Supplementary Information

# Theoretical investigation on the effect of radical substituents on the open-shell character of polycyclic aromatic hydrocarbon

Tomohito Shinozuka,[a] Daiki Shimizu*[a] and Kenji Matsuda*[a,b]

a. Department of Synthetic Chemistry and Biological Chemistry, Graduate School of Engineering, Kyoto University, Katsura, Nishikyo-ku, Kyoto 615-8510, Japan.
b. Fukui Institute for Fundamental Chemistry (FIFC), Kyoto University, Sakyo-ku, Kyoto 606-8103, Japan.

## Contents

# 1. The effect of Mt/Allyl type radicals on PAH's orbital energies

**Table S1** The effect of Mt and Allyl radical substituents on orbital energies of five PAHs subjected in this work. These orbital energies were obtained by simple Hückel molecular orbital theory.

| PAH | PAH with Mt HOMO/LUMO | | With no Radical HOMO/LUMO | | PAH with Allyl HOMO/LUMO |
|---|---|---|---|---|---|
| An | $\varepsilon_L = \alpha - 0.68\beta$<br>$\varepsilon_H = \alpha + 0.68\beta$ | H–L gap $+0.54\beta$ | $\varepsilon_L = \alpha - 0.41\beta$<br>$\varepsilon_H = \alpha + 0.41\beta$ | H–L gap $-0.06\beta$ | $\varepsilon_L = \alpha - 0.38\beta$<br>$\varepsilon_H = \alpha + 0.38\beta$ |
| Pn | $\varepsilon_L = \alpha - 0.49\beta$<br>$\varepsilon_H = \alpha + 0.49\beta$ | H–L gap $+0.54\beta$ | $\varepsilon_L = \alpha - 0.22\beta$<br>$\varepsilon_H = \alpha + 0.22\beta$ | H–L gap $-0.02\beta$ | $\varepsilon_L = \alpha - 0.21\beta$<br>$\varepsilon_H = \alpha + 0.21\beta$ |
| Hp | $\varepsilon_L = \alpha - 0.38\beta$<br>$\varepsilon_H = \alpha + 0.38\beta$ | H–L gap $+0.50\beta$ | $\varepsilon_L = \alpha - 0.13\beta$<br>$\varepsilon_H = \alpha + 0.13\beta$ | H–L gap $-0.00\beta$ | $\varepsilon_L = \alpha - 0.13\beta$<br>$\varepsilon_H = \alpha + 0.13\beta$ |
| Nn | $\varepsilon_L = \alpha - 0.31\beta$<br>$\varepsilon_H = \alpha + 0.31\beta$ | H–L gap $+0.44\beta$ | $\varepsilon_L = \alpha - 0.09\beta$<br>$\varepsilon_H = \alpha + 0.09\beta$ | H–L gap $-0.00\beta$ | $\varepsilon_L = \alpha - 0.09\beta$<br>$\varepsilon_H = \alpha + 0.09\beta$ |
| Tri | $\varepsilon_L = \alpha - 0.39\beta$<br>$\varepsilon_H = \alpha + 0.39\beta$ | H–L gap $+0.78\beta$ | $\varepsilon_L = \alpha - 0.00\beta$<br>$\varepsilon_H = \alpha + 0.00\beta$ | H–L gap $-0.00\beta$ | $\varepsilon_L = \alpha - 0.00\beta$<br>$\varepsilon_H = \alpha + 0.00\beta$ |

**Table S2** The effect of Mt and Allyl radical substituents on orbital energies of five PAHs subjected in this work. These orbital energies were obtained by LC-R(O)BLYP($\mu$=0.33)/6-311G(d,p) level.

| PAH | R = Mt HOMO/LUMO (eV) | | R = H HOMO/LUMO (eV) | | R = Allyl HOMO/LUMO (eV) |
|---|---|---|---|---|---|
| An | $\varepsilon_L = -0.210$<br>$\varepsilon_H = -7.932$ | H–L gap $+0.571$ | $\varepsilon_L = -0.409$<br>$\varepsilon_H = -7.561$ | H–L gap $-0.171$ | $\varepsilon_L = -0.452$<br>$\varepsilon_H = -7.433$ |
| Pn | $\varepsilon_L = -0.719$<br>$\varepsilon_H = -7.563$ | H–L gap $+1.278$ | $\varepsilon_L = -1.213$<br>$\varepsilon_H = -6.779$ | H–L gap $-0.104$ | $\varepsilon_L = -1.238$<br>$\varepsilon_H = -6.700$ |
| Hp | $\varepsilon_L = -0.938$<br>$\varepsilon_H = -7.314$ | H–L gap $+1.892$ | $\varepsilon_L = -1.769$<br>$\varepsilon_H = -6.253$ | H–L gap $-0.090$ | $\varepsilon_L = -1.796$<br>$\varepsilon_H = -6.190$ |
| Nn | $\varepsilon_L = -1.104$<br>$\varepsilon_H = -7.054$ | H–L gap $+2.079$ | $\varepsilon_L = -2.084$<br>$\varepsilon_H = -5.955$ | H–L gap $-0.059$ | $\varepsilon_L = -2.099$<br>$\varepsilon_H = -5.911$ |
| Tri | $\varepsilon_L = -0.964$<br>$\varepsilon_H = -7.208$ | H–L gap $+3.407$ | $\varepsilon_L = -2.609$<br>$\varepsilon_H = -5.446$ | H–L gap $-0.215$ | $\varepsilon_L = -2.586$<br>$\varepsilon_H = -5.208$ |

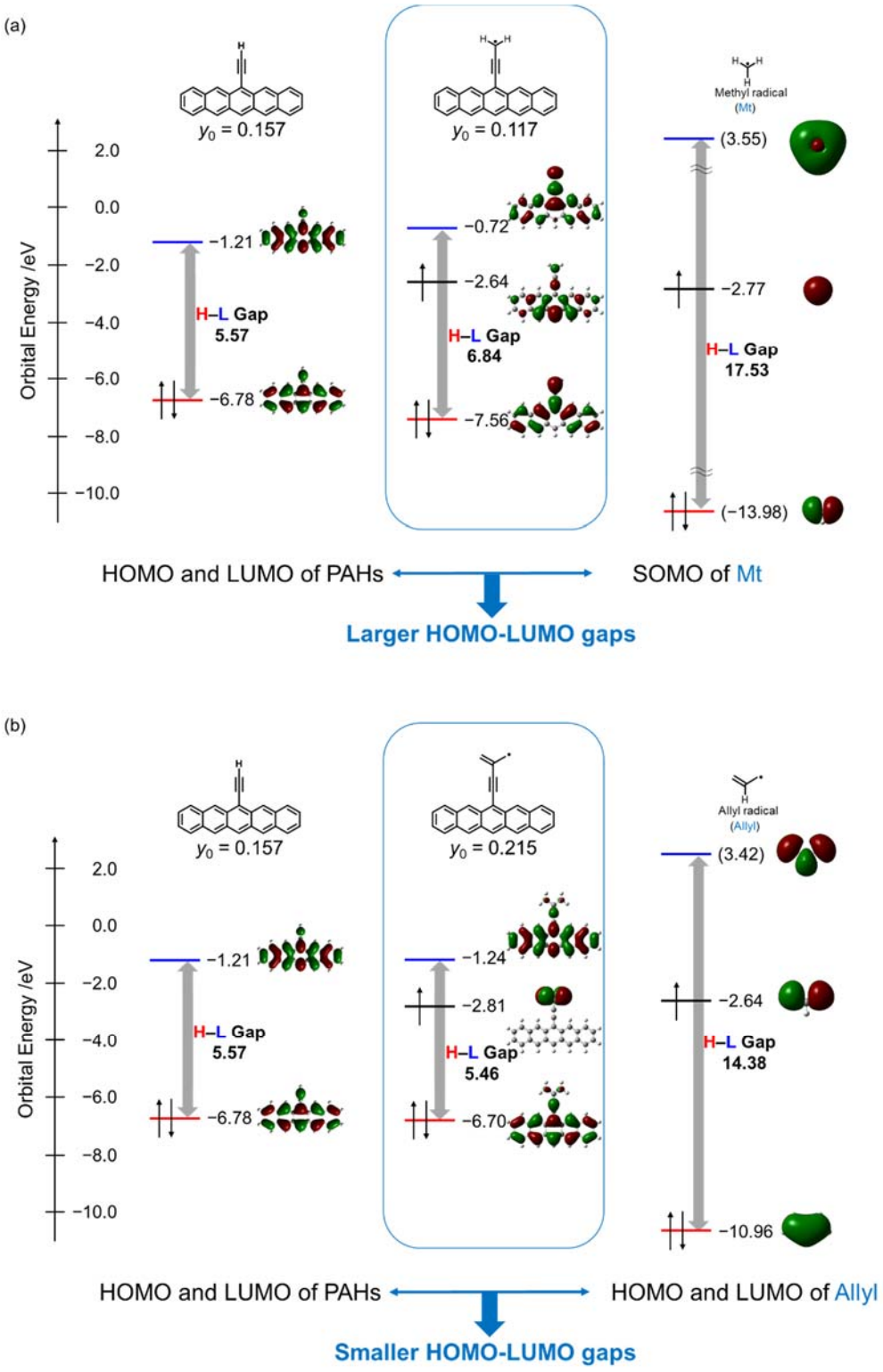


**Fig S1.** The effect of (a)Mt and (b)Allyl radical substituents on orbital energies of PAHs from the viewpoints of Kohn-Sham energies. The results of pentacenes are displayed as a representative of five PAHs. These orbital energies were obtained by LC-R(O)BLYP($\mu$=0.33)/6-311G(d,p) level of theory.

## 2. Plots of $y_0$ *vs.* UDFT HOMO–LUMO gap

Fig. S2 shows a scatter plot of $y_0$ and HOMO–LUMO gaps calculated by unrestricted DFT. Unlike the correlation between $y_0$ and the HOMO–LUMO gap calculated by restricted/restricted-open DFT shown in Fig. 7 in the main text, no clear correlation between the two values were observed.

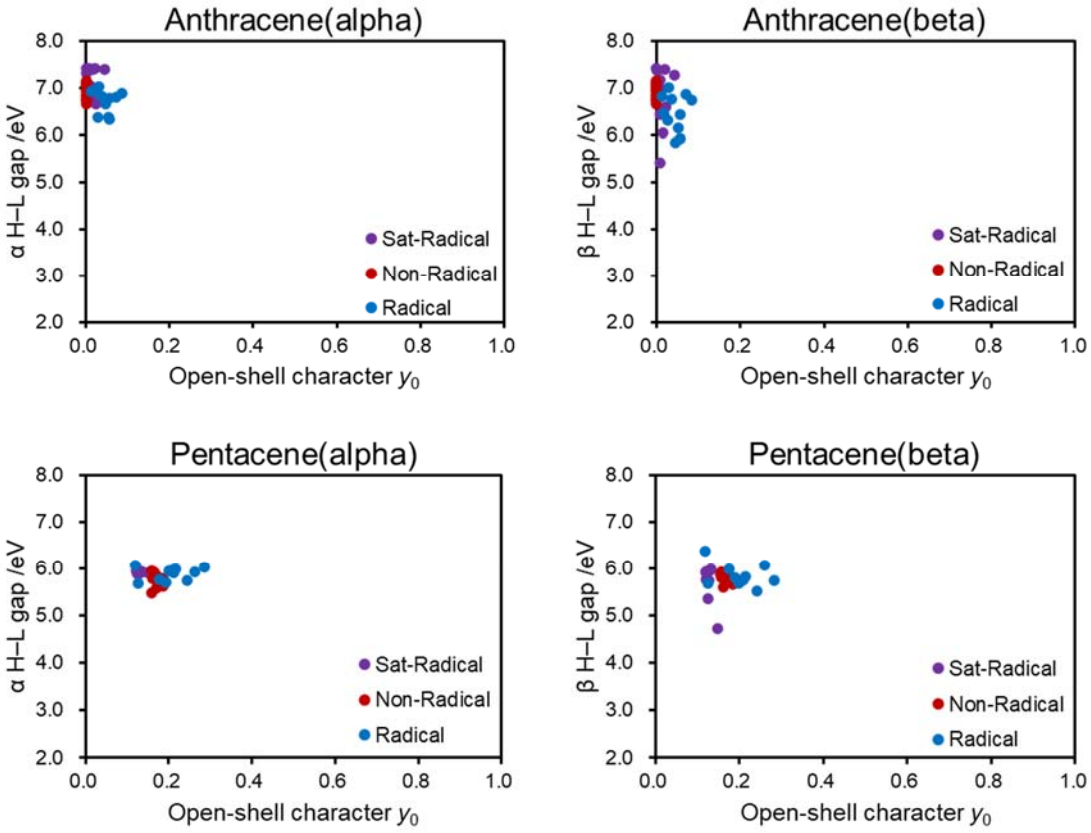


**Fig S2-1.** The scatter plot of $y_0$ and HOMO–LUMO gaps in **An** and **Pn** systems, which were obtained by LC-UBLYP($\mu$=0.33)/6-311G(d,p) level of theory.

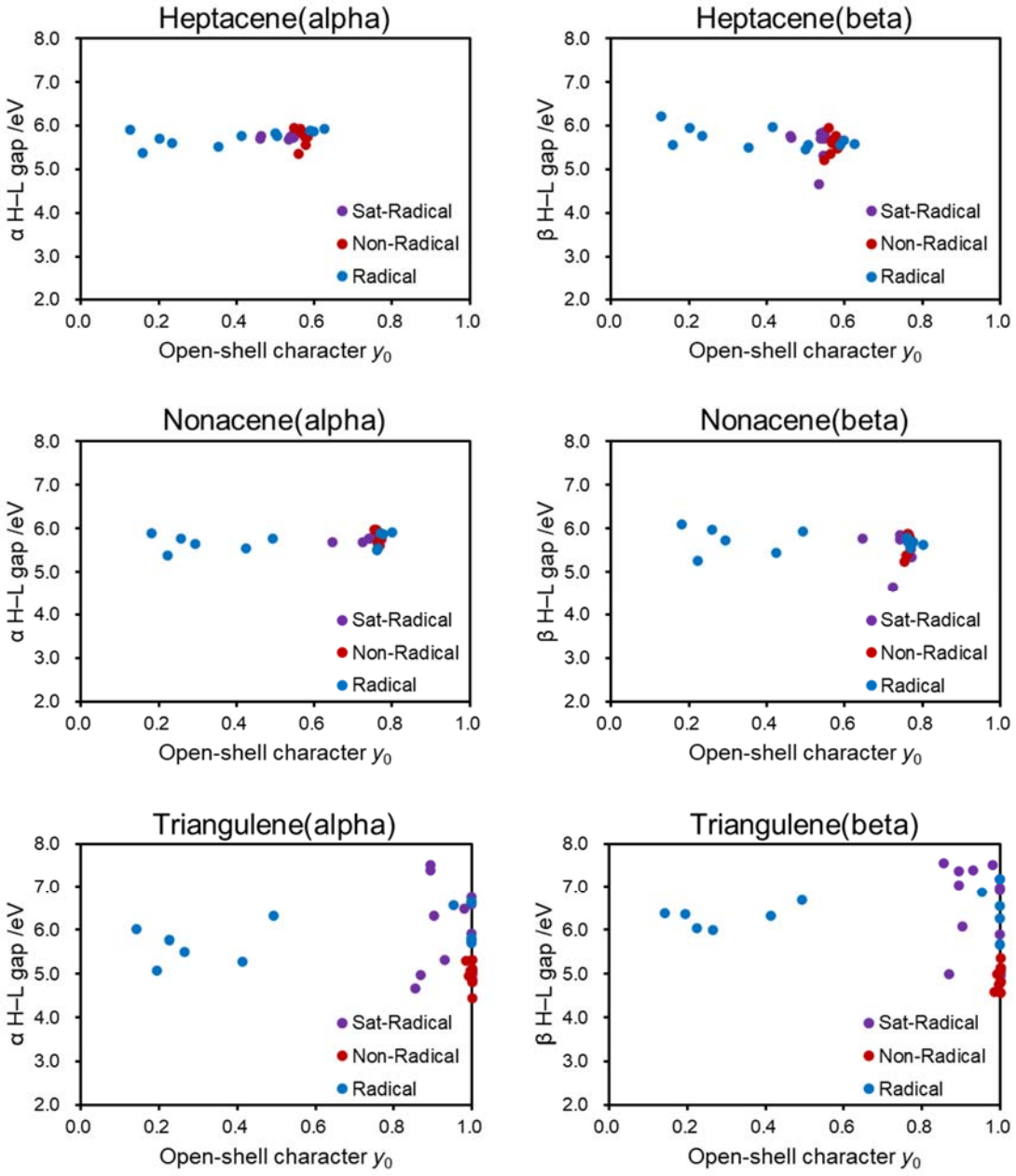


**Fig S2-2.** The scatter plot of $y_0$ and HOMO–LUMO gaps in **Hp**, **Nn** and **Tri** systems, which were obtained by LC-UBLYP($\mu$=0.33)/6-311G(d,p) level of theory.

## 3. Calculated values shown in Fig. 5,7,8 (plots of $y_0$ vs. R(O)DFT HOMO–LUMO gap) in the main text

**Table S3** Calculated open-shell character $y_0$, orbital energies, H–L gaps, and S–T gaps of Non-Radical substituted anthracenes (**An**). Open-shell character $y_0$, orbital energies and S–T gaps were obtained by LC-UBLYP($\mu$=0.33)/6-311G(d,p), LC-RBLYP($\mu$=0.33)/6-311G(d,p) and RAS(4,4)-SF/cc-PVTZ, respectively.

| **An** | $y_0$ | HOMO /eV | SOMO /eV | LUMO /eV | H–L gap /eV | S–T gap /eV |
|---|---|---|---|---|---|---|
| $NO_2$ | 0.000 | -8.068 | - | -1.333 | 6.735 | 2.272 |
| CN | 0.000 | -7.976 | - | -1.047 | 6.929 | 2.323 |
| Cl | 0.000 | -7.580 | - | -0.478 | 7.102 | 2.361 |
| H | 0.000 | -7.561 | - | -0.409 | 7.152 | 2.364 |
| CHO | 0.000 | -7.835 | - | -0.985 | 6.850 | 2.302 |
| $SiMe_3$ | 0.000 | -7.489 | - | -0.423 | 7.067 | 2.338 |
| OMe | 0.000 | -7.199 | - | -0.149 | 7.050 | 2.349 |
| $NH_2$ | 0.000 | -7.031 | - | -0.071 | 6.960 | 2.340 |
| Ph | 0.000 | -7.341 | - | -0.506 | 6.834 | 2.123 |
| BzTh | 0.000 | -7.340 | - | -0.672 | 6.668 | 2.081 |
| Th | 0.000 | -7.304 | - | -0.559 | 6.745 | 2.089 |

**Table S4** Calculated open-shell character $y_0$, orbital energies, H–L gaps, and D–Q gaps of Radical substituted anthracenes (**An**). Open-shell character $y_0$, orbital energies and D–Q gaps were obtained by LC-UBLYP($\mu$=0.33)/6-311G(d,p), LC-ROBLYP($\mu$=0.33)/6-311G(d,p) and RAS(5,5)-SF/cc-PVTZ, respectively.

| **An** | $y_0$ | HOMO /eV | SOMO /eV | LUMO /eV | H–L gap /eV | D–Q gap/eV |
|---|---|---|---|---|---|---|
| Mt | 0.070 | -7.932 | -2.714 | -0.210 | 7.722 | 2.718 |
| DCM | 0.055 | -8.599 | -3.623 | -1.124 | 7.475 | 2.918 |
| DPM | 0.056 | -7.633 | -2.644 | -0.342 | 7.290 | 2.627 |
| Flu | 0.052 | -7.754 | -2.866 | -0.519 | 7.235 | 2.496 |
| PhO | 0.045 | -7.940 | -3.328 | -0.807 | 7.133 | 2.584 |
| NO | 0.035 | -7.647 | -2.826 | -0.345 | 7.302 | 2.396 |
| Allyl | 0.028 | -7.433 | -2.807 | -0.452 | 6.981 | 2.285 |
| IN | 0.012 | -7.544 | -2.770 | -0.630 | 6.914 | 2.317 |
| Phen | 0.026 | -7.352 | -2.637 | -0.523 | 6.829 | 2.091 |
| Ver | 0.018 | -7.519 | -3.025 | -0.633 | 6.886 | 2.083 |
| NN | 0.083 | -7.361 | -2.540 | -0.682 | 6.680 | 1.939 |

**Table S5** Calculated open-shell character $y_0$, orbital energies, and H–L gaps of Sat-Radical substituted anthracenes (**An**). Open-shell character $y_0$ and orbital energies were obtained by LC-UBLYP($\mu$=0.33)/6-311G(d,p) and LC-ROBLYP($\mu$=0.33)/6-311G(d,p), respectively.

| **An** | $y_0$ | HOMO /eV | SOMO /eV | LUMO /eV | H–L gap /eV |
|---|---|---|---|---|---|
| Sat-H | 0.000 | -7.462 | - | -0.044 | 7.417 |
| Sat-Mt | 0.001 | -7.502 | -2.512 | -0.071 | 7.431 |
| Sat-DCM | 0.007 | -7.869 | -4.083 | -0.448 | 7.420 |
| Sat-DPM | 0.011 | -7.503 | -2.449 | -0.088 | 7.415 |
| Sat-Flu | 0.008 | -7.575 | -2.794 | -0.156 | 7.419 |
| Sat-PhO | 0.015 | -7.730 | -3.394 | -0.316 | 7.413 |
| Sat-NO | 0.001 | -7.583 | -2.351 | -0.149 | 7.434 |
| Sat-Allyl | 0.020 | -7.497 | -2.664 | -0.091 | 7.405 |
| Sat-IN | 0.007 | -7.426 | -2.828 | -0.018 | 7.408 |
| Sat-Phen | 0.022 | -7.517 | -2.559 | -0.118 | 7.399 |
| Sat-Ver | 0.012 | -7.517 | -3.012 | -0.113 | 7.404 |
| Sat-NN | 0.043 | -7.401 | -2.597 | -0.005 | 7.396 |

**Table S6** Calculated open-shell character $y_0$, orbital energies, H–L gaps, and S–T gaps of Non-Radical substituted pentacenes (**Pn**). Open-shell character $y_0$, orbital energies and S–T gaps were obtained by LC-UBLYP($\mu$=0.33)/6-311G(d,p), LC-RBLYP($\mu$=0.33)/6-311G(d,p) and RAS(4,4)-SF/cc-PVTZ, respectively.

| **Pn** | $y_0$ | HOMO /eV | SOMO /eV | LUMO /eV | H–L gap /eV | S–T gap /eV |
|---|---|---|---|---|---|---|
| $NO_2$ | 0.156 | -7.188 | - | -1.814 | 5.374 | 1.487 |
| CN | 0.161 | -7.127 | - | -1.678 | 5.449 | 1.136 |
| Cl | 0.158 | -6.808 | - | -1.266 | 5.541 | 1.165 |
| H | 0.157 | -6.779 | - | -1.213 | 5.567 | 1.169 |
| CHO | 0.169 | -7.008 | - | -1.591 | 5.417 | 1.109 |
| $SiMe_3$ | 0.164 | -6.736 | - | -1.214 | 5.523 | 1.154 |
| OMe | 0.167 | -6.530 | - | -1.016 | 5.514 | 1.153 |
| $NH_2$ | 0.176 | -6.420 | - | -0.954 | 5.466 | 1.134 |
| Ph | 0.176 | -6.663 | - | -1.245 | 5.417 | 1.133 |
| BzTh | 0.183 | -6.692 | - | -1.342 | 5.350 | 1.123 |
| Th | 0.184 | -6.651 | - | -1.275 | 5.376 | 1.124 |

**Table S7** Calculated open-shell character $y_0$, orbital energies, H–L gaps, and D–Q gaps of Radical substituted pentacenes (**Pn**). Open-shell character $y_0$, orbital energies and D–Q gaps were obtained by LC-UBLYP($\mu$=0.33)/6-311G(d,p), LC-ROBLYP($\mu$=0.33)/6-311G(d,p) and RAS(5,5)-SF/cc-PVTZ, respectively.

| **Pn** | $y_0$ | HOMO /eV | SOMO /eV | LUMO /eV | H–L gap /eV | D–Q gap /eV |
|---|---|---|---|---|---|---|
| Mt | 0.117 | -7.563 | -2.638 | -0.719 | 6.844 | 1.880 |
| DCM | 0.124 | -8.122 | -3.223 | -1.893 | 6.230 | 2.058 |
| DPM | 0.175 | -7.065 | -2.604 | -1.046 | 6.019 | 1.595 |
| Flu | 0.190 | -7.159 | -2.740 | -1.360 | 5.798 | 1.681 |
| PhO | 0.241 | -7.180 | -3.169 | -1.634 | 5.546 | 1.383 |
| NO | 0.259 | -6.828 | -2.811 | -1.219 | 5.609 | 1.284 |
| Allyl | 0.215 | -6.700 | -2.810 | -1.238 | 5.462 | 1.117 |
| IN | 0.197 | -6.764 | -2.773 | -1.324 | 5.440 | 1.124 |
| Phen | 0.210 | -6.669 | -2.641 | -1.261 | 5.408 | 1.109 |
| Ver | 0.207 | -6.774 | -3.020 | -1.343 | 5.431 | 1.111 |
| NN | 0.284 | -6.647 | -2.537 | -1.348 | 5.298 | 0.940 |

**Table S8** Calculated open-shell character $y_0$, orbital energies, and H–L gaps of Sat-Radical substituted pentacenes (**Pn**). Open-shell character $y_0$ and orbital energies were obtained by LC-UBLYP($\mu$=0.33)/6-311G(d,p) and LC-ROBLYP($\mu$=0.33)/6-311G(d,p), respectively.

| **Pn** | $y_0$ | HOMO /eV | SOMO /eV | LUMO /eV | H–L gap /eV |
|---|---|---|---|---|---|
| Sat-H | 0.120 | -6.680 | - | -0.975 | 5.706 |
| Sat-Mt | 0.131 | -6.713 | -2.523 | -0.996 | 5.717 |
| Sat-DCM | 0.147 | -6.995 | -4.063 | -1.308 | 5.687 |
| Sat-DPM | 0.128 | -6.709 | -2.462 | -1.002 | 5.707 |
| Sat-Flu | 0.128 | -6.772 | -2.803 | -1.063 | 5.709 |
| Sat-PhO | 0.125 | -6.907 | -3.394 | -1.203 | 5.704 |
| Sat-NO | 0.133 | -6.763 | -2.370 | -1.047 | 5.717 |
| Sat-Allyl | 0.122 | -6.711 | -2.676 | -1.011 | 5.700 |
| Sat-IN | 0.121 | -6.628 | -2.856 | -0.928 | 5.700 |
| Sat-Phen | 0.121 | -6.730 | -2.566 | -1.032 | 5.698 |
| Sat-Ver | 0.121 | -6.718 | -3.022 | -1.018 | 5.700 |
| Sat-NN | 0.125 | -6.603 | -2.620 | -0.908 | 5.695 |

**Table S9** Calculated open-shell character $y_0$, orbital energies, H–L gaps, and S–T gaps of Non-Radical substituted heptacenes (**Hp**). Open-shell character $y_0$, orbital energies and S–T gaps were obtained by LC-UBLYP($\mu$=0.33)/6-311G(d,p), LC-RBLYP($\mu$=0.33)/6-311G(d,p) and RAS(4,4)-SF/cc-PVTZ, respectively.

| **Hp** | $y_0$ | HOMO /eV | SOMO /eV | LUMO /eV | H–L gap /eV | S–T gap /eV |
|---|---|---|---|---|---|---|
| $NO_2$ | 0.548 | -6.633 | - | -2.222 | 4.412 | 0.619 |
| CN | 0.559 | -6.572 | - | -2.143 | 4.429 | 0.602 |
| Cl | 0.567 | -6.281 | - | -1.813 | 4.468 | 0.462 |
| H | 0.567 | -6.253 | - | -1.769 | 4.484 | 0.463 |
| CHO | 0.563 | -6.470 | - | -2.057 | 4.412 | 0.459 |
| $SiMe_3$ | 0.571 | -6.221 | - | -1.766 | 4.455 | 0.456 |
| OMe | 0.576 | -6.045 | - | -1.603 | 4.443 | 0.449 |
| $NH_2$ | 0.582 | -5.956 | - | -1.547 | 4.409 | 0.436 |
| Ph | 0.578 | -6.170 | - | -1.786 | 4.385 | 0.443 |
| BzTh | 0.582 | -6.204 | - | -1.861 | 4.343 | 0.438 |
| Th | 0.583 | -6.163 | - | -1.808 | 4.355 | 0.436 |

**Table S10** Calculated open-shell character $y_0$, orbital energies, H–L gaps, and D–Q gaps of Radical substituted heptacenes (**Hp**). Open-shell character $y_0$, orbital energies and D–Q gaps were obtained by LC-UBLYP($\mu$=0.33)/6-311G(d,p), LC-ROBLYP($\mu$=0.33)/6-311G(d,p) and RAS(5,5)-SF/cc-PVTZ, respectively.

| **Hp** | $y_0$ | HOMO /eV | SOMO /eV | LUMO /eV | H–L gap /eV | D–Q gap /eV |
|---|---|---|---|---|---|---|
| Mt | 0.127 | -7.314 | -2.631 | -0.938 | 6.377 | 1.801 |
| DCM | 0.159 | -7.862 | -3.037 | -2.116 | 5.746 | 1.733 |
| DPM | 0.202 | -6.918 | -2.603 | -1.210 | 5.708 | 1.410 |
| Flu | 0.234 | -7.015 | -2.694 | -1.535 | 5.480 | 1.320 |
| PhO | 0.354 | -7.194 | -2.893 | -2.044 | 5.150 | 1.106 |
| NO | 0.414 | -6.878 | -2.666 | -1.392 | 5.486 | 0.668 |
| Allyl | 0.598 | -6.190 | -2.800 | -1.796 | 4.394 | 0.419 |
| IN | 0.500 | -6.326 | -2.763 | -1.747 | 4.579 | 0.605 |
| Phen | 0.505 | -6.262 | -2.641 | -1.700 | 4.562 | 0.600 |
| Ver | 0.589 | -6.261 | -3.003 | -1.873 | 4.388 | 0.425 |
| NN | 0.625 | -6.155 | -2.512 | -1.860 | 4.295 | 0.404 |

**Table S11** Calculated open-shell character $y_0$, orbital energies, and H–L gaps of Sat-Radical substituted heptacenes (**Hp**). Open-shell character $y_0$ and orbital energies were obtained by LC-UBLYP($\mu$=0.33)/6-311G(d,p) and LC-ROBLYP($\mu$=0.33)/6-311G(d,p), respectively.

| **Hp** | $y_0$ | HOMO /eV | SOMO /eV | LUMO /eV | H–L gap /eV |
|---|---|---|---|---|---|
| Sat-H | 0.549 | -6.159 | - | -1.585 | 4.574 |
| Sat-Mt | 0.545 | -6.186 | -2.525 | -1.605 | 4.581 |
| Sat-DCM | 0.534 | -6.451 | -4.028 | -1.859 | 4.592 |
| Sat-DPM | 0.539 | -6.189 | -2.468 | -1.602 | 4.587 |
| Sat-Flu | 0.539 | -6.244 | -2.804 | -1.655 | 4.589 |
| Sat-PhO | 0.546 | -6.361 | -3.385 | -1.785 | 4.576 |
| Sat-NO | 0.545 | -6.224 | -2.380 | -1.643 | 4.581 |
| Sat-Allyl | 0.548 | -6.186 | -2.679 | -1.614 | 4.572 |
| Sat-IN | 0.460 | -6.194 | -2.867 | -1.444 | 4.750 |
| Sat-Phen | 0.548 | -6.203 | -2.569 | -1.634 | 4.569 |
| Sat-Ver | 0.548 | -6.191 | -3.025 | -1.619 | 4.572 |
| Sat-NN | 0.462 | -6.169 | -2.630 | -1.421 | 4.747 |

**Table S12** Calculated open-shell character $y_0$, orbital energies, H–L gaps, and S–T gaps of Non-Radical substituted nonacenes (**Nn**). Open-shell character $y_0$, orbital energies and S–T gaps were obtained by LC-UBLYP($\mu$=0.33)/6-311G(d,p), LC-RBLYP($\mu$=0.33)/6-311G(d,p) and RAS(4,4)-SF/cc-PVTZ, respectively.

| **Nn** | $y_0$ | HOMO /eV | SOMO /eV | LUMO /eV | H–L gap /eV | S–T gap /eV |
|---|---|---|---|---|---|---|
| $NO_2$ | 0.753 | -6.294 | - | -2.476 | 3.818 | 0.264 |
| CN | 0.759 | -6.243 | - | -2.414 | 3.830 | 0.188 |
| Cl | 0.763 | -5.982 | - | -2.123 | 3.859 | 0.190 |
| H | 0.763 | -5.955 | - | -2.084 | 3.871 | 0.192 |
| CHO | 0.760 | -6.151 | - | -2.332 | 3.819 | 0.187 |
| $SiMe_3$ | 0.765 | -5.930 | - | -2.079 | 3.850 | 0.187 |
| OMe | 0.768 | -5.776 | - | -1.936 | 3.840 | 0.184 |
| $NH_2$ | 0.772 | -5.701 | - | -1.884 | 3.817 | 0.176 |
| Ph | 0.768 | -5.893 | - | -2.092 | 3.800 | 0.179 |
| BzTh | 0.770 | -5.927 | - | -2.155 | 3.771 | 0.177 |
| Th | 0.771 | -5.889 | - | -2.109 | 3.780 | 0.177 |

**Table S13** Calculated open-shell character $y_0$, orbital energies, H–L gaps, and D–Q gaps of Radical substituted nonacenes (**Nn**). Open-shell character $y_0$, orbital energies and D–Q gaps were obtained by LC-UBLYP($\mu$=0.33)/6-311G(d,p), LC-ROBLYP($\mu$=0.33)/6-311G(d,p) and RAS(5,5)-SF/cc-PVTZ, respectively..

| **Nn** | $y_0$ | HOMO /eV | SOMO /eV | LUMO /eV | H–L gap /eV | D–Q gap /eV |
|---|---|---|---|---|---|---|
| Mt | 0.182 | -7.054 | -2.639 | -1.104 | 5.951 | 2.000 |
| DCM | 0.223 | -7.385 | -2.961 | -2.216 | 5.169 | 1.390 |
| DPM | 0.258 | -6.775 | -2.615 | -1.330 | 5.445 | 1.284 |
| Flu | 0.293 | -6.873 | -2.688 | -1.638 | 5.234 | 1.516 |
| PhO | 0.424 | -7.052 | -2.850 | -2.139 | 4.913 | 1.013 |
| NO | 0.493 | -6.738 | -2.669 | -1.518 | 5.219 | 1.267 |
| Allyl | 0.776 | -5.911 | -2.796 | -2.099 | 3.812 | 0.170 |
| IN | 0.769 | -5.957 | -2.746 | -2.143 | 3.814 | 0.177 |
| Phen | 0.764 | -5.898 | -2.634 | -2.108 | 3.790 | 0.166 |
| Ver | 0.761 | -5.974 | -2.994 | -2.167 | 3.807 | 0.169 |
| NN | 0.801 | -5.865 | -2.522 | -2.147 | 3.718 | 0.141 |

**Table S14** Calculated open-shell character $y_0$, orbital energies, and H–L gaps of Sat-Radical substituted nonacenes (**Nn**). Open-shell character $y_0$ and orbital energies were obtained by LC-UBLYP($\mu$=0.33)/6-311G(d,p) and LC-ROBLYP($\mu$=0.33)/6-311G(d,p), respectively.

| **Nn** | $y_0$ | HOMO /eV | SOMO /eV | LUMO /eV | H–L gap /eV |
|---|---|---|---|---|---|
| Sat-H | 0.757 | -5.863 | - | -1.935 | 3.928 |
| Sat-Mt | 0.646 | -6.005 | -2.530 | -1.823 | 4.182 |
| Sat-DCM | 0.723 | -6.134 | -4.028 | -2.164 | 3.970 |
| Sat-DPM | 0.742 | -5.889 | -2.470 | -1.952 | 3.936 |
| Sat-Flu | 0.741 | -5.938 | -2.803 | -2.000 | 3.938 |
| Sat-PhO | 0.772 | -6.018 | -3.376 | -2.148 | 3.870 |
| Sat-NO | 0.761 | -5.769 | -2.575 | -2.149 | 3.620 |
| Sat-Allyl | 0.757 | -5.887 | -2.680 | -1.962 | 3.926 |
| Sat-IN | 0.757 | -5.813 | -2.870 | -1.888 | 3.926 |
| Sat-Phen | 0.756 | -5.904 | -2.569 | -1.979 | 3.925 |
| Sat-Ver | 0.756 | -5.891 | -3.026 | -1.965 | 3.926 |
| Sat-NN | 0.757 | -5.791 | -2.634 | -1.868 | 3.923 |

**Table S15** Calculated open-shell character $y_0$, orbital energies, H–L gaps, and S–T gaps of Non-Radical substituted triangulenes (**Tri**). Open-shell character $y_0$, orbital energies and S–T gaps were obtained by LC-UBLYP($\mu$=0.33)/6-311G(d,p), LC-RBLYP($\mu$=0.33)/6-311G(d,p) and RAS(4,4)-SF/cc-PVTZ, respectively.

| **Tri** | $y_0$ | HOMO /eV | SOMO /eV | LUMO /eV | H–L gap /eV | S–T gap /eV |
|---|---|---|---|---|---|---|
| $NO_2$ | 1.000 | -6.081 | - | -3.006 | 3.076 | 0.364 |
| CN | 1.000 | -5.955 | - | -2.957 | 2.998 | 0.340 |
| Cl | 1.000 | -5.265 | - | -2.719 | 2.546 | 0.336 |
| H | 1.000 | -5.446 | - | -2.609 | 2.837 | 0.339 |
| CHO | 0.986 | -5.839 | - | -2.863 | 2.976 | 0.346 |
| $SiMe_3$ | 1.000 | -5.459 | - | -2.634 | 2.825 | 0.335 |
| OMe | 0.991 | -5.160 | - | -2.365 | 2.795 | 0.335 |
| $NH_2$ | 1.000 | -5.015 | - | -2.266 | 2.749 | 0.328 |
| Ph | 1.000 | -5.415 | - | -2.669 | 2.746 | 0.331 |
| BzTh | 0.997 | -5.502 | - | -2.753 | 2.749 | 0.305 |
| Th | 0.998 | -5.412 | - | -2.689 | 2.724 | 0.313 |

**Table S16** Calculated open-shell character $y_0$, orbital energies, H–L gaps, and D–Q gaps of Radical substituted triangulenes (**Tri**). Open-shell character $y_0$, orbital energies and D–Q gaps were obtained by LC-UBLYP($\mu$=0.33)/6-311G(d,p), LC-ROBLYP($\mu$=0.33)/6-311G(d,p) and RAS(5,5)-SF/cc-PVTZ, respectively.

| **Tri** | $y_0$ | HOMO /eV | SOMO /eV | LUMO /eV | H–L gap /eV | D–Q gap /eV |
|---|---|---|---|---|---|---|
| Mt | 0.143 | -7.208 | -2.603 | -0.964 | 6.244 | 1.909 |
| DCM | 0.194 | -7.917 | -2.985 | -2.320 | 5.597 | 1.214 |
| DPM | 0.225 | -6.796 | -2.579 | -1.232 | 5.563 | 1.209 |
| Flu | 0.265 | -6.911 | -2.663 | -1.584 | 5.327 | 1.298 |
| PhO | 0.412 | -7.154 | -2.842 | -2.162 | 4.992 | 0.903 |
| NO | 0.492 | -6.772 | -2.645 | -1.441 | 5.331 | 0.422 |
| Allyl | 0.999 | -5.208 | -3.176 | -2.586 | 2.622 | 0.016 |
| IN | 0.953 | -4.846 | -3.418 | -2.592 | 2.254 | 0.003 |
| Phen | 0.999 | -4.769 | -3.139 | -2.687 | 2.082 | 0.025 |
| Ver | 0.999 | -5.229 | -3.324 | -2.693 | 2.536 | 0.008 |
| NN | 0.998 | -5.157 | -2.909 | -2.672 | 2.485 | 0.030 |

**Table S17** Calculated open-shell character $y_0$, orbital energies, and H–L gaps of Sat-Radical substituted triangulenes (**Tri**). Open-shell character $y_0$ and orbital energies were obtained by LC-UBLYP($\mu$=0.33)/6-311G(d,p) and LC-ROBLYP($\mu$=0.33)/6-311G(d,p), respectively.

| **Tri** | $y_0$ | HOMO /eV | SOMO /eV | LUMO /eV | H–L gap /eV |
|---|---|---|---|---|---|
| Sat-H | 1.000 | -5.190 | - | -2.404 | 2.786 |
| Sat-Mt | 0.894 | -5.629 | -2.570 | -2.076 | 3.553 |
| Sat-DCM | 0.855 | -6.414 | -3.192 | -3.126 | 3.288 |
| Sat-DPM | 0.904 | -5.210 | -2.666 | -2.384 | 2.826 |
| Sat-Flu | 0.870 | -5.495 | -2.718 | -2.592 | 2.903 |
| Sat-PhO | 0.930 | -5.720 | -2.971 | -3.132 | 2.588 |
| Sat-NO | 0.894 | -5.574 | -2.551 | -2.150 | 3.424 |
| Sat-Allyl | 0.998 | -5.222 | -2.934 | -2.420 | 2.802 |
| Sat-IN | 0.980 | -5.255 | -2.699 | -2.627 | 2.628 |
| Sat-Phen | 0.999 | -5.346 | -2.392 | -2.534 | 2.813 |
| Sat-Ver | 0.998 | -5.195 | -3.226 | -2.430 | 2.764 |
| Sat-NN | 0.998 | -5.211 | -2.504 | -2.394 | 2.817 |

## 4. Calculated values shown in Fig. S2 (plots of $y_0$ vs. UDFT HOMO–LUMO gap)

**Table S18** Calculated open-shell character $y_0$, orbital energies, H–L gaps of Non-Radical substituted anthracenes (**An**). All values were obtained by LC-UBLYP($\mu$=0.33)/6-311G(d,p).

| **An** | $y_0$ | αHOMO /eV | αLUMO /eV | αH–L gap /eV | βHOMO /eV | βLUMO /eV | βH–L gap /eV |
|---|---|---|---|---|---|---|---|
| $NO_2$ | 0.000 | -8.068 | -1.333 | 6.735 | -8.068 | -1.333 | 6.735 |
| CN | 0.000 | -7.976 | -1.047 | 6.929 | -7.976 | -1.047 | 6.929 |
| Cl | 0.000 | -7.580 | -0.478 | 7.102 | -7.580 | -0.478 | 7.102 |
| H | 0.000 | -7.561 | -0.409 | 7.152 | -7.561 | -0.409 | 7.152 |
| CHO | 0.000 | -7.835 | -0.985 | 6.850 | -7.835 | -0.985 | 6.850 |
| $SiMe_3$ | 0.000 | -7.489 | -0.423 | 7.067 | -7.489 | -0.423 | 7.067 |
| OMe | 0.000 | -7.199 | -0.149 | 7.050 | -7.199 | -0.149 | 7.050 |
| $NH_2$ | 0.000 | -7.031 | -0.071 | 6.960 | -7.031 | -0.071 | 6.960 |
| Ph | 0.000 | -7.341 | -0.506 | 6.834 | -7.341 | -0.506 | 6.834 |
| BzTh | 0.000 | -7.340 | -0.672 | 6.668 | -7.340 | -0.672 | 6.668 |
| Th | 0.000 | -7.304 | -0.559 | 6.745 | -7.304 | -0.559 | 6.745 |

**Table S19** Calculated open-shell character $y_0$, orbital energies, H–L gaps of Radical substituted anthracenes (**An**). All values were obtained by LC-UBLYP($\mu$=0.33)/6-311G(d,p).

| **An** | $y_0$ | αHOMO /eV | αLUMO /eV | αH–L gap /eV | βHOMO /eV | βLUMO /eV | βH–L gap /eV |
|---|---|---|---|---|---|---|---|
| $NO_2$ | 0.070 | -6.997 | -0.196 | 6.801 | -7.935 | -1.060 | 6.874 |
| CN | 0.055 | -7.932 | -1.144 | 6.788 | -8.530 | -2.614 | 5.916 |
| Cl | 0.056 | -6.677 | -0.346 | 6.331 | -7.655 | -1.226 | 6.428 |
| H | 0.052 | -6.893 | -0.519 | 6.374 | -7.764 | -1.608 | 6.155 |
| CHO | 0.045 | -7.464 | -0.798 | 6.666 | -7.911 | -2.070 | 5.842 |
| $SiMe_3$ | 0.035 | -7.171 | -0.355 | 6.816 | -7.634 | -0.879 | 6.755 |
| OMe | 0.028 | -7.499 | -0.471 | 7.028 | -7.394 | -0.395 | 6.998 |
| $NH_2$ | 0.012 | -7.575 | -0.645 | 6.930 | -7.506 | -0.676 | 6.830 |
| Ph | 0.026 | -6.912 | -0.546 | 6.366 | -7.316 | -0.995 | 6.321 |
| BzTh | 0.018 | -7.591 | -0.654 | 6.937 | -7.484 | -1.022 | 6.462 |
| Th | 0.083 | -7.543 | -0.667 | 6.876 | -7.247 | -0.509 | 6.738 |

**Table S20** Calculated open-shell character $y_0$, orbital energies, H–L gaps of Sat-Radical substituted anthracenes (**An**). All values were obtained by LC-UBLYP($\mu$=0.33)/6-311G(d,p).

| **An** | $y_0$ | αHOMO /eV | αLUMO /eV | αH–L gap /eV | βHOMO /eV | βLUMO /eV | βH–L gap /eV |
|---|---|---|---|---|---|---|---|
| $NO_2$ | 0.000 | -7.462 | -0.044 | 7.417 | -7.462 | -0.044 | 7.417 |
| CN | 0.001 | -7.438 | -0.075 | 7.362 | -7.497 | -0.119 | 7.378 |
| Cl | 0.007 | -7.837 | -0.445 | 7.392 | -7.852 | -2.428 | 5.424 |
| H | 0.011 | -6.885 | -0.090 | 6.796 | -7.498 | -0.504 | 6.995 |
| CHO | 0.008 | -7.192 | -0.152 | 7.039 | -7.566 | -1.127 | 6.438 |
| $SiMe_3$ | 0.015 | -7.693 | -0.305 | 7.388 | -7.714 | -1.674 | 6.040 |
| OMe | 0.001 | -7.477 | -0.153 | 7.324 | -7.578 | -0.200 | 7.378 |
| $NH_2$ | 0.020 | -7.498 | -0.091 | 7.407 | -7.494 | -0.088 | 7.406 |
| Ph | 0.007 | -7.423 | -0.016 | 7.407 | -7.421 | -0.243 | 7.178 |
| BzTh | 0.022 | -6.770 | -0.118 | 6.651 | -7.514 | -0.904 | 6.610 |
| Th | 0.012 | -7.522 | -0.116 | 7.406 | -7.517 | -1.050 | 6.467 |

**Table S21** Calculated open-shell character $y_0$, orbital energies, H–L gaps of Non-Radical substituted pentacenes (**Pn**). All values were obtained by LC-UBLYP($\mu$=0.33)/6-311G(d,p).

| **Pn** | $y_0$ | αHOMO /eV | αLUMO /eV | αH–L gap /eV | βHOMO /eV | βLUMO /eV | βH–L gap /eV |
|---|---|---|---|---|---|---|---|
| $NO_2$ | 0.156 | -7.284 | -1.809 | 5.475 | -7.388 | -1.523 | 5.865 |
| CN | 0.161 | -7.325 | -1.398 | 5.927 | -7.238 | -1.634 | 5.604 |
| Cl | 0.158 | -6.950 | -1.164 | 5.786 | -6.975 | -1.049 | 5.926 |
| H | 0.157 | -6.952 | -1.003 | 5.949 | -6.918 | -1.104 | 5.813 |
| CHO | 0.169 | -7.130 | -1.543 | 5.587 | -7.210 | -1.303 | 5.907 |
| $SiMe_3$ | 0.164 | -6.907 | -0.989 | 5.917 | -6.887 | -1.105 | 5.781 |
| OMe | 0.167 | -6.718 | -0.872 | 5.846 | -6.671 | -0.826 | 5.845 |
| $NH_2$ | 0.176 | -6.550 | -0.767 | 5.783 | -6.635 | -0.792 | 5.844 |
| Ph | 0.176 | -6.846 | -1.146 | 5.699 | -6.818 | -0.995 | 5.823 |
| BzTh | 0.183 | -6.883 | -1.259 | 5.624 | -6.847 | -1.065 | 5.782 |
| Th | 0.184 | -6.806 | -1.011 | 5.795 | -6.846 | -1.175 | 5.671 |

**Table S22** Calculated open-shell character $y_0$, orbital energies, H–L gaps of Radical substituted pentacenes (**Pn**). All values were obtained by LC-UBLYP($\mu$=0.33)/6-311G(d,p).

| **Pn** | $y_0$ | αHOMO /eV | αLUMO /eV | αH–L gap /eV | βHOMO /eV | βLUMO /eV | βH–L gap /eV |
|---|---|---|---|---|---|---|---|
| $NO_2$ | 0.117 | -6.796 | -0.718 | 6.078 | -7.503 | -1.122 | 6.381 |
| CN | 0.124 | -7.430 | -1.742 | 5.688 | -8.041 | -2.355 | 5.686 |
| Cl | 0.175 | -6.646 | -0.882 | 5.764 | -7.209 | -1.207 | 6.002 |
| H | 0.190 | -6.803 | -1.097 | 5.706 | -7.323 | -1.519 | 5.804 |
| CHO | 0.241 | -7.136 | -1.396 | 5.740 | -7.454 | -1.937 | 5.517 |
| $SiMe_3$ | 0.259 | -6.884 | -0.947 | 5.937 | -7.142 | -1.062 | 6.080 |
| OMe | 0.215 | -6.953 | -0.970 | 5.983 | -6.883 | -1.050 | 5.834 |
| $NH_2$ | 0.197 | -6.987 | -1.032 | 5.955 | -6.909 | -1.214 | 5.695 |
| Ph | 0.210 | -6.898 | -0.987 | 5.911 | -6.862 | -1.095 | 5.767 |
| BzTh | 0.207 | -7.025 | -1.061 | 5.964 | -6.947 | -1.194 | 5.753 |
| Th | 0.284 | -7.000 | -0.967 | 6.034 | -6.835 | -1.081 | 5.754 |

**Table S23** Calculated open-shell character $y_0$, orbital energies, H–L gaps of Sat-Radical substituted pentacenes (**Pn**). All values were obtained by LC-UBLYP($\mu$=0.33)/6-311G(d,p).

| **Pn** | $y_0$ | αHOMO /eV | αLUMO /eV | αH–L gap /eV | βHOMO /eV | βLUMO /eV | βH–L gap /eV |
|---|---|---|---|---|---|---|---|
| $NO_2$ | 0.120 | -6.802 | -0.847 | 5.955 | -6.798 | -0.862 | 5.935 |
| CN | 0.131 | -6.817 | -0.877 | 5.939 | -6.845 | -0.870 | 5.975 |
| Cl | 0.147 | -7.096 | -1.192 | 5.904 | -7.149 | -2.423 | 4.726 |
| H | 0.128 | -6.767 | -0.887 | 5.880 | -6.836 | -0.885 | 5.951 |
| CHO | 0.128 | -6.858 | -0.946 | 5.911 | -6.898 | -1.160 | 5.738 |
| $SiMe_3$ | 0.125 | -7.000 | -1.089 | 5.912 | -7.030 | -1.679 | 5.351 |
| OMe | 0.133 | -6.859 | -0.932 | 5.927 | -6.902 | -0.916 | 5.986 |
| $NH_2$ | 0.122 | -6.836 | -0.878 | 5.957 | -6.826 | -0.899 | 5.928 |
| Ph | 0.121 | -6.750 | -0.794 | 5.956 | -6.741 | -0.822 | 5.919 |
| BzTh | 0.121 | -6.783 | -0.898 | 5.885 | -6.845 | -0.922 | 5.923 |
| Th | 0.121 | -6.847 | -0.885 | 5.962 | -6.834 | -1.065 | 5.769 |

**Table S24** Calculated open-shell character $y_0$, orbital energies, H–L gaps of Non-Radical substituted heptacenes (**Hp**). All values were obtained by LC-UBLYP($\mu$=0.33)/6-311G(d,p).

| **Hp** | $y_0$ | αHOMO /eV | αLUMO /eV | αH–L gap /eV | βHOMO /eV | βLUMO /eV | βH–L gap /eV |
|---|---|---|---|---|---|---|---|
| $NO_2$ | 0.548 | -7.317 | -1.362 | 5.955 | -7.105 | -1.897 | 5.208 |
| CN | 0.559 | -7.085 | -1.727 | 5.359 | -7.263 | -1.310 | 5.953 |
| Cl | 0.567 | -6.938 | -1.081 | 5.857 | -6.881 | -1.269 | 5.612 |
| H | 0.567 | -6.918 | -1.048 | 5.870 | -6.852 | -1.214 | 5.638 |
| CHO | 0.563 | -7.157 | -1.226 | 5.931 | -6.999 | -1.639 | 5.360 |
| $SiMe_3$ | 0.571 | -6.875 | -1.032 | 5.843 | -6.832 | -1.214 | 5.618 |
| OMe | 0.576 | -6.730 | -0.990 | 5.740 | -6.652 | -0.933 | 5.720 |
| $NH_2$ | 0.582 | -6.684 | -0.911 | 5.773 | -6.534 | -0.894 | 5.640 |
| Ph | 0.578 | -6.819 | -1.256 | 5.563 | -6.793 | -1.028 | 5.765 |
| BzTh | 0.582 | -6.820 | -1.066 | 5.754 | -6.850 | -1.363 | 5.487 |
| Th | 0.583 | -6.781 | -1.036 | 5.745 | -6.824 | -1.281 | 5.542 |

**Table S25** Calculated open-shell character $y_0$, orbital energies, H–L gaps of Radical substituted heptacenes (**Hp**). All values were obtained by LC-UBLYP($\mu$=0.33)/6-311G(d,p).

| **Hp** | $y_0$ | αHOMO /eV | αLUMO /eV | αH–L gap /eV | βHOMO /eV | βLUMO /eV | βH–L gap /eV |
|---|---|---|---|---|---|---|---|
| $NO_2$ | 0.127 | -6.794 | -0.878 | 5.916 | -7.322 | -1.095 | 6.227 |
| CN | 0.159 | -7.249 | -1.862 | 5.386 | -7.807 | -2.241 | 5.565 |
| Cl | 0.202 | -6.724 | -1.017 | 5.707 | -7.086 | -1.127 | 5.958 |
| H | 0.234 | -6.843 | -1.233 | 5.609 | -7.200 | -1.430 | 5.771 |
| CHO | 0.354 | -7.055 | -1.527 | 5.528 | -7.348 | -1.852 | 5.496 |
| $SiMe_3$ | 0.414 | -6.856 | -1.080 | 5.776 | -7.046 | -1.074 | 5.972 |
| OMe | 0.598 | -6.906 | -1.029 | 5.877 | -6.834 | -1.176 | 5.658 |
| $NH_2$ | 0.500 | -6.897 | -1.064 | 5.832 | -6.798 | -1.327 | 5.472 |
| Ph | 0.505 | -6.824 | -1.057 | 5.767 | -6.794 | -1.225 | 5.569 |
| BzTh | 0.589 | -6.969 | -1.078 | 5.890 | -6.876 | -1.313 | 5.564 |
| Th | 0.625 | -6.921 | -0.990 | 5.930 | -6.785 | -1.208 | 5.577 |

**Table S26** Calculated open-shell character $y_0$, orbital energies, H–L gaps of Sat-Radical substituted heptacenes (**Hp**). All values were obtained by LC-UBLYP($\mu$=0.33)/6-311G(d,p).

| **Hp** | $y_0$ | αHOMO /eV | αLUMO /eV | αH–L gap /eV | βHOMO /eV | βLUMO /eV | βH–L gap /eV |
|---|---|---|---|---|---|---|---|
| $NO_2$ | 0.549 | -6.783 | -0.959 | 5.824 | -6.767 | -0.991 | 5.776 |
| CN | 0.545 | -6.784 | -1.011 | 5.773 | -6.817 | -0.976 | 5.841 |
| Cl | 0.534 | -6.985 | -1.304 | 5.681 | -7.085 | -2.425 | 4.660 |
| H | 0.539 | -6.773 | -1.019 | 5.754 | -6.804 | -0.980 | 5.825 |
| CHO | 0.539 | -6.822 | -1.076 | 5.746 | -6.863 | -1.151 | 5.712 |
| $SiMe_3$ | 0.546 | -6.927 | -1.208 | 5.719 | -6.993 | -1.682 | 5.311 |
| OMe | 0.545 | -6.810 | -1.059 | 5.751 | -6.861 | -1.004 | 5.857 |
| $NH_2$ | 0.548 | -6.813 | -0.981 | 5.831 | -6.788 | -1.026 | 5.762 |
| Ph | 0.460 | -6.682 | -0.965 | 5.717 | -6.693 | -0.929 | 5.764 |
| BzTh | 0.548 | -6.793 | -1.051 | 5.742 | -6.827 | -0.996 | 5.831 |
| Th | 0.548 | -6.820 | -0.983 | 5.837 | -6.791 | -1.078 | 5.713 |

**Table S27** Calculated open-shell character $y_0$, orbital energies, H–L gaps of Non-Radical substituted nonacenes (**Nn**). All values were obtained by LC-UBLYP($\mu$=0.33)/6-311G(d,p).

| **Nn** | $y_0$ | αHOMO /eV | αLUMO /eV | αH–L gap /eV | βHOMO /eV | βLUMO /eV | βH–L gap /eV |
|---|---|---|---|---|---|---|---|
| $NO_2$ | 0.753 | -7.268 | -1.285 | 5.983 | -7.087 | -1.856 | 5.231 |
| CN | 0.759 | -7.229 | -1.260 | 5.969 | -7.073 | -1.689 | 5.384 |
| Cl | 0.763 | -6.903 | -1.261 | 5.642 | -6.951 | -1.078 | 5.873 |
| H | 0.763 | -6.877 | -1.210 | 5.668 | -6.932 | -1.051 | 5.881 |
| CHO | 0.760 | -7.131 | -1.186 | 5.945 | -6.998 | -1.608 | 5.390 |
| $SiMe_3$ | 0.765 | -6.861 | -1.210 | 5.651 | -6.894 | -1.036 | 5.858 |
| OMe | 0.768 | -6.781 | -1.010 | 5.771 | -6.697 | -0.958 | 5.739 |
| $NH_2$ | 0.772 | -6.748 | -0.940 | 5.808 | -6.588 | -0.928 | 5.661 |
| Ph | 0.768 | -6.854 | -1.250 | 5.604 | -6.824 | -1.032 | 5.791 |
| BzTh | 0.770 | -6.846 | -1.061 | 5.785 | -6.880 | -1.351 | 5.529 |
| Th | 0.771 | -6.811 | -1.038 | 5.773 | -6.859 | -1.274 | 5.585 |

**Table S28** Calculated open-shell character $y_0$, orbital energies, H–L gaps of Radical substituted nonacenes (**Nn**). All values were obtained by LC-UBLYP($\mu$=0.33)/6-311G(d,p).

| **Nn** | $y_0$ | αHOMO /eV | αLUMO /eV | αH–L gap /eV | βHOMO /eV | βLUMO /eV | βH–L gap /eV |
|---|---|---|---|---|---|---|---|
| $NO_2$ | 0.182 | -6.837 | -0.936 | 5.901 | -7.164 | -1.074 | 6.091 |
| CN | 0.223 | -7.197 | -1.816 | 5.381 | -7.483 | -2.224 | 5.259 |
| Cl | 0.258 | -6.805 | -1.044 | 5.761 | -7.038 | -1.058 | 5.980 |
| H | 0.293 | -6.896 | -1.238 | 5.658 | -7.143 | -1.409 | 5.734 |
| CHO | 0.424 | -7.050 | -1.508 | 5.542 | -7.280 | -1.843 | 5.437 |
| $SiMe_3$ | 0.493 | -6.883 | -1.102 | 5.781 | -7.014 | -1.072 | 5.942 |
| OMe | 0.776 | -6.917 | -1.037 | 5.880 | -6.863 | -1.179 | 5.684 |
| $NH_2$ | 0.769 | -6.928 | -1.032 | 5.896 | -6.853 | -1.311 | 5.542 |
| Ph | 0.764 | -6.857 | -1.314 | 5.543 | -6.783 | -1.085 | 5.698 |
| BzTh | 0.761 | -6.894 | -1.393 | 5.501 | -6.888 | -1.100 | 5.788 |
| Th | 0.801 | -6.901 | -0.988 | 5.913 | -6.825 | -1.196 | 5.630 |

**Table S29** Calculated open-shell character $y_0$, orbital energies, H–L gaps of Sat-Radical substituted nonacenes (**Nn**). All values were obtained by LC-UBLYP($\mu$=0.33)/6-311G(d,p).

| **Nn** | $y_0$ | αHOMO /eV | αLUMO /eV | αH–L gap /eV | βHOMO /eV | βLUMO /eV | βH–L gap /eV |
|---|---|---|---|---|---|---|---|
| $NO_2$ | 0.757 | -6.822 | -0.980 | 5.841 | -6.807 | -1.014 | 5.794 |
| CN | 0.646 | -6.768 | -1.072 | 5.696 | -6.798 | -1.033 | 5.766 |
| Cl | 0.723 | -6.976 | -1.297 | 5.679 | -7.081 | -2.433 | 4.649 |
| H | 0.742 | -6.819 | -1.038 | 5.781 | -6.840 | -0.996 | 5.844 |
| CHO | 0.741 | -6.856 | -1.089 | 5.767 | -6.894 | -1.151 | 5.743 |
| $SiMe_3$ | 0.772 | -6.950 | -1.207 | 5.742 | -7.019 | -1.687 | 5.332 |
| OMe | 0.761 | -6.845 | -1.069 | 5.776 | -6.890 | -1.014 | 5.876 |
| $NH_2$ | 0.757 | -6.849 | -0.999 | 5.850 | -6.825 | -1.045 | 5.780 |
| Ph | 0.757 | -6.760 | -0.931 | 5.829 | -6.756 | -0.968 | 5.788 |
| BzTh | 0.756 | -6.801 | -1.012 | 5.790 | -6.838 | -1.065 | 5.773 |
| Th | 0.756 | -6.827 | -1.053 | 5.774 | -6.850 | -1.088 | 5.762 |

**Table S30** Calculated open-shell character $y_0$, orbital energies, H–L gaps of Non-Radical substituted triangulenes (**Tri**). All values were obtained by LC-UBLYP($\mu$=0.33)/6-311G(d,p).

| **Tri** | $y_0$ | αHOMO /eV | αLUMO /eV | αH–L gap /eV | βHOMO /eV | βLUMO /eV | βH–L gap /eV |
|---|---|---|---|---|---|---|---|
| $NO_2$ | 1.000 | -6.776 | -2.332 | 4.444 | -7.037 | -1.669 | 5.368 |
| CN | 1.000 | -6.951 | -1.629 | 5.321 | -6.737 | -2.170 | 4.567 |
| Cl | 1.000 | -6.472 | -1.655 | 4.817 | -6.529 | -1.393 | 5.136 |
| H | 1.000 | -6.433 | -1.593 | 4.840 | -6.503 | -1.359 | 5.144 |
| CHO | 0.986 | -6.831 | -1.531 | 5.300 | -6.644 | -2.062 | 4.582 |
| $SiMe_3$ | 1.000 | -6.455 | -1.331 | 5.124 | -6.417 | -1.585 | 4.832 |
| OMe | 0.991 | -6.175 | -1.219 | 4.955 | -6.302 | -1.303 | 4.999 |
| $NH_2$ | 1.000 | -6.038 | -1.164 | 4.874 | -6.261 | -1.192 | 5.068 |
| Ph | 1.000 | -6.366 | -1.309 | 5.057 | -6.419 | -1.611 | 4.808 |
| BzTh | 0.997 | -6.416 | -1.344 | 5.072 | -6.471 | -1.726 | 4.745 |
| Th | 0.998 | -6.363 | -1.312 | 5.050 | -6.437 | -1.635 | 4.801 |

**Table S31** Calculated open-shell character $y_0$, orbital energies, H–L gaps of Radical substituted triangulenes (**Tri**). All values were obtained by LC-UBLYP($\mu$=0.33)/6-311G(d,p).

| **Tri** | $y_0$ | αHOMO /eV | αLUMO /eV | αH–L gap /eV | βHOMO /eV | βLUMO /eV | βH–L gap /eV |
|---|---|---|---|---|---|---|---|
| $NO_2$ | 0.143 | -6.793 | -0.776 | 6.017 | -7.391 | -1.002 | 6.390 |
| CN | 0.194 | -7.344 | -2.269 | 5.075 | -8.252 | -1.888 | 6.364 |
| Cl | 0.225 | -6.784 | -1.011 | 5.773 | -6.988 | -0.952 | 6.036 |
| H | 0.265 | -6.904 | -1.394 | 5.510 | -7.160 | -1.159 | 6.002 |
| CHO | 0.412 | -7.113 | -1.838 | 5.274 | -7.814 | -1.493 | 6.321 |
| $SiMe_3$ | 0.492 | -6.890 | -0.567 | 6.323 | -7.690 | -0.993 | 6.697 |
| OMe | 0.999 | -6.865 | -0.236 | 6.630 | -8.301 | -1.114 | 7.187 |
| $NH_2$ | 0.953 | -6.902 | -0.336 | 6.566 | -8.210 | -1.342 | 6.868 |
| Ph | 0.999 | -6.775 | -1.057 | 5.717 | -6.896 | -1.223 | 5.673 |
| BzTh | 0.999 | -6.916 | -1.092 | 5.824 | -7.889 | -1.345 | 6.544 |
| Th | 0.998 | -6.710 | -0.067 | 6.643 | -7.652 | -1.393 | 6.259 |

**Table S32** Calculated open-shell character $y_0$, orbital energies, H–L gaps of Sat-Radical substituted triangulenes (**Tri**). All values were obtained by LC-UBLYP($\mu$=0.33)/6-311G(d,p).

| **Tri** | $y_0$ | αHOMO /eV | αLUMO /eV | αH–L gap /eV | βHOMO /eV | βLUMO /eV | βH–L gap /eV |
|---|---|---|---|---|---|---|---|
| $NO_2$ | 1.000 | -6.317 | -1.315 | 5.002 | -6.283 | -1.316 | 4.967 |
| CN | 0.894 | -6.826 | 0.567 | 7.394 | -8.206 | -0.842 | 7.363 |
| Cl | 0.855 | -7.089 | -2.417 | 4.672 | -8.754 | -1.209 | 7.545 |
| H | 0.904 | -6.820 | -0.485 | 6.335 | -6.934 | -0.859 | 6.075 |
| CHO | 0.870 | -6.391 | -1.417 | 4.974 | -6.380 | -1.382 | 4.998 |
| $SiMe_3$ | 0.930 | -6.998 | -1.676 | 5.322 | -8.462 | -1.065 | 7.397 |
| OMe | 0.894 | -6.871 | 0.645 | 7.516 | -7.967 | -0.922 | 7.045 |
| $NH_2$ | 0.998 | -6.819 | -0.058 | 6.761 | -8.042 | -0.862 | 7.180 |
| Ph | 0.980 | -6.744 | -0.254 | 6.489 | -8.310 | -0.799 | 7.511 |
| BzTh | 0.999 | -6.838 | -0.919 | 5.919 | -6.782 | -0.885 | 5.897 |
| Th | 0.998 | -6.838 | -1.067 | 5.771 | -7.858 | -0.886 | 6.972 |

# 5. All optimized structures of PAHs with various substituents dealt with in this work.

All PAHs' optimized geometries in this work were obtained with UB3LYP/6-311G(d,p), and it was confirmed by vibrational analysis that they have no imaginary frequencies.

