 1.19185200  | 0.00017600  |
|         | H      | -2.58241000 | -0.57941200 | 0.00045300  |
|         | N      | -0.48167900 | -0.37115600 | 0.00002000  |
|         | H      | -0.35231900 | -1.37718000 | -0.00016600 |
|         | C      | 0.66741800  | 0.36439800  | -0.00000200 |
|         | H      | 0.48669500  | 1.44955600  | -0.00004200 |
|         | O      | 1.79097000  | -0.12654000 | 0.00026000  |
| 'CH₂COMe | C      | 1.35575000  | -0.35350100 | -0.00000300 |
|         | H      | 1.55317400  | -0.97282300 | -0.87997600 |
|         | H      | 2.02893900  | 0.50265400  | -0.00037100 |
|         | H      | 1.55333000  | -0.97215600 | 0.88040900  |
|         | C      | -0.08374700 | 0.11659400  | -0.00000900 |
|         | O      | -0.36863600 | 1.32405000  | 0.00000000  |
|         | C      | -1.12596100 | -0.87400300 | 0.00000000  |
|         | H      | -0.90308500 | -1.93409700 | -0.00001500 |
|         | H      | -2.15951800 | -0.55052100 | 0.00002300  |
| 'CH₂CONH₂ | C     | -1.27937200 | -0.58997800 | -0.00001300 |
|         | H     | -1.33800500 | -1.67127000 | 0.00000100  |
|         | H     | -2.18939700 | -0.00691000 | 0.00019600  |
|         | C     | -0.01107900 | 0.12154500  | -0.00002900 |
|         | O     | 0.04453300  | 1.35990100  | 0.00026000  |
|         | N     | 1.11602700  | -0.64832200 | -0.00019700 |
|         | H     | 2.01792300  | -0.19744100 | 0.00057300  |
|          | H        | CH₂F₂H     | CH₂FH     |
|----------|----------|------------|-----------|
| C        | 1.40351900 | -0.04037500 | -0.10765000 |
| H        | 2.21506600 | 0.16465100  | 0.57553100  |
| H        | 1.59846100 | -0.21723700 | -1.15741700 |
| C        | 0.01107700 | 0.00144700  | 0.36413500  |
| H        | -0.11121600| 0.02936700  | 1.44563300  |
| F        | -0.65203800 | 1.11663700  | -0.15281400 |
| F        | -0.70239400 | -1.08810500 | -0.11414800 |
| C        | 1.23845700 | -0.20604800 | -0.00018200 |
| H        | 1.68360400 | -0.53130000 | -0.93205200 |
| H        | 1.67628900 | -0.54782700 | 0.92927200  |
| C        | -0.02726000| 0.55063700  | 0.00167500  |
| H        | -0.15527900| 1.15726000  | 0.89834300  |
| F        | -1.14640700| -0.36761300 | -0.00147600 |
| H        | -0.15413600| 1.16285200  | -0.89123700 |
| C        | -0.48410700| 0.00001900  | 0.62893700  |
| C        | -2.02723100| 0.67751800  | -0.88769300 |
| C        | -2.02720800| -0.67763800 | -0.88764800 |
| H        | -2.61300800| 1.37876800  | -1.45645400 |
| H        | -2.61295900| -1.37894100 | -1.45637100 |
| N        | -1.08717400| -1.08393800 | 0.04578200  |
| N        | -1.08720900| 1.08391500  | 0.04570400  |
| C        | -0.75181400| -2.47124500 | 0.33595400  |
| H        | -1.47652300| -3.11608800 | -0.15861700 |
| H        | 0.29966300 | -2.70900100 | -0.02847100 |
| H        | -0.78443500| -2.64588800 | 1.41110200  |
| C        | -0.75191100| 2.47125600  | 0.33578500  |
| H        | -0.78472700| 2.64602700  | 1.41090800  |
| C        | -0.49627000| 2.70898200  | -0.02847800 |
| H        | -1.47653800| 3.11603000  | -0.15899400 |
| H        | 1.83112900 | 0.00015600  | 0.88033400  |
| B        | 0.69951700 | 0.00008500  | 1.64290500  |
| H        | 0.77621200 | -1.01822000 | 2.29330500  |
| H        | 0.77609100 | 1.01840000  | 2.29330300  |
| C        | 3.21845500 | 0.00022100  | 0.99777700  |
| H        | 3.64302200 | -0.91503800 | 0.50264200  |
| H        | 3.64265200 | 0.91587300  | 0.50213900  |
| N        | 2.96501800 | -0.00022000 | -1.29058000 |
| H        | 3.24511100 | 0.83236500  | -1.78916200 |
| H        | 3.24555100 | -0.83292400 | -1.78871700 |
| C        | 1.51752500 | -0.15632700 | 0.62784200  |
| C        | 2.66593200 | 0.64394500  | -1.14692900 |
| C        | 2.04963800 | 1.69609900  | -0.55309000 |
| H        | 3.30709400 | 0.60124300  | -2.01015800 |
| H        | 2.05060200 | 2.74287100  | -0.80254400 |
| N        | 1.35280100 | 1.19583500  | 0.53289400  |
| N        | 2.33425700 | -0.48361800 | -0.41640600 |
| C        | 0.51390300 | 1.99629200  | 1.41897100  |
| H        | -0.54132000 | 1.78086800  | 1.24094400  |
| Element | X   | Y     | Z      |
|---------|-----|-------|--------|
| H       | 0.75152800 | 1.77155500 | 2.45764200 |
| H       | 0.70618400 | 3.04922100 | 1.22117200 |
| C       | 2.78831500 | -1.83616000 | -0.72485300 |
| H       | 3.45814900 | -1.78818500 | -1.58137100 |
| H       | 3.31927900 | -2.25810000 | 0.12815200 |
| H       | 1.93901100 | -2.47592600 | -0.96623600 |
| H       | 1.39754300 | -2.19256400 | 1.75669000 |
| H       | 0.49164200 | -0.60844900 | 2.67278900 |
| B       | 0.83621300 | -1.13117700 | 1.64131200 |
| H       | -0.37163300 | -1.45411400 | 1.05051700 |
| C       | -1.68967500 | -1.94355300 | 0.47541900 |
| H       | -1.84311600 | -2.77600100 | 1.15282800 |
| H       | -1.30764800 | -2.22605800 | -0.50033300 |
| C       | -2.66478100 | -0.88981100 | 0.53162500 |
| H       | -3.25138700 | -0.75226600 | 1.43291400 |
| C       | -2.86362200 | 0.03520800 | -0.41689500 |
| F       | -3.73938000 | 1.04636900 | -0.33737100 |
| F       | -2.26059900 | 0.06281500 | -1.61235300 |

**TS3**

| Element | X   | Y     | Z      |
|---------|-----|-------|--------|
| C       | 0.82486000 | 0.10604600 | 0.61225300 |
| C       | 1.77813900 | -1.47417400 | -0.69190100 |
| C       | 2.36735000 | -0.28991600 | -0.99159300 |
| H       | 1.94852300 | -2.46197700 | -1.08342200 |
| H       | 3.14919800 | -0.05207100 | -1.69173100 |
| N       | 1.77676600 | 0.66986200 | -0.18880500 |
| N       | 0.83817000 | -1.22105300 | 0.29156200 |
| C       | 2.11775500 | 2.08934600 | -0.20526300 |
| H       | 2.96188300 | 2.23369400 | -0.87711100 |
| H       | 1.27155500 | 2.68022800 | -0.55762500 |
| H       | 2.38983900 | 2.42145200 | 0.79615200 |
| C       | -0.05312700 | -2.22484400 | 0.86448500 |
| H       | 0.27651200 | -3.20845300 | 0.53454600 |
| H       | -0.01801800 | -2.17574300 | 1.95191400 |
| H       | -1.07909300 | -2.05371700 | 0.53130700 |
| H       | -0.58777300 | 0.12934600 | 2.46708200 |
| H       | 0.23232900 | 1.92536100 | 1.94598300 |
| B       | -0.14508500 | 0.83534700 | 1.59522200 |
| H       | -1.25823600 | 1.09631400 | 0.81226200 |
| C       | -2.56912200 | 1.44750900 | 0.15847300 |
| H       | -2.30056100 | 2.45736800 | -0.13579700 |
| H       | -3.17212900 | 1.39162200 | 1.06121000 |
| C       | -2.83973200 | 0.49765900 | -0.88198900 |
| H       | -2.40172800 | 0.70936600 | -1.85669300 |
| C       | -3.52036300 | -0.66979800 | -0.73713100 |
| H       | -3.98093600 | -0.94402600 | 0.20750600 |
|     | TS4    |     |     |     |
|-----|--------|-----|-----|-----|
| H   | -3.64097800 | -1.35812000 | -1.56500500 |     |
| C   | -3.47766700 | -1.21005600 | 1.34047000  |     |
| H   | -3.62534400 | 0.53527700  | 1.60336900  |     |
| H   | -4.65980300 | -0.27226300 | 0.41865000  |     |
| C   | -2.61549000 | 1.37984400  | -0.82845900 |     |
| H   | -1.74477600 | 1.54186600  | -1.47280000 |     |
| H   | -3.51130600 | 1.54441900  | -1.45047100 |     |
| H   | -2.61435800 | 2.15439800  | -0.05459900 |     |
| C   | -2.86792200 | -1.13101100 | -1.19680300 |     |
| H   | -3.25643700 | -1.26970000 | -1.86083000 |     |
| H   | -1.51981400 | -0.94432300 | -1.83933500 |     |
| H   | -2.22646100 | -2.08114600 | -0.67648800 |     |
| C   | -2.61030600 | -0.00662000 | -0.22778700 |     |
| H   | -1.23305600 | -0.00326000 | 0.61134000  |     |
| B   | -0.19243500 | -0.00636000 | 1.46792700  |     |
| C   | 1.10335700  | 0.00010100  | 0.59148800  |     |
| H   | -0.32675400 | -1.01836400 | 2.10917900  |     |
| H   | -0.32732000 | 1.01581500  | 2.11123700  |     |
| N   | 1.76871300  | 1.08275300  | 0.08627700  |     |
| N   | 1.77045800  | -1.08213700 | 0.08752200  |     |
| C   | 2.81966600  | 0.67839900  | -0.72071800 |     |
| C   | 1.40791900  | 2.47127600  | 0.34596800  |     |
| C   | 2.82059000  | -0.67703500 | -0.72013000 |     |
| C   | 1.40929300  | -2.47092800 | 0.34507700  |     |
| H   | 3.46972700  | 1.38089600  | -1.21279700 |     |
| H   | 2.14405200  | 3.11601300  | -0.13103100 |     |
| H   | 0.41894400  | 2.69013800  | -0.05983500 |     |
| H   | 1.39832000  | 2.66256400  | 1.41893200  |     |
| H   | 3.47140800  | -1.37907500 | -1.21186200 |     |
| H   | 2.15203700  | -3.11511100 | -0.12234100 |     |
| H   | 1.38760400  | -2.66029200 | 1.41811600  |     |
| H   | 0.42544000  | -2.69227700 | -0.07189400 |     |
|     | TS5    |     |     |     |
| C   | 0.78542700  | -0.09236900 | 0.59735900  |     |
| C   | 2.41432900  | 0.19392900  | -0.93843200 |     |
| C   | 1.86592200  | 1.41052400  | -0.69385000 |     |
| H   | 3.21489200  | -0.09587200 | -1.59650200 |     |
| H   | 2.09678300  | 2.37969300  | -1.10035600 |     |
| N   | 0.87195500  | 1.22295100  | 0.24926500  |     |
| N   | 1.74505100  | -0.71757400 | -0.14287300 |     |
| C   | 0.00398200  | 2.27960800  | 0.76046000  |     |
| H   | 0.36645700  | 3.23516300  | 0.38613600  |     |
| H   | -1.02188300 | 2.12119500  | 0.42127800  |     |
| H   | 0.02290800  | 2.28435400  | 1.84935000  |     |
|   | C    | H    | B    | N    |
|---|------|------|------|------|
| C | 2.66256800 | -0.25055200 | -1.75462700 |
| C | 1.94470100 | 0.82247500 | -1.24070800 |
| C | 1.96630500 | 1.12791600 | 0.14253500 |
| C | 2.73951000 | 0.28556300 | 0.97911900 |
| C | 3.45555900 | -0.78635900 | 0.45997200 |
| C | 3.42558200 | -1.06573800 | -0.91090400 |
| H | 2.63306000 | -0.45394100 | -2.82019700 |
| H | 1.36094500 | 1.44818500 | -1.90880500 |
| H | 2.77601700 | 0.49206000 | 2.04423400 |
| H | 4.04554200 | -1.40874600 | 1.12501600 |
| H | 3.98772400 | -1.90032600 | -1.31407500 |
| C | 1.17488700 | 2.20307200 | 0.68672000 |
| H | 0.81207400 | 2.96058100 | -0.00104500 |
| H | 1.43708800 | 2.57606100 | 1.67158900 |
| H | -0.19995000 | 1.63456200 | 1.08228100 |
| B | -1.41179300 | 1.23737200 | 1.58383700 |
| C | -1.89014100 | 0.12207800 | 0.59607200 |
| H | -2.08994600 | 2.23507000 | 1.56035900 |
| H | -1.13471200 | 0.82600700 | 2.68408100 |
| N | -1.57000100 | -1.20418700 | 0.62479000 |
| N | -2.64220000 | 0.27700300 | -0.53255900 |
| C | -2.10538300 | -1.85767400 | -0.47069400 |
| C | -0.74083900 | -1.83799000 | 1.64557700 |
| C | -2.77808300 | -0.92958000 | -1.19585100 |
| C | -3.20704600 | 1.54301800 | -0.99007900 |
| H | -1.96864200 | -2.91243800 | -0.63442300 |
| H | -0.75963600 | -2.91458900 | 1.48637400 |
| H | 0.28724100 | -1.47855300 | 1.57567100 |
| H | -1.13212000 | -1.60987800 | 2.63618400 |
|       |      |      |      |
|-------|------|------|------|
| H     | -3.34011800 | -1.02377100 | -2.10873100 |
| H     | -3.84138800 | 1.34677900  | -1.85255800 |
| H     | -3.80164100 | 1.99528000  | -0.19724300 |
| H     | -2.41288900 | 2.23376700  | -1.27630800 |
|       |      |      |      |
| TS7   | C    | -0.82552200 | 0.01952800  | 0.60215200  |
| C     | -2.35347700 | 0.76344300  | -0.89276300 |
| C     | -2.43314900 | -0.58953600 | -0.86987000 |
| H     | -2.90808900 | 1.48971700  | -1.46127000 |
| H     | -3.07035600 | -1.26499700 | -1.41384800 |
| N     | -1.49747900 | -1.03415700 | 0.04977600  |
| N     | -1.37035100 | 1.12570600  | 0.01352500  |
| H     | 0.47827100  | 0.98371300  | 2.26283500  |
| H     | 0.38101800  | -1.04679200 | 2.27407800  |
| B     | 0.37014300  | -0.03243700 | 1.61346900  |
| H     | 1.49212300  | -0.08754900 | 0.87987500  |
| C     | 2.95515300  | -0.14805200 | 0.15886700  |
| H     | 3.55444600  | -0.30262400 | 1.05500200  |
| C     | 3.09146600  | 1.20732200  | -0.47429300 |
| H     | 2.29024200  | 1.38857600  | -1.20111300 |
| H     | 3.05652900  | 2.00768600  | 0.27088000  |
| H     | 4.04229300  | 1.31278900  | -1.02078200 |
| C     | -1.24385400 | -2.43572400 | 0.36322800  |
| H     | -0.24544600 | -2.72562400 | 0.03169200  |
| H     | -1.31950900 | -2.59859500 | 1.43786400  |
| H     | -1.98543900 | -3.04525500 | -0.15016900 |
| C     | 2.84785900  | -1.33868700 | -0.75095200 |
| H     | 2.64594900  | -2.25841600 | -0.19348300 |
| H     | 2.04401700  | -1.20636200 | -1.48534100 |
| H     | 3.77431000  | -1.50356800 | -1.32397100 |
| C     | -0.94957300 | 2.49656700  | 0.27938400  |
| H     | -1.00413800 | 2.70403700  | 1.34759700  |
| H     | 0.07657600  | 2.65171200  | -0.05806000 |
| H     | -1.61211400 | 3.17372100  | -0.25675900 |
|       |      |      |      |
| TS8   | C    | -0.94320300 | -0.08703500 | 0.58760100  |
| C    | -2.10060600 | 1.30130100  | -0.76833500 |
| C    | -2.56219400 | 0.04466100  | -0.98341600 |
| H    | -2.38755000 | 2.24048600  | -1.20839700 |
| H    | -3.32936400 | -0.31873000 | -1.64473900 |
| N    | -1.84675100 | -0.79581900 | -0.14741200 |
| N    | -1.11207400 | 1.20790000  | 0.19645000  |
| C    | -2.02555800 | -2.24298200 | -0.07375000 |
| H    | -2.82506000 | -2.52727900 | -0.75544300 |
| H    | -1.10635100 | -2.75282500 | -0.36294600 |
| H    | -2.29063100 | -2.53813000 | 0.94119300  |
|     | C       | H       | B       | S       | TS9     |
|-----|---------|---------|---------|---------|---------|
| C   | -0.3307 | 2.3345  | 0.6977  | 0.679   |         |
| H   | -0.7159 | 3.2486  | 0.2499  | 0.221   |         |
| H   | -0.4156 | 2.3965  | 1.7821  | 2.404   |         |
| H   | 0.7194  | 2.2129  | 0.4287  |         |         |
| H   | 0.4866  | 0.1661  | 2.4043  | 0.4911  |         |
| H   | -0.1771 | -1.7241 | 2.0533  |         |         |
| B   | 0.1288  | -0.6509 | 1.5872  | 0.8368  |         |
| H   | 1.2162  | -0.8837 | 0.8368  | 0.4911  |         |
| C   | 2.5953  | -1.2460 | 0.0439  | 0.0379  |         |
| H   | 3.1588  | -1.7529 | 0.8219  |         |         |
| H   | 2.2084  | -1.8954 | -0.7354 |         |         |
| S   | 3.3770  | 0.1910  | -0.6627 |         |         |
| H   | 3.6959  | 0.8144  | 0.4911  |         |         |
| C   | -1.6535 | -0.0001 | 0.4812  | 0.4911  |         |
| C   | -3.4783 | 0.6779  | -0.6691 | 0.4911  |         |
| C   | -3.4784 | -0.6777 | -0.6694 | 0.4911  |         |
| H   | -4.1693 | 1.3813  | -1.1004 | 0.4911  |         |
| H   | -4.1694 | -1.3810 | -1.1007 | 0.4911  |         |
| N   | -2.3578 | -1.0808 | 0.0382  | 0.0379  |         |
| N   | -2.5760 | 1.0808  | 0.0382  | 0.0379  |         |
| C   | -1.9766 | -2.4710 | 0.2676  | 0.2681  |         |
| H   | -2.7445 | -3.1144 | -0.1583 | 0.1238  |         |
| H   | -1.0197 | -2.6865 | 0.2088  | 0.2138  |         |
| H   | -1.8912 | -2.6648 | 1.3364  | 1.3364  |         |
| C   | -1.9762 | 2.4708  | 0.2681  | 0.1238  |         |
| H   | -2.7441 | 3.1144  | -0.1572 | 0.1238  |         |
| H   | -1.8904 | 2.6643  | 1.3370  | 1.3370  |         |
| H   | -1.0194 | 2.6863  | -0.2085 | 0.2138  |         |
| H   | -0.0914 | 1.0153  | 1.8695  | 1.8695  |         |
| H   | -0.0913 | -1.0164 | 1.8687  | 1.8687  |         |
| B   | -0.2777 | -0.0003 | 1.2380  | 0.2138  |         |
| H   | 0.6538  | 0.0001  | 0.2811  | 0.2138  |         |
| C   | 1.9429  | 0.0008  | -0.7625 | 0.2138  |         |
| C   | 3.1651  | -0.0001 | 0.1110  | 0.2138  |         |
| H   | 1.7252  | -0.9107  | -1.3161 | 0.2138  |         |
| H   | 1.7255  | 0.9134  | -1.3146 | 0.2138  |         |
| H   | 3.1473  | -0.8784 | 0.7693  | 0.2138  |         |
| H   | 3.1474  | 0.8768  | 0.7711  | 0.2138  |         |
| C   | 4.5017  | 0.0005  | -0.6623 | 0.2138  |         |
| H   | 4.5352  | 0.8784  | -1.3181 | 0.2138  |         |
| H   | 4.5348  | -0.8756 | -1.3202 | 0.2138  |         |
| C   | 5.7258  | -0.0007 | 0.2598  | 0.2138  |         |
| H   | 6.6579  | -0.0001 | -0.3128 | 0.2138  |         |
| H   | 5.7321  | 0.8817  | 0.9078  | 0.2138  |         |
|     | H   |      |      |      |
|-----|-----|------|------|------|
| **TS10** |     |      |      |      |
|     | C   |      |      |      |
| -1.11582000 | -0.00001900 | 0.48113400 |
| -2.90158900 | 0.67790000 | -0.72880800 |
| -2.90166600 | -0.67770900 | -0.72882300 |
| H   | -3.57788400 | 1.38120400 | -1.18278800 |
| H   | -3.57804200 | -1.38092900 | -1.18281200 |
| N   | -1.80503000 | -1.08078300 | 0.01518300 |
| N   | -1.80490900 | 1.08083400 | 0.01520900 |
|     | C   |      |      |      |
| -1.43099900 | -2.47091700 | 0.25668200 |
| H   | -2.18648300 | -3.11443000 | -0.19039500 |
| H   | -0.46095700 | -2.68695700 | -0.19210400 |
| H   | -1.37615500 | -2.66379500 | 1.32773100 |
| C   | -1.43071500 | 2.47092300 | 0.25672300 |
| H   | -2.18625700 | 3.11452800 | -0.19012000 |
| H   | -1.37559900 | 2.66370400 | 1.32777300 |
| H   | -0.46076200 | 2.68692900 | -0.19227800 |
| H   | 0.39999400 | 1.01581100 | 1.91932100 |
| H   | 0.39989300 | -1.01610800 | 1.91924200 |
| B   | 0.23478800 | -0.00011700 | 1.28243000 |
| H   | 1.19585800 | -0.00011200 | 0.35646200 |
| C   | 2.51938300 | -0.00007100 | -0.64593700 |
| C   | 3.71048900 | 0.00009600 | 0.27024900 |
| H   | 2.32201500 | -0.91250500 | -1.20594400 |
| H   | 2.32185600 | 0.91223700 | -1.20609400 |
| H   | 3.66796700 | -0.87672700 | 0.92751800 |
| H   | 3.66801200 | 0.87720200 | 0.92714300 |
| C   | 5.06576300 | -0.00009800 | -0.46562300 |
| H   | 5.16672700 | 0.88340700 | -1.10328300 |
| H   | 5.89970200 | 0.00002000 | 0.24507700 |
| H   | 5.16666800 | -0.88387400 | -1.10291700 |
| **TS11** |     |      |      |      |
|     | C   |      |      |      |
| 0.96058500 | 0.08495800 | -0.62010200 |
| C   | 2.53576000 | 0.23838500 | 0.98754900 |
| C   | 2.28102900 | -1.07964700 | 0.78963900 |
| H   | 3.22093200 | 0.72923000 | 1.65651300 |
| H   | 2.69997100 | -1.95409700 | 1.25637400 |
| N   | 1.31870200 | -1.15989700 | -0.19926100 |
| N   | 1.72263300 | 0.94059000 | 0.11730600 |
| H   | -0.07066700 | 1.57883900 | -2.08791300 |
| H   | -0.32779800 | -0.40143600 | -2.50310200 |
| B   | -0.14922000 | 0.45161800 | -1.69605600 |
| H   | -1.31281500 | 0.42816400 | -0.96552400 |
| C   | -2.73537600 | 0.46445000 | -0.31103900 |
| H   | -3.29937200 | 0.45760000 | -1.23964800 |
| C   | -2.72691200 | 1.76601400 | 0.46065500 |
|  | X       | Y       | Z       |
|---|---------|---------|---------|
| H | -2.01981000 | 1.72935100 | 1.29244500 |
| H | -2.43900000 | 2.58709200 | -0.19920400 |
| C | 0.72868900 | -2.40810800 | -0.67994200 |
| H | -0.28444100 | -2.52182800 | -0.29081300 |
| H | 0.69797300 | -2.40429500 | -1.76787900 |
| C | 1.67765300 | 2.39838200 | 0.02412600 |
| H | 1.78640000 | 2.70798200 | -1.01379400 |
| H | 0.73095700 | 2.77582300 | 0.41259900 |
| C | -2.81035800 | -0.74593800 | 0.46182900 |
| N | -2.78293000 | 0.98287400 | 1.91886200 |