# 5-1. Core PAH structures

## Anthracene

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -3.654568 | -0.712260 | 0.000000 |
| 2 | 6 | 0 | -3.654568 | 0.712260 | 0.000000 |
| 3 | 6 | 0 | -2.476531 | 1.404834 | 0.000000 |
| 4 | 6 | 0 | -1.221777 | 0.721480 | 0.000000 |
| 5 | 6 | 0 | -1.221777 | -0.721480 | 0.000000 |
| 6 | 6 | 0 | -2.476531 | -1.404834 | 0.000000 |
| 7 | 6 | 0 | 0.000000 | 1.401594 | 0.000000 |
| 8 | 6 | 0 | 1.221777 | 0.721480 | 0.000000 |
| 9 | 6 | 0 | 1.221777 | -0.721480 | 0.000000 |
| 10 | 6 | 0 | 0.000000 | -1.401594 | 0.000000 |
| 11 | 6 | 0 | 2.476531 | 1.404834 | 0.000000 |
| 12 | 6 | 0 | 3.654568 | 0.712260 | 0.000000 |
| 13 | 6 | 0 | 3.654568 | -0.712260 | 0.000000 |
| 14 | 6 | 0 | 2.476531 | -1.404834 | 0.000000 |
| 15 | 1 | 0 | -4.599294 | -1.244189 | 0.000000 |
| 16 | 1 | 0 | -4.599294 | 1.244189 | 0.000000 |
| 17 | 1 | 0 | -2.475602 | 2.489887 | 0.000000 |
| 18 | 1 | 0 | -2.475602 | -2.489887 | 0.000000 |
| 19 | 1 | 0 | 0.000000 | 2.487468 | 0.000000 |
| 20 | 1 | 0 | 0.000000 | -2.487468 | 0.000000 |
| 21 | 1 | 0 | 2.475602 | 2.489887 | 0.000000 |
| 22 | 1 | 0 | 4.599294 | 1.244189 | 0.000000 |
| 23 | 1 | 0 | 4.599294 | -1.244189 | 0.000000 |
| 24 | 1 | 0 | 2.475602 | -2.489887 | 0.000000 |

## Pentacene

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 6.108039 | 0.715883 | 0.000000 |
| 2 | 6 | 0 | 6.108038 | -0.715884 | 0.000000 |
| 3 | 6 | 0 | 4.935282 | -1.408424 | 0.000000 |
| 4 | 6 | 0 | 3.672664 | -0.726753 | 0.000000 |
| 5 | 6 | 0 | 3.672664 | 0.726752 | 0.000000 |
| 6 | 6 | 0 | 4.935283 | 1.408424 | 0.000000 |
| 7 | 6 | 0 | 2.464263 | -1.406066 | 0.000000 |
| 8 | 6 | 0 | 1.224496 | -0.727506 | 0.000000 |
| 9 | 6 | 0 | 1.224496 | 0.727506 | 0.000000 |
| 10 | 6 | 0 | 2.464264 | 1.406067 | 0.000000 |
| 11 | 6 | 0 | 0.000000 | -1.406567 | 0.000000 |
| 12 | 6 | 0 | -1.224496 | -0.727506 | 0.000000 |
| 13 | 6 | 0 | -1.224496 | 0.727506 | 0.000000 |
| 14 | 6 | 0 | 0.000000 | 1.406567 | 0.000000 |
| 15 | 6 | 0 | -2.464263 | -1.406066 | 0.000000 |
| 16 | 6 | 0 | -3.672664 | -0.726753 | 0.000000 |
| 17 | 6 | 0 | -3.672664 | 0.726752 | 0.000000 |
| 18 | 6 | 0 | -2.464264 | 1.406067 | 0.000000 |
| 19 | 6 | 0 | -4.935282 | -1.408424 | 0.000000 |
| 20 | 6 | 0 | -6.108038 | -0.715884 | 0.000000 |
| 21 | 6 | 0 | -6.108039 | 0.715883 | 0.000000 |
| 22 | 6 | 0 | -4.935283 | 1.408424 | 0.000000 |
| 23 | 1 | 0 | 7.054130 | 1.245303 | 0.000000 |
| 24 | 1 | 0 | 7.054130 | -1.245304 | 0.000000 |
| 25 | 1 | 0 | 4.935018 | -2.493429 | 0.000000 |
| 26 | 1 | 0 | 4.935019 | 2.493429 | 0.000000 |
| 27 | 1 | 0 | 2.464833 | -2.491779 | 0.000000 |
| 28 | 1 | 0 | 2.464834 | 2.491780 | 0.000000 |
| 29 | 1 | 0 | 0.000000 | -2.492179 | 0.000000 |
| 30 | 1 | 0 | 0.000000 | 2.492181 | 0.000000 |
| 31 | 1 | 0 | -2.464833 | -2.491779 | 0.000000 |
| 32 | 1 | 0 | -2.464834 | 2.491780 | 0.000000 |
| 33 | 1 | 0 | -4.935018 | -2.493429 | 0.000000 |
| 34 | 1 | 0 | -7.054130 | -1.245304 | 0.000000 |
| 35 | 1 | 0 | -7.054130 | 1.245303 | 0.000000 |
| 36 | 1 | 0 | -4.935019 | 2.493429 | 0.000000 |

## Heptacene

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -8.573888 | -0.713075 | -0.000007 |
| 2 | 6 | 0 | -8.573888 | 0.713075 | -0.000004 |
| 3 | 6 | 0 | -7.396278 | 1.406046 | -0.000001 |
| 4 | 6 | 0 | -6.139625 | 0.724246 | 0.000000 |
| 5 | 6 | 0 | -6.139625 | -0.724246 | -0.000003 |
| 6 | 6 | 0 | -7.396278 | -1.406046 | -0.000007 |
| 7 | 6 | 0 | -4.922831 | 1.404888 | 0.000003 |
| 8 | 6 | 0 | -3.688891 | 0.727553 | 0.000003 |
| 9 | 6 | 0 | -3.688891 | -0.727553 | 0.000001 |
| 10 | 6 | 0 | -4.922831 | -1.404888 | -0.000002 |
| 11 | 6 | 0 | -2.459171 | 1.407481 | 0.000005 |
| 12 | 6 | 0 | -1.230749 | 0.730432 | 0.000004 |
| 13 | 6 | 0 | -1.230749 | -0.730432 | 0.000004 |
| 14 | 6 | 0 | -2.459171 | -1.407481 | 0.000002 |
| 15 | 6 | 0 | 0.000000 | 1.408539 | 0.000004 |
| 16 | 6 | 0 | 1.230749 | 0.730432 | 0.000004 |
| 17 | 6 | 0 | 1.230749 | -0.730432 | 0.000004 |
| 18 | 6 | 0 | 0.000000 | -1.408539 | 0.000004 |
| 19 | 6 | 0 | 2.459171 | 1.407481 | 0.000002 |
| 20 | 6 | 0 | 3.688891 | 0.727553 | 0.000001 |
| 21 | 6 | 0 | 3.688891 | -0.727553 | 0.000003 |
| 22 | 6 | 0 | 2.459171 | -1.407481 | 0.000005 |
| 23 | 6 | 0 | 4.922831 | 1.404888 | -0.000002 |
| 24 | 6 | 0 | 6.139625 | 0.724246 | -0.000003 |
| 25 | 6 | 0 | 6.139625 | -0.724246 | 0.000000 |
| 26 | 6 | 0 | 4.922831 | -1.404888 | 0.000003 |
| 27 | 6 | 0 | 7.396278 | 1.406046 | -0.000007 |
| 28 | 6 | 0 | 8.573888 | 0.713075 | -0.000008 |
| 29 | 6 | 0 | 8.573888 | -0.713075 | -0.000004 |
| 30 | 6 | 0 | 7.396278 | -1.406046 | -0.000001 |
| 31 | 1 | 0 | -9.518746 | -1.244648 | -0.000011 |
| 32 | 1 | 0 | -9.518746 | 1.244648 | -0.000005 |
| 33 | 1 | 0 | -7.396001 | 2.491072 | 0.000002 |
| 34 | 1 | 0 | -7.396001 | -2.491072 | -0.000009 |
| 35 | 1 | 0 | -4.924110 | 2.490607 | 0.000005 |
| 36 | 1 | 0 | -4.924111 | -2.490607 | -0.000004 |
| 37 | 1 | 0 | -2.460091 | 2.493053 | 0.000006 |
| 38 | 1 | 0 | -2.460091 | -2.493053 | 0.000001 |
| 39 | 1 | 0 | 0.000000 | 2.494081 | 0.000005 |
| 40 | 1 | 0 | 0.000000 | -2.494081 | 0.000005 |
| 41 | 1 | 0 | 2.460091 | 2.493053 | 0.000001 |
| 42 | 1 | 0 | 2.460091 | -2.493053 | 0.000006 |
| 43 | 1 | 0 | 4.924110 | 2.490607 | -0.000004 |
| 44 | 1 | 0 | 4.924111 | -2.490607 | 0.000005 |
| 45 | 1 | 0 | 7.396001 | 2.491072 | -0.000009 |
| 46 | 1 | 0 | 9.518746 | 1.244648 | -0.000011 |
| 47 | 1 | 0 | 9.518746 | -1.244648 | -0.000005 |
| 48 | 1 | 0 | 7.396001 | -2.491072 | 0.000002 |

## Nonacene

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 11.036746 | 0.712257 | -0.000011 |
| 2 | 6 | 0 | 11.036746 | -0.712257 | -0.000011 |
| 3 | 6 | 0 | 9.857925 | -1.405280 | -0.000008 |
| 4 | 6 | 0 | 8.603091 | -0.723154 | -0.000005 |
| 5 | 6 | 0 | 8.603091 | 0.723154 | -0.000005 |
| 6 | 6 | 0 | 9.857925 | 1.405280 | -0.000008 |
| 7 | 6 | 0 | 7.383337 | -1.403966 | -0.000002 |
| 8 | 6 | 0 | 6.153335 | -0.726370 | 0.000001 |
| 9 | 6 | 0 | 6.153335 | 0.726370 | 0.000001 |
| 10 | 6 | 0 | 7.383337 | 1.403966 | -0.000002 |
| 11 | 6 | 0 | 4.918094 | -1.406413 | 0.000003 |
| 12 | 6 | 0 | 3.695843 | -0.729625 | 0.000005 |
| 13 | 6 | 0 | 3.695843 | 0.729625 | 0.000005 |
| 14 | 6 | 0 | 4.918094 | 1.406413 | 0.000003 |
| 15 | 6 | 0 | 2.457782 | -1.407707 | 0.000007 |
| 16 | 6 | 0 | 1.232593 | -0.731181 | 0.000007 |
| 17 | 6 | 0 | 1.232593 | 0.731181 | 0.000007 |
| 18 | 6 | 0 | 2.457782 | 1.407707 | 0.000006 |
| 19 | 6 | 0 | 0.000000 | -1.407990 | 0.000008 |
| 20 | 6 | 0 | -1.232593 | -0.731181 | 0.000007 |
| 21 | 6 | 0 | -1.232593 | 0.731181 | 0.000007 |
| 22 | 6 | 0 | 0.000000 | 1.407990 | 0.000008 |
| 23 | 6 | 0 | -2.457782 | -1.407707 | 0.000007 |
| 24 | 6 | 0 | -3.695843 | -0.729625 | 0.000005 |
| 25 | 6 | 0 | -3.695843 | 0.729625 | 0.000005 |
| 26 | 6 | 0 | -2.457782 | 1.407707 | 0.000007 |
| 27 | 6 | 0 | -4.918094 | -1.406413 | 0.000003 |
| 28 | 6 | 0 | -6.153335 | -0.726370 | 0.000001 |
| 29 | 6 | 0 | -6.153335 | 0.726370 | 0.000001 |
| 30 | 6 | 0 | -4.918094 | 1.406413 | 0.000003 |
| 31 | 6 | 0 | -7.383337 | -1.403966 | -0.000002 |
| 32 | 6 | 0 | -8.603091 | -0.723154 | -0.000005 |
| 33 | 6 | 0 | -8.603091 | 0.723154 | -0.000005 |
| 34 | 6 | 0 | -7.383337 | 1.403966 | -0.000002 |
| 35 | 6 | 0 | -9.857925 | -1.405280 | -0.000008 |
| 36 | 6 | 0 | -11.036746 | -0.712257 | -0.000011 |
| 37 | 6 | 0 | -11.036746 | 0.712257 | -0.000011 |
| 38 | 6 | 0 | -9.857925 | 1.405280 | -0.000008 |
| 39 | 1 | 0 | 11.981288 | 1.244387 | -0.000014 |
| 40 | 1 | 0 | 11.981288 | -1.244387 | -0.000014 |
| 41 | 1 | 0 | 9.857548 | -2.490310 | -0.000008 |
| 42 | 1 | 0 | 9.857548 | 2.490310 | -0.000008 |
| 43 | 1 | 0 | 7.384542 | -2.489703 | -0.000002 |

| | | | | | |
|---|---|---|---|---|---|
| 44 | 1 | 0 | 7.384542 | 2.489703 | -0.000001 |
| 45 | 1 | 0 | 4.919059 | -2.492031 | 0.000004 |
| 46 | 1 | 0 | 4.919059 | 2.492031 | 0.000004 |
| 47 | 1 | 0 | 2.458208 | -2.493314 | 0.000008 |
| 48 | 1 | 0 | 2.458208 | 2.493314 | 0.000008 |
| 49 | 1 | 0 | 0.000000 | -2.493601 | 0.000010 |
| 50 | 1 | 0 | 0.000000 | 2.493601 | 0.000009 |
| 51 | 1 | 0 | -2.458208 | -2.493314 | 0.000008 |
| 52 | 1 | 0 | -2.458208 | 2.493314 | 0.000008 |
| 53 | 1 | 0 | -4.919059 | -2.492031 | 0.000004 |
| 54 | 1 | 0 | -4.919059 | 2.492031 | 0.000004 |
| 55 | 1 | 0 | -7.384542 | -2.489703 | -0.000002 |
| 56 | 1 | 0 | -7.384542 | 2.489703 | -0.000001 |
| 57 | 1 | 0 | -9.857548 | -2.490310 | -0.000008 |
| 58 | 1 | 0 | -11.981288 | -1.244387 | -0.000014 |
| 59 | 1 | 0 | -11.981288 | 1.244387 | -0.000014 |
| 60 | 1 | 0 | -9.857548 | 2.490310 | -0.000008 |

## Triangulene

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 0.309235 | 4.230513 | -0.000003 |
| 2 | 6 | 0 | 1.464973 | 3.458626 | -0.000002 |
| 3 | 6 | 0 | 1.392702 | 2.041038 | 0.000000 |
| 4 | 6 | 0 | 0.103697 | 1.418664 | 0.000001 |
| 5 | 6 | 0 | -1.081097 | 2.221858 | 0.000000 |
| 6 | 6 | 0 | -0.946453 | 3.634888 | -0.000002 |
| 7 | 6 | 0 | 0.000000 | 0.000001 | 0.000001 |
| 8 | 6 | 0 | -1.280448 | -0.619531 | 0.000000 |
| 9 | 6 | 0 | -2.463940 | 0.185601 | 0.000002 |
| 10 | 6 | 0 | -2.337639 | 1.587505 | 0.000001 |
| 11 | 6 | 0 | -1.383634 | -2.047190 | -0.000001 |
| 12 | 6 | 0 | -2.674677 | -2.637097 | -0.000004 |
| 13 | 6 | 0 | -3.818347 | -1.847444 | 0.000000 |
| 14 | 6 | 0 | -3.727746 | -0.460608 | 0.000006 |
| 15 | 6 | 0 | 2.543641 | 1.230701 | 0.000001 |
| 16 | 6 | 0 | 2.464739 | -0.174668 | 0.000001 |
| 17 | 6 | 0 | 1.176750 | -0.799145 | 0.000000 |
| 18 | 6 | 0 | 1.071233 | -2.226633 | 0.000000 |
| 19 | 6 | 0 | -0.206002 | -2.818209 | -0.000001 |
| 20 | 6 | 0 | 3.621137 | -0.997789 | 0.000002 |
| 21 | 6 | 0 | 3.509109 | -2.383059 | 0.000001 |
| 22 | 6 | 0 | 2.262768 | -2.998015 | 0.000000 |
| 23 | 1 | 0 | 0.388294 | 5.312045 | -0.000005 |
| 24 | 1 | 0 | 2.439691 | 3.933898 | -0.000003 |
| 25 | 1 | 0 | -1.841697 | 4.246849 | -0.000003 |
| 26 | 1 | 0 | -3.235459 | 2.197215 | 0.000004 |
| 27 | 1 | 0 | -2.757045 | -3.718380 | -0.000009 |
| 28 | 1 | 0 | -4.794511 | -2.319744 | -0.000002 |
| 29 | 1 | 0 | -4.626706 | 0.145882 | 0.000006 |
| 30 | 1 | 0 | 3.520582 | 1.703365 | 0.000003 |
| 31 | 1 | 0 | -0.285127 | -3.900600 | -0.000003 |
| 32 | 1 | 0 | 4.598738 | -0.528476 | 0.000002 |
| 33 | 1 | 0 | 4.406206 | -2.992303 | 0.000001 |
| 34 | 1 | 0 | 2.187023 | -4.079784 | -0.000001 |

# 5-2. Anthracenes(**An**)

## Non-Radical

R=$NO_2$

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 0.664597 | -3.666118 | -0.000002 |
| 2 | 6 | 0 | 2.085491 | -3.654175 | -0.000001 |
| 3 | 6 | 0 | 2.759345 | -2.465601 | -0.000001 |
| 4 | 6 | 0 | 2.053851 | -1.224321 | -0.000001 |
| 5 | 6 | 0 | 0.615399 | -1.237982 | -0.000001 |
| 6 | 6 | 0 | -0.048989 | -2.497335 | -0.000002 |
| 7 | 6 | 0 | 2.728381 | 0.000002 | -0.000001 |
| 8 | 6 | 0 | 2.053849 | 1.224323 | 0.000000 |
| 9 | 6 | 0 | 0.615397 | 1.237983 | 0.000001 |
| 10 | 6 | 0 | -0.084670 | 0.000000 | 0.000000 |
| 11 | 6 | 0 | 2.759342 | 2.465604 | 0.000000 |
| 12 | 6 | 0 | 2.085486 | 3.654177 | 0.000002 |
| 13 | 6 | 0 | 0.664592 | 3.666118 | 0.000004 |
| 14 | 6 | 0 | -0.048993 | 2.497334 | 0.000003 |
| 15 | 6 | 0 | -1.495907 | -0.000001 | 0.000000 |
| 16 | 6 | 0 | -2.703839 | -0.000001 | 0.000000 |
| 17 | 7 | 0 | -4.089032 | -0.000002 | 0.000000 |
| 18 | 8 | 0 | -4.648335 | 1.095057 | -0.000022 |
| 19 | 8 | 0 | -4.648333 | -1.095062 | 0.000021 |
| 20 | 1 | 0 | 0.140390 | -4.614864 | -0.000003 |
| 21 | 1 | 0 | 2.628816 | -4.591851 | -0.000001 |
| 22 | 1 | 0 | 3.843730 | -2.443604 | 0.000000 |
| 23 | 1 | 0 | -1.131708 | -2.519255 | -0.000004 |
| 24 | 1 | 0 | 3.814129 | 0.000002 | -0.000001 |
| 25 | 1 | 0 | 3.843727 | 2.443608 | -0.000001 |
| 26 | 1 | 0 | 2.628810 | 4.591854 | 0.000003 |
| 27 | 1 | 0 | 0.140384 | 4.614863 | 0.000005 |
| 28 | 1 | 0 | -1.131712 | 2.519253 | 0.000003 |

R=CN

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 0.310112 | -3.666573 | 0.000001 |
| 2 | 6 | 0 | 1.731282 | -3.653904 | 0.000000 |
| 3 | 6 | 0 | 2.404210 | -2.465141 | -0.000001 |
| 4 | 6 | 0 | 1.699696 | -1.222912 | 0.000000 |
| 5 | 6 | 0 | 0.260793 | -1.236679 | 0.000000 |
| 6 | 6 | 0 | -0.402217 | -2.497716 | 0.000001 |
| 7 | 6 | 0 | 2.375636 | 0.000038 | -0.000001 |
| 8 | 6 | 0 | 1.699657 | 1.222966 | 0.000000 |
| 9 | 6 | 0 | 0.260753 | 1.236687 | 0.000000 |
| 10 | 6 | 0 | -0.440047 | -0.000008 | 0.000001 |
| 11 | 6 | 0 | 2.404130 | 2.465217 | -0.000001 |
| 12 | 6 | 0 | 1.731163 | 3.653959 | 0.000000 |
| 13 | 6 | 0 | 0.309994 | 3.666582 | 0.000001 |
| 14 | 6 | 0 | -0.402298 | 2.497701 | 0.000001 |
| 15 | 6 | 0 | -1.853698 | -0.000031 | 0.000001 |
| 16 | 6 | 0 | -3.067508 | -0.000051 | 0.000000 |
| 17 | 6 | 0 | -4.430471 | -0.000074 | -0.000001 |
| 18 | 7 | 0 | -5.591195 | -0.000078 | -0.000002 |
| 19 | 1 | 0 | -0.213819 | -4.615511 | 0.000002 |
| 20 | 1 | 0 | 2.275208 | -4.591277 | 0.000000 |
| 21 | 1 | 0 | 3.488625 | -2.442943 | -0.000002 |
| 22 | 1 | 0 | -1.484788 | -2.520583 | 0.000002 |
| 23 | 1 | 0 | 3.461254 | 0.000055 | -0.000002 |
| 24 | 1 | 0 | 3.488546 | 2.443054 | -0.000002 |
| 25 | 1 | 0 | 2.275059 | 4.591349 | 0.000000 |
| 26 | 1 | 0 | -0.213969 | 4.615503 | 0.000002 |
| 27 | 1 | 0 | -1.484869 | 2.520534 | 0.000002 |

R=Cl

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 0.425339 | 3.664427 | 0.000002 |
| 2 | 6 | 0 | 1.847287 | 3.653458 | -0.000001 |
| 3 | 6 | 0 | 2.522436 | 2.466111 | -0.000002 |
| 4 | 6 | 0 | 1.822349 | 1.220735 | -0.000001 |
| 5 | 6 | 0 | 0.382401 | 1.231792 | 0.000001 |
| 6 | 6 | 0 | -0.282447 | 2.493743 | 0.000004 |
| 7 | 6 | 0 | 2.501514 | 0.000016 | -0.000001 |
| 8 | 6 | 0 | 1.822365 | -1.220713 | -0.000001 |
| 9 | 6 | 0 | 0.382418 | -1.231790 | 0.000001 |
| 10 | 6 | 0 | -0.321257 | -0.000003 | 0.000000 |
| 11 | 6 | 0 | 2.522468 | -2.466079 | -0.000001 |
| 12 | 6 | 0 | 1.847334 | -3.653435 | 0.000000 |
| 13 | 6 | 0 | 0.425387 | -3.664424 | 0.000002 |
| 14 | 6 | 0 | -0.282414 | -2.493748 | 0.000002 |
| 15 | 6 | 0 | -1.744336 | -0.000012 | -0.000001 |
| 16 | 6 | 0 | -2.950600 | -0.000017 | -0.000001 |
| 17 | 17 | 0 | -4.598415 | -0.000026 | -0.000001 |
| 18 | 1 | 0 | -0.100090 | 4.612738 | 0.000004 |
| 19 | 1 | 0 | 2.390215 | 4.591723 | -0.000002 |
| 20 | 1 | 0 | 3.607122 | 2.447058 | -0.000004 |
| 21 | 1 | 0 | -1.365105 | 2.509542 | 0.000007 |
| 22 | 1 | 0 | 3.587121 | 0.000023 | -0.000002 |
| 23 | 1 | 0 | 3.607154 | -2.447013 | -0.000002 |
| 24 | 1 | 0 | 2.390275 | -4.591693 | 0.000000 |
| 25 | 1 | 0 | -0.100030 | -4.612742 | 0.000003 |
| 26 | 1 | 0 | -1.365072 | -2.509560 | 0.000003 |

R=H

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -3.664172 | -0.274085 | -0.000002 |
| 2 | 6 | 0 | -3.653295 | 1.147965 | -0.000002 |
| 3 | 6 | 0 | -2.466003 | 1.823144 | 0.000000 |
| 4 | 6 | 0 | -1.220719 | 1.122862 | 0.000001 |
| 5 | 6 | 0 | -1.231647 | -0.317241 | 0.000002 |
| 6 | 6 | 0 | -2.493784 | -0.982295 | 0.000000 |
| 7 | 6 | 0 | -0.000001 | 1.801905 | 0.000001 |
| 8 | 6 | 0 | 1.220717 | 1.122863 | 0.000001 |
| 9 | 6 | 0 | 1.231646 | -0.317240 | 0.000000 |
| 10 | 6 | 0 | 0.000000 | -1.020418 | 0.000002 |
| 11 | 6 | 0 | 2.466000 | 1.823147 | 0.000000 |
| 12 | 6 | 0 | 3.653293 | 1.147969 | -0.000002 |
| 13 | 6 | 0 | 3.664171 | -0.274081 | -0.000002 |
| 14 | 6 | 0 | 2.493784 | -0.982293 | -0.000001 |
| 15 | 6 | 0 | 0.000002 | -2.445233 | 0.000005 |
| 16 | 6 | 0 | 0.000008 | -3.650877 | -0.000002 |
| 17 | 1 | 0 | -4.612658 | -0.799297 | -0.000005 |
| 18 | 1 | 0 | -4.591599 | 1.690886 | -0.000003 |
| 19 | 1 | 0 | -2.446888 | 2.907851 | 0.000000 |
| 20 | 1 | 0 | -2.508219 | -2.064895 | 0.000000 |
| 21 | 1 | 0 | -0.000002 | 2.887557 | 0.000003 |
| 22 | 1 | 0 | 2.446884 | 2.907854 | 0.000002 |
| 23 | 1 | 0 | 4.591596 | 1.690891 | -0.000001 |
| 24 | 1 | 0 | 4.612658 | -0.799292 | -0.000005 |
| 25 | 1 | 0 | 2.508221 | -2.064892 | 0.000000 |
| 26 | 1 | 0 | 0.000013 | -4.713202 | -0.000004 |

R=CHO

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 2.475039 | -2.845231 | 0.000003 |
| 2 | 6 | 0 | 3.626635 | -2.012273 | -0.000001 |
| 3 | 6 | 0 | 3.486980 | -0.653263 | -0.000003 |
| 4 | 6 | 0 | 2.193252 | -0.048538 | -0.000002 |
| 5 | 6 | 0 | 1.027710 | -0.892188 | 0.000000 |
| 6 | 6 | 0 | 1.217692 | -2.303857 | 0.000003 |
| 7 | 6 | 0 | 2.035806 | 1.340170 | -0.000001 |
| 8 | 6 | 0 | 0.776337 | 1.945812 | 0.000000 |
| 9 | 6 | 0 | -0.404198 | 1.123069 | -0.000002 |
| 10 | 6 | 0 | -0.260991 | -0.292467 | -0.000002 |
| 11 | 6 | 0 | 0.631338 | 3.366524 | 0.000004 |
| 12 | 6 | 0 | -0.606393 | 3.944688 | 0.000004 |
| 13 | 6 | 0 | -1.771774 | 3.131110 | 0.000000 |
| 14 | 6 | 0 | -1.675920 | 1.765430 | -0.000003 |
| 15 | 6 | 0 | -1.419980 | -1.101569 | -0.000003 |
| 16 | 6 | 0 | -2.441926 | -1.756522 | 0.000000 |
| 17 | 6 | 0 | -3.665127 | -2.506165 | 0.000004 |
| 18 | 8 | 0 | -4.768823 | -2.001252 | -0.000003 |
| 19 | 1 | 0 | 2.597599 | -3.922375 | 0.000007 |
| 20 | 1 | 0 | 4.612914 | -2.461633 | -0.000002 |
| 21 | 1 | 0 | 4.358500 | -0.007468 | -0.000007 |
| 22 | 1 | 0 | 0.345680 | -2.945698 | 0.000006 |
| 23 | 1 | 0 | 2.920942 | 1.968955 | -0.000002 |
| 24 | 1 | 0 | 1.527895 | 3.977085 | 0.000006 |
| 25 | 1 | 0 | -0.706604 | 5.023905 | 0.000006 |
| 26 | 1 | 0 | -2.748802 | 3.600641 | -0.000002 |
| 27 | 1 | 0 | -2.569498 | 1.153954 | -0.000006 |
| 28 | 1 | 0 | -3.534918 | -3.605740 | 0.000014 |

R=$SiMe_3$

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -1.366214 | -3.664214 | 0.001318 |
| 2 | 6 | 0 | -2.788107 | -3.650591 | 0.000005 |
| 3 | 6 | 0 | -3.460870 | -2.461839 | -0.001104 |
| 4 | 6 | 0 | -2.758141 | -1.217914 | -0.001022 |
| 5 | 6 | 0 | -1.318277 | -1.231641 | 0.000001 |
| 6 | 6 | 0 | -0.656023 | -2.494810 | 0.001287 |
| 7 | 6 | 0 | -3.435250 | 0.003993 | -0.001714 |
| 8 | 6 | 0 | -2.753755 | 1.223463 | -0.001051 |
| 9 | 6 | 0 | -1.313865 | 1.231985 | 0.000049 |
| 10 | 6 | 0 | -0.610401 | -0.001104 | -0.000144 |
| 11 | 6 | 0 | -3.451978 | 2.469920 | -0.001221 |
| 12 | 6 | 0 | -2.774899 | 3.656224 | -0.000066 |
| 13 | 6 | 0 | -1.352966 | 3.664699 | 0.001430 |
| 14 | 6 | 0 | -0.646989 | 2.492736 | 0.001463 |
| 15 | 6 | 0 | 0.811704 | -0.003337 | -0.000850 |
| 16 | 6 | 0 | 2.029028 | -0.004423 | -0.002268 |
| 17 | 14 | 0 | 3.871461 | -0.003122 | -0.000861 |

| | | | | | |
|---|---|---|---|---|---|
| 18 | 6 | 0 | 4.467960 | 1.636872 | 0.712939 |
| 19 | 6 | 0 | 4.480832 | -0.204707 | -1.773682 |
| 20 | 6 | 0 | 4.472595 | -1.438286 | 1.063911 |
| 21 | 1 | 0 | -0.842789 | -4.613721 | 0.002574 |
| 22 | 1 | 0 | -3.332999 | -4.587779 | 0.000027 |
| 23 | 1 | 0 | -4.545559 | -2.440576 | -0.001962 |
| 24 | 1 | 0 | 0.426557 | -2.510153 | 0.002745 |
| 25 | 1 | 0 | -4.520902 | 0.005939 | -0.002590 |
| 26 | 1 | 0 | -4.536737 | 2.452589 | -0.002177 |
| 27 | 1 | 0 | -3.316394 | 4.595381 | -0.000127 |
| 28 | 1 | 0 | -0.826091 | 4.612294 | 0.002788 |
| 29 | 1 | 0 | 0.435648 | 2.504215 | 0.003116 |
| 30 | 1 | 0 | 4.104451 | 1.779086 | 1.734225 |
| 31 | 1 | 0 | 5.561689 | 1.673993 | 0.737002 |
| 32 | 1 | 0 | 4.118023 | 2.480972 | 0.112271 |
| 33 | 1 | 0 | 4.127601 | -1.143497 | -2.208865 |
| 34 | 1 | 0 | 5.574956 | -0.207619 | -1.809620 |
| 35 | 1 | 0 | 4.125445 | 0.611201 | -2.408818 |
| 36 | 1 | 0 | 5.566458 | -1.466432 | 1.094491 |
| 37 | 1 | 0 | 4.109616 | -1.347220 | 2.091177 |
| 38 | 1 | 0 | 4.124268 | -2.397105 | 0.670117 |

R=OMe

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -2.139358 | -3.107515 | -0.000003 |
| 2 | 6 | 0 | -3.390083 | -2.431035 | 0.000004 |
| 3 | 6 | 0 | -3.429925 | -1.065643 | 0.000007 |
| 4 | 6 | 0 | -2.228835 | -0.291468 | 0.000004 |
| 5 | 6 | 0 | -0.961805 | -0.976384 | -0.000003 |
| 6 | 6 | 0 | -0.966646 | -2.403055 | -0.000006 |
| 7 | 6 | 0 | -2.259978 | 1.105039 | 0.000007 |
| 8 | 6 | 0 | -1.086055 | 1.861812 | 0.000003 |
| 9 | 6 | 0 | 0.191216 | 1.196033 | -0.000004 |
| 10 | 6 | 0 | 0.241054 | -0.222292 | -0.000006 |
| 11 | 6 | 0 | -1.117886 | 3.290497 | 0.000006 |
| 12 | 6 | 0 | 0.034705 | 4.023591 | 0.000001 |
| 13 | 6 | 0 | 1.296060 | 3.367059 | -0.000007 |
| 14 | 6 | 0 | 1.368950 | 2.000996 | -0.000010 |
| 15 | 6 | 0 | 1.496596 | -0.893701 | -0.000010 |
| 16 | 6 | 0 | 2.550641 | -1.481991 | -0.000011 |
| 17 | 8 | 0 | 3.657184 | -2.161331 | -0.000012 |
| 18 | 6 | 0 | 4.872358 | -1.374736 | 0.000027 |
| 19 | 1 | 0 | -2.119011 | -4.191553 | -0.000006 |
| 20 | 1 | 0 | -4.309947 | -3.004979 | 0.000007 |
| 21 | 1 | 0 | -4.379682 | -0.541054 | 0.000013 |
| 22 | 1 | 0 | -0.016881 | -2.922952 | -0.000012 |
| 23 | 1 | 0 | -3.218784 | 1.613948 | 0.000013 |
| 24 | 1 | 0 | -2.084748 | 3.782850 | 0.000012 |
| 25 | 1 | 0 | -0.005919 | 5.107029 | 0.000003 |
| 26 | 1 | 0 | 2.205064 | 3.958227 | -0.000012 |
| 27 | 1 | 0 | 2.331612 | 1.505281 | -0.000016 |
| 28 | 1 | 0 | 5.687667 | -2.094494 | 0.000094 |
| 29 | 1 | 0 | 4.913595 | -0.752473 | -0.896473 |
| 30 | 1 | 0 | 4.913501 | -0.752412 | 0.896488 |

R=$NH_2$

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 3.665448 | -0.086266 | -0.010196 |
| 2 | 6 | 0 | 3.653871 | -1.507951 | 0.003106 |
| 3 | 6 | 0 | 2.466172 | -2.182932 | 0.010487 |
| 4 | 6 | 0 | 1.218453 | -1.486209 | 0.005662 |
| 5 | 6 | 0 | 1.229964 | -0.046195 | -0.006011 |
| 6 | 6 | 0 | 2.492277 | 0.617721 | -0.014504 |
| 7 | 6 | 0 | 0.000000 | -2.169462 | 0.012100 |
| 8 | 6 | 0 | -1.218453 | -1.486209 | 0.005662 |
| 9 | 6 | 0 | -1.229964 | -0.046195 | -0.006011 |
| 10 | 6 | 0 | 0.000000 | 0.664469 | -0.008985 |
| 11 | 6 | 0 | -2.466172 | -2.182931 | 0.010487 |
| 12 | 6 | 0 | -3.653871 | -1.507950 | 0.003106 |
| 13 | 6 | 0 | -3.665448 | -0.086265 | -0.010196 |
| 14 | 6 | 0 | -2.492277 | 0.617721 | -0.014504 |
| 15 | 6 | 0 | 0.000000 | 2.084794 | -0.013535 |
| 16 | 6 | 0 | 0.000001 | 3.294891 | 0.004504 |
| 17 | 7 | 0 | 0.000001 | 4.639565 | -0.051796 |
| 18 | 1 | 0 | 4.613405 | 0.440025 | -0.018147 |
| 19 | 1 | 0 | 4.591881 | -2.051803 | 0.006461 |
| 20 | 1 | 0 | 2.448520 | -3.267788 | 0.019639 |
| 21 | 1 | 0 | 2.505830 | 1.700510 | -0.027148 |
| 22 | 1 | 0 | 0.000000 | -3.254821 | 0.021503 |
| 23 | 1 | 0 | -2.448521 | -3.267787 | 0.019639 |
| 24 | 1 | 0 | -4.591882 | -2.051802 | 0.006461 |
| 25 | 1 | 0 | -4.613405 | 0.440026 | -0.018147 |
| 26 | 1 | 0 | -2.505830 | 1.700511 | -0.027148 |
| 27 | 1 | 0 | -0.841237 | 5.094891 | 0.276204 |
| 28 | 1 | 0 | 0.841239 | 5.094891 | 0.276205 |

R=Ph

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -1.535015 | -3.665603 | 0.000033 |
| 2 | 6 | 0 | -2.956567 | -3.653621 | 0.000032 |
| 3 | 6 | 0 | -3.630180 | -2.465266 | 0.000021 |
| 4 | 6 | 0 | -2.929005 | -1.220493 | 0.000010 |
| 5 | 6 | 0 | -1.489383 | -1.232247 | 0.000010 |
| 6 | 6 | 0 | -0.826975 | -2.494632 | 0.000023 |
| 7 | 6 | 0 | -3.608831 | 0.000000 | 0.000001 |
| 8 | 6 | 0 | -2.929004 | 1.220493 | -0.000009 |
| 9 | 6 | 0 | -1.489382 | 1.232247 | -0.000011 |
| 10 | 6 | 0 | -0.780977 | 0.000000 | -0.000001 |
| 11 | 6 | 0 | -3.630179 | 2.465267 | -0.000019 |
| 12 | 6 | 0 | -2.956565 | 3.653621 | -0.000031 |
| 13 | 6 | 0 | -1.535013 | 3.665604 | -0.000034 |
| 14 | 6 | 0 | -0.826974 | 2.494631 | -0.000025 |
| 15 | 6 | 0 | 0.637638 | 0.000000 | -0.000002 |
| 16 | 6 | 0 | 1.850152 | 0.000000 | -0.000002 |
| 17 | 6 | 0 | 3.272261 | 0.000000 | -0.000001 |
| 18 | 6 | 0 | 3.990557 | -1.210603 | -0.000123 |
| 19 | 6 | 0 | 5.379686 | -1.205766 | -0.000121 |
| 20 | 6 | 0 | 6.080137 | 0.000000 | 0.000002 |
| 21 | 6 | 0 | 5.379686 | 1.205766 | 0.000123 |
| 22 | 6 | 0 | 3.990557 | 1.210602 | 0.000122 |
| 23 | 1 | 0 | -1.010106 | -4.614278 | 0.000043 |
| 24 | 1 | 0 | -3.500667 | -4.591267 | 0.000040 |
| 25 | 1 | 0 | -4.714885 | -2.444982 | 0.000021 |
| 26 | 1 | 0 | 0.255481 | -2.509755 | 0.000025 |
| 27 | 1 | 0 | -4.694420 | 0.000001 | 0.000002 |
| 28 | 1 | 0 | -4.714884 | 2.444983 | -0.000017 |
| 29 | 1 | 0 | -3.500665 | 4.591268 | -0.000038 |
| 30 | 1 | 0 | -1.010104 | 4.614278 | -0.000045 |
| 31 | 1 | 0 | 0.255482 | 2.509755 | -0.000029 |
| 32 | 1 | 0 | 3.446900 | -2.147543 | -0.000219 |
| 33 | 1 | 0 | 5.918574 | -2.146541 | -0.000216 |
| 34 | 1 | 0 | 7.164068 | 0.000000 | 0.000002 |
| 35 | 1 | 0 | 5.918574 | 2.146540 | 0.000219 |
| 36 | 1 | 0 | 3.446900 | 2.147542 | 0.000218 |

R=BzTh

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -2.711115 | 3.701777 | 0.000031 |
| 2 | 6 | 0 | -4.132110 | 3.667674 | 0.000033 |
| 3 | 6 | 0 | -4.787174 | 2.468905 | 0.000023 |
| 4 | 6 | 0 | -4.066570 | 1.235426 | 0.000010 |
| 5 | 6 | 0 | -2.627637 | 1.270067 | 0.000008 |
| 6 | 6 | 0 | -1.984560 | 2.541959 | 0.000019 |
| 7 | 6 | 0 | -4.727080 | 0.004191 | 0.000000 |
| 8 | 6 | 0 | -4.029066 | -1.206202 | -0.000012 |
| 9 | 6 | 0 | -2.589732 | -1.196687 | -0.000014 |
| 10 | 6 | 0 | -1.901438 | 0.047619 | -0.000004 |
| 11 | 6 | 0 | -4.711520 | -2.461175 | -0.000023 |
| 12 | 6 | 0 | -4.019811 | -3.639178 | -0.000035 |
| 13 | 6 | 0 | -2.598454 | -3.629670 | -0.000038 |
| 14 | 6 | 0 | -1.907731 | -2.448187 | -0.000028 |
| 15 | 6 | 0 | -0.485795 | 0.068412 | -0.000007 |
| 16 | 6 | 0 | 0.728044 | 0.091359 | -0.000009 |
| 17 | 6 | 0 | 2.130265 | 0.093121 | -0.000006 |
| 18 | 6 | 0 | 2.980238 | 1.167270 | -0.000067 |
| 19 | 6 | 0 | 4.363854 | 0.806368 | -0.000045 |
| 20 | 6 | 0 | 4.551398 | -0.598096 | 0.000036 |
| 21 | 16 | 0 | 3.017048 | -1.445586 | 0.000083 |
| 22 | 6 | 0 | 5.497750 | 1.640072 | -0.000092 |
| 23 | 6 | 0 | 6.761794 | 1.076665 | -0.000059 |
| 24 | 6 | 0 | 6.926385 | -0.319007 | 0.000022 |
| 25 | 6 | 0 | 5.826680 | -1.165657 | 0.000070 |
| 26 | 1 | 0 | -2.201016 | 4.658448 | 0.000040 |
| 27 | 1 | 0 | -4.690684 | 4.596712 | 0.000043 |
| 28 | 1 | 0 | -5.871385 | 2.431651 | 0.000025 |
| 29 | 1 | 0 | -0.902393 | 2.575321 | 0.000018 |
| 30 | 1 | 0 | -5.812510 | -0.012479 | 0.000002 |
| 31 | 1 | 0 | -5.796365 | -2.457229 | -0.000021 |
| 32 | 1 | 0 | -4.549529 | -4.584968 | -0.000043 |
| 33 | 1 | 0 | -2.058873 | -4.569960 | -0.000048 |
| 34 | 1 | 0 | -0.825057 | -2.449729 | -0.000030 |
| 35 | 1 | 0 | 2.623381 | 2.188417 | -0.000126 |
| 36 | 1 | 0 | 5.373603 | 2.717337 | -0.000154 |
| 37 | 1 | 0 | 7.636642 | 1.716504 | -0.000095 |
| 38 | 1 | 0 | 7.924528 | -0.741437 | 0.000047 |
| 39 | 1 | 0 | 5.957192 | -2.241376 | 0.000132 |

R=Th

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -1.814057 | -3.644404 | -0.000003 |
| 2 | 6 | 0 | -3.230467 | -3.524567 | -0.000007 |
| 3 | 6 | 0 | -3.812140 | -2.288517 | -0.000006 |
| 4 | 6 | 0 | -3.018887 | -1.100358 | -0.000002 |
| 5 | 6 | 0 | -1.584596 | -1.221800 | 0.000000 |
| 6 | 6 | 0 | -1.019296 | -2.530304 | 0.000000 |
| 7 | 6 | 0 | -3.604244 | 0.168307 | 0.000000 |
| 8 | 6 | 0 | -2.833791 | 1.333894 | 0.000002 |

| | | | | | |
|---|---|---|---|---|---|
| 9 | 6 | 0 | -1.397576 | 1.237176 | 0.000002 |
| 10 | 6 | 0 | -0.785288 | -0.046023 | 0.000002 |
| 11 | 6 | 0 | -3.438393 | 2.628272 | 0.000004 |
| 12 | 6 | 0 | -2.676509 | 3.762150 | 0.000004 |
| 13 | 6 | 0 | -1.258263 | 3.666588 | 0.000002 |
| 14 | 6 | 0 | -0.640954 | 2.445227 | 0.000001 |
| 15 | 6 | 0 | 0.627005 | -0.153154 | 0.000004 |
| 16 | 6 | 0 | 1.837118 | -0.249658 | 0.000005 |
| 17 | 6 | 0 | 3.236353 | -0.347916 | 0.000004 |
| 18 | 6 | 0 | 4.023908 | -1.481099 | 0.000018 |
| 19 | 6 | 0 | 5.413897 | -1.200332 | 0.000012 |
| 20 | 6 | 0 | 5.687611 | 0.139300 | -0.000006 |
| 21 | 16 | 0 | 4.244675 | 1.092983 | -0.000016 |
| 22 | 1 | 0 | -1.362486 | -4.630070 | -0.000003 |
| 23 | 1 | 0 | -3.844129 | -4.418224 | -0.000011 |
| 24 | 1 | 0 | -4.892185 | -2.186196 | -0.000009 |
| 25 | 1 | 0 | 0.058956 | -2.628384 | 0.000002 |
| 26 | 1 | 0 | -4.686661 | 0.250616 | 0.000000 |
| 27 | 1 | 0 | -4.521497 | 2.690352 | 0.000007 |
| 28 | 1 | 0 | -3.148011 | 4.738311 | 0.000007 |
| 29 | 1 | 0 | -0.662638 | 4.572450 | 0.000000 |
| 30 | 1 | 0 | 0.439809 | 2.380483 | -0.000001 |
| 31 | 1 | 0 | 3.602887 | -2.477031 | 0.000032 |
| 32 | 1 | 0 | 6.181684 | -1.962472 | 0.000022 |
| 33 | 1 | 0 | 6.650889 | 0.625748 | -0.000013 |

---

## Radical

R=Mt

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 0.000051 | 3.344995 | 0.000003 |
| 2 | 6 | 0 | 0.000020 | 2.103784 | -0.000006 |
| 3 | 6 | 0 | 0.000072 | 4.688179 | 0.000008 |
| 4 | 6 | 0 | -3.676464 | -0.058947 | -0.000004 |
| 5 | 6 | 0 | -3.660041 | -1.474597 | 0.000001 |
| 6 | 6 | 0 | -2.465064 | -2.144422 | 0.000004 |
| 7 | 6 | 0 | -1.226579 | -1.438728 | 0.000002 |
| 8 | 6 | 0 | -1.245248 | -0.004425 | -0.000003 |
| 9 | 6 | 0 | -2.500606 | 0.652597 | -0.000006 |
| 10 | 6 | 0 | -0.000025 | -2.119944 | 0.000004 |
| 11 | 6 | 0 | 1.226543 | -1.438753 | 0.000002 |
| 12 | 6 | 0 | 1.245241 | -0.004451 | -0.000001 |
| 13 | 6 | 0 | 0.000004 | 0.721967 | -0.000004 |
| 14 | 6 | 0 | 2.465015 | -2.144472 | 0.000003 |
| 15 | 6 | 0 | 3.660005 | -1.474671 | 0.000000 |
| 16 | 6 | 0 | 3.676457 | -0.059021 | -0.000003 |
| 17 | 6 | 0 | 2.500612 | 0.652546 | -0.000004 |
| 18 | 1 | 0 | -0.927427 | 5.249215 | 0.000012 |
| 19 | 1 | 0 | 0.927589 | 5.249186 | 0.000013 |
| 20 | 1 | 0 | -4.624828 | 0.466225 | -0.000007 |
| 21 | 1 | 0 | -4.594598 | -2.023959 | 0.000003 |
| 22 | 1 | 0 | -2.440967 | -3.229010 | 0.000009 |
| 23 | 1 | 0 | -2.519602 | 1.735407 | -0.000009 |
| 24 | 1 | 0 | -0.000036 | -3.205260 | 0.000008 |
| 25 | 1 | 0 | 2.440896 | -3.229059 | 0.000004 |
| 26 | 1 | 0 | 4.594551 | -2.024051 | 0.000000 |
| 27 | 1 | 0 | 4.624831 | 0.466132 | -0.000005 |
| 28 | 1 | 0 | 2.519630 | 1.735356 | -0.000008 |

R=DCM

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -1.070459 | -3.673903 | 0.000014 |
| 2 | 6 | 0 | -2.485621 | -3.657935 | -0.000003 |
| 3 | 6 | 0 | -3.156326 | -2.463105 | -0.000015 |
| 4 | 6 | 0 | -2.447461 | -1.227656 | -0.000011 |
| 5 | 6 | 0 | -1.013021 | -1.246276 | 0.000005 |
| 6 | 6 | 0 | -0.354442 | -2.500142 | 0.000018 |
| 7 | 6 | 0 | -3.124934 | 0.000003 | -0.000020 |
| 8 | 6 | 0 | -2.447458 | 1.227660 | -0.000010 |
| 9 | 6 | 0 | -1.013018 | 1.246277 | 0.000008 |
| 10 | 6 | 0 | -0.296385 | -0.000001 | 0.000009 |
| 11 | 6 | 0 | -3.156320 | 2.463111 | -0.000014 |
| 12 | 6 | 0 | -2.485613 | 3.657939 | 0.000001 |
| 13 | 6 | 0 | -1.070450 | 3.673904 | 0.000022 |
| 14 | 6 | 0 | -0.354436 | 2.500141 | 0.000024 |
| 15 | 6 | 0 | 1.089485 | -0.000002 | 0.000011 |
| 16 | 6 | 0 | 2.318636 | -0.000002 | 0.000005 |
| 17 | 6 | 0 | 3.689784 | -0.000005 | -0.000003 |
| 18 | 6 | 0 | 4.409759 | 1.222987 | -0.000014 |
| 19 | 6 | 0 | 4.409759 | -1.222991 | -0.000005 |
| 20 | 7 | 0 | 4.981804 | 2.230011 | -0.000025 |
| 21 | 7 | 0 | 4.981794 | -2.230016 | 0.000001 |
| 22 | 1 | 0 | -0.545668 | -4.622070 | 0.000025 |
| 23 | 1 | 0 | -3.033687 | -4.592740 | -0.000006 |
| 24 | 1 | 0 | -4.240521 | -2.438084 | -0.000028 |
| 25 | 1 | 0 | 0.727979 | -2.527271 | 0.000031 |
| 26 | 1 | 0 | -4.210301 | 0.000004 | -0.000036 |
| 27 | 1 | 0 | -4.240516 | 2.438092 | -0.000029 |
| 28 | 1 | 0 | -3.033676 | 4.592747 | -0.000002 |
| 29 | 1 | 0 | -0.545657 | 4.622069 | 0.000036 |
| 30 | 1 | 0 | 0.727985 | 2.527268 | 0.000039 |

R=DPM

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -2.599561 | -3.650708 | -0.399609 |
| 2 | 6 | 0 | -4.017278 | -3.637948 | -0.379751 |
| 3 | 6 | 0 | -4.688449 | -2.452744 | -0.247693 |
| 4 | 6 | 0 | -3.984663 | -1.217912 | -0.123277 |
| 5 | 6 | 0 | -2.548177 | -1.233259 | -0.131857 |
| 6 | 6 | 0 | -1.889061 | -2.482706 | -0.280687 |
| 7 | 6 | 0 | -4.665304 | 0.000003 | 0.000003 |
| 8 | 6 | 0 | -3.984657 | 1.217914 | 0.123283 |
| 9 | 6 | 0 | -2.548171 | 1.233255 | 0.131861 |
| 10 | 6 | 0 | -1.829297 | -0.000004 | 0.000002 |
| 11 | 6 | 0 | -4.688438 | 2.452750 | 0.247697 |
| 12 | 6 | 0 | -4.017261 | 3.637951 | 0.379752 |
| 13 | 6 | 0 | -2.599545 | 3.650705 | 0.399608 |
| 14 | 6 | 0 | -1.889049 | 2.482700 | 0.280689 |
| 15 | 6 | 0 | -0.433455 | -0.000006 | 0.000001 |
| 16 | 6 | 0 | 0.795986 | -0.000006 | 0.000000 |
| 17 | 6 | 0 | 2.173465 | -0.000004 | -0.000001 |
| 18 | 6 | 0 | 2.883361 | 1.284107 | -0.106406 |
| 19 | 6 | 0 | 4.134043 | 1.488154 | 0.509629 |
| 20 | 6 | 0 | 4.134068 | -1.488136 | -0.509603 |
| 21 | 6 | 0 | 2.883370 | -1.284110 | 0.106404 |
| 22 | 6 | 0 | 4.775695 | -2.718606 | -0.433002 |
| 23 | 6 | 0 | 4.192886 | -3.777969 | 0.261465 |
| 24 | 6 | 0 | 2.953431 | -3.594693 | 0.874932 |
| 25 | 6 | 0 | 2.306014 | -2.368631 | 0.796680 |
| 26 | 6 | 0 | 2.306012 | 2.368612 | -0.796712 |
| 27 | 6 | 0 | 2.953420 | 3.594679 | -0.874964 |
| 28 | 6 | 0 | 4.192856 | 3.777977 | -0.261468 |
| 29 | 6 | 0 | 4.775659 | 2.718629 | 0.433028 |
| 30 | 1 | 0 | -2.074216 | -4.592054 | -0.514333 |
| 31 | 1 | 0 | -4.564765 | -4.568847 | -0.474235 |
| 32 | 1 | 0 | -5.773070 | -2.431082 | -0.237181 |
| 33 | 1 | 0 | -0.806679 | -2.499593 | -0.308420 |
| 34 | 1 | 0 | -5.750724 | 0.000005 | 0.000006 |
| 35 | 1 | 0 | -5.773059 | 2.431092 | 0.237189 |
| 36 | 1 | 0 | -4.564745 | 4.568852 | 0.474235 |
| 37 | 1 | 0 | -2.074195 | 4.592049 | 0.514328 |
| 38 | 1 | 0 | -0.806668 | 2.499582 | 0.308422 |
| 39 | 1 | 0 | 4.587792 | 0.682995 | 1.073638 |
| 40 | 1 | 0 | 4.587824 | -0.682965 | -1.073589 |
| 41 | 1 | 0 | 5.731857 | -2.854027 | -0.926350 |
| 42 | 1 | 0 | 4.697358 | -4.735477 | 0.322415 |
| 43 | 1 | 0 | 2.493155 | -4.409492 | 1.422860 |
| 44 | 1 | 0 | 1.350227 | -2.229415 | 1.287691 |
| 45 | 1 | 0 | 1.350241 | 2.229379 | -1.287748 |
| 46 | 1 | 0 | 2.493148 | 4.409467 | -1.422915 |
| 47 | 1 | 0 | 4.697320 | 4.735489 | -0.322420 |
| 48 | 1 | 0 | 5.731808 | 2.854068 | 0.926397 |

R=Flu

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 2.791472 | 3.669032 | -0.146281 |
| 2 | 6 | 0 | 4.209435 | 3.654234 | -0.137194 |
| 3 | 6 | 0 | 4.879511 | 2.462459 | -0.088465 |
| 4 | 6 | 0 | 4.174174 | 1.223050 | -0.043805 |
| 5 | 6 | 0 | 2.737546 | 1.238885 | -0.047238 |
| 6 | 6 | 0 | 2.080523 | 2.496627 | -0.103164 |
| 7 | 6 | 0 | 4.854183 | 0.000002 | 0.000002 |
| 8 | 6 | 0 | 4.174176 | -1.223047 | 0.043806 |
| 9 | 6 | 0 | 2.737548 | -1.238886 | 0.047236 |
| 10 | 6 | 0 | 2.018978 | -0.000001 | -0.000001 |
| 11 | 6 | 0 | 4.879517 | -2.462455 | 0.088467 |
| 12 | 6 | 0 | 4.209443 | -3.654231 | 0.137191 |
| 13 | 6 | 0 | 2.791479 | -3.669033 | 0.146275 |
| 14 | 6 | 0 | 2.080528 | -2.496629 | 0.103158 |
| 15 | 6 | 0 | 0.621594 | -0.000002 | 0.000001 |
| 16 | 6 | 0 | -0.606574 | -0.000003 | 0.000002 |
| 17 | 6 | 0 | -1.979422 | -0.000002 | 0.000004 |
| 18 | 6 | 0 | -2.847533 | -1.168696 | -0.056539 |
| 19 | 6 | 0 | -4.200159 | -0.732203 | -0.035434 |
| 20 | 6 | 0 | -4.200157 | 0.732204 | 0.035428 |
| 21 | 6 | 0 | -2.847531 | 1.168694 | 0.056543 |
| 22 | 6 | 0 | -5.233806 | 1.658746 | 0.081818 |
| 23 | 6 | 0 | -4.921796 | 3.019758 | 0.150323 |
| 24 | 6 | 0 | -3.591124 | 3.449428 | 0.174177 |
| 25 | 6 | 0 | -2.545691 | 2.529053 | 0.128464 |
| 26 | 6 | 0 | -2.545696 | -2.529056 | -0.128451 |
| 27 | 6 | 0 | -3.591130 | -3.449429 | -0.174168 |
| 28 | 6 | 0 | -4.921802 | -3.019756 | -0.150326 |
| 29 | 6 | 0 | -5.233809 | -1.658743 | -0.081828 |
| 30 | 1 | 0 | 2.267034 | 4.616837 | -0.189207 |
| 31 | 1 | 0 | 4.757070 | 4.589071 | -0.171121 |
| 32 | 1 | 0 | 5.964037 | 2.438687 | -0.084035 |
| 33 | 1 | 0 | 0.998327 | 2.515118 | -0.116395 |
| 34 | 1 | 0 | 5.939592 | 0.000003 | 0.000004 |
| 35 | 1 | 0 | 5.964042 | -2.438680 | 0.084039 |
| 36 | 1 | 0 | 4.757080 | -4.589068 | 0.171117 |
| 37 | 1 | 0 | 2.267044 | -4.616840 | 0.189197 |
| 38 | 1 | 0 | 0.998333 | -2.515122 | 0.116385 |
| 39 | 1 | 0 | -6.269924 | 1.338481 | 0.066410 |
| 40 | 1 | 0 | -5.721010 | 3.751390 | 0.186924 |
| 41 | 1 | 0 | -3.371892 | 4.509635 | 0.230000 |
| 42 | 1 | 0 | -1.515073 | 2.864154 | 0.152998 |
| 43 | 1 | 0 | -1.515078 | -2.864159 | -0.152976 |
| 44 | 1 | 0 | -3.371900 | -4.509637 | -0.229984 |
| 45 | 1 | 0 | -5.721017 | -3.751387 | -0.186930 |
| 46 | 1 | 0 | -6.269926 | -1.338476 | -0.066429 |

R=PhO

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 1.872748 | -3.669689 | -0.000005 |
| 2 | 6 | 0 | 3.291616 | -3.655430 | -0.000003 |
| 3 | 6 | 0 | 3.962542 | -2.463820 | -0.000001 |
| 4 | 6 | 0 | 3.256523 | -1.223728 | 0.000000 |
| 5 | 6 | 0 | 1.819241 | -1.238644 | -0.000001 |
| 6 | 6 | 0 | 1.160499 | -2.498159 | -0.000004 |
| 7 | 6 | 0 | 3.934778 | 0.000000 | 0.000001 |
| 8 | 6 | 0 | 3.256523 | 1.223728 | 0.000002 |
| 9 | 6 | 0 | 1.819241 | 1.238644 | 0.000001 |

| | | | | | |
|---|---|---|---|---|---|
| 10 | 6 | 0 | 1.106198 | 0.000000 | -0.000001 |
| 11 | 6 | 0 | 3.962542 | 2.463820 | 0.000003 |
| 12 | 6 | 0 | 3.291615 | 3.655430 | 0.000004 |
| 13 | 6 | 0 | 1.872748 | 3.669689 | 0.000003 |
| 14 | 6 | 0 | 1.160498 | 2.498159 | 0.000001 |
| 15 | 6 | 0 | -0.296632 | 0.000000 | -0.000001 |
| 16 | 6 | 0 | -1.518815 | 0.000000 | -0.000001 |
| 17 | 6 | 0 | -2.912181 | 0.000000 | -0.000001 |
| 18 | 6 | 0 | -3.642407 | -1.231352 | 0.000013 |
| 19 | 6 | 0 | -5.004698 | -1.239150 | 0.000014 |
| 20 | 6 | 0 | -5.777652 | 0.000000 | 0.000001 |
| 21 | 6 | 0 | -5.004698 | 1.239149 | -0.000014 |
| 22 | 6 | 0 | -3.642407 | 1.231352 | -0.000014 |
| 23 | 8 | 0 | -7.018005 | 0.000000 | 0.000002 |
| 24 | 1 | 0 | 1.348838 | -4.618693 | -0.000007 |
| 25 | 1 | 0 | 3.837961 | -4.591470 | -0.000004 |
| 26 | 1 | 0 | 5.046963 | -2.440132 | 0.000000 |
| 27 | 1 | 0 | 0.078180 | -2.518750 | -0.000005 |
| 28 | 1 | 0 | 5.020266 | 0.000000 | 0.000002 |
| 29 | 1 | 0 | 5.046963 | 2.440133 | 0.000004 |
| 30 | 1 | 0 | 3.837960 | 4.591470 | 0.000006 |
| 31 | 1 | 0 | 1.348838 | 4.618693 | 0.000004 |
| 32 | 1 | 0 | 0.078180 | 2.518750 | 0.000001 |
| 33 | 1 | 0 | -3.084329 | -2.160626 | 0.000023 |
| 34 | 1 | 0 | -5.569190 | -2.164281 | 0.000025 |
| 35 | 1 | 0 | -5.569190 | 2.164281 | -0.000025 |
| 36 | 1 | 0 | -3.084329 | 2.160626 | -0.000025 |

R=NO

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -0.883811 | 3.659404 | 0.000006 |
| 2 | 6 | 0 | -2.301894 | 3.582409 | -0.000004 |
| 3 | 6 | 0 | -2.920799 | 2.363465 | -0.000008 |
| 4 | 6 | 0 | -2.164734 | 1.152224 | -0.000004 |
| 5 | 6 | 0 | -0.728753 | 1.230932 | 0.000004 |
| 6 | 6 | 0 | -0.124275 | 2.519442 | 0.000010 |
| 7 | 6 | 0 | -2.789063 | -0.099385 | -0.000006 |
| 8 | 6 | 0 | -2.054383 | -1.289802 | -0.000002 |
| 9 | 6 | 0 | -0.617171 | -1.239563 | 0.000003 |
| 10 | 6 | 0 | 0.035537 | 0.028798 | 0.000005 |
| 11 | 6 | 0 | -2.698799 | -2.563838 | -0.000002 |
| 12 | 6 | 0 | -1.971372 | -3.721284 | 0.000001 |
| 13 | 6 | 0 | -0.552229 | -3.669838 | 0.000005 |
| 14 | 6 | 0 | 0.103984 | -2.467212 | 0.000005 |
| 15 | 6 | 0 | 1.442108 | 0.076641 | 0.000005 |
| 16 | 6 | 0 | 2.658558 | 0.063212 | 0.000002 |
| 17 | 7 | 0 | 3.990183 | -0.004093 | -0.000002 |
| 18 | 8 | 0 | 4.599873 | -1.133062 | -0.000013 |
| 19 | 6 | 0 | 4.812883 | 1.214685 | -0.000001 |
| 20 | 1 | 0 | -0.401834 | 4.630514 | 0.000012 |
| 21 | 1 | 0 | -2.888600 | 4.493914 | -0.000007 |
| 22 | 1 | 0 | -4.003439 | 2.294444 | -0.000016 |
| 23 | 1 | 0 | 0.956778 | 2.585957 | 0.000018 |
| 24 | 1 | 0 | -3.873382 | -0.148283 | -0.000011 |
| 25 | 1 | 0 | -3.783259 | -2.592700 | -0.000005 |
| 26 | 1 | 0 | -2.473099 | -4.682254 | 0.000001 |
| 27 | 1 | 0 | 0.016021 | -4.592934 | 0.000008 |
| 28 | 1 | 0 | 1.186741 | -2.438407 | 0.000008 |
| 29 | 1 | 0 | 4.171467 | 2.094715 | 0.000023 |
| 30 | 1 | 0 | 5.443824 | 1.203206 | 0.890124 |
| 31 | 1 | 0 | 5.443791 | 1.203231 | -0.890150 |

R=Allyl

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 2.717586 | 0.000007 | 0.000001 |
| 2 | 6 | 0 | 1.506729 | 0.000006 | 0.000004 |
| 3 | 6 | 0 | 4.151383 | 0.000008 | -0.000003 |
| 4 | 6 | 0 | -0.665561 | -3.664505 | 0.061515 |
| 5 | 6 | 0 | -2.087296 | -3.653109 | 0.055755 |
| 6 | 6 | 0 | -2.761590 | -2.465361 | 0.034977 |
| 7 | 6 | 0 | -2.060891 | -1.220432 | 0.017222 |
| 8 | 6 | 0 | -0.621105 | -1.231686 | 0.019215 |
| 9 | 6 | 0 | 0.042329 | -2.493736 | 0.044371 |
| 10 | 6 | 0 | -2.740537 | -0.000007 | -0.000004 |
| 11 | 6 | 0 | -2.060898 | 1.220422 | -0.017227 |
| 12 | 6 | 0 | -0.621113 | 1.231685 | -0.019212 |
| 13 | 6 | 0 | 0.085889 | 0.000001 | 0.000002 |
| 14 | 6 | 0 | -2.761605 | 2.465347 | -0.034983 |
| 15 | 6 | 0 | -2.087318 | 3.653098 | -0.055755 |
| 16 | 6 | 0 | -0.665584 | 3.664504 | -0.061507 |
| 17 | 6 | 0 | 0.042313 | 2.493739 | -0.044362 |
| 18 | 6 | 0 | 4.827370 | 1.144693 | 0.422115 |
| 19 | 6 | 0 | 4.827372 | -1.144675 | -0.422123 |
| 20 | 1 | 0 | -0.140479 | -4.612884 | 0.081018 |
| 21 | 1 | 0 | -2.630901 | -4.590940 | 0.069331 |
| 22 | 1 | 0 | -3.846303 | -2.445698 | 0.032353 |
| 23 | 1 | 0 | 1.124839 | -2.508188 | 0.053104 |
| 24 | 1 | 0 | -3.826154 | -0.000011 | -0.000008 |
| 25 | 1 | 0 | -3.846318 | 2.445677 | -0.032367 |
| 26 | 1 | 0 | -2.630930 | 4.590927 | -0.069333 |
| 27 | 1 | 0 | -0.140508 | 4.612886 | -0.081003 |
| 28 | 1 | 0 | 1.124824 | 2.508197 | -0.053089 |
| 29 | 1 | 0 | 5.910037 | 1.169446 | 0.425130 |
| 30 | 1 | 0 | 4.293506 | 2.022929 | 0.757259 |
| 31 | 1 | 0 | 5.910038 | -1.169422 | -0.425147 |
| 32 | 1 | 0 | 4.293509 | -2.022914 | -0.757258 |

R=IN

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 2.999014 | 3.662032 | 0.055802 |
| 2 | 6 | 0 | 4.410366 | 3.490707 | 0.063477 |
| 3 | 6 | 0 | 4.947961 | 2.234812 | 0.048189 |
| 4 | 6 | 0 | 4.110929 | 1.077683 | 0.024275 |
| 5 | 6 | 0 | 2.682539 | 1.252498 | 0.016639 |
| 6 | 6 | 0 | 2.162106 | 2.579357 | 0.033298 |
| 7 | 6 | 0 | 4.645573 | -0.213536 | 0.008119 |
| 8 | 6 | 0 | 3.834640 | -1.351655 | -0.015887 |
| 9 | 6 | 0 | 2.403256 | -1.201833 | -0.023917 |
| 10 | 6 | 0 | 1.846386 | 0.105387 | -0.006666 |
| 11 | 6 | 0 | 4.391287 | -2.666906 | -0.032852 |
| 12 | 6 | 0 | 3.584877 | -3.769432 | -0.056796 |
| 13 | 6 | 0 | 2.171147 | -3.619210 | -0.065496 |
| 14 | 6 | 0 | 1.595953 | -2.377104 | -0.049739 |
| 15 | 6 | 0 | 0.439154 | 0.254418 | -0.012359 |
| 16 | 6 | 0 | -0.766556 | 0.351947 | -0.016089 |
| 17 | 6 | 0 | -2.178704 | 0.392043 | -0.025604 |
| 18 | 7 | 0 | -2.924432 | 1.444209 | 0.000207 |
| 19 | 6 | 0 | -4.342794 | 1.018327 | -0.145279 |
| 20 | 6 | 0 | -4.345881 | -0.526820 | 0.178429 |
| 21 | 7 | 0 | -2.895289 | -0.822662 | -0.063754 |
| 22 | 6 | 0 | -4.612996 | -0.859068 | 1.657520 |
| 23 | 6 | 0 | -5.206371 | -1.419293 | -0.714498 |
| 24 | 6 | 0 | -4.724891 | 1.327543 | -1.606682 |
| 25 | 6 | 0 | -5.214325 | 1.864666 | 0.788000 |
| 26 | 8 | 0 | -2.405239 | -1.985460 | -0.073582 |
| 27 | 1 | 0 | 2.583969 | 4.663469 | 0.067924 |
| 28 | 1 | 0 | 5.055387 | 4.361734 | 0.081473 |
| 29 | 1 | 0 | 6.023533 | 2.093453 | 0.053881 |
| 30 | 1 | 0 | 1.087813 | 2.717077 | 0.027712 |
| 31 | 1 | 0 | 5.724358 | -0.336266 | 0.014161 |
| 32 | 1 | 0 | 5.471148 | -2.770560 | -0.026465 |
| 33 | 1 | 0 | 4.017826 | -4.763223 | -0.069567 |
| 34 | 1 | 0 | 1.541633 | -4.501545 | -0.085203 |
| 35 | 1 | 0 | 0.517217 | -2.273957 | -0.057664 |
| 36 | 1 | 0 | -4.376072 | -1.911126 | 1.828603 |
| 37 | 1 | 0 | -3.993440 | -0.257594 | 2.325165 |
| 38 | 1 | 0 | -5.661715 | -0.692890 | 1.911298 |
| 39 | 1 | 0 | -6.265981 | -1.211777 | -0.546851 |
| 40 | 1 | 0 | -4.986444 | -1.280620 | -1.772495 |
| 41 | 1 | 0 | -5.016418 | -2.465071 | -0.466536 |
| 42 | 1 | 0 | -4.550485 | 2.387728 | -1.797814 |
| 43 | 1 | 0 | -4.115553 | 0.757470 | -2.310867 |
| 44 | 1 | 0 | -5.778585 | 1.108648 | -1.797167 |
| 45 | 1 | 0 | -6.267168 | 1.577926 | 0.710695 |
| 46 | 1 | 0 | -4.903913 | 1.776097 | 1.828920 |
| 47 | 1 | 0 | -5.123179 | 2.914492 | 0.502982 |

R=Phen

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -3.286906 | -3.657893 | -0.235699 |
| 2 | 6 | 0 | -4.708471 | -3.646362 | -0.230212 |
| 3 | 6 | 0 | -5.382257 | -2.460612 | -0.153009 |
| 4 | 6 | 0 | -4.681196 | -1.218193 | -0.075658 |
| 5 | 6 | 0 | -3.241572 | -1.229743 | -0.077974 |
| 6 | 6 | 0 | -2.578890 | -2.489220 | -0.162416 |
| 7 | 6 | 0 | -5.360963 | -0.000001 | -0.000003 |
| 8 | 6 | 0 | -4.681198 | 1.218191 | 0.075654 |
| 9 | 6 | 0 | -3.241574 | 1.229742 | 0.077976 |
| 10 | 6 | 0 | -2.533533 | 0.000000 | 0.000002 |
| 11 | 6 | 0 | -5.382260 | 2.460609 | 0.153002 |
| 12 | 6 | 0 | -4.708476 | 3.646359 | 0.230208 |
| 13 | 6 | 0 | -3.286911 | 3.657892 | 0.235701 |
| 14 | 6 | 0 | -2.578894 | 2.489221 | 0.162420 |
| 15 | 6 | 0 | -1.114600 | 0.000001 | 0.000006 |
| 16 | 6 | 0 | 0.097618 | 0.000002 | 0.000006 |
| 17 | 6 | 0 | 1.521037 | 0.000002 | 0.000004 |
| 18 | 6 | 0 | 2.229314 | -1.197074 | 0.186585 |
| 19 | 6 | 0 | 3.640749 | -1.221264 | 0.190192 |
| 20 | 6 | 0 | 4.357629 | 0.000001 | 0.000000 |
| 21 | 6 | 0 | 3.640749 | 1.221265 | -0.190190 |
| 22 | 6 | 0 | 2.229314 | 1.197076 | -0.186578 |
| 23 | 6 | 0 | 4.373786 | -2.420670 | 0.377742 |
| 24 | 6 | 0 | 5.763070 | -2.411341 | 0.376510 |
| 25 | 6 | 0 | 6.467483 | -1.227014 | 0.191543 |
| 26 | 6 | 0 | 5.785436 | 0.000000 | -0.000002 |
| 27 | 6 | 0 | 6.467483 | 1.227013 | -0.191550 |
| 28 | 6 | 0 | 5.763071 | 2.411341 | -0.376515 |
| 29 | 6 | 0 | 4.373787 | 2.420671 | -0.377742 |
| 30 | 1 | 0 | -2.761985 | -4.604390 | -0.299824 |
| 31 | 1 | 0 | -5.252447 | -4.582246 | -0.288715 |

| | | | | | |
|---|---|---|---|---|---|
| 32 | 1 | 0 | -6.466959 | -2.440649 | -0.149713 |
| 33 | 1 | 0 | -1.496423 | -2.503751 | -0.170321 |
| 34 | 1 | 0 | -6.446555 | -0.000002 | -0.000006 |
| 35 | 1 | 0 | -6.466963 | 2.440645 | 0.149702 |
| 36 | 1 | 0 | -5.252454 | 4.582243 | 0.288709 |
| 37 | 1 | 0 | -2.761992 | 4.604390 | 0.299827 |
| 38 | 1 | 0 | -1.496427 | 2.503753 | 0.170330 |
| 39 | 1 | 0 | 1.682666 | -2.120714 | 0.334654 |
| 40 | 1 | 0 | 1.682667 | 2.120718 | -0.334646 |
| 41 | 1 | 0 | 3.833363 | -3.349476 | 0.523025 |
| 42 | 1 | 0 | 6.304664 | -3.339464 | 0.521650 |
| 43 | 1 | 0 | 7.551935 | -1.230869 | 0.192218 |
| 44 | 1 | 0 | 7.551935 | 1.230868 | -0.192229 |
| 45 | 1 | 0 | 6.304665 | 3.339464 | -0.521656 |
| 46 | 1 | 0 | 3.833364 | 3.349478 | -0.523023 |