**TS12**

|  | X       | Y       | Z       |
|---|---------|---------|---------|
| C | 2.53779900 | -0.00647000 | 0.46182900 |
| C | 4.30074500 | 0.69449900 | -0.77018400 |
| H | 4.96426700 | 1.40439400 | -1.23264000 |
| H | 4.99182500 | -1.35776000 | -1.23211500 |
| N | 3.23127600 | -1.07452400 | -0.01196600 |
| N | 3.20973800 | 1.08659200 | -0.01253800 |
| C | 2.87330600 | -2.46860200 | 0.23309400 |
| H | 2.82388000 | -2.65973100 | 1.30458000 |
| H | 1.90456900 | -2.69615200 | -0.21280400 |
| H | 3.63466200 | -3.10439200 | -0.21495700 |
| C | 2.82454000 | 2.47336600 | 0.23245200 |
| H | 1.84900900 | 2.68014600 | -0.20864700 |
| H | 2.77686600 | 2.66528300 | 1.30390900 |
| H | 3.57028000 | 3.12390200 | -0.22067800 |
| H | 1.04900400 | -1.03140700 | 1.91886200 |
| H | 1.03035200 | 1.00048400 | 1.92041600 |
| B | 1.19701700 | -0.01356800 | 1.28130200 |
| C | -1.10210100 | -0.03226300 | -0.62858500 |
| H | -0.91802900 | -0.96016800 | -1.16574100 |
| H | -0.90182800 | 0.86523000 | -1.20979200 |
| C | -2.27997800 | 0.00017800 | 0.30229900 |
| H | -2.23040300 | 0.89729900 | 0.93175200 |
| H | -2.23804700 | -0.85892900 | 0.98331500 |
| H | 0.22663800 | -0.02133900 | 0.36665200 |
| C | -3.64030100 | -0.01553400 | -0.42404000 |
| H | -3.71927300 | -0.91307400 | -1.04412200 |
| H | -3.71273300 | 0.84539600 | -1.09475600 |
| C | -4.81794800 | 0.01737500 | 0.57571800 |
| H | -4.76393700 | 0.91420400 | 1.20078300 |
| H | -4.77151300 | -0.84400400 | 1.24936800 |
|    | C   | N   | TS13  |    | C   | N   | TS14  |
|----|-----|-----|-------|----|-----|-----|-------|
|    | -6.1196800 | 0.00485600 | -0.08269600 |    | -7.14024600 | -0.00552100 | -0.62265300 |
| C  | 3.79282200 | -0.67810300 | -0.58107500 | H  | 4.50413500 | -1.38149300 | -0.97762100 |
| N  | 2.63976600 | 1.08037900 | 0.07105100 | C  | 2.24778500 | 2.47142600 | 0.28044200 |
| H  | 1.32300700 | 2.69016400 | -0.25423000 | H  | 2.09706600 | 2.66187400 | 1.34241000 |
| C  | 3.79297900 | 0.67769400 | -0.58116000 | H  | 3.04217400 | 3.11373000 | -0.09510000 |
| H  | 2.63952900 | -1.08044100 | 0.07120800 | N  | 2.63952900 | -1.08044100 | 0.07120800 |
| C  | 2.24715300 | -2.47136800 | 0.28065100 | C  | 2.24715300 | -2.47136800 | 0.28065100 |
| H  | 3.04160500 | -3.11390000 | -0.09436600 | H  | 3.04160500 | -3.11390000 | -0.09436600 |
| H  | 2.09584700 | -2.66158300 | 1.34257400 | H  | 2.09584700 | -2.66158300 | 1.34257400 |
| C  | 0.50700700 | 0.00026700 | 1.17721400 | H  | -0.38199600 | 0.00014800 | 0.18655700 |
| H  | -1.64754000 | -0.00014000 | -0.89228000 | C  | -1.64754000 | -0.00014000 | -0.89228000 |
| H  | -1.42538800 | 0.91379700 | -1.43791900 | H  | -1.42525800 | -0.91422800 | -1.43760900 |
| C  | -2.86579300 | -0.00065000 | -0.01854600 | H  | -2.86588300 | 0.87892300 | 0.63324000 |
| H  | -2.86599500 | -0.87904900 | 0.63324300 | H  | -2.86599500 | -0.87904900 | 0.63324300 |
| C  | -4.19072600 | 0.00002400 | -0.83688000 | H  | -4.23609100 | 0.88000000 | -1.48452100 |
| H  | -4.23621500 | -0.87994100 | -1.48452600 | C  | -5.37719200 | 0.00010600 | 0.01508000 |
| N  | -6.29527100 | 0.00016600 | 0.71565400 | H  | 0.29469800 | -1.01526000 | 1.79957800 |
| H  | 0.50700700 | 0.00026700 | 1.17721400 | B  | -0.38199600 | 0.00014800 | 0.18655700 |
| C  | -1.64754000 | -0.00014000 | -0.89228000 | H  | -1.42538800 | 0.91379700 | -1.43791900 |
| H  | -1.42525800 | -0.91422800 | -1.43760900 | C  | -2.86579300 | -0.00065000 | -0.01854600 |
| H  | -2.86588300 | 0.87892300 | 0.63324000 | H  | -2.86599500 | -0.87904900 | 0.63324300 |
| C  | -4.19072600 | 0.00002400 | -0.83688000 | H  | -4.23609100 | 0.88000000 | -1.48452100 |
| H  | -4.23621500 | -0.87994100 | -1.48452600 | C  | -5.37719200 | 0.00010600 | 0.01508000 |
| C  | 0.53798200 | 0.00002000 | 0.45854900 |
| C  | 2.41721300 | -0.67746100 | -0.60130900 |
| C  | 2.41697500 | 0.67807400 | -0.60136400 |
| H  | 3.12883400 | -1.38044100 | -0.99809800 |
| H  | 3.12834600 | 1.38127100 | -0.99821600 |
| N  | 1.26309300 | 1.08105600 | 0.05044800 |
| N  | 1.26347000 | -1.08079200 | 0.05052800 |
| C  | 0.87047300 | 2.47109400 | 0.25986100 |
| H  | 1.66138000 | 3.11452100 | -0.12135700 |
| H  | -0.05816900 | 2.68789300 | -0.26913400 |
| H  | 0.72537600 | 2.66360000 | 1.32250200 |
| C  | 0.87131900 | -2.47094300 | 0.26006700 |
|   | 1.66219800  | -3.11414500  | -0.12158800  |
|---|------------|--------------|--------------|
| H | 0.72680000  | -2.66355800  | 1.32277100   |
| H | -0.05753000  | -2.68793800  | -0.26847700  |
| H | -1.08787800  | -1.01597100  | 1.77076400   |
| H | -1.08497700  | 1.01556600   | 1.77039500   |
| B | -0.87211800  | -0.00024700  | 1.14859400   |
| H | -1.76005300  | -0.00073700  | 0.15066200   |
| C | -3.01459600  | -0.00137100  | -0.93085600  |
| C | -4.25913000  | 0.00064700   | -0.09005500  |
| H | -2.78060400  | -0.91398400  | -1.47440600  |
| H | -2.77932500  | 0.90939800   | -1.47694200  |
| H | -4.30510100  | 0.88489200   | 0.55377400   |
| H | -5.17622600  | 0.00045700   | -0.69795700  |
| H | -4.30631800  | -0.88179800  | 0.55615200   |