R=Ver

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 3.965205 | -3.664761 | 0.057000 |
| 2 | 6 | 0 | 5.386833 | -3.653815 | 0.043952 |
| 3 | 6 | 0 | 6.062344 | -2.466458 | 0.035238 |
| 4 | 6 | 0 | 5.361487 | -1.221764 | 0.038610 |
| 5 | 6 | 0 | 3.922229 | -1.233848 | 0.049546 |
| 6 | 6 | 0 | 3.256041 | -2.494333 | 0.059392 |
| 7 | 6 | 0 | 6.039713 | 0.000001 | 0.032239 |
| 8 | 6 | 0 | 5.361485 | 1.221765 | 0.038646 |
| 9 | 6 | 0 | 3.922227 | 1.233846 | 0.049582 |
| 10 | 6 | 0 | 3.218997 | -0.000002 | 0.051637 |
| 11 | 6 | 0 | 6.062340 | 2.466460 | 0.035311 |
| 12 | 6 | 0 | 5.386827 | 3.653816 | 0.044061 |
| 13 | 6 | 0 | 3.965199 | 3.664759 | 0.057108 |
| 14 | 6 | 0 | 3.256037 | 2.494330 | 0.059464 |
| 15 | 6 | 0 | 1.801743 | -0.000003 | 0.054383 |
| 16 | 6 | 0 | 0.592470 | -0.000003 | 0.054268 |
| 17 | 6 | 0 | -0.832818 | -0.000001 | 0.057352 |
| 18 | 7 | 0 | -1.425296 | -1.194565 | 0.066453 |
| 19 | 7 | 0 | -2.789228 | -1.173200 | 0.069382 |
| 20 | 6 | 0 | -3.560972 | 0.000001 | 0.025964 |
| 21 | 7 | 0 | -2.789226 | 1.173201 | 0.069369 |
| 22 | 7 | 0 | -1.425294 | 1.194564 | 0.066441 |
| 23 | 8 | 0 | -4.768271 | 0.000002 | -0.039850 |
| 24 | 6 | 0 | -3.408537 | 2.468463 | -0.011417 |
| 25 | 6 | 0 | -3.408542 | -2.468461 | -0.011385 |
| 26 | 6 | 0 | -2.758934 | -3.466176 | -0.742479 |
| 27 | 6 | 0 | -3.311232 | -4.739888 | -0.812842 |
| 28 | 6 | 0 | -4.507489 | -5.026730 | -0.158846 |
| 29 | 6 | 0 | -5.146465 | -4.028026 | 0.571882 |
| 30 | 6 | 0 | -4.605247 | -2.748693 | 0.652791 |
| 31 | 6 | 0 | -2.758926 | 3.466166 | -0.742526 |
| 32 | 6 | 0 | -3.311222 | 4.739878 | -0.812909 |
| 33 | 6 | 0 | -4.507480 | 5.026731 | -0.158921 |
| 34 | 6 | 0 | -5.146459 | 4.028040 | 0.571822 |
| 35 | 6 | 0 | -4.605243 | 2.748706 | 0.652751 |
| 36 | 1 | 0 | 3.439884 | -4.613060 | 0.066415 |
| 37 | 1 | 0 | 5.929708 | -4.592109 | 0.042010 |
| 38 | 1 | 0 | 7.146977 | -2.447329 | 0.026441 |
| 39 | 1 | 0 | 2.173252 | -2.509979 | 0.071761 |
| 40 | 1 | 0 | 7.125341 | 0.000002 | 0.023391 |
| 41 | 1 | 0 | 7.146974 | 2.447333 | 0.026514 |
| 42 | 1 | 0 | 5.929700 | 4.592110 | 0.042148 |
| 43 | 1 | 0 | 3.439877 | 4.613056 | 0.066551 |
| 44 | 1 | 0 | 2.173248 | 2.509973 | 0.071833 |
| 45 | 1 | 0 | -1.825262 | -3.236237 | -1.236283 |
| 46 | 1 | 0 | -2.804076 | -5.508299 | -1.384842 |
| 47 | 1 | 0 | -4.937301 | -6.019950 | -0.217243 |
| 48 | 1 | 0 | -6.074734 | -4.241516 | 1.089068 |
| 49 | 1 | 0 | -5.111226 | -1.979036 | 1.214538 |
| 50 | 1 | 0 | -1.825253 | 3.236217 | -1.236324 |
| 51 | 1 | 0 | -2.804062 | 5.508278 | -1.384920 |
| 52 | 1 | 0 | -4.937290 | 6.019951 | -0.217333 |
| 53 | 1 | 0 | -6.074729 | 4.241538 | 1.089001 |
| 54 | 1 | 0 | -5.111224 | 1.979058 | 1.214508 |

R=NN

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 2.709828 | 3.664487 | 0.061758 |
| 2 | 6 | 0 | 4.131299 | 3.654044 | 0.061503 |
| 3 | 6 | 0 | 4.808659 | 2.467456 | 0.041488 |
| 4 | 6 | 0 | 4.108337 | 1.222925 | 0.020450 |
| 5 | 6 | 0 | 2.669733 | 1.236285 | 0.020528 |
| 6 | 6 | 0 | 1.999715 | 2.494135 | 0.042095 |
| 7 | 6 | 0 | 4.785742 | 0.000001 | 0.000001 |
| 8 | 6 | 0 | 4.108339 | -1.222923 | -0.020449 |
| 9 | 6 | 0 | 2.669735 | -1.236285 | -0.020529 |
| 10 | 6 | 0 | 1.968924 | 0.000000 | -0.000001 |
| 11 | 6 | 0 | 4.808662 | -2.467453 | -0.041485 |
| 12 | 6 | 0 | 4.131303 | -3.654042 | -0.061501 |
| 13 | 6 | 0 | 2.709833 | -3.664487 | -0.061760 |
| 14 | 6 | 0 | 1.999718 | -2.494136 | -0.042098 |
| 15 | 6 | 0 | 0.558229 | -0.000001 | -0.000002 |
| 16 | 6 | 0 | -0.653498 | -0.000002 | -0.000002 |
| 17 | 6 | 0 | -2.044046 | -0.000001 | -0.000002 |
| 18 | 7 | 0 | -2.822642 | -1.115535 | -0.030790 |
| 19 | 6 | 0 | -4.276153 | -0.763055 | 0.182930 |
| 20 | 6 | 0 | -4.276153 | 0.763054 | -0.182928 |
| 21 | 7 | 0 | -2.822641 | 1.115534 | 0.030788 |
| 22 | 8 | 0 | -2.418232 | 2.315108 | 0.050967 |
| 23 | 8 | 0 | -2.418234 | -2.315110 | -0.050969 |
| 24 | 6 | 0 | -4.566436 | -1.055817 | 1.664796 |
| 25 | 6 | 0 | -5.144079 | -1.653917 | -0.703159 |
| 26 | 6 | 0 | -4.566439 | 1.055817 | -1.664794 |
| 27 | 6 | 0 | -5.144076 | 1.653917 | 0.703162 |
| 28 | 1 | 0 | 2.183447 | 4.611995 | 0.077926 |
| 29 | 1 | 0 | 4.673493 | 4.592656 | 0.077391 |
| 30 | 1 | 0 | 5.893364 | 2.449403 | 0.041323 |
| 31 | 1 | 0 | 0.916121 | 2.511625 | 0.043138 |
| 32 | 1 | 0 | 5.871463 | 0.000002 | 0.000002 |
| 33 | 1 | 0 | 5.893367 | -2.449399 | -0.041318 |
| 34 | 1 | 0 | 4.673498 | -4.592653 | -0.077387 |
| 35 | 1 | 0 | 2.183452 | -4.611996 | -0.077928 |
| 36 | 1 | 0 | 0.916124 | -2.511627 | -0.043143 |
| 37 | 1 | 0 | -5.617117 | -0.875275 | 1.899622 |
| 38 | 1 | 0 | -4.340085 | -2.105272 | 1.858889 |
| 39 | 1 | 0 | -3.949504 | -0.446084 | 2.327510 |
| 40 | 1 | 0 | -4.977627 | -2.695248 | -0.427598 |
| 41 | 1 | 0 | -6.200321 | -1.417239 | -0.554246 |
| 42 | 1 | 0 | -4.904684 | -1.545760 | -1.760228 |
| 43 | 1 | 0 | -5.617121 | 0.875275 | -1.899618 |
| 44 | 1 | 0 | -4.340089 | 2.105272 | -1.858886 |
| 45 | 1 | 0 | -3.949509 | 0.446083 | -2.327509 |
| 46 | 1 | 0 | -4.977624 | 2.695248 | 0.427600 |
| 47 | 1 | 0 | -6.200318 | 1.417239 | 0.554254 |
| 48 | 1 | 0 | -4.904678 | 1.545761 | 1.760231 |

# Sat-Radical

R=Sat-H

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 3.668134 | 0.167474 | -0.110712 |
| 2 | 6 | 0 | 3.650787 | -1.242663 | 0.068391 |
| 3 | 6 | 0 | 2.457872 | -1.902095 | 0.139601 |
| 4 | 6 | 0 | 1.216451 | -1.201722 | 0.037321 |
| 5 | 6 | 0 | 1.222762 | 0.229897 | -0.155546 |
| 6 | 6 | 0 | 2.501823 | 0.873279 | -0.218850 |
| 7 | 6 | 0 | 0.000000 | -1.878223 | 0.123135 |
| 8 | 6 | 0 | -1.216452 | -1.201722 | 0.037320 |
| 9 | 6 | 0 | -1.222762 | 0.229897 | -0.155547 |
| 10 | 6 | 0 | 0.000000 | 0.933413 | -0.266580 |
| 11 | 6 | 0 | -2.457873 | -1.902095 | 0.139601 |
| 12 | 6 | 0 | -3.650788 | -1.242662 | 0.068392 |
| 13 | 6 | 0 | -3.668134 | 0.167475 | -0.110712 |
| 14 | 6 | 0 | -2.501823 | 0.873280 | -0.218850 |
| 15 | 6 | 0 | 0.000001 | 2.436155 | -0.472052 |
| 16 | 6 | 0 | 0.000002 | 3.235295 | 0.844438 |
| 17 | 1 | 0 | 4.618585 | 0.686984 | -0.161097 |
| 18 | 1 | 0 | 4.585299 | -1.786197 | 0.149194 |
| 19 | 1 | 0 | 2.429256 | -2.977824 | 0.278919 |
| 20 | 1 | 0 | 2.553490 | 1.945932 | -0.347591 |
| 21 | 1 | 0 | -0.000001 | -2.954396 | 0.266188 |
| 22 | 1 | 0 | -2.429257 | -2.977823 | 0.278920 |
| 23 | 1 | 0 | -4.585300 | -1.786196 | 0.149196 |
| 24 | 1 | 0 | -4.618585 | 0.686985 | -0.161097 |
| 25 | 1 | 0 | -2.553490 | 1.945933 | -0.347591 |
| 26 | 1 | 0 | 0.865544 | 2.726660 | -1.070496 |
| 27 | 1 | 0 | -0.865545 | 2.726662 | -1.070492 |
| 28 | 1 | 0 | 0.000003 | 4.311097 | 0.646462 |
| 29 | 1 | 0 | -0.881276 | 3.001143 | 1.446694 |
| 30 | 1 | 0 | 0.881279 | 3.001142 | 1.446695 |

R=Sat-Mt

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -1.223257 | -0.072125 | -0.193725 |
| 2 | 6 | 0 | -1.216629 | -1.492757 | 0.067520 |
| 3 | 6 | 0 | 0.000002 | -2.164149 | 0.185837 |
| 4 | 6 | 0 | 1.216633 | -1.492755 | 0.067520 |
| 5 | 6 | 0 | 1.223257 | -0.072122 | -0.193725 |
| 6 | 6 | 0 | 0.000000 | 0.625073 | -0.338699 |
| 7 | 6 | 0 | -2.502203 | 0.567080 | -0.288633 |
| 8 | 6 | 0 | -3.668475 | -0.132951 | -0.146527 |
| 9 | 6 | 0 | -3.650921 | -1.532620 | 0.100779 |
| 10 | 6 | 0 | -2.457840 | -2.187648 | 0.203532 |
| 11 | 6 | 0 | 2.457845 | -2.187644 | 0.203531 |
| 12 | 6 | 0 | 3.650924 | -1.532614 | 0.100779 |
| 13 | 6 | 0 | 3.668476 | -0.132945 | -0.146526 |
| 14 | 6 | 0 | 2.502202 | 0.567085 | -0.288632 |
| 15 | 6 | 0 | -0.000002 | 2.114479 | -0.609662 |
| 16 | 6 | 0 | -0.000005 | 2.975709 | 0.697342 |
| 17 | 6 | 0 | -0.000006 | 4.439658 | 0.432811 |
| 18 | 1 | 0 | 0.000003 | -3.232106 | 0.380894 |
| 19 | 1 | 0 | -2.554320 | 1.631882 | -0.471145 |
| 20 | 1 | 0 | -4.618981 | 0.383259 | -0.222772 |
| 21 | 1 | 0 | -4.585319 | -2.071767 | 0.207765 |
| 22 | 1 | 0 | -2.428984 | -3.255393 | 0.394502 |
| 23 | 1 | 0 | 2.428990 | -3.255389 | 0.394500 |
| 24 | 1 | 0 | 4.585324 | -2.071759 | 0.207763 |
| 25 | 1 | 0 | 4.618981 | 0.383268 | -0.222771 |
| 26 | 1 | 0 | 2.554318 | 1.631887 | -0.471144 |
| 27 | 1 | 0 | 0.866831 | 2.391819 | -1.211133 |
| 28 | 1 | 0 | -0.866833 | 2.391817 | -1.211135 |
| 29 | 1 | 0 | -0.878682 | 2.693214 | 1.286581 |
| 30 | 1 | 0 | 0.878670 | 2.693217 | 1.286585 |
| 31 | 1 | 0 | -0.926233 | 4.976764 | 0.265169 |
| 32 | 1 | 0 | 0.926222 | 4.976773 | 0.265205 |

R=Sat-DCM

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 1.059219 | 3.669580 | 0.153333 |
| 2 | 6 | 0 | 2.453798 | 3.651248 | -0.117244 |
| 3 | 6 | 0 | 3.106888 | 2.457444 | -0.228141 |
| 4 | 6 | 0 | 2.412887 | 1.218066 | -0.078518 |
| 5 | 6 | 0 | 0.997460 | 1.226016 | 0.207319 |
| 6 | 6 | 0 | 0.359676 | 2.504191 | 0.310688 |
| 7 | 6 | 0 | 3.080287 | -0.000005 | -0.208023 |
| 8 | 6 | 0 | 2.412880 | -1.218073 | -0.078527 |
| 9 | 6 | 0 | 0.997454 | -1.226017 | 0.207312 |
| 10 | 6 | 0 | 0.307888 | 0.000001 | 0.366059 |
| 11 | 6 | 0 | 3.106873 | -2.457454 | -0.228161 |
| 12 | 6 | 0 | 2.453776 | -3.651255 | -0.117272 |
| 13 | 6 | 0 | 1.059199 | -3.669581 | 0.153310 |
| 14 | 6 | 0 | 0.359662 | -2.504189 | 0.310676 |
| 15 | 6 | 0 | -1.172540 | 0.000004 | 0.667936 |
| 16 | 6 | 0 | -2.034758 | 0.000002 | -0.637058 |
| 17 | 6 | 0 | -3.509433 | 0.000003 | -0.338242 |
| 18 | 6 | 0 | -4.193730 | 1.208157 | -0.150310 |
| 19 | 6 | 0 | -4.193718 | -1.208148 | -0.150251 |
| 20 | 7 | 0 | -4.719562 | 2.235312 | -0.005859 |
| 21 | 7 | 0 | -4.719539 | -2.235302 | -0.005751 |
| 22 | 1 | 0 | 0.544287 | 4.619877 | 0.236860 |
| 23 | 1 | 0 | 2.990941 | 4.585220 | -0.234825 |
| 24 | 1 | 0 | 4.171291 | 2.427399 | -0.435693 |
| 25 | 1 | 0 | -0.701282 | 2.563518 | 0.513662 |
| 26 | 1 | 0 | 4.144378 | -0.000007 | -0.422673 |
| 27 | 1 | 0 | 4.171276 | -2.427414 | -0.435716 |
| 28 | 1 | 0 | 2.990914 | -4.585230 | -0.234862 |
| 29 | 1 | 0 | 0.544262 | -4.619876 | 0.236834 |
| 30 | 1 | 0 | -0.701295 | -2.563512 | 0.513655 |
| 31 | 1 | 0 | -1.444217 | -0.869482 | 1.266896 |
| 32 | 1 | 0 | -1.444215 | 0.869492 | 1.266893 |
| 33 | 1 | 0 | -1.787618 | 0.883134 | -1.229541 |
| 34 | 1 | 0 | -1.787619 | -0.883134 | -1.229536 |

R=Sat-DPM

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -2.452936 | -1.265731 | -0.397185 |
| 2 | 6 | 0 | -3.863449 | -1.298983 | -0.084864 |
| 3 | 6 | 0 | -4.526382 | -0.113713 | 0.231121 |
| 4 | 6 | 0 | -3.858468 | 1.110268 | 0.253157 |
| 5 | 6 | 0 | -2.448407 | 1.156981 | -0.055550 |
| 6 | 6 | 0 | -1.755095 | -0.033978 | -0.381513 |
| 7 | 6 | 0 | -1.828949 | -2.516556 | -0.712985 |
| 8 | 6 | 0 | -2.529121 | -3.691471 | -0.716974 |
| 9 | 6 | 0 | -3.915593 | -3.712639 | -0.405067 |
| 10 | 6 | 0 | -4.558305 | -2.547652 | -0.101020 |
| 11 | 6 | 0 | -4.547161 | 2.319206 | 0.578692 |
| 12 | 6 | 0 | -3.896664 | 3.518920 | 0.605877 |
| 13 | 6 | 0 | -2.508938 | 3.575758 | 0.303996 |
| 14 | 6 | 0 | -1.813785 | 2.441102 | -0.013137 |
| 15 | 6 | 0 | -0.267988 | 0.011342 | -0.664488 |
| 16 | 6 | 0 | 0.597755 | -0.089381 | 0.629499 |
| 17 | 6 | 0 | 2.079928 | -0.011685 | 0.358926 |
| 18 | 6 | 0 | 2.637609 | 1.296527 | 0.004018 |
| 19 | 6 | 0 | 2.894321 | -1.203592 | 0.395274 |
| 20 | 6 | 0 | 3.610492 | 1.433649 | -1.012202 |
| 21 | 6 | 0 | 4.107757 | 2.678206 | -1.376657 |
| 22 | 6 | 0 | 3.658873 | 3.834402 | -0.738610 |
| 23 | 6 | 0 | 2.696543 | 3.726508 | 0.264376 |
| 24 | 6 | 0 | 2.188133 | 2.483833 | 0.623508 |
| 25 | 6 | 0 | 4.304726 | -1.142352 | 0.560194 |
| 26 | 6 | 0 | 5.079195 | -2.289680 | 0.625576 |
| 27 | 6 | 0 | 4.491424 | -3.553011 | 0.530005 |
| 28 | 6 | 0 | 3.106733 | -3.645512 | 0.382719 |
| 29 | 6 | 0 | 2.323902 | -2.502296 | 0.324301 |
| 30 | 1 | 0 | -5.585577 | -0.144853 | 0.467129 |
| 31 | 1 | 0 | -0.777428 | -2.540383 | -0.963645 |
| 32 | 1 | 0 | -2.023471 | -4.618354 | -0.963812 |
| 33 | 1 | 0 | -4.455000 | -4.652917 | -0.413180 |
| 34 | 1 | 0 | -5.617134 | -2.547164 | 0.136156 |
| 35 | 1 | 0 | -5.606716 | 2.260282 | 0.805078 |
| 36 | 1 | 0 | -4.431217 | 4.428782 | 0.854254 |
| 37 | 1 | 0 | -1.997374 | 4.531650 | 0.323358 |
| 38 | 1 | 0 | -0.759528 | 2.525042 | -0.238847 |
| 39 | 1 | 0 | 0.018909 | -0.791168 | -1.344699 |
| 40 | 1 | 0 | -0.008326 | 0.933670 | -1.185958 |
| 41 | 1 | 0 | 0.296108 | 0.725121 | 1.294374 |
| 42 | 1 | 0 | 0.345885 | -1.008782 | 1.159926 |
| 43 | 1 | 0 | 3.951606 | 0.550048 | -1.537154 |
| 44 | 1 | 0 | 4.842923 | 2.747537 | -2.171024 |
| 45 | 1 | 0 | 4.050056 | 4.804810 | -1.021647 |
| 46 | 1 | 0 | 2.343397 | 4.615685 | 0.775248 |
| 47 | 1 | 0 | 1.456040 | 2.429303 | 1.419858 |
| 48 | 1 | 0 | 4.781213 | -0.177463 | 0.672774 |
| 49 | 1 | 0 | 6.151030 | -2.200799 | 0.766089 |
| 50 | 1 | 0 | 5.100152 | -4.448296 | 0.579711 |
| 51 | 1 | 0 | 2.633584 | -4.618963 | 0.312470 |
| 52 | 1 | 0 | 1.253961 | -2.613621 | 0.207621 |

R=Sat-Flu

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -2.608086 | 1.223512 | 0.226824 |
| 2 | 6 | 0 | -4.026548 | 1.216699 | -0.046020 |
| 3 | 6 | 0 | -4.695971 | -0.000007 | -0.173705 |
| 4 | 6 | 0 | -4.026542 | -1.216708 | -0.046007 |
| 5 | 6 | 0 | -2.608079 | -1.223511 | 0.226837 |
| 6 | 6 | 0 | -1.910386 | 0.000003 | 0.367535 |
| 7 | 6 | 0 | -1.973077 | 2.503065 | 0.340526 |
| 8 | 6 | 0 | -2.673821 | 3.669149 | 0.199176 |
| 9 | 6 | 0 | -4.069733 | 3.651080 | -0.067921 |
| 10 | 6 | 0 | -4.721530 | 2.457534 | -0.184584 |
| 11 | 6 | 0 | -4.721518 | -2.457548 | -0.184558 |
| 12 | 6 | 0 | -4.069715 | -3.651089 | -0.067882 |
| 13 | 6 | 0 | -2.673803 | -3.669149 | 0.199214 |

| | | | | | |
|---|---|---|---|---|---|
| 14 | 6 | 0 | -1.973065 | -2.503061 | 0.340552 |
| 15 | 6 | 0 | -0.417997 | 0.000008 | 0.620426 |
| 16 | 6 | 0 | 0.416200 | 0.000006 | -0.699722 |
| 17 | 6 | 0 | 1.886848 | 0.000004 | -0.450419 |
| 18 | 6 | 0 | 2.720831 | -1.158764 | -0.269150 |
| 19 | 6 | 0 | 4.052700 | -0.732588 | 0.027273 |
| 20 | 6 | 0 | 4.052700 | 0.732588 | 0.027283 |
| 21 | 6 | 0 | 2.720832 | 1.158769 | -0.269134 |
| 22 | 6 | 0 | 5.055777 | 1.664061 | 0.244216 |
| 23 | 6 | 0 | 4.746145 | 3.027826 | 0.166937 |
| 24 | 6 | 0 | 3.446283 | 3.452094 | -0.128291 |
| 25 | 6 | 0 | 2.427907 | 2.526921 | -0.348392 |
| 26 | 6 | 0 | 2.427906 | -2.526914 | -0.348426 |
| 27 | 6 | 0 | 3.446281 | -3.452091 | -0.128338 |
| 28 | 6 | 0 | 4.746143 | -3.027827 | 0.166895 |
| 29 | 6 | 0 | 5.055776 | -1.664063 | 0.244193 |
| 30 | 1 | 0 | -5.761599 | -0.000011 | -0.380943 |
| 31 | 1 | 0 | -0.912868 | 2.556864 | 0.547345 |
| 32 | 1 | 0 | -2.161323 | 4.619962 | 0.294123 |
| 33 | 1 | 0 | -4.609022 | 4.585225 | -0.175831 |
| 34 | 1 | 0 | -5.787138 | 2.428009 | -0.386838 |
| 35 | 1 | 0 | -5.787126 | -2.428031 | -0.386811 |
| 36 | 1 | 0 | -4.609000 | -4.585238 | -0.175781 |
| 37 | 1 | 0 | -2.161301 | -4.619958 | 0.294171 |
| 38 | 1 | 0 | -0.912855 | -2.556853 | 0.547371 |
| 39 | 1 | 0 | -0.129897 | 0.866112 | 1.216850 |
| 40 | 1 | 0 | -0.129892 | -0.866089 | 1.216856 |
| 41 | 1 | 0 | 0.132943 | -0.876411 | -1.290126 |
| 42 | 1 | 0 | 0.132945 | 0.876423 | -1.290127 |
| 43 | 1 | 0 | 6.069355 | 1.350316 | 0.470074 |
| 44 | 1 | 0 | 5.524135 | 3.763902 | 0.334856 |
| 45 | 1 | 0 | 3.231060 | 4.512934 | -0.188569 |
| 46 | 1 | 0 | 1.426148 | 2.867414 | -0.587415 |
| 47 | 1 | 0 | 1.426146 | -2.867403 | -0.587453 |
| 48 | 1 | 0 | 3.231057 | -4.512929 | -0.188631 |
| 49 | 1 | 0 | 5.524133 | -3.763906 | 0.334804 |
| 50 | 1 | 0 | 6.069354 | -1.350323 | 0.470055 |

R=Sat-PhO

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -1.749514 | 1.223910 | -0.206499 |
| 2 | 6 | 0 | -3.171710 | 1.216931 | 0.045854 |
| 3 | 6 | 0 | -3.842872 | 0.000004 | 0.161749 |
| 4 | 6 | 0 | -3.171715 | -1.216926 | 0.045855 |
| 5 | 6 | 0 | -1.749519 | -1.223911 | -0.206498 |
| 6 | 6 | 0 | -1.052083 | -0.000002 | -0.341998 |
| 7 | 6 | 0 | -1.111836 | 2.503397 | -0.303391 |
| 8 | 6 | 0 | -1.814191 | 3.669172 | -0.168334 |
| 9 | 6 | 0 | -3.214578 | 3.651017 | 0.073863 |
| 10 | 6 | 0 | -3.868685 | 2.457426 | 0.176091 |
| 11 | 6 | 0 | -3.868695 | -2.457418 | 0.176091 |
| 12 | 6 | 0 | -3.214592 | -3.651011 | 0.073864 |
| 13 | 6 | 0 | -1.814206 | -3.669172 | -0.168333 |
| 14 | 6 | 0 | -1.111846 | -2.503400 | -0.303389 |
| 15 | 6 | 0 | 0.441457 | -0.000005 | -0.591494 |
| 16 | 6 | 0 | 1.271361 | 0.000004 | 0.727166 |
| 17 | 6 | 0 | 2.753149 | 0.000001 | 0.471399 |
| 18 | 6 | 0 | 3.460510 | -1.217243 | 0.327632 |
| 19 | 6 | 0 | 4.804517 | -1.233807 | 0.050774 |
| 20 | 6 | 0 | 5.553696 | -0.000005 | -0.106248 |
| 21 | 6 | 0 | 4.804521 | 1.233801 | 0.050772 |
| 22 | 6 | 0 | 3.460515 | 1.217242 | 0.327631 |
| 23 | 8 | 0 | 6.778191 | -0.000007 | -0.358812 |
| 24 | 1 | 0 | -4.911675 | 0.000006 | 0.351684 |
| 25 | 1 | 0 | -0.047410 | 2.558179 | -0.487394 |
| 26 | 1 | 0 | -1.299332 | 4.620054 | -0.248083 |
| 27 | 1 | 0 | -3.754983 | 4.585098 | 0.175702 |
| 28 | 1 | 0 | -4.937363 | 2.427703 | 0.361013 |
| 29 | 1 | 0 | -4.937373 | -2.427691 | 0.361013 |
| 30 | 1 | 0 | -3.755001 | -4.585090 | 0.175703 |
| 31 | 1 | 0 | -1.299350 | -4.620056 | -0.248082 |
| 32 | 1 | 0 | -0.047419 | -2.558186 | -0.487393 |
| 33 | 1 | 0 | 0.728846 | -0.866332 | -1.188963 |
| 34 | 1 | 0 | 0.728847 | 0.866314 | -1.188974 |
| 35 | 1 | 0 | 0.993316 | 0.878765 | 1.315636 |
| 36 | 1 | 0 | 0.993315 | -0.878750 | 1.315648 |
| 37 | 1 | 0 | 2.921695 | -2.152025 | 0.449508 |
| 38 | 1 | 0 | 5.357270 | -2.159925 | -0.055686 |
| 39 | 1 | 0 | 5.357278 | 2.159917 | -0.055689 |
| 40 | 1 | 0 | 2.921703 | 2.152026 | 0.449506 |

R=Sat-NO

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -0.437824 | -1.252125 | 0.184890 |
| 2 | 6 | 0 | -1.833584 | -1.518100 | -0.070321 |
| 3 | 6 | 0 | -2.726368 | -0.451941 | -0.183069 |
| 4 | 6 | 0 | -2.301554 | 0.871183 | -0.065870 |
| 5 | 6 | 0 | -0.907696 | 1.151304 | 0.191872 |
| 6 | 6 | 0 | 0.008571 | 0.083144 | 0.333196 |
| 7 | 6 | 0 | 0.442013 | -2.380476 | 0.272006 |
| 8 | 6 | 0 | -0.022709 | -3.659308 | 0.130158 |
| 9 | 6 | 0 | -1.401111 | -3.912651 | -0.106711 |
| 10 | 6 | 0 | -2.276589 | -2.869715 | -0.204396 |
| 11 | 6 | 0 | -3.222449 | 1.955783 | -0.198993 |
| 12 | 6 | 0 | -2.809274 | 3.252633 | -0.096916 |
| 13 | 6 | 0 | -1.438420 | 3.539210 | 0.147135 |
| 14 | 6 | 0 | -0.526810 | 2.529454 | 0.286719 |
| 15 | 6 | 0 | 1.470934 | 0.348893 | 0.612270 |
| 16 | 6 | 0 | 2.326218 | 0.385518 | -0.676103 |
| 17 | 7 | 0 | 3.760886 | 0.357807 | -0.379202 |
| 18 | 6 | 0 | 4.509021 | 1.598227 | -0.187173 |
| 19 | 8 | 0 | 4.226670 | -0.707241 | 0.154728 |
| 20 | 1 | 0 | -3.775462 | -0.656771 | -0.372926 |
| 21 | 1 | 0 | 1.500461 | -2.227132 | 0.437486 |
| 22 | 1 | 0 | 0.668941 | -4.491453 | 0.197587 |
| 23 | 1 | 0 | -1.749465 | -4.933848 | -0.211901 |
| 24 | 1 | 0 | -3.330726 | -3.048441 | -0.389207 |
| 25 | 1 | 0 | -4.265150 | 1.722106 | -0.387311 |
| 26 | 1 | 0 | -3.518407 | 4.065811 | -0.201501 |
| 27 | 1 | 0 | -1.114977 | 4.571335 | 0.223768 |
| 28 | 1 | 0 | 0.508242 | 2.786553 | 0.468512 |
| 29 | 1 | 0 | 1.597375 | 1.282949 | 1.161457 |
| 30 | 1 | 0 | 1.885273 | -0.432872 | 1.249556 |
| 31 | 1 | 0 | 2.115543 | -0.495590 | -1.284760 |
| 32 | 1 | 0 | 2.104428 | 1.274362 | -1.271255 |
| 33 | 1 | 0 | 5.567695 | 1.359542 | -0.277389 |
| 34 | 1 | 0 | 4.226054 | 2.329389 | -0.946666 |
| 35 | 1 | 0 | 4.326405 | 2.021141 | 0.808957 |

R=Sat-Allyl

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 0.634884 | 1.223019 | 0.206077 |
| 2 | 6 | 0 | 2.050042 | 1.216554 | -0.083708 |
| 3 | 6 | 0 | 2.718620 | -0.000005 | -0.216947 |
| 4 | 6 | 0 | 2.050037 | -1.216561 | -0.083708 |
| 5 | 6 | 0 | 0.634879 | -1.223021 | 0.206077 |
| 6 | 6 | 0 | -0.060160 | 0.000001 | 0.360933 |
| 7 | 6 | 0 | -0.001092 | 2.502254 | 0.319035 |
| 8 | 6 | 0 | 0.696520 | 3.668460 | 0.165544 |
| 9 | 6 | 0 | 2.090432 | 3.650881 | -0.112643 |
| 10 | 6 | 0 | 2.742447 | 2.457749 | -0.232108 |
| 11 | 6 | 0 | 2.742436 | -2.457759 | -0.232108 |
| 12 | 6 | 0 | 2.090417 | -3.650888 | -0.112642 |
| 13 | 6 | 0 | 0.696505 | -3.668461 | 0.165546 |
| 14 | 6 | 0 | -0.001102 | -2.502253 | 0.319037 |
| 15 | 6 | 0 | -1.546588 | 0.000003 | 0.654808 |
| 16 | 6 | 0 | -2.421805 | 0.000004 | -0.624602 |
| 17 | 6 | 0 | -3.908495 | 0.000006 | -0.307552 |
| 18 | 6 | 0 | -4.568114 | -1.211240 | -0.152024 |
| 19 | 6 | 0 | -4.568111 | 1.211253 | -0.152016 |
| 20 | 1 | 0 | 3.782271 | -0.000007 | -0.434280 |
| 21 | 1 | 0 | -1.061046 | 2.554378 | 0.527478 |
| 22 | 1 | 0 | 0.183034 | 4.619101 | 0.257112 |
| 23 | 1 | 0 | 2.627647 | 4.585283 | -0.228842 |
| 24 | 1 | 0 | 3.805947 | 2.428807 | -0.445422 |
| 25 | 1 | 0 | 3.805937 | -2.428822 | -0.445422 |
| 26 | 1 | 0 | 2.627628 | -4.585293 | -0.228841 |
| 27 | 1 | 0 | 0.183015 | -4.619100 | 0.257116 |
| 28 | 1 | 0 | -1.061056 | -2.554372 | 0.527482 |
| 29 | 1 | 0 | -1.812723 | -0.865660 | 1.263738 |
| 30 | 1 | 0 | -1.812720 | 0.865667 | 1.263739 |
| 31 | 1 | 0 | -2.171162 | 0.876547 | -1.228326 |
| 32 | 1 | 0 | -2.171165 | -0.876540 | -1.228326 |
| 33 | 1 | 0 | -5.620027 | -1.247514 | 0.106425 |
| 34 | 1 | 0 | -4.058035 | -2.156193 | -0.296044 |
| 35 | 1 | 0 | -5.620023 | 1.247529 | 0.106435 |
| 36 | 1 | 0 | -4.058030 | 2.156206 | -0.296029 |

R=Sat-IN

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 2.297017 | -1.199877 | 0.161811 |
| 2 | 6 | 0 | 3.716735 | -1.338938 | -0.062763 |
| 3 | 6 | 0 | 4.512437 | -0.196934 | -0.156710 |
| 4 | 6 | 0 | 3.967381 | 1.082645 | -0.053044 |
| 5 | 6 | 0 | 2.548752 | 1.235427 | 0.173553 |
| 6 | 6 | 0 | 1.730647 | 0.089094 | 0.300717 |
| 7 | 6 | 0 | 1.518785 | -2.402398 | 0.225840 |
| 8 | 6 | 0 | 2.099965 | -3.633747 | 0.093293 |
| 9 | 6 | 0 | 3.500999 | -3.762394 | -0.110482 |
| 10 | 6 | 0 | 4.281902 | -2.645296 | -0.186948 |
| 11 | 6 | 0 | 4.788310 | 2.246469 | -0.169455 |
| 12 | 6 | 0 | 4.255381 | 3.500150 | -0.083162 |
| 13 | 6 | 0 | 2.858371 | 3.660906 | 0.125906 |
| 14 | 6 | 0 | 2.039426 | 2.572795 | 0.250650 |
| 15 | 6 | 0 | 0.246588 | 0.231785 | 0.565888 |
| 16 | 6 | 0 | -0.596252 | 0.274922 | -0.735387 |
| 17 | 6 | 0 | -2.060986 | 0.339772 | -0.451110 |
| 18 | 7 | 0 | -2.721942 | -0.803487 | 0.022176 |
| 19 | 6 | 0 | -4.200445 | -0.553526 | 0.030253 |
| 20 | 6 | 0 | -4.180668 | 1.024211 | -0.063433 |

| | | | | | |
|---|---|---|---|---|---|
| 21 | 7 | 0 | -2.822997 | 1.363644 | -0.576628 |
| 22 | 6 | 0 | -5.231657 | 1.618321 | -1.006403 |
| 23 | 6 | 0 | -4.295879 | 1.711263 | 1.310608 |
| 24 | 6 | 0 | -4.818649 | -1.166654 | 1.286039 |
| 25 | 6 | 0 | -4.765148 | -1.254252 | -1.218337 |
| 26 | 8 | 0 | -2.197572 | -1.941479 | 0.213554 |
| 27 | 1 | 0 | 5.579847 | -0.306525 | -0.322255 |
| 28 | 1 | 0 | 0.446637 | -2.345291 | 0.363326 |
| 29 | 1 | 0 | 1.483928 | -4.524716 | 0.141541 |
| 30 | 1 | 0 | 3.941764 | -4.748119 | -0.208390 |
| 31 | 1 | 0 | 5.351789 | -2.728533 | -0.347793 |
| 32 | 1 | 0 | 5.852161 | 2.108906 | -0.332971 |
| 33 | 1 | 0 | 4.889348 | 4.374665 | -0.175760 |
| 34 | 1 | 0 | 2.439329 | 4.659205 | 0.185155 |
| 35 | 1 | 0 | 0.980182 | 2.734375 | 0.399933 |
| 36 | 1 | 0 | -0.101684 | -0.597495 | 1.181293 |
| 37 | 1 | 0 | 0.048440 | 1.136837 | 1.141840 |
| 38 | 1 | 0 | -0.332255 | 1.149953 | -1.330138 |
| 39 | 1 | 0 | -0.388328 | -0.621212 | -1.325943 |
| 40 | 1 | 0 | -5.117518 | 2.703873 | -1.025367 |
| 41 | 1 | 0 | -5.116214 | 1.256264 | -2.027873 |
| 42 | 1 | 0 | -6.244729 | 1.385940 | -0.665389 |
| 43 | 1 | 0 | -5.288172 | 1.570090 | 1.746277 |
| 44 | 1 | 0 | -3.549475 | 1.334751 | 2.013066 |
| 45 | 1 | 0 | -4.122834 | 2.781373 | 1.183224 |
| 46 | 1 | 0 | -4.643680 | -2.244066 | 1.282377 |
| 47 | 1 | 0 | -4.387397 | -0.760560 | 2.200482 |
| 48 | 1 | 0 | -5.897249 | -0.992606 | 1.301247 |
| 49 | 1 | 0 | -5.848597 | -1.134074 | -1.276979 |
| 50 | 1 | 0 | -4.321861 | -0.864640 | -2.136494 |
| 51 | 1 | 0 | -4.536353 | -2.320117 | -1.155610 |

R=Sat-Phen

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 3.085611 | 1.223100 | -0.211579 |
| 2 | 6 | 0 | 4.514447 | 1.216557 | 0.000630 |
| 3 | 6 | 0 | 5.189194 | -0.000020 | 0.097473 |
| 4 | 6 | 0 | 4.514428 | -1.216586 | 0.000619 |
| 5 | 6 | 0 | 3.085591 | -1.223105 | -0.211589 |
| 6 | 6 | 0 | 2.383128 | 0.000004 | -0.327638 |
| 7 | 6 | 0 | 2.444780 | 2.502439 | -0.290409 |
| 8 | 6 | 0 | 3.149880 | 3.668588 | -0.175461 |
| 9 | 6 | 0 | 4.556761 | 3.650877 | 0.026918 |
| 10 | 6 | 0 | 5.214076 | 2.457645 | 0.111032 |
| 11 | 6 | 0 | 5.214038 | -2.457686 | 0.111009 |
| 12 | 6 | 0 | 4.556705 | -3.650906 | 0.026885 |
| 13 | 6 | 0 | 3.149823 | -3.668594 | -0.175492 |
| 14 | 6 | 0 | 2.444741 | -2.502434 | -0.290429 |
| 15 | 6 | 0 | 0.882537 | 0.000019 | -0.536493 |
| 16 | 6 | 0 | 0.082468 | 0.000048 | 0.793525 |
| 17 | 6 | 0 | -1.413683 | 0.000033 | 0.571665 |
| 18 | 6 | 0 | -2.112241 | 1.201729 | 0.450223 |
| 19 | 6 | 0 | -3.505703 | 1.234214 | 0.202239 |
| 20 | 6 | 0 | -4.212032 | 0.000003 | 0.075077 |
| 21 | 6 | 0 | -3.505682 | -1.234192 | 0.202270 |
| 22 | 6 | 0 | -2.112221 | -1.201679 | 0.450250 |
| 23 | 6 | 0 | -5.618796 | -0.000011 | -0.173010 |
| 24 | 6 | 0 | -6.290067 | -1.242010 | -0.290523 |
| 25 | 6 | 0 | -5.595714 | -2.439657 | -0.164556 |
| 26 | 6 | 0 | -4.227134 | -2.447485 | 0.078855 |
| 27 | 6 | 0 | -4.227173 | 2.447491 | 0.078791 |
| 28 | 6 | 0 | -5.595754 | 2.439635 | -0.164621 |
| 29 | 6 | 0 | -6.290087 | 1.241974 | -0.290557 |
| 30 | 1 | 0 | 6.263055 | -0.000029 | 0.256791 |
| 31 | 1 | 0 | 1.375280 | 2.554848 | -0.442335 |
| 32 | 1 | 0 | 2.632444 | 4.619305 | -0.239940 |
| 33 | 1 | 0 | 5.099625 | 4.585207 | 0.113521 |
| 34 | 1 | 0 | 6.287592 | 2.428549 | 0.266158 |
| 35 | 1 | 0 | 6.287554 | -2.428607 | 0.266135 |
| 36 | 1 | 0 | 5.099555 | -4.585245 | 0.113479 |
| 37 | 1 | 0 | 2.632373 | -4.619303 | -0.239979 |
| 38 | 1 | 0 | 1.375239 | -2.554825 | -0.442353 |
| 39 | 1 | 0 | 0.581267 | 0.865522 | -1.128910 |
| 40 | 1 | 0 | 0.581244 | -0.865491 | -1.128887 |
| 41 | 1 | 0 | 0.370899 | -0.876373 | 1.380892 |
| 42 | 1 | 0 | 0.370888 | 0.876503 | 1.380847 |
| 43 | 1 | 0 | -1.582219 | 2.143488 | 0.557004 |
| 44 | 1 | 0 | -1.582183 | -2.143426 | 0.557049 |
| 45 | 1 | 0 | -7.357971 | -1.246884 | -0.479709 |
| 46 | 1 | 0 | -6.128419 | -3.379761 | -0.256674 |
| 47 | 1 | 0 | -3.695615 | -3.387884 | 0.176444 |
| 48 | 1 | 0 | -3.695670 | 3.387901 | 0.176356 |
| 49 | 1 | 0 | -6.128474 | 3.379728 | -0.256764 |
| 50 | 1 | 0 | -7.357991 | 1.246825 | -0.479743 |

R=Sat-Ver

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 3.725928 | 1.223760 | -0.239968 |
| 2 | 6 | 0 | 5.157919 | 1.217073 | -0.051322 |
| 3 | 6 | 0 | 5.834122 | -0.000006 | 0.031497 |
| 4 | 6 | 0 | 5.157922 | -1.217086 | -0.051339 |
| 5 | 6 | 0 | 3.725932 | -1.223775 | -0.239986 |
| 6 | 6 | 0 | 3.025247 | -0.000007 | -0.351978 |
| 7 | 6 | 0 | 3.079582 | 2.501642 | -0.298681 |
| 8 | 6 | 0 | 3.786114 | 3.667695 | -0.190805 |
| 9 | 6 | 0 | 5.197047 | 3.650943 | -0.017915 |
| 10 | 6 | 0 | 5.858071 | 2.458591 | 0.049593 |
| 11 | 6 | 0 | 5.858078 | -2.458603 | 0.049561 |
| 12 | 6 | 0 | 5.197057 | -3.650956 | -0.017963 |
| 13 | 6 | 0 | 3.786124 | -3.667711 | -0.190856 |
| 14 | 6 | 0 | 3.079590 | -2.501657 | -0.298717 |
| 15 | 6 | 0 | 1.525899 | -0.000007 | -0.563133 |
| 16 | 6 | 0 | 0.726762 | -0.000014 | 0.763793 |
| 17 | 6 | 0 | -0.759271 | -0.000006 | 0.516750 |
| 18 | 7 | 0 | -1.338652 | 1.186355 | 0.388859 |
| 19 | 7 | 0 | -2.678817 | 1.171743 | 0.110833 |
| 20 | 6 | 0 | -3.443730 | 0.000007 | 0.000211 |
| 21 | 7 | 0 | -2.678830 | -1.171739 | 0.110841 |
| 22 | 7 | 0 | -1.338665 | -1.186362 | 0.388865 |
| 23 | 6 | 0 | -3.296233 | -2.468050 | 0.062030 |
| 24 | 6 | 0 | -2.786763 | -3.474634 | 0.887154 |
| 25 | 6 | 0 | -3.335712 | -4.750857 | 0.840283 |
| 26 | 6 | 0 | -4.390845 | -5.033563 | -0.024399 |
| 27 | 6 | 0 | -4.890681 | -4.027043 | -0.846955 |
| 28 | 6 | 0 | -4.350952 | -2.745000 | -0.812327 |
| 29 | 6 | 0 | -3.296206 | 2.468062 | 0.062014 |
| 30 | 6 | 0 | -4.350908 | 2.745024 | -0.812357 |
| 31 | 6 | 0 | -4.890622 | 4.027074 | -0.846993 |
| 32 | 6 | 0 | -4.390784 | 5.033587 | -0.024429 |
| 33 | 6 | 0 | -3.335666 | 4.750868 | 0.840267 |
| 34 | 6 | 0 | -2.786733 | 3.474638 | 0.887146 |
| 35 | 8 | 0 | -4.640970 | 0.000012 | -0.175702 |
| 36 | 1 | 0 | 6.910855 | -0.000006 | 0.170417 |
| 37 | 1 | 0 | 2.005870 | 2.554023 | -0.420161 |
| 38 | 1 | 0 | 3.265665 | 4.617772 | -0.237034 |
| 39 | 1 | 0 | 5.740144 | 4.585800 | 0.061629 |
| 40 | 1 | 0 | 6.934314 | 2.430732 | 0.184830 |
| 41 | 1 | 0 | 6.934320 | -2.430743 | 0.184800 |
| 42 | 1 | 0 | 5.740156 | -4.585813 | 0.061571 |
| 43 | 1 | 0 | 3.265678 | -4.617788 | -0.237098 |
| 44 | 1 | 0 | 2.005878 | -2.554039 | -0.420200 |
| 45 | 1 | 0 | 1.226382 | 0.868757 | -1.151214 |
| 46 | 1 | 0 | 1.226383 | -0.868766 | -1.151223 |
| 47 | 1 | 0 | 0.986141 | -0.883777 | 1.349307 |
| 48 | 1 | 0 | 0.986151 | 0.883736 | 1.349321 |
| 49 | 1 | 0 | -1.960884 | -3.248864 | 1.546692 |
| 50 | 1 | 0 | -2.937451 | -5.524607 | 1.486555 |
| 51 | 1 | 0 | -4.818923 | -6.028703 | -0.057265 |
| 52 | 1 | 0 | -5.708157 | -4.236255 | -1.527251 |
| 53 | 1 | 0 | -4.751296 | -1.969921 | -1.446751 |
| 54 | 1 | 0 | -4.751252 | 1.969950 | -1.446788 |
| 55 | 1 | 0 | -5.708085 | 4.236296 | -1.527301 |
| 56 | 1 | 0 | -4.818850 | 6.028732 | -0.057300 |
| 57 | 1 | 0 | -2.937405 | 5.524613 | 1.486546 |
| 58 | 1 | 0 | -1.960866 | 3.248858 | 1.546694 |

R=Sat-NN

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 2.573544 | -3.663227 | 0.024939 |
| 2 | 6 | 0 | 3.983346 | -3.651065 | -0.158291 |
| 3 | 6 | 0 | 4.652976 | -2.462177 | -0.200334 |
| 4 | 6 | 0 | 3.962445 | -1.219292 | -0.059125 |
| 5 | 6 | 0 | 2.533425 | -1.223446 | 0.149675 |
| 6 | 6 | 0 | 1.875178 | -2.496758 | 0.175199 |
| 7 | 6 | 0 | 4.643798 | -0.003445 | -0.120818 |
| 8 | 6 | 0 | 3.974875 | 1.215473 | -0.006704 |
| 9 | 6 | 0 | 2.545859 | 1.225149 | 0.202091 |
| 10 | 6 | 0 | 1.845171 | 0.001585 | 0.308203 |
| 11 | 6 | 0 | 4.678066 | 2.456209 | -0.094423 |
| 12 | 6 | 0 | 4.020704 | 3.649033 | -0.001498 |
| 13 | 6 | 0 | 2.610980 | 3.667744 | 0.181828 |
| 14 | 6 | 0 | 1.900994 | 2.502967 | 0.281831 |
| 15 | 6 | 0 | 0.356906 | 0.002765 | 0.579198 |
| 16 | 6 | 0 | -0.495044 | 0.033245 | -0.717958 |
| 17 | 6 | 0 | -1.945083 | 0.017064 | -0.418489 |
| 18 | 7 | 0 | -2.705075 | 1.113975 | -0.245852 |
| 19 | 6 | 0 | -4.167970 | 0.755286 | -0.111114 |
| 20 | 6 | 0 | -4.071687 | -0.773833 | 0.245540 |
| 21 | 7 | 0 | -2.673397 | -1.097636 | -0.230032 |
| 22 | 6 | 0 | -4.083132 | -1.074748 | 1.753115 |
| 23 | 6 | 0 | -5.066831 | -1.685519 | -0.470278 |
| 24 | 6 | 0 | -4.801008 | 1.049677 | -1.480942 |
| 25 | 6 | 0 | -4.805943 | 1.645069 | 0.954076 |
| 26 | 8 | 0 | -2.311417 | 2.321038 | -0.336479 |
| 27 | 8 | 0 | -2.238945 | -2.293959 | -0.274838 |
| 28 | 1 | 0 | 2.045529 | -4.610038 | 0.041014 |
| 29 | 1 | 0 | 4.518790 | -4.587153 | -0.269883 |
| 30 | 1 | 0 | 5.727788 | -2.438259 | -0.347522 |
| 31 | 1 | 0 | 0.800107 | -2.546589 | 0.291414 |
| 32 | 1 | 0 | 5.719095 | -0.005686 | -0.270998 |
| 33 | 1 | 0 | 5.752646 | 2.427624 | -0.242465 |
| 34 | 1 | 0 | 4.565726 | 4.583512 | -0.072811 |
| 35 | 1 | 0 | 2.092604 | 4.618323 | 0.238229 |

```
   36         1          0       0.826454    2.558492    0.399573
   37         1          0       0.080093   -0.879933    1.156705
   38         1          0       0.087643    0.862533    1.193834
   39         1          0      -0.274115    0.937199   -1.288261
   40         1          0      -0.265433   -0.841075   -1.330106
   41         1          0      -5.074254   -0.904858    2.177836
   42         1          0      -3.815350   -2.122398    1.896828
   43         1          0      -3.360947   -0.461777    2.295520
   44         1          0      -4.820509   -2.722254   -0.240446
   45         1          0      -6.082816   -1.482012   -0.123735
   46         1          0      -5.034493   -1.566578   -1.552539
   47         1          0      -4.636956    2.102299   -1.716172
   48         1          0      -4.350908    0.450154   -2.274208
   49         1          0      -5.875591    0.858124   -1.464293
   50         1          0      -4.706498    2.686342    0.647494
   51         1          0      -5.868077    1.409924    1.055685
   52         1          0      -4.327745    1.536538    1.926701
-----------------------------------------------------------------
```

# 5-3. Pentacenes(**Pn**)

## Non-Radical

R=$NO_2$

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 6.118856 | -0.292413 | -0.000005 |
| 2 | 6 | 0 | 6.103304 | -1.722374 | -0.000004 |
| 3 | 6 | 0 | 4.921932 | -2.401148 | -0.000001 |
| 4 | 6 | 0 | 3.671828 | -1.699443 | 0.000000 |
| 5 | 6 | 0 | 3.687169 | -0.249592 | -0.000001 |
| 6 | 6 | 0 | 4.954499 | 0.417291 | -0.000004 |
| 7 | 6 | 0 | 2.450751 | -2.355830 | 0.000002 |
| 8 | 6 | 0 | 1.226906 | -1.650976 | 0.000002 |
| 9 | 6 | 0 | 1.242490 | -0.200307 | 0.000001 |
| 10 | 6 | 0 | 2.486544 | 0.453743 | 0.000000 |
| 11 | 6 | 0 | 0.000002 | -2.323842 | 0.000003 |
| 12 | 6 | 0 | -1.226904 | -1.650977 | 0.000003 |
| 13 | 6 | 0 | -1.242489 | -0.200308 | 0.000000 |
| 14 | 6 | 0 | 0.000001 | 0.502053 | 0.000001 |
| 15 | 6 | 0 | -2.450748 | -2.355831 | 0.000003 |
| 16 | 6 | 0 | -3.671826 | -1.699446 | 0.000001 |
| 17 | 6 | 0 | -3.687168 | -0.249595 | -0.000001 |
| 18 | 6 | 0 | -2.486543 | 0.453741 | -0.000002 |
| 19 | 6 | 0 | -4.921929 | -2.401152 | 0.000002 |
| 20 | 6 | 0 | -6.103302 | -1.722378 | -0.000001 |
| 21 | 6 | 0 | -6.118854 | -0.292418 | -0.000004 |
| 22 | 6 | 0 | -4.954498 | 0.417287 | -0.000004 |
| 23 | 6 | 0 | 0.000000 | 1.907401 | 0.000001 |
| 24 | 6 | 0 | -0.000003 | 3.117123 | 0.000000 |
| 25 | 7 | 0 | -0.000005 | 4.498470 | 0.000002 |
| 26 | 8 | 0 | -1.095956 | 5.060328 | -0.000016 |
| 27 | 8 | 0 | 1.095946 | 5.060330 | 0.000019 |
| 28 | 1 | 0 | 7.070904 | 0.225920 | -0.000007 |
| 29 | 1 | 0 | 7.043150 | -2.262349 | -0.000005 |
| 30 | 1 | 0 | 4.906633 | -3.485814 | 0.000000 |
| 31 | 1 | 0 | 4.967652 | 1.501657 | -0.000004 |
| 32 | 1 | 0 | 2.426419 | -3.440921 | 0.000002 |
| 33 | 1 | 0 | 2.512581 | 1.537190 | -0.000002 |
| 34 | 1 | 0 | 0.000002 | -3.409544 | 0.000005 |
| 35 | 1 | 0 | -2.426415 | -3.440923 | 0.000005 |
| 36 | 1 | 0 | -2.512581 | 1.537189 | -0.000003 |
| 37 | 1 | 0 | -4.906629 | -3.485817 | 0.000004 |
| 38 | 1 | 0 | -7.043147 | -2.262354 | 0.000000 |
| 39 | 1 | 0 | -7.070903 | 0.225915 | -0.000006 |
| 40 | 1 | 0 | -4.967652 | 1.501654 | -0.000006 |

R=CN

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 6.119629 | 0.021567 | 0.000004 |
| 2 | 6 | 0 | 6.103547 | 1.451968 | -0.000001 |
| 3 | 6 | 0 | 4.922205 | 2.130354 | -0.000004 |
| 4 | 6 | 0 | 3.671596 | 1.428891 | -0.000002 |
| 5 | 6 | 0 | 3.687314 | -0.021185 | 0.000003 |
| 6 | 6 | 0 | 4.955530 | -0.687754 | 0.000006 |
| 7 | 6 | 0 | 2.450889 | 2.084928 | -0.000004 |
| 8 | 6 | 0 | 1.225585 | 1.381849 | -0.000002 |
| 9 | 6 | 0 | 1.241034 | -0.069295 | 0.000002 |
| 10 | 6 | 0 | 2.487029 | -0.722937 | 0.000005 |
| 11 | 6 | 0 | 0.000001 | 2.056145 | -0.000005 |
| 12 | 6 | 0 | -1.225584 | 1.381850 | -0.000002 |
| 13 | 6 | 0 | -1.241033 | -0.069295 | 0.000002 |
| 14 | 6 | 0 | 0.000000 | -0.771437 | 0.000004 |
| 15 | 6 | 0 | -2.450888 | 2.084929 | -0.000004 |
| 16 | 6 | 0 | -3.671595 | 1.428892 | -0.000002 |
| 17 | 6 | 0 | -3.687313 | -0.021184 | 0.000003 |
| 18 | 6 | 0 | -2.487028 | -0.722936 | 0.000005 |
| 19 | 6 | 0 | -4.922204 | 2.130355 | -0.000004 |
| 20 | 6 | 0 | -6.103546 | 1.451969 | -0.000001 |
| 21 | 6 | 0 | -6.119629 | 0.021569 | 0.000004 |
| 22 | 6 | 0 | -4.955530 | -0.687753 | 0.000006 |
| 23 | 6 | 0 | 0.000000 | -2.180414 | 0.000008 |
| 24 | 6 | 0 | -0.000002 | -3.395653 | 0.000003 |
| 25 | 6 | 0 | -0.000004 | -4.757700 | -0.000007 |
| 26 | 7 | 0 | -0.000003 | -5.918962 | -0.000016 |
| 27 | 1 | 0 | 7.071854 | -0.496480 | 0.000006 |
| 28 | 1 | 0 | 7.043292 | 1.992171 | -0.000003 |
| 29 | 1 | 0 | 4.906833 | 3.215044 | -0.000008 |
| 30 | 1 | 0 | 4.969301 | -1.772229 | 0.000010 |
| 31 | 1 | 0 | 2.426980 | 3.170054 | -0.000008 |
| 32 | 1 | 0 | 2.513665 | -1.806210 | 0.000009 |
| 33 | 1 | 0 | 0.000001 | 3.141681 | -0.000009 |
| 34 | 1 | 0 | -2.426978 | 3.170054 | -0.000008 |
| 35 | 1 | 0 | -2.513665 | -1.806210 | 0.000009 |
| 36 | 1 | 0 | -4.906831 | 3.215045 | -0.000008 |
| 37 | 1 | 0 | -7.043291 | 1.992173 | -0.000003 |
| 38 | 1 | 0 | -7.071853 | -0.496478 | 0.000006 |
| 39 | 1 | 0 | -4.969301 | -1.772228 | 0.000010 |

R=Cl

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 6.117653 | -0.102340 | -0.000009 |
| 2 | 6 | 0 | 6.104579 | -1.533399 | -0.000003 |
| 3 | 6 | 0 | 4.925100 | -2.214866 | 0.000003 |
| 4 | 6 | 0 | 3.671237 | -1.518250 | 0.000000 |
| 5 | 6 | 0 | 3.683765 | -0.067551 | -0.000005 |
| 6 | 6 | 0 | 4.951288 | 0.602367 | -0.000009 |
| 7 | 6 | 0 | 2.453031 | -2.178279 | 0.000003 |
| 8 | 6 | 0 | 1.223508 | -1.481391 | 0.000003 |
| 9 | 6 | 0 | 1.235548 | -0.029178 | -0.000005 |
| 10 | 6 | 0 | 2.482203 | 0.628589 | -0.000009 |
| 11 | 6 | 0 | 0.000018 | -2.158997 | 0.000012 |
| 12 | 6 | 0 | -1.223479 | -1.481402 | 0.000008 |
| 13 | 6 | 0 | -1.235533 | -0.029190 | -0.000001 |
| 14 | 6 | 0 | 0.000004 | 0.674794 | -0.000004 |
| 15 | 6 | 0 | -2.452995 | -2.178300 | 0.000013 |
| 16 | 6 | 0 | -3.671208 | -1.518282 | 0.000005 |
| 17 | 6 | 0 | -3.683749 | -0.067584 | -0.000008 |
| 18 | 6 | 0 | -2.482191 | 0.628567 | -0.000011 |
| 19 | 6 | 0 | -4.925065 | -2.214909 | 0.000010 |
| 20 | 6 | 0 | -6.104550 | -1.533453 | 0.000001 |
| 21 | 6 | 0 | -6.117638 | -0.102394 | -0.000013 |
| 22 | 6 | 0 | -4.951278 | 0.602323 | -0.000018 |
| 23 | 6 | 0 | 0.000002 | 2.094745 | -0.000005 |
| 24 | 6 | 0 | -0.000027 | 3.301734 | -0.000009 |
| 25 | 17 | 0 | -0.000088 | 4.949416 | 0.000018 |
| 26 | 1 | 0 | 7.068670 | 0.418123 | -0.000013 |
| 27 | 1 | 0 | 7.045682 | -2.071554 | 0.000003 |
| 28 | 1 | 0 | 4.913396 | -3.299742 | 0.000015 |
| 29 | 1 | 0 | 4.961095 | 1.687109 | -0.000010 |
| 30 | 1 | 0 | 2.434024 | -3.263654 | 0.000016 |
| 31 | 1 | 0 | 2.500928 | 1.711974 | -0.000003 |
| 32 | 1 | 0 | 0.000021 | -3.244419 | 0.000022 |
| 33 | 1 | 0 | -2.433979 | -3.263675 | 0.000022 |
| 34 | 1 | 0 | -2.500923 | 1.711951 | -0.000021 |
| 35 | 1 | 0 | -4.913350 | -3.299785 | 0.000020 |
| 36 | 1 | 0 | -7.045649 | -2.071616 | 0.000004 |
| 37 | 1 | 0 | -7.068659 | 0.418058 | -0.000021 |
| 38 | 1 | 0 | -4.961095 | 1.687065 | -0.000029 |

R=H

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 6.117512 | -0.402420 | 0.000000 |
| 2 | 6 | 0 | 6.104439 | 1.028695 | 0.000000 |
| 3 | 6 | 0 | 4.924956 | 1.710122 | 0.000000 |
| 4 | 6 | 0 | 3.671001 | 1.013580 | 0.000000 |
| 5 | 6 | 0 | 3.683373 | -0.437203 | 0.000000 |
| 6 | 6 | 0 | 4.951116 | -1.106999 | 0.000000 |
| 7 | 6 | 0 | 2.452882 | 1.673652 | 0.000000 |
| 8 | 6 | 0 | 1.223465 | 0.976520 | 0.000000 |
| 9 | 6 | 0 | 1.235315 | -0.475820 | 0.000000 |
| 10 | 6 | 0 | 2.482202 | -1.133838 | 0.000000 |
| 11 | 6 | 0 | 0.000000 | 1.654053 | 0.000000 |
| 12 | 6 | 0 | -1.223465 | 0.976520 | 0.000000 |
| 13 | 6 | 0 | -1.235315 | -0.475820 | 0.000000 |
| 14 | 6 | 0 | 0.000000 | -1.179333 | 0.000000 |
| 15 | 6 | 0 | -2.452882 | 1.673652 | 0.000000 |
| 16 | 6 | 0 | -3.671001 | 1.013580 | 0.000000 |
| 17 | 6 | 0 | -3.683373 | -0.437203 | 0.000000 |
| 18 | 6 | 0 | -2.482202 | -1.133838 | 0.000000 |
| 19 | 6 | 0 | -4.924955 | 1.710123 | 0.000000 |
| 20 | 6 | 0 | -6.104438 | 1.028696 | 0.000000 |
| 21 | 6 | 0 | -6.117512 | -0.402420 | 0.000001 |
| 22 | 6 | 0 | -4.951116 | -1.106999 | 0.000001 |
| 23 | 6 | 0 | -0.000001 | -2.601147 | -0.000001 |
| 24 | 6 | 0 | -0.000002 | -3.807494 | 0.000000 |
| 25 | 1 | 0 | 7.068558 | -0.922881 | 0.000000 |
| 26 | 1 | 0 | 7.045547 | 1.566888 | 0.000001 |
| 27 | 1 | 0 | 4.913279 | 2.795021 | 0.000000 |
| 28 | 1 | 0 | 4.960821 | -2.191751 | 0.000000 |
| 29 | 1 | 0 | 2.433823 | 2.759045 | 0.000000 |
| 30 | 1 | 0 | 2.499629 | -2.217174 | 0.000000 |
| 31 | 1 | 0 | 0.000000 | 2.739515 | 0.000000 |
| 32 | 1 | 0 | -2.433823 | 2.759045 | 0.000000 |
| 33 | 1 | 0 | -2.499628 | -2.217174 | 0.000000 |
| 34 | 1 | 0 | -4.913279 | 2.795022 | 0.000000 |
| 35 | 1 | 0 | -7.045547 | 1.566889 | 0.000000 |
| 36 | 1 | 0 | -7.068558 | -0.922880 | 0.000001 |
| 37 | 1 | 0 | -4.960821 | -2.191751 | 0.000001 |
| 38 | 1 | 0 | -0.000005 | -4.869790 | -0.000001 |

R=CHO

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -6.182129 | 0.168349 | -0.000019 |
| 2 | 6 | 0 | -6.220586 | -1.261519 | -0.000011 |
| 3 | 6 | 0 | -5.065649 | -1.984171 | -0.000001 |

| | | | | | |
|---|---|---|---|---|---|
| 4 | 6 | 0 | -3.789116 | -1.331185 | 0.000001 |
| 5 | 6 | 0 | -3.749339 | 0.118413 | -0.000006 |
| 6 | 6 | 0 | -4.991483 | 0.832350 | -0.000016 |
| 7 | 6 | 0 | -2.594180 | -2.033509 | 0.000009 |
| 8 | 6 | 0 | -1.343242 | -1.377342 | 0.000011 |
| 9 | 6 | 0 | -1.302800 | 0.073205 | 0.000004 |
| 10 | 6 | 0 | -2.522793 | 0.773394 | -0.000005 |
| 11 | 6 | 0 | -0.143698 | -2.097762 | 0.000020 |
| 12 | 6 | 0 | 1.106778 | -1.470554 | 0.000015 |
| 13 | 6 | 0 | 1.176208 | -0.021075 | 0.000000 |
| 14 | 6 | 0 | -0.037486 | 0.730393 | 0.000001 |
| 15 | 6 | 0 | 2.304566 | -2.219683 | 0.000021 |
| 16 | 6 | 0 | 3.548726 | -1.608992 | 0.000008 |
| 17 | 6 | 0 | 3.617855 | -0.160472 | -0.000013 |
| 18 | 6 | 0 | 2.444998 | 0.586644 | -0.000015 |
| 19 | 6 | 0 | 4.772843 | -2.355757 | 0.000012 |
| 20 | 6 | 0 | 5.978198 | -1.720800 | -0.000005 |
| 21 | 6 | 0 | 6.046917 | -0.291973 | -0.000028 |
| 22 | 6 | 0 | 4.909449 | 0.459500 | -0.000032 |
| 23 | 6 | 0 | 0.030101 | 2.137143 | 0.000008 |
| 24 | 6 | 0 | 0.144017 | 3.347082 | 0.000008 |
| 25 | 6 | 0 | 0.317105 | 4.768809 | 0.000010 |
| 26 | 8 | 0 | 1.399953 | 5.320153 | 0.000029 |
| 27 | 1 | 0 | -7.113932 | 0.722394 | -0.000028 |
| 28 | 1 | 0 | -7.180162 | -1.765711 | -0.000012 |
| 29 | 1 | 0 | -5.091659 | -3.068702 | 0.000006 |
| 30 | 1 | 0 | -4.963924 | 1.916653 | -0.000023 |
| 31 | 1 | 0 | -2.611991 | -3.118799 | 0.000014 |
| 32 | 1 | 0 | -2.503821 | 1.856843 | -0.000012 |
| 33 | 1 | 0 | -0.185086 | -3.182621 | 0.000030 |
| 34 | 1 | 0 | 2.240361 | -3.303225 | 0.000034 |
| 35 | 1 | 0 | 2.508971 | 1.668326 | -0.000035 |
| 36 | 1 | 0 | 4.718008 | -3.439221 | 0.000029 |
| 37 | 1 | 0 | 6.897527 | -2.295210 | -0.000002 |
| 38 | 1 | 0 | 7.017519 | 0.190814 | -0.000043 |
| 39 | 1 | 0 | 4.961531 | 1.542736 | -0.000050 |
| 40 | 1 | 0 | -0.624520 | 5.351564 | -0.000001 |

R=$SiMe_3$

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -6.127743 | -0.799459 | 0.000000 |
| 2 | 6 | 0 | -6.122545 | -2.230523 | 0.000000 |
| 3 | 6 | 0 | -4.946741 | -2.918409 | 0.000000 |
| 4 | 6 | 0 | -3.689005 | -2.228800 | 0.000000 |
| 5 | 6 | 0 | -3.693389 | -0.778117 | -0.000001 |
| 6 | 6 | 0 | -4.957284 | -0.101442 | -0.000001 |
| 7 | 6 | 0 | -2.474367 | -2.895437 | 0.000000 |
| 8 | 6 | 0 | -1.241183 | -2.204987 | 0.000000 |
| 9 | 6 | 0 | -1.245109 | -0.752777 | -0.000001 |
| 10 | 6 | 0 | -2.487981 | -0.088323 | -0.000001 |
| 11 | 6 | 0 | -0.021614 | -2.889699 | 0.000000 |
| 12 | 6 | 0 | 1.205702 | -2.218970 | 0.000000 |
| 13 | 6 | 0 | 1.226091 | -0.766949 | 0.000000 |
| 14 | 6 | 0 | -0.005502 | -0.053704 | 0.000000 |
| 15 | 6 | 0 | 2.430989 | -2.923338 | 0.000000 |
| 16 | 6 | 0 | 3.653090 | -2.270443 | 0.000000 |
| 17 | 6 | 0 | 3.673880 | -0.819906 | 0.000000 |
| 18 | 6 | 0 | 2.476355 | -0.116456 | 0.000000 |
| 19 | 6 | 0 | 4.902970 | -2.974192 | 0.000000 |
| 20 | 6 | 0 | 6.086438 | -2.299562 | 0.000000 |
| 21 | 6 | 0 | 6.107781 | -0.868647 | -0.000001 |
| 22 | 6 | 0 | 4.945283 | -0.157423 | -0.000001 |
| 23 | 6 | 0 | 0.003653 | 1.364975 | 0.000000 |
| 24 | 6 | 0 | 0.014241 | 2.583066 | 0.000000 |
| 25 | 14 | 0 | 0.039294 | 4.424789 | 0.000001 |
| 26 | 6 | 0 | -0.843593 | 5.043539 | 1.546910 |
| 27 | 6 | 0 | -0.843520 | 5.043539 | -1.546951 |
| 28 | 6 | 0 | 1.836265 | 4.996194 | 0.000041 |
| 29 | 1 | 0 | -7.075878 | -0.273699 | 0.000000 |
| 30 | 1 | 0 | -7.066583 | -2.763576 | 0.000001 |
| 31 | 1 | 0 | -4.941051 | -4.003366 | 0.000001 |
| 32 | 1 | 0 | -4.961073 | 0.983363 | -0.000001 |
| 33 | 1 | 0 | -2.461206 | -3.980932 | 0.000000 |
| 34 | 1 | 0 | -2.498319 | 0.995116 | -0.000002 |
| 35 | 1 | 0 | -0.027834 | -3.975141 | 0.000001 |
| 36 | 1 | 0 | 2.405562 | -4.008617 | 0.000001 |
| 37 | 1 | 0 | 2.499066 | 0.966806 | 0.000000 |
| 38 | 1 | 0 | 4.885075 | -4.059016 | 0.000001 |
| 39 | 1 | 0 | 7.024411 | -2.843226 | 0.000000 |
| 40 | 1 | 0 | 7.061787 | -0.353615 | -0.000001 |
| 41 | 1 | 0 | 4.961176 | 0.927260 | -0.000001 |
| 42 | 1 | 0 | -0.352823 | 4.679867 | 2.453655 |
| 43 | 1 | 0 | -0.845984 | 6.137725 | 1.580476 |
| 44 | 1 | 0 | -1.883017 | 4.705027 | 1.572158 |
| 45 | 1 | 0 | -0.352702 | 4.679873 | -2.453671 |
| 46 | 1 | 0 | -0.845913 | 6.137726 | -1.580514 |
| 47 | 1 | 0 | -1.882942 | 4.705024 | -1.572253 |
| 48 | 1 | 0 | 1.895339 | 6.089191 | 0.000039 |
| 49 | 1 | 0 | 2.366890 | 4.632328 | 0.884180 |
| 50 | 1 | 0 | 2.366932 | 4.632322 | -0.884070 |

R=OMe

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 6.174841 | 0.119209 | -0.000002 |
| 2 | 6 | 0 | 6.214367 | -1.311422 | 0.000001 |
| 3 | 6 | 0 | 5.060976 | -2.036475 | 0.000003 |
| 4 | 6 | 0 | 3.781512 | -1.387758 | 0.000001 |
| 5 | 6 | 0 | 3.740894 | 0.062235 | -0.000002 |
| 6 | 6 | 0 | 4.982467 | 0.779119 | -0.000003 |
| 7 | 6 | 0 | 2.588497 | -2.092428 | 0.000003 |
| 8 | 6 | 0 | 1.332589 | -1.443601 | 0.000001 |
| 9 | 6 | 0 | 1.291862 | 0.008469 | -0.000001 |
| 10 | 6 | 0 | 2.513767 | 0.711824 | -0.000003 |
| 11 | 6 | 0 | 0.136112 | -2.167747 | 0.000003 |
| 12 | 6 | 0 | -1.109295 | -1.531711 | 0.000001 |
| 13 | 6 | 0 | -1.173566 | -0.080365 | -0.000001 |
| 14 | 6 | 0 | 0.033292 | 0.672809 | -0.000002 |
| 15 | 6 | 0 | -2.315164 | -2.269516 | 0.000002 |
| 16 | 6 | 0 | -3.556283 | -1.653653 | 0.000001 |
| 17 | 6 | 0 | -3.621171 | -0.204507 | -0.000002 |
| 18 | 6 | 0 | -2.443807 | 0.531319 | -0.000002 |
| 19 | 6 | 0 | -4.785137 | -2.393805 | 0.000001 |
| 20 | 6 | 0 | -5.988576 | -1.755292 | 0.000000 |
| 21 | 6 | 0 | -6.053316 | -0.325587 | -0.000002 |
| 22 | 6 | 0 | -4.912026 | 0.419222 | -0.000003 |
| 23 | 6 | 0 | -0.012955 | 2.092653 | -0.000004 |
| 24 | 6 | 0 | -0.028968 | 3.300332 | -0.000004 |
| 25 | 8 | 0 | 0.009481 | 4.597594 | -0.000005 |
| 26 | 6 | 0 | -1.277134 | 5.261665 | 0.000013 |
| 27 | 1 | 0 | 7.105862 | 0.674754 | -0.000004 |
| 28 | 1 | 0 | 7.174774 | -1.814611 | 0.000002 |
| 29 | 1 | 0 | 5.090181 | -3.121123 | 0.000005 |
| 30 | 1 | 0 | 4.951167 | 1.863592 | -0.000006 |
| 31 | 1 | 0 | 2.610635 | -3.177858 | 0.000005 |
| 32 | 1 | 0 | 2.491105 | 1.795082 | -0.000005 |
| 33 | 1 | 0 | 0.175152 | -3.252288 | 0.000005 |
| 34 | 1 | 0 | -2.258594 | -3.353693 | 0.000004 |
| 35 | 1 | 0 | -2.499193 | 1.613468 | -0.000004 |
| 36 | 1 | 0 | -4.734981 | -3.477674 | 0.000003 |
| 37 | 1 | 0 | -6.909661 | -2.327202 | 0.000000 |
| 38 | 1 | 0 | -7.022366 | 0.160663 | -0.000004 |
| 39 | 1 | 0 | -4.960952 | 1.503221 | -0.000005 |
| 40 | 1 | 0 | -1.057210 | 6.326693 | 0.000016 |
| 41 | 1 | 0 | -1.837224 | 4.988147 | -0.896652 |
| 42 | 1 | 0 | -1.837203 | 4.988138 | 0.896688 |

R=$NH_2$

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -6.118889 | 0.151111 | -0.015679 |
| 2 | 6 | 0 | -6.106363 | -1.279798 | -0.000627 |
| 3 | 6 | 0 | -4.927190 | -1.962280 | 0.009092 |
| 4 | 6 | 0 | -3.671870 | -1.268007 | 0.004848 |
| 5 | 6 | 0 | -3.684141 | 0.182224 | -0.009335 |
| 6 | 6 | 0 | -4.950694 | 0.853258 | -0.019998 |
| 7 | 6 | 0 | -2.454036 | -1.929097 | 0.012722 |
| 8 | 6 | 0 | -1.221395 | -1.236915 | 0.008017 |
| 9 | 6 | 0 | -1.234020 | 0.215540 | -0.003753 |
| 10 | 6 | 0 | -2.480068 | 0.874004 | -0.012869 |
| 11 | 6 | 0 | -0.000001 | -1.918371 | 0.014662 |
| 12 | 6 | 0 | 1.221393 | -1.236916 | 0.008015 |
| 13 | 6 | 0 | 1.234019 | 0.215539 | -0.003753 |
| 14 | 6 | 0 | 0.000000 | 0.926552 | -0.005854 |
| 15 | 6 | 0 | 2.454033 | -1.929099 | 0.012717 |
| 16 | 6 | 0 | 3.671867 | -1.268010 | 0.004845 |
| 17 | 6 | 0 | 3.684140 | 0.182221 | -0.009333 |
| 18 | 6 | 0 | 2.480067 | 0.874002 | -0.012865 |
| 19 | 6 | 0 | 4.927188 | -1.962284 | 0.009086 |
| 20 | 6 | 0 | 6.106361 | -1.279803 | -0.000629 |
| 21 | 6 | 0 | 6.118887 | 0.151107 | -0.015675 |
| 22 | 6 | 0 | 4.950694 | 0.853255 | -0.019992 |
| 23 | 6 | 0 | 0.000000 | 2.343228 | -0.008145 |
| 24 | 6 | 0 | 0.000005 | 3.554137 | 0.013392 |
| 25 | 7 | 0 | 0.000007 | 4.897378 | -0.038387 |
| 26 | 1 | 0 | -7.069382 | 0.672623 | -0.024099 |
| 27 | 1 | 0 | -7.047792 | -1.817670 | 0.002520 |
| 28 | 1 | 0 | -4.917136 | -3.047237 | 0.019920 |
| 29 | 1 | 0 | -4.959187 | 1.938258 | -0.032222 |
| 30 | 1 | 0 | -2.437707 | -3.014613 | 0.022067 |
| 31 | 1 | 0 | -2.496374 | 1.957517 | -0.025641 |
| 32 | 1 | 0 | -0.000002 | -3.003456 | 0.024395 |
| 33 | 1 | 0 | 2.437703 | -3.014615 | 0.022058 |
| 34 | 1 | 0 | 2.496374 | 1.957516 | -0.025633 |
| 35 | 1 | 0 | 4.917132 | -3.047241 | 0.019910 |
| 36 | 1 | 0 | 7.047790 | -1.817675 | 0.002517 |
| 37 | 1 | 0 | 7.069381 | 0.672618 | -0.024092 |
| 38 | 1 | 0 | 4.959187 | 1.938255 | -0.032211 |
| 39 | 1 | 0 | 0.842282 | 5.355236 | 0.282895 |
| 40 | 1 | 0 | -0.842229 | 5.355242 | 0.282992 |

R=Ph

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 6.119127 | -0.965003 | -0.000028 |
| 2 | 6 | 0 | 6.104749 | -2.395787 | -0.000020 |
| 3 | 6 | 0 | 4.924426 | -3.076125 | -0.000012 |
| 4 | 6 | 0 | 3.671294 | -2.378416 | -0.000011 |
| 5 | 6 | 0 | 3.685061 | -0.928211 | -0.000017 |
| 6 | 6 | 0 | 4.952847 | -0.259645 | -0.000027 |
| 7 | 6 | 0 | 2.451988 | -3.036707 | -0.000004 |
| 8 | 6 | 0 | 1.223293 | -2.338434 | -0.000002 |
| 9 | 6 | 0 | 1.236367 | -0.886484 | -0.000005 |
| 10 | 6 | 0 | 2.483192 | -0.231407 | -0.000015 |
| 11 | 6 | 0 | 0.000000 | -3.016573 | 0.000000 |
| 12 | 6 | 0 | -1.223292 | -2.338434 | 0.000002 |
| 13 | 6 | 0 | -1.236366 | -0.886485 | 0.000005 |
| 14 | 6 | 0 | 0.000000 | -0.177169 | 0.000000 |
| 15 | 6 | 0 | -2.451987 | -3.036707 | 0.000004 |
| 16 | 6 | 0 | -3.671293 | -2.378417 | 0.000011 |
| 17 | 6 | 0 | -3.685060 | -0.928212 | 0.000017 |
| 18 | 6 | 0 | -2.483192 | -0.231408 | 0.000014 |
| 19 | 6 | 0 | -4.924425 | -3.076126 | 0.000013 |
| 20 | 6 | 0 | -6.104748 | -2.395789 | 0.000021 |
| 21 | 6 | 0 | -6.119126 | -0.965004 | 0.000028 |
| 22 | 6 | 0 | -4.952846 | -0.259646 | 0.000026 |
| 23 | 6 | 0 | 0.000000 | 1.237399 | 0.000000 |
| 24 | 6 | 0 | -0.000001 | 2.450944 | 0.000000 |
| 25 | 6 | 0 | -0.000001 | 3.871943 | 0.000000 |
| 26 | 6 | 0 | -1.210722 | 4.590950 | -0.000205 |
| 27 | 6 | 0 | -1.205789 | 5.979883 | -0.000204 |
| 28 | 6 | 0 | -0.000001 | 6.680515 | 0.000000 |
| 29 | 6 | 0 | 1.205788 | 5.979883 | 0.000204 |
| 30 | 6 | 0 | 1.210721 | 4.590950 | 0.000205 |
| 31 | 1 | 0 | 7.070532 | -0.445200 | -0.000035 |
| 32 | 1 | 0 | 7.045319 | -2.934935 | -0.000021 |
| 33 | 1 | 0 | 4.911757 | -4.161018 | -0.000007 |
| 34 | 1 | 0 | 4.963875 | 0.825152 | -0.000033 |
| 35 | 1 | 0 | 2.431545 | -4.122083 | -0.000001 |
| 36 | 1 | 0 | 2.501764 | 0.851798 | -0.000022 |
| 37 | 1 | 0 | 0.000000 | -4.101961 | 0.000000 |
| 38 | 1 | 0 | -2.431544 | -4.122083 | 0.000002 |
| 39 | 1 | 0 | -2.501764 | 0.851797 | 0.000021 |
| 40 | 1 | 0 | -4.911756 | -4.161019 | 0.000007 |
| 41 | 1 | 0 | -7.045318 | -2.934936 | 0.000022 |
| 42 | 1 | 0 | -7.070532 | -0.445201 | 0.000035 |
| 43 | 1 | 0 | -4.963875 | 0.825151 | 0.000032 |
| 44 | 1 | 0 | -2.147710 | 4.047421 | -0.000367 |
| 45 | 1 | 0 | -2.146547 | 6.518811 | -0.000363 |
| 46 | 1 | 0 | -0.000001 | 7.764421 | 0.000000 |
| 47 | 1 | 0 | 2.146546 | 6.518810 | 0.000364 |
| 48 | 1 | 0 | 2.147709 | 4.047421 | 0.000367 |

R=BzTh

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -1.588750 | -6.145108 | 0.000026 |
| 2 | 6 | 0 | -3.018241 | -6.203808 | 0.000013 |
| 3 | 6 | 0 | -3.758137 | -5.059809 | 0.000003 |
| 4 | 6 | 0 | -3.124956 | -3.773004 | 0.000004 |
| 5 | 6 | 0 | -1.676132 | -3.712984 | 0.000018 |
| 6 | 6 | 0 | -0.943344 | -4.944470 | 0.000029 |
| 7 | 6 | 0 | -3.844445 | -2.588583 | -0.000005 |
| 8 | 6 | 0 | -3.209256 | -1.326287 | -0.000003 |
| 9 | 6 | 0 | -1.758822 | -1.265992 | 0.000009 |
| 10 | 6 | 0 | -1.040917 | -2.477003 | 0.000020 |
| 11 | 6 | 0 | -3.948553 | -0.138738 | -0.000011 |
| 12 | 6 | 0 | -3.334433 | 1.118113 | -0.000008 |
| 13 | 6 | 0 | -1.885430 | 1.206428 | 0.000003 |
| 14 | 6 | 0 | -1.114613 | 0.006547 | 0.000011 |
| 15 | 6 | 0 | -4.095259 | 2.308899 | -0.000016 |
| 16 | 6 | 0 | -3.500698 | 3.560689 | -0.000013 |
| 17 | 6 | 0 | -2.053319 | 3.649183 | -0.000002 |
| 18 | 6 | 0 | -1.295195 | 2.484525 | 0.000005 |
| 19 | 6 | 0 | -4.262309 | 4.775908 | -0.000022 |
| 20 | 6 | 0 | -3.643766 | 5.989813 | -0.000019 |
| 21 | 6 | 0 | -2.215800 | 6.077821 | -0.000006 |
| 22 | 6 | 0 | -1.451004 | 4.949465 | 0.000001 |
| 23 | 6 | 0 | 0.294866 | 0.077339 | 0.000017 |
| 24 | 6 | 0 | 1.508433 | 0.141698 | 0.000018 |
| 25 | 6 | 0 | 2.908372 | 0.189822 | 0.000014 |
| 26 | 6 | 0 | 3.724071 | 1.291247 | 0.000075 |
| 27 | 6 | 0 | 5.118211 | 0.975489 | 0.000047 |
| 28 | 6 | 0 | 5.351702 | -0.422273 | -0.000040 |
| 29 | 16 | 0 | 3.845689 | -1.319376 | -0.000085 |
| 30 | 6 | 0 | 6.224569 | 1.845645 | 0.000092 |
| 31 | 6 | 0 | 7.506279 | 1.323718 | 0.000051 |
| 32 | 6 | 0 | 7.716357 | -0.065808 | -0.000035 |
| 33 | 6 | 0 | 6.644662 | -0.947858 | -0.000081 |
| 34 | 1 | 0 | -1.021082 | -7.068717 | 0.000035 |
| 35 | 1 | 0 | -3.508623 | -7.170682 | 0.000012 |
| 36 | 1 | 0 | -4.842240 | -5.102446 | -0.000007 |
| 37 | 1 | 0 | 0.140489 | -4.899861 | 0.000038 |
| 38 | 1 | 0 | -4.929433 | -2.623134 | -0.000014 |
| 39 | 1 | 0 | 0.042017 | -2.443166 | 0.000030 |
| 40 | 1 | 0 | -5.032510 | -0.194227 | -0.000020 |
| 41 | 1 | 0 | -5.178095 | 2.232395 | -0.000024 |
| 42 | 1 | 0 | -0.214351 | 2.560217 | 0.000012 |
| 43 | 1 | 0 | -5.345069 | 4.707185 | -0.000031 |
| 44 | 1 | 0 | -4.230661 | 6.901316 | -0.000026 |
| 45 | 1 | 0 | -1.745721 | 7.054734 | -0.000003 |
| 46 | 1 | 0 | -0.368252 | 5.016530 | 0.000010 |
| 47 | 1 | 0 | 3.334461 | 2.300314 | 0.000141 |
| 48 | 1 | 0 | 6.065456 | 2.918301 | 0.000158 |
| 49 | 1 | 0 | 8.359788 | 1.991764 | 0.000086 |
| 50 | 1 | 0 | 8.727720 | -0.455505 | -0.000065 |
| 51 | 1 | 0 | 6.810207 | -2.018751 | -0.000147 |

R=Th

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -5.849941 | -1.789120 | -0.000003 |
| 2 | 6 | 0 | -5.639262 | -3.204283 | -0.000001 |
| 3 | 6 | 0 | -4.376759 | -3.716382 | 0.000000 |
| 4 | 6 | 0 | -3.231359 | -2.853228 | 0.000000 |
| 5 | 6 | 0 | -3.444365 | -1.418834 | -0.000002 |
| 6 | 6 | 0 | -4.791572 | -0.930141 | -0.000003 |
| 7 | 6 | 0 | -1.933088 | -3.337873 | 0.000001 |
| 8 | 6 | 0 | -0.811839 | -2.477692 | 0.000000 |
| 9 | 6 | 0 | -1.024925 | -1.041601 | -0.000001 |
| 10 | 6 | 0 | -2.349348 | -0.563503 | -0.000002 |
| 11 | 6 | 0 | 0.493177 | -2.981332 | 0.000001 |
| 12 | 6 | 0 | 1.611933 | -2.141613 | 0.000001 |
| 13 | 6 | 0 | 1.426238 | -0.701753 | 0.000000 |
| 14 | 6 | 0 | 0.103365 | -0.169559 | -0.000001 |
| 15 | 6 | 0 | 2.924921 | -2.664234 | 0.000001 |
| 16 | 6 | 0 | 4.042382 | -1.844665 | 0.000001 |
| 17 | 6 | 0 | 3.857075 | -0.406426 | 0.000000 |
| 18 | 6 | 0 | 2.570615 | 0.118653 | 0.000000 |
| 19 | 6 | 0 | 5.379365 | -2.363761 | 0.000002 |
| 20 | 6 | 0 | 6.455172 | -1.527809 | 0.000002 |
| 21 | 6 | 0 | 6.273011 | -0.108713 | 0.000001 |
| 22 | 6 | 0 | 5.020847 | 0.429875 | 0.000000 |
| 23 | 6 | 0 | -0.091062 | 1.228979 | -0.000001 |
| 24 | 6 | 0 | -0.254560 | 2.433028 | -0.000002 |
| 25 | 6 | 0 | -0.456676 | 3.819735 | -0.000002 |
| 26 | 6 | 0 | 0.482405 | 4.831888 | -0.000014 |
| 27 | 6 | 0 | -0.088545 | 6.129485 | -0.000010 |
| 28 | 6 | 0 | -1.455922 | 6.111331 | 0.000004 |
| 29 | 16 | 0 | -2.079982 | 4.498082 | 0.000013 |
| 30 | 1 | 0 | -6.863667 | -1.404815 | -0.000004 |
| 31 | 1 | 0 | -6.496931 | -3.867436 | -0.000001 |
| 32 | 1 | 0 | -4.215371 | -4.789272 | 0.000001 |
| 33 | 1 | 0 | -4.951043 | 0.142875 | -0.000004 |
| 34 | 1 | 0 | -1.763839 | -4.410158 | 0.000001 |
| 35 | 1 | 0 | -2.518633 | 0.506678 | -0.000003 |
| 36 | 1 | 0 | 0.642243 | -4.056393 | 0.000002 |
| 37 | 1 | 0 | 3.053823 | -3.742113 | 0.000002 |
| 38 | 1 | 0 | 2.441207 | 1.194407 | -0.000001 |
| 39 | 1 | 0 | 5.515745 | -3.440116 | 0.000003 |
| 40 | 1 | 0 | 7.460832 | -1.932763 | 0.000002 |
| 41 | 1 | 0 | 7.144018 | 0.536814 | 0.000001 |
| 42 | 1 | 0 | 4.882806 | 1.505913 | -0.000001 |
| 43 | 1 | 0 | 1.545242 | 4.633308 | -0.000025 |
| 44 | 1 | 0 | 0.492118 | 7.042283 | -0.000018 |
| 45 | 1 | 0 | -2.136537 | 6.948750 | 0.000010 |

## Radical

R=Mt

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 0.000004 | 3.605814 | 0.000018 |
| 2 | 6 | 0 | 0.000001 | 2.354671 | 0.000005 |
| 3 | 6 | 0 | 0.000008 | 4.935005 | 0.000033 |
| 4 | 6 | 0 | 6.142248 | 0.152358 | -0.000023 |
| 5 | 6 | 0 | 6.121114 | -1.266467 | -0.000008 |
| 6 | 6 | 0 | 4.929071 | -1.943347 | 0.000006 |
| 7 | 6 | 0 | 3.690427 | -1.239258 | 0.000004 |
| 8 | 6 | 0 | 3.712722 | 0.198438 | -0.000011 |
| 9 | 6 | 0 | 4.968178 | 0.863528 | -0.000024 |
| 10 | 6 | 0 | 2.450348 | -1.891187 | 0.000015 |
| 11 | 6 | 0 | 1.236815 | -1.186764 | 0.000013 |
| 12 | 6 | 0 | 1.264304 | 0.259350 | 0.000000 |
| 13 | 6 | 0 | 2.491733 | 0.902245 | -0.000012 |
| 14 | 6 | 0 | -0.000001 | -1.865135 | 0.000021 |
| 15 | 6 | 0 | -1.236816 | -1.186764 | 0.000013 |
| 16 | 6 | 0 | -1.264305 | 0.259349 | 0.000001 |
| 17 | 6 | 0 | 0.000000 | 1.001286 | 0.000000 |
| 18 | 6 | 0 | -2.450350 | -1.891185 | 0.000016 |
| 19 | 6 | 0 | -3.690429 | -1.239256 | 0.000004 |
| 20 | 6 | 0 | -3.712723 | 0.198440 | -0.000010 |
| 21 | 6 | 0 | -2.491733 | 0.902246 | -0.000011 |
| 22 | 6 | 0 | -4.929073 | -1.943345 | 0.000006 |
| 23 | 6 | 0 | -6.121115 | -1.266464 | -0.000008 |
| 24 | 6 | 0 | -6.142249 | 0.152361 | -0.000023 |
| 25 | 6 | 0 | -4.968179 | 0.863531 | -0.000024 |
| 26 | 1 | 0 | 0.926744 | 5.498258 | 0.000039 |
| 27 | 1 | 0 | -0.926723 | 5.498266 | 0.000040 |
| 28 | 1 | 0 | 7.093391 | 0.672377 | -0.000034 |
| 29 | 1 | 0 | 7.056960 | -1.813833 | -0.000007 |
| 30 | 1 | 0 | 4.912060 | -3.028166 | 0.000017 |
| 31 | 1 | 0 | 4.982803 | 1.948336 | -0.000036 |
| 32 | 1 | 0 | 2.423762 | -2.976394 | 0.000026 |
| 33 | 1 | 0 | 2.518247 | 1.986112 | -0.000022 |
| 34 | 1 | 0 | -0.000001 | -2.950111 | 0.000031 |
| 35 | 1 | 0 | -2.423765 | -2.976393 | 0.000026 |
| 36 | 1 | 0 | -2.518246 | 1.986113 | -0.000022 |
| 37 | 1 | 0 | -4.912061 | -3.028163 | 0.000017 |
| 38 | 1 | 0 | -7.056962 | -1.813830 | -0.000007 |
| 39 | 1 | 0 | -7.093393 | 0.672379 | -0.000034 |
| 40 | 1 | 0 | -4.982804 | 1.948339 | -0.000036 |

R=DCM

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -6.129922 | -0.599134 | 0.000016 |
| 2 | 6 | 0 | -6.113306 | -2.019520 | 0.000005 |
| 3 | 6 | 0 | -4.925863 | -2.702448 | -0.000004 |
| 4 | 6 | 0 | -3.684610 | -2.001995 | -0.000003 |
| 5 | 6 | 0 | -3.702681 | -0.561957 | 0.000008 |
| 6 | 6 | 0 | -4.956323 | 0.109857 | 0.000017 |
| 7 | 6 | 0 | -2.449671 | -2.659626 | -0.000010 |
| 8 | 6 | 0 | -1.233218 | -1.958478 | -0.000009 |
| 9 | 6 | 0 | -1.256370 | -0.511502 | 0.000000 |
| 10 | 6 | 0 | -2.484781 | 0.139200 | 0.000008 |
| 11 | 6 | 0 | -0.000006 | -2.637399 | -0.000013 |
| 12 | 6 | 0 | 1.233210 | -1.958482 | -0.000008 |
| 13 | 6 | 0 | 1.256367 | -0.511506 | 0.000000 |
| 14 | 6 | 0 | -0.000003 | 0.218369 | -0.000001 |
| 15 | 6 | 0 | 2.449660 | -2.659633 | -0.000009 |
| 16 | 6 | 0 | 3.684601 | -2.002004 | -0.000002 |
| 17 | 6 | 0 | 3.702677 | -0.561967 | 0.000006 |
| 18 | 6 | 0 | 2.484777 | 0.139193 | 0.000007 |
| 19 | 6 | 0 | 4.925852 | -2.702461 | -0.000003 |
| 20 | 6 | 0 | 6.113298 | -2.019536 | 0.000004 |
| 21 | 6 | 0 | 6.129917 | -0.599151 | 0.000012 |
| 22 | 6 | 0 | 4.956319 | 0.109843 | 0.000013 |
| 23 | 6 | 0 | 0.000002 | 1.586055 | -0.000004 |
| 24 | 6 | 0 | 0.000005 | 2.820706 | -0.000007 |
| 25 | 6 | 0 | 0.000011 | 4.183103 | -0.000007 |
| 26 | 6 | 0 | -1.226178 | 4.902376 | -0.000009 |
| 27 | 7 | 0 | -2.235804 | 5.468921 | -0.000013 |
| 28 | 6 | 0 | 1.226207 | 4.902367 | -0.000002 |
| 29 | 7 | 0 | 2.235837 | 5.468904 | 0.000004 |
| 30 | 1 | 0 | -7.079664 | -0.077219 | 0.000023 |
| 31 | 1 | 0 | -7.051615 | -2.562194 | 0.000004 |
| 32 | 1 | 0 | -4.913532 | -3.787001 | -0.000012 |
| 33 | 1 | 0 | -4.967073 | 1.194250 | 0.000025 |
| 34 | 1 | 0 | -2.427263 | -3.744637 | -0.000017 |
| 35 | 1 | 0 | -2.511406 | 1.222784 | 0.000015 |
| 36 | 1 | 0 | -0.000007 | -3.722277 | -0.000021 |
| 37 | 1 | 0 | 2.427250 | -3.744644 | -0.000015 |
| 38 | 1 | 0 | 2.511406 | 1.222778 | 0.000012 |
| 39 | 1 | 0 | 4.913519 | -3.787014 | -0.000010 |
| 40 | 1 | 0 | 7.051604 | -2.562213 | 0.000003 |
| 41 | 1 | 0 | 7.079660 | -0.077238 | 0.000018 |
| 42 | 1 | 0 | 4.967073 | 1.194236 | 0.000020 |

R=DPM

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -2.450365 | -3.980864 | -0.060815 |
| 2 | 6 | 0 | -3.686197 | -3.327253 | -0.110632 |
| 3 | 6 | 0 | -3.705356 | -1.887930 | -0.138216 |
| 4 | 6 | 0 | -2.487606 | -1.185510 | -0.104838 |
| 5 | 6 | 0 | -1.258082 | -1.830890 | -0.041551 |
| 6 | 6 | 0 | -1.234303 | -3.278421 | -0.030426 |
| 7 | 6 | 0 | 0.000012 | -1.097976 | 0.000004 |
| 8 | 6 | 0 | 1.258120 | -1.830865 | 0.041557 |
| 9 | 6 | 0 | 1.234370 | -3.278396 | 0.030412 |
| 10 | 6 | 0 | 0.000040 | -3.956731 | -0.000012 |
| 11 | 6 | 0 | 2.487631 | -1.185462 | 0.104857 |
| 12 | 6 | 0 | 3.705395 | -1.887858 | 0.138229 |
| 13 | 6 | 0 | 3.686265 | -3.327181 | 0.110623 |
| 14 | 6 | 0 | 2.450446 | -3.980816 | 0.060794 |
| 15 | 6 | 0 | 4.960712 | -1.221321 | 0.201722 |
| 16 | 6 | 0 | 6.133789 | -1.930946 | 0.231886 |
| 17 | 6 | 0 | 6.115806 | -3.351161 | 0.201040 |
| 18 | 6 | 0 | 4.927109 | -4.029223 | 0.142713 |
| 19 | 6 | 0 | -4.927027 | -4.029320 | -0.142729 |
| 20 | 6 | 0 | -6.115738 | -3.351280 | -0.201041 |
| 21 | 6 | 0 | -6.133749 | -1.931065 | -0.231865 |
| 22 | 6 | 0 | -4.960687 | -1.221418 | -0.201694 |
| 23 | 6 | 0 | -0.000001 | 0.268796 | 0.000006 |
| 24 | 6 | 0 | -0.000014 | 1.509020 | 0.000004 |
| 25 | 6 | 0 | -0.000028 | 2.867201 | 0.000001 |
| 26 | 6 | 0 | 1.281385 | 3.588300 | -0.138798 |
| 27 | 6 | 0 | 1.502938 | 4.817274 | 0.509192 |
| 28 | 6 | 0 | -1.503046 | 4.817227 | -0.509217 |
| 29 | 6 | 0 | -1.281458 | 3.588272 | 0.138797 |
| 30 | 6 | 0 | 2.333567 | 3.042147 | -0.897111 |
| 31 | 6 | 0 | 3.554137 | 3.697681 | -1.003170 |
| 32 | 6 | 0 | 3.758610 | 4.914352 | -0.352540 |
| 33 | 6 | 0 | 2.727360 | 5.467937 | 0.404562 |
| 34 | 6 | 0 | -2.727483 | 5.467861 | -0.404590 |
| 35 | 6 | 0 | -3.758713 | 4.914266 | 0.352534 |
| 36 | 6 | 0 | -3.554204 | 3.697614 | 1.003186 |
| 37 | 6 | 0 | -2.333619 | 3.042108 | 0.897130 |
| 38 | 1 | 0 | -2.425805 | -5.066099 | -0.049415 |
| 39 | 1 | 0 | -2.513163 | -0.102360 | -0.138645 |
| 40 | 1 | 0 | 0.000051 | -5.041807 | -0.000020 |
| 41 | 1 | 0 | 2.513166 | -0.102312 | 0.138681 |
| 42 | 1 | 0 | 2.425908 | -5.066052 | 0.049378 |
| 43 | 1 | 0 | 4.972304 | -0.136767 | 0.226668 |
| 44 | 1 | 0 | 7.083511 | -1.410470 | 0.280300 |
| 45 | 1 | 0 | 7.052430 | -3.896690 | 0.225158 |
| 46 | 1 | 0 | 4.912310 | -5.113891 | 0.120999 |
| 47 | 1 | 0 | -4.912207 | -5.113988 | -0.121032 |
| 48 | 1 | 0 | -7.052351 | -3.896828 | -0.225164 |
| 49 | 1 | 0 | -7.083482 | -1.410608 | -0.280268 |
| 50 | 1 | 0 | -4.972300 | -0.136863 | -0.226623 |
| 51 | 1 | 0 | 0.716812 | 5.249160 | 1.116040 |
| 52 | 1 | 0 | -0.716936 | 5.249120 | -1.116081 |
| 53 | 1 | 0 | 2.174007 | 2.106198 | -1.419419 |
| 54 | 1 | 0 | 4.345411 | 3.263311 | -1.604189 |
| 55 | 1 | 0 | 4.710541 | 5.426093 | -0.436454 |
| 56 | 1 | 0 | 2.879100 | 6.408269 | 0.922876 |
| 57 | 1 | 0 | -2.879252 | 6.408179 | -0.922922 |
| 58 | 1 | 0 | -4.710656 | 5.425985 | 0.436445 |
| 59 | 1 | 0 | -4.345461 | 3.263237 | 1.604222 |
| 60 | 1 | 0 | -2.174030 | 2.106173 | 1.419455 |

R=Flu

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 4.122783 | -2.449069 | -0.000005 |
| 2 | 6 | 0 | 3.470563 | -3.685260 | -0.000006 |
| 3 | 6 | 0 | 2.030353 | -3.706112 | -0.000004 |
| 4 | 6 | 0 | 1.327609 | -2.489791 | -0.000001 |
| 5 | 6 | 0 | 1.970895 | -1.256569 | 0.000000 |
| 6 | 6 | 0 | 3.418794 | -1.233047 | -0.000002 |
| 7 | 6 | 0 | 1.237923 | 0.000000 | 0.000001 |
| 8 | 6 | 0 | 1.970896 | 1.256567 | 0.000001 |
| 9 | 6 | 0 | 3.418795 | 1.233045 | -0.000001 |
| 10 | 6 | 0 | 4.097309 | -0.000001 | -0.000003 |
| 11 | 6 | 0 | 1.327611 | 2.489791 | 0.000005 |
| 12 | 6 | 0 | 2.030356 | 3.706111 | 0.000006 |
| 13 | 6 | 0 | 3.470566 | 3.685257 | 0.000003 |
| 14 | 6 | 0 | 4.122785 | 2.449066 | -0.000001 |
| 15 | 6 | 0 | 1.365295 | 4.964465 | 0.000012 |
| 16 | 6 | 0 | 2.076051 | 6.136414 | 0.000013 |
| 17 | 6 | 0 | 3.497197 | 6.116059 | 0.000010 |
| 18 | 6 | 0 | 4.174257 | 4.926045 | 0.000005 |
| 19 | 6 | 0 | 4.174253 | -4.926048 | -0.000009 |
| 20 | 6 | 0 | 3.497192 | -6.116061 | -0.000010 |
| 21 | 6 | 0 | 2.076046 | -6.136415 | -0.000008 |
| 22 | 6 | 0 | 1.365291 | -4.964466 | -0.000005 |
| 23 | 6 | 0 | -0.133000 | 0.000000 | 0.000003 |
| 24 | 6 | 0 | -1.371087 | 0.000001 | 0.000003 |
| 25 | 6 | 0 | -2.727816 | 0.000001 | 0.000003 |

| | | | | | |
|---|---|---|---|---|---|
| 26 | 6 | 0 | -3.603007 | 1.172478 | -0.000007 |
| 27 | 6 | 0 | -4.952492 | 0.733049 | -0.000006 |
| 28 | 6 | 0 | -4.952493 | -0.733046 | 0.000004 |
| 29 | 6 | 0 | -3.603007 | -1.172475 | 0.000009 |
| 30 | 6 | 0 | -3.304728 | 2.534041 | -0.000017 |
| 31 | 6 | 0 | -4.351804 | 3.453895 | -0.000026 |
| 32 | 6 | 0 | -5.681575 | 3.021094 | -0.000025 |
| 33 | 6 | 0 | -5.989610 | 1.658726 | -0.000015 |
| 34 | 6 | 0 | -5.989611 | -1.658722 | 0.000009 |
| 35 | 6 | 0 | -5.681577 | -3.021090 | 0.000020 |
| 36 | 6 | 0 | -4.351806 | -3.453892 | 0.000026 |
| 37 | 6 | 0 | -3.304729 | -2.534039 | 0.000021 |
| 38 | 1 | 0 | 5.207936 | -2.422671 | -0.000007 |
| 39 | 1 | 0 | 0.244383 | -2.516036 | -0.000001 |
| 40 | 1 | 0 | 5.182331 | -0.000002 | -0.000005 |
| 41 | 1 | 0 | 0.244384 | 2.516036 | 0.000009 |
| 42 | 1 | 0 | 5.207938 | 2.422668 | -0.000003 |
| 43 | 1 | 0 | 0.280614 | 4.979928 | 0.000015 |
| 44 | 1 | 0 | 1.556580 | 7.087817 | 0.000018 |
| 45 | 1 | 0 | 4.043214 | 7.052609 | 0.000011 |
| 46 | 1 | 0 | 5.259019 | 4.909245 | 0.000002 |
| 47 | 1 | 0 | 5.259016 | -4.909249 | -0.000010 |
| 48 | 1 | 0 | 4.043209 | -7.052611 | -0.000012 |
| 49 | 1 | 0 | 1.556574 | -7.087818 | -0.000009 |
| 50 | 1 | 0 | 0.280610 | -4.979928 | -0.000005 |
| 51 | 1 | 0 | -2.274740 | 2.871987 | -0.000019 |
| 52 | 1 | 0 | -4.134632 | 4.516048 | -0.000034 |
| 53 | 1 | 0 | -6.482304 | 3.752003 | -0.000032 |
| 54 | 1 | 0 | -7.024654 | 1.334710 | -0.000015 |
| 55 | 1 | 0 | -7.024654 | -1.334706 | 0.000005 |
| 56 | 1 | 0 | -6.482307 | -3.751999 | 0.000024 |
| 57 | 1 | 0 | -4.134635 | -4.516045 | 0.000034 |
| 58 | 1 | 0 | -2.274742 | -2.871985 | 0.000026 |

R=PhO

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 6.129599 | -1.243908 | -0.000005 |
| 2 | 6 | 0 | 6.111544 | -2.667317 | 0.000002 |
| 3 | 6 | 0 | 4.924579 | -3.346360 | 0.000006 |
| 4 | 6 | 0 | 3.680975 | -2.644296 | 0.000003 |
| 5 | 6 | 0 | 3.699330 | -1.201535 | -0.000003 |
| 6 | 6 | 0 | 4.959154 | -0.534364 | -0.000007 |
| 7 | 6 | 0 | 2.449442 | -3.299271 | 0.000005 |
| 8 | 6 | 0 | 1.230743 | -2.596371 | 0.000002 |
| 9 | 6 | 0 | 1.250928 | -1.147730 | -0.000001 |
| 10 | 6 | 0 | 2.486827 | -0.499847 | -0.000004 |
| 11 | 6 | 0 | 0.000144 | -3.274454 | 0.000000 |
| 12 | 6 | 0 | -1.230513 | -2.596478 | -0.000002 |
| 13 | 6 | 0 | -1.250824 | -1.147838 | 0.000000 |
| 14 | 6 | 0 | 0.000021 | -0.422971 | -0.000001 |
| 15 | 6 | 0 | -2.449151 | -3.299483 | -0.000004 |
| 16 | 6 | 0 | -3.680741 | -2.644613 | -0.000003 |
| 17 | 6 | 0 | -3.699222 | -1.201856 | 0.000002 |
| 18 | 6 | 0 | -2.486778 | -0.500063 | 0.000002 |
| 19 | 6 | 0 | -4.924284 | -3.346786 | -0.000004 |
| 20 | 6 | 0 | -6.111308 | -2.667845 | -0.000001 |
| 21 | 6 | 0 | -6.129486 | -1.244437 | 0.000004 |
| 22 | 6 | 0 | -4.959101 | -0.534793 | 0.000005 |
| 23 | 6 | 0 | -0.000040 | 0.959304 | -0.000001 |
| 24 | 6 | 0 | -0.000097 | 2.188971 | 0.000000 |
| 25 | 6 | 0 | -0.000159 | 3.568832 | 0.000000 |
| 26 | 6 | 0 | -1.233952 | 4.305651 | -0.000005 |
| 27 | 6 | 0 | -1.241105 | 5.664142 | -0.000005 |
| 28 | 6 | 0 | -0.000289 | 6.441896 | 0.000000 |
| 29 | 6 | 0 | 1.240597 | 5.664254 | 0.000005 |
| 30 | 6 | 0 | 1.233568 | 4.305762 | 0.000004 |
| 31 | 8 | 0 | -0.000344 | 7.678099 | 0.000001 |
| 32 | 1 | 0 | 7.080743 | -0.724118 | -0.000008 |
| 33 | 1 | 0 | 7.049460 | -3.210764 | 0.000005 |
| 34 | 1 | 0 | 4.909509 | -4.431027 | 0.000011 |
| 35 | 1 | 0 | 4.972987 | 0.550216 | -0.000012 |
| 36 | 1 | 0 | 2.425037 | -4.384365 | 0.000008 |
| 37 | 1 | 0 | 2.511686 | 0.583454 | -0.000007 |
| 38 | 1 | 0 | 0.000191 | -4.359559 | 0.000001 |
| 39 | 1 | 0 | -2.424653 | -4.384575 | -0.000006 |
| 40 | 1 | 0 | -2.511731 | 0.583237 | 0.000005 |
| 41 | 1 | 0 | -4.909121 | -4.431452 | -0.000008 |
| 42 | 1 | 0 | -7.049177 | -3.211372 | -0.000003 |
| 43 | 1 | 0 | -7.080674 | -0.724730 | 0.000007 |
| 44 | 1 | 0 | -4.973030 | 0.549786 | 0.000010 |
| 45 | 1 | 0 | -2.163520 | 3.747523 | -0.000008 |
| 46 | 1 | 0 | -2.166175 | 6.228938 | -0.000008 |
| 47 | 1 | 0 | 2.165618 | 6.229133 | 0.000009 |
| 48 | 1 | 0 | 2.163187 | 3.747718 | 0.000008 |

R=NO

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -6.157622 | -0.255195 | 0.000001 |
| 2 | 6 | 0 | -6.158452 | -1.679942 | 0.000001 |
| 3 | 6 | 0 | -4.980886 | -2.373667 | 0.000000 |
| 4 | 6 | 0 | -3.726049 | -1.689332 | 0.000000 |
| 5 | 6 | 0 | -3.725279 | -0.245208 | 0.000000 |
| 6 | 6 | 0 | -4.978266 | 0.437691 | 0.000001 |
| 7 | 6 | 0 | -2.505266 | -2.361538 | -0.000001 |
| 8 | 6 | 0 | -1.274067 | -1.678259 | -0.000001 |
| 9 | 6 | 0 | -1.275191 | -0.228744 | 0.000000 |
| 10 | 6 | 0 | -2.504433 | 0.437663 | 0.000000 |
| 11 | 6 | 0 | -0.052729 | -2.372273 | -0.000002 |
| 12 | 6 | 0 | 1.185602 | -1.709096 | -0.000001 |
| 13 | 6 | 0 | 1.223038 | -0.260301 | 0.000001 |
| 14 | 6 | 0 | -0.018304 | 0.473237 | 0.000001 |
| 15 | 6 | 0 | 2.399138 | -2.423298 | -0.000002 |
| 16 | 6 | 0 | 3.635823 | -1.780718 | -0.000001 |
| 17 | 6 | 0 | 3.669838 | -0.337087 | 0.000002 |
| 18 | 6 | 0 | 2.467404 | 0.378175 | 0.000003 |
| 19 | 6 | 0 | 4.873738 | -2.495129 | -0.000002 |
| 20 | 6 | 0 | 6.067060 | -1.828786 | -0.000001 |
| 21 | 6 | 0 | 6.100251 | -0.404378 | 0.000003 |
| 22 | 6 | 0 | 4.938106 | 0.317079 | 0.000004 |
| 23 | 7 | 0 | 0.270183 | 4.393189 | -0.000005 |
| 24 | 8 | 0 | 1.433852 | 4.932515 | -0.000004 |
| 25 | 6 | 0 | -0.891202 | 5.298492 | 0.000002 |
| 26 | 6 | 0 | 0.107615 | 3.080856 | -0.000001 |
| 27 | 6 | 0 | 0.016965 | 1.861078 | 0.000001 |
| 28 | 1 | 0 | -7.101993 | 0.277127 | 0.000002 |
| 29 | 1 | 0 | -7.103537 | -2.211043 | 0.000001 |
| 30 | 1 | 0 | -4.980073 | -3.458592 | 0.000000 |
| 31 | 1 | 0 | -4.977840 | 1.522684 | 0.000001 |
| 32 | 1 | 0 | -2.497352 | -3.447017 | -0.000002 |
| 33 | 1 | 0 | -2.514556 | 1.521723 | 0.000001 |
| 34 | 1 | 0 | -0.066560 | -3.457295 | -0.000003 |
| 35 | 1 | 0 | 2.364205 | -3.508270 | -0.000004 |
| 36 | 1 | 0 | 2.506929 | 1.461574 | 0.000005 |
| 37 | 1 | 0 | 4.847397 | -3.579762 | -0.000005 |
| 38 | 1 | 0 | 6.999402 | -2.382102 | -0.000002 |
| 39 | 1 | 0 | 7.057024 | 0.105245 | 0.000004 |
| 40 | 1 | 0 | 4.961321 | 1.401522 | 0.000006 |
| 41 | 1 | 0 | -0.831518 | 5.926477 | -0.889937 |
| 42 | 1 | 0 | -1.814387 | 4.720919 | -0.000031 |
| 43 | 1 | 0 | -0.831551 | 5.926429 | 0.889978 |

R=Allyl

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 0.000000 | 3.129530 | 0.000000 |
| 2 | 6 | 0 | 0.000000 | 1.917357 | 0.000000 |
| 3 | 6 | 0 | -0.000001 | 4.561572 | -0.000001 |
| 4 | 6 | 0 | -6.119252 | -0.284326 | -0.025590 |
| 5 | 6 | 0 | -6.105265 | -1.714698 | -0.018017 |
| 6 | 6 | 0 | -4.924805 | -2.395387 | -0.009888 |
| 7 | 6 | 0 | -3.671906 | -1.698042 | -0.008317 |
| 8 | 6 | 0 | -3.685279 | -0.248144 | -0.014783 |
| 9 | 6 | 0 | -4.952500 | 0.420812 | -0.024149 |
| 10 | 6 | 0 | -2.452251 | -2.356935 | -0.002549 |
| 11 | 6 | 0 | -1.223752 | -1.659095 | -0.001214 |
| 12 | 6 | 0 | -1.236473 | -0.207127 | -0.003380 |
| 13 | 6 | 0 | -2.482809 | 0.448594 | -0.012567 |
| 14 | 6 | 0 | 0.000000 | -2.337194 | -0.000001 |
| 15 | 6 | 0 | 1.223752 | -1.659094 | 0.001212 |
| 16 | 6 | 0 | 1.236473 | -0.207126 | 0.003380 |
| 17 | 6 | 0 | 0.000000 | 0.501289 | 0.000000 |
| 18 | 6 | 0 | 2.452252 | -2.356934 | 0.002546 |
| 19 | 6 | 0 | 3.671906 | -1.698041 | 0.008316 |
| 20 | 6 | 0 | 3.685279 | -0.248144 | 0.014785 |
| 21 | 6 | 0 | 2.482809 | 0.448594 | 0.012569 |
| 22 | 6 | 0 | 4.924805 | -2.395387 | 0.009886 |
| 23 | 6 | 0 | 6.105266 | -1.714698 | 0.018017 |
| 24 | 6 | 0 | 6.119252 | -0.284326 | 0.025593 |
| 25 | 6 | 0 | 4.952501 | 0.420813 | 0.024152 |
| 26 | 6 | 0 | 1.174097 | 5.239113 | -0.331330 |
| 27 | 6 | 0 | -1.174098 | 5.239113 | 0.331327 |
| 28 | 1 | 0 | -7.070423 | 0.235851 | -0.032710 |
| 29 | 1 | 0 | -7.045888 | -2.253749 | -0.019171 |
| 30 | 1 | 0 | -4.912462 | -3.480272 | -0.004660 |
| 31 | 1 | 0 | -4.963138 | 1.505588 | -0.030408 |
| 32 | 1 | 0 | -2.432303 | -3.442317 | 0.000000 |
| 33 | 1 | 0 | -2.500918 | 1.531819 | -0.021151 |
| 34 | 1 | 0 | 0.000000 | -3.422598 | -0.000003 |
| 35 | 1 | 0 | 2.432304 | -3.442317 | -0.000004 |
| 36 | 1 | 0 | 2.500918 | 1.531820 | 0.021155 |
| 37 | 1 | 0 | 4.912463 | -3.480272 | 0.004656 |
| 38 | 1 | 0 | 7.045888 | -2.253749 | 0.019171 |
| 39 | 1 | 0 | 7.070423 | 0.235851 | 0.032715 |
| 40 | 1 | 0 | 4.963138 | 1.505588 | 0.030415 |
| 41 | 1 | 0 | 2.076508 | 4.706348 | -0.596612 |
| 42 | 1 | 0 | 1.197888 | 6.321759 | -0.332535 |
| 43 | 1 | 0 | -1.197889 | 6.321759 | 0.332530 |
| 44 | 1 | 0 | -2.076509 | 4.706348 | 0.596610 |

R=IN

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|

| | | | | | |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -0.712719 | 6.076653 | -0.039250 |
| 2 | 6 | 0 | 0.596474 | 6.653577 | -0.031222 |
| 3 | 6 | 0 | 1.703860 | 5.859717 | -0.020370 |
| 4 | 6 | 0 | 1.584510 | 4.430671 | -0.016688 |
| 5 | 6 | 0 | 0.257401 | 3.845856 | -0.024669 |
| 6 | 6 | 0 | -0.875732 | 4.723174 | -0.036089 |
| 7 | 6 | 0 | 2.687630 | 3.591024 | -0.006099 |
| 8 | 6 | 0 | 2.554203 | 2.184411 | -0.002885 |
| 9 | 6 | 0 | 1.225180 | 1.601455 | -0.010514 |
| 10 | 6 | 0 | 0.111726 | 2.463364 | -0.021475 |
| 11 | 6 | 0 | 3.672879 | 1.343552 | 0.007236 |
| 12 | 6 | 0 | 3.559355 | -0.051456 | 0.009556 |
| 13 | 6 | 0 | 2.241550 | -0.659418 | 0.001271 |
| 14 | 6 | 0 | 1.093252 | 0.182080 | -0.007886 |
| 15 | 6 | 0 | 4.700046 | -0.884895 | 0.019678 |
| 16 | 6 | 0 | 4.597787 | -2.267419 | 0.021723 |
| 17 | 6 | 0 | 3.280380 | -2.874035 | 0.013145 |
| 18 | 6 | 0 | 2.150800 | -2.064168 | 0.003382 |
| 19 | 6 | 0 | 5.747551 | -3.124299 | 0.031984 |
| 20 | 6 | 0 | 5.610166 | -4.479864 | 0.033614 |
| 21 | 6 | 0 | 4.310966 | -5.078583 | 0.025088 |
| 22 | 6 | 0 | 3.189160 | -4.304121 | 0.015206 |
| 23 | 6 | 0 | -0.199489 | -0.381685 | -0.014475 |
| 24 | 6 | 0 | -1.326429 | -0.824882 | -0.019360 |
| 25 | 6 | 0 | -2.670107 | -1.255213 | -0.030300 |
| 26 | 7 | 0 | -3.098715 | -2.472680 | -0.030754 |
| 27 | 6 | 0 | -4.579895 | -2.449428 | -0.168175 |
| 28 | 6 | 0 | -5.005826 | -0.973849 | 0.196892 |
| 29 | 7 | 0 | -3.695231 | -0.284070 | -0.039053 |
| 30 | 6 | 0 | -6.086762 | -0.331159 | -0.670742 |
| 31 | 6 | 0 | -5.341908 | -0.766849 | 1.684755 |
| 32 | 6 | 0 | -5.181033 | -3.526876 | 0.739911 |
| 33 | 6 | 0 | -4.870308 | -2.812293 | -1.638355 |
| 34 | 8 | 0 | -3.545031 | 0.969083 | -0.019289 |
| 35 | 1 | 0 | -1.578370 | 6.729290 | -0.048040 |
| 36 | 1 | 0 | 0.699592 | 7.732854 | -0.033972 |
| 37 | 1 | 0 | 2.697211 | 6.296041 | -0.014410 |
| 38 | 1 | 0 | -1.866369 | 4.281768 | -0.042334 |
| 39 | 1 | 0 | 3.685312 | 4.018828 | -0.000414 |
| 40 | 1 | 0 | -0.886190 | 2.039065 | -0.028184 |
| 41 | 1 | 0 | 4.663088 | 1.788520 | 0.013250 |
| 42 | 1 | 0 | 5.681933 | -0.422037 | 0.026016 |
| 43 | 1 | 0 | 1.169980 | -2.525565 | -0.002815 |
| 44 | 1 | 0 | 6.731991 | -2.668298 | 0.038433 |
| 45 | 1 | 0 | 6.487153 | -5.117140 | 0.041415 |
| 46 | 1 | 0 | 4.226344 | -6.159400 | 0.026592 |
| 47 | 1 | 0 | 2.203900 | -4.757718 | 0.008801 |
| 48 | 1 | 0 | -6.192332 | 0.719267 | -0.393828 |
| 49 | 1 | 0 | -5.845172 | -0.375134 | -1.732179 |
| 50 | 1 | 0 | -7.045996 | -0.828800 | -0.508927 |
| 51 | 1 | 0 | -6.302187 | -1.222221 | 1.934449 |
| 52 | 1 | 0 | -4.575191 | -1.191753 | 2.335103 |
| 53 | 1 | 0 | -5.402582 | 0.304874 | 1.884736 |
| 54 | 1 | 0 | -4.807710 | -4.503594 | 0.426305 |
| 55 | 1 | 0 | -4.900412 | -3.384684 | 1.783337 |
| 56 | 1 | 0 | -6.272622 | -3.537411 | 0.668876 |
| 57 | 1 | 0 | -5.944552 | -2.887262 | -1.825185 |
| 58 | 1 | 0 | -4.445449 | -2.077405 | -2.325080 |
| 59 | 1 | 0 | -4.411515 | -3.777740 | -1.858313 |

R=Phen

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 2.453399 | 6.118373 | -0.112260 |
| 2 | 6 | 0 | 3.883924 | 6.104126 | -0.105548 |
| 3 | 6 | 0 | 4.564266 | 4.923856 | -0.081061 |
| 4 | 6 | 0 | 3.866555 | 3.671127 | -0.061153 |
| 5 | 6 | 0 | 2.416579 | 3.684783 | -0.066838 |
| 6 | 6 | 0 | 1.748024 | 4.952041 | -0.093674 |
| 7 | 6 | 0 | 4.524936 | 2.451717 | -0.038200 |
| 8 | 6 | 0 | 3.826711 | 1.223393 | -0.019008 |
| 9 | 6 | 0 | 2.374813 | 1.236467 | -0.021055 |
| 10 | 6 | 0 | 1.719698 | 2.482729 | -0.047092 |
| 11 | 6 | 0 | 4.504840 | 0.000001 | 0.000000 |
| 12 | 6 | 0 | 3.826711 | -1.223391 | 0.019007 |
| 13 | 6 | 0 | 2.374814 | -1.236467 | 0.021055 |
| 14 | 6 | 0 | 1.665571 | 0.000000 | 0.000000 |
| 15 | 6 | 0 | 4.524938 | -2.451714 | 0.038200 |
| 16 | 6 | 0 | 3.866558 | -3.671125 | 0.061153 |
| 17 | 6 | 0 | 2.416581 | -3.684782 | 0.066838 |
| 18 | 6 | 0 | 1.719699 | -2.482729 | 0.047092 |
| 19 | 6 | 0 | 4.564269 | -4.923853 | 0.081061 |
| 20 | 6 | 0 | 3.883929 | -6.104124 | 0.105549 |
| 21 | 6 | 0 | 2.453403 | -6.118372 | 0.112261 |
| 22 | 6 | 0 | 1.748027 | -4.952040 | 0.093675 |
| 23 | 6 | 0 | 0.251153 | 0.000000 | -0.000002 |
| 24 | 6 | 0 | -0.962273 | -0.000001 | -0.000002 |
| 25 | 6 | 0 | -2.384223 | -0.000001 | -0.000001 |
| 26 | 6 | 0 | -3.093418 | 1.195846 | 0.195393 |
| 27 | 6 | 0 | -4.504656 | 1.219874 | 0.199265 |
| 28 | 6 | 0 | -5.221689 | -0.000001 | 0.000000 |
| 29 | 6 | 0 | -4.504656 | -1.219876 | -0.199265 |
| 30 | 6 | 0 | -3.093418 | -1.195848 | -0.195395 |
| 31 | 6 | 0 | -6.649341 | -0.000001 | 0.000000 |
| 32 | 6 | 0 | -7.331514 | -1.225549 | -0.200707 |
| 33 | 6 | 0 | -6.627139 | -2.408438 | -0.394527 |
| 34 | 6 | 0 | -5.237834 | -2.417767 | -0.395805 |
| 35 | 6 | 0 | -5.237834 | 2.417765 | 0.395805 |
| 36 | 6 | 0 | -6.627139 | 2.408436 | 0.394528 |
| 37 | 6 | 0 | -7.331514 | 1.225547 | 0.200708 |
| 38 | 1 | 0 | 1.933529 | 7.069524 | -0.132583 |
| 39 | 1 | 0 | 4.423150 | 7.044526 | -0.120524 |
| 40 | 1 | 0 | 5.649147 | 4.911263 | -0.076412 |
| 41 | 1 | 0 | 0.663241 | 4.962936 | -0.099318 |
| 42 | 1 | 0 | 5.610307 | 2.431371 | -0.035677 |
| 43 | 1 | 0 | 0.636490 | 2.501200 | -0.054300 |
| 44 | 1 | 0 | 5.590225 | 0.000001 | 0.000000 |
| 45 | 1 | 0 | 5.610309 | -2.431368 | 0.035676 |
| 46 | 1 | 0 | 0.636492 | -2.501200 | 0.054300 |
| 47 | 1 | 0 | 5.649150 | -4.911260 | 0.076412 |
| 48 | 1 | 0 | 4.423155 | -7.044524 | 0.120525 |
| 49 | 1 | 0 | 1.933534 | -7.069523 | 0.132585 |
| 50 | 1 | 0 | 0.663245 | -4.962937 | 0.099320 |
| 51 | 1 | 0 | -2.547011 | 2.118500 | 0.350193 |
| 52 | 1 | 0 | -2.547011 | -2.118501 | -0.350196 |
| 53 | 1 | 0 | -8.415959 | -1.229338 | -0.201414 |
| 54 | 1 | 0 | -7.168732 | -3.335440 | -0.546650 |
| 55 | 1 | 0 | -4.697535 | -3.345524 | -0.548135 |
| 56 | 1 | 0 | -4.697535 | 3.345522 | 0.548135 |
| 57 | 1 | 0 | -7.168732 | 3.335438 | 0.546651 |
| 58 | 1 | 0 | -8.415959 | 1.229336 | 0.201415 |

R=Ver

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -4.570425 | 6.105217 | -0.033186 |
| 2 | 6 | 0 | -3.140228 | 6.118191 | -0.059732 |
| 3 | 6 | 0 | -2.435194 | 4.951415 | -0.065529 |
| 4 | 6 | 0 | -3.105126 | 3.684862 | -0.045129 |
| 5 | 6 | 0 | -4.555022 | 3.672203 | -0.020182 |
| 6 | 6 | 0 | -5.251860 | 4.925412 | -0.014391 |
| 7 | 6 | 0 | -2.407369 | 2.482769 | -0.049786 |
| 8 | 6 | 0 | -3.065708 | 1.238266 | -0.033094 |
| 9 | 6 | 0 | -4.517006 | 1.224880 | -0.011943 |
| 10 | 6 | 0 | -5.215024 | 2.453171 | -0.004608 |
| 11 | 6 | 0 | -2.361286 | 0.000000 | -0.038023 |
| 12 | 6 | 0 | -3.065708 | -1.238266 | -0.033099 |
| 13 | 6 | 0 | -4.517005 | -1.224880 | -0.011948 |
| 14 | 6 | 0 | -5.193596 | 0.000000 | -0.000115 |
| 15 | 6 | 0 | -2.407368 | -2.482769 | -0.049796 |
| 16 | 6 | 0 | -3.105126 | -3.684862 | -0.045144 |
| 17 | 6 | 0 | -4.555021 | -3.672204 | -0.020197 |
| 18 | 6 | 0 | -5.215024 | -2.453172 | -0.004618 |
| 19 | 6 | 0 | -2.435194 | -4.951415 | -0.065550 |
| 20 | 6 | 0 | -3.140227 | -6.118191 | -0.059758 |
| 21 | 6 | 0 | -4.570424 | -6.105217 | -0.033212 |
| 22 | 6 | 0 | -5.251860 | -4.925412 | -0.014411 |
| 23 | 6 | 0 | -0.948836 | 0.000000 | -0.045498 |
| 24 | 6 | 0 | 0.261690 | 0.000000 | -0.047594 |
| 25 | 6 | 0 | 1.685225 | 0.000000 | -0.052918 |
| 26 | 7 | 0 | 2.278685 | -1.195048 | -0.062792 |
| 27 | 7 | 0 | 3.642574 | -1.173025 | -0.069559 |
| 28 | 6 | 0 | 4.414554 | 0.000000 | -0.030993 |
| 29 | 7 | 0 | 3.642575 | 1.173025 | -0.069568 |
| 30 | 7 | 0 | 2.278686 | 1.195047 | -0.062801 |
| 31 | 8 | 0 | 5.622328 | 0.000000 | 0.027905 |
| 32 | 6 | 0 | 4.262628 | -2.467728 | 0.012949 |
| 33 | 6 | 0 | 4.262628 | 2.467728 | 0.012931 |
| 34 | 6 | 0 | 3.619901 | 3.461227 | 0.755679 |
| 35 | 6 | 0 | 4.173275 | 4.734364 | 0.828703 |
| 36 | 6 | 0 | 5.363768 | 5.024611 | 0.165695 |
| 37 | 6 | 0 | 5.995963 | 4.029990 | -0.576431 |
| 38 | 6 | 0 | 5.453536 | 2.751310 | -0.659957 |
| 39 | 6 | 0 | 5.453536 | -2.751315 | -0.659936 |
| 40 | 6 | 0 | 5.995963 | -4.029994 | -0.576401 |
| 41 | 6 | 0 | 5.363768 | -5.024610 | 0.165733 |
| 42 | 6 | 0 | 4.173275 | -4.734358 | 0.828739 |
| 43 | 6 | 0 | 3.619901 | -3.461221 | 0.755705 |
| 44 | 1 | 0 | -5.108756 | 7.046221 | -0.028937 |
| 45 | 1 | 0 | -2.619837 | 7.069118 | -0.076079 |
| 46 | 1 | 0 | -1.350742 | 4.960399 | -0.087243 |
| 47 | 1 | 0 | -6.336567 | 4.913715 | 0.004782 |
| 48 | 1 | 0 | -1.323956 | 2.501686 | -0.070064 |
| 49 | 1 | 0 | -6.300250 | 2.433780 | 0.012285 |
| 50 | 1 | 0 | -6.278950 | 0.000000 | 0.016891 |
| 51 | 1 | 0 | -1.323956 | -2.501686 | -0.070074 |
| 52 | 1 | 0 | -6.300249 | -2.433781 | 0.012275 |
| 53 | 1 | 0 | -1.350742 | -4.960399 | -0.087263 |
| 54 | 1 | 0 | -2.619837 | -7.069118 | -0.076109 |
| 55 | 1 | 0 | -5.108755 | -7.046222 | -0.028966 |
| 56 | 1 | 0 | -6.336566 | -4.913716 | 0.004762 |
| 57 | 1 | 0 | 2.691020 | 3.228189 | 1.257118 |
| 58 | 1 | 0 | 3.672012 | 5.499440 | 1.410326 |
| 59 | 1 | 0 | 5.794562 | 6.017281 | 0.226219 |
| 60 | 1 | 0 | 6.919772 | 4.246230 | -1.100411 |
| 61 | 1 | 0 | 5.954155 | 1.984496 | -1.230423 |
| 62 | 1 | 0 | 5.954155 | -1.984505 | -1.230408 |
| 63 | 1 | 0 | 6.919773 | -4.246237 | -1.100379 |

| | | | | | |
|---|---|---|---|---|---|
| 64 | 1 | 0 | 5.794563 | -6.017279 | 0.226265 |
| 65 | 1 | 0 | 3.672012 | -5.499430 | 1.410367 |
| 66 | 1 | 0 | 2.691019 | -3.228180 | 1.257141 |

R=NN

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -1.957632 | 3.686826 | -0.019705 |
| 2 | 6 | 0 | -3.406586 | 3.674828 | -0.019957 |
| 3 | 6 | 0 | -4.068611 | 2.454676 | -0.013295 |
| 4 | 6 | 0 | -3.371309 | 1.227165 | -0.006351 |
| 5 | 6 | 0 | -1.920800 | 1.242277 | -0.006036 |
| 6 | 6 | 0 | -1.259097 | 2.482634 | -0.012908 |
| 7 | 6 | 0 | -4.047315 | 0.000006 | 0.000000 |
| 8 | 6 | 0 | -3.371313 | -1.227156 | 0.006351 |
| 9 | 6 | 0 | -1.920804 | -1.242272 | 0.006036 |
| 10 | 6 | 0 | -1.217214 | 0.000001 | -0.000001 |
| 11 | 6 | 0 | -4.068619 | -2.454665 | 0.013295 |
| 12 | 6 | 0 | -3.406598 | -3.674819 | 0.019958 |
| 13 | 6 | 0 | -1.957644 | -3.686821 | 0.019705 |
| 14 | 6 | 0 | -1.259105 | -2.482632 | 0.012908 |
| 15 | 6 | 0 | -4.102147 | -4.927581 | 0.027287 |
| 16 | 6 | 0 | -3.418655 | -6.107443 | 0.033912 |
| 17 | 6 | 0 | -1.989441 | -6.119142 | 0.033736 |
| 18 | 6 | 0 | -1.285142 | -4.950665 | 0.026862 |
| 19 | 6 | 0 | -1.285124 | 4.950667 | -0.026862 |
| 20 | 6 | 0 | -1.989419 | 6.119146 | -0.033736 |
| 21 | 6 | 0 | -3.418633 | 6.107452 | -0.033912 |
| 22 | 6 | 0 | -4.102130 | 4.927592 | -0.027286 |
| 23 | 6 | 0 | 0.185812 | -0.000001 | -0.000001 |
| 24 | 6 | 0 | 1.399867 | -0.000003 | -0.000001 |
| 25 | 6 | 0 | 2.786760 | -0.000004 | -0.000001 |
| 26 | 7 | 0 | 3.568159 | 1.116181 | -0.010745 |
| 27 | 6 | 0 | 5.020318 | 0.758866 | 0.199526 |
| 28 | 6 | 0 | 5.020317 | -0.758880 | -0.199525 |
| 29 | 7 | 0 | 3.568157 | -1.116190 | 0.010744 |
| 30 | 8 | 0 | 3.163767 | -2.316372 | 0.007813 |
| 31 | 8 | 0 | 3.163770 | 2.316364 | -0.007813 |
| 32 | 6 | 0 | 5.307448 | 1.018181 | 1.688288 |
| 33 | 6 | 0 | 5.891690 | 1.667713 | -0.664640 |
| 34 | 6 | 0 | 5.307448 | -1.018195 | -1.688287 |
| 35 | 6 | 0 | 5.891686 | -1.667728 | 0.664641 |
| 36 | 1 | 0 | -5.154012 | 2.436478 | -0.013627 |
| 37 | 1 | 0 | -0.174769 | 2.503396 | -0.013304 |
| 38 | 1 | 0 | -5.132838 | 0.000007 | 0.000000 |
| 39 | 1 | 0 | -5.154020 | -2.436464 | 0.013628 |
| 40 | 1 | 0 | -0.174777 | -2.503397 | 0.013302 |
| 41 | 1 | 0 | -5.187072 | -4.917283 | 0.027516 |
| 42 | 1 | 0 | -3.956500 | -7.048796 | 0.039473 |
| 43 | 1 | 0 | -1.467431 | -7.069300 | 0.039246 |
| 44 | 1 | 0 | -0.200553 | -4.956646 | 0.026901 |
| 45 | 1 | 0 | -0.200535 | 4.956645 | -0.026902 |
| 46 | 1 | 0 | -1.467406 | 7.069302 | -0.039246 |
| 47 | 1 | 0 | -3.956475 | 7.048807 | -0.039472 |
| 48 | 1 | 0 | -5.187055 | 4.917298 | -0.027515 |
| 49 | 1 | 0 | 6.357634 | 0.832516 | 1.921400 |
| 50 | 1 | 0 | 5.080576 | 2.062980 | 1.905635 |
| 51 | 1 | 0 | 4.689102 | 0.393558 | 2.335650 |
| 52 | 1 | 0 | 5.727190 | 2.702960 | -0.365946 |
| 53 | 1 | 0 | 6.947170 | 1.425403 | -0.519383 |
| 54 | 1 | 0 | 5.653781 | 1.584004 | -1.724260 |
| 55 | 1 | 0 | 6.357633 | -0.832531 | -1.921399 |
| 56 | 1 | 0 | 5.080574 | -2.062994 | -1.905634 |
| 57 | 1 | 0 | 4.689101 | -0.393573 | -2.335650 |
| 58 | 1 | 0 | 5.727185 | -2.702974 | 0.365947 |
| 59 | 1 | 0 | 6.947167 | -1.425420 | 0.519384 |
| 60 | 1 | 0 | 5.653777 | -1.584019 | 1.724261 |

## Sat-Radical

R=Sat-H

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -6.121031 | 0.323051 | -0.064120 |
| 2 | 6 | 0 | -6.101136 | -1.101895 | 0.074118 |
| 3 | 6 | 0 | -4.918503 | -1.775754 | 0.122756 |
| 4 | 6 | 0 | -3.667906 | -1.078085 | 0.036851 |
| 5 | 6 | 0 | -3.686308 | 0.364868 | -0.104694 |
| 6 | 6 | 0 | -4.958127 | 1.027439 | -0.149729 |
| 7 | 6 | 0 | -2.445653 | -1.725792 | 0.086722 |
| 8 | 6 | 0 | -1.219104 | -1.027698 | 0.004342 |
| 9 | 6 | 0 | -1.225772 | 0.421074 | -0.149011 |
| 10 | 6 | 0 | -2.489282 | 1.061213 | -0.192506 |
| 11 | 6 | 0 | 0.000000 | -1.705238 | 0.070377 |
| 12 | 6 | 0 | 1.219103 | -1.027698 | 0.004342 |
| 13 | 6 | 0 | 1.225771 | 0.421074 | -0.149011 |
| 14 | 6 | 0 | 0.000000 | 1.126997 | -0.240779 |
| 15 | 6 | 0 | 2.445653 | -1.725792 | 0.086722 |
| 16 | 6 | 0 | 3.667905 | -1.078086 | 0.036851 |
| 17 | 6 | 0 | 3.686307 | 0.364868 | -0.104695 |
| 18 | 6 | 0 | 2.489282 | 1.061213 | -0.192506 |
| 19 | 6 | 0 | 4.918502 | -1.775755 | 0.122756 |
| 20 | 6 | 0 | 6.101135 | -1.101896 | 0.074118 |
| 21 | 6 | 0 | 6.121031 | 0.323051 | -0.064120 |
| 22 | 6 | 0 | 4.958127 | 1.027438 | -0.149729 |
| 23 | 6 | 0 | 0.000001 | 2.633520 | -0.403586 |
| 24 | 6 | 0 | 0.000005 | 3.396493 | 0.934840 |
| 25 | 1 | 0 | -7.074392 | 0.838050 | -0.100413 |
| 26 | 1 | 0 | -7.039631 | -1.640656 | 0.140216 |
| 27 | 1 | 0 | -4.901273 | -2.855492 | 0.228264 |
| 28 | 1 | 0 | -4.974139 | 2.107323 | -0.254935 |
| 29 | 1 | 0 | -2.418773 | -2.805685 | 0.196158 |
| 30 | 1 | 0 | -2.542524 | 2.137639 | -0.290781 |
| 31 | 1 | 0 | -0.000001 | -2.784819 | 0.182466 |
| 32 | 1 | 0 | 2.418771 | -2.805686 | 0.196158 |
| 33 | 1 | 0 | 2.542523 | 2.137638 | -0.290781 |
| 34 | 1 | 0 | 4.901271 | -2.855493 | 0.228264 |
| 35 | 1 | 0 | 7.039630 | -1.640657 | 0.140216 |
| 36 | 1 | 0 | 7.074391 | 0.838049 | -0.100413 |
| 37 | 1 | 0 | 4.974138 | 2.107322 | -0.254935 |
| 38 | 1 | 0 | 0.865490 | 2.940687 | -0.993908 |
| 39 | 1 | 0 | -0.865492 | 2.940688 | -0.993902 |
| 40 | 1 | 0 | 0.000005 | 4.477221 | 0.765795 |
| 41 | 1 | 0 | -0.881301 | 3.146107 | 1.530333 |
| 42 | 1 | 0 | 0.881312 | 3.146106 | 1.530329 |