**TS15**

|   | -3.17937500  | 0.68506200   | -0.76219200  |
|---|-------------|--------------|--------------|
| C | -3.84808500  | 1.39164800   | -1.22213900  |
| H | -3.18478100  | -0.67033300  | -0.76305400  |
| H | -3.85908900  | -1.37154500  | -1.22396400  |
| N | -2.09778400  | -1.07761400  | -0.00839000  |
| C | -1.72994300  | -2.47083600  | 0.23304200   |
| H | -0.76320300  | -2.69166100  | -0.22006000  |
| H | -1.67306100  | -2.66220900  | 1.30379800   |
| H | -2.49074400  | -3.10982800  | -0.21104700  |
| N | -2.08916800  | 1.08211600   | -0.00700300  |
| C | -1.71061000  | 2.47207200   | 0.23658900   |
| H | -2.46469600  | 3.11761100   | -0.20948600  |
| H | -1.65553900  | 2.66230700   | 1.30765900   |
| H | -0.74067300  | 2.68517500   | -0.21332200  |
| C | -1.41150100  | -0.00076300  | 0.46323700   |
| H | 0.08173600   | 1.00741200   | 1.93364400   |
| B | -0.07079500  | -0.00660400  | 1.29182600   |
| H | 0.89609900   | -0.00964500  | 0.39097000   |
| C | 2.27680000   | -0.01222100  | -0.57801400  |
| H | 2.13907800   | -0.93441600  | -1.13319700  |
| H | 2.13204800   | 0.89988600   | -1.14788900  |
| C | 3.38013800   | 0.00030900   | 0.45352700   |
| H | 3.30588600   | 0.88384100   | 1.09565000   |
| H | 3.31302800   | -0.87357400  | 1.10950700   |
| C | 4.71612200   | 0.00091100   | -0.15195500  |
| N | 5.75357000   | 0.00108000   | -0.66158600  |
| H | 0.07376300   | -1.02266600  | 1.93221400   |

**TS16**

|   | -0.44758000  | -0.00004800  | 0.63025100   |
|---|--------------|--------------|--------------|
| C | -2.00602000  | 0.67813000   | -0.85734400  |
| C | -2.00618000  | -0.67765600  | -0.85743600  |
| Element | X     | Y     | Z     |
|---------|-------|-------|-------|
| H       | -2.59893400 | 1.38099600 | -1.41629300 |
| H       | -2.59925900 | -1.38030600 | -1.41648400 |
| N       | -1.05083900 | -1.08029700 | 0.06008500 |
| N       | -1.05058500 | 1.08042100 | 0.06023100 |
| C       | -0.70891200 | -2.47160100 | 0.34335700 |
| H       | -1.45511300 | -3.11325600 | -0.12164300 |
| H       | 0.27601900  | -2.71121900 | -0.05993100 |
| H       | -0.70287700 | -2.63936600 | 1.41897200 |
| C       | -0.70831600 | 2.47160600 | 0.34367600 |
| H       | -1.45432700 | 3.11350000 | -0.12129700 |
| H       | -0.70230200 | 2.63925400 | 1.41931000 |
| H       | 0.27669800  | 2.71101500 | -0.05953400 |
| H       | 0.80796900  | 1.01544700 | 2.30435000 |
| H       | 0.80772100  | -1.01602000 | 2.30434000 |
| B       | 0.75192100  | -0.00024900 | 1.64964700 |
| C       | -0.51066400 | -0.10313500 | 0.53802900 |
| C       | -1.78602100 | 1.34247000 | -0.64602400 |
| C       | -2.33441000 | 0.11056700 | -0.78362000 |
| H       | -2.08865900 | 2.29488100 | -1.04544400 |
| H       | -3.20600200 | -0.21361400 | -1.32547500 |
| N       | -1.54789900 | -0.76594500 | -0.05389600 |
| N       | -0.67226500 | 1.20053400 | 0.16498200 |
| C       | -1.77812800 | -2.20343200 | 0.04188200 |
| C       | -2.74263800 | -2.43118000 | -0.40872100 |
| H       | -0.99558900 | -2.75233700 | -0.48452300 |
| H       | -1.78308600 | -2.51096100 | 1.08684200 |
| C       | 0.22570300  | 2.28536800 | 0.54512000 |
| H       | -0.14239300 | 3.21010400 | 0.10430700 |
| H       | 0.25653600  | 2.38754000 | 1.63014000 |
| H       | 1.23322800  | 2.08393000 | 0.17850200 |
| H       | 1.15694000  | 0.07270400 | 2.14650300 |
| H       | 0.42097500  | -1.79784900 | 1.83169800 |
| B       | 0.67365200  | -0.71260100 | 1.36112700 |
| H       | 1.65609100  | -0.92746700 | 0.46241500 |
| C       | 2.97614100  | -1.07705900 | -0.47567400 |
| H       | 3.62649300  | -1.70423500 | 0.13409200 |
| H       | 2.58844800  | -1.53481200 | -1.38067100 |
| O       | 3.45209900  | 0.20530400 | -0.73788100 |
| H       | 3.82002200  | 0.57306300 | 0.07333200 |

TS17

| Element | X     | Y     | Z     |
|---------|-------|-------|-------|
| C       | -0.51066400 | -0.10313500 | 0.53802900 |
| C       | -1.78602100 | 1.34247000 | -0.64602400 |
| C       | -2.33441000 | 0.11056700 | -0.78362000 |
| H       | -2.08865900 | 2.29488100 | -1.04544400 |
| H       | -3.20600200 | -0.21361400 | -1.32547500 |
| N       | -1.54789900 | -0.76594500 | -0.05389600 |
| N       | -0.67226500 | 1.20053400 | 0.16498200 |
| C       | -1.77812800 | -2.20343200 | 0.04188200 |
| C       | -2.74263800 | -2.43118000 | -0.40872100 |
| H       | -0.99558900 | -2.75233700 | -0.48452300 |
| H       | -1.78308600 | -2.51096100 | 1.08684200 |
| C       | 0.22570300  | 2.28536800 | 0.54512000 |
| H       | -0.14239300 | 3.21010400 | 0.10430700 |
| H       | 0.25653600  | 2.38754000 | 1.63014000 |
| H       | 1.23322800  | 2.08393000 | 0.17850200 |
| H       | 1.15694000  | 0.07270400 | 2.14650300 |
| H       | 0.42097500  | -1.79784900 | 1.83169800 |
| B       | 0.67365200  | -0.71260100 | 1.36112700 |
| H       | 1.65609100  | -0.92746700 | 0.46241500 |
| C       | 2.97614100  | -1.07705900 | -0.47567400 |
| H       | 3.62649300  | -1.70423500 | 0.13409200 |
| H       | 2.58844800  | -1.53481200 | -1.38067100 |
| O       | 3.45209900  | 0.20530400 | -0.73788100 |
| H       | 3.82002200  | 0.57306300 | 0.07333200 |
| TS18 | C   | 0.02908100  | -0.00001200  | 0.46415800  |
|      | C   | 1.89805500  | -0.67780100  | -0.60841900 |
|      | C   | 1.89798000  | 0.67797800   | -0.60842100 |
|      | H   | 2.60627000  | -1.38127200  | -1.01030800 |
|      | H   | 2.60612100  | 1.38152500   | -1.01030700 |
|      | N   | 0.74914000  | 1.07995500   | 0.05193600  |
|      | C   | 0.57104000  | 2.47117200   | 0.26383000  |
|      | H   | 1.14718000  | 3.11366200   | -0.12179600 |
|      | H   | -0.57280800 | 2.68716400   | -0.26418700 |
|      | H   | 0.21590200  | 2.66334700   | 1.32528100  |
|      | C   | 0.35735300  | -2.47116100  | 0.26234500  |
|      | H   | -0.57236000 | -2.68731600  | -0.26448700 |
|      | H   | 0.21586000  | -2.66329600  | 1.32520900  |
|      | B   | -1.37761400 | -0.00008600  | 1.17330900  |
|      | H   | -2.69180000 | -0.00094000  | 0.19652000  |
|      | C   | -3.52272000 | -0.00010300  | -0.94128800 |
|      | H   | -4.39036600 | -0.00130800  | -0.28911000 |
|      | H   | -4.39837300 | 0.92268100   | -1.47509900 |
|      | H   | -3.32596400 | -0.92168200  | -1.47665000 |

| TS19 | C   | -0.73065800 | -0.15439100 | 0.59133000 |
|      | C   | -2.30139500 | 0.32114100  | -0.95394600 |
|      | C   | -1.70174800 | 1.48829000  | -0.60812200 |
|      | H   | -3.09906800 | 0.11844400  | -1.64723600 |
|      | H   | -1.87418000 | 2.49507400  | -0.94687000 |
|      | N   | -0.74549100 | 1.18258400  | 0.34174700  |
|      | N   | -1.69775900 | -0.67615300 | -0.21083200 |
|      | C   | 0.16857500  | 2.15792600  | 0.93479300  |
|      | H   | -0.25939600 | 3.15146600  | 0.81494500  |
|      | H   | 0.29515600  | 1.93972600  | 1.99285300  |
|      | H   | 1.13943700  | 2.11571800  | 0.43830000  |
|      | C   | -2.04137600 | -2.09492600 | -0.30030400 |
|      | H   | -1.22793200 | -2.65366500 | -0.76397100 |
|      | H   | -2.22954300 | -2.49547800 | 0.69398300  |
|      | H   | -2.93869000 | -2.19256200 | -0.90804400 |
|      | H   | 0.62958700  | -0.28275600 | 2.48418800  |
|      | H   | -0.13639900 | -2.04789200 | 1.82019600  |
|      | B   | 0.24941600  | -0.93923200 | 1.54535200  |
|      | H   | 1.35391500  | -1.12350400 | 0.82039600  |
|      | C   | 3.08161900  | -0.22716800 | -0.63862000 |
|      | N   | 3.27518100  | 0.78501900  | -1.18444100 |
|   |   |   |   |
|---|---|---|---|
| C | 2.76892000 | -1.40500500 | 0.05200800 |
| H | 2.45013000 | -2.25240700 | -0.54299500 |
| H | 3.36275500 | -1.63136300 | 0.92934700 |
| **TS20** |   |   |   |
| C | -0.81804700 | -0.15276000 | 0.54539000 |
| C | -1.76465000 | 1.57003800 | -0.55325700 |
| C | -2.49978400 | 0.46099000 | -0.82172100 |
| H | -1.88318000 | 2.58844400 | -0.87989000 |
| H | -3.38261200 | 0.33034700 | -1.42290500 |
| N | -1.90815100 | -0.58666100 | -0.14118700 |
| N | -0.74103800 | 1.17899000 | 0.28801500 |
| C | -2.38904800 | -1.96822000 | -0.17572100 |
| H | -1.88318000 | 2.58844400 | -0.87989000 |
| H | -3.38261200 | 0.33034700 | -1.42290500 |
| H | -3.34332100 | -1.98473600 | -0.69836700 |
| C | 0.31519500 | 2.06701900 | 0.77577400 |
| H | -0.00492300 | 3.09656400 | 0.62701500 |
| H | 0.48037400 | 1.88658300 | 1.83620900 |
| H | 1.24198900 | 1.88552500 | 0.22923500 |
| H | 0.65863800 | -0.40727200 | 2.33382600 |
| B | 0.19012200 | -1.01697700 | 1.40246500 |
| H | 1.22782700 | -1.21178500 | 0.61299600 |
| C | 2.47597200 | -1.48665600 | -0.42223900 |
| H | 2.73803200 | -2.44966000 | -0.00040700 |
| H | 1.83365500 | -1.48357100 | -1.29593000 |
| C | 3.36188600 | -0.38775900 | -0.22485600 |
| O | 3.27794600 | 0.70787300 | -0.80882600 |
| H | -0.23146500 | -2.11330200 | 1.67152400 |
| H | 4.14647800 | -0.53099000 | 0.54115400 |
| **TS21** |   |   |   |
| C | -1.17296200 | -0.16370800 | 0.52775200 |
| C | -2.29430600 | 1.50547700 | -0.48713400 |
| C | -2.97700700 | 0.35541700 | -0.71824100 |
| H | -2.49553900 | 2.51680900 | -0.79470600 |
| H | -3.88760500 | 0.17545100 | -1.26251600 |
| N | -2.27744900 | -0.65897000 | -0.09063200 |
| N | -1.19356100 | 1.17159500 | 0.27869400 |
| C | -2.67415800 | -2.06714300 | -0.10293200 |
| H | -1.91311300 | -2.66939000 | -0.59812700 |
| H | -2.80990400 | -2.42771600 | 0.91556400 |
| H | -3.61264100 | -2.15321500 | -0.64690500 |
| C | -0.16638200 | 2.11845300 | 0.71485500 |
| H | -0.51290800 | 3.12604100 | 0.49329800 |
| H | -0.00420800 | 2.01644900 | 1.78666400 |
| H | 0.76903000 | 1.92760300 | 0.18719700 |
| H | 0.43470600 | -0.32263800 | 2.20524300 |
|   |   |   |   |
|---|---|---|---|
| B | -0.05986900 | -0.96792000 | 1.31141600 |
| H | 0.91706900 | -1.12820400 | 0.44943800 |
| C | 2.15828100 | -1.33821700 | -0.67379200 |
| H | 2.48089100 | -2.30200800 | -0.30518100 |
| H | 1.50641500 | -1.31097400 | -1.53516300 |
| H | 0.91706900 | -1.12820400 | 0.44943800 |
| C | 2.84339600 | 0.92113200 | -0.95866000 |
| O | 3.97333100 | -0.40628100 | 0.47634200 |
| H | 4.44558800 | 0.43197300 | 0.59116500 |
| H | -0.41318700 | -2.07752100 | 1.62560700 |
| TS22 |   |   |   |
| C | -0.80196200 | -0.00653600 | 0.62833500 |
| C | -2.35939500 | 0.47387500 | -0.93161600 |
| C | -2.19265700 | -0.87210300 | -0.92323900 |
| H | -3.00608300 | 1.09903900 | -1.52218900 |
| H | -2.66606600 | -1.64294100 | -1.50593200 |
| N | -1.23706700 | -1.15205700 | 0.03764600 |
| N | -1.50235300 | 0.99083700 | 0.02431100 |
| C | -0.74308800 | -2.49039700 | 0.35494500 |
| H | -1.29335200 | -3.21229100 | -0.24539900 |
| H | 0.32011500 | -2.56314000 | 0.12535200 |
| H | -0.89501700 | -2.70409400 | 1.41222200 |
| C | -1.35493000 | 2.41414100 | 0.32213600 |
| H | -2.08903700 | 2.96542100 | -0.26237000 |
| H | -1.52493200 | 2.59321600 | 1.38273900 |
| H | -0.35317500 | 2.75377800 | 0.05839900 |
| H | 0.26599500 | 1.17313900 | 2.32884600 |
| H | 0.42580700 | -0.85008300 | 2.41442600 |
| B | 0.33271800 | 0.13334800 | 1.71597800 |
| H | 1.45961800 | 0.18651700 | 1.03566300 |
| C | 2.87865400 | 0.22071900 | 0.10649600 |
| H | 3.79254100 | 0.40593100 | 0.67211800 |
| F | 2.93141600 | -0.98375700 | -0.52713500 |
| F | 2.68149500 | 1.18588100 | -0.83395400 |
| TS23 |   |   |   |
| C | -1.42418700 | 0.02365900 | 0.67521700 |
| C | -2.61362600 | 0.37273100 | -1.20745700 |
| C | -2.40329600 | -0.96306200 | -1.09899800 |
| H | -3.13694300 | 0.94403900 | -1.95145000 |
| H | -2.70873400 | -1.77702200 | -1.73311000 |
| N | -1.67613500 | -1.16156300 | 0.06070900 |
| N | -2.00934300 | 0.96362200 | -0.11250600 |
| C | -1.20603900 | -2.46421700 | 0.53071400 |
| H | -1.68740500 | -3.23892000 | -0.06301000 |
| H | -0.12429200 | -2.53704400 | 0.41625400 |
| H | -1.46572900 | -2.59356200 | 1.57966700 |
|     | C     | H     | B     | F     |
|-----|-------|-------|-------|-------|
| C   | -1.98176300 | 2.40347400 | 0.14161900 |     |
| H   | -2.59353700 | 2.89694500 | -0.61099300 |     |
| H   | -2.38077900 | 2.61515000 | 1.13227800 |     |
| H   | -0.96008200 | 2.77819200 | 0.07963400 |     |
| H   | -0.86087000 | 1.30268000 | 2.53594600 |     |
| H   | -0.57236100 | -0.69657500 | 2.71862200 |     |
| B   | -0.57002600 | 0.26573400 | 1.98621800 |     |
| H   | 0.65774900  | 0.40517900 | 1.58909300 |     |
| C   | 2.37400200  | 0.62151500 | 1.17978200 |     |
| H   | 2.44657300  | 1.69567000 | 1.28453100 |     |
| H   | 2.81633400  | 0.00617100 | 1.95155900 |     |
| C   | 2.46957600  | 0.10359500 | 0.19755200 |     |
| F   | 2.13472000  | -1.21414200 | -1.06638000 |     |
| F   | 1.67343200  | 0.77216100 | -1.06638000 |     |
| F   | 3.73968700  | 0.18307600 | -0.73149100 |     |