R=Sat-Mt

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -1.226423 | 0.202895 | -0.194043 |
| 2 | 6 | 0 | -1.219348 | -1.236422 | 0.030701 |
| 3 | 6 | 0 | 0.000000 | -1.909652 | 0.130238 |
| 4 | 6 | 0 | 1.219348 | -1.236422 | 0.030701 |
| 5 | 6 | 0 | 1.226423 | 0.202895 | -0.194043 |
| 6 | 6 | 0 | 0.000000 | 0.903249 | -0.321556 |
| 7 | 6 | 0 | -2.489702 | 0.839669 | -0.269430 |
| 8 | 6 | 0 | -3.686865 | 0.148242 | -0.146917 |
| 9 | 6 | 0 | -3.668159 | -1.285702 | 0.066268 |
| 10 | 6 | 0 | -2.445582 | -1.929872 | 0.147833 |
| 11 | 6 | 0 | 2.445583 | -1.929872 | 0.147833 |
| 12 | 6 | 0 | 3.668160 | -1.285702 | 0.066268 |
| 13 | 6 | 0 | 3.686866 | 0.148242 | -0.146917 |
| 14 | 6 | 0 | 2.489702 | 0.839669 | -0.269430 |
| 15 | 6 | 0 | 0.000000 | 2.397492 | -0.551027 |
| 16 | 6 | 0 | -0.000001 | 3.223537 | 0.780655 |
| 17 | 6 | 0 | -0.000001 | 4.693481 | 0.555863 |
| 18 | 6 | 0 | 4.918440 | -1.978588 | 0.186822 |
| 19 | 6 | 0 | 6.101296 | -1.308271 | 0.104402 |
| 20 | 6 | 0 | 6.121459 | 0.107820 | -0.104960 |
| 21 | 6 | 0 | 4.958618 | 0.807404 | -0.225403 |
| 22 | 6 | 0 | -4.958618 | 0.807403 | -0.225403 |
| 23 | 6 | 0 | -6.121459 | 0.107820 | -0.104960 |
| 24 | 6 | 0 | -6.101295 | -1.308271 | 0.104402 |
| 25 | 6 | 0 | -4.918440 | -1.978588 | 0.186822 |
| 26 | 1 | 0 | 0.000000 | -2.982276 | 0.296106 |
| 27 | 1 | 0 | -2.543489 | 1.909546 | -0.423280 |
| 28 | 1 | 0 | -2.418375 | -3.003007 | 0.310561 |
| 29 | 1 | 0 | 2.418375 | -3.003007 | 0.310560 |
| 30 | 1 | 0 | 2.543489 | 1.909546 | -0.423280 |
| 31 | 1 | 0 | 0.866878 | 2.691851 | -1.144326 |
| 32 | 1 | 0 | -0.866877 | 2.691851 | -1.144327 |
| 33 | 1 | 0 | -0.878918 | 2.924635 | 1.361166 |
| 34 | 1 | 0 | 0.878915 | 2.924636 | 1.361169 |
| 35 | 1 | 0 | -0.926135 | 5.234917 | 0.402142 |
| 36 | 1 | 0 | 0.926134 | 5.234923 | 0.402174 |
| 37 | 1 | 0 | 4.900937 | -3.051698 | 0.346088 |
| 38 | 1 | 0 | 7.039657 | -1.843286 | 0.197216 |
| 39 | 1 | 0 | 7.074896 | 0.620162 | -0.167241 |
| 40 | 1 | 0 | 4.974962 | 1.880649 | -0.384559 |
| 41 | 1 | 0 | -4.974962 | 1.880649 | -0.384560 |
| 42 | 1 | 0 | -7.074896 | 0.620161 | -0.167241 |
| 43 | 1 | 0 | -7.039657 | -1.843287 | 0.197216 |
| 44 | 1 | 0 | -4.900937 | -3.051698 | 0.346089 |

R=Sat-DCM

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -6.120277 | -0.598072 | 0.098236 |
| 2 | 6 | 0 | -6.100051 | -2.007765 | -0.140188 |
| 3 | 6 | 0 | -4.916517 | -2.678326 | -0.228063 |
| 4 | 6 | 0 | -3.669219 | -1.988000 | -0.083684 |
| 5 | 6 | 0 | -3.688592 | -0.560429 | 0.160376 |
| 6 | 6 | 0 | -4.957509 | 0.099560 | 0.242790 |
| 7 | 6 | 0 | -2.444366 | -2.631216 | -0.171864 |
| 8 | 6 | 0 | -1.221240 | -1.939617 | -0.033086 |
| 9 | 6 | 0 | -1.229667 | -0.507399 | 0.228468 |
| 10 | 6 | 0 | -2.490015 | 0.128796 | 0.309396 |
| 11 | 6 | 0 | 0.000003 | -2.608926 | -0.147923 |
| 12 | 6 | 0 | 1.221244 | -1.939616 | -0.033085 |
| 13 | 6 | 0 | 1.229669 | -0.507397 | 0.228466 |
| 14 | 6 | 0 | 0.000001 | 0.185019 | 0.382870 |
| 15 | 6 | 0 | 2.444371 | -2.631214 | -0.171861 |
| 16 | 6 | 0 | 3.669223 | -1.987996 | -0.083682 |
| 17 | 6 | 0 | 3.688594 | -0.560424 | 0.160373 |
| 18 | 6 | 0 | 2.490016 | 0.128800 | 0.309392 |
| 19 | 6 | 0 | 4.916522 | -2.678321 | -0.228058 |
| 20 | 6 | 0 | 6.100056 | -2.007758 | -0.140185 |
| 21 | 6 | 0 | 6.120279 | -0.598064 | 0.098234 |
| 22 | 6 | 0 | 4.957510 | 0.099567 | 0.242785 |
| 23 | 6 | 0 | 0.000000 | 1.664273 | 0.656522 |
| 24 | 6 | 0 | -0.000008 | 2.508235 | -0.668876 |
| 25 | 6 | 0 | -0.000006 | 3.983980 | -0.394163 |
| 26 | 6 | 0 | 1.210112 | 4.664067 | -0.205907 |
| 27 | 7 | 0 | 2.242208 | 5.180650 | -0.060557 |
| 28 | 6 | 0 | -1.210122 | 4.664068 | -0.205906 |
| 29 | 7 | 0 | -2.242218 | 5.180653 | -0.060552 |
| 30 | 1 | 0 | -7.073309 | -0.085769 | 0.163401 |
| 31 | 1 | 0 | -7.037999 | -2.539635 | -0.251352 |
| 32 | 1 | 0 | -4.898547 | -3.747617 | -0.409985 |
| 33 | 1 | 0 | -4.974580 | 1.169074 | 0.423233 |
| 34 | 1 | 0 | -2.415992 | -3.700416 | -0.357451 |
| 35 | 1 | 0 | -2.549449 | 1.194417 | 0.489238 |
| 36 | 1 | 0 | 0.000003 | -3.676765 | -0.341970 |
| 37 | 1 | 0 | 2.415999 | -3.700414 | -0.357445 |
| 38 | 1 | 0 | 2.549449 | 1.194421 | 0.489231 |
| 39 | 1 | 0 | 4.898553 | -3.747613 | -0.409975 |
| 40 | 1 | 0 | 7.038003 | -2.539628 | -0.251346 |
| 41 | 1 | 0 | 7.073310 | -0.085759 | 0.163396 |
| 42 | 1 | 0 | 4.974580 | 1.169082 | 0.423224 |
| 43 | 1 | 0 | -0.869766 | 1.949954 | 1.248060 |
| 44 | 1 | 0 | 0.869770 | 1.949957 | 1.248053 |
| 45 | 1 | 0 | 0.883505 | 2.246326 | -1.254410 |
| 46 | 1 | 0 | -0.883528 | 2.246327 | -1.254399 |

R=Sat-DPM

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 1.534797 | 1.570390 | -0.281825 |
| 2 | 6 | 0 | 1.734545 | 2.980969 | 0.025803 |
| 3 | 6 | 0 | 0.625291 | 3.803736 | 0.230748 |
| 4 | 6 | 0 | -0.678449 | 3.310805 | 0.147144 |
| 5 | 6 | 0 | -0.892561 | 1.903019 | -0.158786 |
| 6 | 6 | 0 | 0.219279 | 1.047867 | -0.371473 |
| 7 | 6 | 0 | 2.696508 | 0.783674 | -0.479691 |
| 8 | 6 | 0 | 3.980662 | 1.302821 | -0.391446 |
| 9 | 6 | 0 | 4.166792 | 2.706525 | -0.081065 |
| 10 | 6 | 0 | 3.047689 | 3.497002 | 0.115176 |
| 11 | 6 | 0 | -1.791621 | 4.156526 | 0.356460 |
| 12 | 6 | 0 | -3.094060 | 3.693234 | 0.281644 |
| 13 | 6 | 0 | -3.318525 | 2.293949 | -0.023410 |
| 14 | 6 | 0 | -2.233839 | 1.452364 | -0.229123 |
| 15 | 6 | 0 | -0.006251 | -0.422325 | -0.644603 |
| 16 | 6 | 0 | -0.155244 | -1.266235 | 0.661602 |
| 17 | 6 | 0 | -0.430168 | -2.723708 | 0.390609 |
| 18 | 6 | 0 | 0.623904 | -3.702762 | 0.490274 |
| 19 | 6 | 0 | -1.785944 | -3.085183 | -0.041028 |
| 20 | 6 | 0 | 0.348141 | -5.093032 | 0.605143 |
| 21 | 6 | 0 | 1.363551 | -6.027200 | 0.731753 |
| 22 | 6 | 0 | 2.701926 | -5.627920 | 0.751778 |
| 23 | 6 | 0 | 3.003634 | -4.268443 | 0.657385 |
| 24 | 6 | 0 | 1.993340 | -3.326532 | 0.536354 |
| 25 | 6 | 0 | -2.006169 | -3.996991 | -1.097172 |
| 26 | 6 | 0 | -3.289115 | -4.306955 | -1.531029 |
| 27 | 6 | 0 | -4.401188 | -3.725091 | -0.923131 |
| 28 | 6 | 0 | -4.209809 | -2.820475 | 0.120444 |
| 29 | 6 | 0 | -2.926792 | -2.498120 | 0.547875 |
| 30 | 6 | 0 | 5.503588 | 3.219446 | 0.007110 |
| 31 | 6 | 0 | 6.579196 | 2.409408 | -0.198008 |
| 32 | 6 | 0 | 6.397075 | 1.023635 | -0.508196 |
| 33 | 6 | 0 | 5.145930 | 0.492539 | -0.601110 |
| 34 | 6 | 0 | -4.671358 | 1.823329 | -0.105214 |
| 35 | 6 | 0 | -5.721562 | 2.666459 | 0.101473 |

| | | | | | |
|---|---|---|---|---|---|
| 36 | 6 | 0 | -5.498339 | 4.047398 | 0.406033 |
| 37 | 6 | 0 | -4.231769 | 4.541247 | 0.492062 |
| 38 | 1 | 0 | 0.780584 | 4.852661 | 0.462439 |
| 39 | 1 | 0 | 2.599794 | -0.267009 | -0.718836 |
| 40 | 1 | 0 | 3.173183 | 4.550666 | 0.345136 |
| 41 | 1 | 0 | -1.609988 | 5.202916 | 0.582146 |
| 42 | 1 | 0 | -2.442681 | 0.414770 | -0.453783 |
| 43 | 1 | 0 | 0.809188 | -0.834226 | -1.239733 |
| 44 | 1 | 0 | -0.901925 | -0.562639 | -1.251722 |
| 45 | 1 | 0 | -0.974772 | -0.833370 | 1.241643 |
| 46 | 1 | 0 | 0.739371 | -1.141510 | 1.273500 |
| 47 | 1 | 0 | -0.680760 | -5.426755 | 0.628767 |
| 48 | 1 | 0 | 1.110899 | -7.077434 | 0.829918 |
| 49 | 1 | 0 | 3.493638 | -6.361418 | 0.850112 |
| 50 | 1 | 0 | 4.037299 | -3.940585 | 0.679791 |
| 51 | 1 | 0 | 2.266016 | -2.281918 | 0.465736 |
| 52 | 1 | 0 | -1.153421 | -4.440516 | -1.596275 |
| 53 | 1 | 0 | -3.421519 | -4.999941 | -2.354718 |
| 54 | 1 | 0 | -5.401847 | -3.971040 | -1.259347 |
| 55 | 1 | 0 | -5.065072 | -2.368528 | 0.611061 |
| 56 | 1 | 0 | -2.808362 | -1.807719 | 1.374146 |
| 57 | 1 | 0 | 5.639233 | 4.270227 | 0.240952 |
| 58 | 1 | 0 | 7.584676 | 2.808880 | -0.128838 |
| 59 | 1 | 0 | 7.268046 | 0.398620 | -0.670001 |
| 60 | 1 | 0 | 5.008936 | -0.557255 | -0.839141 |
| 61 | 1 | 0 | -4.839454 | 0.777361 | -0.339514 |
| 62 | 1 | 0 | -6.738732 | 2.297030 | 0.035145 |
| 63 | 1 | 0 | -6.350111 | 4.698611 | 0.566814 |
| 64 | 1 | 0 | -4.060735 | 5.587907 | 0.721220 |

R=Sat-Flu

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -1.885502 | -1.226680 | 0.221276 |
| 2 | 6 | 0 | -3.316153 | -1.219308 | -0.053514 |
| 3 | 6 | 0 | -3.984214 | 0.000132 | -0.181598 |
| 4 | 6 | 0 | -3.316067 | 1.219525 | -0.053504 |
| 5 | 6 | 0 | -1.885416 | 1.226794 | 0.221285 |
| 6 | 6 | 0 | -1.187713 | 0.000032 | 0.360448 |
| 7 | 6 | 0 | -1.256075 | -2.490734 | 0.335777 |
| 8 | 6 | 0 | -1.945932 | -3.687675 | 0.200995 |
| 9 | 6 | 0 | -3.369452 | -3.668208 | -0.072652 |
| 10 | 6 | 0 | -4.006925 | -2.445027 | -0.189707 |
| 11 | 6 | 0 | -4.006754 | 2.445293 | -0.189687 |
| 12 | 6 | 0 | -3.369195 | 3.668429 | -0.072623 |
| 13 | 6 | 0 | -1.945675 | 3.687794 | 0.201025 |
| 14 | 6 | 0 | -1.255901 | 2.490803 | 0.335797 |
| 15 | 6 | 0 | 0.303698 | -0.000021 | 0.606434 |
| 16 | 6 | 0 | 1.133094 | -0.000052 | -0.718995 |
| 17 | 6 | 0 | 2.603953 | -0.000091 | -0.474567 |
| 18 | 6 | 0 | 3.438108 | -1.158841 | -0.293381 |
| 19 | 6 | 0 | 4.769463 | -0.732703 | 0.005260 |
| 20 | 6 | 0 | 4.769507 | 0.732410 | 0.005230 |
| 21 | 6 | 0 | 3.438177 | 1.158615 | -0.293427 |
| 22 | 6 | 0 | 5.772721 | 1.663780 | 0.222218 |
| 23 | 6 | 0 | 5.464052 | 3.027522 | 0.141772 |
| 24 | 6 | 0 | 4.165058 | 3.451858 | -0.157253 |
| 25 | 6 | 0 | 3.146425 | 2.526787 | -0.376653 |
| 26 | 6 | 0 | 3.146273 | -2.526998 | -0.376552 |
| 27 | 6 | 0 | 4.164850 | -3.452122 | -0.157115 |
| 28 | 6 | 0 | 5.463870 | -3.027851 | 0.141894 |
| 29 | 6 | 0 | 5.772621 | -1.664125 | 0.222286 |
| 30 | 6 | 0 | -1.294741 | 4.960043 | 0.326524 |
| 31 | 6 | 0 | -1.991911 | 6.122499 | 0.189451 |
| 32 | 6 | 0 | -3.396983 | 6.101608 | -0.084008 |
| 33 | 6 | 0 | -4.059708 | 4.918285 | -0.209554 |
| 34 | 6 | 0 | -4.060051 | -4.918015 | -0.209594 |
| 35 | 6 | 0 | -3.397410 | -6.101386 | -0.084059 |
| 36 | 6 | 0 | -1.992339 | -6.122377 | 0.189399 |
| 37 | 6 | 0 | -1.295087 | -4.959971 | 0.326483 |
| 38 | 1 | 0 | -5.049529 | 0.000170 | -0.389214 |
| 39 | 1 | 0 | -0.195148 | -2.546406 | 0.541574 |
| 40 | 1 | 0 | -5.073085 | -2.416897 | -0.392904 |
| 41 | 1 | 0 | -5.072915 | 2.417239 | -0.392885 |
| 42 | 1 | 0 | -0.194970 | 2.546400 | 0.541595 |
| 43 | 1 | 0 | 0.595338 | 0.866093 | 1.201164 |
| 44 | 1 | 0 | 0.595276 | -0.866155 | 1.201165 |
| 45 | 1 | 0 | 0.846859 | -0.876823 | -1.307247 |
| 46 | 1 | 0 | 0.846907 | 0.876726 | -1.307259 |
| 47 | 1 | 0 | 6.785836 | 1.349886 | 0.449911 |
| 48 | 1 | 0 | 6.242229 | 3.763496 | 0.309212 |
| 49 | 1 | 0 | 3.951173 | 4.512716 | -0.222133 |
| 50 | 1 | 0 | 2.145882 | 2.867135 | -0.620825 |
| 51 | 1 | 0 | 2.145709 | -2.867295 | -0.620710 |
| 52 | 1 | 0 | 3.950901 | -4.512970 | -0.221951 |
| 53 | 1 | 0 | 6.242002 | -3.763865 | 0.309364 |
| 54 | 1 | 0 | 6.785755 | -1.350283 | 0.449967 |
| 55 | 1 | 0 | -0.230456 | 4.977103 | 0.537257 |
| 56 | 1 | 0 | -1.486069 | 7.076323 | 0.287993 |
| 57 | 1 | 0 | -3.929941 | 7.039770 | -0.189406 |
| 58 | 1 | 0 | -5.124805 | 4.900106 | -0.415484 |
| 59 | 1 | 0 | -5.125148 | -4.899760 | -0.415524 |
| 60 | 1 | 0 | -3.930433 | -7.039510 | -0.189464 |
| 61 | 1 | 0 | -1.486562 | -7.076237 | 0.287933 |
| 62 | 1 | 0 | -0.230803 | -4.977107 | 0.537215 |

R=Sat-PhO

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -1.227470 | -1.109424 | -0.210135 |
| 2 | 6 | 0 | -1.220214 | -2.544646 | 0.038975 |
| 3 | 6 | 0 | -0.000746 | -3.215328 | 0.152164 |
| 4 | 6 | 0 | 1.219016 | -2.545185 | 0.038952 |
| 5 | 6 | 0 | 1.226901 | -1.109966 | -0.210153 |
| 6 | 6 | 0 | -0.000131 | -0.412192 | -0.343501 |
| 7 | 6 | 0 | -2.491418 | -0.476439 | -0.303040 |
| 8 | 6 | 0 | -3.688318 | -1.167426 | -0.173073 |
| 9 | 6 | 0 | -3.668797 | -2.596716 | 0.068716 |
| 10 | 6 | 0 | -2.445589 | -3.237496 | 0.165923 |
| 11 | 6 | 0 | 2.444086 | -3.238578 | 0.165874 |
| 12 | 6 | 0 | 3.667576 | -2.598340 | 0.068650 |
| 13 | 6 | 0 | 3.687725 | -1.169056 | -0.173129 |
| 14 | 6 | 0 | 2.491129 | -0.477539 | -0.303072 |
| 15 | 6 | 0 | 0.000198 | 1.080725 | -0.582809 |
| 16 | 6 | 0 | 0.000384 | 1.902406 | 0.743197 |
| 17 | 6 | 0 | 0.000784 | 3.385185 | 0.497580 |
| 18 | 6 | 0 | 1.218062 | 4.093446 | 0.358308 |
| 19 | 6 | 0 | 1.235030 | 5.439025 | 0.089417 |
| 20 | 6 | 0 | 0.001547 | 6.189585 | -0.063917 |
| 21 | 6 | 0 | -1.232350 | 5.439525 | 0.088555 |
| 22 | 6 | 0 | -1.216115 | 4.093944 | 0.357459 |
| 23 | 8 | 0 | 0.001881 | 7.415458 | -0.309411 |
| 24 | 6 | 0 | -4.960645 | -0.512446 | -0.272328 |
| 25 | 6 | 0 | -6.122655 | -1.211772 | -0.142768 |
| 26 | 6 | 0 | -6.101572 | -2.622947 | 0.096731 |
| 27 | 6 | 0 | -4.918119 | -3.289451 | 0.198233 |
| 28 | 6 | 0 | 4.916594 | -3.291628 | 0.198140 |
| 29 | 6 | 0 | 6.100339 | -2.625646 | 0.096623 |
| 30 | 6 | 0 | 6.122043 | -1.214478 | -0.142864 |
| 31 | 6 | 0 | 4.960339 | -0.514638 | -0.272399 |
| 32 | 1 | 0 | -0.000981 | -4.284570 | 0.338361 |
| 33 | 1 | 0 | -2.547949 | 0.589223 | -0.483057 |
| 34 | 1 | 0 | -2.417262 | -4.307511 | 0.347377 |
| 35 | 1 | 0 | 2.415289 | -4.308582 | 0.347323 |
| 36 | 1 | 0 | 2.548129 | 0.588100 | -0.483079 |
| 37 | 1 | 0 | 0.866635 | 1.372737 | -1.177933 |
| 38 | 1 | 0 | -0.866113 | 1.373119 | -1.177931 |
| 39 | 1 | 0 | -0.878769 | 1.619826 | 1.328771 |
| 40 | 1 | 0 | 0.879352 | 1.619359 | 1.328819 |
| 41 | 1 | 0 | 2.152712 | 3.553876 | 0.478038 |
| 42 | 1 | 0 | 2.161332 | 5.992279 | -0.012874 |
| 43 | 1 | 0 | -2.158355 | 5.993156 | -0.014382 |
| 44 | 1 | 0 | -2.151068 | 3.554756 | 0.476544 |
| 45 | 1 | 0 | -4.978916 | 0.556883 | -0.455573 |
| 46 | 1 | 0 | -7.076551 | -0.702636 | -0.221183 |
| 47 | 1 | 0 | -7.039561 | -3.157188 | 0.196306 |
| 48 | 1 | 0 | -4.899410 | -4.358978 | 0.379384 |
| 49 | 1 | 0 | 4.897415 | -4.361148 | 0.379281 |
| 50 | 1 | 0 | 7.038094 | -3.160303 | 0.196178 |
| 51 | 1 | 0 | 7.076162 | -0.705764 | -0.221292 |
| 52 | 1 | 0 | 4.979080 | 0.554684 | -0.455639 |

R=Sat-NO

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 1.150488 | -0.294337 | 0.196591 |
| 2 | 6 | 0 | 1.091812 | -1.730553 | -0.034137 |
| 3 | 6 | 0 | -0.152189 | -2.357757 | -0.136350 |
| 4 | 6 | 0 | -1.346867 | -1.641685 | -0.034865 |
| 5 | 6 | 0 | -1.303200 | -0.204001 | 0.199080 |
| 6 | 6 | 0 | -0.051448 | 0.446434 | 0.331645 |
| 7 | 6 | 0 | 2.433201 | 0.303196 | 0.271351 |
| 8 | 6 | 0 | 3.604663 | -0.431421 | 0.144613 |
| 9 | 6 | 0 | 3.536617 | -1.863772 | -0.068982 |
| 10 | 6 | 0 | 2.292652 | -2.466318 | -0.152654 |
| 11 | 6 | 0 | -2.597145 | -2.289668 | -0.158296 |
| 12 | 6 | 0 | -3.796127 | -1.602946 | -0.074113 |
| 13 | 6 | 0 | -3.764241 | -0.170613 | 0.149141 |
| 14 | 6 | 0 | -2.543359 | 0.476595 | 0.277555 |
| 15 | 6 | 0 | 0.025128 | 1.933152 | 0.585477 |
| 16 | 6 | 0 | 0.203271 | 2.753468 | -0.715578 |
| 17 | 7 | 0 | 0.591594 | 4.138165 | -0.436315 |
| 18 | 6 | 0 | -0.419688 | 5.177933 | -0.259204 |
| 19 | 8 | 0 | 1.738692 | 4.326769 | 0.097607 |
| 20 | 6 | 0 | -5.069899 | -2.250337 | -0.201327 |
| 21 | 6 | 0 | -6.228603 | -1.539566 | -0.115546 |
| 22 | 6 | 0 | -6.198844 | -0.125243 | 0.104453 |
| 23 | 6 | 0 | -5.012300 | 0.532073 | 0.231335 |
| 24 | 6 | 0 | 4.897303 | 0.186005 | 0.219041 |
| 25 | 6 | 0 | 6.035329 | -0.553169 | 0.096737 |
| 26 | 6 | 0 | 5.966925 | -1.967926 | -0.110627 |
| 27 | 6 | 0 | 4.762329 | -2.598832 | -0.190807 |
| 28 | 1 | 0 | -0.191583 | -3.429114 | -0.305899 |
| 29 | 1 | 0 | 2.526354 | 1.372339 | 0.415913 |
| 30 | 1 | 0 | 2.228715 | -3.537477 | -0.318024 |
| 31 | 1 | 0 | -2.608145 | -3.361921 | -0.328399 |

| | | | | | |
|---|---|---|---|---|---|
| 32 | 1 | 0 | -2.560174 | 1.546796 | 0.439784 |
| 33 | 1 | 0 | -0.859397 | 2.282735 | 1.119674 |
| 34 | 1 | 0 | 0.875763 | 2.165057 | 1.227535 |
| 35 | 1 | 0 | 1.002706 | 2.319888 | -1.318771 |
| 36 | 1 | 0 | -0.713313 | 2.754716 | -1.309751 |
| 37 | 1 | 0 | 0.078991 | 6.140691 | -0.360673 |
| 38 | 1 | 0 | -1.197181 | 5.079267 | -1.018940 |
| 39 | 1 | 0 | -0.876533 | 5.120474 | 0.737022 |
| 40 | 1 | 0 | -5.089868 | -3.322236 | -0.368116 |
| 41 | 1 | 0 | -7.185106 | -2.040394 | -0.213182 |
| 42 | 1 | 0 | -7.133699 | 0.419862 | 0.170246 |
| 43 | 1 | 0 | -4.991728 | 1.603934 | 0.399629 |
| 44 | 1 | 0 | 4.947685 | 1.258214 | 0.375868 |
| 45 | 1 | 0 | 7.005639 | -0.073241 | 0.155936 |
| 46 | 1 | 0 | 6.886651 | -2.534323 | -0.204362 |
| 47 | 1 | 0 | 4.708690 | -3.670848 | -0.349346 |

R=Sat-Allyl

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -1.226094 | -0.222175 | -0.211299 |
| 2 | 6 | 0 | -1.219206 | -1.654045 | 0.057263 |
| 3 | 6 | 0 | 0.000005 | -2.323561 | 0.179247 |
| 4 | 6 | 0 | 1.219214 | -1.654042 | 0.057262 |
| 5 | 6 | 0 | 1.226099 | -0.222172 | -0.211300 |
| 6 | 6 | 0 | 0.000002 | 0.474981 | -0.354484 |
| 7 | 6 | 0 | -2.489888 | 0.410579 | -0.312876 |
| 8 | 6 | 0 | -3.686810 | -0.277713 | -0.173745 |
| 9 | 6 | 0 | -3.668013 | -1.703938 | 0.086760 |
| 10 | 6 | 0 | -2.445448 | -2.344179 | 0.193196 |
| 11 | 6 | 0 | 2.445458 | -2.344173 | 0.193196 |
| 12 | 6 | 0 | 3.668022 | -1.703929 | 0.086760 |
| 13 | 6 | 0 | 3.686815 | -0.277703 | -0.173743 |
| 14 | 6 | 0 | 2.489892 | 0.410585 | -0.312875 |
| 15 | 6 | 0 | -0.000001 | 1.964961 | -0.621064 |
| 16 | 6 | 0 | -0.000006 | 2.817644 | 0.674423 |
| 17 | 6 | 0 | -0.000017 | 4.309519 | 0.383317 |
| 18 | 6 | 0 | 1.211188 | 4.971851 | 0.239415 |
| 19 | 6 | 0 | -1.211232 | 4.971838 | 0.239438 |
| 20 | 6 | 0 | 4.918340 | -2.393557 | 0.225142 |
| 21 | 6 | 0 | 6.101285 | -1.727524 | 0.115198 |
| 22 | 6 | 0 | 6.121630 | -0.319233 | -0.142047 |
| 23 | 6 | 0 | 4.958943 | 0.377032 | -0.280669 |
| 24 | 6 | 0 | -4.958939 | 0.377018 | -0.280672 |
| 25 | 6 | 0 | -6.121625 | -0.319249 | -0.142050 |
| 26 | 6 | 0 | -6.101276 | -1.727539 | 0.115196 |
| 27 | 6 | 0 | -4.918329 | -2.393569 | 0.225141 |
| 28 | 1 | 0 | 0.000007 | -3.390405 | 0.378971 |
| 29 | 1 | 0 | -2.543798 | 1.474359 | -0.503951 |
| 30 | 1 | 0 | -2.418081 | -3.411644 | 0.389679 |
| 31 | 1 | 0 | 2.418094 | -3.411637 | 0.389679 |
| 32 | 1 | 0 | 2.543799 | 1.474366 | -0.503948 |
| 33 | 1 | 0 | 0.865602 | 2.242303 | -1.225204 |
| 34 | 1 | 0 | -0.865602 | 2.242298 | -1.225211 |
| 35 | 1 | 0 | -0.876665 | 2.556313 | 1.273271 |
| 36 | 1 | 0 | 0.876659 | 2.556327 | 1.273268 |
| 37 | 1 | 0 | 1.247558 | 6.028123 | -0.000518 |
| 38 | 1 | 0 | 2.156052 | 4.459552 | 0.375861 |
| 39 | 1 | 0 | -1.247617 | 6.028108 | -0.000494 |
| 40 | 1 | 0 | -2.156085 | 4.459524 | 0.375899 |
| 41 | 1 | 0 | 4.900653 | -3.460740 | 0.420169 |
| 42 | 1 | 0 | 7.039643 | -2.259958 | 0.221793 |
| 43 | 1 | 0 | 7.075217 | 0.189679 | -0.226259 |
| 44 | 1 | 0 | 4.975627 | 1.444143 | -0.476743 |
| 45 | 1 | 0 | -4.975626 | 1.444129 | -0.476747 |
| 46 | 1 | 0 | -7.075212 | 0.189661 | -0.226263 |
| 47 | 1 | 0 | -7.039632 | -2.259976 | 0.221791 |
| 48 | 1 | 0 | -4.900640 | -3.460752 | 0.420169 |

R=Sat-IN

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 1.050030 | 1.658255 | 0.167697 |
| 2 | 6 | 0 | 2.335048 | 2.312576 | -0.034656 |
| 3 | 6 | 0 | 3.494292 | 1.536914 | -0.109973 |
| 4 | 6 | 0 | 3.453906 | 0.144298 | -0.012906 |
| 5 | 6 | 0 | 2.174480 | -0.522831 | 0.190368 |
| 6 | 6 | 0 | 0.992079 | 0.248671 | 0.302060 |
| 7 | 6 | 0 | -0.103433 | 2.480691 | 0.211902 |
| 8 | 6 | 0 | -0.035920 | 3.861184 | 0.082576 |
| 9 | 6 | 0 | 1.249615 | 4.506538 | -0.100118 |
| 10 | 6 | 0 | 2.387975 | 3.720128 | -0.153877 |
| 11 | 6 | 0 | 4.633704 | -0.628295 | -0.111601 |
| 12 | 6 | 0 | 4.619053 | -2.010359 | -0.035382 |
| 13 | 6 | 0 | 3.348937 | -2.684868 | 0.151210 |
| 14 | 6 | 0 | 2.184210 | -1.938274 | 0.258390 |
| 15 | 6 | 0 | -0.342141 | -0.422606 | 0.543307 |
| 16 | 6 | 0 | -1.102260 | -0.744729 | -0.770078 |
| 17 | 6 | 0 | -2.462902 | -1.305215 | -0.513862 |
| 18 | 7 | 0 | -3.477342 | -0.460992 | -0.036798 |
| 19 | 6 | 0 | -4.665119 | -1.285306 | 0.360863 |
| 20 | 6 | 0 | -4.294029 | -2.626358 | -0.389671 |
| 21 | 7 | 0 | -2.833294 | -2.523276 | -0.666956 |
| 22 | 6 | 0 | -4.558495 | -3.901353 | 0.417530 |
| 23 | 6 | 0 | -4.974107 | -2.755994 | -1.766001 |
| 24 | 6 | 0 | -5.948675 | -0.579287 | -0.074688 |
| 25 | 6 | 0 | -4.629051 | -1.388703 | 1.895983 |
| 26 | 8 | 0 | -3.360795 | 0.775431 | 0.217276 |
| 27 | 6 | 0 | 3.343572 | -4.118052 | 0.219014 |
| 28 | 6 | 0 | 4.499945 | -4.830697 | 0.115238 |
| 29 | 6 | 0 | 5.753609 | -4.163189 | -0.065891 |
| 30 | 6 | 0 | 5.809515 | -2.804277 | -0.138632 |
| 31 | 6 | 0 | 1.288436 | 5.935209 | -0.224526 |
| 32 | 6 | 0 | 0.144334 | 6.672902 | -0.176043 |
| 33 | 6 | 0 | -1.126072 | 6.036215 | -0.000627 |
| 34 | 6 | 0 | -1.211999 | 4.682132 | 0.123166 |
| 35 | 1 | 0 | 4.450888 | 2.028612 | -0.256283 |
| 36 | 1 | 0 | -1.083445 | 2.036128 | 0.332713 |
| 37 | 1 | 0 | 3.355783 | 4.191087 | -0.297026 |
| 38 | 1 | 0 | 5.578043 | -0.112551 | -0.256966 |
| 39 | 1 | 0 | 1.254596 | -2.477504 | 0.388332 |
| 40 | 1 | 0 | -0.207369 | -1.347523 | 1.105760 |
| 41 | 1 | 0 | -0.969400 | 0.217241 | 1.164265 |
| 42 | 1 | 0 | -1.206581 | 0.171476 | -1.357317 |
| 43 | 1 | 0 | -0.546463 | -1.470744 | -1.364000 |
| 44 | 1 | 0 | -4.241759 | -4.764783 | -0.170630 |
| 45 | 1 | 0 | -4.000871 | -3.916618 | 1.353927 |
| 46 | 1 | 0 | -5.623073 | -4.012240 | 0.643141 |
| 47 | 1 | 0 | -6.053324 | -2.896848 | -1.666950 |
| 48 | 1 | 0 | -4.791566 | -1.878438 | -2.389452 |
| 49 | 1 | 0 | -4.557575 | -3.622490 | -2.282587 |
| 50 | 1 | 0 | -6.011445 | 0.390198 | 0.422887 |
| 51 | 1 | 0 | -5.981641 | -0.406695 | -1.149922 |
| 52 | 1 | 0 | -6.821845 | -1.170581 | 0.211274 |
| 53 | 1 | 0 | -5.476944 | -1.966983 | 2.267929 |
| 54 | 1 | 0 | -3.708283 | -1.856476 | 2.249110 |
| 55 | 1 | 0 | -4.683128 | -0.382754 | 2.317225 |
| 56 | 1 | 0 | 2.393782 | -4.624554 | 0.355837 |
| 57 | 1 | 0 | 4.479695 | -5.913355 | 0.169124 |
| 58 | 1 | 0 | 6.660460 | -4.751998 | -0.145627 |
| 59 | 1 | 0 | 6.758320 | -2.296506 | -0.277332 |
| 60 | 1 | 0 | 2.251542 | 6.416419 | -0.359565 |
| 61 | 1 | 0 | 0.186937 | 7.752122 | -0.271616 |
| 62 | 1 | 0 | -2.022804 | 6.644723 | 0.032611 |
| 63 | 1 | 0 | -2.172922 | 4.196148 | 0.254568 |

R=Sat-Phen

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -2.263480 | 1.226200 | -0.204810 |
| 2 | 6 | 0 | -3.704307 | 1.219211 | 0.010551 |
| 3 | 6 | 0 | -4.377769 | -0.000006 | 0.108017 |
| 4 | 6 | 0 | -3.704302 | -1.219220 | 0.010548 |
| 5 | 6 | 0 | -2.263475 | -1.226204 | -0.204813 |
| 6 | 6 | 0 | -1.561435 | -0.000001 | -0.321109 |
| 7 | 6 | 0 | -1.627880 | 2.490146 | -0.283921 |
| 8 | 6 | 0 | -2.321119 | 3.687007 | -0.171008 |
| 9 | 6 | 0 | -3.755834 | 3.667995 | 0.037477 |
| 10 | 6 | 0 | -4.399226 | 2.445303 | 0.120794 |
| 11 | 6 | 0 | -4.399217 | -2.445315 | 0.120789 |
| 12 | 6 | 0 | -3.755820 | -3.668005 | 0.037470 |
| 13 | 6 | 0 | -2.321105 | -3.687011 | -0.171015 |
| 14 | 6 | 0 | -1.627871 | -2.490148 | -0.283926 |
| 15 | 6 | 0 | -0.062111 | 0.000002 | -0.527566 |
| 16 | 6 | 0 | 0.736500 | 0.000000 | 0.804317 |
| 17 | 6 | 0 | 2.232790 | 0.000002 | 0.584286 |
| 18 | 6 | 0 | 2.931601 | -1.201667 | 0.463878 |
| 19 | 6 | 0 | 4.325364 | -1.234199 | 0.217687 |
| 20 | 6 | 0 | 5.031825 | 0.000006 | 0.091208 |
| 21 | 6 | 0 | 4.325357 | 1.234209 | 0.217668 |
| 22 | 6 | 0 | 2.931595 | 1.201673 | 0.463859 |
| 23 | 6 | 0 | 6.438888 | 0.000008 | -0.155113 |
| 24 | 6 | 0 | 7.110351 | 1.241985 | -0.271704 |
| 25 | 6 | 0 | 6.415930 | 2.439641 | -0.146292 |
| 26 | 6 | 0 | 5.047070 | 2.447465 | 0.095500 |
| 27 | 6 | 0 | 5.047084 | -2.447454 | 0.095538 |
| 28 | 6 | 0 | 6.415943 | -2.439626 | -0.146254 |
| 29 | 6 | 0 | 7.110358 | -1.241967 | -0.271686 |
| 30 | 6 | 0 | -1.663403 | -4.959274 | -0.255400 |
| 31 | 6 | 0 | -2.364582 | -6.121826 | -0.142866 |
| 32 | 6 | 0 | -3.781197 | -6.101241 | 0.063524 |
| 33 | 6 | 0 | -4.450400 | -4.918153 | 0.150082 |
| 34 | 6 | 0 | -4.450418 | 4.918140 | 0.150091 |
| 35 | 6 | 0 | -3.781219 | 6.101231 | 0.063534 |
| 36 | 6 | 0 | -2.364604 | 6.121821 | -0.142856 |
| 37 | 6 | 0 | -1.663421 | 4.959272 | -0.255392 |
| 38 | 1 | 0 | -5.451199 | -0.000008 | 0.268568 |
| 39 | 1 | 0 | -0.558020 | 2.544441 | -0.437186 |
| 40 | 1 | 0 | -5.473179 | 2.417709 | 0.277878 |
| 41 | 1 | 0 | -5.473171 | -2.417725 | 0.277873 |
| 42 | 1 | 0 | -0.558011 | -2.544438 | -0.437190 |
| 43 | 1 | 0 | 0.240376 | -0.865446 | -1.119582 |
| 44 | 1 | 0 | 0.240374 | 0.865453 | -1.119579 |
| 45 | 1 | 0 | 0.447200 | 0.876568 | 1.390880 |
| 46 | 1 | 0 | 0.447203 | -0.876573 | 1.390875 |
| 47 | 1 | 0 | 2.401560 | -2.143387 | 0.570844 |

| | | | | | |
|---|---|---|---|---|---|
| 48 | 1 | 0 | 2.401548 | 2.143392 | 0.570811 |
| 49 | 1 | 0 | 8.178483 | 1.246840 | -0.459560 |
| 50 | 1 | 0 | 6.948818 | 3.379728 | -0.237457 |
| 51 | 1 | 0 | 4.515603 | 3.387907 | 0.192985 |
| 52 | 1 | 0 | 4.515622 | -3.387897 | 0.193038 |
| 53 | 1 | 0 | 6.948836 | -3.379711 | -0.237405 |
| 54 | 1 | 0 | 8.178490 | -1.246820 | -0.459541 |
| 55 | 1 | 0 | -0.589981 | -4.976230 | -0.413306 |
| 56 | 1 | 0 | -1.853310 | -7.075527 | -0.209633 |
| 57 | 1 | 0 | -4.317383 | -7.039500 | 0.150181 |
| 58 | 1 | 0 | -5.523930 | -4.900223 | 0.306347 |
| 59 | 1 | 0 | -5.523948 | 4.900206 | 0.306357 |
| 60 | 1 | 0 | -4.317409 | 7.039488 | 0.150193 |
| 61 | 1 | 0 | -1.853336 | 7.075525 | -0.209622 |
| 62 | 1 | 0 | -0.589999 | 4.976232 | -0.413298 |

R=Sat-Ver

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -2.914404 | -1.226759 | -0.227734 |
| 2 | 6 | 0 | -4.358650 | -1.219866 | -0.038352 |
| 3 | 6 | 0 | -5.033848 | -0.000061 | 0.043337 |
| 4 | 6 | 0 | -4.358700 | 1.219769 | -0.038365 |
| 5 | 6 | 0 | -2.914454 | 1.226720 | -0.227748 |
| 6 | 6 | 0 | -2.214428 | -0.000006 | -0.340699 |
| 7 | 6 | 0 | -2.272496 | -2.488888 | -0.283700 |
| 8 | 6 | 0 | -2.966405 | -3.685921 | -0.176174 |
| 9 | 6 | 0 | -4.405725 | -3.668399 | -0.000905 |
| 10 | 6 | 0 | -5.053642 | -2.446687 | 0.062636 |
| 11 | 6 | 0 | -5.053741 | 2.446563 | 0.062611 |
| 12 | 6 | 0 | -4.405873 | 3.668301 | -0.000942 |
| 13 | 6 | 0 | -2.966554 | 3.685880 | -0.176212 |
| 14 | 6 | 0 | -2.272597 | 2.488873 | -0.283726 |
| 15 | 6 | 0 | -0.716696 | 0.000022 | -0.550926 |
| 16 | 6 | 0 | 0.082591 | 0.000046 | 0.776703 |
| 17 | 6 | 0 | 1.568149 | 0.000042 | 0.528583 |
| 18 | 7 | 0 | 2.147363 | 1.186422 | 0.399821 |
| 19 | 7 | 0 | 3.487091 | 1.171768 | 0.119778 |
| 20 | 6 | 0 | 4.251723 | 0.000035 | 0.006883 |
| 21 | 7 | 0 | 3.487080 | -1.171694 | 0.119755 |
| 22 | 7 | 0 | 2.147352 | -1.186341 | 0.399794 |
| 23 | 6 | 0 | 4.104477 | -2.467973 | 0.071137 |
| 24 | 6 | 0 | 5.155870 | -2.746408 | -0.806661 |
| 25 | 6 | 0 | 5.695576 | -4.028492 | -0.840917 |
| 26 | 6 | 0 | 5.198977 | -5.033452 | -0.014496 |
| 27 | 6 | 0 | 4.147246 | -4.749193 | 0.853867 |
| 28 | 6 | 0 | 3.598335 | -3.472906 | 0.900353 |
| 29 | 6 | 0 | 4.104498 | 2.468043 | 0.071180 |
| 30 | 6 | 0 | 3.598364 | 3.472965 | 0.900414 |
| 31 | 6 | 0 | 4.147284 | 4.749249 | 0.853949 |
| 32 | 6 | 0 | 5.199016 | 5.033515 | -0.014411 |
| 33 | 6 | 0 | 5.695607 | 4.028565 | -0.840849 |
| 34 | 6 | 0 | 5.155891 | 2.746484 | -0.806615 |
| 35 | 8 | 0 | 5.448418 | 0.000032 | -0.172436 |
| 36 | 6 | 0 | -2.303442 | 4.956907 | -0.233908 |
| 37 | 6 | 0 | -3.004935 | 6.120082 | -0.129644 |
| 38 | 6 | 0 | -4.426280 | 6.101277 | 0.041655 |
| 39 | 6 | 0 | -5.100211 | 4.919298 | 0.103694 |
| 40 | 6 | 0 | -5.100013 | -4.919423 | 0.103743 |
| 41 | 6 | 0 | -4.426034 | -6.101376 | 0.041716 |
| 42 | 6 | 0 | -3.004688 | -6.120124 | -0.129581 |
| 43 | 6 | 0 | -2.303241 | -4.956923 | -0.233856 |
| 44 | 1 | 0 | -6.110476 | -0.000082 | 0.181201 |
| 45 | 1 | 0 | -1.198093 | -2.542437 | -0.404169 |
| 46 | 1 | 0 | -6.130579 | -2.420763 | 0.198202 |
| 47 | 1 | 0 | -6.130677 | 2.420598 | 0.198178 |
| 48 | 1 | 0 | -1.198196 | 2.542464 | -0.404197 |
| 49 | 1 | 0 | -0.416770 | -0.868692 | -1.139057 |
| 50 | 1 | 0 | -0.416804 | 0.868740 | -1.139068 |
| 51 | 1 | 0 | -0.176784 | 0.883885 | 1.361970 |
| 52 | 1 | 0 | -0.176785 | -0.883773 | 1.362002 |
| 53 | 1 | 0 | 5.553673 | -1.972417 | -1.444046 |
| 54 | 1 | 0 | 6.510489 | -4.238963 | -1.523883 |
| 55 | 1 | 0 | 5.627152 | -6.028561 | -0.046989 |
| 56 | 1 | 0 | 3.752040 | -5.521549 | 1.503682 |
| 57 | 1 | 0 | 2.775510 | -3.245722 | 1.563260 |
| 58 | 1 | 0 | 2.775538 | 3.245775 | 1.563319 |
| 59 | 1 | 0 | 3.752084 | 5.521596 | 1.503778 |
| 60 | 1 | 0 | 5.627198 | 6.028621 | -0.046887 |
| 61 | 1 | 0 | 6.510521 | 4.239041 | -1.523813 |
| 62 | 1 | 0 | 5.553689 | 1.972501 | -1.444012 |
| 63 | 1 | 0 | -1.226443 | 4.971290 | -0.364719 |
| 64 | 1 | 0 | -2.490160 | 7.073097 | -0.176593 |
| 65 | 1 | 0 | -4.962434 | 7.040169 | 0.121895 |
| 66 | 1 | 0 | -6.177223 | 4.902952 | 0.234165 |
| 67 | 1 | 0 | -6.177025 | -4.903119 | 0.234212 |
| 68 | 1 | 0 | -4.962149 | -7.040288 | 0.121965 |
| 69 | 1 | 0 | -2.489874 | -7.073120 | -0.176521 |
| 70 | 1 | 0 | -1.226242 | -4.971263 | -0.364666 |

R=Sat-NN

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -2.010793 | -6.092416 | 0.068103 |
| 2 | 6 | 0 | -3.433629 | -6.052173 | -0.086663 |
| 3 | 6 | 0 | -4.091696 | -4.860525 | -0.133519 |
| 4 | 6 | 0 | -3.378773 | -3.620110 | -0.027438 |
| 5 | 6 | 0 | -1.938418 | -3.659946 | 0.136578 |
| 6 | 6 | 0 | -1.291728 | -4.940176 | 0.174543 |
| 7 | 6 | 0 | -4.009325 | -2.388792 | -0.084758 |
| 8 | 6 | 0 | -3.295278 | -1.172862 | 0.014893 |
| 9 | 6 | 0 | -1.851713 | -1.204015 | 0.205403 |
| 10 | 6 | 0 | -1.225438 | -2.474587 | 0.249937 |
| 11 | 6 | 0 | -3.949159 | 0.058826 | -0.068701 |
| 12 | 6 | 0 | -3.252408 | 1.267692 | 0.000843 |
| 13 | 6 | 0 | -1.808682 | 1.250256 | 0.191637 |
| 14 | 6 | 0 | -1.135308 | 0.011621 | 0.325704 |
| 15 | 6 | 0 | -3.923296 | 2.506730 | -0.112954 |
| 16 | 6 | 0 | -3.249786 | 3.715678 | -0.069230 |
| 17 | 6 | 0 | -1.808978 | 3.706636 | 0.095224 |
| 18 | 6 | 0 | -1.137938 | 2.498376 | 0.222444 |
| 19 | 6 | 0 | -3.918556 | 4.979153 | -0.189700 |
| 20 | 6 | 0 | -3.218897 | 6.147327 | -0.155802 |
| 21 | 6 | 0 | -1.795559 | 6.139189 | -0.000644 |
| 22 | 6 | 0 | -1.117529 | 4.963609 | 0.119170 |
| 23 | 6 | 0 | 0.353169 | -0.012602 | 0.584117 |
| 24 | 6 | 0 | 1.196841 | -0.032376 | -0.719501 |
| 25 | 6 | 0 | 2.647904 | -0.043909 | -0.426526 |
| 26 | 7 | 0 | 3.398421 | 1.056096 | -0.238511 |
| 27 | 6 | 0 | 4.791888 | 0.704177 | 0.231440 |
| 28 | 6 | 0 | 4.856593 | -0.826409 | -0.126847 |
| 29 | 7 | 0 | 3.386475 | -1.155644 | -0.256434 |
| 30 | 8 | 0 | 2.967831 | -2.354664 | -0.345362 |
| 31 | 8 | 0 | 2.987188 | 2.260827 | -0.279249 |
| 32 | 6 | 0 | 5.478699 | -1.132077 | -1.499221 |
| 33 | 6 | 0 | 5.480801 | -1.729369 | 0.935396 |
| 34 | 6 | 0 | 4.815050 | 1.003380 | 1.739219 |
| 35 | 6 | 0 | 5.802278 | 1.596395 | -0.487539 |
| 36 | 1 | 0 | -1.508783 | -7.052882 | 0.099210 |
| 37 | 1 | 0 | -3.983883 | -6.982821 | -0.168509 |
| 38 | 1 | 0 | -5.169568 | -4.828269 | -0.253929 |
| 39 | 1 | 0 | -0.213328 | -4.968706 | 0.289364 |
| 40 | 1 | 0 | -5.086115 | -2.346731 | -0.217758 |
| 41 | 1 | 0 | -0.149551 | -2.545854 | 0.351758 |
| 42 | 1 | 0 | -5.026249 | 0.076961 | -0.202287 |
| 43 | 1 | 0 | -5.000894 | 2.501049 | -0.245947 |
| 44 | 1 | 0 | -0.060230 | 2.533161 | 0.324502 |
| 45 | 1 | 0 | -4.996871 | 4.983553 | -0.310408 |
| 46 | 1 | 0 | -3.736020 | 7.095798 | -0.248437 |
| 47 | 1 | 0 | -1.260053 | 7.081682 | 0.019888 |
| 48 | 1 | 0 | -0.038808 | 4.955161 | 0.234105 |
| 49 | 1 | 0 | 0.645164 | 0.856855 | 1.174438 |
| 50 | 1 | 0 | 0.616128 | -0.885826 | 1.182450 |
| 51 | 1 | 0 | 0.958431 | -0.922787 | -1.303888 |
| 52 | 1 | 0 | 0.977811 | 0.855925 | -1.314858 |
| 53 | 1 | 0 | 6.556939 | -0.962060 | -1.486256 |
| 54 | 1 | 0 | 5.292939 | -2.181005 | -1.734827 |
| 55 | 1 | 0 | 5.037831 | -0.523008 | -2.290383 |
| 56 | 1 | 0 | 5.360751 | -2.768243 | 0.628068 |
| 57 | 1 | 0 | 6.547521 | -1.514586 | 1.033802 |
| 58 | 1 | 0 | 5.007890 | -1.612826 | 1.909672 |
| 59 | 1 | 0 | 4.568880 | 2.056032 | 1.884932 |
| 60 | 1 | 0 | 4.082865 | 0.404486 | 2.283932 |
| 61 | 1 | 0 | 5.804201 | 0.813351 | 2.159954 |
| 62 | 1 | 0 | 5.578253 | 2.637656 | -0.255391 |
| 63 | 1 | 0 | 6.815345 | 1.371766 | -0.145561 |
| 64 | 1 | 0 | 5.762958 | 1.479516 | -1.569789 |

# 5-4. Heptacenes(**Hp**)

## Non-Radical

R=$NO_2$

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 8.581109 | -0.082889 | -0.000002 |
| 2 | 6 | 0 | 8.567055 | -1.509510 | -0.000001 |
| 3 | 6 | 0 | 7.384157 | -2.191867 | -0.000001 |
| 4 | 6 | 0 | 6.134006 | -1.496921 | 0.000000 |
| 5 | 6 | 0 | 6.148526 | -0.048004 | -0.000001 |
| 6 | 6 | 0 | 7.411425 | 0.622298 | -0.000002 |
| 7 | 6 | 0 | 4.911852 | -2.165502 | 0.000000 |
| 8 | 6 | 0 | 3.686540 | -1.471581 | 0.000001 |
| 9 | 6 | 0 | 3.701381 | -0.019047 | 0.000000 |
| 10 | 6 | 0 | 4.939861 | 0.646715 | -0.000001 |
| 11 | 6 | 0 | 2.447725 | -2.129984 | 0.000001 |
| 12 | 6 | 0 | 1.231696 | -1.430026 | 0.000001 |
| 13 | 6 | 0 | 1.248342 | 0.026894 | 0.000001 |
| 14 | 6 | 0 | 2.480326 | 0.681632 | 0.000001 |
| 15 | 6 | 0 | 0.000000 | -2.102710 | 0.000001 |
| 16 | 6 | 0 | -1.231696 | -1.430026 | 0.000001 |
| 17 | 6 | 0 | -1.248341 | 0.026894 | 0.000001 |
| 18 | 6 | 0 | 0.000000 | 0.731344 | 0.000001 |
| 19 | 6 | 0 | -2.447724 | -2.129985 | 0.000001 |
| 20 | 6 | 0 | -3.686539 | -1.471582 | 0.000000 |
| 21 | 6 | 0 | -3.701380 | -0.019047 | 0.000000 |
| 22 | 6 | 0 | -2.480326 | 0.681631 | 0.000000 |
| 23 | 6 | 0 | -4.911852 | -2.165503 | 0.000000 |
| 24 | 6 | 0 | -6.134005 | -1.496922 | 0.000000 |
| 25 | 6 | 0 | -6.148526 | -0.048005 | -0.000001 |
| 26 | 6 | 0 | -4.939860 | 0.646714 | 0.000000 |
| 27 | 6 | 0 | -7.384156 | -2.191868 | -0.000001 |
| 28 | 6 | 0 | -8.567054 | -1.509511 | -0.000001 |
| 29 | 6 | 0 | -8.581109 | -0.082890 | -0.000001 |
| 30 | 6 | 0 | -7.411425 | 0.622297 | -0.000001 |
| 31 | 6 | 0 | 0.000000 | 2.133550 | 0.000001 |
| 32 | 6 | 0 | -0.000001 | 3.344225 | 0.000002 |
| 33 | 7 | 0 | -0.000002 | 4.724545 | 0.000000 |
| 34 | 8 | 0 | -1.096464 | 5.286880 | -0.000005 |
| 35 | 8 | 0 | 1.096458 | 5.286883 | 0.000004 |
| 36 | 1 | 0 | 9.531307 | 0.438740 | -0.000002 |
| 37 | 1 | 0 | 9.507019 | -2.049495 | -0.000001 |
| 38 | 1 | 0 | 7.373517 | -3.276659 | 0.000000 |
| 39 | 1 | 0 | 7.421377 | 1.706971 | -0.000002 |
| 40 | 1 | 0 | 4.900655 | -3.250959 | 0.000001 |
| 41 | 1 | 0 | 4.951249 | 1.731929 | -0.000001 |
| 42 | 1 | 0 | 2.426124 | -3.215019 | 0.000001 |
| 43 | 1 | 0 | 2.504236 | 1.765199 | 0.000000 |
| 44 | 1 | 0 | 0.000001 | -3.188196 | 0.000001 |
| 45 | 1 | 0 | -2.426123 | -3.215020 | 0.000001 |
| 46 | 1 | 0 | -2.504236 | 1.765199 | 0.000001 |
| 47 | 1 | 0 | -4.900654 | -3.250960 | 0.000000 |
| 48 | 1 | 0 | -4.951248 | 1.731928 | 0.000000 |
| 49 | 1 | 0 | -7.373516 | -3.276660 | 0.000000 |
| 50 | 1 | 0 | -9.507018 | -2.049496 | -0.000001 |
| 51 | 1 | 0 | -9.531307 | 0.438739 | -0.000002 |
| 52 | 1 | 0 | -7.421377 | 1.706970 | -0.000001 |

R=CN

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 8.583765 | 0.132009 | 0.000000 |
| 2 | 6 | 0 | 8.568737 | -1.294125 | 0.000000 |
| 3 | 6 | 0 | 7.384834 | -1.975524 | 0.000000 |
| 4 | 6 | 0 | 6.135542 | -1.279891 | 0.000000 |
| 5 | 6 | 0 | 6.151025 | 0.168499 | 0.000000 |
| 6 | 6 | 0 | 7.414037 | 0.837829 | 0.000000 |
| 7 | 6 | 0 | 4.912132 | -1.947699 | 0.000000 |
| 8 | 6 | 0 | 3.687654 | -1.253495 | 0.000000 |
| 9 | 6 | 0 | 3.703271 | 0.198651 | 0.000000 |
| 10 | 6 | 0 | 4.941852 | 0.863578 | 0.000000 |
| 11 | 6 | 0 | 2.447646 | -1.911084 | 0.000000 |
| 12 | 6 | 0 | 1.231212 | -1.212418 | 0.000000 |
| 13 | 6 | 0 | 1.248032 | 0.244825 | 0.000000 |
| 14 | 6 | 0 | 2.481324 | 0.898519 | 0.000000 |
| 15 | 6 | 0 | -0.000001 | -1.886155 | 0.000000 |
| 16 | 6 | 0 | -1.231213 | -1.212418 | 0.000000 |
| 17 | 6 | 0 | -1.248033 | 0.244825 | 0.000000 |
| 18 | 6 | 0 | -0.000001 | 0.948989 | 0.000000 |
| 19 | 6 | 0 | -2.447648 | -1.911084 | 0.000000 |
| 20 | 6 | 0 | -3.687655 | -1.253493 | 0.000000 |
| 21 | 6 | 0 | -3.703273 | 0.198652 | 0.000000 |
| 22 | 6 | 0 | -2.481325 | 0.898520 | 0.000000 |
| 23 | 6 | 0 | -4.912134 | -1.947698 | 0.000000 |
| 24 | 6 | 0 | -6.135544 | -1.279889 | 0.000000 |
| 25 | 6 | 0 | -6.151026 | 0.168502 | 0.000000 |
| 26 | 6 | 0 | -4.941853 | 0.863580 | 0.000000 |
| 27 | 6 | 0 | -7.384836 | -1.975522 | 0.000000 |
| 28 | 6 | 0 | -8.568739 | -1.294121 | 0.000000 |
| 29 | 6 | 0 | -8.583767 | 0.132012 | 0.000000 |
| 30 | 6 | 0 | -7.414038 | 0.837831 | 0.000000 |
| 31 | 6 | 0 | 0.000000 | 2.354138 | 0.000000 |
| 32 | 6 | 0 | 0.000002 | 3.570587 | 0.000000 |
| 33 | 6 | 0 | 0.000005 | 4.931923 | 0.000000 |
| 34 | 7 | 0 | 0.000017 | 6.093508 | 0.000001 |
| 35 | 1 | 0 | 9.534197 | 0.653256 | 0.000000 |
| 36 | 1 | 0 | 9.508185 | -1.835030 | 0.000000 |
| 37 | 1 | 0 | 7.373414 | -3.060336 | 0.000000 |
| 38 | 1 | 0 | 7.424903 | 1.922565 | 0.000000 |
| 39 | 1 | 0 | 4.900388 | -3.033176 | 0.000000 |
| 40 | 1 | 0 | 4.954496 | 1.948892 | 0.000000 |
| 41 | 1 | 0 | 2.426008 | -2.996141 | 0.000000 |
| 42 | 1 | 0 | 2.506519 | 1.981884 | 0.000000 |
| 43 | 1 | 0 | -0.000001 | -2.971502 | 0.000000 |
| 44 | 1 | 0 | -2.426010 | -2.996141 | 0.000000 |
| 45 | 1 | 0 | -2.506520 | 1.981885 | 0.000000 |
| 46 | 1 | 0 | -4.900390 | -3.033174 | 0.000000 |
| 47 | 1 | 0 | -4.954496 | 1.948893 | 0.000000 |
| 48 | 1 | 0 | -7.373416 | -3.060333 | 0.000000 |
| 49 | 1 | 0 | -9.508188 | -1.835026 | 0.000000 |
| 50 | 1 | 0 | -9.534198 | 0.653260 | 0.000000 |
| 51 | 1 | 0 | -7.424903 | 1.922568 | 0.000000 |

R=Cl

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 8.583727 | 0.066251 | -0.000007 |
| 2 | 6 | 0 | 8.570911 | -1.359480 | -0.000002 |
| 3 | 6 | 0 | 7.387250 | -2.042220 | 0.000001 |
| 4 | 6 | 0 | 6.137000 | -1.349003 | 0.000000 |
| 5 | 6 | 0 | 6.150157 | 0.098987 | -0.000004 |
| 6 | 6 | 0 | 7.412119 | 0.769771 | -0.000008 |
| 7 | 6 | 0 | 4.913767 | -2.018701 | 0.000003 |
| 8 | 6 | 0 | 3.688138 | -1.327423 | 0.000002 |
| 9 | 6 | 0 | 3.701132 | 0.124810 | -0.000002 |
| 10 | 6 | 0 | 4.938853 | 0.791413 | -0.000005 |
| 11 | 6 | 0 | 2.448618 | -1.987698 | 0.000005 |
| 12 | 6 | 0 | 1.229960 | -1.293210 | 0.000004 |
| 13 | 6 | 0 | 1.243362 | 0.164905 | 0.000000 |
| 14 | 6 | 0 | 2.477277 | 0.821061 | -0.000002 |
| 15 | 6 | 0 | 0.000002 | -1.969694 | 0.000007 |
| 16 | 6 | 0 | -1.229958 | -1.293210 | 0.000004 |
| 17 | 6 | 0 | -1.243360 | 0.164904 | 0.000001 |
| 18 | 6 | 0 | 0.000001 | 0.870205 | 0.000000 |
| 19 | 6 | 0 | -2.448615 | -1.987699 | 0.000004 |
| 20 | 6 | 0 | -3.688135 | -1.327425 | 0.000001 |
| 21 | 6 | 0 | -3.701130 | 0.124808 | -0.000001 |
| 22 | 6 | 0 | -2.477275 | 0.821059 | -0.000001 |
| 23 | 6 | 0 | -4.913764 | -2.018704 | 0.000001 |
| 24 | 6 | 0 | -6.136997 | -1.349006 | -0.000001 |
| 25 | 6 | 0 | -6.150155 | 0.098983 | -0.000003 |
| 26 | 6 | 0 | -4.938850 | 0.791410 | -0.000003 |
| 27 | 6 | 0 | -7.387247 | -2.042223 | -0.000001 |
| 28 | 6 | 0 | -8.570908 | -1.359483 | -0.000003 |
| 29 | 6 | 0 | -8.583724 | 0.066247 | -0.000005 |
| 30 | 6 | 0 | -7.412116 | 0.769768 | -0.000005 |
| 31 | 6 | 0 | -0.000001 | 2.286554 | -0.000004 |
| 32 | 6 | 0 | -0.000004 | 3.494482 | 0.000013 |
| 33 | 17 | 0 | -0.000013 | 5.141723 | 0.000004 |
| 34 | 1 | 0 | 9.533233 | 0.589390 | -0.000010 |
| 35 | 1 | 0 | 9.510989 | -1.899445 | -0.000001 |
| 36 | 1 | 0 | 7.377397 | -3.127160 | 0.000005 |
| 37 | 1 | 0 | 7.421280 | 1.854690 | -0.000011 |
| 38 | 1 | 0 | 4.904210 | -3.104322 | 0.000007 |
| 39 | 1 | 0 | 4.949429 | 1.876916 | -0.000008 |
| 40 | 1 | 0 | 2.430342 | -3.072955 | 0.000008 |
| 41 | 1 | 0 | 2.496260 | 1.904436 | -0.000005 |
| 42 | 1 | 0 | 0.000002 | -3.055007 | 0.000010 |
| 43 | 1 | 0 | -2.430338 | -3.072956 | 0.000005 |
| 44 | 1 | 0 | -2.496260 | 1.904433 | -0.000003 |
| 45 | 1 | 0 | -4.904206 | -3.104325 | 0.000003 |
| 46 | 1 | 0 | -4.949428 | 1.876913 | -0.000004 |
| 47 | 1 | 0 | -7.377394 | -3.127164 | 0.000000 |
| 48 | 1 | 0 | -9.510987 | -1.899449 | -0.000004 |
| 49 | 1 | 0 | -9.533231 | 0.589386 | -0.000007 |
| 50 | 1 | 0 | -7.421278 | 1.854687 | -0.000006 |

R=H

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 8.583654 | 0.460690 | 0.000007 |
| 2 | 6 | 0 | 8.570850 | -0.965040 | 0.000010 |
| 3 | 6 | 0 | 7.387153 | -1.647753 | 0.000010 |
| 4 | 6 | 0 | 6.136866 | -0.954601 | 0.000005 |
| 5 | 6 | 0 | 6.149989 | 0.493389 | 0.000003 |
| 6 | 6 | 0 | 7.411986 | 1.164136 | 0.000004 |
| 7 | 6 | 0 | 4.913615 | -1.624287 | 0.000003 |
| 8 | 6 | 0 | 3.687950 | -0.933054 | -0.000001 |
| 9 | 6 | 0 | 3.700773 | 0.519233 | -0.000002 |
| 10 | 6 | 0 | 4.938646 | 1.185736 | 0.000000 |
| 11 | 6 | 0 | 2.448464 | -1.593363 | -0.000004 |

| | | | | | |
|---|---|---|---|---|---|
| 12 | 6 | 0 | 1.229917 | -0.898687 | -0.000007 |
| 13 | 6 | 0 | 1.243129 | 0.559558 | -0.000007 |
| 14 | 6 | 0 | 2.477225 | 1.215965 | -0.000005 |
| 15 | 6 | 0 | 0.000001 | -1.575160 | -0.000009 |
| 16 | 6 | 0 | -1.229916 | -0.898688 | -0.000008 |
| 17 | 6 | 0 | -1.243128 | 0.559557 | -0.000003 |
| 18 | 6 | 0 | 0.000000 | 1.264408 | -0.000006 |
| 19 | 6 | 0 | -2.448463 | -1.593364 | -0.000011 |
| 20 | 6 | 0 | -3.687949 | -0.933054 | -0.000006 |
| 21 | 6 | 0 | -3.700772 | 0.519233 | 0.000003 |
| 22 | 6 | 0 | -2.477224 | 1.215964 | 0.000003 |
| 23 | 6 | 0 | -4.913614 | -1.624288 | -0.000009 |
| 24 | 6 | 0 | -6.136866 | -0.954602 | -0.000002 |
| 25 | 6 | 0 | -6.149988 | 0.493389 | 0.000010 |
| 26 | 6 | 0 | -4.938646 | 1.185735 | 0.000012 |
| 27 | 6 | 0 | -7.387152 | -1.647754 | -0.000005 |
| 28 | 6 | 0 | -8.570849 | -0.965041 | 0.000003 |
| 29 | 6 | 0 | -8.583653 | 0.460689 | 0.000015 |
| 30 | 6 | 0 | -7.411985 | 1.164135 | 0.000018 |
| 31 | 6 | 0 | -0.000002 | 2.682662 | -0.000006 |
| 32 | 6 | 0 | -0.000008 | 3.889911 | -0.000021 |
| 33 | 1 | 0 | 9.533156 | 0.983861 | 0.000008 |
| 34 | 1 | 0 | 9.510925 | -1.505031 | 0.000013 |
| 35 | 1 | 0 | 7.377307 | -2.732705 | 0.000013 |
| 36 | 1 | 0 | 7.421123 | 2.249073 | 0.000002 |
| 37 | 1 | 0 | 4.904084 | -2.709921 | 0.000007 |
| 38 | 1 | 0 | 4.949150 | 2.271241 | 0.000000 |
| 39 | 1 | 0 | 2.430160 | -2.678634 | -0.000001 |
| 40 | 1 | 0 | 2.494929 | 2.299290 | -0.000001 |
| 41 | 1 | 0 | 0.000001 | -2.660504 | -0.000011 |
| 42 | 1 | 0 | -2.430160 | -2.678634 | -0.000016 |
| 43 | 1 | 0 | -2.494928 | 2.299289 | 0.000009 |
| 44 | 1 | 0 | -4.904083 | -2.709922 | -0.000017 |
| 45 | 1 | 0 | -4.949149 | 2.271240 | 0.000020 |
| 46 | 1 | 0 | -7.377307 | -2.732706 | -0.000014 |
| 47 | 1 | 0 | -9.510924 | -1.505031 | 0.000001 |
| 48 | 1 | 0 | -9.533155 | 0.983861 | 0.000022 |
| 49 | 1 | 0 | -7.421122 | 2.249072 | 0.000027 |
| 50 | 1 | 0 | -0.000014 | 4.952239 | -0.000034 |

R=CHO

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 8.631934 | 0.205837 | -0.000007 |
| 2 | 6 | 0 | 8.635282 | -1.220361 | -0.000005 |
| 3 | 6 | 0 | 7.460094 | -1.916709 | -0.000003 |
| 4 | 6 | 0 | 6.201855 | -1.237314 | -0.000001 |
| 5 | 6 | 0 | 6.198646 | 0.211088 | -0.000003 |
| 6 | 6 | 0 | 7.453082 | 0.896368 | -0.000006 |
| 7 | 6 | 0 | 4.987067 | -1.920720 | 0.000001 |
| 8 | 6 | 0 | 3.753608 | -1.242624 | 0.000002 |
| 9 | 6 | 0 | 3.750272 | 0.209659 | 0.000000 |
| 10 | 6 | 0 | 4.980332 | 0.890120 | -0.000002 |
| 11 | 6 | 0 | 2.522121 | -1.916459 | 0.000004 |
| 12 | 6 | 0 | 1.297062 | -1.233312 | 0.000004 |
| 13 | 6 | 0 | 1.294533 | 0.223958 | 0.000003 |
| 14 | 6 | 0 | 2.518864 | 0.893105 | 0.000001 |
| 15 | 6 | 0 | 0.074168 | -1.922912 | 0.000006 |
| 16 | 6 | 0 | -1.165613 | -1.264841 | 0.000005 |
| 17 | 6 | 0 | -1.199880 | 0.191980 | 0.000002 |
| 18 | 6 | 0 | 0.039134 | 0.915024 | 0.000002 |
| 19 | 6 | 0 | -2.373080 | -1.979051 | 0.000006 |
| 20 | 6 | 0 | -3.620869 | -1.335987 | 0.000003 |
| 21 | 6 | 0 | -3.653195 | 0.115880 | -0.000001 |
| 22 | 6 | 0 | -2.440290 | 0.831614 | -0.000001 |
| 23 | 6 | 0 | -4.837315 | -2.044119 | 0.000003 |
| 24 | 6 | 0 | -6.068261 | -1.389995 | 0.000000 |
| 25 | 6 | 0 | -6.100192 | 0.058089 | -0.000004 |
| 26 | 6 | 0 | -4.898978 | 0.767025 | -0.000005 |
| 27 | 6 | 0 | -7.309716 | -2.099495 | 0.000000 |
| 28 | 6 | 0 | -8.501261 | -1.431388 | -0.000003 |
| 29 | 6 | 0 | -8.532445 | -0.005557 | -0.000008 |
| 30 | 6 | 0 | -7.370576 | 0.713250 | -0.000008 |
| 31 | 6 | 0 | 0.006709 | 2.319099 | 0.000003 |
| 32 | 6 | 0 | -0.078298 | 3.532557 | 0.000006 |
| 33 | 6 | 0 | -0.221237 | 4.956882 | 0.000010 |
| 34 | 8 | 0 | -1.293422 | 5.530038 | -0.000003 |
| 35 | 1 | 0 | 9.575587 | 0.739328 | -0.000009 |
| 36 | 1 | 0 | 9.581568 | -1.749239 | -0.000006 |
| 37 | 1 | 0 | 7.462546 | -3.001602 | -0.000002 |
| 38 | 1 | 0 | 7.450132 | 1.981229 | -0.000007 |
| 39 | 1 | 0 | 4.989412 | -3.006287 | 0.000002 |
| 40 | 1 | 0 | 4.979052 | 1.975586 | -0.000003 |
| 41 | 1 | 0 | 2.514921 | -3.001742 | 0.000005 |
| 42 | 1 | 0 | 2.525652 | 1.976762 | -0.000001 |
| 43 | 1 | 0 | 0.088221 | -3.008266 | 0.000008 |
| 44 | 1 | 0 | -2.338415 | -3.063823 | 0.000008 |
| 45 | 1 | 0 | -2.475696 | 1.914678 | -0.000004 |
| 46 | 1 | 0 | -4.813492 | -3.129443 | 0.000007 |
| 47 | 1 | 0 | -4.922613 | 1.852068 | -0.000008 |
| 48 | 1 | 0 | -7.286209 | -3.184152 | 0.000004 |
| 49 | 1 | 0 | -9.434553 | -1.982943 | -0.000003 |
| 50 | 1 | 0 | -9.488677 | 0.505017 | -0.000011 |
| 51 | 1 | 0 | -7.393139 | 1.797792 | -0.000012 |
| 52 | 1 | 0 | 0.731728 | 5.520578 | 0.000027 |

R=$SiMe_3$

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -8.588176 | -0.524144 | -0.005198 |
| 2 | 6 | 0 | -8.576449 | -1.949828 | -0.002889 |
| 3 | 6 | 0 | -7.393204 | -2.633379 | -0.000530 |
| 4 | 6 | 0 | -6.142416 | -1.941174 | -0.000316 |
| 5 | 6 | 0 | -6.154457 | -0.493252 | -0.002617 |
| 6 | 6 | 0 | -7.415903 | 0.178387 | -0.005059 |
| 7 | 6 | 0 | -4.919575 | -2.611732 | 0.001908 |
| 8 | 6 | 0 | -3.693476 | -1.921376 | 0.001964 |
| 9 | 6 | 0 | -3.705202 | -0.469198 | -0.000186 |
| 10 | 6 | 0 | -4.942403 | 0.198111 | -0.002460 |
| 11 | 6 | 0 | -2.454267 | -2.582399 | 0.003767 |
| 12 | 6 | 0 | -1.235336 | -1.888455 | 0.003446 |
| 13 | 6 | 0 | -1.247522 | -0.430374 | 0.001599 |
| 14 | 6 | 0 | -2.480650 | 0.226440 | -0.000128 |
| 15 | 6 | 0 | -0.006089 | -2.566354 | 0.004660 |
| 16 | 6 | 0 | 1.224573 | -1.891036 | 0.003433 |
| 17 | 6 | 0 | 1.239684 | -0.433024 | 0.001282 |
| 18 | 6 | 0 | -0.003207 | 0.276045 | 0.001408 |
| 19 | 6 | 0 | 2.442114 | -2.587426 | 0.003990 |
| 20 | 6 | 0 | 3.682640 | -1.928848 | 0.002000 |
| 21 | 6 | 0 | 3.697236 | -0.476701 | -0.000906 |
| 22 | 6 | 0 | 2.474084 | 0.221425 | -0.001000 |
| 23 | 6 | 0 | 4.907393 | -2.621595 | 0.002454 |
| 24 | 6 | 0 | 6.131530 | -1.953393 | 0.000021 |
| 25 | 6 | 0 | 6.146389 | -0.505495 | -0.003218 |
| 26 | 6 | 0 | 4.935700 | 0.188267 | -0.003614 |
| 27 | 6 | 0 | 7.380978 | -2.648019 | 0.000493 |
| 28 | 6 | 0 | 8.565541 | -1.966753 | -0.002087 |
| 29 | 6 | 0 | 8.580038 | -0.541093 | -0.005361 |
| 30 | 6 | 0 | 7.409130 | 0.163713 | -0.005918 |
| 31 | 6 | 0 | -0.000821 | 1.690810 | 0.001656 |
| 32 | 6 | 0 | 0.003709 | 2.910016 | 0.002578 |
| 33 | 14 | 0 | 0.017822 | 4.752220 | 0.002050 |
| 34 | 6 | 0 | 1.761304 | 5.334752 | -0.417712 |
| 35 | 6 | 0 | -0.481618 | 5.364244 | 1.714030 |
| 36 | 6 | 0 | -1.207143 | 5.364460 | -1.293901 |
| 37 | 1 | 0 | -9.537268 | -0.000221 | -0.007098 |
| 38 | 1 | 0 | -9.516913 | -2.489148 | -0.003047 |
| 39 | 1 | 0 | -7.384152 | -3.718343 | 0.001194 |
| 40 | 1 | 0 | -7.424278 | 1.263345 | -0.006864 |
| 41 | 1 | 0 | -4.910832 | -3.697380 | 0.003532 |
| 42 | 1 | 0 | -4.952202 | 1.283633 | -0.004291 |
| 43 | 1 | 0 | -2.436622 | -3.667694 | 0.005228 |
| 44 | 1 | 0 | -2.496501 | 1.309808 | -0.001926 |
| 45 | 1 | 0 | -0.007244 | -3.651698 | 0.006276 |
| 46 | 1 | 0 | 2.422306 | -3.672685 | 0.005813 |
| 47 | 1 | 0 | 2.492191 | 1.304763 | -0.003311 |
| 48 | 1 | 0 | 4.896554 | -3.707224 | 0.004702 |
| 49 | 1 | 0 | 4.947515 | 1.273758 | -0.006262 |
| 50 | 1 | 0 | 7.369833 | -3.732963 | 0.002946 |
| 51 | 1 | 0 | 9.504959 | -2.507897 | -0.001685 |
| 52 | 1 | 0 | 9.530146 | -0.019015 | -0.007433 |
| 53 | 1 | 0 | 7.419566 | 1.248648 | -0.008461 |
| 54 | 1 | 0 | 2.075142 | 4.968542 | -1.398968 |
| 55 | 1 | 0 | 1.810598 | 6.428086 | -0.435780 |
| 56 | 1 | 0 | 2.485491 | 4.979880 | 0.320803 |
| 57 | 1 | 0 | -1.483425 | 5.017623 | 1.981894 |
| 58 | 1 | 0 | -0.483753 | 6.458407 | 1.748978 |
| 59 | 1 | 0 | 0.210893 | 5.004294 | 2.479657 |
| 60 | 1 | 0 | -1.222048 | 6.458544 | -1.326354 |
| 61 | 1 | 0 | -0.942213 | 5.001717 | -2.290632 |
| 62 | 1 | 0 | -2.222017 | 5.022413 | -1.073152 |

R=OMe

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 8.627597 | 0.160002 | -0.000005 |
| 2 | 6 | 0 | 8.631063 | -1.265582 | -0.000001 |
| 3 | 6 | 0 | 7.454846 | -1.961498 | 0.000001 |
| 4 | 6 | 0 | 6.196771 | -1.282834 | 0.000000 |
| 5 | 6 | 0 | 6.193389 | 0.165016 | -0.000003 |
| 6 | 6 | 0 | 7.447606 | 0.849843 | -0.000006 |
| 7 | 6 | 0 | 4.980809 | -1.966334 | 0.000003 |
| 8 | 6 | 0 | 3.747472 | -1.289245 | 0.000002 |
| 9 | 6 | 0 | 3.743894 | 0.162825 | -0.000002 |
| 10 | 6 | 0 | 4.973701 | 0.843352 | -0.000004 |
| 11 | 6 | 0 | 2.514894 | -1.963088 | 0.000004 |
| 12 | 6 | 0 | 1.287912 | -1.283407 | 0.000003 |
| 13 | 6 | 0 | 1.284613 | 0.175015 | 0.000000 |
| 14 | 6 | 0 | 2.511285 | 0.844361 | -0.000002 |
| 15 | 6 | 0 | 0.066880 | -1.975836 | 0.000005 |
| 16 | 6 | 0 | -1.169368 | -1.311063 | 0.000003 |
| 17 | 6 | 0 | -1.199161 | 0.147248 | 0.000000 |
| 18 | 6 | 0 | 0.034457 | 0.871019 | -0.000001 |
| 19 | 6 | 0 | -2.380695 | -2.018301 | 0.000005 |
| 20 | 6 | 0 | -3.628546 | -1.373259 | 0.000002 |
| 21 | 6 | 0 | -3.658711 | 0.078588 | -0.000002 |

| | | | | | |
|---|---|---|---|---|---|
| 22 | 6 | 0 | -2.441484 | 0.787132 | -0.000003 |
| 23 | 6 | 0 | -4.845832 | -2.078804 | 0.000004 |
| 24 | 6 | 0 | -6.077601 | -1.424255 | 0.000001 |
| 25 | 6 | 0 | -6.108214 | 0.023254 | -0.000004 |
| 26 | 6 | 0 | -4.904467 | 0.729522 | -0.000005 |
| 27 | 6 | 0 | -7.319322 | -2.132364 | 0.000002 |
| 28 | 6 | 0 | -8.511740 | -1.464577 | -0.000002 |
| 29 | 6 | 0 | -8.541781 | -0.039337 | -0.000006 |
| 30 | 6 | 0 | -7.378324 | 0.678092 | -0.000007 |
| 31 | 6 | 0 | 0.023628 | 2.287697 | -0.000003 |
| 32 | 6 | 0 | 0.037488 | 3.496372 | -0.000003 |
| 33 | 8 | 0 | 0.108926 | 4.791674 | -0.000004 |
| 34 | 6 | 0 | -1.160148 | 5.489566 | 0.000018 |
| 35 | 1 | 0 | 9.571000 | 0.694199 | -0.000007 |
| 36 | 1 | 0 | 9.577148 | -1.795071 | 0.000000 |
| 37 | 1 | 0 | 7.457285 | -3.046560 | 0.000004 |
| 38 | 1 | 0 | 7.444326 | 1.934882 | -0.000009 |
| 39 | 1 | 0 | 4.983692 | -3.052079 | 0.000006 |
| 40 | 1 | 0 | 4.971812 | 1.928991 | -0.000007 |
| 41 | 1 | 0 | 2.509127 | -3.048585 | 0.000007 |
| 42 | 1 | 0 | 2.517482 | 1.927783 | -0.000005 |
| 43 | 1 | 0 | 0.078972 | -3.060987 | 0.000008 |
| 44 | 1 | 0 | -2.350149 | -3.103370 | 0.000008 |
| 45 | 1 | 0 | -2.471931 | 1.870200 | -0.000005 |
| 46 | 1 | 0 | -4.823196 | -3.164301 | 0.000007 |
| 47 | 1 | 0 | -4.929010 | 1.815056 | -0.000008 |
| 48 | 1 | 0 | -7.296066 | -3.217164 | 0.000005 |
| 49 | 1 | 0 | -9.445044 | -2.016227 | -0.000001 |
| 50 | 1 | 0 | -9.497510 | 0.472503 | -0.000009 |
| 51 | 1 | 0 | -7.401103 | 1.762981 | -0.000011 |
| 52 | 1 | 0 | -0.912017 | 6.548328 | 0.000017 |
| 53 | 1 | 0 | -1.726856 | 5.230659 | -0.896741 |
| 54 | 1 | 0 | -1.726828 | 5.230654 | 0.896794 |

R=$NH_2$

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -8.586420 | 0.260199 | -0.020774 |
| 2 | 6 | 0 | -8.572743 | -1.165134 | -0.005345 |
| 3 | 6 | 0 | -7.387982 | -1.846460 | 0.005381 |
| 4 | 6 | 0 | -6.138229 | -1.152700 | 0.001555 |
| 5 | 6 | 0 | -6.152254 | 0.294882 | -0.013833 |
| 6 | 6 | 0 | -7.414671 | 0.964155 | -0.024885 |
| 7 | 6 | 0 | -4.913912 | -1.821251 | 0.011608 |
| 8 | 6 | 0 | -3.688744 | -1.129635 | 0.007645 |
| 9 | 6 | 0 | -3.702538 | 0.322205 | -0.006652 |
| 10 | 6 | 0 | -4.940335 | 0.987406 | -0.017551 |
| 11 | 6 | 0 | -2.448073 | -1.788753 | 0.015942 |
| 12 | 6 | 0 | -1.228612 | -1.095744 | 0.011600 |
| 13 | 6 | 0 | -1.242828 | 0.362476 | -0.000013 |
| 14 | 6 | 0 | -2.476819 | 1.016785 | -0.009582 |
| 15 | 6 | 0 | 0.000000 | -1.774887 | 0.018280 |
| 16 | 6 | 0 | 1.228612 | -1.095744 | 0.011598 |
| 17 | 6 | 0 | 1.242828 | 0.362476 | -0.000012 |
| 18 | 6 | 0 | 0.000000 | 1.073834 | -0.001118 |
| 19 | 6 | 0 | 2.448074 | -1.788752 | 0.015938 |
| 20 | 6 | 0 | 3.688744 | -1.129634 | 0.007642 |
| 21 | 6 | 0 | 3.702538 | 0.322205 | -0.006650 |
| 22 | 6 | 0 | 2.476819 | 1.016786 | -0.009578 |
| 23 | 6 | 0 | 4.913912 | -1.821251 | 0.011602 |
| 24 | 6 | 0 | 6.138229 | -1.152700 | 0.001552 |
| 25 | 6 | 0 | 6.152254 | 0.294882 | -0.013830 |
| 26 | 6 | 0 | 4.940335 | 0.987406 | -0.017546 |
| 27 | 6 | 0 | 7.387982 | -1.846459 | 0.005376 |
| 28 | 6 | 0 | 8.572743 | -1.165134 | -0.005347 |
| 29 | 6 | 0 | 8.586420 | 0.260199 | -0.020771 |
| 30 | 6 | 0 | 7.414672 | 0.964156 | -0.024879 |
| 31 | 6 | 0 | 0.000000 | 2.486260 | -0.001512 |
| 32 | 6 | 0 | -0.000001 | 3.698263 | 0.022670 |
| 33 | 7 | 0 | -0.000006 | 5.040513 | -0.026533 |
| 34 | 1 | 0 | -9.536173 | 0.783008 | -0.029452 |
| 35 | 1 | 0 | -9.512298 | -1.706113 | -0.002379 |
| 36 | 1 | 0 | -7.377173 | -2.931424 | 0.016883 |
| 37 | 1 | 0 | -7.424835 | 2.049169 | -0.036942 |
| 38 | 1 | 0 | -4.903690 | -2.906912 | 0.022422 |
| 39 | 1 | 0 | -4.952187 | 2.073068 | -0.029739 |
| 40 | 1 | 0 | -2.429960 | -2.874090 | 0.025199 |
| 41 | 1 | 0 | -2.495945 | 2.100170 | -0.022225 |
| 42 | 1 | 0 | 0.000000 | -2.859995 | 0.027707 |
| 43 | 1 | 0 | 2.429960 | -2.874090 | 0.025192 |
| 44 | 1 | 0 | 2.495945 | 2.100170 | -0.022216 |
| 45 | 1 | 0 | 4.903690 | -2.906912 | 0.022413 |
| 46 | 1 | 0 | 4.952187 | 2.073068 | -0.029730 |
| 47 | 1 | 0 | 7.377173 | -2.931424 | 0.016873 |
| 48 | 1 | 0 | 9.512298 | -1.706112 | -0.002383 |
| 49 | 1 | 0 | 9.536173 | 0.783008 | -0.029446 |
| 50 | 1 | 0 | 7.424835 | 2.049169 | -0.036932 |
| 51 | 1 | 0 | 0.843018 | 5.500324 | 0.289658 |
| 52 | 1 | 0 | -0.842990 | 5.500321 | 0.289770 |

R=Ph

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -8.585593 | -0.638891 | -0.000001 |
| 2 | 6 | 0 | -8.571099 | -2.064442 | 0.000000 |
| 3 | 6 | 0 | -7.386436 | -2.745627 | 0.000001 |
| 4 | 6 | 0 | -6.137085 | -2.050946 | 0.000000 |
| 5 | 6 | 0 | -6.151966 | -0.603203 | -0.000001 |
| 6 | 6 | 0 | -7.414596 | 0.065919 | -0.000001 |
| 7 | 6 | 0 | -4.912771 | -2.719057 | 0.000000 |
| 8 | 6 | 0 | -3.688275 | -2.026156 | 0.000000 |
| 9 | 6 | 0 | -3.702887 | -0.574361 | -0.000001 |
| 10 | 6 | 0 | -4.940943 | 0.090451 | -0.000002 |
| 11 | 6 | 0 | -2.447277 | -2.684049 | 0.000000 |
| 12 | 6 | 0 | -1.229939 | -1.987559 | -0.000001 |
| 13 | 6 | 0 | -1.244746 | -0.529706 | -0.000001 |
| 14 | 6 | 0 | -2.478695 | 0.123037 | -0.000001 |
| 15 | 6 | 0 | 0.000000 | -2.664324 | -0.000002 |
| 16 | 6 | 0 | 1.229939 | -1.987559 | -0.000002 |
| 17 | 6 | 0 | 1.244745 | -0.529706 | 0.000000 |
| 18 | 6 | 0 | 0.000000 | 0.181441 | 0.000000 |
| 19 | 6 | 0 | 2.447277 | -2.684049 | -0.000003 |
| 20 | 6 | 0 | 3.688275 | -2.026156 | -0.000001 |
| 21 | 6 | 0 | 3.702887 | -0.574361 | 0.000002 |
| 22 | 6 | 0 | 2.478694 | 0.123038 | 0.000002 |
| 23 | 6 | 0 | 4.912771 | -2.719057 | -0.000002 |
| 24 | 6 | 0 | 6.137085 | -2.050946 | 0.000000 |
| 25 | 6 | 0 | 6.151966 | -0.603203 | 0.000004 |
| 26 | 6 | 0 | 4.940943 | 0.090451 | 0.000005 |
| 27 | 6 | 0 | 7.386436 | -2.745627 | -0.000001 |
| 28 | 6 | 0 | 8.571099 | -2.064442 | 0.000001 |
| 29 | 6 | 0 | 8.585593 | -0.638892 | 0.000005 |
| 30 | 6 | 0 | 7.414596 | 0.065919 | 0.000007 |
| 31 | 6 | 0 | 0.000000 | 1.591203 | -0.000001 |
| 32 | 6 | 0 | 0.000000 | 2.806137 | -0.000001 |
| 33 | 6 | 0 | 0.000000 | 4.226045 | -0.000001 |
| 34 | 6 | 0 | -1.211062 | 4.945340 | 0.000025 |
| 35 | 6 | 0 | -1.205972 | 6.334081 | 0.000025 |
| 36 | 6 | 0 | 0.000000 | 7.034665 | -0.000001 |
| 37 | 6 | 0 | 1.205972 | 6.334081 | -0.000026 |
| 38 | 6 | 0 | 1.211062 | 4.945339 | -0.000026 |
| 39 | 1 | 0 | -9.535683 | -0.116771 | -0.000001 |
| 40 | 1 | 0 | -9.510482 | -2.605638 | 0.000001 |
| 41 | 1 | 0 | -7.375208 | -3.830571 | 0.000002 |
| 42 | 1 | 0 | -7.425188 | 1.150875 | -0.000002 |
| 43 | 1 | 0 | -4.901782 | -3.804682 | 0.000001 |
| 44 | 1 | 0 | -4.953258 | 1.175988 | -0.000002 |
| 45 | 1 | 0 | -2.426998 | -3.769292 | 0.000000 |
| 46 | 1 | 0 | -2.498147 | 1.206228 | -0.000002 |
| 47 | 1 | 0 | 0.000000 | -3.749620 | -0.000003 |
| 48 | 1 | 0 | 2.426997 | -3.769292 | -0.000004 |
| 49 | 1 | 0 | 2.498147 | 1.206228 | 0.000005 |
| 50 | 1 | 0 | 4.901782 | -3.804682 | -0.000005 |
| 51 | 1 | 0 | 4.953258 | 1.175988 | 0.000007 |
| 52 | 1 | 0 | 7.375208 | -3.830571 | -0.000004 |
| 53 | 1 | 0 | 9.510482 | -2.605639 | 0.000000 |
| 54 | 1 | 0 | 9.535683 | -0.116771 | 0.000008 |
| 55 | 1 | 0 | 7.425188 | 1.150874 | 0.000010 |
| 56 | 1 | 0 | -2.147996 | 4.401748 | 0.000045 |
| 57 | 1 | 0 | -2.146617 | 6.873172 | 0.000045 |
| 58 | 1 | 0 | 0.000001 | 8.118555 | -0.000001 |
| 59 | 1 | 0 | 2.146618 | 6.873172 | -0.000046 |
| 60 | 1 | 0 | 2.147996 | 4.401747 | -0.000047 |

R=BzTh

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -8.499147 | -1.639518 | 0.000005 |
| 2 | 6 | 0 | -8.450427 | -3.064281 | 0.000004 |
| 3 | 6 | 0 | -7.249869 | -3.717021 | 0.000003 |
| 4 | 6 | 0 | -6.017619 | -2.992476 | 0.000003 |
| 5 | 6 | 0 | -6.067306 | -1.545566 | 0.000004 |
| 6 | 6 | 0 | -7.345456 | -0.906721 | 0.000005 |
| 7 | 6 | 0 | -4.777636 | -3.631127 | 0.000002 |
| 8 | 6 | 0 | -3.570383 | -2.908762 | 0.000002 |
| 9 | 6 | 0 | -3.620275 | -1.457943 | 0.000002 |
| 10 | 6 | 0 | -4.873415 | -0.822623 | 0.000003 |
| 11 | 6 | 0 | -2.313672 | -3.536376 | 0.000002 |
| 12 | 6 | 0 | -1.113811 | -2.810394 | 0.000002 |
| 13 | 6 | 0 | -1.164721 | -1.353674 | 0.000002 |
| 14 | 6 | 0 | -2.413152 | -0.730746 | 0.000002 |
| 15 | 6 | 0 | 0.132517 | -3.456876 | 0.000002 |
| 16 | 6 | 0 | 1.346369 | -2.751258 | 0.000002 |
| 17 | 6 | 0 | 1.327324 | -1.293734 | 0.000001 |
| 18 | 6 | 0 | 0.064297 | -0.613257 | 0.000001 |
| 19 | 6 | 0 | 2.579690 | -3.418753 | 0.000002 |
| 20 | 6 | 0 | 3.804871 | -2.731624 | 0.000001 |
| 21 | 6 | 0 | 3.785200 | -1.280042 | -0.000001 |
| 22 | 6 | 0 | 2.544480 | -0.611730 | -0.000001 |
| 23 | 6 | 0 | 5.045307 | -3.395412 | 0.000000 |
| 24 | 6 | 0 | 6.253450 | -2.698431 | -0.000002 |
| 25 | 6 | 0 | 6.233999 | -1.250814 | -0.000004 |
| 26 | 6 | 0 | 5.006807 | -0.585996 | -0.000004 |
| 27 | 6 | 0 | 7.518862 | -3.363366 | -0.000003 |
| 28 | 6 | 0 | 8.686981 | -2.654209 | -0.000005 |
| 29 | 6 | 0 | 8.667646 | -1.228751 | -0.000008 |

| | | | | | |
|---|---|---|---|---|---|
| 30 | 6 | 0 | 7.480290 | -0.551861 | -0.000007 |
| 31 | 6 | 0 | 0.029250 | 0.792069 | 0.000002 |
| 32 | 6 | 0 | 0.002839 | 2.008763 | 0.000003 |
| 33 | 6 | 0 | -0.052495 | 3.406668 | 0.000003 |
| 34 | 6 | 0 | 0.987163 | 4.301528 | 0.000037 |
| 35 | 6 | 0 | 0.570569 | 5.668351 | 0.000026 |
| 36 | 6 | 0 | -0.840695 | 5.799357 | -0.000020 |
| 37 | 16 | 0 | -1.626236 | 4.232155 | -0.000047 |
| 38 | 6 | 0 | 1.357940 | 6.835281 | 0.000053 |
| 39 | 6 | 0 | 0.744053 | 8.075481 | 0.000035 |
| 40 | 6 | 0 | -0.657137 | 8.183668 | -0.000010 |
| 41 | 6 | 0 | -1.458906 | 7.050563 | -0.000038 |
| 42 | 1 | 0 | -9.461491 | -1.140383 | 0.000006 |
| 43 | 1 | 0 | -9.376584 | -3.627807 | 0.000005 |
| 44 | 1 | 0 | -7.212686 | -4.801371 | 0.000003 |
| 45 | 1 | 0 | -7.381829 | 0.177618 | 0.000005 |
| 46 | 1 | 0 | -4.740523 | -4.716154 | 0.000002 |
| 47 | 1 | 0 | -4.911422 | 0.262232 | 0.000004 |
| 48 | 1 | 0 | -2.266889 | -4.620775 | 0.000002 |
| 49 | 1 | 0 | -2.461485 | 0.351663 | 0.000003 |
| 50 | 1 | 0 | 0.158622 | -4.541835 | 0.000003 |
| 51 | 1 | 0 | 2.585035 | -4.504143 | 0.000003 |
| 52 | 1 | 0 | 2.539561 | 0.471769 | -0.000002 |
| 53 | 1 | 0 | 5.060003 | -4.480970 | 0.000002 |
| 54 | 1 | 0 | 4.993365 | 0.499515 | -0.000005 |
| 55 | 1 | 0 | 7.533378 | -4.448252 | -0.000001 |
| 56 | 1 | 0 | 9.638943 | -3.172926 | -0.000006 |
| 57 | 1 | 0 | 9.605085 | -0.684273 | -0.000010 |
| 58 | 1 | 0 | 7.465166 | 0.533023 | -0.000009 |
| 59 | 1 | 0 | 2.021904 | 3.986411 | 0.000070 |
| 60 | 1 | 0 | 2.439318 | 6.754652 | 0.000088 |
| 61 | 1 | 0 | 1.348068 | 8.975422 | 0.000056 |
| 62 | 1 | 0 | -1.119475 | 9.163944 | -0.000024 |
| 63 | 1 | 0 | -2.538986 | 7.137813 | -0.000073 |

R=Th

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 8.661089 | -0.458045 | -0.000009 |
| 2 | 6 | 0 | 8.677298 | -1.883483 | -0.000002 |
| 3 | 6 | 0 | 7.507516 | -2.590018 | 0.000002 |
| 4 | 6 | 0 | 6.243587 | -1.922364 | 0.000000 |
| 5 | 6 | 0 | 6.227307 | -0.474766 | -0.000007 |
| 6 | 6 | 0 | 7.475114 | 0.221394 | -0.000011 |
| 7 | 6 | 0 | 5.033794 | -2.616682 | 0.000003 |
| 8 | 6 | 0 | 3.794829 | -1.950268 | 0.000001 |
| 9 | 6 | 0 | 3.778339 | -0.498654 | -0.000004 |
| 10 | 6 | 0 | 5.001439 | 0.192687 | -0.000008 |
| 11 | 6 | 0 | 2.568042 | -2.634759 | 0.000001 |
| 12 | 6 | 0 | 1.336024 | -1.964883 | -0.000001 |
| 13 | 6 | 0 | 1.320184 | -0.507257 | 0.000001 |
| 14 | 6 | 0 | 2.538925 | 0.172174 | -0.000003 |
| 15 | 6 | 0 | 0.120689 | -2.668009 | -0.000006 |
| 16 | 6 | 0 | -1.123965 | -2.018223 | -0.000005 |
| 17 | 6 | 0 | -1.171287 | -0.561285 | 0.000007 |
| 18 | 6 | 0 | 0.059088 | 0.176459 | 0.000007 |
| 19 | 6 | 0 | -2.325799 | -2.740910 | -0.000013 |
| 20 | 6 | 0 | -3.581088 | -2.110210 | -0.000006 |
| 21 | 6 | 0 | -3.627459 | -0.659278 | 0.000013 |
| 22 | 6 | 0 | -2.418343 | 0.064682 | 0.000018 |
| 23 | 6 | 0 | -4.790080 | -2.829556 | -0.000015 |
| 24 | 6 | 0 | -6.028663 | -2.187980 | -0.000005 |
| 25 | 6 | 0 | -6.074881 | -0.741016 | 0.000016 |
| 26 | 6 | 0 | -4.879086 | -0.021047 | 0.000024 |
| 27 | 6 | 0 | -7.262620 | -2.909528 | -0.000013 |
| 28 | 6 | 0 | -8.461740 | -2.254017 | -0.000003 |
| 29 | 6 | 0 | -8.507051 | -0.829203 | 0.000018 |
| 30 | 6 | 0 | -7.351503 | -0.099214 | 0.000027 |
| 31 | 6 | 0 | 0.028016 | 1.582542 | 0.000013 |
| 32 | 6 | 0 | 0.004739 | 2.799137 | 0.000016 |
| 33 | 6 | 0 | -0.035796 | 4.198132 | 0.000018 |
| 34 | 6 | 0 | 1.014868 | 5.095571 | 0.000107 |
| 35 | 6 | 0 | 0.598090 | 6.449893 | 0.000078 |
| 36 | 6 | 0 | -0.762565 | 6.590356 | -0.000031 |
| 37 | 16 | 0 | -1.570029 | 5.060685 | -0.000103 |
| 38 | 1 | 0 | 9.599699 | 0.084440 | -0.000012 |
| 39 | 1 | 0 | 9.628097 | -2.404358 | 0.000000 |
| 40 | 1 | 0 | 7.519636 | -3.674950 | 0.000007 |
| 41 | 1 | 0 | 7.462351 | 1.306327 | -0.000016 |
| 42 | 1 | 0 | 5.046148 | -3.702288 | 0.000008 |
| 43 | 1 | 0 | 4.990345 | 1.278244 | -0.000013 |
| 44 | 1 | 0 | 2.571190 | -3.720179 | 0.000002 |
| 45 | 1 | 0 | 2.536122 | 1.255688 | -0.000004 |
| 46 | 1 | 0 | 0.144226 | -3.753014 | -0.000011 |
| 47 | 1 | 0 | -2.281861 | -3.825448 | -0.000023 |
| 48 | 1 | 0 | -2.463621 | 1.147232 | 0.000030 |
| 49 | 1 | 0 | -4.755601 | -3.914687 | -0.000030 |
| 50 | 1 | 0 | -4.914553 | 1.063933 | 0.000039 |
| 51 | 1 | 0 | -7.227990 | -3.993978 | -0.000029 |
| 52 | 1 | 0 | -9.389207 | -2.815405 | -0.000009 |
| 53 | 1 | 0 | -9.468184 | -0.327708 | 0.000026 |
| 54 | 1 | 0 | -7.385333 | 0.985235 | 0.000042 |
| 55 | 1 | 0 | 2.047483 | 4.775067 | 0.000191 |
| 56 | 1 | 0 | 1.280412 | 7.289407 | 0.000136 |
| 57 | 1 | 0 | -1.341203 | 7.501239 | -0.000074 |

# Radical

R=Mt

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 0.000000 | 3.753937 | -0.000028 |
| 2 | 6 | 0 | 0.000000 | 2.499970 | -0.000022 |
| 3 | 6 | 0 | 0.000002 | 5.079208 | -0.000037 |
| 4 | 6 | 0 | 8.600852 | 0.254943 | 0.000034 |
| 5 | 6 | 0 | 8.579470 | -1.167083 | 0.000016 |
| 6 | 6 | 0 | 7.389629 | -1.843044 | 0.000000 |
| 7 | 6 | 0 | 6.146605 | -1.141810 | 0.000002 |
| 8 | 6 | 0 | 6.169198 | 0.301234 | 0.000019 |
| 9 | 6 | 0 | 7.430271 | 0.965225 | 0.000035 |
| 10 | 6 | 0 | 4.913909 | -1.804608 | -0.000013 |
| 11 | 6 | 0 | 3.699605 | -1.104160 | -0.000012 |
| 12 | 6 | 0 | 3.724623 | 0.341883 | 0.000005 |
| 13 | 6 | 0 | 4.954115 | 1.001600 | 0.000020 |
| 14 | 6 | 0 | 2.444586 | -1.751328 | -0.000024 |
| 15 | 6 | 0 | 1.238753 | -1.045363 | -0.000021 |
| 16 | 6 | 0 | 1.270865 | 0.408781 | -0.000008 |
| 17 | 6 | 0 | 2.488258 | 1.046709 | 0.000006 |
| 18 | 6 | 0 | 0.000000 | -1.718405 | -0.000029 |
| 19 | 6 | 0 | -1.238753 | -1.045364 | -0.000020 |
| 20 | 6 | 0 | -1.270866 | 0.408780 | -0.000009 |
| 21 | 6 | 0 | 0.000000 | 1.154397 | -0.000013 |
| 22 | 6 | 0 | -2.444586 | -1.751328 | -0.000020 |
| 23 | 6 | 0 | -3.699605 | -1.104160 | -0.000009 |
| 24 | 6 | 0 | -3.724622 | 0.341883 | 0.000003 |
| 25 | 6 | 0 | -2.488258 | 1.046709 | 0.000002 |
| 26 | 6 | 0 | -4.913909 | -1.804608 | -0.000008 |
| 27 | 6 | 0 | -6.146605 | -1.141810 | 0.000005 |
| 28 | 6 | 0 | -6.169198 | 0.301234 | 0.000017 |
| 29 | 6 | 0 | -4.954114 | 1.001600 | 0.000015 |
| 30 | 6 | 0 | -7.389630 | -1.843044 | 0.000006 |
| 31 | 6 | 0 | -8.579471 | -1.167083 | 0.000019 |
| 32 | 6 | 0 | -8.600853 | 0.254943 | 0.000031 |
| 33 | 6 | 0 | -7.430271 | 0.965225 | 0.000029 |
| 34 | 1 | 0 | -0.926536 | 5.643080 | -0.000038 |
| 35 | 1 | 0 | 0.926550 | 5.643064 | -0.000039 |
| 36 | 1 | 0 | 9.552688 | 0.773791 | 0.000047 |
| 37 | 1 | 0 | 9.515697 | -1.713769 | 0.000015 |
| 38 | 1 | 0 | 7.373251 | -2.927903 | -0.000013 |
| 39 | 1 | 0 | 7.445481 | 2.050126 | 0.000048 |
| 40 | 1 | 0 | 4.897332 | -2.890142 | -0.000027 |
| 41 | 1 | 0 | 4.971241 | 2.087130 | 0.000032 |
| 42 | 1 | 0 | 2.414983 | -2.836348 | -0.000036 |
| 43 | 1 | 0 | 2.517564 | 2.130614 | 0.000017 |
| 44 | 1 | 0 | 0.000000 | -2.803518 | -0.000040 |
| 45 | 1 | 0 | -2.414983 | -2.836347 | -0.000029 |
| 46 | 1 | 0 | -2.517564 | 2.130614 | 0.000011 |
| 47 | 1 | 0 | -4.897332 | -2.890142 | -0.000017 |
| 48 | 1 | 0 | -4.971240 | 2.087130 | 0.000024 |
| 49 | 1 | 0 | -7.373252 | -2.927903 | -0.000003 |
| 50 | 1 | 0 | -9.515697 | -1.713769 | 0.000020 |
| 51 | 1 | 0 | -9.552689 | 0.773791 | 0.000041 |
| 52 | 1 | 0 | -7.445482 | 2.050127 | 0.000038 |

R=DCM

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 8.584438 | -0.320531 | 0.000059 |
| 2 | 6 | 0 | 8.573084 | -1.743450 | 0.000027 |
| 3 | 6 | 0 | 7.390085 | -2.430581 | -0.000001 |
| 4 | 6 | 0 | 6.141634 | -1.739104 | 0.000002 |
| 5 | 6 | 0 | 6.154226 | -0.294499 | 0.000034 |
| 6 | 6 | 0 | 7.409922 | 0.381370 | 0.000062 |
| 7 | 6 | 0 | 4.915851 | -2.413420 | -0.000025 |
| 8 | 6 | 0 | 3.695274 | -1.723302 | -0.000021 |
| 9 | 6 | 0 | 3.711578 | -0.275753 | 0.000010 |
| 10 | 6 | 0 | 4.936984 | 0.397009 | 0.000037 |
| 11 | 6 | 0 | 2.447184 | -2.381118 | -0.000044 |
| 12 | 6 | 0 | 1.235127 | -1.684541 | -0.000038 |
| 13 | 6 | 0 | 1.260396 | -0.229607 | -0.000011 |
| 14 | 6 | 0 | 2.477629 | 0.421314 | 0.000012 |
| 15 | 6 | 0 | 0.000000 | -2.360745 | -0.000054 |
| 16 | 6 | 0 | -1.235127 | -1.684541 | -0.000038 |
| 17 | 6 | 0 | -1.260395 | -0.229607 | -0.000011 |
| 18 | 6 | 0 | 0.000000 | 0.504834 | -0.000011 |
| 19 | 6 | 0 | -2.447184 | -2.381118 | -0.000044 |
| 20 | 6 | 0 | -3.695274 | -1.723303 | -0.000021 |
| 21 | 6 | 0 | -3.711578 | -0.275753 | 0.000010 |
| 22 | 6 | 0 | -2.477629 | 0.421314 | 0.000012 |
| 23 | 6 | 0 | -4.915851 | -2.413420 | -0.000025 |
| 24 | 6 | 0 | -6.141634 | -1.739104 | 0.000002 |
| 25 | 6 | 0 | -6.154226 | -0.294499 | 0.000034 |
| 26 | 6 | 0 | -4.936984 | 0.397009 | 0.000037 |
| 27 | 6 | 0 | -7.390085 | -2.430581 | -0.000001 |
| 28 | 6 | 0 | -8.573083 | -1.743450 | 0.000026 |
| 29 | 6 | 0 | -8.584438 | -0.320531 | 0.000058 |
| 30 | 6 | 0 | -7.409922 | 0.381370 | 0.000062 |
| 31 | 6 | 0 | 0.000000 | 1.866382 | -0.000012 |
| 32 | 6 | 0 | 0.000000 | 3.103072 | -0.000018 |
| 33 | 6 | 0 | 0.000000 | 4.462085 | -0.000023 |
| 34 | 6 | 0 | -1.227211 | 5.181527 | -0.000027 |
| 35 | 6 | 0 | 1.227211 | 5.181527 | -0.000027 |
| 36 | 7 | 0 | -2.237262 | 5.746908 | -0.000029 |
| 37 | 7 | 0 | 2.237263 | 5.746908 | -0.000031 |
| 38 | 1 | 0 | 9.532571 | 0.204487 | 0.000080 |
| 39 | 1 | 0 | 9.513808 | -2.282106 | 0.000024 |
| 40 | 1 | 0 | 7.383435 | -3.515278 | -0.000025 |
| 41 | 1 | 0 | 7.415695 | 1.465975 | 0.000086 |
| 42 | 1 | 0 | 4.909345 | -3.498793 | -0.000048 |
| 43 | 1 | 0 | 4.943696 | 1.482307 | 0.000060 |
| 44 | 1 | 0 | 2.426567 | -3.466085 | -0.000065 |
| 45 | 1 | 0 | 2.501991 | 1.505142 | 0.000034 |
| 46 | 1 | 0 | 0.000000 | -3.445527 | -0.000076 |
| 47 | 1 | 0 | -2.426566 | -3.466085 | -0.000065 |
| 48 | 1 | 0 | -2.501991 | 1.505142 | 0.000034 |
| 49 | 1 | 0 | -4.909345 | -3.498792 | -0.000048 |
| 50 | 1 | 0 | -4.943696 | 1.482307 | 0.000060 |
| 51 | 1 | 0 | -7.383435 | -3.515278 | -0.000025 |
| 52 | 1 | 0 | -9.513808 | -2.282106 | 0.000024 |
| 53 | 1 | 0 | -9.532571 | 0.204487 | 0.000080 |
| 54 | 1 | 0 | -7.415695 | 1.465975 | 0.000086 |

R=DPM

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 8.597778 | -1.503522 | -0.152854 |
| 2 | 6 | 0 | 8.578305 | -2.925352 | -0.115627 |
| 3 | 6 | 0 | 7.389489 | -3.601869 | -0.076915 |
| 4 | 6 | 0 | 6.145579 | -2.902015 | -0.072601 |
| 5 | 6 | 0 | 6.166064 | -1.458937 | -0.109310 |
| 6 | 6 | 0 | 7.426671 | -0.794433 | -0.149724 |
| 7 | 6 | 0 | 4.914192 | -3.565576 | -0.035723 |
| 8 | 6 | 0 | 3.698660 | -2.866592 | -0.031961 |
| 9 | 6 | 0 | 3.721378 | -1.420198 | -0.064599 |
| 10 | 6 | 0 | 4.951144 | -0.759625 | -0.104376 |
| 11 | 6 | 0 | 2.445302 | -3.515278 | -0.005776 |
| 12 | 6 | 0 | 1.237970 | -2.811015 | -0.002607 |
| 13 | 6 | 0 | 1.267026 | -1.355997 | -0.015600 |
| 14 | 6 | 0 | 2.486398 | -0.716370 | -0.057513 |
| 15 | 6 | 0 | 0.000002 | -3.484349 | 0.000003 |
| 16 | 6 | 0 | -1.237967 | -2.811015 | 0.002609 |
| 17 | 6 | 0 | -1.267023 | -1.355997 | 0.015597 |
| 18 | 6 | 0 | 0.000001 | -0.618501 | -0.000002 |
| 19 | 6 | 0 | -2.445299 | -3.515279 | 0.005781 |
| 20 | 6 | 0 | -3.698657 | -2.866593 | 0.031963 |
| 21 | 6 | 0 | -3.721376 | -1.420199 | 0.064595 |
| 22 | 6 | 0 | -2.486396 | -0.716371 | 0.057506 |
| 23 | 6 | 0 | -4.914189 | -3.565578 | 0.035728 |
| 24 | 6 | 0 | -6.145576 | -2.902016 | 0.072603 |
| 25 | 6 | 0 | -6.166062 | -1.458939 | 0.109306 |
| 26 | 6 | 0 | -4.951142 | -0.759626 | 0.104370 |
| 27 | 6 | 0 | -7.389487 | -3.601871 | 0.076920 |
| 28 | 6 | 0 | -8.578302 | -2.925354 | 0.115630 |
| 29 | 6 | 0 | -8.597775 | -1.503524 | 0.152851 |
| 30 | 6 | 0 | -7.426669 | -0.794434 | 0.149718 |
| 31 | 6 | 0 | 0.000001 | 0.737474 | -0.000003 |
| 32 | 6 | 0 | 0.000001 | 1.981932 | -0.000003 |
| 33 | 6 | 0 | 0.000000 | 3.332989 | -0.000001 |
| 34 | 6 | 0 | -1.279971 | 4.058151 | -0.152073 |
| 35 | 6 | 0 | 1.279968 | 4.058155 | 0.152073 |
| 36 | 6 | 0 | -1.509266 | 5.278829 | 0.507225 |
| 37 | 6 | 0 | -2.730993 | 5.932912 | 0.390615 |
| 38 | 6 | 0 | -3.749860 | 5.390550 | -0.390802 |
| 39 | 6 | 0 | -3.536263 | 4.182508 | -1.054161 |
| 40 | 6 | 0 | -2.318301 | 3.523659 | -0.936006 |
| 41 | 6 | 0 | 1.509258 | 5.278835 | -0.507224 |
| 42 | 6 | 0 | 2.730982 | 5.932923 | -0.390612 |
| 43 | 6 | 0 | 3.749850 | 5.390565 | 0.390806 |
| 44 | 6 | 0 | 3.536258 | 4.182522 | 1.054164 |
| 45 | 6 | 0 | 2.318299 | 3.523668 | 0.936007 |
| 46 | 1 | 0 | 9.548853 | -0.984153 | -0.184214 |
| 47 | 1 | 0 | 9.515083 | -3.471103 | -0.118564 |
| 48 | 1 | 0 | 7.374431 | -4.686422 | -0.049083 |
| 49 | 1 | 0 | 7.440403 | 0.290107 | -0.179038 |
| 50 | 1 | 0 | 4.898992 | -4.650882 | -0.010861 |
| 51 | 1 | 0 | 4.966272 | 0.325571 | -0.132542 |
| 52 | 1 | 0 | 2.417275 | -4.600309 | 0.006621 |
| 53 | 1 | 0 | 2.515793 | 0.366703 | -0.094713 |
| 54 | 1 | 0 | 0.000002 | -4.569533 | 0.000005 |
| 55 | 1 | 0 | -2.417271 | -4.600310 | -0.006611 |
| 56 | 1 | 0 | -2.515792 | 0.366703 | 0.094703 |
| 57 | 1 | 0 | -4.898988 | -4.650884 | 0.010870 |
| 58 | 1 | 0 | -4.966270 | 0.325570 | 0.132531 |
| 59 | 1 | 0 | -7.374428 | -4.686424 | 0.049092 |
| 60 | 1 | 0 | -9.515080 | -3.471106 | 0.118569 |
| 61 | 1 | 0 | -9.548850 | -0.984155 | 0.184210 |
| 62 | 1 | 0 | -7.440401 | 0.290106 | 0.179028 |
| 63 | 1 | 0 | -0.731650 | 5.702220 | 1.130909 |
| 64 | 1 | 0 | -2.889966 | 6.867133 | 0.917681 |
| 65 | 1 | 0 | -4.699286 | 5.905244 | -0.484610 |
| 66 | 1 | 0 | -4.317442 | 3.757935 | -1.675033 |
| 67 | 1 | 0 | -2.150268 | 2.594946 | -1.468527 |

| | | | | | |
|---|---|---|---|---|---|
| 68 | 1 | 0 | 0.731641 | 5.702222 | -1.130909 |
| 69 | 1 | 0 | 2.889951 | 6.867146 | -0.917677 |
| 70 | 1 | 0 | 4.699273 | 5.905264 | 0.484616 |
| 71 | 1 | 0 | 4.317438 | 3.757952 | 1.675036 |
| 72 | 1 | 0 | 2.150270 | 2.594953 | 1.468527 |

R=Flu

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 8.597120 | -1.616309 | -0.000127 |
| 2 | 6 | 0 | 8.576637 | -3.038821 | -0.000036 |
| 3 | 6 | 0 | 7.387625 | -3.715753 | 0.000029 |
| 4 | 6 | 0 | 6.143888 | -3.015447 | 0.000008 |
| 5 | 6 | 0 | 6.165414 | -1.571658 | -0.000083 |
| 6 | 6 | 0 | 7.426627 | -0.906717 | -0.000150 |
| 7 | 6 | 0 | 4.912389 | -3.679159 | 0.000072 |
| 8 | 6 | 0 | 3.696874 | -2.979839 | 0.000050 |
| 9 | 6 | 0 | 3.720177 | -1.532939 | -0.000039 |
| 10 | 6 | 0 | 4.951161 | -0.872369 | -0.000104 |
| 11 | 6 | 0 | 2.443840 | -3.628027 | 0.000107 |
| 12 | 6 | 0 | 1.236473 | -2.923509 | 0.000082 |
| 13 | 6 | 0 | 1.264858 | -1.468176 | 0.000006 |
| 14 | 6 | 0 | 2.486375 | -0.829726 | -0.000056 |
| 15 | 6 | 0 | -0.000002 | -3.597601 | 0.000125 |
| 16 | 6 | 0 | -1.236475 | -2.923508 | 0.000081 |
| 17 | 6 | 0 | -1.264860 | -1.468175 | 0.000008 |
| 18 | 6 | 0 | -0.000001 | -0.729656 | 0.000000 |
| 19 | 6 | 0 | -2.443843 | -3.628026 | 0.000103 |
| 20 | 6 | 0 | -3.696876 | -2.979837 | 0.000048 |
| 21 | 6 | 0 | -3.720178 | -1.532937 | -0.000034 |
| 22 | 6 | 0 | -2.486376 | -0.829725 | -0.000050 |
| 23 | 6 | 0 | -4.912392 | -3.679156 | 0.000067 |
| 24 | 6 | 0 | -6.143890 | -3.015443 | 0.000007 |
| 25 | 6 | 0 | -6.165416 | -1.571654 | -0.000078 |
| 26 | 6 | 0 | -4.951162 | -0.872366 | -0.000096 |
| 27 | 6 | 0 | -7.387628 | -3.715749 | 0.000025 |
| 28 | 6 | 0 | -8.576639 | -3.038816 | -0.000036 |
| 29 | 6 | 0 | -8.597122 | -1.616305 | -0.000120 |
| 30 | 6 | 0 | -7.426628 | -0.906713 | -0.000140 |
| 31 | 6 | 0 | 0.000000 | 0.630111 | -0.000003 |
| 32 | 6 | 0 | 0.000002 | 1.872640 | 0.000009 |
| 33 | 6 | 0 | 0.000002 | 3.222294 | 0.000021 |
| 34 | 6 | 0 | -1.173683 | 4.100467 | 0.000023 |
| 35 | 6 | 0 | 1.173688 | 4.100466 | 0.000028 |
| 36 | 6 | 0 | -2.534769 | 3.803181 | 0.000026 |
| 37 | 6 | 0 | -3.453990 | 4.850994 | 0.000025 |
| 38 | 6 | 0 | -3.020189 | 6.180303 | 0.000021 |
| 39 | 6 | 0 | -1.657931 | 6.486965 | 0.000019 |
| 40 | 6 | 0 | -0.733159 | 5.448498 | 0.000020 |
| 41 | 6 | 0 | 0.733164 | 5.448497 | 0.000023 |
| 42 | 6 | 0 | 1.657936 | 6.486965 | 0.000027 |
| 43 | 6 | 0 | 3.020194 | 6.180303 | 0.000035 |
| 44 | 6 | 0 | 3.453994 | 4.850994 | 0.000042 |
| 45 | 6 | 0 | 2.534774 | 3.803180 | 0.000039 |
| 46 | 1 | 0 | 9.548721 | -1.097113 | -0.000178 |
| 47 | 1 | 0 | 9.513325 | -3.584639 | -0.000019 |
| 48 | 1 | 0 | 7.372099 | -4.800579 | 0.000098 |
| 49 | 1 | 0 | 7.441249 | 0.178142 | -0.000219 |
| 50 | 1 | 0 | 4.896658 | -4.764658 | 0.000139 |
| 51 | 1 | 0 | 4.968348 | 0.213072 | -0.000173 |
| 52 | 1 | 0 | 2.415123 | -4.713017 | 0.000167 |
| 53 | 1 | 0 | 2.515037 | 0.253600 | -0.000124 |
| 54 | 1 | 0 | -0.000002 | -4.682670 | 0.000184 |
| 55 | 1 | 0 | -2.415127 | -4.713016 | 0.000161 |
| 56 | 1 | 0 | -2.515038 | 0.253602 | -0.000114 |
| 57 | 1 | 0 | -4.896662 | -4.764655 | 0.000130 |
| 58 | 1 | 0 | -4.968349 | 0.213075 | -0.000159 |
| 59 | 1 | 0 | -7.372103 | -4.800575 | 0.000089 |
| 60 | 1 | 0 | -9.513328 | -3.584634 | -0.000022 |
| 61 | 1 | 0 | -9.548722 | -1.097108 | -0.000168 |
| 62 | 1 | 0 | -7.441250 | 0.178146 | -0.000204 |
| 63 | 1 | 0 | -2.873505 | 2.773435 | 0.000033 |
| 64 | 1 | 0 | -4.516303 | 4.634624 | 0.000028 |
| 65 | 1 | 0 | -3.750449 | 6.981624 | 0.000020 |
| 66 | 1 | 0 | -1.332701 | 7.521598 | 0.000018 |
| 67 | 1 | 0 | 1.332706 | 7.521598 | 0.000024 |
| 68 | 1 | 0 | 3.750454 | 6.981623 | 0.000037 |
| 69 | 1 | 0 | 4.516308 | 4.634623 | 0.000051 |
| 70 | 1 | 0 | 2.873510 | 2.773435 | 0.000050 |

R=PhO

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -8.590168 | -0.867610 | 0.000022 |
| 2 | 6 | 0 | -8.573647 | -2.290958 | 0.000005 |
| 3 | 6 | 0 | -7.387584 | -2.972068 | -0.000006 |
| 4 | 6 | 0 | -6.141264 | -2.275493 | -0.000002 |
| 5 | 6 | 0 | -6.158760 | -0.830559 | 0.000015 |
| 6 | 6 | 0 | -7.418547 | -0.161235 | 0.000027 |
| 7 | 6 | 0 | -4.913208 | -2.943484 | -0.000013 |
| 8 | 6 | 0 | -3.694216 | -2.248265 | -0.000009 |
| 9 | 6 | 0 | -3.713582 | -0.800192 | 0.000007 |
| 10 | 6 | 0 | -4.944376 | -0.134944 | 0.000019 |
| 11 | 6 | 0 | -2.445413 | -2.901497 | -0.000019 |
| 12 | 6 | 0 | -1.234745 | -2.200686 | -0.000015 |
| 13 | 6 | 0 | -1.259171 | -0.745163 | 0.000000 |
| 14 | 6 | 0 | -2.481938 | -0.099965 | 0.000011 |
| 15 | 6 | 0 | 0.000001 | -2.875920 | -0.000023 |
| 16 | 6 | 0 | 1.234746 | -2.200686 | -0.000015 |
| 17 | 6 | 0 | 1.259172 | -0.745162 | 0.000000 |
| 18 | 6 | 0 | 0.000000 | -0.013199 | 0.000002 |
| 19 | 6 | 0 | 2.445415 | -2.901496 | -0.000021 |
| 20 | 6 | 0 | 3.694217 | -2.248264 | -0.000010 |
| 21 | 6 | 0 | 3.713583 | -0.800191 | 0.000007 |
| 22 | 6 | 0 | 2.481939 | -0.099965 | 0.000011 |
| 23 | 6 | 0 | 4.913209 | -2.943482 | -0.000015 |
| 24 | 6 | 0 | 6.141265 | -2.275492 | -0.000003 |
| 25 | 6 | 0 | 6.158760 | -0.830557 | 0.000015 |
| 26 | 6 | 0 | 4.944377 | -0.134943 | 0.000020 |
| 27 | 6 | 0 | 7.387585 | -2.972066 | -0.000008 |
| 28 | 6 | 0 | 8.573648 | -2.290956 | 0.000005 |
| 29 | 6 | 0 | 8.590169 | -0.867608 | 0.000023 |
| 30 | 6 | 0 | 7.418548 | -0.161233 | 0.000028 |
| 31 | 6 | 0 | 0.000000 | 1.356597 | 0.000004 |
| 32 | 6 | 0 | 0.000000 | 2.591354 | 0.000002 |
| 33 | 6 | 0 | -0.000001 | 3.962000 | -0.000002 |
| 34 | 6 | 0 | -1.236040 | 4.702961 | -0.000007 |
| 35 | 6 | 0 | -1.242603 | 6.058678 | -0.000012 |
| 36 | 6 | 0 | -0.000003 | 6.839110 | -0.000013 |
| 37 | 6 | 0 | 1.242599 | 6.058680 | -0.000008 |
| 38 | 6 | 0 | 1.236038 | 4.702962 | -0.000003 |
| 39 | 8 | 0 | -0.000003 | 8.072317 | -0.000018 |
| 40 | 1 | 0 | -9.540438 | -0.346198 | 0.000031 |
| 41 | 1 | 0 | -9.512170 | -2.833480 | 0.000002 |
| 42 | 1 | 0 | -7.375737 | -4.056831 | -0.000019 |
| 43 | 1 | 0 | -7.429848 | 0.923537 | 0.000039 |
| 44 | 1 | 0 | -4.901340 | -4.028922 | -0.000026 |
| 45 | 1 | 0 | -4.957417 | 0.950466 | 0.000031 |
| 46 | 1 | 0 | -2.420827 | -3.986481 | -0.000031 |
| 47 | 1 | 0 | -2.507073 | 0.983536 | 0.000023 |
| 48 | 1 | 0 | 0.000001 | -3.960920 | -0.000035 |
| 49 | 1 | 0 | 2.420828 | -3.986480 | -0.000033 |
| 50 | 1 | 0 | 2.507074 | 0.983536 | 0.000023 |
| 51 | 1 | 0 | 4.901342 | -4.028920 | -0.000029 |
| 52 | 1 | 0 | 4.957417 | 0.950468 | 0.000033 |
| 53 | 1 | 0 | 7.375739 | -4.056829 | -0.000022 |
| 54 | 1 | 0 | 9.512171 | -2.833477 | 0.000001 |
| 55 | 1 | 0 | 9.540438 | -0.346196 | 0.000033 |
| 56 | 1 | 0 | 7.429848 | 0.923539 | 0.000042 |
| 57 | 1 | 0 | -2.165515 | 4.144423 | -0.000007 |
| 58 | 1 | 0 | -2.167329 | 6.624119 | -0.000016 |
| 59 | 1 | 0 | 2.167324 | 6.624122 | -0.000009 |
| 60 | 1 | 0 | 2.165512 | 4.144425 | 0.000001 |

R=NO

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 8.613850 | -0.091851 | -0.000015 |
| 2 | 6 | 0 | 8.601816 | -1.515362 | -0.000004 |
| 3 | 6 | 0 | 7.417131 | -2.198845 | 0.000003 |
| 4 | 6 | 0 | 6.168428 | -1.505979 | 0.000000 |
| 5 | 6 | 0 | 6.181207 | -0.060910 | -0.000010 |
| 6 | 6 | 0 | 7.439903 | 0.610898 | -0.000018 |
| 7 | 6 | 0 | 4.942210 | -2.176627 | 0.000007 |
| 8 | 6 | 0 | 3.720149 | -1.485454 | 0.000005 |
| 9 | 6 | 0 | 3.734143 | -0.036701 | -0.000006 |
| 10 | 6 | 0 | 4.964536 | 0.630732 | -0.000013 |
| 11 | 6 | 0 | 2.474524 | -2.143983 | 0.000012 |
| 12 | 6 | 0 | 1.259457 | -1.449624 | 0.000010 |
| 13 | 6 | 0 | 1.277304 | 0.006278 | 0.000001 |
| 14 | 6 | 0 | 2.499408 | 0.657424 | -0.000008 |
| 15 | 6 | 0 | 0.027081 | -2.129794 | 0.000015 |
| 16 | 6 | 0 | -1.210787 | -1.459875 | 0.000010 |
| 17 | 6 | 0 | -1.240766 | -0.004543 | 0.000002 |
| 18 | 6 | 0 | 0.016413 | 0.724076 | 0.000002 |
| 19 | 6 | 0 | -2.419797 | -2.164876 | 0.000013 |
| 20 | 6 | 0 | -3.670448 | -1.515834 | 0.000006 |
| 21 | 6 | 0 | -3.694963 | -0.067387 | -0.000004 |
| 22 | 6 | 0 | -2.467264 | 0.639224 | -0.000005 |
| 23 | 6 | 0 | -4.887143 | -2.216279 | 0.000009 |
| 24 | 6 | 0 | -6.117949 | -1.553849 | 0.000001 |
| 25 | 6 | 0 | -6.140709 | -0.108862 | -0.000011 |
| 26 | 6 | 0 | -4.929481 | 0.592370 | -0.000013 |
| 27 | 6 | 0 | -7.361824 | -2.255269 | 0.000003 |
| 28 | 6 | 0 | -8.550999 | -1.579537 | -0.000006 |
| 29 | 6 | 0 | -8.572830 | -0.156138 | -0.000017 |
| 30 | 6 | 0 | -7.403769 | 0.554731 | -0.000020 |
| 31 | 6 | 0 | -0.007620 | 2.099519 | 0.000003 |
| 32 | 6 | 0 | -0.089328 | 3.324791 | 0.000005 |
| 33 | 7 | 0 | -0.246112 | 4.630069 | 0.000011 |
| 34 | 8 | 0 | -1.401917 | 5.183579 | 0.000017 |
| 35 | 6 | 0 | 0.923625 | 5.527617 | 0.000012 |
| 36 | 1 | 0 | 9.562591 | 0.432642 | -0.000020 |
| 37 | 1 | 0 | 9.541785 | -2.055498 | -0.000002 |
| 38 | 1 | 0 | 7.407783 | -3.283767 | 0.000011 |
| 39 | 1 | 0 | 7.448594 | 1.695901 | -0.000026 |

| | | | | | |
|---|---|---|---|---|---|
| 40 | 1 | 0 | 4.933055 | -3.262222 | 0.000015 |
| 41 | 1 | 0 | 4.975369 | 1.716436 | -0.000021 |
| 42 | 1 | 0 | 2.455273 | -3.229192 | 0.000018 |
| 43 | 1 | 0 | 2.521287 | 1.741427 | -0.000018 |
| 44 | 1 | 0 | 0.031870 | -3.214898 | 0.000022 |
| 45 | 1 | 0 | -2.391404 | -3.249930 | 0.000021 |
| 46 | 1 | 0 | -2.500754 | 1.722974 | -0.000011 |
| 47 | 1 | 0 | -4.870394 | -3.301825 | 0.000017 |
| 48 | 1 | 0 | -4.945903 | 1.677707 | -0.000021 |
| 49 | 1 | 0 | -7.345268 | -3.340137 | 0.000012 |
| 50 | 1 | 0 | -9.487333 | -2.126051 | -0.000004 |
| 51 | 1 | 0 | -9.525114 | 0.361875 | -0.000024 |
| 52 | 1 | 0 | -7.418964 | 1.639516 | -0.000028 |
| 53 | 1 | 0 | 1.843395 | 4.944679 | 0.000012 |
| 54 | 1 | 0 | 0.864597 | 6.155376 | -0.889842 |
| 55 | 1 | 0 | 0.864595 | 6.155374 | 0.889868 |

R=Allyl

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 0.000000 | 3.361862 | 0.000000 |
| 2 | 6 | 0 | 0.000000 | 2.147137 | -0.000001 |
| 3 | 6 | 0 | 0.000000 | 4.789883 | 0.000000 |
| 4 | 6 | 0 | 8.586619 | -0.083272 | 0.000013 |
| 5 | 6 | 0 | 8.572037 | -1.508363 | 0.000007 |
| 6 | 6 | 0 | 7.387029 | -2.189554 | 0.000002 |
| 7 | 6 | 0 | 6.138159 | -1.494756 | 0.000002 |
| 8 | 6 | 0 | 6.153179 | -0.047561 | 0.000008 |
| 9 | 6 | 0 | 7.415273 | 0.621611 | 0.000013 |
| 10 | 6 | 0 | 4.913101 | -2.162899 | -0.000003 |
| 11 | 6 | 0 | 3.689387 | -1.469885 | -0.000002 |
| 12 | 6 | 0 | 3.704284 | -0.018558 | 0.000003 |
| 13 | 6 | 0 | 4.941358 | 0.646263 | 0.000008 |
| 14 | 6 | 0 | 2.447305 | -2.127543 | -0.000005 |
| 15 | 6 | 0 | 1.230677 | -1.430883 | -0.000003 |
| 16 | 6 | 0 | 1.245989 | 0.026832 | -0.000002 |
| 17 | 6 | 0 | 2.478912 | 0.679083 | 0.000003 |
| 18 | 6 | 0 | 0.000000 | -2.107465 | -0.000001 |
| 19 | 6 | 0 | -1.230677 | -1.430883 | 0.000001 |
| 20 | 6 | 0 | -1.245989 | 0.026832 | 0.000000 |
| 21 | 6 | 0 | 0.000000 | 0.738821 | -0.000001 |
| 22 | 6 | 0 | -2.447305 | -2.127543 | 0.000002 |
| 23 | 6 | 0 | -3.689387 | -1.469885 | 0.000001 |
| 24 | 6 | 0 | -3.704284 | -0.018558 | -0.000004 |
| 25 | 6 | 0 | -2.478912 | 0.679083 | -0.000004 |
| 26 | 6 | 0 | -4.913101 | -2.162899 | 0.000002 |
| 27 | 6 | 0 | -6.138159 | -1.494756 | -0.000001 |
| 28 | 6 | 0 | -6.153179 | -0.047561 | -0.000006 |
| 29 | 6 | 0 | -4.941358 | 0.646263 | -0.000008 |
| 30 | 6 | 0 | -7.387029 | -2.189554 | 0.000000 |
| 31 | 6 | 0 | -8.572037 | -1.508363 | -0.000004 |
| 32 | 6 | 0 | -8.586619 | -0.083272 | -0.000009 |
| 33 | 6 | 0 | -7.415273 | 0.621610 | -0.000010 |
| 34 | 6 | 0 | -1.220558 | 5.469680 | 0.000179 |
| 35 | 6 | 0 | 1.220557 | 5.469681 | -0.000179 |
| 36 | 1 | 0 | 9.536636 | 0.438968 | 0.000017 |
| 37 | 1 | 0 | 9.511308 | -2.049755 | 0.000007 |
| 38 | 1 | 0 | 7.375758 | -3.274496 | -0.000003 |
| 39 | 1 | 0 | 7.425866 | 1.706564 | 0.000018 |
| 40 | 1 | 0 | 4.902071 | -3.248522 | -0.000007 |
| 41 | 1 | 0 | 4.953731 | 1.731801 | 0.000013 |
| 42 | 1 | 0 | 2.426833 | -3.212783 | -0.000006 |
| 43 | 1 | 0 | 2.498619 | 1.762298 | 0.000010 |
| 44 | 1 | 0 | 0.000000 | -3.192758 | -0.000001 |
| 45 | 1 | 0 | -2.426833 | -3.212783 | 0.000004 |
| 46 | 1 | 0 | -2.498619 | 1.762298 | -0.000011 |
| 47 | 1 | 0 | -4.902071 | -3.248522 | 0.000006 |
| 48 | 1 | 0 | -4.953731 | 1.731801 | -0.000012 |
| 49 | 1 | 0 | -7.375758 | -3.274496 | 0.000004 |
| 50 | 1 | 0 | -9.511308 | -2.049755 | -0.000003 |
| 51 | 1 | 0 | -9.536636 | 0.438967 | -0.000012 |
| 52 | 1 | 0 | -7.425866 | 1.706563 | -0.000014 |
| 53 | 1 | 0 | -1.242482 | 6.552306 | 0.000180 |
| 54 | 1 | 0 | -2.161774 | 4.938111 | 0.000324 |
| 55 | 1 | 0 | 1.242481 | 6.552306 | -0.000179 |
| 56 | 1 | 0 | 2.161773 | 4.938111 | -0.000325 |