**TS24**

|     | C     | H     | N     |
|-----|-------|-------|-------|
| C   | -0.89976600 | -0.10293300 | 0.63528600 |
| C   | -2.00024700 | 1.21458500  | -0.83005000 |
| C   | -2.36049600 | -0.06770900 | -1.08507000 |
| H   | -2.30050400 | 2.13557500  | -1.29861000 |
| H   | -3.03587300 | -0.47597900 | -1.81661600 |
| N   | -1.68055400 | -0.86380500 | -0.17955200 |
| N   | -1.10765400 | 1.17853700  | 0.22678300  |
| C   | -1.77324300 | -2.32110200 | -0.12516000 |
| H   | -2.52937500 | -2.64495500 | -0.83777600 |
| H   | -0.81527000 | -2.77186700 | -0.38544800 |
| H   | -2.05656800 | -2.64033200 | 0.87667000  |
| C   | -0.44245600 | 2.34976500  | 0.79258000  |
| H   | -0.87846200 | 3.24290900  | 0.34907400  |
| H   | -0.58354600 | 2.37217000  | 1.87202000  |
| H   | 0.62539000  | 2.31950700  | 0.57250500  |
| H   | 0.27158200  | 0.22935600  | 2.61664100  |
| H   | -0.18471900 | -1.69885400 | 2.17129000  |
| B   | 0.09554900  | -0.59952800 | 1.75293700  |
| H   | 1.26229600  | -0.72548000 | 1.14724200  |
| C   | 2.79977200  | -0.91996100 | 0.48597200  |
| H   | 3.44569600  | -0.65307800 | 1.31662200  |
| H   | 2.79651000  | -1.95555700 | 0.16780200  |
| Cl  | 3.00477400  | 0.18501400  | -0.88736400 |

**TS25**

|     | C     | H     | N     |
|-----|-------|-------|-------|
| C   | -0.93597300 | -0.04293200 | 0.51834900 |
| C   | -2.43015600 | 1.18658400  | -0.65519400 |
| C   | -2.84730600 | -0.10254600 | -0.69222300 |
| H   | -2.85850800 | 2.07612000  | -1.08333700 |
| H   | -3.70827400 | -0.54933900 | -1.15834400 |
| N   | -1.92725600 | -0.84600000 | 0.02898600  |
|   | X         | Y         | Z         |
|---|-----------|-----------|-----------|
| N | -1.261362 | 1.212199  | 0.087989  |
| C | -1.997290 | -2.289462 | 0.226008  |
| H | -2.908590 | -2.658937 | -0.241034 |
| H | -1.135016 | -2.777589 | -0.229896 |
| H | -2.013870 | -2.524310 | 1.290324  |
| C | -0.471988 | 2.409340  | 0.354973  |
| H | -0.991123 | 3.267904  | -0.067478 |
| H | -0.353122 | 2.549439  | 1.429355  |
| H | 0.514964  | 2.322618  | -0.101459 |
| H | 0.837118  | 0.411327  | 1.949327  |
| H | 0.218048  | -1.526237 | 1.886288  |
| B | 0.351243  | -0.480480 | 1.292474  |
| O | 3.276458  | 0.047070  | -0.839651 |
| C | 4.148182  | 0.222635  | 0.273710  |
| C | 4.804793  | -0.648591 | 0.390800  |
| H | 4.752126  | 1.107091  | 0.072824  |
| H | 3.575692  | 0.367357  | 1.195150  |
|   |           |           |           |
|TS26|          |           |           |
| C | -1.280756 | -0.059311 | 0.574812  |
| C | -2.438729 | 1.396895  | -0.709623 |
| C | -3.042442 | 0.188038  | -0.820872 |
| H | -2.679582 | 2.346239  | -1.155513 |
| H | -3.909748 | -0.115471 | -1.381083 |
| N | -2.326641 | -0.694698 | -0.029356 |
| N | -1.364204 | 1.234064  | 0.148162  |
| C | -2.636323 | -2.113406 | 0.118446  |
| H | -3.587337 | -2.312749 | -0.372216 |
| H | -1.858127 | -2.724466 | -0.341025 |
| H | -2.710705 | -2.370557 | 1.174230  |
| C | -0.424628 | 2.289341  | 0.514222  |
| H | -0.772151 | 3.226583  | 0.083240  |
| H | -0.372955 | 2.384825  | 1.598479  |
| H | 0.569946  | 2.058938  | 0.128669  |
| H | 0.344621  | 0.097744  | 2.230156  |
| H | -0.485246 | -1.742904 | 1.972099  |
| B | -0.159309 | -0.694117 | 1.467199  |
| H | 0.832335  | -1.002929 | 0.600090  |
| C | 2.034901  | -1.435454 | -0.386103 |
| H | 2.552097  | -2.189403 | 0.204613  |
| H | 1.453759  | -1.832514 | -1.123999 |
| S | 3.027194  | -0.061274 | -0.895793 |
|   | C    | H    | N    | C    | H    | N    | C    | H    | N    | C    | H    | N    |
|---|------|------|------|------|------|------|------|------|------|------|------|------|
| C | 3.89020500 | 0.33236300 | 0.66565600 |
| H | 4.49246200 | -0.51733100 | 0.99064700 |
| H | 4.54386800 | 1.18176400 | 0.46698600 |
| H | 3.17075600 | 0.59684800 | 1.44041700 |
| TS27 | C | -0.96601200 | -0.05880800 | 0.59914900 |
|     | C | -2.09091600 | 1.34886500 | -0.77662400 |
|     | C | -2.59935200 | 0.10682200 | -0.96467400 |
|     | H | -2.34994400 | 2.28941900 | -1.23115000 |
|     | H | -3.38617900 | -0.23863300 | -1.61264700 |
|     | N | -1.90877600 | -0.74702800 | -0.11928200 |
|     | N | -1.09751500 | 1.24030400 | 0.18329700 |
|     | C | -2.13878800 | -2.18190300 | -0.01762400 |
|     | H | -2.97815000 | -2.44604200 | -0.65891900 |
|     | H | -1.25379400 | -2.73465800 | -0.33724100 |
|     | H | -2.36986500 | -2.45992200 | 1.01245900 |
|     | C | -0.26635300 | 2.34233800 | 0.64728200 |
|     | H | -0.29711300 | 2.40435200 | 1.73514100 |
|     | H | 0.76882200 | 2.19644100 | 0.33197900 |
|     | H | -0.64672600 | 3.26905600 | 0.22065400 |
|     | H | 1.17100600 | -0.96172500 | 0.77548100 |
|     | B | 0.10206500 | -0.64415700 | 1.57032700 |
|     | H | -0.21988300 | -1.69965500 | 2.06799500 |
|     | H | 0.54466300 | 0.16737700 | 2.35114800 |
|     | C | 2.47160500 | -1.38490500 | -0.03020400 |
|     | H | 2.06190700 | -2.22356200 | -0.58583000 |
|     | H | 3.11294300 | -1.66361900 | 0.80725100 |
|     | N | 2.91071900 | -0.31414800 | -0.82634000 |
|     | H | 3.00405800 | -0.52421700 | -1.81034800 |
|     | C | 3.96819700 | 0.53783100 | -0.30579000 |
|     | H | 4.16834500 | 1.34846900 | -1.00894500 |
|     | H | 3.64974300 | 0.98388000 | 0.64011200 |
|     | H | 4.90855700 | -0.00643600 | -0.12160400 |
| TS28 | C | 1.20476800 | 0.21144300 | 0.60885200 |
|     | C | 1.90955400 | -1.57455100 | -0.58495800 |
|     | C | 2.40122600 | -0.46384500 | -1.18721800 |
|     | H | 2.01632300 | -2.61554600 | -0.83575800 |
|     | H | 3.02001200 | -0.35409600 | -2.06077700 |
|     | N | 1.96615900 | 0.62260400 | -0.44736000 |
|     | N | 1.18372400 | -1.15039400 | 0.51488700 |
|     | C | 2.26304800 | 2.01566000 | -0.76542800 |
|     | H | 2.95444100 | 2.03880000 | -1.60576300 |
|     | H | 1.35001200 | 2.54805900 | -1.03538800 |
|     | H | 2.71812500 | 2.50741300 | 0.09374700 |
|     | C | 0.46255900 | -2.03676000 | 1.42263700 |
|        | C          | O          | H          |
|--------|------------|------------|------------|
|        | 0.72355400 | -1.80439000| 2.45415000 |
|        | -0.61473800| -1.92078300| 1.29316400 |
|        | 0.74331900 | -3.06438700| 1.19886600 |
|        | -0.76615500| 1.36591900 | 1.07734600 |
|        | 0.44178300 | 1.11264000 | 1.63851400 |
|        | 0.93975100 | 2.20506100 | 1.77933800 |
|        | 0.17418700 | 0.54112300 | 2.66923600 |
|        | -2.22147000| 1.70642800 | 0.52217600 |
|        | -1.95319800| 2.30969100 | -0.33858500|
|        | -2.65897400| 2.24438000 | 1.35469800 |
|        | -2.88669500| 0.50821500 | 0.20186900 |
|        | -3.35159900| 0.00705200 | 0.95003300 |
|        | -2.80799300| -0.15052900| -0.97866300|
|        | -2.27016300| 0.41737000 | -1.75417200|
|        | -3.29328600| -1.26236500| -1.19285800|

**TS29**

|        | C          | O          | H          |
|--------|------------|------------|------------|
|        | -1.17436300| -0.17813800| 0.52109700 |
|        | -2.32006300| 1.50659200 | -0.43894300|
|        | -3.00902900| 0.36030500 | -0.67077200|
|        | -2.52831200| 2.52248000 | -0.72621200|
|        | -3.93347700| 0.18925000 | -1.19439600|
|        | -2.29460700| -0.66398500| -0.07730300|
|        | -1.20071000| 1.16124300 | 0.29371500 |
|        | -2.69242200| -2.07158100| -0.10197600|
|        | -1.94744800| -2.66554900| -0.63060700|
|        | -2.79768100| -2.44977600| 0.91376900 |
|        | -3.64707400| -2.14809800| -0.61857100|
|        | -0.16048800| 2.10075800 | 0.71489900 |
|        | -0.51685800| 3.11215600 | 0.52903000 |
|        | 0.03849200 | 1.97480700 | 1.77798700 |
|        | 0.75669500 | 1.92392500 | 0.15099200 |
|        | 0.47692100 | -0.37129000| 2.15456400 |
|        | -0.04155700| -0.99336400| 1.25860100 |
|        | 0.92806300 | -1.11004500| 0.36203400 |
|        | 2.08706700 | -1.24901500| -0.77539600|
|        | 2.37043800 | -2.26036300| -0.50990300|
|        | 1.40066700 | -1.13263000| -1.60607900|
|        | 2.98098400 | -0.16040400| -0.49426500|
|        | 2.81231600 | 0.97374400 | -0.98494500|
|        | 0.36829500 | -2.11844800| 1.54147200 |
|        | 4.09584200 | -0.38853400| 0.51100400 |
|        | 3.73375700 | -0.11414300| 1.50880000 |
|        | 4.41947100 | -1.43018900| 0.54908400 |
|        | 4.94580200 | 0.25407500 | 0.27582300 |

**TS30**

|        | C          | O          | H          |
|--------|------------|------------|------------|
|        | 1.16496100 | 0.17503000 | 0.52755000 |
|      |        |        |        |        |
|------|--------|--------|--------|--------|
|  C   | 2.27830300 | -1.52341200 | -0.44960200 |        |
|  C   | 2.97864900  | -0.38600700 | -0.68867000 |        |
|  H   | 2.47016800  | -2.54155300 | -0.74024200 |        |
|  H   | 3.89841000  | -0.22572700 | -1.22366500 |        |
|  N   | 2.28499600  | 0.64681300  | -0.08426300 |        |
|  N   | 1.17221100  | -1.16499700 | 0.29777900  |        |
|  C   | 2.69846900  | 2.04903800  | -0.11531500 |        |
|  H   | 1.96437300  | 2.64857800  | -0.65332800 |        |
|  H   | 2.79986400  | 2.43285000  | 0.89871800  |        |
|  H   | 3.65792500  | 2.11170800  | -0.62499400 |        |
|  C   | 0.12431300  | -2.09143200 | 0.72725600  |        |
|  H   | 0.46611200  | -3.10713800 | 0.53672800  |        |
|  H   | -0.06315800 | -1.96483600 | 1.79246400  |        |
|  H   | -0.79572100 | -1.90183300 | 0.17168100  |        |
|  H   | -0.47722600 | 0.38574400  | 2.16675200  |        |
|  B   | 0.05033800  | 1.00496600  | 1.27298900  |        |
|  H   | -0.91916700 | 1.15405300  | 0.37541300  |        |
|  C   | -2.14197700 | 1.33896500  | -0.70002100 |        |
|  H   | -2.47439600 | 2.31254100  | -0.35889900 |        |
|  H   | -1.52353900 | 1.31680200  | -1.58741000 |        |
|  C   | -2.97235200 | 0.17325900  | -0.46411400 |        |
|  O   | -2.78441900 | -0.92016900 | -1.02856400 |        |
|  H   | 0.40423500  | 2.11959100  | 1.56909700  |        |
|  N   | -3.98721600 | 0.31614400  | 0.45407000  |        |
|  H   | -4.02037800 | 1.12150800  | 1.05932800  |        |
|  H   | -4.43596700 | -0.52413600 | 0.78630500  |        |

|      |        |        |        |        |
|------|--------|--------|--------|--------|
|  C   | 1.22357800  | -0.11308500 | 0.64846500 |        |
|  C   | 2.47447700  | -0.23425200 | -1.22470500 |        |
|  C   | 2.21744500  | 1.07674000  | -0.98935900 |        |
|  H   | 3.03804500  | -0.71138900 | -2.00741800 |        |
|  H   | 2.51044600  | 1.95928200  | -1.53087000 |        |
|  N   | 1.45454400  | 1.13565000  | 0.16261500  |        |
|  N   | 1.85903600  | -0.95150700 | -0.21379000 |        |
|  C   | 0.91411100  | 2.36600600  | 0.73707600  |        |
|  H   | 1.42457200  | 3.21347100  | 0.28328700  |        |
|  H   | -0.15591400 | 2.43323600  | 0.53781200  |        |
|  H   | 1.08076600  | 2.37235400  | 1.81252900  |        |
|  C   | 1.89142200  | -2.40846300 | -0.09593100 |        |
|  H   | 2.48356400  | -2.80552700 | -0.91809900 |        |
|  H   | 2.34325200  | -2.69939700 | 0.85151400  |        |
|  H   | 0.88173500  | -2.81477000 | -0.14923400 |        |
|  H   | 0.56643100  | -1.62156200 | 2.29690000  |        |
|  H   | 0.36366100  | 0.34455400  | 2.76154300  |        |
|  B   | 0.34190700  | -0.50333200 | 1.89912900  |        |
|   | X         | Y         | Z         |
|---|-----------|-----------|-----------|
| H | -0.90491000 | -0.51010600 | 1.46937600 |
| C | -2.55748800 | -0.53350900 | 1.05818000 |
| H | -2.79491900 | -1.53271800 | 1.40308800 |
| H | -2.92697100 | 0.29099500  | 1.65800300 |
| C | -2.54776700 | -0.33882700 | -0.39348200 |
| F | -1.97502400 | 0.87931100  | -0.73873900 |
| F | -3.85495100 | -0.26403800 | -0.93718900 |
| H | -2.03924200 | -1.11589500 | -0.96395600 |