R=IN

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 8.916535 | -0.331368 | -0.009239 |
| 2 | 6 | 0 | 9.075085 | -1.755567 | -0.018974 |
| 3 | 6 | 0 | 7.987085 | -2.573310 | -0.021841 |
| 4 | 6 | 0 | 6.655764 | -2.034960 | -0.015232 |
| 5 | 6 | 0 | 6.494734 | -0.588222 | -0.005335 |
| 6 | 6 | 0 | 7.675490 | 0.228163 | -0.002689 |
| 7 | 6 | 0 | 5.531965 | -2.842500 | -0.017977 |
| 8 | 6 | 0 | 4.223034 | -2.301554 | -0.011430 |
| 9 | 6 | 0 | 4.061302 | -0.854033 | -0.001629 |
| 10 | 6 | 0 | 5.221004 | -0.044106 | 0.001128 |
| 11 | 6 | 0 | 3.083102 | -3.103317 | -0.013971 |
| 12 | 6 | 0 | 1.786195 | -2.556238 | -0.007399 |
| 13 | 6 | 0 | 1.624825 | -1.107551 | 0.002055 |
| 14 | 6 | 0 | 2.774898 | -0.306493 | 0.004598 |
| 15 | 6 | 0 | 0.649886 | -3.374384 | -0.009615 |
| 16 | 6 | 0 | -0.649540 | -2.853465 | -0.002888 |
| 17 | 6 | 0 | -0.839686 | -1.408389 | 0.005825 |
| 18 | 6 | 0 | 0.308626 | -0.560526 | 0.007580 |
| 19 | 6 | 0 | -1.777535 | -3.695943 | -0.003995 |
| 20 | 6 | 0 | -3.075990 | -3.189633 | 0.003546 |
| 21 | 6 | 0 | -3.263823 | -1.745408 | 0.012732 |
| 22 | 6 | 0 | -2.147458 | -0.903469 | 0.013522 |
| 23 | 6 | 0 | -4.218851 | -4.026362 | 0.003035 |
| 24 | 6 | 0 | -5.502135 | -3.508226 | 0.011255 |
| 25 | 6 | 0 | -5.689658 | -2.064513 | 0.020714 |
| 26 | 6 | 0 | -4.582159 | -1.232678 | 0.021120 |
| 27 | 6 | 0 | -6.667764 | -4.347162 | 0.011038 |
| 28 | 6 | 0 | -7.918746 | -3.810971 | 0.019556 |
| 29 | 6 | 0 | -8.103252 | -2.389861 | 0.028986 |
| 30 | 6 | 0 | -7.030451 | -1.551763 | 0.029515 |
| 31 | 6 | 0 | 0.121076 | 0.835567 | 0.014926 |
| 32 | 6 | 0 | -0.087227 | 2.028929 | 0.020389 |
| 33 | 6 | 0 | -0.422511 | 3.399130 | 0.031219 |
| 34 | 7 | 0 | -1.787942 | 3.763932 | 0.035335 |
| 35 | 6 | 0 | -1.885359 | 5.241390 | -0.201792 |
| 36 | 6 | 0 | -0.407178 | 5.651200 | 0.170883 |
| 37 | 7 | 0 | 0.389200 | 4.402098 | 0.035269 |
| 38 | 6 | 0 | 0.199547 | 6.729248 | -0.732802 |
| 39 | 6 | 0 | -0.257546 | 6.087112 | 1.642340 |
| 40 | 6 | 0 | -3.003617 | 5.826289 | 0.659365 |
| 41 | 6 | 0 | -2.229210 | 5.418873 | -1.691737 |
| 42 | 8 | 0 | -2.776904 | 2.979709 | 0.010720 |
| 43 | 1 | 0 | 9.798676 | 0.298820 | -0.007138 |
| 44 | 1 | 0 | 10.074107 | -2.176542 | -0.024048 |
| 45 | 1 | 0 | 8.106448 | -3.651659 | -0.029206 |
| 46 | 1 | 0 | 7.555607 | 1.306347 | 0.004666 |
| 47 | 1 | 0 | 5.650450 | -3.921629 | -0.025338 |
| 48 | 1 | 0 | 5.101990 | 1.034695 | 0.008423 |
| 49 | 1 | 0 | 3.193212 | -4.183090 | -0.021218 |
| 50 | 1 | 0 | 2.663620 | 0.771610 | 0.011652 |
| 51 | 1 | 0 | 0.781626 | -4.451934 | -0.016472 |
| 52 | 1 | 0 | -1.625643 | -4.770654 | -0.010431 |
| 53 | 1 | 0 | -2.302106 | 0.169730 | 0.020959 |
| 54 | 1 | 0 | -4.078055 | -5.102836 | -0.003815 |
| 55 | 1 | 0 | -4.719154 | -0.156127 | 0.028290 |
| 56 | 1 | 0 | -6.527947 | -5.423079 | 0.003973 |
| 57 | 1 | 0 | -8.789177 | -4.457313 | 0.019335 |
| 58 | 1 | 0 | -9.109870 | -1.987352 | 0.035773 |
| 59 | 1 | 0 | -7.169069 | -0.475874 | 0.036742 |
| 60 | 1 | 0 | 1.225735 | 6.922250 | -0.414349 |
| 61 | 1 | 0 | 0.230073 | 6.417379 | -1.776599 |
| 62 | 1 | 0 | -0.363455 | 7.664605 | -0.662694 |
| 63 | 1 | 0 | -0.756952 | 7.041436 | 1.827977 |
| 64 | 1 | 0 | -0.664443 | 5.339524 | 2.326259 |
| 65 | 1 | 0 | 0.804138 | 6.201373 | 1.867606 |
| 66 | 1 | 0 | -3.952416 | 5.366542 | 0.377087 |
| 67 | 1 | 0 | -2.845753 | 5.643525 | 1.721735 |
| 68 | 1 | 0 | -3.080725 | 6.904096 | 0.496996 |
| 69 | 1 | 0 | -2.341937 | 6.475420 | -1.942484 |
| 70 | 1 | 0 | -1.462169 | 4.987489 | -2.337413 |
| 71 | 1 | 0 | -3.173136 | 4.909783 | -1.896951 |

R=Phen

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 8.573855 | -1.920165 | -0.080523 |
| 2 | 6 | 0 | 8.558642 | -3.353168 | -0.071784 |
| 3 | 6 | 0 | 7.379659 | -4.033010 | -0.056565 |
| 4 | 6 | 0 | 6.123056 | -3.337720 | -0.048770 |
| 5 | 6 | 0 | 6.138595 | -1.882008 | -0.057282 |
| 6 | 6 | 0 | 7.409573 | -1.214774 | -0.073546 |
| 7 | 6 | 0 | 4.909947 | -4.003321 | -0.034069 |
| 8 | 6 | 0 | 3.675662 | -3.308404 | -0.026560 |
| 9 | 6 | 0 | 3.690392 | -1.852228 | -0.033626 |
| 10 | 6 | 0 | 4.939807 | -1.188644 | -0.049629 |
| 11 | 6 | 0 | 2.446916 | -3.965034 | -0.014417 |
| 12 | 6 | 0 | 1.224701 | -3.266208 | -0.007217 |
| 13 | 6 | 0 | 1.238502 | -1.807913 | -0.009703 |
| 14 | 6 | 0 | 2.479274 | -1.154801 | -0.025227 |
| 15 | 6 | 0 | -0.000006 | -3.943229 | 0.000002 |
| 16 | 6 | 0 | -1.224710 | -3.266205 | 0.007219 |
| 17 | 6 | 0 | -1.238508 | -1.807910 | 0.009704 |
| 18 | 6 | 0 | -0.000002 | -1.098771 | 0.000000 |
| 19 | 6 | 0 | -2.446927 | -3.965028 | 0.014420 |
| 20 | 6 | 0 | -3.675672 | -3.308395 | 0.026562 |
| 21 | 6 | 0 | -3.690398 | -1.852219 | 0.033625 |
| 22 | 6 | 0 | -2.479279 | -1.154795 | 0.025226 |
| 23 | 6 | 0 | -4.909959 | -4.003309 | 0.034070 |
| 24 | 6 | 0 | -6.123065 | -3.337706 | 0.048770 |
| 25 | 6 | 0 | -6.138601 | -1.881993 | 0.057279 |
| 26 | 6 | 0 | -4.939812 | -1.188632 | 0.049626 |
| 27 | 6 | 0 | -7.379670 | -4.032992 | 0.056565 |
| 28 | 6 | 0 | -8.558652 | -3.353148 | 0.071782 |
| 29 | 6 | 0 | -8.573862 | -1.920144 | 0.080519 |
| 30 | 6 | 0 | -7.409578 | -1.214756 | 0.073541 |
| 31 | 6 | 0 | 0.000000 | 0.314363 | 0.000001 |

| | | | | | |
|---|---|---|---|---|---|
| 32 | 6 | 0 | 0.000002 | 1.528064 | 0.000000 |
| 33 | 6 | 0 | 0.000005 | 2.950073 | 0.000000 |
| 34 | 6 | 0 | -1.187163 | 3.659320 | -0.242280 |
| 35 | 6 | 0 | -1.211034 | 5.070384 | -0.247050 |
| 36 | 6 | 0 | 0.000009 | 5.787458 | 0.000000 |
| 37 | 6 | 0 | 1.211050 | 5.070380 | 0.247051 |
| 38 | 6 | 0 | 1.187174 | 3.659316 | 0.242281 |
| 39 | 6 | 0 | 0.000011 | 7.215192 | 0.000000 |
| 40 | 6 | 0 | 1.216664 | 7.897323 | 0.248802 |
| 41 | 6 | 0 | 2.391081 | 7.192873 | 0.489091 |
| 42 | 6 | 0 | 2.400388 | 5.803699 | 0.490713 |
| 43 | 6 | 0 | -2.400370 | 5.803707 | -0.490713 |
| 44 | 6 | 0 | -2.391058 | 7.192880 | -0.489090 |
| 45 | 6 | 0 | -1.216639 | 7.897327 | -0.248802 |
| 46 | 1 | 0 | 9.525765 | -1.401464 | -0.092915 |
| 47 | 1 | 0 | 9.499265 | -3.892163 | -0.077570 |
| 48 | 1 | 0 | 7.367705 | -5.117896 | -0.050109 |
| 49 | 1 | 0 | 7.421345 | -0.129901 | -0.080395 |
| 50 | 1 | 0 | 4.897314 | -5.088883 | -0.028405 |
| 51 | 1 | 0 | 4.952839 | -0.103205 | -0.056451 |
| 52 | 1 | 0 | 2.425298 | -5.050231 | -0.011580 |
| 53 | 1 | 0 | 2.498781 | -0.071727 | -0.033660 |
| 54 | 1 | 0 | -0.000007 | -5.028577 | 0.000004 |
| 55 | 1 | 0 | -2.425312 | -5.050226 | 0.011584 |
| 56 | 1 | 0 | -2.498783 | -0.071721 | 0.033657 |
| 57 | 1 | 0 | -4.897328 | -5.088871 | 0.028409 |
| 58 | 1 | 0 | -4.952841 | -0.103193 | 0.056447 |
| 59 | 1 | 0 | -7.367719 | -5.117878 | 0.050111 |
| 60 | 1 | 0 | -9.499276 | -3.892140 | 0.077570 |
| 61 | 1 | 0 | -9.525770 | -1.401441 | 0.092909 |
| 62 | 1 | 0 | -7.421348 | -0.129883 | 0.080388 |
| 63 | 1 | 0 | -2.102827 | 3.112841 | -0.433986 |
| 64 | 1 | 0 | 2.102836 | 3.112834 | 0.433988 |
| 65 | 1 | 0 | 1.220459 | 8.981764 | 0.249690 |
| 66 | 1 | 0 | 3.311333 | 7.734518 | 0.677668 |
| 67 | 1 | 0 | 3.321388 | 5.263379 | 0.679591 |
| 68 | 1 | 0 | -3.321372 | 5.263389 | -0.679591 |
| 69 | 1 | 0 | -3.311309 | 7.734528 | -0.677668 |
| 70 | 1 | 0 | -1.220431 | 8.981768 | -0.249689 |

R=Ver

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -8.584285 | -2.569548 | 0.075577 |
| 2 | 6 | 0 | -8.571753 | -3.994381 | 0.037443 |
| 3 | 6 | 0 | -7.388093 | -4.677005 | 0.009516 |
| 4 | 6 | 0 | -6.138066 | -3.983982 | 0.017474 |
| 5 | 6 | 0 | -6.151014 | -2.536995 | 0.055272 |
| 6 | 6 | 0 | -7.412211 | -1.866310 | 0.084193 |
| 7 | 6 | 0 | -4.914476 | -4.653700 | -0.008728 |
| 8 | 6 | 0 | -3.689504 | -3.962430 | -0.000120 |
| 9 | 6 | 0 | -3.702811 | -2.511201 | 0.035167 |
| 10 | 6 | 0 | -4.938913 | -1.844470 | 0.062760 |
| 11 | 6 | 0 | -2.448934 | -4.622288 | -0.022164 |
| 12 | 6 | 0 | -1.231487 | -3.926876 | -0.011534 |
| 13 | 6 | 0 | -1.246994 | -2.469906 | 0.018862 |
| 14 | 6 | 0 | -2.477898 | -1.813653 | 0.041877 |
| 15 | 6 | 0 | 0.000004 | -4.602297 | -0.028362 |
| 16 | 6 | 0 | 1.231494 | -3.926874 | -0.011534 |
| 17 | 6 | 0 | 1.247000 | -2.469904 | 0.018863 |
| 18 | 6 | 0 | 0.000002 | -1.762470 | 0.025870 |
| 19 | 6 | 0 | 2.448942 | -4.622285 | -0.022164 |
| 20 | 6 | 0 | 3.689511 | -3.962425 | -0.000121 |
| 21 | 6 | 0 | 3.702817 | -2.511196 | 0.035166 |
| 22 | 6 | 0 | 2.477902 | -1.813650 | 0.041877 |
| 23 | 6 | 0 | 4.914484 | -4.653694 | -0.008728 |
| 24 | 6 | 0 | 6.138074 | -3.983973 | 0.017473 |
| 25 | 6 | 0 | 6.151020 | -2.536987 | 0.055270 |
| 26 | 6 | 0 | 4.938917 | -1.844463 | 0.062759 |
| 27 | 6 | 0 | 7.388102 | -4.676995 | 0.009514 |
| 28 | 6 | 0 | 8.571761 | -3.994369 | 0.037440 |
| 29 | 6 | 0 | 8.584291 | -2.569537 | 0.075575 |
| 30 | 6 | 0 | 7.412216 | -1.866300 | 0.084191 |
| 31 | 6 | 0 | 0.000002 | -0.356666 | 0.036996 |
| 32 | 6 | 0 | 0.000001 | 0.855965 | 0.041238 |
| 33 | 6 | 0 | -0.000001 | 2.276473 | 0.048334 |
| 34 | 7 | 0 | 1.196127 | 2.871135 | 0.058798 |
| 35 | 7 | 0 | 1.173237 | 4.234743 | 0.067868 |
| 36 | 6 | 0 | -0.000005 | 5.006562 | 0.031309 |
| 37 | 7 | 0 | -1.173245 | 4.234739 | 0.067867 |
| 38 | 7 | 0 | -1.196131 | 2.871131 | 0.058797 |
| 39 | 6 | 0 | -2.467455 | 4.856042 | -0.015617 |
| 40 | 6 | 0 | 2.467445 | 4.856050 | -0.015614 |
| 41 | 8 | 0 | -0.000007 | 6.214314 | -0.024533 |
| 42 | 6 | 0 | -2.752900 | 6.041840 | 0.665153 |
| 43 | 6 | 0 | -4.030655 | 6.586208 | 0.579923 |
| 44 | 6 | 0 | -5.022318 | 5.960630 | -0.171735 |
| 45 | 6 | 0 | -4.730144 | 4.775038 | -0.842631 |
| 46 | 6 | 0 | -3.457798 | 4.219941 | -0.767973 |
| 47 | 6 | 0 | 3.457791 | 4.219953 | -0.767971 |
| 48 | 6 | 0 | 4.730134 | 4.775055 | -0.842627 |
| 49 | 6 | 0 | 5.022304 | 5.960647 | -0.171729 |
| 50 | 6 | 0 | 4.030638 | 6.586221 | 0.579929 |
| 51 | 6 | 0 | 2.752885 | 6.041848 | 0.665157 |
| 52 | 1 | 0 | -9.533587 | -2.046528 | 0.098199 |
| 53 | 1 | 0 | -9.511857 | -4.534279 | 0.031165 |
| 54 | 1 | 0 | -7.378554 | -5.761568 | -0.018980 |
| 55 | 1 | 0 | -7.420793 | -0.781815 | 0.114079 |
| 56 | 1 | 0 | -4.905183 | -5.738984 | -0.035657 |
| 57 | 1 | 0 | -4.948389 | -0.759421 | 0.092141 |
| 58 | 1 | 0 | -2.430252 | -5.707262 | -0.046224 |
| 59 | 1 | 0 | -2.497179 | -0.730344 | 0.069003 |
| 60 | 1 | 0 | 0.000005 | -5.687374 | -0.052297 |
| 61 | 1 | 0 | 2.430262 | -5.707259 | -0.046224 |
| 62 | 1 | 0 | 2.497182 | -0.730341 | 0.069003 |
| 63 | 1 | 0 | 4.905193 | -5.738978 | -0.035658 |
| 64 | 1 | 0 | 4.948393 | -0.759414 | 0.092140 |
| 65 | 1 | 0 | 7.378564 | -5.761558 | -0.018981 |
| 66 | 1 | 0 | 9.511865 | -4.534266 | 0.031162 |
| 67 | 1 | 0 | 9.533592 | -2.046515 | 0.098196 |
| 68 | 1 | 0 | 7.420797 | -0.781805 | 0.114077 |
| 69 | 1 | 0 | -1.988118 | 6.537184 | 1.243031 |
| 70 | 1 | 0 | -4.248549 | 7.506172 | 1.109932 |
| 71 | 1 | 0 | -6.014246 | 6.392927 | -0.233676 |
| 72 | 1 | 0 | -5.492872 | 4.279314 | -1.432044 |
| 73 | 1 | 0 | -3.223104 | 3.294913 | -1.275831 |
| 74 | 1 | 0 | 3.223100 | 3.294925 | -1.275829 |
| 75 | 1 | 0 | 5.492865 | 4.279334 | -1.432039 |
| 76 | 1 | 0 | 6.014231 | 6.392948 | -0.233669 |
| 77 | 1 | 0 | 4.248529 | 7.506185 | 1.109938 |
| 78 | 1 | 0 | 1.988101 | 6.537189 | 1.243035 |

R=NN

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -8.584940 | -1.526039 | -0.021278 |
| 2 | 6 | 0 | -8.573945 | -2.950942 | -0.021485 |
| 3 | 6 | 0 | -7.390779 | -3.635619 | -0.018098 |
| 4 | 6 | 0 | -6.140261 | -2.944091 | -0.014301 |
| 5 | 6 | 0 | -6.151774 | -1.497171 | -0.014029 |
| 6 | 6 | 0 | -7.411558 | -0.824231 | -0.017649 |
| 7 | 6 | 0 | -4.916722 | -3.615960 | -0.011063 |
| 8 | 6 | 0 | -3.691825 | -2.925824 | -0.007630 |
| 9 | 6 | 0 | -3.704658 | -1.474754 | -0.007247 |
| 10 | 6 | 0 | -4.938205 | -0.805343 | -0.010432 |
| 11 | 6 | 0 | -2.450458 | -3.587230 | -0.004896 |
| 12 | 6 | 0 | -1.233505 | -2.892125 | -0.002084 |
| 13 | 6 | 0 | -1.251355 | -1.435739 | -0.001594 |
| 14 | 6 | 0 | -2.478082 | -0.776551 | -0.004179 |
| 15 | 6 | 0 | -0.000007 | -3.566897 | -0.000002 |
| 16 | 6 | 0 | 1.233493 | -2.892128 | 0.002078 |
| 17 | 6 | 0 | 1.251347 | -1.435742 | 0.001583 |
| 18 | 6 | 0 | -0.000003 | -0.727985 | -0.000008 |
| 19 | 6 | 0 | 2.450444 | -3.587236 | 0.004895 |
| 20 | 6 | 0 | 3.691812 | -2.925834 | 0.007630 |
| 21 | 6 | 0 | 3.704650 | -1.474763 | 0.007242 |
| 22 | 6 | 0 | 2.478075 | -0.776557 | 0.004169 |
| 23 | 6 | 0 | 4.916708 | -3.615973 | 0.011067 |
| 24 | 6 | 0 | 6.140249 | -2.944107 | 0.014307 |
| 25 | 6 | 0 | 6.151766 | -1.497187 | 0.014030 |
| 26 | 6 | 0 | 4.938198 | -0.805356 | 0.010428 |
| 27 | 6 | 0 | 7.390765 | -3.635639 | 0.018109 |
| 28 | 6 | 0 | 8.573933 | -2.950964 | 0.021498 |
| 29 | 6 | 0 | 8.584931 | -1.526062 | 0.021286 |
| 30 | 6 | 0 | 7.411551 | -0.824250 | 0.017653 |
| 31 | 6 | 0 | -0.000001 | 0.666354 | -0.000010 |
| 32 | 6 | 0 | 0.000002 | 1.883585 | -0.000010 |
| 33 | 6 | 0 | 0.000007 | 3.265514 | -0.000005 |
| 34 | 7 | 0 | -1.117005 | 4.050985 | -0.003473 |
| 35 | 6 | 0 | -0.756308 | 5.501624 | 0.208717 |
| 36 | 6 | 0 | 0.756335 | 5.501621 | -0.208711 |
| 37 | 7 | 0 | 1.117023 | 4.050977 | 0.003467 |
| 38 | 6 | 0 | 0.996013 | 5.783359 | -1.701845 |
| 39 | 6 | 0 | 1.674087 | 6.377867 | 0.640844 |
| 40 | 6 | 0 | -0.995985 | 5.783351 | 1.701852 |
| 41 | 6 | 0 | -1.674054 | 6.377883 | -0.640832 |
| 42 | 8 | 0 | -2.317004 | 3.647020 | 0.007876 |
| 43 | 8 | 0 | 2.317019 | 3.647004 | -0.007883 |
| 44 | 1 | 0 | -9.533574 | -1.001301 | -0.024072 |
| 45 | 1 | 0 | -9.514634 | -3.489954 | -0.024407 |
| 46 | 1 | 0 | -7.382618 | -4.720604 | -0.018310 |
| 47 | 1 | 0 | -7.418192 | 0.260641 | -0.017560 |
| 48 | 1 | 0 | -4.908769 | -4.701624 | -0.011382 |
| 49 | 1 | 0 | -4.944741 | 0.280037 | -0.010381 |
| 50 | 1 | 0 | -2.432523 | -4.672513 | -0.005315 |
| 51 | 1 | 0 | -2.499506 | 0.307836 | -0.004268 |
| 52 | 1 | 0 | -0.000008 | -4.652265 | -0.000001 |
| 53 | 1 | 0 | 2.432506 | -4.672519 | 0.005317 |
| 54 | 1 | 0 | 2.499502 | 0.307829 | 0.004254 |
| 55 | 1 | 0 | 4.908752 | -4.701637 | 0.011390 |
| 56 | 1 | 0 | 4.944737 | 0.280024 | 0.010374 |
| 57 | 1 | 0 | 7.382601 | -4.720623 | 0.018324 |
| 58 | 1 | 0 | 9.514620 | -3.489978 | 0.024423 |
| 59 | 1 | 0 | 9.533567 | -1.001326 | 0.024082 |
| 60 | 1 | 0 | 7.418188 | 0.260622 | 0.017560 |
| 61 | 1 | 0 | 0.807004 | 6.832624 | -1.936378 |
| 62 | 1 | 0 | 2.037952 | 5.556182 | -1.932347 |
| 63 | 1 | 0 | 0.363025 | 5.162583 | -2.338716 |

```
   64         1          0       2.705868    6.215854    0.329073
   65         1          0       1.426776    7.432214    0.495830
   66         1          0       1.605027    6.142668    1.702124
   67         1          0      -0.806967    6.832613    1.936394
   68         1          0      -2.037927    5.556181    1.932351
   69         1          0      -0.363004    5.162565    2.338720
   70         1          0      -2.705836    6.215874   -0.329062
   71         1          0      -1.426735    7.432227   -0.495809
   72         1          0      -1.604995    6.142692   -1.702113
-------------------------------------------------------------------
```

## Sat-Radical

R=Sat-H

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 8.586525 | 0.391040 | -0.021176 |
| 2 | 6 | 0 | 8.566683 | -1.030573 | 0.088627 |
| 3 | 6 | 0 | 7.379637 | -1.706540 | 0.122404 |
| 4 | 6 | 0 | 6.132716 | -1.011019 | 0.049008 |
| 5 | 6 | 0 | 6.152888 | 0.433014 | -0.062509 |
| 6 | 6 | 0 | 7.418563 | 1.096684 | -0.094168 |
| 7 | 6 | 0 | 4.906326 | -1.673599 | 0.081483 |
| 8 | 6 | 0 | 3.684248 | -0.979327 | 0.008811 |
| 9 | 6 | 0 | 3.702982 | 0.467705 | -0.104358 |
| 10 | 6 | 0 | 4.945468 | 1.127411 | -0.135428 |
| 11 | 6 | 0 | 2.440763 | -1.627878 | 0.044533 |
| 12 | 6 | 0 | 1.225586 | -0.929965 | -0.025214 |
| 13 | 6 | 0 | 1.232807 | 0.527349 | -0.151146 |
| 14 | 6 | 0 | 2.484121 | 1.166621 | -0.180354 |
| 15 | 6 | 0 | 0.000001 | -1.607125 | 0.026838 |
| 16 | 6 | 0 | -1.225584 | -0.929965 | -0.025215 |
| 17 | 6 | 0 | -1.232806 | 0.527348 | -0.151146 |
| 18 | 6 | 0 | 0.000000 | 1.234673 | -0.231800 |
| 19 | 6 | 0 | -2.440762 | -1.627879 | 0.044531 |
| 20 | 6 | 0 | -3.684247 | -0.979327 | 0.008809 |
| 21 | 6 | 0 | -3.702981 | 0.467705 | -0.104357 |
| 22 | 6 | 0 | -2.484120 | 1.166621 | -0.180352 |
| 23 | 6 | 0 | -4.906325 | -1.673600 | 0.081480 |
| 24 | 6 | 0 | -6.132715 | -1.011020 | 0.049006 |
| 25 | 6 | 0 | -6.152887 | 0.433013 | -0.062507 |
| 26 | 6 | 0 | -4.945467 | 1.127411 | -0.135425 |
| 27 | 6 | 0 | -7.379636 | -1.706541 | 0.122400 |
| 28 | 6 | 0 | -8.566681 | -1.030574 | 0.088625 |
| 29 | 6 | 0 | -8.586524 | 0.391039 | -0.021175 |
| 30 | 6 | 0 | -7.418562 | 1.096683 | -0.094165 |
| 31 | 6 | 0 | -0.000001 | 2.742640 | -0.368119 |
| 32 | 6 | 0 | -0.000011 | 3.482511 | 0.983667 |
| 33 | 1 | 0 | 9.538510 | 0.909136 | -0.046395 |
| 34 | 1 | 0 | 9.503930 | -1.572531 | 0.145254 |
| 35 | 1 | 0 | 7.364318 | -2.788247 | 0.205917 |
| 36 | 1 | 0 | 7.433425 | 2.178414 | -0.177760 |
| 37 | 1 | 0 | 4.890736 | -2.755918 | 0.165858 |
| 38 | 1 | 0 | 4.962872 | 2.209823 | -0.219685 |
| 39 | 1 | 0 | 2.414112 | -2.709506 | 0.133275 |
| 40 | 1 | 0 | 2.537807 | 2.244534 | -0.258613 |
| 41 | 1 | 0 | 0.000001 | -2.688604 | 0.118283 |
| 42 | 1 | 0 | -2.414111 | -2.709507 | 0.133271 |
| 43 | 1 | 0 | -2.537806 | 2.244534 | -0.258608 |
| 44 | 1 | 0 | -4.890735 | -2.755919 | 0.165853 |
| 45 | 1 | 0 | -4.962871 | 2.209823 | -0.219680 |
| 46 | 1 | 0 | -7.364317 | -2.788249 | 0.205911 |
| 47 | 1 | 0 | -9.503928 | -1.572533 | 0.145251 |
| 48 | 1 | 0 | -9.538509 | 0.909135 | -0.046393 |
| 49 | 1 | 0 | -7.433424 | 2.178414 | -0.177755 |
| 50 | 1 | 0 | 0.865669 | 3.059949 | -0.952913 |
| 51 | 1 | 0 | -0.865664 | 3.059947 | -0.952924 |
| 52 | 1 | 0 | -0.000011 | 4.565879 | 0.832803 |
| 53 | 1 | 0 | -0.881360 | 3.222105 | 1.574684 |
| 54 | 1 | 0 | 0.881328 | 3.222106 | 1.574699 |

R=Sat-Mt

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 0.000000 | 3.753937 | -0.000028 |
| 2 | 6 | 0 | 0.000000 | 2.499970 | -0.000022 |
| 3 | 6 | 0 | 0.000002 | 5.079208 | -0.000037 |
| 4 | 6 | 0 | 8.600852 | 0.254943 | 0.000034 |
| 5 | 6 | 0 | 8.579470 | -1.167083 | 0.000016 |
| 6 | 6 | 0 | 7.389629 | -1.843044 | 0.000000 |
| 7 | 6 | 0 | 6.146605 | -1.141810 | 0.000002 |
| 8 | 6 | 0 | 6.169198 | 0.301234 | 0.000019 |
| 9 | 6 | 0 | 7.430271 | 0.965225 | 0.000035 |
| 10 | 6 | 0 | 4.913909 | -1.804608 | -0.000013 |
| 11 | 6 | 0 | 3.699605 | -1.104160 | -0.000012 |
| 12 | 6 | 0 | 3.724623 | 0.341883 | 0.000005 |
| 13 | 6 | 0 | 4.954115 | 1.001600 | 0.000020 |
| 14 | 6 | 0 | 2.444586 | -1.751328 | -0.000024 |
| 15 | 6 | 0 | 1.238753 | -1.045363 | -0.000021 |
| 16 | 6 | 0 | 1.270865 | 0.408781 | -0.000008 |
| 17 | 6 | 0 | 2.488258 | 1.046709 | 0.000006 |
| 18 | 6 | 0 | 0.000000 | -1.718405 | -0.000029 |
| 19 | 6 | 0 | -1.238753 | -1.045364 | -0.000020 |
| 20 | 6 | 0 | -1.270866 | 0.408780 | -0.000009 |
| 21 | 6 | 0 | 0.000000 | 1.154397 | -0.000013 |
| 22 | 6 | 0 | -2.444586 | -1.751328 | -0.000020 |
| 23 | 6 | 0 | -3.699605 | -1.104160 | -0.000009 |
| 24 | 6 | 0 | -3.724622 | 0.341883 | 0.000003 |
| 25 | 6 | 0 | -2.488258 | 1.046709 | 0.000002 |
| 26 | 6 | 0 | -4.913909 | -1.804608 | -0.000008 |
| 27 | 6 | 0 | -6.146605 | -1.141810 | 0.000005 |
| 28 | 6 | 0 | -6.169198 | 0.301234 | 0.000017 |
| 29 | 6 | 0 | -4.954114 | 1.001600 | 0.000015 |
| 30 | 6 | 0 | -7.389630 | -1.843044 | 0.000006 |
| 31 | 6 | 0 | -8.579471 | -1.167083 | 0.000019 |
| 32 | 6 | 0 | -8.600853 | 0.254943 | 0.000031 |
| 33 | 6 | 0 | -7.430271 | 0.965225 | 0.000029 |
| 34 | 1 | 0 | -0.926536 | 5.643080 | -0.000038 |
| 35 | 1 | 0 | 0.926550 | 5.643064 | -0.000039 |
| 36 | 1 | 0 | 9.552688 | 0.773791 | 0.000047 |
| 37 | 1 | 0 | 9.515697 | -1.713769 | 0.000015 |
| 38 | 1 | 0 | 7.373251 | -2.927903 | -0.000013 |
| 39 | 1 | 0 | 7.445481 | 2.050126 | 0.000048 |
| 40 | 1 | 0 | 4.897332 | -2.890142 | -0.000027 |
| 41 | 1 | 0 | 4.971241 | 2.087130 | 0.000032 |
| 42 | 1 | 0 | 2.414983 | -2.836348 | -0.000036 |
| 43 | 1 | 0 | 2.517564 | 2.130614 | 0.000017 |
| 44 | 1 | 0 | 0.000000 | -2.803518 | -0.000040 |
| 45 | 1 | 0 | -2.414983 | -2.836347 | -0.000029 |
| 46 | 1 | 0 | -2.517564 | 2.130614 | 0.000011 |
| 47 | 1 | 0 | -4.897332 | -2.890142 | -0.000017 |
| 48 | 1 | 0 | -4.971240 | 2.087130 | 0.000024 |
| 49 | 1 | 0 | -7.373252 | -2.927903 | -0.000003 |
| 50 | 1 | 0 | -9.515697 | -1.713769 | 0.000020 |
| 51 | 1 | 0 | -9.552689 | 0.773791 | 0.000041 |
| 52 | 1 | 0 | -7.445482 | 2.050127 | 0.000038 |

R=Sat-DCM

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 8.584438 | -0.320531 | 0.000059 |
| 2 | 6 | 0 | 8.573084 | -1.743450 | 0.000027 |
| 3 | 6 | 0 | 7.390085 | -2.430581 | -0.000001 |
| 4 | 6 | 0 | 6.141634 | -1.739104 | 0.000002 |
| 5 | 6 | 0 | 6.154226 | -0.294499 | 0.000034 |
| 6 | 6 | 0 | 7.409922 | 0.381370 | 0.000062 |
| 7 | 6 | 0 | 4.915851 | -2.413420 | -0.000025 |
| 8 | 6 | 0 | 3.695274 | -1.723302 | -0.000021 |
| 9 | 6 | 0 | 3.711578 | -0.275753 | 0.000010 |
| 10 | 6 | 0 | 4.936984 | 0.397009 | 0.000037 |
| 11 | 6 | 0 | 2.447184 | -2.381118 | -0.000044 |
| 12 | 6 | 0 | 1.235127 | -1.684541 | -0.000038 |
| 13 | 6 | 0 | 1.260396 | -0.229607 | -0.000011 |
| 14 | 6 | 0 | 2.477629 | 0.421314 | 0.000012 |
| 15 | 6 | 0 | 0.000000 | -2.360745 | -0.000054 |
| 16 | 6 | 0 | -1.235127 | -1.684541 | -0.000038 |
| 17 | 6 | 0 | -1.260395 | -0.229607 | -0.000011 |
| 18 | 6 | 0 | 0.000000 | 0.504834 | -0.000011 |
| 19 | 6 | 0 | -2.447184 | -2.381118 | -0.000044 |
| 20 | 6 | 0 | -3.695274 | -1.723303 | -0.000021 |
| 21 | 6 | 0 | -3.711578 | -0.275753 | 0.000010 |
| 22 | 6 | 0 | -2.477629 | 0.421314 | 0.000012 |
| 23 | 6 | 0 | -4.915851 | -2.413420 | -0.000025 |
| 24 | 6 | 0 | -6.141634 | -1.739104 | 0.000002 |
| 25 | 6 | 0 | -6.154226 | -0.294499 | 0.000034 |
| 26 | 6 | 0 | -4.936984 | 0.397009 | 0.000037 |
| 27 | 6 | 0 | -7.390085 | -2.430581 | -0.000001 |
| 28 | 6 | 0 | -8.573083 | -1.743450 | 0.000026 |
| 29 | 6 | 0 | -8.584438 | -0.320531 | 0.000058 |
| 30 | 6 | 0 | -7.409922 | 0.381370 | 0.000062 |
| 31 | 6 | 0 | 0.000000 | 1.866382 | -0.000012 |
| 32 | 6 | 0 | 0.000000 | 3.103072 | -0.000018 |
| 33 | 6 | 0 | 0.000000 | 4.462085 | -0.000023 |
| 34 | 6 | 0 | -1.227211 | 5.181527 | -0.000027 |
| 35 | 6 | 0 | 1.227211 | 5.181527 | -0.000027 |
| 36 | 7 | 0 | -2.237262 | 5.746908 | -0.000029 |
| 37 | 7 | 0 | 2.237263 | 5.746908 | -0.000031 |
| 38 | 1 | 0 | 9.532571 | 0.204487 | 0.000080 |
| 39 | 1 | 0 | 9.513808 | -2.282106 | 0.000024 |
| 40 | 1 | 0 | 7.383435 | -3.515278 | -0.000025 |
| 41 | 1 | 0 | 7.415695 | 1.465975 | 0.000086 |
| 42 | 1 | 0 | 4.909345 | -3.498793 | -0.000048 |
| 43 | 1 | 0 | 4.943696 | 1.482307 | 0.000060 |
| 44 | 1 | 0 | 2.426567 | -3.466085 | -0.000065 |
| 45 | 1 | 0 | 2.501991 | 1.505142 | 0.000034 |
| 46 | 1 | 0 | 0.000000 | -3.445527 | -0.000076 |
| 47 | 1 | 0 | -2.426566 | -3.466085 | -0.000065 |
| 48 | 1 | 0 | -2.501991 | 1.505142 | 0.000034 |
| 49 | 1 | 0 | -4.909345 | -3.498792 | -0.000048 |
| 50 | 1 | 0 | -4.943696 | 1.482307 | 0.000060 |
| 51 | 1 | 0 | -7.383435 | -3.515278 | -0.000025 |
| 52 | 1 | 0 | -9.513808 | -2.282106 | 0.000024 |
| 53 | 1 | 0 | -9.532571 | 0.204487 | 0.000080 |
| 54 | 1 | 0 | -7.415695 | 1.465975 | 0.000086 |

R=Sat-DPM

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 8.597778 | -1.503522 | -0.152854 |
| 2 | 6 | 0 | 8.578305 | -2.925352 | -0.115627 |
| 3 | 6 | 0 | 7.389489 | -3.601869 | -0.076915 |
| 4 | 6 | 0 | 6.145579 | -2.902015 | -0.072601 |
| 5 | 6 | 0 | 6.166064 | -1.458937 | -0.109310 |
| 6 | 6 | 0 | 7.426671 | -0.794433 | -0.149724 |
| 7 | 6 | 0 | 4.914192 | -3.565576 | -0.035723 |

| | | | | | |
|---|---|---|---|---|---|
| 8 | 6 | 0 | 3.698660 | -2.866592 | -0.031961 |
| 9 | 6 | 0 | 3.721378 | -1.420198 | -0.064599 |
| 10 | 6 | 0 | 4.951144 | -0.759625 | -0.104376 |
| 11 | 6 | 0 | 2.445302 | -3.515278 | -0.005776 |
| 12 | 6 | 0 | 1.237970 | -2.811015 | -0.002607 |
| 13 | 6 | 0 | 1.267026 | -1.355997 | -0.015600 |
| 14 | 6 | 0 | 2.486398 | -0.716370 | -0.057513 |
| 15 | 6 | 0 | 0.000002 | -3.484349 | 0.000003 |
| 16 | 6 | 0 | -1.237967 | -2.811015 | 0.002609 |
| 17 | 6 | 0 | -1.267023 | -1.355997 | 0.015597 |
| 18 | 6 | 0 | 0.000001 | -0.618501 | -0.000002 |
| 19 | 6 | 0 | -2.445299 | -3.515279 | 0.005781 |
| 20 | 6 | 0 | -3.698657 | -2.866593 | 0.031963 |
| 21 | 6 | 0 | -3.721376 | -1.420199 | 0.064595 |
| 22 | 6 | 0 | -2.486396 | -0.716371 | 0.057506 |
| 23 | 6 | 0 | -4.914189 | -3.565578 | 0.035728 |
| 24 | 6 | 0 | -6.145576 | -2.902016 | 0.072603 |
| 25 | 6 | 0 | -6.166062 | -1.458939 | 0.109306 |
| 26 | 6 | 0 | -4.951142 | -0.759626 | 0.104370 |
| 27 | 6 | 0 | -7.389487 | -3.601871 | 0.076920 |
| 28 | 6 | 0 | -8.578302 | -2.925354 | 0.115630 |
| 29 | 6 | 0 | -8.597775 | -1.503524 | 0.152851 |
| 30 | 6 | 0 | -7.426669 | -0.794434 | 0.149718 |
| 31 | 6 | 0 | 0.000001 | 0.737474 | -0.000003 |
| 32 | 6 | 0 | 0.000001 | 1.981932 | -0.000003 |
| 33 | 6 | 0 | 0.000000 | 3.332989 | -0.000001 |
| 34 | 6 | 0 | -1.279971 | 4.058151 | -0.152073 |
| 35 | 6 | 0 | 1.279968 | 4.058155 | 0.152073 |
| 36 | 6 | 0 | -1.509266 | 5.278829 | 0.507225 |
| 37 | 6 | 0 | -2.730993 | 5.932912 | 0.390615 |
| 38 | 6 | 0 | -3.749860 | 5.390550 | -0.390802 |
| 39 | 6 | 0 | -3.536263 | 4.182508 | -1.054161 |
| 40 | 6 | 0 | -2.318301 | 3.523659 | -0.936006 |
| 41 | 6 | 0 | 1.509258 | 5.278835 | -0.507224 |
| 42 | 6 | 0 | 2.730982 | 5.932923 | -0.390612 |
| 43 | 6 | 0 | 3.749850 | 5.390565 | 0.390806 |
| 44 | 6 | 0 | 3.536258 | 4.182522 | 1.054164 |
| 45 | 6 | 0 | 2.318299 | 3.523668 | 0.936007 |
| 46 | 1 | 0 | 9.548853 | -0.984153 | -0.184214 |
| 47 | 1 | 0 | 9.515083 | -3.471103 | -0.118564 |
| 48 | 1 | 0 | 7.374431 | -4.686422 | -0.049083 |
| 49 | 1 | 0 | 7.440403 | 0.290107 | -0.179038 |
| 50 | 1 | 0 | 4.898992 | -4.650882 | -0.010861 |
| 51 | 1 | 0 | 4.966272 | 0.325571 | -0.132542 |
| 52 | 1 | 0 | 2.417275 | -4.600309 | 0.006621 |
| 53 | 1 | 0 | 2.515793 | 0.366703 | -0.094713 |
| 54 | 1 | 0 | 0.000002 | -4.569533 | 0.000005 |
| 55 | 1 | 0 | -2.417271 | -4.600310 | -0.006611 |
| 56 | 1 | 0 | -2.515792 | 0.366703 | 0.094703 |
| 57 | 1 | 0 | -4.898988 | -4.650884 | 0.010870 |
| 58 | 1 | 0 | -4.966270 | 0.325570 | 0.132531 |
| 59 | 1 | 0 | -7.374428 | -4.686424 | 0.049092 |
| 60 | 1 | 0 | -9.515080 | -3.471106 | 0.118569 |
| 61 | 1 | 0 | -9.548850 | -0.984155 | 0.184210 |
| 62 | 1 | 0 | -7.440401 | 0.290106 | 0.179028 |
| 63 | 1 | 0 | -0.731650 | 5.702220 | 1.130909 |
| 64 | 1 | 0 | -2.889966 | 6.867133 | 0.917681 |
| 65 | 1 | 0 | -4.699286 | 5.905244 | -0.484610 |
| 66 | 1 | 0 | -4.317442 | 3.757935 | -1.675033 |
| 67 | 1 | 0 | -2.150268 | 2.594946 | -1.468527 |
| 68 | 1 | 0 | 0.731641 | 5.702222 | -1.130909 |
| 69 | 1 | 0 | 2.889951 | 6.867146 | -0.917677 |
| 70 | 1 | 0 | 4.699273 | 5.905264 | 0.484616 |
| 71 | 1 | 0 | 4.317438 | 3.757952 | 1.675036 |
| 72 | 1 | 0 | 2.150270 | 2.594953 | 1.468527 |

R=Sat-Flu

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 8.597120 | -1.616309 | -0.000127 |
| 2 | 6 | 0 | 8.576637 | -3.038821 | -0.000036 |
| 3 | 6 | 0 | 7.387625 | -3.715753 | 0.000029 |
| 4 | 6 | 0 | 6.143888 | -3.015447 | 0.000008 |
| 5 | 6 | 0 | 6.165414 | -1.571658 | -0.000083 |
| 6 | 6 | 0 | 7.426627 | -0.906717 | -0.000150 |
| 7 | 6 | 0 | 4.912389 | -3.679159 | 0.000072 |
| 8 | 6 | 0 | 3.696874 | -2.979839 | 0.000050 |
| 9 | 6 | 0 | 3.720177 | -1.532939 | -0.000039 |
| 10 | 6 | 0 | 4.951161 | -0.872369 | -0.000104 |
| 11 | 6 | 0 | 2.443840 | -3.628027 | 0.000107 |
| 12 | 6 | 0 | 1.236473 | -2.923509 | 0.000082 |
| 13 | 6 | 0 | 1.264858 | -1.468176 | 0.000006 |
| 14 | 6 | 0 | 2.486375 | -0.829726 | -0.000056 |
| 15 | 6 | 0 | -0.000002 | -3.597601 | 0.000125 |
| 16 | 6 | 0 | -1.236475 | -2.923508 | 0.000081 |
| 17 | 6 | 0 | -1.264860 | -1.468175 | 0.000008 |
| 18 | 6 | 0 | -0.000001 | -0.729656 | 0.000000 |
| 19 | 6 | 0 | -2.443843 | -3.628026 | 0.000103 |
| 20 | 6 | 0 | -3.696876 | -2.979837 | 0.000048 |
| 21 | 6 | 0 | -3.720178 | -1.532937 | -0.000034 |
| 22 | 6 | 0 | -2.486376 | -0.829725 | -0.000050 |
| 23 | 6 | 0 | -4.912392 | -3.679156 | 0.000067 |
| 24 | 6 | 0 | -6.143890 | -3.015443 | 0.000007 |
| 25 | 6 | 0 | -6.165416 | -1.571654 | -0.000078 |
| 26 | 6 | 0 | -4.951162 | -0.872366 | -0.000096 |
| 27 | 6 | 0 | -7.387628 | -3.715749 | 0.000025 |
| 28 | 6 | 0 | -8.576639 | -3.038816 | -0.000036 |
| 29 | 6 | 0 | -8.597122 | -1.616305 | -0.000120 |
| 30 | 6 | 0 | -7.426628 | -0.906713 | -0.000140 |
| 31 | 6 | 0 | 0.000000 | 0.630111 | -0.000003 |
| 32 | 6 | 0 | 0.000002 | 1.872640 | 0.000009 |
| 33 | 6 | 0 | 0.000002 | 3.222294 | 0.000021 |
| 34 | 6 | 0 | -1.173683 | 4.100467 | 0.000023 |
| 35 | 6 | 0 | 1.173688 | 4.100466 | 0.000028 |
| 36 | 6 | 0 | -2.534769 | 3.803181 | 0.000026 |
| 37 | 6 | 0 | -3.453990 | 4.850994 | 0.000025 |
| 38 | 6 | 0 | -3.020189 | 6.180303 | 0.000021 |
| 39 | 6 | 0 | -1.657931 | 6.486965 | 0.000019 |
| 40 | 6 | 0 | -0.733159 | 5.448498 | 0.000020 |
| 41 | 6 | 0 | 0.733164 | 5.448497 | 0.000023 |
| 42 | 6 | 0 | 1.657936 | 6.486965 | 0.000027 |
| 43 | 6 | 0 | 3.020194 | 6.180303 | 0.000035 |
| 44 | 6 | 0 | 3.453994 | 4.850994 | 0.000042 |
| 45 | 6 | 0 | 2.534774 | 3.803180 | 0.000039 |
| 46 | 1 | 0 | 9.548721 | -1.097113 | -0.000178 |
| 47 | 1 | 0 | 9.513325 | -3.584639 | -0.000019 |
| 48 | 1 | 0 | 7.372099 | -4.800579 | 0.000098 |
| 49 | 1 | 0 | 7.441249 | 0.178142 | -0.000219 |
| 50 | 1 | 0 | 4.896658 | -4.764658 | 0.000139 |
| 51 | 1 | 0 | 4.968348 | 0.213072 | -0.000173 |
| 52 | 1 | 0 | 2.415123 | -4.713017 | 0.000167 |
| 53 | 1 | 0 | 2.515037 | 0.253600 | -0.000124 |
| 54 | 1 | 0 | -0.000002 | -4.682670 | 0.000184 |
| 55 | 1 | 0 | -2.415127 | -4.713016 | 0.000161 |
| 56 | 1 | 0 | -2.515038 | 0.253602 | -0.000114 |
| 57 | 1 | 0 | -4.896662 | -4.764655 | 0.000130 |
| 58 | 1 | 0 | -4.968349 | 0.213075 | -0.000159 |
| 59 | 1 | 0 | -7.372103 | -4.800575 | 0.000089 |
| 60 | 1 | 0 | -9.513328 | -3.584634 | -0.000022 |
| 61 | 1 | 0 | -9.548722 | -1.097108 | -0.000168 |
| 62 | 1 | 0 | -7.441250 | 0.178146 | -0.000204 |
| 63 | 1 | 0 | -2.873505 | 2.773435 | 0.000033 |
| 64 | 1 | 0 | -4.516303 | 4.634624 | 0.000028 |
| 65 | 1 | 0 | -3.750449 | 6.981624 | 0.000020 |
| 66 | 1 | 0 | -1.332701 | 7.521598 | 0.000018 |
| 67 | 1 | 0 | 1.332706 | 7.521598 | 0.000024 |
| 68 | 1 | 0 | 3.750454 | 6.981623 | 0.000037 |
| 69 | 1 | 0 | 4.516308 | 4.634623 | 0.000051 |
| 70 | 1 | 0 | 2.873510 | 2.773435 | 0.000050 |

R=Sat-PhO

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -8.590168 | -0.867610 | 0.000022 |
| 2 | 6 | 0 | -8.573647 | -2.290958 | 0.000005 |
| 3 | 6 | 0 | -7.387584 | -2.972068 | -0.000006 |
| 4 | 6 | 0 | -6.141264 | -2.275493 | -0.000002 |
| 5 | 6 | 0 | -6.158760 | -0.830559 | 0.000015 |
| 6 | 6 | 0 | -7.418547 | -0.161235 | 0.000027 |
| 7 | 6 | 0 | -4.913208 | -2.943484 | -0.000013 |
| 8 | 6 | 0 | -3.694216 | -2.248265 | -0.000009 |
| 9 | 6 | 0 | -3.713582 | -0.800192 | 0.000007 |
| 10 | 6 | 0 | -4.944376 | -0.134944 | 0.000019 |
| 11 | 6 | 0 | -2.445413 | -2.901497 | -0.000019 |
| 12 | 6 | 0 | -1.234745 | -2.200686 | -0.000015 |
| 13 | 6 | 0 | -1.259171 | -0.745163 | 0.000000 |
| 14 | 6 | 0 | -2.481938 | -0.099965 | 0.000011 |
| 15 | 6 | 0 | 0.000001 | -2.875920 | -0.000023 |
| 16 | 6 | 0 | 1.234746 | -2.200686 | -0.000015 |
| 17 | 6 | 0 | 1.259172 | -0.745162 | 0.000000 |
| 18 | 6 | 0 | 0.000000 | -0.013199 | 0.000002 |
| 19 | 6 | 0 | 2.445415 | -2.901496 | -0.000021 |
| 20 | 6 | 0 | 3.694217 | -2.248264 | -0.000010 |
| 21 | 6 | 0 | 3.713583 | -0.800191 | 0.000007 |
| 22 | 6 | 0 | 2.481939 | -0.099965 | 0.000011 |
| 23 | 6 | 0 | 4.913209 | -2.943482 | -0.000015 |
| 24 | 6 | 0 | 6.141265 | -2.275492 | -0.000003 |
| 25 | 6 | 0 | 6.158760 | -0.830557 | 0.000015 |
| 26 | 6 | 0 | 4.944377 | -0.134943 | 0.000020 |
| 27 | 6 | 0 | 7.387585 | -2.972066 | -0.000008 |
| 28 | 6 | 0 | 8.573648 | -2.290956 | 0.000005 |
| 29 | 6 | 0 | 8.590169 | -0.867608 | 0.000023 |
| 30 | 6 | 0 | 7.418548 | -0.161233 | 0.000028 |
| 31 | 6 | 0 | 0.000000 | 1.356597 | 0.000004 |
| 32 | 6 | 0 | 0.000000 | 2.591354 | 0.000002 |
| 33 | 6 | 0 | -0.000001 | 3.962000 | -0.000002 |
| 34 | 6 | 0 | -1.236040 | 4.702961 | -0.000007 |
| 35 | 6 | 0 | -1.242603 | 6.058678 | -0.000012 |
| 36 | 6 | 0 | -0.000003 | 6.839110 | -0.000013 |
| 37 | 6 | 0 | 1.242599 | 6.058680 | -0.000008 |
| 38 | 6 | 0 | 1.236038 | 4.702962 | -0.000003 |
| 39 | 8 | 0 | -0.000003 | 8.072317 | -0.000018 |
| 40 | 1 | 0 | -9.540438 | -0.346198 | 0.000031 |
| 41 | 1 | 0 | -9.512170 | -2.833480 | 0.000002 |
| 42 | 1 | 0 | -7.375737 | -4.056831 | -0.000019 |
| 43 | 1 | 0 | -7.429848 | 0.923537 | 0.000039 |
| 44 | 1 | 0 | -4.901340 | -4.028922 | -0.000026 |
| 45 | 1 | 0 | -4.957417 | 0.950466 | 0.000031 |

| | | | | | |
|---|---|---|---|---|---|
| 46 | 1 | 0 | -2.420827 | -3.986481 | -0.000031 |
| 47 | 1 | 0 | -2.507073 | 0.983536 | 0.000023 |
| 48 | 1 | 0 | 0.000001 | -3.960920 | -0.000035 |
| 49 | 1 | 0 | 2.420828 | -3.986480 | -0.000033 |
| 50 | 1 | 0 | 2.507074 | 0.983536 | 0.000023 |
| 51 | 1 | 0 | 4.901342 | -4.028920 | -0.000029 |
| 52 | 1 | 0 | 4.957417 | 0.950468 | 0.000033 |
| 53 | 1 | 0 | 7.375739 | -4.056829 | -0.000022 |
| 54 | 1 | 0 | 9.512171 | -2.833477 | 0.000001 |
| 55 | 1 | 0 | 9.540438 | -0.346196 | 0.000033 |
| 56 | 1 | 0 | 7.429848 | 0.923539 | 0.000042 |
| 57 | 1 | 0 | -2.165515 | 4.144423 | -0.000007 |
| 58 | 1 | 0 | -2.167329 | 6.624119 | -0.000016 |
| 59 | 1 | 0 | 2.167324 | 6.624122 | -0.000009 |
| 60 | 1 | 0 | 2.165512 | 4.144425 | 0.000001 |

R=Sat-NO

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 8.613850 | -0.091851 | -0.000015 |
| 2 | 6 | 0 | 8.601816 | -1.515362 | -0.000004 |
| 3 | 6 | 0 | 7.417131 | -2.198845 | 0.000003 |
| 4 | 6 | 0 | 6.168428 | -1.505979 | 0.000000 |
| 5 | 6 | 0 | 6.181207 | -0.060910 | -0.000010 |
| 6 | 6 | 0 | 7.439903 | 0.610898 | -0.000018 |
| 7 | 6 | 0 | 4.942210 | -2.176627 | 0.000007 |
| 8 | 6 | 0 | 3.720149 | -1.485454 | 0.000005 |
| 9 | 6 | 0 | 3.734143 | -0.036701 | -0.000006 |
| 10 | 6 | 0 | 4.964536 | 0.630732 | -0.000013 |
| 11 | 6 | 0 | 2.474524 | -2.143983 | 0.000012 |
| 12 | 6 | 0 | 1.259457 | -1.449624 | 0.000010 |
| 13 | 6 | 0 | 1.277304 | 0.006278 | 0.000001 |
| 14 | 6 | 0 | 2.499408 | 0.657424 | -0.000008 |
| 15 | 6 | 0 | 0.027081 | -2.129794 | 0.000015 |
| 16 | 6 | 0 | -1.210787 | -1.459875 | 0.000010 |
| 17 | 6 | 0 | -1.240766 | -0.004543 | 0.000002 |
| 18 | 6 | 0 | 0.016413 | 0.724076 | 0.000002 |
| 19 | 6 | 0 | -2.419797 | -2.164876 | 0.000013 |
| 20 | 6 | 0 | -3.670448 | -1.515834 | 0.000006 |
| 21 | 6 | 0 | -3.694963 | -0.067387 | -0.000004 |
| 22 | 6 | 0 | -2.467264 | 0.639224 | -0.000005 |
| 23 | 6 | 0 | -4.887143 | -2.216279 | 0.000009 |
| 24 | 6 | 0 | -6.117949 | -1.553849 | 0.000001 |
| 25 | 6 | 0 | -6.140709 | -0.108862 | -0.000011 |
| 26 | 6 | 0 | -4.929481 | 0.592370 | -0.000013 |
| 27 | 6 | 0 | -7.361824 | -2.255269 | 0.000003 |
| 28 | 6 | 0 | -8.550999 | -1.579537 | -0.000006 |
| 29 | 6 | 0 | -8.572830 | -0.156138 | -0.000017 |
| 30 | 6 | 0 | -7.403769 | 0.554731 | -0.000020 |
| 31 | 6 | 0 | -0.007620 | 2.099519 | 0.000003 |
| 32 | 6 | 0 | -0.089328 | 3.324791 | 0.000005 |
| 33 | 7 | 0 | -0.246112 | 4.630069 | 0.000011 |
| 34 | 8 | 0 | -1.401917 | 5.183579 | 0.000017 |
| 35 | 6 | 0 | 0.923625 | 5.527617 | 0.000012 |
| 36 | 1 | 0 | 9.562591 | 0.432642 | -0.000020 |
| 37 | 1 | 0 | 9.541785 | -2.055498 | -0.000002 |
| 38 | 1 | 0 | 7.407783 | -3.283767 | 0.000011 |
| 39 | 1 | 0 | 7.448594 | 1.695901 | -0.000026 |
| 40 | 1 | 0 | 4.933055 | -3.262222 | 0.000015 |
| 41 | 1 | 0 | 4.975369 | 1.716436 | -0.000021 |
| 42 | 1 | 0 | 2.455273 | -3.229192 | 0.000018 |
| 43 | 1 | 0 | 2.521287 | 1.741427 | -0.000018 |
| 44 | 1 | 0 | 0.031870 | -3.214898 | 0.000022 |
| 45 | 1 | 0 | -2.391404 | -3.249930 | 0.000021 |
| 46 | 1 | 0 | -2.500754 | 1.722974 | -0.000011 |
| 47 | 1 | 0 | -4.870394 | -3.301825 | 0.000017 |
| 48 | 1 | 0 | -4.945903 | 1.677707 | -0.000021 |
| 49 | 1 | 0 | -7.345268 | -3.340137 | 0.000012 |
| 50 | 1 | 0 | -9.487333 | -2.126051 | -0.000004 |
| 51 | 1 | 0 | -9.525114 | 0.361875 | -0.000024 |
| 52 | 1 | 0 | -7.418964 | 1.639516 | -0.000028 |
| 53 | 1 | 0 | 1.843395 | 4.944679 | 0.000012 |
| 54 | 1 | 0 | 0.864597 | 6.155376 | -0.889842 |
| 55 | 1 | 0 | 0.864595 | 6.155374 | 0.889868 |

R=Sat-Allyl

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 0.000000 | 3.361862 | 0.000000 |
| 2 | 6 | 0 | 0.000000 | 2.147137 | -0.000001 |
| 3 | 6 | 0 | 0.000000 | 4.789883 | 0.000000 |
| 4 | 6 | 0 | 8.586619 | -0.083272 | 0.000013 |
| 5 | 6 | 0 | 8.572037 | -1.508363 | 0.000007 |
| 6 | 6 | 0 | 7.387029 | -2.189554 | 0.000002 |
| 7 | 6 | 0 | 6.138159 | -1.494756 | 0.000002 |
| 8 | 6 | 0 | 6.153179 | -0.047561 | 0.000008 |
| 9 | 6 | 0 | 7.415273 | 0.621611 | 0.000013 |
| 10 | 6 | 0 | 4.913101 | -2.162899 | -0.000003 |
| 11 | 6 | 0 | 3.689387 | -1.469885 | -0.000002 |
| 12 | 6 | 0 | 3.704284 | -0.018558 | 0.000003 |
| 13 | 6 | 0 | 4.941358 | 0.646263 | 0.000008 |
| 14 | 6 | 0 | 2.447305 | -2.127543 | -0.000005 |
| 15 | 6 | 0 | 1.230677 | -1.430883 | -0.000003 |
| 16 | 6 | 0 | 1.245989 | 0.026832 | -0.000002 |
| 17 | 6 | 0 | 2.478912 | 0.679083 | 0.000003 |
| 18 | 6 | 0 | 0.000000 | -2.107465 | -0.000001 |
| 19 | 6 | 0 | -1.230677 | -1.430883 | 0.000001 |
| 20 | 6 | 0 | -1.245989 | 0.026832 | 0.000000 |
| 21 | 6 | 0 | 0.000000 | 0.738821 | -0.000001 |
| 22 | 6 | 0 | -2.447305 | -2.127543 | 0.000002 |
| 23 | 6 | 0 | -3.689387 | -1.469885 | 0.000001 |
| 24 | 6 | 0 | -3.704284 | -0.018558 | -0.000004 |
| 25 | 6 | 0 | -2.478912 | 0.679083 | -0.000004 |
| 26 | 6 | 0 | -4.913101 | -2.162899 | 0.000002 |
| 27 | 6 | 0 | -6.138159 | -1.494756 | -0.000001 |
| 28 | 6 | 0 | -6.153179 | -0.047561 | -0.000006 |
| 29 | 6 | 0 | -4.941358 | 0.646263 | -0.000008 |
| 30 | 6 | 0 | -7.387029 | -2.189554 | 0.000000 |
| 31 | 6 | 0 | -8.572037 | -1.508363 | -0.000004 |
| 32 | 6 | 0 | -8.586619 | -0.083272 | -0.000009 |
| 33 | 6 | 0 | -7.415273 | 0.621610 | -0.000010 |
| 34 | 6 | 0 | -1.220558 | 5.469680 | 0.000179 |
| 35 | 6 | 0 | 1.220557 | 5.469681 | -0.000179 |
| 36 | 1 | 0 | 9.536636 | 0.438968 | 0.000017 |
| 37 | 1 | 0 | 9.511308 | -2.049755 | 0.000007 |
| 38 | 1 | 0 | 7.375758 | -3.274496 | -0.000003 |
| 39 | 1 | 0 | 7.425866 | 1.706564 | 0.000018 |
| 40 | 1 | 0 | 4.902071 | -3.248522 | -0.000007 |
| 41 | 1 | 0 | 4.953731 | 1.731801 | 0.000013 |
| 42 | 1 | 0 | 2.426833 | -3.212783 | -0.000006 |
| 43 | 1 | 0 | 2.498619 | 1.762298 | 0.000010 |
| 44 | 1 | 0 | 0.000000 | -3.192758 | -0.000001 |
| 45 | 1 | 0 | -2.426833 | -3.212783 | 0.000004 |
| 46 | 1 | 0 | -2.498619 | 1.762298 | -0.000011 |
| 47 | 1 | 0 | -4.902071 | -3.248522 | 0.000006 |
| 48 | 1 | 0 | -4.953731 | 1.731801 | -0.000012 |
| 49 | 1 | 0 | -7.375758 | -3.274496 | 0.000004 |
| 50 | 1 | 0 | -9.511308 | -2.049755 | -0.000003 |
| 51 | 1 | 0 | -9.536636 | 0.438967 | -0.000012 |
| 52 | 1 | 0 | -7.425866 | 1.706563 | -0.000014 |
| 53 | 1 | 0 | -1.242482 | 6.552306 | 0.000180 |
| 54 | 1 | 0 | -2.161774 | 4.938111 | 0.000324 |
| 55 | 1 | 0 | 1.242481 | 6.552306 | -0.000179 |
| 56 | 1 | 0 | 2.161773 | 4.938111 | -0.000325 |

R=Sat-IN

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 8.916535 | -0.331368 | -0.009239 |
| 2 | 6 | 0 | 9.075085 | -1.755567 | -0.018974 |
| 3 | 6 | 0 | 7.987085 | -2.573310 | -0.021841 |
| 4 | 6 | 0 | 6.655764 | -2.034960 | -0.015232 |
| 5 | 6 | 0 | 6.494734 | -0.588222 | -0.005335 |
| 6 | 6 | 0 | 7.675490 | 0.228163 | -0.002689 |
| 7 | 6 | 0 | 5.531965 | -2.842500 | -0.017977 |
| 8 | 6 | 0 | 4.223034 | -2.301554 | -0.011430 |
| 9 | 6 | 0 | 4.061302 | -0.854033 | -0.001629 |
| 10 | 6 | 0 | 5.221004 | -0.044106 | 0.001128 |
| 11 | 6 | 0 | 3.083102 | -3.103317 | -0.013971 |
| 12 | 6 | 0 | 1.786195 | -2.556238 | -0.007399 |
| 13 | 6 | 0 | 1.624825 | -1.107551 | 0.002055 |
| 14 | 6 | 0 | 2.774898 | -0.306493 | 0.004598 |
| 15 | 6 | 0 | 0.649886 | -3.374384 | -0.009615 |
| 16 | 6 | 0 | -0.649540 | -2.853465 | -0.002888 |
| 17 | 6 | 0 | -0.839686 | -1.408389 | 0.005825 |
| 18 | 6 | 0 | 0.308626 | -0.560526 | 0.007580 |
| 19 | 6 | 0 | -1.777535 | -3.695943 | -0.003995 |
| 20 | 6 | 0 | -3.075990 | -3.189633 | 0.003546 |
| 21 | 6 | 0 | -3.263823 | -1.745408 | 0.012732 |
| 22 | 6 | 0 | -2.147458 | -0.903469 | 0.013522 |
| 23 | 6 | 0 | -4.218851 | -4.026362 | 0.003035 |
| 24 | 6 | 0 | -5.502135 | -3.508226 | 0.011255 |
| 25 | 6 | 0 | -5.689658 | -2.064513 | 0.020714 |
| 26 | 6 | 0 | -4.582159 | -1.232678 | 0.021120 |
| 27 | 6 | 0 | -6.667764 | -4.347162 | 0.011038 |
| 28 | 6 | 0 | -7.918746 | -3.810971 | 0.019556 |
| 29 | 6 | 0 | -8.103252 | -2.389861 | 0.028986 |
| 30 | 6 | 0 | -7.030451 | -1.551763 | 0.029515 |
| 31 | 6 | 0 | 0.121076 | 0.835567 | 0.014926 |
| 32 | 6 | 0 | -0.087227 | 2.028929 | 0.020389 |
| 33 | 6 | 0 | -0.422511 | 3.399130 | 0.031219 |
| 34 | 7 | 0 | -1.787942 | 3.763932 | 0.035335 |
| 35 | 6 | 0 | -1.885359 | 5.241390 | -0.201792 |
| 36 | 6 | 0 | -0.407178 | 5.651200 | 0.170883 |
| 37 | 7 | 0 | 0.389200 | 4.402098 | 0.035269 |
| 38 | 6 | 0 | 0.199547 | 6.729248 | -0.732802 |
| 39 | 6 | 0 | -0.257546 | 6.087112 | 1.642340 |
| 40 | 6 | 0 | -3.003617 | 5.826289 | 0.659365 |
| 41 | 6 | 0 | -2.229210 | 5.418873 | -1.691737 |
| 42 | 8 | 0 | -2.776904 | 2.979709 | 0.010720 |
| 43 | 1 | 0 | 9.798676 | 0.298820 | -0.007138 |
| 44 | 1 | 0 | 10.074107 | -2.176542 | -0.024048 |
| 45 | 1 | 0 | 8.106448 | -3.651659 | -0.029206 |
| 46 | 1 | 0 | 7.555607 | 1.306347 | 0.004666 |
| 47 | 1 | 0 | 5.650450 | -3.921629 | -0.025338 |
| 48 | 1 | 0 | 5.101990 | 1.034695 | 0.008423 |

| | | | | | |
|---|---|---|---|---|---|
| 49 | 1 | 0 | 3.193212 | -4.183090 | -0.021218 |
| 50 | 1 | 0 | 2.663620 | 0.771610 | 0.011652 |
| 51 | 1 | 0 | 0.781626 | -4.451934 | -0.016472 |
| 52 | 1 | 0 | -1.625643 | -4.770654 | -0.010431 |
| 53 | 1 | 0 | -2.302106 | 0.169730 | 0.020959 |
| 54 | 1 | 0 | -4.078055 | -5.102836 | -0.003815 |
| 55 | 1 | 0 | -4.719154 | -0.156127 | 0.028290 |
| 56 | 1 | 0 | -6.527947 | -5.423079 | 0.003973 |
| 57 | 1 | 0 | -8.789177 | -4.457313 | 0.019335 |
| 58 | 1 | 0 | -9.109870 | -1.987352 | 0.035773 |
| 59 | 1 | 0 | -7.169069 | -0.475874 | 0.036742 |
| 60 | 1 | 0 | 1.225735 | 6.922250 | -0.414349 |
| 61 | 1 | 0 | 0.230073 | 6.417379 | -1.776599 |
| 62 | 1 | 0 | -0.363455 | 7.664605 | -0.662694 |
| 63 | 1 | 0 | -0.756952 | 7.041436 | 1.827977 |
| 64 | 1 | 0 | -0.664443 | 5.339524 | 2.326259 |
| 65 | 1 | 0 | 0.804138 | 6.201373 | 1.867606 |
| 66 | 1 | 0 | -3.952416 | 5.366542 | 0.377087 |
| 67 | 1 | 0 | -2.845753 | 5.643525 | 1.721735 |
| 68 | 1 | 0 | -3.080725 | 6.904096 | 0.496996 |
| 69 | 1 | 0 | -2.341937 | 6.475420 | -1.942484 |
| 70 | 1 | 0 | -1.462169 | 4.987489 | -2.337413 |
| 71 | 1 | 0 | -3.173136 | 4.909783 | -1.896951 |

R=Sat-Phen

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 8.573855 | -1.920165 | -0.080523 |
| 2 | 6 | 0 | 8.558642 | -3.353168 | -0.071784 |
| 3 | 6 | 0 | 7.379659 | -4.033010 | -0.056565 |
| 4 | 6 | 0 | 6.123056 | -3.337720 | -0.048770 |
| 5 | 6 | 0 | 6.138595 | -1.882008 | -0.057282 |
| 6 | 6 | 0 | 7.409573 | -1.214774 | -0.073546 |
| 7 | 6 | 0 | 4.909947 | -4.003321 | -0.034069 |
| 8 | 6 | 0 | 3.675662 | -3.308404 | -0.026560 |
| 9 | 6 | 0 | 3.690392 | -1.852228 | -0.033626 |
| 10 | 6 | 0 | 4.939807 | -1.188644 | -0.049629 |
| 11 | 6 | 0 | 2.446916 | -3.965034 | -0.014417 |
| 12 | 6 | 0 | 1.224701 | -3.266208 | -0.007217 |
| 13 | 6 | 0 | 1.238502 | -1.807913 | -0.009703 |
| 14 | 6 | 0 | 2.479274 | -1.154801 | -0.025227 |
| 15 | 6 | 0 | -0.000006 | -3.943229 | 0.000002 |
| 16 | 6 | 0 | -1.224710 | -3.266205 | 0.007219 |
| 17 | 6 | 0 | -1.238508 | -1.807910 | 0.009704 |
| 18 | 6 | 0 | -0.000002 | -1.098771 | 0.000000 |
| 19 | 6 | 0 | -2.446927 | -3.965028 | 0.014420 |
| 20 | 6 | 0 | -3.675672 | -3.308395 | 0.026562 |
| 21 | 6 | 0 | -3.690398 | -1.852219 | 0.033625 |
| 22 | 6 | 0 | -2.479279 | -1.154795 | 0.025226 |
| 23 | 6 | 0 | -4.909959 | -4.003309 | 0.034070 |
| 24 | 6 | 0 | -6.123065 | -3.337706 | 0.048770 |
| 25 | 6 | 0 | -6.138601 | -1.881993 | 0.057279 |
| 26 | 6 | 0 | -4.939812 | -1.188632 | 0.049626 |
| 27 | 6 | 0 | -7.379670 | -4.032992 | 0.056565 |
| 28 | 6 | 0 | -8.558652 | -3.353148 | 0.071782 |
| 29 | 6 | 0 | -8.573862 | -1.920144 | 0.080519 |
| 30 | 6 | 0 | -7.409578 | -1.214756 | 0.073541 |
| 31 | 6 | 0 | 0.000000 | 0.314363 | 0.000001 |
| 32 | 6 | 0 | 0.000002 | 1.528064 | 0.000000 |
| 33 | 6 | 0 | 0.000005 | 2.950073 | 0.000000 |
| 34 | 6 | 0 | -1.187163 | 3.659320 | -0.242280 |
| 35 | 6 | 0 | -1.211034 | 5.070384 | -0.247050 |
| 36 | 6 | 0 | 0.000009 | 5.787458 | 0.000000 |
| 37 | 6 | 0 | 1.211050 | 5.070380 | 0.247051 |
| 38 | 6 | 0 | 1.187174 | 3.659316 | 0.242281 |
| 39 | 6 | 0 | 0.000011 | 7.215192 | 0.000000 |
| 40 | 6 | 0 | 1.216664 | 7.897323 | 0.248802 |
| 41 | 6 | 0 | 2.391081 | 7.192873 | 0.489091 |
| 42 | 6 | 0 | 2.400388 | 5.803699 | 0.490713 |
| 43 | 6 | 0 | -2.400370 | 5.803707 | -0.490713 |
| 44 | 6 | 0 | -2.391058 | 7.192880 | -0.489090 |
| 45 | 6 | 0 | -1.216639 | 7.897327 | -0.248802 |
| 46 | 1 | 0 | 9.525765 | -1.401464 | -0.092915 |
| 47 | 1 | 0 | 9.499265 | -3.892163 | -0.077570 |
| 48 | 1 | 0 | 7.367705 | -5.117896 | -0.050109 |
| 49 | 1 | 0 | 7.421345 | -0.129901 | -0.080395 |
| 50 | 1 | 0 | 4.897314 | -5.088883 | -0.028405 |
| 51 | 1 | 0 | 4.952839 | -0.103205 | -0.056451 |
| 52 | 1 | 0 | 2.425298 | -5.050231 | -0.011580 |
| 53 | 1 | 0 | 2.498781 | -0.071727 | -0.033660 |
| 54 | 1 | 0 | -0.000007 | -5.028577 | 0.000004 |
| 55 | 1 | 0 | -2.425312 | -5.050226 | 0.011584 |
| 56 | 1 | 0 | -2.498783 | -0.071721 | 0.033657 |
| 57 | 1 | 0 | -4.897328 | -5.088871 | 0.028409 |
| 58 | 1 | 0 | -4.952841 | -0.103193 | 0.056447 |
| 59 | 1 | 0 | -7.367719 | -5.117878 | 0.050111 |
| 60 | 1 | 0 | -9.499276 | -3.892140 | 0.077570 |
| 61 | 1 | 0 | -9.525770 | -1.401441 | 0.092909 |
| 62 | 1 | 0 | -7.421348 | -0.129883 | 0.080388 |
| 63 | 1 | 0 | -2.102827 | 3.112841 | -0.433986 |
| 64 | 1 | 0 | 2.102836 | 3.112834 | 0.433988 |
| 65 | 1 | 0 | 1.220459 | 8.981764 | 0.249690 |
| 66 | 1 | 0 | 3.311333 | 7.734518 | 0.677668 |
| 67 | 1 | 0 | 3.321388 | 5.263379 | 0.679591 |
| 68 | 1 | 0 | -3.321372 | 5.263389 | -0.679591 |
| 69 | 1 | 0 | -3.311309 | 7.734528 | -0.677668 |
| 70 | 1 | 0 | -1.220431 | 8.981768 | -0.249689 |