| TS32                  |   |   |   |
|-----------------------|---|---|---|
| C | 1.07227900 | -0.02934300 | 0.49058900 |
| C | 2.92252000 | -0.37467400 | -0.75570500 |
| C | 2.69879900 | 0.96249300  | -0.72019200 |
| H | 3.69908300 | -0.94528300 | -1.23415900 |
| H | 3.24386500 | 1.77856300  | -1.16173100 |
| N | 1.56435100 | 1.16025800  | 0.04742000  |
| N | 1.92058100 | -0.96982800 | -0.00890400 |
| C | 0.96381600 | 2.46431400  | 0.31870100  |
| H | 1.63739300 | 2.37318300  | -0.04651200 |
| H | 0.00272100 | 2.55300000  | -0.18909500 |
| H | 0.81316800 | 2.58234000  | 1.38905000  |
| C | 1.78039500 | -2.41073700 | 0.18978400  |
| H | 2.67147800 | -2.90049400 | -0.19815000 |
| H | 1.67631300 | -2.63031700 | 1.25103000  |
| H | 0.90293700 | -2.78434700 | -0.33930700 |
| H | -0.23666000| -1.31959600 | 1.91961900  |
| H | -0.55507400| 0.68647300  | 1.99205900  |
| B | -0.24347300| -0.26972300 | 1.32164500  |
| H | -1.21391800| -0.38868800 | 0.41771600  |
| C | -2.51992100| -0.54870100 | -0.60396100 |
| H | -2.14428100| 0.00645600  | -1.45791400 |
| H | -2.52479100| -1.62843700 | -0.71379500 |
| C | -3.59618300| 0.06397000  | 0.19155800  |
| F | -4.87393700| 0.03886000  | -0.52138100 |
| H | -3.42075200| 1.12025800  | 0.39874300  |
| H | -3.79177400| -0.47108000 | 1.12153500  |

| TS33                  |   |   |   |
|-----------------------|---|---|---|
| C | -0.54495900 | -0.17975500 | 0.30435600 |
| C | -2.60507200 | 0.57215500  | -0.23397700 |
| C | -2.28301100 | -0.40036500 | -1.12062600 |
| H | -3.49069900 | 1.17678000  | -0.14463200 |
| H | -2.83502700 | -0.80720100 | -1.94987800 |
| N | -1.01740500| -0.85105600 | -0.78625300 |
| N | -1.53590600| 0.69818900  | 0.63642800  |
| C | -0.29500600| -1.88906900 | -1.51681900 |
| H | -0.79867900| -2.05459000 | -2.46750000 |
| H | 0.72764500 | -1.56421000 | -1.70466900 |
| H | -0.27481900| -2.82008400 | -0.94978800 |

|   | X         | Y         | Z         |
|---|-----------|-----------|-----------|
| H | -0.90491000 | -0.51010600 | 1.46937600 |
| C | -2.55748800 | -0.53350900 | 1.05818000 |
| H | -2.79491900 | -1.53271800 | 1.40308800 |
| H | -2.92697100 | 0.29099500  | 1.65800300 |
| C | -2.54776700 | -0.33882700 | -0.39348200 |
| F | -1.97502400 | 0.87931100  | -0.73873900 |
| F | -3.85495100 | -0.26403800 | -0.93718900 |
| H | -2.03924200 | -1.11589500 | -0.96395600 |
|       | TS34          |       |       |       |
|-------|---------------|-------|-------|-------|
|       | C  | 1.29292600   | -0.32196500 | 0.23379500 |
|       | H  | 1.27050400   | -2.53450600 | -0.18395200 |
|       | C  | 1.37530300   | -1.89198900 | -1.37908000 |
|       | H  | 1.22816700   | -3.58460100 | 0.04120400  |
|       | H  | 1.44263900   | -2.27526100 | -2.38215000 |
|       | N  | 1.38345800   | -0.53651700 | -1.10763700 |
|       | N  | 1.22172600   | -1.56200600 | 0.79184500  |
|       | C  | 1.47152400   | 0.50430000  | -2.13197600 |
|       | H  | 1.31609500   | 0.04055700  | -3.10398600 |
|       | H  | 0.69967800   | 1.25415600  | -1.96639700 |
|       | H  | 2.45002700   | 0.98324700  | -2.10922500 |
|       | C  | 1.10415500   | -1.84397500 | 2.22246400  |
|       | H  | 1.15587300   | -2.92178500 | 2.36136800  |
|       | H  | 1.91960800   | -1.36859300 | 2.76548600  |
|       | H  | 0.15263500   | -1.47647500 | 2.60625200  |
|       | H  | 1.29257700   | 0.91522200  | 2.20127600  |
|       | B  | 1.17877800   | 1.03818900  | 1.01330900  |
|       | H  | -0.14391600  | 1.42557600  | 0.86974200  |
|       | C  | -1.55165400  | 1.95050000  | 0.76497000  |
|       | C  | 2.00979400   | 2.23876400  | 0.47254600  |
|       | N  | 2.60088200   | 3.16987900  | 0.10782600  |
|       | H  | -1.50984600  | 2.64332500  | 1.59801000  |
|       | H  | -1.45136800  | 2.41670000  | -0.20988100 |
|       | C  | -2.47114600  | 0.85322500  | 0.89269500  |
|       | H  | -2.79367700  | 0.53421900  | 1.87709400  |
|       | C  | -2.92372700  | 0.10709800  | -0.12300200 |
|       | F  | -3.73869000  | -0.94477900 | -0.00029800 |
|       | F  | -2.65696800  | 0.31750800  | -1.41485600 |
|       |       |       |       |       |
|       | TS35          |       |       |       |
|       | C  | 0.89231800   | -0.31752200 | -0.10604100 |
|       | C  | 2.67839800   | 0.96566300  | 0.38157900  |
|       | C  | 1.97998100   | 0.78357000  | 1.52966000  |
|  | X   | Y   | Z   |       |       |
|---|-----|-----|-----|-------|-------|
| H | 3.58675200 | 1.50955900 | 0.19009800 |       |       |
| H | 2.16373800 | 1.13940300 | 2.52833900 |       |       |
| N | 0.88582400 | -0.00190900 | 1.21819900 |       |       |
| N | 2.00217000 | 0.28629200 | -0.61446500 |       |       |
| C | -0.14735400 | -0.38991500 | 2.17890100 |       |       |
| H | 0.09160700 | 0.06496000 | 3.13795700 |       |       |
| H | -1.11997500 | -0.02872500 | 1.84219800 |       |       |
| H | -0.17807600 | -1.47258300 | 2.28923500 |       |       |
| C | 2.43530400 | 0.22926800 | -2.01066900 |       |       |
| H | 3.39015200 | 0.74459800 | -2.09167100 |       |       |
| H | 2.55507900 | -0.80704000 | -2.32355000 |       |       |
| H | 1.70609400 | 0.71839500 | -2.65609000 |       |       |
| H | 0.17692400 | -1.36767400 | -2.05418900 |       |       |
| B | -0.18439800 | -1.09860700 | -0.94261700 |       |       |
| H | -1.20184000 | -0.17356000 | -1.14991200 |       |       |
| C | -2.36971000 | 0.68788100 | -1.49849100 |       |       |
| C | -0.88480100 | -2.30498500 | -0.25178600 |       |       |
| N | -1.44400500 | -3.20853500 | 0.21759900 |       |       |
| C | -1.71814300 | -2.08336100 | 1.48395900 |       |       |
| H | -0.79724700 | -2.62481700 | 1.26564400 |       |       |
| H | -1.65340900 | -1.65542200 | 2.48335400 |       |       |
| H | -2.55991600 | -2.77149800 | 1.43827900 |       |       |
| C | -1.21282800 | 2.01747700 | -1.25596900 |       |       |
| H | -1.39025300 | 2.84473700 | -0.56904400 |       |       |
| H | -0.14379300 | 1.93419600 | -1.44712200 |       |       |
| H | -1.73102800 | 2.20669000 | -2.19410700 |       |       |
| H | 0.30456300 | -0.30781100 | 2.09079200 |       |       |
| B | 0.19955600 | 0.35946000 | 1.09536300 |       |       |
| C | 0.49725200 | 1.86169500 | 1.40499100 |       |       |
| N | 0.76374100 | 2.96383500 | 1.65961700 |       |       |

TS36

|  | X   | Y   | Z   |       |       |
|---|-----|-----|-----|-------|-------|
| C | -1.14387000 | 0.06810100 | 0.32490800 |       |       |
| C | -2.85000500 | 0.11249600 | -1.14983800 |       |       |
| C | -2.98567700 | -1.01097800 | -0.40441000 |       |       |
| H | -3.45197000 | 0.50188700 | -1.95226800 |       |       |
| H | -3.72787900 | -1.78944200 | -0.43404800 |       |       |
| N | -1.93660100 | -1.02672600 | 0.49812500 |       |       |
| N | -1.71607700 | 0.76409300 | -0.69711100 |       |       |
| C | -1.71814300 | -2.08336100 | 1.48395900 |       |       |
| H | -0.79724700 | -2.62481700 | 1.26564400 |       |       |
| H | -1.65340900 | -1.65542200 | 2.48335400 |       |       |
| H | -2.55991600 | -2.77149800 | 1.43827900 |       |       |
| C | -1.21282800 | 2.01747700 | -1.25596900 |       |       |
| H | -1.39025300 | 2.84473700 | -0.56904400 |       |       |
| H | -0.14379300 | 1.93419600 | -1.44712200 |       |       |
| H | -1.73102800 | 2.20669000 | -2.19410700 |       |       |
| H | 0.30456300 | -0.30781100 | 2.09079200 |       |       |
| B | 0.19955600 | 0.35946000 | 1.09536300 |       |       |
| C | 0.49725200 | 1.86169500 | 1.40499100 |       |       |
| N | 0.76374100 | 2.96383500 | 1.65961700 |       |       |
|   |   |   |   |
|---|---|---|---|
| H | 1.20809100 | -0.06855800 | 0.31165100 |
| C | 2.49110400 | -0.64641900 | -0.44613700 |
| C | 3.58837300 | -0.38751800 | 0.55211000 |
| H | 4.56003700 | -0.74266900 | 0.17192200 |
| H | 3.69560700 | 0.68030900 | 0.76486900 |
| H | 3.40218800 | 0.68030900 | 0.76486900 |
| C | 2.49110400 | -0.64641900 | -0.44613700 |
| H | 1.93155800 | -2.58906400 | 0.32164300 |
| H | 1.19758900 | -2.18682400 | -1.24268500 |
| H | 2.90041300 | -2.64806200 | -1.15447800 |
| C | 2.53296200 | 0.19028400 | -1.69782100 |
| H | 1.62852200 | 0.06028400 | -2.30076800 |
| H | 2.64452900 | 1.25450900 | -1.46838300 |
| H | 3.38682600 | -0.09366000 | -2.33439000 |
| TS37 |   |   |   |
| C | -0.75919200 | -0.08512500 | 0.31669100 |
| C | -2.29066100 | -1.00719100 | -1.04953300 |
| C | -1.89943400 | -1.96308000 | -0.17031000 |
| H | -3.00177600 | -1.04236800 | -1.85621000 |
| H | -2.20391200 | -2.98983100 | -0.06697900 |
| N | -0.96120000 | -1.38497900 | 0.66332600 |
| N | -1.58055000 | 0.13794200 | -0.74428000 |
| C | -0.26664500 | -2.95559000 | 1.73677200 |
| H | -0.72914500 | -3.07341500 | 1.85300400 |
| H | 0.78777900 | -2.22053200 | 1.48664400 |
| H | -0.35352900 | -1.54000600 | 2.66869000 |
| C | -1.68828800 | 1.39939100 | -1.47617900 |
| H | -2.24829300 | 1.20762700 | -2.39780300 |
| H | -2.24063900 | 2.13703900 | -0.88124600 |
| H | -0.71354000 | 1.78295300 | -1.71955400 |
| B | 0.30037100 | 0.87928800 | 0.96640900 |
| H | 1.38019700 | 0.82987900 | 0.10446100 |
| C | 2.63868800 | 0.78930700 | -0.66367300 |
| H | 2.37957900 | 1.54116700 | -1.40313900 |
| H | 3.29478500 | 1.13256100 | 0.14259500 |
| C | 3.40344600 | -1.36761800 | -0.41398300 |
| H | 3.48526600 | -2.39039500 | -0.77063700 |
| H | 3.87338200 | -1.11852300 | 0.54423800 |
| N | 2.78212700 | -0.49122100 | -1.13923700 |
| H | 0.75683700 | 0.46492200 | 1.99410300 |
| C | -0.06607200 | 2.39000700 | 1.05647900 |
| N | -0.28502000 | 3.52707000 | 1.14193500 |
| TS38 |   |   |   |
| C | 1.20439900 | -2.63757400 | 0.18999400 |
| H | 0.84976600 | -3.61034600 | 0.48244600 |
| C | 1.87609600 | -2.23508100 | -0.91699800 |
| Atom | X       | Y       | Z       |
|------|---------|---------|---------|
| H    | 2.22158300 | -2.79107700 | -1.77092700 |
| N    | 2.08267300 | -0.87374700 | -0.79199900 |
| C    | 2.75816900 | -0.05075300 | -1.79513700 |
| H    | 2.14456900 | 0.81546000 | -2.03887900 |
| H    | 3.72624300 | 0.28631400 | -1.42625200 |
| H    | 2.89990000 | -0.65187900 | -2.69092400 |
| N    | 1.01653500 | -1.51770000 | 0.97815200 |
| C    | 0.30810800 | -1.52343900 | 2.25798900 |
| H    | 0.10637000 | -2.55731100 | 2.53087300 |
| H    | 0.92404900 | -1.05943500 | 3.02643600 |
| H    | -0.63390000 | -0.98062600 | 2.17225600 |
| C    | 1.55611500 | -0.42115100 | 0.37903500 |
| H    | 1.14356500 | 1.11032800 | 2.07585300 |
| B    | 1.45431500 | 1.05359500 | 0.91802500 |
| C    | 2.63778900 | 2.01499400 | 0.59542500 |
| N    | 3.48565300 | 2.77873800 | 0.37900500 |
| H    | 0.36489200 | 1.58800100 | 0.28285200 |
| C    | -0.87357800 | 2.26519100 | -0.30260900 |
| H    | -0.93227100 | 3.06445500 | 0.42948100 |
| C    | -1.93455100 | 1.28642300 | -0.31902900 |
| C    | -2.76687400 | 1.08831200 | 0.80828600 |
| C    | -2.14006900 | 0.44348000 | -1.43687600 |
| C    | -3.75462000 | 0.11064400 | 0.81030200 |
| H    | -2.63202500 | 1.72020700 | 1.68039000 |
| C    | -3.12939500 | -0.53255300 | -1.43025400 |
| H    | -1.51698200 | 0.57276300 | -2.31624600 |
| C    | -3.94532400 | -0.70812200 | -0.30768500 |
| H    | -4.38409700 | -0.01403000 | 1.68513600 |
| H    | -3.27079900 | -1.15932600 | -2.3047300 |
| H    | -4.71875900 | -1.46761300 | -0.30547100 |
| H    | -0.43529800 | 2.55288100 | -1.25342500 |

**TS39**

| Atom | X       | Y       | Z       |
|------|---------|---------|---------|
| C    | -0.91101400 | 0.09679700 | 0.27977200 |
| C    | -2.69259300 | 0.05111100 | -1.10034900 |
| C    | -2.84816500 | -0.95061400 | -0.20055300 |
| H    | -3.31688600 | 0.36536800 | -1.91849100 |
| H    | -3.63383900 | -1.67685600 | -0.08596400 |
| N    | -1.75082700 | -0.91091500 | 0.64226200 |
| N    | -1.49842700 | 0.68181500 | -0.79943400 |
| C    | -1.53073800 | -1.84103600 | 1.74909400 |
| H    | -0.69496900 | -2.50584500 | 1.52874700 |
| H    | -1.31808400 | -1.28899700 | 2.66270400 |
| H    | -2.43485800 | -2.43119800 | 1.88431700 |
| C    | -0.95125100 | 1.81225900 | -1.54786200 |
| H    | -1.10972100 | 2.74584100 | -1.00767800 |
| H   | 0.11622000 | 1.66507900 | -1.70283900 |
| H   | -1.45087100 | 1.86086300 | -2.51358900 |
| H   | 0.68154900  | -0.18856300 | 1.94342900  |
| B   | 0.49357800  | 0.42050000  | 0.92370800  |
| C   | 0.80217600  | 1.94079500  | 1.12099100  |
| N   | 1.07656400  | 3.05886700  | 1.27784800  |
| H   | 1.42279900  | -0.03395500 | 0.07183600  |
| C   | 2.63683300  | -0.63524000 | -0.80643200 |
| C   | 2.18988800  | -2.04175400 | -1.08674200 |
| H   | 2.93609500  | -2.59326200 | -1.67951700 |
| H   | 2.04594200  | -2.60512900 | -0.15745800 |
| H   | 1.25059700  | -2.06701800 | -1.64722800 |
| H   | 2.56204100  | 0.05231700  | -1.64848900 |
| C   | 3.83784900  | -0.43808800 | 0.07395600  |
| N   | 4.75591600  | -0.81159600 | -0.40593400 |
| H   | 4.00081100  | 0.61768800  | 0.30750900  |
| H   | 3.73028700  | -0.98128000 | 1.01952900  |

**TS40**

| C   | -0.88148100 | 0.03133800 | 0.27972500 |
| C   | -2.12261900 | 1.82900800 | -0.26786900 |
| C   | -2.26167400 | 0.91897400 | -1.26305900 |
| H   | -2.54612700 | 2.81083200 | -0.14809300 |
| H   | -2.83300800 | 0.95422400 | -2.17417400 |
| N   | -1.49134700 | -0.17652000 | -0.91782600 |
| N   | -1.27553100 | 1.27184000 | 0.67319100 |
| C   | -1.35625400 | -1.37952700 | -1.73865100 |
| H   | -1.70093200 | -1.14974800 | -2.74496600 |
| H   | -0.31108800 | -1.68094200 | -1.77789000 |
| H   | -1.95033600 | -2.19522400 | -1.32667000 |
| C   | -0.85030500 | 1.94967700 | 1.89774100 |
| H   | -1.43387600 | 2.86203400 | 2.00217500 |
| H   | -1.02381200 | 1.30711900 | 2.75898300 |
| H   | 0.20893400  | 2.20221300 | 1.84337700 |
| H   | 0.40041100  | -0.50892900 | 2.13936600 |
| B   | 0.15432300  | -0.89681900 | 1.02873300 |
| H   | 1.31276700  | -0.76998700 | 0.36236700 |
| C   | 2.75848700  | -0.63263800 | -0.32182600 |
| H   | 3.37252600  | -1.17927400 | 0.38696200 |
| H   | 2.58719000  | -1.13929100 | -1.26646700 |
| S   | 3.19492300  | 1.06988600  | -0.57727500 |
| H   | 3.40970800  | 1.40029600  | 0.71292200 |
| C   | -0.17926100 | -2.42369400 | 1.02930900 |
| N   | -0.37942000 | -3.56763800 | 1.04929900 |

**TS41**

| C   | -1.40192700 | -0.21668900 | 0.23167700 |
| C   | -2.50964900 | -1.37757200 | -1.34916800 |
|   |   |   |   |
|---|---|---|---|
| C | -2.21158700 | -2.23766000 | -0.34458700 |
| H | -3.03020900 | -1.53291900 | -2.27802900 |
| H | -2.42075600 | -3.28699400 | -0.23171800 |
| N | -1.53321800 | -1.51288300 | 0.61964700 |
| N | -2.00136900 | -0.14335500 | -0.98621400 |
| C | -1.02206400 | -2.08216700 | 1.86693400 |
| H | -1.39070100 | -3.10246800 | 1.95201700 |
| H | 0.06797300 | -2.09101900 | 1.86305700 |
| H | -2.90100000 | 1.70957700 | -1.44571200 |
| C | -1.15712700 | 1.60581700 | -1.76896200 |
| H | -0.28397200 | 0.57641900 | 2.10539900 |
| B | -0.61453700 | 0.91950500 | 1.00153300 |
| C | 1.99152700 | 1.37825700 | -0.34289300 |
| C | 2.80010000 | 0.16377200 | 0.01139100 |
| H | 1.69409200 | 1.49724300 | -1.38291500 |
| H | 2.24170600 | 2.31197000 | 0.15577400 |
| H | 2.30895500 | -0.73684800 | -0.37975900 |
| H | 2.83464700 | 0.04868500 | 1.10216600 |
| C | 4.24971100 | 0.19533300 | -0.52105000 |
| H | 4.75311800 | 1.08818700 | -0.13325000 |
| H | 4.22891000 | 0.30261100 | -1.61171900 |
| C | -1.33543000 | 2.30811400 | 1.04315400 |
| N | -1.82948200 | 3.35832200 | 1.08976900 |
| C | 5.05034800 | -1.05452700 | -0.14077900 |
| H | 6.07196800 | -1.00602700 | -0.52848800 |
| H | 5.11152300 | -1.16797000 | 0.94633400 |
| H | 4.58411600 | -1.95978900 | -0.54302800 |

| TS42   |   |   |   |
|---|---|---|---|
| C | -1.16366300 | -0.06285000 | 0.21995600 |
| C | -2.88726500 | -0.07485600 | -1.22996300 |
| C | -2.97729600 | -1.20014100 | 0.47952800 |
| H | -3.51116400 | 0.29260400 | -2.02599000 |
| H | -3.69438300 | -2.00205700 | -0.49766700 |
| N | -1.91489400 | -1.18007200 | 0.40730000 |
| N | -1.76738000 | 0.61057200 | -0.79463300 |
| C | -1.64846100 | -2.22795200 | 1.39358900 |
| H | -2.48577400 | -2.92286100 | 1.38660500 |
| H | -0.73279200 | -2.76356000 | 1.14328300 |
| H | -1.54909000 | -1.78965300 | 2.38510900 |
| C | -1.32124800 | 1.87933000 | -1.35767200 |
| H | -1.79671000 | 2.02803100 | -2.31762500 |
|   |   |   |
|---|---|---|
| H | -1.55039500 | 2.70654900 | -0.69124200 |
| H | -0.22842700 | 1.84373500 | -1.50639800 |
| H | 0.40461000 | -0.43817400 | 1.88989800 |
| C | 0.19181500 | 0.28905600 | 0.95653700 |
| H | 1.16336000 | 0.04114600 | 0.08186200 |
| B | 2.44366200 | -0.30446500 | -0.88877000 |
| C | 3.59202300 | -0.56822100 | 0.04337200 |
| H | 2.02809900 | -1.15591200 | -1.42457800 |
| H | 2.47447500 | 0.61433700 | -1.47113700 |
| H | 3.33719500 | -1.39383900 | 0.71793100 |
| H | 3.75979700 | 0.30933100 | 0.67832000 |
| C | 4.90771900 | -0.91117200 | -0.68471800 |
| C | 5.21835900 | -0.09248700 | -1.34047600 |
| H | 5.71497400 | -1.09419700 | 0.03234600 |
| C | 4.79383700 | -1.80812200 | -1.30079200 |
| C | 0.35601800 | 1.78892300 | 1.37347100 |
| N | 0.51492200 | 2.89353900 | 1.69296700 |
| TS43 | C | -0.97357300 | 0.18166400 | 0.32678700 |
| C | -2.70749800 | -0.35283200 | -1.00075100 |
| C | -2.72035400 | -1.20717800 | 0.05313500 |
| H | -3.36202200 | -0.27476300 | -1.85101200 |
| H | -3.38752000 | -2.01590600 | 0.29478400 |
| N | -1.65268200 | -0.86705900 | 0.86055700 |
| N | -1.62916400 | 0.49139400 | -0.82240900 |
| C | -1.30731200 | -1.56462500 | 2.10101400 |
| H | -0.37062000 | -2.10875000 | 1.98185700 |
| H | -1.21091600 | -0.84932800 | 2.91557200 |
| H | -2.10595600 | -2.26740500 | 2.32820100 |
| C | -1.25665500 | 1.55589500 | -1.75622100 |
| H | -1.46452800 | 2.53354400 | -1.32309600 |
| H | -0.19722800 | 1.48421900 | -1.99687300 |
| H | -1.83884000 | 1.42981100 | -2.66663000 |
| H | 0.60182800 | 0.44058300 | 2.02188600 |
| B | 0.35377400 | 0.80801300 | 0.90806100 |
| C | 0.52804400 | 2.35029400 | 0.75539600 |
| N | 0.70830000 | 3.49281600 | 0.65882600 |
| H | 1.36338000 | 0.26414300 | 0.16928700 |
| C | 2.62967200 | -0.27574500 | -0.53151200 |
| H | 2.68148200 | 0.47947400 | -1.31165500 |
| C | 3.68430400 | -0.19475900 | 0.54999200 |
| H | 4.67671000 | -0.43256400 | 0.15171900 |
| H | 3.72112800 | 0.81667700 | 0.95923200 |
| H | 3.47186400 | -0.88969200 | 1.36479100 |
| C | 2.23777800 | -1.54805800 | -1.00098000 |
|       | TS44       | TS45       |
|-------|------------|------------|
| N     | 1.85445600 | 1.85101200 |
| C     | 4.18728600 | -1.85101200|
| H     | 4.87180300 | -1.84895200|
| C     | 4.12342100 | -2.22556500|
| H     | 4.74185000 | -2.61596800|
| N     | 3.04208900 | -2.01591800|
| C     | 2.61970300 | -2.28773100|
| H     | 1.53708600 | -2.34148900|
| H     | 2.92352000 | 1.48125200 |
| N     | 3.14799500 | -3.23872600|
| C     | 2.86365000 | 1.02740000 |
| H     | 3.67192000 | 0.11202500 |
| H     | 2.80589600 | -1.21716100|
| C     | 1.92158500 | -1.07471900|
| C     | 2.43727100 | -0.98534300|
| H     | 0.90024400 | -2.37602800|
| H     | 1.11663000 | -2.36442700|
| H     | 1.02740000 | -2.27605500|
| N     | 0.91387800 | -3.74381300|
| C     | 0.11202500 | -3.78086800|
| N     | -1.21716100| -3.87627700|
| C     | -0.98534300| -4.90350600|
| H     | -2.27605500| -4.89529400|
| C     | -3.74381300| -4.79174400|
| H     | -3.78086800| -6.21229000|
| H     | -3.87627700| -7.23872600|
| N     | -1.85101200| -1.85101200|
| C     | -2.22556500| -2.22556500|
| H     | -2.61596800| -2.61596800|
| N     | -2.01591800| -2.01591800|
| C     | -2.28773100| -2.28773100|
| H     | -1.48125200| -1.48125200|
| H     | -3.23040700| -3.23040700|
| H     | -2.34148900| -2.34148900|
|   | X       | Y       | Z       |
|---|---------|---------|---------|
| N | -1.42651400 | -1.58689700 | -0.70228400 |
| C | -0.92434900 | -1.96916500 | -2.02300200 |
| H | -1.07770000 | -3.03900700 | -2.14818100 |
| H | -1.46715100 | -3.03900700 | -2.14818100 |
| H | -1.39071000 | -1.96916500 | -2.14818100 |
| C | -2.08355000 | 3.16001200 | -0.76464900 |
| H | 0.08464700 | 1.37234400 | -0.43986800 |
| C | -1.57161400 | 1.84756200 | 0.07639700 |
| H | 1.75345100 | 2.64065800 | -0.64393400 |
| H | 1.32339300 | 2.19434800 | 1.07627800 |
| C | 2.40068900 | 0.60397000 | -0.03980600 |
| H | 2.38227000 | 0.22934100 | -1.06784000 |
| C | 1.99431600 | -0.18687100 | 0.59819600 |
| C | 3.88542500 | 0.83958900 | 0.36427400 |
| H | 4.33467500 | 1.60651700 | -0.27247900 |
| H | 3.94650700 | 1.19853100 | 1.39526000 |
| C | 4.68967600 | -0.37494900 | 0.25484400 |
| H | 5.29656700 | -1.35208900 | 0.15872700 |
| C | -0.70960800 | -0.04346800 | 0.22114200 |
| C | -2.55681800 | 0.53754500 | -0.92955800 |
| C | -2.79713800 | -0.66516400 | -0.35224600 |
| H | -3.17797600 | 1.15522800 | -1.55442400 |
| H | -3.66771100 | -1.29684400 | -0.37921800 |
| N | -1.65650300 | -1.01013600 | 0.35162500 |
| N | -1.27076900 | 0.90435900 | -0.57550900 |
| C | -1.50398100 | -2.25099400 | 1.11214400 |
| H | -0.76172200 | -2.89668600 | 0.64292500 |
| H | -1.19334100 | -2.02776100 | 2.13129700 |
| H | -2.46536800 | -2.76039300 | 1.12924100 |
| C | -0.61637000 | 2.13859100 | -1.00847700 |
| H | -0.61809000 | 2.87710400 | -0.20662900 |
| H | 0.41094500 | 1.92448900 | -1.29749500 |
| H | -1.15658000 | 2.53206400 | -1.86740900 |
| H | 0.92263300 | -1.00441800 | 1.56275300 |
| B | 0.76578700 | -0.09752900 | 0.78901600 |
| C | 1.29493100 | 1.24508700 | 1.39340500 |
| N | 1.73387200 | 2.22001000 | 1.84323800 |
| H | 1.55575800 | -0.37456700 | -0.24683200 |
| C | 2.62945100 | -0.79513800 | -1.41285000 |
| H | 2.02376900 | -1.52677500 | -1.94252100 |
|   |   |   |   |   |
|---|---|---|---|---|
| H | 2.71698600 | 0.16143500 | -1.92234000 |
| C | 3.83476300 | -1.29770400 | -0.67315200 |
| H | 4.63290900 | -1.61786700 | -1.35894900 |
| H | 4.26134800 | -0.52353500 | -0.02818200 |
| H | 3.58993000 | -2.15992400 | -0.04522700 |
| C | 3.24169100 | -1.19960200 | -0.53494100 |
| H | 3.97247000 | -1.98892600 | -0.55758000 |
| C | 3.11330100 | -0.08778100 | -1.30057000 |
| H | 3.71049800 | 0.27809500 | -2.11747400 |
| N | 1.99325100 | 0.58436600 | -0.84786200 |
| C | 1.49840100 | 1.83903000 | -1.41616600 |
| H | 0.41848200 | 1.78409700 | -1.54091700 |
| H | 1.74460600 | 2.67732200 | -0.76481200 |
| H | 1.96514100 | 1.98306700 | -2.38838000 |
| N | 2.20126300 | -1.18377500 | 0.37644700 |
| C | 1.97776600 | -2.22162500 | 1.38530500 |
| H | 2.81658400 | -2.91364900 | 1.35161300 |
| H | 1.91739700 | -1.77254700 | 2.37497000 |
| H | 1.05525500 | -2.76258900 | 1.17632700 |
| C | 1.42833800 | -0.08353500 | 0.19008500 |
| H | -0.08956600 | -0.45681300 | 1.90925200 |
| B | 0.09064200 | 0.26741000 | 0.96743000 |
| C | -0.05353800 | 1.76991000 | 1.38612400 |
| N | -0.20400800 | 2.87516600 | 1.70743200 |
| H | -0.90043300 | 0.01938300 | 0.13122400 |
| C | -2.25031000 | -0.33753700 | -0.76661200 |
| H | -2.22547300 | 0.46139600 | -1.50050200 |
| H | -1.98084500 | -1.32078700 | -1.13858400 |
| C | -3.35462800 | -0.27873200 | 0.26329300 |
| H | -3.17249900 | -0.98932300 | 1.07566900 |
| H | -3.41590900 | 0.71545400 | 0.71665400 |
| C | -4.66727800 | 0.58775100 | -0.31285200 |
| N | -5.68641700 | -0.83654200 | -0.79696100 |

|   |   |   |   |   |
|---|---|---|---|---|
| C | 0.62352400 | 0.30081600 | -0.00410700 |
| C | -2.66221800 | -0.64806300 | 0.07414300 |
| C | -1.92431700 | -1.18038500 | 1.07968800 |
| H | -3.67874200 | -0.83281400 | -0.22597000 |
| H | -2.17504000 | -1.91604200 | 1.82368200 |
| N | -0.67554400 | -0.59152600 | 1.01812500 |
| N | -1.85233600 | 0.26182300 | -0.58146300 |
| C | 0.43675300 | -0.91423700 | 1.91389900 |
| H | 0.14466100 | -1.76356600 | 2.52806900 |
| H | 1.31464200 | -1.17896000 | 1.32582000 |
| H | 0.66782000 | -0.06452200 | 2.55514400 |
|   | C    |        |        |        |        |        |        |        |        |
|---|------|--------|--------|--------|--------|--------|--------|--------|--------|
|   |      | -2.27446800 | 1.04786200 | -1.74233500 |
| H |      | -3.35177300 | 0.94157000 | -1.85258300 |
| H |      | -2.02787200 | 2.09651200 | -1.58971700 |
| H |      | -1.78136700 | 0.68870500 | -2.64580500 |
| H |      | 0.34283700  | 1.89991200 | -1.38951500 |
| B |      | 0.62594300  | 1.13850900 | -0.50392300 |
| H |      | 1.47082100  | 0.26836500 | -1.04188100 |
| C |      | 2.53697200  | -0.81208200 | -1.67610900 |
| H |      | 2.14394800  | -1.05175900 | -2.65959500 |
| H |      | 3.50177700  | -0.31967400 | -1.60385200 |
| F |      | 2.45862100  | -1.89563900 | -0.82519100 |
| C |      | 1.42606800  | 1.86839100 | 0.62672500 |
| N |      | 2.05350700  | 2.41922700 | 1.43349800 |

**TS49**

|   | C    |        |        |        |        |        |        |        |        |
|---|------|--------|--------|--------|--------|--------|--------|--------|--------|
|   |      | 0.57793400 | 0.07656900 | 0.27289700 |
| C |      | 2.56814600 | -0.85083100 | -0.23557600 |
| C |      | 2.42078500 | 0.24906900 | -1.01356200 |
| H |      | 3.37057000 | -1.56477200 | -0.17219100 |
| H |      | 3.07130800 | 0.67825500 | -1.75545100 |
| N |      | 1.19424600 | 0.80594400 | -0.69716300 |
| N |      | 1.43272700 | -0.94554300 | 0.55017100 |
| C |      | 0.64284400 | 2.00147500 | -1.33302200 |
| H |      | 1.22730700 | 2.21751300 | -2.22528400 |
| H |      | -0.39291100 | 1.82199700 | -1.61788400 |
| H |      | 0.68553500 | 2.85336600 | -0.65454700 |
| C |      | 1.19354300 | -2.01080400 | 1.52277200 |
| C |      | 1.90345000 | 2.60073200 | 1.61337600 |
| H |      | 0.94169000 | -1.58155900 | 2.49118800 |
| H |      | 0.37780100 | -2.65370700 | 1.19085500 |
| H |      | -1.06914900 | -0.44461600 | 1.82185100 |
| B |      | -0.86530200 | 0.27084100 | 0.87674400 |
| H |      | -1.72934900 | -0.16087700 | -0.06353800 |
| C |      | -2.82355200 | -0.82632000 | -1.03740600 |
| H |      | -3.74820500 | -0.39613200 | -0.65493900 |
| H |      | -2.50457900 | -0.48429200 | -2.01693000 |
| O |      | -2.70465500 | -2.20333000 | -0.92961900 |
| H |      | -3.08215600 | -2.48997700 | -0.09041300 |
| C |      | -1.27936500 | 1.74415300 | 1.18994300 |
| N |      | -1.63976900 | 2.82218300 | 1.43140100 |

**TS50**

|   | C    |        |        |        |        |        |        |        |        |
|---|------|--------|--------|--------|--------|--------|--------|--------|--------|
|   |      | 0.34508700 | -0.10321800 | -0.16777000 |
| C |      | 1.90875400 | 1.38775400 | 0.46265800 |
| C |      | 2.54900800 | 0.23977400 | 0.13012400 |
| H |      | 2.29059600 | 2.33208700 | 0.80960300 |
| H |      | 3.59856400 | -0.00878600 | 0.13389100 |
| N |      | 1.57740300 | -0.66650000 | -0.25571600 |
|   |   |   |   |
|---|---|---|---|
| N | 0.55680200 | 1.16060900 | 0.28081900 |
| C | 1.85842100 | -2.03860800 | -0.68259700 |
| H | 1.46001600 | -1.16060900 | -0.28081900 |
| H | 1.41129500 | -2.22507300 | -1.65735700 |
| H | 2.93773200 | -2.15865300 | -0.74943600 |
| C | -0.48883300 | 2.15143400 | 0.53789500 |
| H | -0.83272400 | 2.56979400 | -0.39563000 |
| H | -1.32802200 | 1.67360800 | 1.03968000 |
| H | -0.07822900 | 2.92610900 | 1.18246000 |
| B | -0.89511600 | -1.91420300 | -0.92540300 |
| N | -2.88170600 | 0.60895200 | -1.83878700 |
| C | 2.52681200 | -0.93365200 | -0.23587400 |
| H | 3.34630300 | -1.60706700 | -0.05531900 |
| C | 2.15804400 | -0.26618200 | -1.35846200 |
| H | 2.59545300 | -0.24660000 | -2.34126200 |
| N | 1.02532500 | 0.45698900 | -1.04205100 |
| C | 0.30336900 | 1.31104600 | -1.98739500 |
| H | -0.76745800 | 1.14548800 | -1.88741900 |
| H | 0.52693300 | 2.36117500 | -1.80096900 |
| H | 0.61359000 | 1.04441100 | -2.99551100 |
| N | 1.61605400 | -0.60151700 | 0.74772400 |
| C | 1.65306500 | -1.13276800 | 2.11273100 |
| H | 2.57782800 | -1.69281100 | 2.23258200 |
| H | 1.62813900 | -0.31596200 | 2.83126000 |
| H | 0.80489900 | -1.79491600 | 2.28410900 |
| C | 0.68768500 | 0.25856200 | 0.25747300 |
| H | -0.53304500 | 0.56773900 | 2.1665600 |
| B | -0.56670000 | 0.81881100 | 1.04492700 |
| C | -0.92344900 | 2.31822300 | 0.78728300 |
| N | -1.22892500 | 3.42498600 | 0.62094800 |
| H | -1.62005100 | 0.12068200 | 0.59344300 |
| C | -2.95052200 | -0.65573300 | 0.18744400 |
| H | -3.40817600 | -0.69248900 | 1.16924000 |
| H | -3.35924900 | 0.07548700 | -0.50050800 |
| C | -2.54111800 | -1.88038000 | -0.36293900 |
| N | -2.13459300 | -2.87627200 | -0.80840700 |

**TS52**

|   |   |   |   |
|---|---|---|---|
| C | -0.81000800 | -0.31204700 | 0.07114800 |
|      | X       | Y       | Z       |
|------|---------|---------|---------|
| C    | -2.6206 | 0.9874  | -0.2044 |
| C    | -1.8903 | 1.0581  | -1.3481 |
| H    | -3.5603 | 1.4535  | 0.0614  |
| H    | -2.0544 | 1.6030  | -2.2569 |
| N    | -0.7800 | 0.2560  | -1.1605 |
| N    | -2.0800 | 0.1189  | -2.1344 |
| C    | 0.3094  | 0.6404  | -1.7732 |
| C    | -3.9445 | 0.2281  | 2.1449  |
| C    | -2.9812 | -1.2813 | 2.1054  |
| H    | -1.7263 | 0.1885  | 2.7519  |
| H    | -0.0434 | -1.6171 | 1.8460  |
| B    | 0.2745  | -1.2492 | 0.7528  |
| C    | 2.6807  | 0.2879  | 1.2198  |
| C    | 2.7734  | 0.0319  | 2.2697  |
| H    | 3.2506  | -0.313  | 0.5184  |
| C    | 2.4238  | 1.6839  | 0.8878  |
| O    | 2.5110  | 1.2393  | -0.2673 |
| H    | 2.0815  | 2.3090  | 1.7043  |
| C    | 0.8161  | -2.4173 | -0.1261 |
| N    | 1.2471  | -3.2957 | -0.7489 |

|      | X       | Y       | Z       |
|------|---------|---------|---------|
| C    | 1.1061  | -0.1227 | 0.2978  |
| C    | 2.1719  | -2.0706 | -0.0457 |
| C    | 2.8420  | -1.1106 | -0.7314 |
| H    | 2.3563  | -3.1264 | 0.0478  |
| H    | 3.7237  | -1.1695 | -1.2154 |
| N    | 2.1734  | 0.0790  | -0.5163 |
| N    | 1.1097  | -1.4499 | 0.5811  |
| C    | 2.5766  | 1.3590  | -1.1045 |
| H    | 3.3360  | 1.1612  | -1.8578 |
| H    | 1.7205  | 1.8373  | -1.5765 |
| H    | 2.9849  | 2.0189  | -0.3404 |
| C    | 0.1096  | -2.1498 | 1.3930  |
| H    | 0.4282  | -3.1840 | 1.5036  |
| H    | 0.0383  | -1.6854 | 2.3750  |
| H    | -0.8621 | -2.1168 | 0.8998  |
| H    | -0.5791 | 0.5145  | 1.7621  |
| B    | -0.0120 | 0.8956  | 0.7749  |
| H    | -0.9481 | 0.8508  | -0.1551 |
| C    | -2.1395 | 0.6620  | -1.2587 |
| Atom | X       | Y       | Z       |
|------|---------|---------|---------|
| H    | -2.41587100 | 1.70450400 | -1.34396400 |
| H    | -1.50732000 | 0.23721300 | -2.02597500 |
| C    | -3.03047600 | -0.24478700 | -0.57995800 |
| O    | -2.93426300 | -1.46788500 | -0.56199200 |
| O    | -4.00610500 | 0.39393900 | 0.13026700 |
| H    | -4.52341700 | -0.28649100 | 0.58641400 |
| C    | 0.40483100  | 2.39550700  | 0.91615700  |
| N    | 0.65730600  | 3.52074700  | 1.03933000  |

**TS54**

| Atom | X       | Y       | Z       |
|------|---------|---------|---------|
| C    | 0.85859400 | 0.17077500 | 0.25041500 |
| C    | 2.72319000 | -0.73782400 | -0.61717500 |
| C    | 2.17633400 | 0.06001000 | -1.56807700 |
| H    | 3.61052000 | -1.34603200 | -0.63393400 |
| H    | 2.49732500 | 0.28167900 | -2.57085600 |
| N    | 1.03077500 | 0.60776400 | -1.02288600 |
| N    | 1.90486000 | -0.65823100 | 0.49455400 |
| C    | 0.13135500 | 1.51981600 | -1.73253300 |
| H    | 0.39892000 | 1.51171500 | -2.78703100 |
| H    | -0.89746600 | 1.18124000 | -1.62033100 |
| H    | 0.22712100 | 2.53145000 | -1.33951800 |

**TS55**

| Atom | X       | Y       | Z       |
|------|---------|---------|---------|
| C    | 1.33575000 | -0.02652800 | 0.22064700 |
| C    | 2.28758600 | -1.96241000 | -0.40657700 |
| C    | 2.12991700 | -1.20378000 | -1.52028600 |
| H    | 2.70035200 | -2.94785100 | -0.27969000 |
| H    | 2.38095900 | -1.40071800 | -2.54783200 |
| N    | 1.54024700 | -0.02063600 | -1.11973600 |
| N    | 1.79626400 | -1.22587300 | 0.65469800 |
| C    | 1.18736600 | 1.07344600 | -2.02686600 |
| H    | 1.18609100 | 0.68767000 | -3.04418200 |
| H    | 0.19328900 | 1.44301500 | -1.78376600 |
| H    | 1.90893400 | 1.88577100 | -1.94364400 |
| C    | 1.76610200 | -1.70218400 | 2.04021800 |
|        |        |        |        |        |
|--------|--------|--------|--------|--------|
|        |        |        |        |        |
|        |        |        |        |        |
| H      | 2.31954200 | -2.63741500 | 2.08926100 |
| H      | 2.23282500 | -0.96977300 | 2.69567100 |
| H      | 0.73826300 | -1.87263600 | 2.35904200 |
| H      | 0.70506500 | 0.83988100  | 2.28435400 |
| B      | 0.62725800 | 1.08413200 | 1.11143400 |
| H      | -0.64764200 | 1.04096500 | 0.83364700 |
| C      | -2.34534100 | 1.04198900 | 0.64981300 |
| H      | -2.63918000 | 1.08991300 | 1.69029100 |
| H      | -2.47708100 | 1.93411400 | 0.05120400 |
| C      | 1.08743500 | 2.55445100 | 0.81813200 |
| N      | 1.39800900 | 3.65604900 | 0.62962900 |
| C      | -2.62481100 | -0.22881200 | -0.03109800 |
| F      | -2.20612200 | -1.31140900 | -1.25440900 |
| F      | -3.96485800 | -0.44963700 | -0.26670000 |
| TS56   | -0.87577100 | 0.10830200 | 0.23938400 |
| C      | -2.10158100 | -0.77178100 | -1.42895600 |
| C      | -2.34783200 | -1.50025400 | -0.31178600 |
| H      | -2.48602300 | -0.86472100 | -2.42970300 |
| H      | -2.98685000 | -2.35131000 | -0.15285400 |
| N      | -1.58984500 | -0.94820000 | 0.70456200 |
| N      | -1.19241200 | 0.20819000 | -1.07688100 |
| C      | -1.55822600 | -1.46059100 | 2.07595900 |
| H      | -2.31480300 | -2.23731000 | 2.16480800 |
| H      | -0.57898400 | -1.88263400 | 2.30038900 |
| H      | -1.77643200 | -0.65893300 | 2.77895100 |
| C      | -0.65123600 | 1.20263200 | -2.00403800 |
| H      | -0.80373000 | 0.84460600 | -3.02017100 |
| H      | -1.15341100 | 2.16139900 | -1.87472300 |
| H      | 0.41491500  | 1.32618500 | -1.82429100 |
| B      | 0.17254600 | 0.96731100 | 1.06269500 |
| H      | 1.36973100 | 0.59288900 | 0.64305000 |
| C      | 2.90475100 | 0.14985100 | 0.24046200 |
| H      | 3.17471800 | 0.87488000 | -0.51787700 |
| H      | 3.41221700 | 0.20820000 | 1.19551200 |
| Cl     | 2.87547700 | -1.49846700 | -0.39582400 |
| H      | 0.15058000 | 0.71163000 | 2.23626800 |
| C      | 0.09343000 | 2.51311000 | 0.82528500 |
| N      | 0.07523700 | 3.66356700 | 0.67207700 |
| TS57   | 0.95735600 | -0.06997500 | 0.27302000 |
| C      | 2.56472600 | -1.56239800 | -0.24854300 |
| C      | 2.81745500 | -0.43004100 | -0.94905400 |
| H      | 3.09015000 | -2.50082100 | -0.21466500 |
| H      | 3.60623900 | -0.19126600 | -1.64087500 |
|  |  |  |  |
|---|---|---|---|
|  |  |  |  |
|  |  |  |  |
| H | 2.41127800 | 1.89511200 | -2.02661800 |
| H | 0.70419800 | 1.99256400 | -0.43324000 |
| H | 1.96670900 | 2.57269400 | 0.49804000 |
| H | 0.67369300 | -1.88869200 | 1.38644000 |
| H | -0.16147100 | -2.62699700 | 1.74807300 |
| H | -0.83067500 | -0.11515600 | 0.84849300 |
| B | -0.37636100 | 0.53982100 | -0.14548000 |
| C | -2.45151900 | -0.91856700 | -1.02785900 |
| H | -3.05295000 | -1.08472000 | 1.22661400 |
| O | -3.09732100 | 0.71755000 | -0.12871200 |
| C | -0.33089100 | 2.05424500 | 1.51425000 |
| N | -0.35562900 | 3.17993000 | 1.54250000 |
| N | -0.00687000 | -0.89761000 | 1.09270000 |
| H | -4.77981800 | -0.13567500 | -0.08280500 |
| H | -4.47035500 | -1.88210300 | 0.12092700 |
| H | -3.47769100 | -0.69118700 | 1.00688900 |
| B | 0.08606700 | 0.81000700 | 0.89435700 |
| C | 1.21393600 | -0.11861900 | -0.62588100 |
| N | 1.82241500 | 0.47566900 | -0.62588100 |
| N | 1.42281500 | -1.32942400 | 0.49804000 |
| C | 1.71816700 | 1.81994200 | -1.19103000 |
| H | 2.41127800 | 1.89511200 | -1.19103000 |
| C | 0.80720900 | -2.31405900 | 1.38644000 |
| H | 1.46696500 | 1.99256400 | -1.19103000 |
| C | -4.00687000 | 0.71755000 | -1.02785900 |
| H | -4.77981800 | -0.13567500 | -0.08280500 |
| H | -4.47035500 | -1.88210300 | 0.12092700 |
| H | -3.47769100 | -0.69118700 | 1.00688900 |
| C | 1.21393600 | -0.11861900 | 0.30108700 |
| C | 2.11461400 | -0.91856700 | -0.12871200 |
| C | 2.27761800 | 1.44971100 | -1.34426100 |
| H | 2.86048400 | 1.29961900 | -2.25085800 |
| H | 1.30172800 | 1.85357400 | -1.60843400 |
| C | 0.64556300 | -2.19036800 | 1.59856800 |
| H | 1.10109000 | -3.17636600 | 1.69712800 |
| H | 0.67160100 | -1.88210300 | 2.56003800 |
| H | -0.39029600 | -2.30221700 | 1.27734300 |
| H | -0.42761600 | 0.34177600 | 1.87479400 |
| B | 0.08606700 | 0.81000700 | 0.89435700 |
| H | -0.90412900 | 0.81571800 | -0.02755500 |
| C | -2.11772300 | 0.81931900 | -1.06196700 |
| H | -2.61939200 | 1.74721500 | -0.95636000 |
| H | -1.56783400 | 0.85136500 | -1.99841900 |
|      | S          | C          | N          | C          | H          | H          | H          | C          | N          | C          | H          | H          | H          | C          |
|------|------------|------------|------------|------------|------------|------------|------------|------------|------------|------------|------------|------------|------------|------------|
|      | -3.09202200 | -0.64415600 | -0.92632700 |           |            |            |            |            |            |            |            |            |            |
|      | 0.47017800  | 2.30591200  | 1.12348900  |            |            |            |            |            |            |            |            |            |            |
|      | 0.69909500  | 3.43021500  | 1.30597100  |            |            |            |            |            |            |            |            |            |            |
|      | -3.97323700 | -0.32655900 | 0.64197100  |            |            |            |            |            |            |            |            |            |            |
|      | -4.58486200 | 0.57244000  | 0.55662600  |            |            |            |            |            |            |            |            |            |            |
|      | -4.61761000 | -1.18585500 | 0.82686600  |            |            |            |            |            |            |            |            |            |            |
|      | -3.26230000 | -0.21965900 | 1.46095100  |            |            |            |            |            |            |            |            |            |            |
|      |            |            |            |            |            |            |            |            |            |            |            |            |            |
| **TS59** |            |            |            |            |            |            |            |            |            |            |            |            |            |
|      | 0.91478600  | -0.11809600 | 0.30225900  |            |            |            |            |            |            |            |            |            |            |
|      | 2.01061500  | -2.01243200 | -0.25759800 |            |            |            |            |            |            |            |            |            |            |
|      | 2.37214100  | -1.05610500 | -1.14661300 |            |            |            |            |            |            |            |            |            |            |
|      | 2.30679700  | -3.04372800 | -0.17652100 |            |            |            |            |            |            |            |            |            |            |
|      | 3.04478000  | -1.0490100  | -1.98564300 |            |            |            |            |            |            |            |            |            |            |
|      | 1.69217500  | 0.09910100  | -0.79956700 |            |            |            |            |            |            |            |            |            |            |
|      | 1.12047500  | -1.42851700 | 0.62762500  |            |            |            |            |            |            |            |            |            |            |
|      | 1.79120400  | 1.36227000  | -1.52522700 |            |            |            |            |            |            |            |            |            |            |
|      | 2.28782600  | 1.17595600  | -2.47570200 |            |            |            |            |            |            |            |            |            |            |
|      | 0.79423900  | 1.75897700  | -1.71362500 |            |            |            |            |            |            |            |            |            |            |
|      | 2.36315700  | 2.09368200  | -0.95385900 |            |            |            |            |            |            |            |            |            |            |
|      | 0.47836100  | -2.13259200 | 1.73341400  |            |            |            |            |            |            |            |            |            |            |
|      | 0.62895600  | -1.58526500 | 2.66309800  |            |            |            |            |            |            |            |            |            |            |
|      | -0.59187400 | -2.23720700 | 1.55002600  |            |            |            |            |            |            |            |            |            |            |
|      | 0.92726500  | -3.12048400 | 1.81805700  |            |            |            |            |            |            |            |            |            |            |
|      | -1.21897900 | 0.87057400  | 0.19205300  |            |            |            |            |            |            |            |            |            |            |
|      | -0.10188300 | 0.85349400  | 0.99420100  |            |            |            |            |            |            |            |            |            |            |
|      | -0.50922100 | 0.43484300  | 2.04560300  |            |            |            |            |            |            |            |            |            |            |
|      | -2.54763300 | 0.90908600  | -0.63394700 |            |            |            |            |            |            |            |            |            |            |
|      | -2.21107000 | 1.50882600  | -1.47480200 |            |            |            |            |            |            |            |            |            |            |
|      | -3.16990800 | 1.43970200  | 0.08594300  |            |            |            |            |            |            |            |            |            |            |
|      | -2.94649700 | -0.38932100 | -0.95528300 |            |            |            |            |            |            |            |            |            |            |
|      | -2.96694300 | -0.61533100 | -1.93858500 |            |            |            |            |            |            |            |            |            |            |
|      | 0.32969500  | 2.34747700  | 1.11116300  |            |            |            |            |            |            |            |            |            |            |
|      | 0.59430000  | 3.47524600  | 1.21538100  |            |            |            |            |            |            |            |            |            |            |
|      | -3.96699600 | -1.04437700 | -0.15374400 |            |            |            |            |            |            |            |            |            |            |
|      | -4.09093800 | -2.07564200 | -0.48829800 |            |            |            |            |            |            |            |            |            |            |
|      | -3.65750000 | -1.06555400 | 0.89446000  |            |            |            |            |            |            |            |            |            |            |
|      | -4.94338300 | -0.53887200 | -0.20855000 |            |            |            |            |            |            |            |            |            |            |
| **TS60** |            |            |            |            |            |            |            |            |            |            |            |            |            |
|      | 1.03572600  | -0.29425500 | 0.28878500  |            |            |            |            |            |            |            |            |            |            |
|      | 1.23718700  | -2.50634200 | -0.08769000 |            |            |            |            |            |            |            |            |            |            |
|      | 1.69199100  | -1.86212500 | -1.19029100 |            |            |            |            |            |            |            |            |            |            |
|      | 1.16319000  | -3.55686800 | 0.13269800  |            |            |            |            |            |            |            |            |            |            |
|      | 2.09375200  | -2.24361500 | -2.11263700 |            |            |            |            |            |            |            |            |            |            |
|      | 1.55795000  | -0.50656600 | -0.95010700 |            |            |            |            |            |            |            |            |            |            |
|      | 0.84001200  | -1.53493200 | 0.81316300  |            |            |            |            |            |            |            |            |            |            |
|      | 1.92864300  | 0.53722400  | -1.90511200 |            |            |            |            |            |            |            |            |            |            |
|   |   |   |   |
|---|---|---|---|
| H | 2.04631400 | 0.07940300 | -2.88543100 |
| H | 1.14249700 | 1.28883400 | -1.95297700 |
| H | 2.86335400 | 1.01438900 | -1.61080000 |
| C | 0.27111700 | -1.82116900 | 2.13002700 |
| H | 0.80764600 | -1.26464300 | 2.89647100 |
| H | -0.78388400 | -1.54727400 | 2.15694400 |
| H | 0.37102700 | -2.88792600 | 2.31956400 |
| H | -0.53722400 | 1.46046700 | 0.40071800 |
| B | 0.63222000 | 1.06995400 | 0.96810500 |
| H | 0.35580000 | 0.94391500 | 2.13054300 |
| C | -1.93984800 | 1.94493600 | -0.13073000 |
| H | -1.70354300 | 2.09894300 | -1.17825200 |
| H | -2.08614000 | 2.84334100 | 0.45683400 |
| N | -2.89192500 | 0.93946500 | 0.10644800 |
| H | -3.31444500 | 0.88666400 | 1.02623500 |
| C | 1.61164600 | 2.26554000 | 0.74731100 |
| N | 2.30146300 | 3.18952800 | 0.60673300 |
| C | -3.18324200 | -0.08559300 | -0.73298000 |
| H | -2.68516000 | 0.00435200 | -1.71132300 |
| O | -3.93326400 | -1.01893900 | -0.45733600 |
|   |   |   |   |
| TS61  |   |   |   |
| C | -1.06966300 | 0.10466400 | -0.17279400 |
| C | -2.35183000 | -1.63240400 | 0.44783700 |
| C | -1.88383000 | -1.04242000 | 1.57723400 |
| H | -2.99863500 | -2.48173400 | 0.31418000 |
| H | -2.03925200 | -1.28459700 | 2.61396200 |
| N | -1.10101100 | 0.02282800 | 1.18110300 |
| N | -1.84381500 | -0.91755500 | -0.61900000 |
| C | -0.34130900 | 0.87308200 | 2.10334700 |
| H | 0.71586600 | 0.60467500 | 2.06389600 |
| H | -0.47177800 | 1.91908900 | 1.83488100 |
| H | -0.72472900 | 0.71091400 | 3.10867500 |
| C | -2.12025500 | -1.23036400 | -2.02361700 |
| H | -2.86744300 | -2.02042200 | -2.05418200 |
| H | -2.50450400 | -0.34903400 | -2.53328200 |
| H | -1.21329500 | -1.57152400 | -2.52170400 |
| H | -0.41289900 | 0.93584400 | -2.25065600 |
| B | -0.24101200 | 1.10871200 | -1.07731600 |
| H | 1.05204700 | 0.79957900 | -0.87143500 |
| C | 2.59209000 | 0.62475300 | -0.67906000 |
| H | 2.85451500 | 0.64590300 | -1.73125200 |
| H | 2.73887000 | 1.54520300 | -0.12516900 |
| C | 2.72218500 | -0.61482800 | 0.05157600 |
| O | 2.66924800 | -0.64938100 | 1.29249600 |
| C | -0.35629500 | 2.61904900 | -0.69245800 |

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|     |   X     |   Y     |   Z      |
|-----|--------|--------|----------|
| N   | -0.41009100 | 3.74851700 | -0.43274900 |
| C   | 2.87875100  | -1.89333600 | -0.75088600 |
| H   | 2.18123500  | -1.91897000 | -1.59305500 |
| H   | 3.88932600  | -1.94791800 | -1.16922400 |
| H   | 2.71710400  | -2.76122200 | -0.11158300 |
| TS62 |
| C   | 1.09997000  | -0.12271000 | 0.30699600  |
| C   | 2.11467300  | -2.10122200 | -0.02157500 |
| C   | 2.81800200  | -1.16285400 | -0.70337500 |
| H   | 2.26767700  | -3.16171200 | 0.07587600  |
| H   | 3.70337400  | -1.24837600 | -1.30874600 |
| N   | 2.18099900  | 0.04634100  | -0.49781500 |
| N   | 1.06421900  | -1.44910000 | 0.59381300  |
| C   | 2.62372100  | 1.31188600  | -1.08765500 |
| H   | 1.78667100  | 1.80720900  | -1.57625100 |
| H   | 3.03564700  | 1.96776500  | -0.32192000 |
| H   | 3.38986300  | 1.09123100  | -1.82778600 |
| C   | 0.03263600  | -2.11882300 | 1.39160200  |
| H   | -0.92967100 | -2.05987100 | 0.88124300  |
| H   | -0.57224400 | 0.57068100  | 1.75935200  |
| B   | 0.00386500  | 0.92448400  | 0.76649600  |
| H   | -0.93623500 | 0.88105100  | -0.16915600 |
| C   | -2.12760500 | 0.69907300  | -1.25323900 |
| H   | -2.41448100 | 1.74081300  | -1.34249600 |
| H   | -1.50605300 | 0.29241400  | -2.04010000 |
| C   | -3.01328600 | -0.24388200 | -0.58239500 |
| O   | -2.83157400 | -1.47316700 | -0.61647400 |
| N   | -4.03986100 | 0.29387600  | 0.14297200  |
| H   | -4.19622400 | 1.28673900  | 0.20011500  |
| H   | -4.64099400 | -0.31926600 | 0.67076400  |
| C   | 0.44551500  | 2.41867800  | 0.88516800  |
| N   | 0.70927100  | 3.54370200  | 0.99008000  |
| TS63 |
| C   | -1.37323100 | 0.00147900  | -0.24520900 |
| C   | -3.15993700 | -0.60524000 | 0.97764600  |
| C   | -2.56798600 | 0.44008300  | 1.60767900  |
| H   | -4.03260400 | -1.17984800 | 1.23424700  |
| H   | -2.82696000 | 0.95271000  | 2.51752400  |
| N   | -1.47047500 | 0.79844400  | 0.84848800  |
| N   | -2.41624000 | -0.86299600 | -0.15856900 |
| C   | -0.54972100 | 1.88399300  | 1.19557700  |
| H   | -0.73678700 | 2.17043200  | 2.22846300  |
| H   | 0.47763600  | 1.53853000  | 1.09964000  |
| H   | -0.71113000 | 2.74260300  | 0.54451600  |
|   |   |   |   |
|---|---|---|---|
| C | -2.71948400 | -1.93392900 | -1.11081600 |
| H | -3.67245900 | -2.37695100 | -0.82950100 |
| H | -2.79099700 | -1.52823000 | -2.11808700 |
| H | -1.94300400 | -2.69788900 | -1.08200500 |
| H | -0.54604600 | -0.71329900 | -2.29402700 |
| B | -0.24461600 | -0.01829000 | -1.36177300 |
| H | 0.80606700 | -0.60615300 | -0.82985800 |
| C | 2.15473100 | -1.46681000 | -0.32606100 |
| H | 1.71444300 | -2.09267200 | 0.44310000 |
| H | 2.39339400 | -1.94606300 | -1.26808800 |
| C | 0.23774600 | 1.38778700 | -1.85558800 |
| N | 0.62986900 | 2.40528900 | -2.25195200 |
| C | 3.09762000 | -0.43517600 | 0.12837000 |
| F | 2.57669200 | 0.28069800 | 1.19864200 |
| F | 4.28619000 | -0.99987600 | 0.63456300 |
| H | 3.40508500 | 0.28260700 | -0.63125500 |

|   |   |   |   |
|---|---|---|---|
| C | -1.12093100 | -0.06014700 | -0.22001700 |
| C | -2.93392900 | -1.20496100 | 0.45822800 |
| C | -2.84993400 | -0.08495400 | 1.21841200 |
| H | -3.64995800 | -2.00795000 | 0.46598600 |
| H | -3.47895700 | 0.27505400 | 2.01378300 |
| N | -1.72986200 | 0.60512100 | 0.79454500 |
| N | -1.86703300 | -1.17628000 | -0.42126300 |
| C | -1.27778300 | 1.87472900 | 1.36564000 |
| H | -1.77623100 | 2.01776300 | 2.32210900 |
| H | -0.20125100 | 1.84347200 | 1.52300000 |
| H | -1.52175500 | 2.70187800 | 0.69937000 |
| C | -1.59232200 | -2.21817700 | -1.41351000 |
| H | -2.43246100 | -2.90936900 | -1.42184600 |
| H | -1.47999600 | -1.77204400 | -2.39980300 |
| H | -0.68222600 | -2.75902400 | -1.15507300 |
| H | 0.46747400 | -0.42314700 | -1.87941900 |
| B | 0.23435000 | 0.30758200 | -0.95544000 |
| H | 1.20334600 | 0.07798300 | -0.07572500 |
| C | 2.45148000 | -0.25869700 | 0.94048200 |
| H | 2.52748300 | 0.69403000 | 1.45505100 |
| H | 1.99497700 | -1.06313000 | 1.5901900 |
| C | 0.37813000 | 1.80844000 | -1.37501100 |
| N | 0.52885100 | 2.91351200 | -1.69638100 |
| C | 3.53119800 | -0.61454000 | -0.00192900 |
| F | 4.74536700 | -0.97649200 | 0.71131500 |
| H | 3.29073200 | -1.48894900 | -0.60781100 |
| H | 3.81961400 | 0.21734000 | -0.64534900 |