R=Sat-Ver

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -8.584285 | -2.569548 | 0.075577 |
| 2 | 6 | 0 | -8.571753 | -3.994381 | 0.037443 |
| 3 | 6 | 0 | -7.388093 | -4.677005 | 0.009516 |
| 4 | 6 | 0 | -6.138066 | -3.983982 | 0.017474 |
| 5 | 6 | 0 | -6.151014 | -2.536995 | 0.055272 |
| 6 | 6 | 0 | -7.412211 | -1.866310 | 0.084193 |
| 7 | 6 | 0 | -4.914476 | -4.653700 | -0.008728 |
| 8 | 6 | 0 | -3.689504 | -3.962430 | -0.000120 |
| 9 | 6 | 0 | -3.702811 | -2.511201 | 0.035167 |
| 10 | 6 | 0 | -4.938913 | -1.844470 | 0.062760 |
| 11 | 6 | 0 | -2.448934 | -4.622288 | -0.022164 |
| 12 | 6 | 0 | -1.231487 | -3.926876 | -0.011534 |
| 13 | 6 | 0 | -1.246994 | -2.469906 | 0.018862 |
| 14 | 6 | 0 | -2.477898 | -1.813653 | 0.041877 |
| 15 | 6 | 0 | 0.000004 | -4.602297 | -0.028362 |
| 16 | 6 | 0 | 1.231494 | -3.926874 | -0.011534 |
| 17 | 6 | 0 | 1.247000 | -2.469904 | 0.018863 |
| 18 | 6 | 0 | 0.000002 | -1.762470 | 0.025870 |
| 19 | 6 | 0 | 2.448942 | -4.622285 | -0.022164 |
| 20 | 6 | 0 | 3.689511 | -3.962425 | -0.000121 |
| 21 | 6 | 0 | 3.702817 | -2.511196 | 0.035166 |
| 22 | 6 | 0 | 2.477902 | -1.813650 | 0.041877 |
| 23 | 6 | 0 | 4.914484 | -4.653694 | -0.008728 |
| 24 | 6 | 0 | 6.138074 | -3.983973 | 0.017473 |
| 25 | 6 | 0 | 6.151020 | -2.536987 | 0.055270 |
| 26 | 6 | 0 | 4.938917 | -1.844463 | 0.062759 |
| 27 | 6 | 0 | 7.388102 | -4.676995 | 0.009514 |
| 28 | 6 | 0 | 8.571761 | -3.994369 | 0.037440 |
| 29 | 6 | 0 | 8.584291 | -2.569537 | 0.075575 |
| 30 | 6 | 0 | 7.412216 | -1.866300 | 0.084191 |
| 31 | 6 | 0 | 0.000002 | -0.356666 | 0.036996 |
| 32 | 6 | 0 | 0.000001 | 0.855965 | 0.041238 |
| 33 | 6 | 0 | -0.000001 | 2.276473 | 0.048334 |
| 34 | 7 | 0 | 1.196127 | 2.871135 | 0.058798 |
| 35 | 7 | 0 | 1.173237 | 4.234743 | 0.067868 |
| 36 | 6 | 0 | -0.000005 | 5.006562 | 0.031309 |
| 37 | 7 | 0 | -1.173245 | 4.234739 | 0.067867 |
| 38 | 7 | 0 | -1.196131 | 2.871131 | 0.058797 |
| 39 | 6 | 0 | -2.467455 | 4.856042 | -0.015617 |
| 40 | 6 | 0 | 2.467445 | 4.856050 | -0.015614 |
| 41 | 8 | 0 | -0.000007 | 6.214314 | -0.024533 |
| 42 | 6 | 0 | -2.752900 | 6.041840 | 0.665153 |
| 43 | 6 | 0 | -4.030655 | 6.586208 | 0.579923 |
| 44 | 6 | 0 | -5.022318 | 5.960630 | -0.171735 |
| 45 | 6 | 0 | -4.730144 | 4.775038 | -0.842631 |
| 46 | 6 | 0 | -3.457798 | 4.219941 | -0.767973 |
| 47 | 6 | 0 | 3.457791 | 4.219953 | -0.767971 |
| 48 | 6 | 0 | 4.730134 | 4.775055 | -0.842627 |
| 49 | 6 | 0 | 5.022304 | 5.960647 | -0.171729 |
| 50 | 6 | 0 | 4.030638 | 6.586221 | 0.579929 |
| 51 | 6 | 0 | 2.752885 | 6.041848 | 0.665157 |
| 52 | 1 | 0 | -9.533587 | -2.046528 | 0.098199 |
| 53 | 1 | 0 | -9.511857 | -4.534279 | 0.031165 |
| 54 | 1 | 0 | -7.378554 | -5.761568 | -0.018980 |
| 55 | 1 | 0 | -7.420793 | -0.781815 | 0.114079 |
| 56 | 1 | 0 | -4.905183 | -5.738984 | -0.035657 |
| 57 | 1 | 0 | -4.948389 | -0.759421 | 0.092141 |
| 58 | 1 | 0 | -2.430252 | -5.707262 | -0.046224 |
| 59 | 1 | 0 | -2.497179 | -0.730344 | 0.069003 |
| 60 | 1 | 0 | 0.000005 | -5.687374 | -0.052297 |
| 61 | 1 | 0 | 2.430262 | -5.707259 | -0.046224 |
| 62 | 1 | 0 | 2.497182 | -0.730341 | 0.069003 |
| 63 | 1 | 0 | 4.905193 | -5.738978 | -0.035658 |
| 64 | 1 | 0 | 4.948393 | -0.759414 | 0.092140 |
| 65 | 1 | 0 | 7.378564 | -5.761558 | -0.018981 |
| 66 | 1 | 0 | 9.511865 | -4.534266 | 0.031162 |
| 67 | 1 | 0 | 9.533592 | -2.046515 | 0.098196 |
| 68 | 1 | 0 | 7.420797 | -0.781805 | 0.114077 |
| 69 | 1 | 0 | -1.988118 | 6.537184 | 1.243031 |
| 70 | 1 | 0 | -4.248549 | 7.506172 | 1.109932 |
| 71 | 1 | 0 | -6.014246 | 6.392927 | -0.233676 |
| 72 | 1 | 0 | -5.492872 | 4.279314 | -1.432044 |
| 73 | 1 | 0 | -3.223104 | 3.294913 | -1.275831 |
| 74 | 1 | 0 | 3.223100 | 3.294925 | -1.275829 |
| 75 | 1 | 0 | 5.492865 | 4.279334 | -1.432039 |
| 76 | 1 | 0 | 6.014231 | 6.392948 | -0.233669 |
| 77 | 1 | 0 | 4.248529 | 7.506185 | 1.109938 |
| 78 | 1 | 0 | 1.988101 | 6.537189 | 1.243035 |

R=Sat-NN

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -8.584940 | -1.526039 | -0.021278 |
| 2 | 6 | 0 | -8.573945 | -2.950942 | -0.021485 |
| 3 | 6 | 0 | -7.390779 | -3.635619 | -0.018098 |

| | | | | | |
|---|---|---|---|---|---|
| 4 | 6 | 0 | -6.140261 | -2.944091 | -0.014301 |
| 5 | 6 | 0 | -6.151774 | -1.497171 | -0.014029 |
| 6 | 6 | 0 | -7.411558 | -0.824231 | -0.017649 |
| 7 | 6 | 0 | -4.916722 | -3.615960 | -0.011063 |
| 8 | 6 | 0 | -3.691825 | -2.925824 | -0.007630 |
| 9 | 6 | 0 | -3.704658 | -1.474754 | -0.007247 |
| 10 | 6 | 0 | -4.938205 | -0.805343 | -0.010432 |
| 11 | 6 | 0 | -2.450458 | -3.587230 | -0.004896 |
| 12 | 6 | 0 | -1.233505 | -2.892125 | -0.002084 |
| 13 | 6 | 0 | -1.251355 | -1.435739 | -0.001594 |
| 14 | 6 | 0 | -2.478082 | -0.776551 | -0.004179 |
| 15 | 6 | 0 | -0.000007 | -3.566897 | -0.000002 |
| 16 | 6 | 0 | 1.233493 | -2.892128 | 0.002078 |
| 17 | 6 | 0 | 1.251347 | -1.435742 | 0.001583 |
| 18 | 6 | 0 | -0.000003 | -0.727985 | -0.000008 |
| 19 | 6 | 0 | 2.450444 | -3.587236 | 0.004895 |
| 20 | 6 | 0 | 3.691812 | -2.925834 | 0.007630 |
| 21 | 6 | 0 | 3.704650 | -1.474763 | 0.007242 |
| 22 | 6 | 0 | 2.478075 | -0.776557 | 0.004169 |
| 23 | 6 | 0 | 4.916708 | -3.615973 | 0.011067 |
| 24 | 6 | 0 | 6.140249 | -2.944107 | 0.014307 |
| 25 | 6 | 0 | 6.151766 | -1.497187 | 0.014030 |
| 26 | 6 | 0 | 4.938198 | -0.805356 | 0.010428 |
| 27 | 6 | 0 | 7.390765 | -3.635639 | 0.018109 |
| 28 | 6 | 0 | 8.573933 | -2.950964 | 0.021498 |
| 29 | 6 | 0 | 8.584931 | -1.526062 | 0.021286 |
| 30 | 6 | 0 | 7.411551 | -0.824250 | 0.017653 |
| 31 | 6 | 0 | -0.000001 | 0.666354 | -0.000010 |
| 32 | 6 | 0 | 0.000002 | 1.883585 | -0.000010 |
| 33 | 6 | 0 | 0.000007 | 3.265514 | -0.000005 |
| 34 | 7 | 0 | -1.117005 | 4.050985 | -0.003473 |
| 35 | 6 | 0 | -0.756308 | 5.501624 | 0.208717 |
| 36 | 6 | 0 | 0.756335 | 5.501621 | -0.208711 |
| 37 | 7 | 0 | 1.117023 | 4.050977 | 0.003467 |
| 38 | 6 | 0 | 0.996013 | 5.783359 | -1.701845 |
| 39 | 6 | 0 | 1.674087 | 6.377867 | 0.640844 |
| 40 | 6 | 0 | -0.995985 | 5.783351 | 1.701852 |
| 41 | 6 | 0 | -1.674054 | 6.377883 | -0.640832 |
| 42 | 8 | 0 | -2.317004 | 3.647020 | 0.007876 |
| 43 | 8 | 0 | 2.317019 | 3.647004 | -0.007883 |
| 44 | 1 | 0 | -9.533574 | -1.001301 | -0.024072 |
| 45 | 1 | 0 | -9.514634 | -3.489954 | -0.024407 |
| 46 | 1 | 0 | -7.382618 | -4.720604 | -0.018310 |
| 47 | 1 | 0 | -7.418192 | 0.260641 | -0.017560 |
| 48 | 1 | 0 | -4.908769 | -4.701624 | -0.011382 |
| 49 | 1 | 0 | -4.944741 | 0.280037 | -0.010381 |
| 50 | 1 | 0 | -2.432523 | -4.672513 | -0.005315 |
| 51 | 1 | 0 | -2.499506 | 0.307836 | -0.004268 |
| 52 | 1 | 0 | -0.000008 | -4.652265 | -0.000001 |
| 53 | 1 | 0 | 2.432506 | -4.672519 | 0.005317 |
| 54 | 1 | 0 | 2.499502 | 0.307829 | 0.004254 |
| 55 | 1 | 0 | 4.908752 | -4.701637 | 0.011390 |
| 56 | 1 | 0 | 4.944737 | 0.280024 | 0.010374 |
| 57 | 1 | 0 | 7.382601 | -4.720623 | 0.018324 |
| 58 | 1 | 0 | 9.514620 | -3.489978 | 0.024423 |
| 59 | 1 | 0 | 9.533567 | -1.001326 | 0.024082 |
| 60 | 1 | 0 | 7.418188 | 0.260622 | 0.017560 |
| 61 | 1 | 0 | 0.807004 | 6.832624 | -1.936378 |
| 62 | 1 | 0 | 2.037952 | 5.556182 | -1.932347 |
| 63 | 1 | 0 | 0.363025 | 5.162583 | -2.338716 |
| 64 | 1 | 0 | 2.705868 | 6.215854 | 0.329073 |
| 65 | 1 | 0 | 1.426776 | 7.432214 | 0.495830 |
| 66 | 1 | 0 | 1.605027 | 6.142668 | 1.702124 |
| 67 | 1 | 0 | -0.806967 | 6.832613 | 1.936394 |
| 68 | 1 | 0 | -2.037927 | 5.556181 | 1.932351 |
| 69 | 1 | 0 | -0.363004 | 5.162565 | 2.338720 |
| 70 | 1 | 0 | -2.705836 | 6.215874 | -0.329062 |
| 71 | 1 | 0 | -1.426735 | 7.432227 | -0.495809 |
| 72 | 1 | 0 | -1.604995 | 6.142692 | -1.702113 |

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# 5-5. Nonacenes(**Nn**)

## Non-Radical

R=$NO_2$

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 11.041964 | 0.062266 | -0.000003 |
| 2 | 6 | 0 | 11.032561 | -1.362679 | -0.000004 |
| 3 | 6 | 0 | 9.850454 | -2.049185 | -0.000004 |
| 4 | 6 | 0 | 8.599568 | -1.359069 | -0.000002 |
| 5 | 6 | 0 | 8.609323 | 0.087691 | -0.000001 |
| 6 | 6 | 0 | 9.868229 | 0.762864 | -0.000002 |
| 7 | 6 | 0 | 7.376781 | -2.032952 | -0.000001 |
| 8 | 6 | 0 | 6.150498 | -1.347470 | 0.000000 |
| 9 | 6 | 0 | 6.161174 | 0.105308 | 0.000001 |
| 10 | 6 | 0 | 7.394949 | 0.776353 | 0.000000 |
| 11 | 6 | 0 | 4.911809 | -2.019573 | 0.000001 |
| 12 | 6 | 0 | 3.695466 | -1.331360 | 0.000002 |
| 13 | 6 | 0 | 3.707805 | 0.125111 | 0.000002 |
| 14 | 6 | 0 | 4.932004 | 0.795392 | 0.000002 |
| 15 | 6 | 0 | 2.449481 | -1.990841 | 0.000002 |
| 16 | 6 | 0 | 1.233669 | -1.296464 | 0.000002 |
| 17 | 6 | 0 | 1.249901 | 0.162427 | 0.000003 |
| 18 | 6 | 0 | 2.476939 | 0.820735 | 0.000003 |
| 19 | 6 | 0 | 0.000000 | -1.968227 | 0.000002 |
| 20 | 6 | 0 | -1.233668 | -1.296464 | 0.000002 |
| 21 | 6 | 0 | -1.249901 | 0.162427 | 0.000003 |
| 22 | 6 | 0 | 0.000000 | 0.865839 | 0.000003 |
| 23 | 6 | 0 | -2.449480 | -1.990841 | 0.000001 |
| 24 | 6 | 0 | -3.695466 | -1.331360 | 0.000001 |
| 25 | 6 | 0 | -3.707805 | 0.125111 | 0.000002 |
| 26 | 6 | 0 | -2.476939 | 0.820735 | 0.000002 |
| 27 | 6 | 0 | -4.911809 | -2.019573 | 0.000000 |
| 28 | 6 | 0 | -6.150497 | -1.347470 | 0.000000 |
| 29 | 6 | 0 | -6.161174 | 0.105308 | 0.000000 |
| 30 | 6 | 0 | -4.932004 | 0.795392 | 0.000001 |
| 31 | 6 | 0 | -7.376781 | -2.032952 | -0.000001 |
| 32 | 6 | 0 | -8.599568 | -1.359069 | -0.000002 |
| 33 | 6 | 0 | -8.609322 | 0.087691 | -0.000001 |
| 34 | 6 | 0 | -7.394949 | 0.776353 | 0.000000 |
| 35 | 6 | 0 | -9.850453 | -2.049185 | -0.000003 |
| 36 | 6 | 0 | -11.032561 | -1.362679 | -0.000003 |
| 37 | 6 | 0 | -11.041964 | 0.062266 | -0.000003 |
| 38 | 6 | 0 | -9.868229 | 0.762864 | -0.000001 |
| 39 | 6 | 0 | 0.000000 | 2.268901 | 0.000003 |
| 40 | 6 | 0 | 0.000000 | 3.479288 | 0.000003 |
| 41 | 7 | 0 | -0.000001 | 4.860493 | -0.000001 |
| 42 | 8 | 0 | 1.096310 | 5.422208 | 0.000004 |
| 43 | 8 | 0 | -1.096313 | 5.422205 | -0.000009 |
| 44 | 1 | 0 | 11.990004 | 0.587855 | -0.000004 |
| 45 | 1 | 0 | 11.973938 | -1.900273 | -0.000006 |
| 46 | 1 | 0 | 9.843824 | -3.134057 | -0.000004 |
| 47 | 1 | 0 | 9.874208 | 1.847699 | -0.000001 |
| 48 | 1 | 0 | 7.371657 | -3.118532 | -0.000002 |
| 49 | 1 | 0 | 7.401944 | 1.861843 | 0.000001 |
| 50 | 1 | 0 | 4.904491 | -3.104988 | 0.000000 |
| 51 | 1 | 0 | 4.938851 | 1.880650 | 0.000003 |
| 52 | 1 | 0 | 2.431026 | -3.075961 | 0.000001 |
| 53 | 1 | 0 | 2.497334 | 1.904466 | 0.000003 |
| 54 | 1 | 0 | 0.000000 | -3.053613 | 0.000002 |
| 55 | 1 | 0 | -2.431026 | -3.075961 | 0.000001 |
| 56 | 1 | 0 | -2.497334 | 1.904466 | 0.000003 |
| 57 | 1 | 0 | -4.904491 | -3.104988 | 0.000000 |
| 58 | 1 | 0 | -4.938851 | 1.880650 | 0.000002 |
| 59 | 1 | 0 | -7.371657 | -3.118533 | -0.000002 |
| 60 | 1 | 0 | -7.401944 | 1.861843 | 0.000001 |
| 61 | 1 | 0 | -9.843824 | -3.134058 | -0.000003 |
| 62 | 1 | 0 | -11.973938 | -1.900274 | -0.000004 |
| 63 | 1 | 0 | -11.990004 | 0.587855 | -0.000003 |
| 64 | 1 | 0 | -9.874208 | 1.847699 | -0.000001 |

R=CN

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 11.044799 | 0.233515 | 0.000005 |
| 2 | 6 | 0 | 11.032980 | -1.191269 | 0.000001 |
| 3 | 6 | 0 | 9.849442 | -1.875486 | -0.000002 |
| 4 | 6 | 0 | 8.599909 | -1.183097 | 0.000000 |
| 5 | 6 | 0 | 8.612094 | 0.263453 | 0.000004 |
| 6 | 6 | 0 | 9.872153 | 0.936198 | 0.000006 |
| 7 | 6 | 0 | 7.375629 | -1.854611 | -0.000003 |
| 8 | 6 | 0 | 6.150778 | -1.166885 | -0.000001 |
| 9 | 6 | 0 | 6.163737 | 0.285732 | 0.000003 |
| 10 | 6 | 0 | 7.398587 | 0.954262 | 0.000005 |
| 11 | 6 | 0 | 4.910604 | -1.836717 | -0.000004 |
| 12 | 6 | 0 | 3.695588 | -1.146548 | -0.000002 |
| 13 | 6 | 0 | 3.709707 | 0.309740 | 0.000002 |
| 14 | 6 | 0 | 4.935012 | 0.977561 | 0.000004 |
| 15 | 6 | 0 | 2.448445 | -1.804039 | -0.000004 |
| 16 | 6 | 0 | 1.232976 | -1.109246 | -0.000003 |
| 17 | 6 | 0 | 1.249735 | 0.349884 | 0.000001 |
| 18 | 6 | 0 | 2.478657 | 1.005717 | 0.000003 |
| 19 | 6 | 0 | 0.000001 | -1.781773 | -0.000005 |
| 20 | 6 | 0 | -1.232974 | -1.109246 | -0.000003 |
| 21 | 6 | 0 | -1.249734 | 0.349884 | 0.000001 |
| 22 | 6 | 0 | 0.000001 | 1.053184 | 0.000002 |
| 23 | 6 | 0 | -2.448443 | -1.804040 | -0.000004 |
| 24 | 6 | 0 | -3.695586 | -1.146549 | -0.000002 |
| 25 | 6 | 0 | -3.709705 | 0.309739 | 0.000002 |
| 26 | 6 | 0 | -2.478655 | 1.005716 | 0.000003 |
| 27 | 6 | 0 | -4.910602 | -1.836718 | -0.000004 |
| 28 | 6 | 0 | -6.150777 | -1.166886 | -0.000001 |
| 29 | 6 | 0 | -6.163735 | 0.285730 | 0.000003 |
| 30 | 6 | 0 | -4.935010 | 0.977560 | 0.000004 |
| 31 | 6 | 0 | -7.375627 | -1.854613 | -0.000003 |
| 32 | 6 | 0 | -8.599907 | -1.183099 | 0.000000 |
| 33 | 6 | 0 | -8.612092 | 0.263451 | 0.000004 |
| 34 | 6 | 0 | -7.398586 | 0.954260 | 0.000005 |
| 35 | 6 | 0 | -9.849440 | -1.875488 | -0.000002 |
| 36 | 6 | 0 | -11.032978 | -1.191272 | 0.000001 |
| 37 | 6 | 0 | -11.044798 | 0.233512 | 0.000005 |
| 38 | 6 | 0 | -9.872152 | 0.936196 | 0.000006 |
| 39 | 6 | 0 | 0.000001 | 2.458592 | 0.000004 |
| 40 | 6 | 0 | -0.000002 | 3.674972 | 0.000002 |
| 41 | 6 | 0 | -0.000007 | 5.036367 | -0.000002 |
| 42 | 7 | 0 | -0.000021 | 6.197889 | -0.000023 |
| 43 | 1 | 0 | 11.993726 | 0.757548 | 0.000006 |
| 44 | 1 | 0 | 11.973359 | -1.730616 | 0.000000 |
| 45 | 1 | 0 | 9.840735 | -2.960365 | -0.000005 |
| 46 | 1 | 0 | 9.880216 | 2.021053 | 0.000009 |
| 47 | 1 | 0 | 7.368393 | -2.940201 | -0.000006 |
| 48 | 1 | 0 | 7.407907 | 2.039788 | 0.000008 |
| 49 | 1 | 0 | 4.901317 | -2.922140 | -0.000007 |
| 50 | 1 | 0 | 4.944490 | 2.062887 | 0.000007 |
| 51 | 1 | 0 | 2.428660 | -2.889164 | -0.000007 |
| 52 | 1 | 0 | 2.501392 | 2.089223 | 0.000005 |
| 53 | 1 | 0 | 0.000001 | -2.867085 | -0.000008 |
| 54 | 1 | 0 | -2.428658 | -2.889165 | -0.000007 |
| 55 | 1 | 0 | -2.501391 | 2.089223 | 0.000005 |
| 56 | 1 | 0 | -4.901315 | -2.922141 | -0.000007 |
| 57 | 1 | 0 | -4.944489 | 2.062885 | 0.000007 |
| 58 | 1 | 0 | -7.368391 | -2.940203 | -0.000006 |
| 59 | 1 | 0 | -7.407906 | 2.039786 | 0.000008 |
| 60 | 1 | 0 | -9.840733 | -2.960367 | -0.000005 |
| 61 | 1 | 0 | -11.973357 | -1.730619 | 0.000000 |
| 62 | 1 | 0 | -11.993724 | 0.757546 | 0.000006 |
| 63 | 1 | 0 | -9.880215 | 2.021051 | 0.000009 |

R=Cl

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 11.045340 | 0.172041 | 0.000014 |
| 2 | 6 | 0 | 11.033563 | -1.252622 | 0.000011 |
| 3 | 6 | 0 | 9.849502 | -1.936197 | 0.000006 |
| 4 | 6 | 0 | 8.600008 | -1.243799 | 0.000005 |
| 5 | 6 | 0 | 8.612080 | 0.202583 | 0.000009 |
| 6 | 6 | 0 | 9.872426 | 0.874655 | 0.000013 |
| 7 | 6 | 0 | 7.375235 | -1.914742 | 0.000001 |
| 8 | 6 | 0 | 6.150504 | -1.226956 | 0.000000 |
| 9 | 6 | 0 | 6.163025 | 0.225646 | 0.000004 |
| 10 | 6 | 0 | 7.398172 | 0.893338 | 0.000008 |
| 11 | 6 | 0 | 4.909899 | -1.896562 | -0.000004 |
| 12 | 6 | 0 | 3.694804 | -1.206796 | -0.000005 |
| 13 | 6 | 0 | 3.707639 | 0.249793 | -0.000001 |
| 14 | 6 | 0 | 4.933429 | 0.916863 | 0.000003 |
| 15 | 6 | 0 | 2.447909 | -1.865402 | -0.000009 |
| 16 | 6 | 0 | 1.231472 | -1.172365 | -0.000010 |
| 17 | 6 | 0 | 1.245154 | 0.287503 | -0.000006 |
| 18 | 6 | 0 | 2.475558 | 0.943782 | -0.000002 |
| 19 | 6 | 0 | 0.000000 | -1.847414 | -0.000014 |
| 20 | 6 | 0 | -1.231472 | -1.172365 | -0.000012 |
| 21 | 6 | 0 | -1.245154 | 0.287503 | -0.000007 |
| 22 | 6 | 0 | 0.000000 | 0.991940 | -0.000005 |
| 23 | 6 | 0 | -2.447909 | -1.865402 | -0.000014 |
| 24 | 6 | 0 | -3.694803 | -1.206797 | -0.000010 |
| 25 | 6 | 0 | -3.707638 | 0.249792 | -0.000002 |
| 26 | 6 | 0 | -2.475558 | 0.943781 | -0.000001 |
| 27 | 6 | 0 | -4.909897 | -1.896563 | -0.000011 |
| 28 | 6 | 0 | -6.150503 | -1.226957 | -0.000005 |
| 29 | 6 | 0 | -6.163024 | 0.225645 | 0.000004 |
| 30 | 6 | 0 | -4.933428 | 0.916862 | 0.000005 |
| 31 | 6 | 0 | -7.375233 | -1.914743 | -0.000006 |
| 32 | 6 | 0 | -8.600007 | -1.243800 | 0.000002 |
| 33 | 6 | 0 | -8.612079 | 0.202582 | 0.000012 |
| 34 | 6 | 0 | -7.398170 | 0.893337 | 0.000012 |
| 35 | 6 | 0 | -9.849501 | -1.936198 | 0.000002 |
| 36 | 6 | 0 | -11.033562 | -1.252623 | 0.000010 |
| 37 | 6 | 0 | -11.045339 | 0.172040 | 0.000020 |
| 38 | 6 | 0 | -9.872425 | 0.874654 | 0.000020 |
| 39 | 6 | 0 | -0.000001 | 2.408183 | -0.000003 |
| 40 | 6 | 0 | -0.000002 | 3.616147 | -0.000009 |
| 41 | 17 | 0 | -0.000005 | 5.263244 | -0.000013 |
| 42 | 1 | 0 | 11.994260 | 0.696263 | 0.000017 |
| 43 | 1 | 0 | 11.973799 | -1.792315 | 0.000011 |

| | | | | | |
|---|---|---|---|---|---|
| 44 | 1 | 0 | 9.840389 | -3.021158 | 0.000004 |
| 45 | 1 | 0 | 9.880761 | 1.959618 | 0.000016 |
| 46 | 1 | 0 | 7.367627 | -3.000419 | -0.000002 |
| 47 | 1 | 0 | 7.407967 | 1.978982 | 0.000010 |
| 48 | 1 | 0 | 4.900721 | -2.982089 | -0.000007 |
| 49 | 1 | 0 | 4.942935 | 2.002300 | 0.000005 |
| 50 | 1 | 0 | 2.429696 | -2.950693 | -0.000012 |
| 51 | 1 | 0 | 2.493642 | 2.027228 | 0.000001 |
| 52 | 1 | 0 | 0.000000 | -2.932769 | -0.000017 |
| 53 | 1 | 0 | -2.429695 | -2.950693 | -0.000018 |
| 54 | 1 | 0 | -2.493642 | 2.027227 | 0.000004 |
| 55 | 1 | 0 | -4.900720 | -2.982089 | -0.000017 |
| 56 | 1 | 0 | -4.942934 | 2.002298 | 0.000011 |
| 57 | 1 | 0 | -7.367626 | -3.000420 | -0.000012 |
| 58 | 1 | 0 | -7.407965 | 1.978981 | 0.000019 |
| 59 | 1 | 0 | -9.840388 | -3.021159 | -0.000005 |
| 60 | 1 | 0 | -11.973798 | -1.792316 | 0.000010 |
| 61 | 1 | 0 | -11.994259 | 0.696262 | 0.000027 |
| 62 | 1 | 0 | -9.880760 | 1.959617 | 0.000028 |

R=H

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 11.045303 | 0.495434 | 0.000005 |
| 2 | 6 | 0 | 11.033492 | -0.929223 | 0.000004 |
| 3 | 6 | 0 | 9.849376 | -1.612729 | 0.000002 |
| 4 | 6 | 0 | 8.599885 | -0.920325 | 0.000001 |
| 5 | 6 | 0 | 8.611987 | 0.526053 | 0.000003 |
| 6 | 6 | 0 | 9.872374 | 1.198048 | 0.000005 |
| 7 | 6 | 0 | 7.375069 | -1.591215 | 0.000000 |
| 8 | 6 | 0 | 6.150333 | -0.903431 | 0.000000 |
| 9 | 6 | 0 | 6.162856 | 0.549181 | 0.000001 |
| 10 | 6 | 0 | 7.398059 | 1.216799 | 0.000002 |
| 11 | 6 | 0 | 4.909691 | -1.572978 | -0.000002 |
| 12 | 6 | 0 | 3.694593 | -0.883193 | -0.000002 |
| 13 | 6 | 0 | 3.707279 | 0.573446 | -0.000001 |
| 14 | 6 | 0 | 4.933244 | 1.240371 | 0.000000 |
| 15 | 6 | 0 | 2.447730 | -1.541803 | -0.000003 |
| 16 | 6 | 0 | 1.231406 | -0.848571 | -0.000003 |
| 17 | 6 | 0 | 1.244921 | 0.611423 | -0.000003 |
| 18 | 6 | 0 | 2.475512 | 1.267934 | -0.000002 |
| 19 | 6 | 0 | 0.000000 | -1.523650 | -0.000003 |
| 20 | 6 | 0 | -1.231406 | -0.848571 | -0.000003 |
| 21 | 6 | 0 | -1.244921 | 0.611423 | -0.000003 |
| 22 | 6 | 0 | 0.000000 | 1.315421 | -0.000004 |
| 23 | 6 | 0 | -2.447730 | -1.541804 | -0.000002 |
| 24 | 6 | 0 | -3.694593 | -0.883194 | -0.000002 |
| 25 | 6 | 0 | -3.707279 | 0.573445 | -0.000002 |
| 26 | 6 | 0 | -2.475513 | 1.267933 | -0.000002 |
| 27 | 6 | 0 | -4.909691 | -1.572979 | -0.000001 |
| 28 | 6 | 0 | -6.150333 | -0.903431 | 0.000000 |
| 29 | 6 | 0 | -6.162855 | 0.549181 | 0.000000 |
| 30 | 6 | 0 | -4.933244 | 1.240371 | 0.000000 |
| 31 | 6 | 0 | -7.375069 | -1.591216 | 0.000001 |
| 32 | 6 | 0 | -8.599884 | -0.920325 | 0.000002 |
| 33 | 6 | 0 | -8.611986 | 0.526053 | 0.000002 |
| 34 | 6 | 0 | -7.398059 | 1.216799 | 0.000002 |
| 35 | 6 | 0 | -9.849376 | -1.612729 | 0.000003 |
| 36 | 6 | 0 | -11.033492 | -0.929223 | 0.000004 |
| 37 | 6 | 0 | -11.045303 | 0.495435 | 0.000004 |
| 38 | 6 | 0 | -9.872373 | 1.198049 | 0.000004 |
| 39 | 6 | 0 | 0.000000 | 2.733567 | -0.000004 |
| 40 | 6 | 0 | -0.000001 | 3.940839 | -0.000003 |
| 41 | 1 | 0 | 11.994234 | 1.019652 | 0.000006 |
| 42 | 1 | 0 | 11.973704 | -1.468967 | 0.000004 |
| 43 | 1 | 0 | 9.840218 | -2.697696 | 0.000001 |
| 44 | 1 | 0 | 9.880740 | 2.283023 | 0.000006 |
| 45 | 1 | 0 | 7.367437 | -2.676900 | -0.000001 |
| 46 | 1 | 0 | 7.407894 | 2.302456 | 0.000003 |
| 47 | 1 | 0 | 4.900494 | -2.658515 | -0.000003 |
| 48 | 1 | 0 | 4.942730 | 2.325805 | 0.000001 |
| 49 | 1 | 0 | 2.429477 | -2.627107 | -0.000004 |
| 50 | 1 | 0 | 2.492350 | 2.351327 | -0.000002 |
| 51 | 1 | 0 | 0.000000 | -2.609031 | -0.000004 |
| 52 | 1 | 0 | -2.429476 | -2.627107 | -0.000003 |
| 53 | 1 | 0 | -2.492350 | 2.351327 | -0.000002 |
| 54 | 1 | 0 | -4.900494 | -2.658516 | -0.000001 |
| 55 | 1 | 0 | -4.942730 | 2.325804 | 0.000000 |
| 56 | 1 | 0 | -7.367437 | -2.676900 | 0.000000 |
| 57 | 1 | 0 | -7.407893 | 2.302455 | 0.000002 |
| 58 | 1 | 0 | -9.840218 | -2.697696 | 0.000002 |
| 59 | 1 | 0 | -11.973705 | -1.468966 | 0.000005 |
| 60 | 1 | 0 | -11.994234 | 1.019653 | 0.000005 |
| 61 | 1 | 0 | -9.880739 | 2.283024 | 0.000004 |
| 62 | 1 | 0 | -0.000002 | 5.003191 | -0.000003 |

R=CHO

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 11.003348 | 0.144234 | -0.000022 |
| 2 | 6 | 0 | 10.984625 | -1.280487 | -0.000020 |
| 3 | 6 | 0 | 9.797753 | -1.958941 | -0.000011 |
| 4 | 6 | 0 | 8.551489 | -1.260622 | -0.000005 |
| 5 | 6 | 0 | 8.570693 | 0.185850 | -0.000007 |
| 6 | 6 | 0 | 9.834024 | 0.852468 | -0.000016 |
| 7 | 6 | 0 | 7.323963 | -1.926210 | 0.000001 |
| 8 | 6 | 0 | 6.102415 | -1.232575 | 0.000006 |
| 9 | 6 | 0 | 6.122500 | 0.219981 | 0.000006 |
| 10 | 6 | 0 | 7.360554 | 0.882554 | -0.000002 |
| 11 | 6 | 0 | 4.858925 | -1.896398 | 0.000009 |
| 12 | 6 | 0 | 3.647458 | -1.199998 | 0.000012 |
| 13 | 6 | 0 | 3.668922 | 0.256204 | 0.000013 |
| 14 | 6 | 0 | 4.897336 | 0.918183 | 0.000011 |
| 15 | 6 | 0 | 2.396768 | -1.850929 | 0.000012 |
| 16 | 6 | 0 | 1.185639 | -1.148450 | 0.000010 |
| 17 | 6 | 0 | 1.210395 | 0.310465 | 0.000008 |
| 18 | 6 | 0 | 2.442412 | 0.960258 | 0.000015 |
| 19 | 6 | 0 | -0.051489 | -1.813572 | 0.000011 |
| 20 | 6 | 0 | -1.280510 | -1.133197 | 0.000008 |
| 21 | 6 | 0 | -1.287495 | 0.326006 | 0.000007 |
| 22 | 6 | 0 | -0.034867 | 1.024477 | 0.000007 |
| 23 | 6 | 0 | -2.500128 | -1.820556 | 0.000007 |
| 24 | 6 | 0 | -3.743055 | -1.154918 | 0.000004 |
| 25 | 6 | 0 | -3.747761 | 0.301557 | 0.000005 |
| 26 | 6 | 0 | -2.511696 | 0.989160 | 0.000006 |
| 27 | 6 | 0 | -4.962588 | -1.837216 | 0.000000 |
| 28 | 6 | 0 | -6.198469 | -1.159694 | -0.000002 |
| 29 | 6 | 0 | -6.202269 | 0.292981 | 0.000002 |
| 30 | 6 | 0 | -4.968930 | 0.976657 | 0.000005 |
| 31 | 6 | 0 | -7.427828 | -1.839654 | -0.000008 |
| 32 | 6 | 0 | -8.647799 | -1.160640 | -0.000009 |
| 33 | 6 | 0 | -8.650915 | 0.286016 | -0.000004 |
| 34 | 6 | 0 | -7.433090 | 0.969018 | 0.000001 |
| 35 | 6 | 0 | -9.901802 | -1.845152 | -0.000015 |
| 36 | 6 | 0 | -11.081071 | -1.153731 | -0.000016 |
| 37 | 6 | 0 | -11.083964 | 0.271187 | -0.000010 |
| 38 | 6 | 0 | -9.906942 | 0.966436 | -0.000004 |
| 39 | 6 | 0 | -0.011704 | 2.429082 | 0.000004 |
| 40 | 6 | 0 | 0.065234 | 3.642948 | 0.000000 |
| 41 | 6 | 0 | 0.199952 | 5.068534 | -0.000005 |
| 42 | 8 | 0 | 1.269146 | 5.646831 | -0.000002 |
| 43 | 1 | 0 | 11.954783 | 0.663741 | -0.000030 |
| 44 | 1 | 0 | 11.922384 | -1.824435 | -0.000024 |
| 45 | 1 | 0 | 9.783821 | -3.043795 | -0.000008 |
| 46 | 1 | 0 | 9.847148 | 1.937281 | -0.000018 |
| 47 | 1 | 0 | 7.311528 | -3.011786 | 0.000003 |
| 48 | 1 | 0 | 7.374739 | 1.968002 | -0.000001 |
| 49 | 1 | 0 | 4.844391 | -2.981805 | 0.000012 |
| 50 | 1 | 0 | 4.910998 | 2.003368 | 0.000015 |
| 51 | 1 | 0 | 2.370968 | -2.935985 | 0.000019 |
| 52 | 1 | 0 | 2.468438 | 2.043662 | 0.000013 |
| 53 | 1 | 0 | -0.058356 | -2.898955 | 0.000015 |
| 54 | 1 | 0 | -2.487625 | -2.905821 | 0.000010 |
| 55 | 1 | 0 | -2.523171 | 2.072860 | 0.000006 |
| 56 | 1 | 0 | -4.960220 | -2.922695 | -0.000001 |
| 57 | 1 | 0 | -4.971675 | 2.062090 | 0.000007 |
| 58 | 1 | 0 | -7.427333 | -2.925285 | -0.000011 |
| 59 | 1 | 0 | -7.435789 | 2.054648 | 0.000005 |
| 60 | 1 | 0 | -9.899791 | -2.930082 | -0.000019 |
| 61 | 1 | 0 | -12.024789 | -1.687235 | -0.000021 |
| 62 | 1 | 0 | -12.029619 | 0.801152 | -0.000011 |
| 63 | 1 | 0 | -9.908327 | 2.051367 | 0.000000 |
| 64 | 1 | 0 | -0.755851 | 5.627173 | -0.000013 |

R=$SiMe_3$

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -11.049640 | -0.328353 | -0.000005 |
| 2 | 6 | 0 | -11.038193 | -1.753035 | -0.000004 |
| 3 | 6 | 0 | -9.854246 | -2.436795 | -0.000002 |
| 4 | 6 | 0 | -8.604542 | -1.744708 | -0.000001 |
| 5 | 6 | 0 | -8.616276 | -0.298318 | -0.000002 |
| 6 | 6 | 0 | -9.876537 | 0.373951 | -0.000004 |
| 7 | 6 | 0 | -7.379916 | -2.415854 | 0.000001 |
| 8 | 6 | 0 | -6.154968 | -1.728366 | 0.000001 |
| 9 | 6 | 0 | -6.167121 | -0.275768 | 0.000000 |
| 10 | 6 | 0 | -7.402171 | 0.392092 | -0.000001 |
| 11 | 6 | 0 | -4.914487 | -2.398171 | 0.000003 |
| 12 | 6 | 0 | -3.699252 | -1.708625 | 0.000003 |
| 13 | 6 | 0 | -3.711535 | -0.252054 | 0.000002 |
| 14 | 6 | 0 | -4.937200 | 0.415030 | 0.000001 |
| 15 | 6 | 0 | -2.452426 | -2.367349 | 0.000003 |
| 16 | 6 | 0 | -1.236034 | -1.674227 | 0.000003 |
| 17 | 6 | 0 | -1.249181 | -0.214378 | 0.000002 |
| 18 | 6 | 0 | -2.479128 | 0.441924 | 0.000002 |
| 19 | 6 | 0 | -0.005051 | -2.350194 | 0.000003 |
| 20 | 6 | 0 | 1.226776 | -1.675779 | 0.000001 |
| 21 | 6 | 0 | 1.241592 | -0.215998 | 0.000000 |
| 22 | 6 | 0 | -0.003390 | 0.491717 | 0.000001 |
| 23 | 6 | 0 | 2.442381 | -2.370297 | 0.000002 |
| 24 | 6 | 0 | 3.689949 | -1.712944 | 0.000001 |
| 25 | 6 | 0 | 3.703841 | -0.256392 | 0.000000 |
| 26 | 6 | 0 | 2.472233 | 0.439039 | -0.000001 |
| 27 | 6 | 0 | 4.904448 | -2.403796 | 0.000001 |
| 28 | 6 | 0 | 6.145633 | -1.735281 | 0.000000 |
| 29 | 6 | 0 | 6.159328 | -0.282692 | -0.000001 |

| | | | | | |
|---|---|---|---|---|---|
| 30 | 6 | 0 | 4.930172 | 0.409478 | -0.000001 |
| 31 | 6 | 0 | 7.369861 | -2.424061 | 0.000000 |
| 32 | 6 | 0 | 8.595187 | -1.754196 | -0.000001 |
| 33 | 6 | 0 | 8.608445 | -0.307815 | -0.000002 |
| 34 | 6 | 0 | 7.395076 | 0.383885 | -0.000002 |
| 35 | 6 | 0 | 9.844169 | -2.447593 | 0.000000 |
| 36 | 6 | 0 | 11.028830 | -1.765073 | -0.000001 |
| 37 | 6 | 0 | 11.041777 | -0.340401 | -0.000003 |
| 38 | 6 | 0 | 9.869412 | 0.363135 | -0.000003 |
| 39 | 6 | 0 | -0.001343 | 1.906359 | 0.000001 |
| 40 | 6 | 0 | 0.003595 | 3.125587 | 0.000002 |
| 41 | 14 | 0 | 0.020311 | 4.968136 | 0.000001 |
| 42 | 6 | 0 | -0.865512 | 5.581066 | -1.547300 |
| 43 | 6 | 0 | 1.814798 | 5.546734 | 0.000017 |
| 44 | 6 | 0 | -0.865539 | 5.581068 | 1.547286 |
| 45 | 1 | 0 | -11.998442 | 0.196109 | -0.000006 |
| 46 | 1 | 0 | -11.978541 | -2.292550 | -0.000004 |
| 47 | 1 | 0 | -9.845337 | -3.521770 | -0.000001 |
| 48 | 1 | 0 | -9.884659 | 1.458938 | -0.000005 |
| 49 | 1 | 0 | -7.372522 | -3.501545 | 0.000001 |
| 50 | 1 | 0 | -7.411806 | 1.477766 | -0.000002 |
| 51 | 1 | 0 | -4.905519 | -3.483717 | 0.000003 |
| 52 | 1 | 0 | -4.946544 | 1.500477 | 0.000000 |
| 53 | 1 | 0 | -2.434293 | -3.452669 | 0.000004 |
| 54 | 1 | 0 | -2.494608 | 1.525354 | 0.000001 |
| 55 | 1 | 0 | -0.005755 | -3.435582 | 0.000003 |
| 56 | 1 | 0 | 2.423024 | -3.455600 | 0.000002 |
| 57 | 1 | 0 | 2.489080 | 1.522456 | -0.000002 |
| 58 | 1 | 0 | 4.894343 | -3.489334 | 0.000002 |
| 59 | 1 | 0 | 4.940548 | 1.494903 | -0.000002 |
| 60 | 1 | 0 | 7.361333 | -3.509746 | 0.000001 |
| 61 | 1 | 0 | 7.405800 | 1.469545 | -0.000003 |
| 62 | 1 | 0 | 9.834125 | -3.532559 | 0.000001 |
| 63 | 1 | 0 | 11.968612 | -2.305577 | -0.000001 |
| 64 | 1 | 0 | 11.991131 | 0.183063 | -0.000004 |
| 65 | 1 | 0 | 9.878656 | 1.448111 | -0.000004 |
| 66 | 1 | 0 | -1.903327 | 5.237691 | -1.572327 |
| 67 | 1 | 0 | -0.873024 | 6.675197 | -1.581480 |
| 68 | 1 | 0 | -0.373034 | 5.219285 | -2.453856 |
| 69 | 1 | 0 | 2.346875 | 5.185187 | 0.884231 |
| 70 | 1 | 0 | 1.869223 | 6.639960 | 0.000025 |
| 71 | 1 | 0 | 2.346886 | 5.185200 | -0.884196 |
| 72 | 1 | 0 | -0.873057 | 6.675198 | 1.581460 |
| 73 | 1 | 0 | -1.903353 | 5.237688 | 1.572299 |
| 74 | 1 | 0 | -0.373073 | 5.219293 | 2.453850 |

R=OMe

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -11.012669 | 0.100231 | -0.000015 |
| 2 | 6 | 0 | -10.991083 | -1.324271 | -0.000009 |
| 3 | 6 | 0 | -9.801978 | -1.999153 | -0.000003 |
| 4 | 6 | 0 | -8.557310 | -1.298109 | -0.000003 |
| 5 | 6 | 0 | -8.579280 | 0.148102 | -0.000009 |
| 6 | 6 | 0 | -9.844514 | 0.810924 | -0.000015 |
| 7 | 6 | 0 | -7.327655 | -1.960122 | 0.000003 |
| 8 | 6 | 0 | -6.107687 | -1.263919 | 0.000003 |
| 9 | 6 | 0 | -6.129883 | 0.188590 | -0.000003 |
| 10 | 6 | 0 | -7.369911 | 0.847067 | -0.000008 |
| 11 | 6 | 0 | -4.862265 | -1.924719 | 0.000007 |
| 12 | 6 | 0 | -3.651836 | -1.226933 | 0.000007 |
| 13 | 6 | 0 | -3.673651 | 0.229581 | 0.000003 |
| 14 | 6 | 0 | -4.904230 | 0.887397 | -0.000002 |
| 15 | 6 | 0 | -2.400399 | -1.877051 | 0.000010 |
| 16 | 6 | 0 | -1.187837 | -1.177230 | 0.000009 |
| 17 | 6 | 0 | -1.208976 | 0.282891 | 0.000007 |
| 18 | 6 | 0 | -2.444378 | 0.929372 | 0.000003 |
| 19 | 6 | 0 | 0.045771 | -1.847915 | 0.000010 |
| 20 | 6 | 0 | 1.272487 | -1.164675 | 0.000008 |
| 21 | 6 | 0 | 1.278641 | 0.295381 | 0.000008 |
| 22 | 6 | 0 | 0.030934 | 0.998079 | 0.000008 |
| 23 | 6 | 0 | 2.492155 | -1.852061 | 0.000007 |
| 24 | 6 | 0 | 3.736482 | -1.188410 | 0.000005 |
| 25 | 6 | 0 | 3.742511 | 0.268141 | 0.000005 |
| 26 | 6 | 0 | 2.506484 | 0.956023 | 0.000007 |
| 27 | 6 | 0 | 4.954325 | -1.873202 | 0.000003 |
| 28 | 6 | 0 | 6.192297 | -1.198549 | 0.000000 |
| 29 | 6 | 0 | 6.198369 | 0.254112 | 0.000000 |
| 30 | 6 | 0 | 4.965440 | 0.939969 | 0.000003 |
| 31 | 6 | 0 | 7.419907 | -1.881231 | -0.000003 |
| 32 | 6 | 0 | 8.642031 | -1.205452 | -0.000006 |
| 33 | 6 | 0 | 8.647848 | 0.240935 | -0.000006 |
| 34 | 6 | 0 | 7.430894 | 0.926536 | -0.000003 |
| 35 | 6 | 0 | 9.894500 | -1.892503 | -0.000010 |
| 36 | 6 | 0 | 11.075907 | -1.204254 | -0.000013 |
| 37 | 6 | 0 | 11.081568 | 0.220430 | -0.000013 |
| 38 | 6 | 0 | 9.905547 | 0.917985 | -0.000010 |
| 39 | 6 | 0 | 0.028908 | 2.414501 | 0.000009 |
| 40 | 6 | 0 | 0.050439 | 3.623147 | 0.000015 |
| 41 | 8 | 0 | 0.130317 | 4.917749 | 0.000021 |
| 42 | 6 | 0 | -1.134101 | 5.624372 | -0.000012 |
| 43 | 1 | 0 | -11.965204 | 0.617975 | -0.000020 |
| 44 | 1 | 0 | -11.927462 | -1.870667 | -0.000010 |
| 45 | 1 | 0 | -9.785052 | -3.084069 | 0.000001 |
| 46 | 1 | 0 | -9.860693 | 1.895892 | -0.000020 |
| 47 | 1 | 0 | -7.312261 | -3.045766 | 0.000007 |
| 48 | 1 | 0 | -7.387846 | 1.932749 | -0.000013 |
| 49 | 1 | 0 | -4.845598 | -3.010212 | 0.000011 |
| 50 | 1 | 0 | -4.922123 | 1.972947 | -0.000006 |
| 51 | 1 | 0 | -2.375506 | -2.962288 | 0.000012 |
| 52 | 1 | 0 | -2.468213 | 2.012641 | 0.000000 |
| 53 | 1 | 0 | 0.051195 | -2.933215 | 0.000011 |
| 54 | 1 | 0 | 2.478611 | -2.937516 | 0.000007 |
| 55 | 1 | 0 | 2.519467 | 2.039420 | 0.000007 |
| 56 | 1 | 0 | 4.949588 | -2.958829 | 0.000003 |
| 57 | 1 | 0 | 4.970502 | 2.025486 | 0.000003 |
| 58 | 1 | 0 | 7.416657 | -2.966992 | -0.000003 |
| 59 | 1 | 0 | 7.436313 | 2.012269 | -0.000003 |
| 60 | 1 | 0 | 9.889781 | -2.977551 | -0.000010 |
| 61 | 1 | 0 | 12.018373 | -1.740116 | -0.000016 |
| 62 | 1 | 0 | 12.028240 | 0.748812 | -0.000016 |
| 63 | 1 | 0 | 9.909366 | 2.003032 | -0.000010 |
| 64 | 1 | 0 | -0.878636 | 6.681372 | 0.000000 |
| 65 | 1 | 0 | -1.702395 | 5.369308 | -0.896835 |
| 66 | 1 | 0 | -1.702446 | 5.369299 | 0.896776 |

R=$NH_2$

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -11.048538 | 0.322628 | -0.024733 |
| 2 | 6 | 0 | -11.033946 | -1.101910 | -0.009623 |
| 3 | 6 | 0 | -9.848117 | -1.782426 | 0.001156 |
| 4 | 6 | 0 | -8.600002 | -1.087471 | -0.002381 |
| 5 | 6 | 0 | -8.614857 | 0.358765 | -0.017624 |
| 6 | 6 | 0 | -9.876921 | 1.027586 | -0.028595 |
| 7 | 6 | 0 | -7.373584 | -1.755279 | 0.008145 |
| 8 | 6 | 0 | -6.150270 | -1.064900 | 0.004540 |
| 9 | 6 | 0 | -6.165297 | 0.387606 | -0.010434 |
| 10 | 6 | 0 | -7.402147 | 1.051901 | -0.021211 |
| 11 | 6 | 0 | -4.908039 | -1.731600 | 0.014444 |
| 12 | 6 | 0 | -3.694403 | -1.039456 | 0.010808 |
| 13 | 6 | 0 | -3.709155 | 0.416961 | -0.002973 |
| 14 | 6 | 0 | -4.936224 | 1.080624 | -0.013716 |
| 15 | 6 | 0 | -2.446039 | -1.695616 | 0.018915 |
| 16 | 6 | 0 | -1.230063 | -1.001824 | 0.014937 |
| 17 | 6 | 0 | -1.244711 | 0.458013 | 0.004062 |
| 18 | 6 | 0 | -2.476014 | 1.110744 | -0.005351 |
| 19 | 6 | 0 | 0.000000 | -1.679176 | 0.021240 |
| 20 | 6 | 0 | 1.230063 | -1.001824 | 0.014934 |
| 21 | 6 | 0 | 1.244712 | 0.458012 | 0.004064 |
| 22 | 6 | 0 | 0.000001 | 1.168273 | 0.003672 |
| 23 | 6 | 0 | 2.446040 | -1.695614 | 0.018909 |
| 24 | 6 | 0 | 3.694404 | -1.039454 | 0.010804 |
| 25 | 6 | 0 | 3.709156 | 0.416963 | -0.002969 |
| 26 | 6 | 0 | 2.476013 | 1.110745 | -0.005344 |
| 27 | 6 | 0 | 4.908040 | -1.731598 | 0.014438 |
| 28 | 6 | 0 | 6.150271 | -1.064899 | 0.004537 |
| 29 | 6 | 0 | 6.165298 | 0.387608 | -0.010429 |
| 30 | 6 | 0 | 4.936225 | 1.080626 | -0.013707 |
| 31 | 6 | 0 | 7.373585 | -1.755278 | 0.008139 |
| 32 | 6 | 0 | 8.600003 | -1.087470 | -0.002383 |
| 33 | 6 | 0 | 8.614859 | 0.358766 | -0.017621 |
| 34 | 6 | 0 | 7.402148 | 1.051902 | -0.021204 |
| 35 | 6 | 0 | 9.848118 | -1.782426 | 0.001151 |
| 36 | 6 | 0 | 11.033947 | -1.101910 | -0.009627 |
| 37 | 6 | 0 | 11.048539 | 0.322628 | -0.024731 |
| 38 | 6 | 0 | 9.876922 | 1.027587 | -0.028590 |
| 39 | 6 | 0 | -0.000001 | 2.580347 | 0.004431 |
| 40 | 6 | 0 | -0.000005 | 3.792429 | 0.030062 |
| 41 | 7 | 0 | -0.000012 | 5.134480 | -0.017551 |
| 42 | 1 | 0 | -11.998524 | 0.845000 | -0.033284 |
| 43 | 1 | 0 | -11.972978 | -1.643758 | -0.006836 |
| 44 | 1 | 0 | -9.836427 | -2.867374 | 0.012542 |
| 45 | 1 | 0 | -9.887773 | 2.112564 | -0.040256 |
| 46 | 1 | 0 | -7.363368 | -2.840950 | 0.019298 |
| 47 | 1 | 0 | -7.414773 | 2.137585 | -0.032909 |
| 48 | 1 | 0 | -4.896493 | -2.817136 | 0.024786 |
| 49 | 1 | 0 | -4.948735 | 2.166156 | -0.025491 |
| 50 | 1 | 0 | -2.426390 | -2.780951 | 0.027741 |
| 51 | 1 | 0 | -2.495644 | 2.194150 | -0.017438 |
| 52 | 1 | 0 | 0.000001 | -2.764408 | 0.029925 |
| 53 | 1 | 0 | 2.426393 | -2.780950 | 0.027732 |
| 54 | 1 | 0 | 2.495642 | 2.194151 | -0.017423 |
| 55 | 1 | 0 | 4.896494 | -2.817134 | 0.024774 |
| 56 | 1 | 0 | 4.948736 | 2.166158 | -0.025476 |
| 57 | 1 | 0 | 7.363368 | -2.840949 | 0.019288 |
| 58 | 1 | 0 | 7.414775 | 2.137586 | -0.032897 |
| 59 | 1 | 0 | 9.836427 | -2.867373 | 0.012534 |
| 60 | 1 | 0 | 11.972979 | -1.643758 | -0.006841 |
| 61 | 1 | 0 | 11.998525 | 0.845000 | -0.033282 |
| 62 | 1 | 0 | 9.887775 | 2.112565 | -0.040248 |
| 63 | 1 | 0 | -0.843170 | 5.594482 | 0.297915 |
| 64 | 1 | 0 | 0.843166 | 5.594490 | 0.297849 |

R=Ph

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|

| | | | | | |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -11.047095 | -0.425427 | 0.000002 |
| 2 | 6 | 0 | -11.033283 | -1.850128 | 0.000000 |
| 3 | 6 | 0 | -9.848222 | -2.531864 | -0.000001 |
| 4 | 6 | 0 | -8.599628 | -1.837667 | 0.000000 |
| 5 | 6 | 0 | -8.613765 | -0.391280 | 0.000001 |
| 6 | 6 | 0 | -9.875203 | 0.278839 | 0.000002 |
| 7 | 6 | 0 | -7.373946 | -2.506700 | -0.000001 |
| 8 | 6 | 0 | -6.150117 | -1.817112 | -0.000001 |
| 9 | 6 | 0 | -6.164691 | -0.364585 | 0.000001 |
| 10 | 6 | 0 | -7.400837 | 0.301133 | 0.000002 |
| 11 | 6 | 0 | -4.908523 | -2.484773 | -0.000002 |
| 12 | 6 | 0 | -3.694600 | -1.793005 | -0.000001 |
| 13 | 6 | 0 | -3.709319 | -0.336732 | 0.000000 |
| 14 | 6 | 0 | -4.935723 | 0.328181 | 0.000001 |
| 15 | 6 | 0 | -2.446337 | -2.448926 | -0.000001 |
| 16 | 6 | 0 | -1.231334 | -1.753498 | -0.000001 |
| 17 | 6 | 0 | -1.246537 | -0.293843 | 0.000000 |
| 18 | 6 | 0 | -2.477127 | 0.358701 | 0.000000 |
| 19 | 6 | 0 | 0.000000 | -2.428723 | 0.000000 |
| 20 | 6 | 0 | 1.231335 | -1.753498 | 0.000000 |
| 21 | 6 | 0 | 1.246537 | -0.293843 | 0.000000 |
| 22 | 6 | 0 | 0.000000 | 0.416472 | 0.000000 |
| 23 | 6 | 0 | 2.446338 | -2.448926 | 0.000001 |
| 24 | 6 | 0 | 3.694601 | -1.793005 | 0.000001 |
| 25 | 6 | 0 | 3.709320 | -0.336731 | 0.000000 |
| 26 | 6 | 0 | 2.477127 | 0.358701 | -0.000001 |
| 27 | 6 | 0 | 4.908524 | -2.484773 | 0.000002 |
| 28 | 6 | 0 | 6.150117 | -1.817112 | 0.000001 |
| 29 | 6 | 0 | 6.164691 | -0.364585 | -0.000001 |
| 30 | 6 | 0 | 4.935723 | 0.328182 | -0.000001 |
| 31 | 6 | 0 | 7.373946 | -2.506700 | 0.000002 |
| 32 | 6 | 0 | 8.599629 | -1.837666 | 0.000001 |
| 33 | 6 | 0 | 8.613765 | -0.391280 | -0.000001 |
| 34 | 6 | 0 | 7.400838 | 0.301133 | -0.000002 |
| 35 | 6 | 0 | 9.848223 | -2.531863 | 0.000001 |
| 36 | 6 | 0 | 11.033283 | -1.850127 | 0.000000 |
| 37 | 6 | 0 | 11.047095 | -0.425426 | -0.000002 |
| 38 | 6 | 0 | 9.875203 | 0.278839 | -0.000002 |
| 39 | 6 | 0 | 0.000000 | 1.826047 | -0.000001 |
| 40 | 6 | 0 | 0.000000 | 3.041039 | -0.000001 |
| 41 | 6 | 0 | -0.000001 | 4.460964 | 0.000000 |
| 42 | 6 | 0 | -1.211111 | 5.180120 | -0.000012 |
| 43 | 6 | 0 | -1.206026 | 6.568854 | -0.000011 |
| 44 | 6 | 0 | -0.000002 | 7.269347 | 0.000001 |
| 45 | 6 | 0 | 1.206023 | 6.568855 | 0.000012 |
| 46 | 6 | 0 | 1.211109 | 5.180121 | 0.000012 |
| 47 | 1 | 0 | -11.996782 | 0.097438 | 0.000003 |
| 48 | 1 | 0 | -11.972734 | -2.391201 | 0.000000 |
| 49 | 1 | 0 | -9.837464 | -3.616822 | -0.000002 |
| 50 | 1 | 0 | -9.885183 | 1.363816 | 0.000004 |
| 51 | 1 | 0 | -7.364667 | -3.592376 | -0.000002 |
| 52 | 1 | 0 | -7.412398 | 1.386802 | 0.000003 |
| 53 | 1 | 0 | -4.897591 | -3.570296 | -0.000002 |
| 54 | 1 | 0 | -4.947292 | 1.413640 | 0.000002 |
| 55 | 1 | 0 | -2.425814 | -3.534196 | -0.000002 |
| 56 | 1 | 0 | -2.495966 | 1.441953 | 0.000001 |
| 57 | 1 | 0 | 0.000000 | -3.514073 | 0.000000 |
| 58 | 1 | 0 | 2.425815 | -3.534196 | 0.000002 |
| 59 | 1 | 0 | 2.495966 | 1.441953 | -0.000002 |
| 60 | 1 | 0 | 4.897592 | -3.570296 | 0.000003 |
| 61 | 1 | 0 | 4.947292 | 1.413640 | -0.000003 |
| 62 | 1 | 0 | 7.364668 | -3.592375 | 0.000003 |
| 63 | 1 | 0 | 7.412398 | 1.386802 | -0.000003 |
| 64 | 1 | 0 | 9.837464 | -3.616821 | 0.000003 |
| 65 | 1 | 0 | 11.972734 | -2.391200 | 0.000001 |
| 66 | 1 | 0 | 11.996783 | 0.097439 | -0.000002 |
| 67 | 1 | 0 | 9.885183 | 1.363817 | -0.000004 |
| 68 | 1 | 0 | -2.148008 | 4.636476 | -0.000021 |
| 69 | 1 | 0 | -2.146626 | 7.107999 | -0.000020 |
| 70 | 1 | 0 | -0.000002 | 8.353234 | 0.000001 |
| 71 | 1 | 0 | 2.146622 | 7.108001 | 0.000021 |
| 72 | 1 | 0 | 2.148006 | 4.636478 | 0.000021 |

R=BzTh

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -11.097895 | -1.033159 | -0.000010 |
| 2 | 6 | 0 | -11.094645 | -2.457961 | -0.000005 |
| 3 | 6 | 0 | -9.914767 | -3.148537 | -0.000001 |
| 4 | 6 | 0 | -8.661028 | -2.463602 | -0.000002 |
| 5 | 6 | 0 | -8.664457 | -1.017126 | -0.000006 |
| 6 | 6 | 0 | -9.920873 | -0.337594 | -0.000010 |
| 7 | 6 | 0 | -7.440443 | -3.141764 | 0.000002 |
| 8 | 6 | 0 | -6.211506 | -2.461255 | 0.000001 |
| 9 | 6 | 0 | -6.215386 | -1.008702 | -0.000003 |
| 10 | 6 | 0 | -7.446486 | -0.333743 | -0.000007 |
| 11 | 6 | 0 | -4.974949 | -3.138128 | 0.000004 |
| 12 | 6 | 0 | -3.755984 | -2.455328 | 0.000003 |
| 13 | 6 | 0 | -3.760199 | -0.999103 | 0.000000 |
| 14 | 6 | 0 | -4.981321 | -0.325015 | -0.000004 |
| 15 | 6 | 0 | -2.512504 | -3.120403 | 0.000004 |
| 16 | 6 | 0 | -1.292509 | -2.433960 | 0.000002 |
| 17 | 6 | 0 | -1.297857 | -0.974457 | 0.000002 |
| 18 | 6 | 0 | -2.522629 | -0.312627 | -0.000001 |
| 19 | 6 | 0 | -0.065817 | -3.117940 | 0.000000 |
| 20 | 6 | 0 | 1.171066 | -2.452600 | -0.000002 |
| 21 | 6 | 0 | 1.198405 | -0.993393 | 0.000001 |
| 22 | 6 | 0 | -0.044417 | -0.274096 | 0.000002 |
| 23 | 6 | 0 | 2.380562 | -3.157445 | -0.000005 |
| 24 | 6 | 0 | 3.633902 | -2.511130 | -0.000002 |
| 25 | 6 | 0 | 3.659937 | -1.055189 | 0.000003 |
| 26 | 6 | 0 | 2.432997 | -0.350004 | 0.000004 |
| 27 | 6 | 0 | 4.842513 | -3.212082 | -0.000004 |
| 28 | 6 | 0 | 6.088937 | -2.553507 | 0.000000 |
| 29 | 6 | 0 | 6.114318 | -1.101166 | 0.000007 |
| 30 | 6 | 0 | 4.890720 | -0.398917 | 0.000008 |
| 31 | 6 | 0 | 7.307655 | -3.252133 | -0.000001 |
| 32 | 6 | 0 | 8.538103 | -2.592008 | 0.000004 |
| 33 | 6 | 0 | 8.562888 | -1.145741 | 0.000011 |
| 34 | 6 | 0 | 7.355191 | -0.444354 | 0.000013 |
| 35 | 6 | 0 | 9.781602 | -3.295352 | 0.000003 |
| 36 | 6 | 0 | 10.971517 | -2.622205 | 0.000008 |
| 37 | 6 | 0 | 10.995800 | -1.197607 | 0.000016 |
| 38 | 6 | 0 | 9.829160 | -0.484761 | 0.000017 |
| 39 | 6 | 0 | -0.032386 | 1.131408 | 0.000003 |
| 40 | 6 | 0 | -0.025503 | 2.348448 | 0.000004 |
| 41 | 6 | 0 | 0.007830 | 3.746997 | 0.000004 |
| 42 | 6 | 0 | -1.046005 | 4.625188 | 0.000086 |
| 43 | 6 | 0 | -0.651165 | 5.998427 | 0.000059 |
| 44 | 6 | 0 | 0.757845 | 6.151744 | -0.000048 |
| 45 | 16 | 0 | 1.568237 | 4.597309 | -0.000113 |
| 46 | 6 | 0 | -1.457036 | 7.152668 | 0.000125 |
| 47 | 6 | 0 | -0.862925 | 8.402420 | 0.000082 |
| 48 | 6 | 0 | 0.536406 | 8.532786 | -0.000025 |
| 49 | 6 | 0 | 1.356114 | 7.412637 | -0.000091 |
| 50 | 1 | 0 | -12.043690 | -0.503309 | -0.000013 |
| 51 | 1 | 0 | -12.038103 | -2.991997 | -0.000005 |
| 52 | 1 | 0 | -9.912096 | -4.233531 | 0.000002 |
| 53 | 1 | 0 | -9.922795 | 0.747415 | -0.000014 |
| 54 | 1 | 0 | -7.439245 | -4.227463 | 0.000005 |
| 55 | 1 | 0 | -7.449963 | 0.751972 | -0.000011 |
| 56 | 1 | 0 | -4.972038 | -4.223683 | 0.000007 |
| 57 | 1 | 0 | -4.984787 | 0.760496 | -0.000007 |
| 58 | 1 | 0 | -2.499896 | -4.205763 | 0.000005 |
| 59 | 1 | 0 | -2.534790 | 0.770872 | -0.000004 |
| 60 | 1 | 0 | -0.074057 | -4.203232 | -0.000001 |
| 61 | 1 | 0 | 2.351538 | -4.242497 | -0.000007 |
| 62 | 1 | 0 | 2.462790 | 0.733128 | 0.000009 |
| 63 | 1 | 0 | 4.823504 | -4.297479 | -0.000009 |
| 64 | 1 | 0 | 4.909927 | 0.686358 | 0.000013 |
| 65 | 1 | 0 | 7.290459 | -4.337702 | -0.000007 |
| 66 | 1 | 0 | 7.374453 | 0.641153 | 0.000018 |
| 67 | 1 | 0 | 9.762962 | -4.380193 | -0.000003 |
| 68 | 1 | 0 | 11.907006 | -3.170097 | 0.000007 |
| 69 | 1 | 0 | 11.949303 | -0.681760 | 0.000020 |
| 70 | 1 | 0 | 9.846972 | 0.600088 | 0.000023 |
| 71 | 1 | 0 | -2.075591 | 4.293620 | 0.000165 |
| 72 | 1 | 0 | -2.536988 | 7.054844 | 0.000208 |
| 73 | 1 | 0 | -1.481105 | 9.292678 | 0.000133 |
| 74 | 1 | 0 | 0.983098 | 9.520287 | -0.000057 |
| 75 | 1 | 0 | 2.434660 | 7.517076 | -0.000173 |

R=Th

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -10.990667 | -0.532093 | 0.000012 |
| 2 | 6 | 0 | -10.963897 | -1.956630 | 0.000001 |
| 3 | 6 | 0 | -9.772730 | -2.627595 | -0.000005 |
| 4 | 6 | 0 | -8.530473 | -1.922070 | -0.000001 |
| 5 | 6 | 0 | -8.557771 | -0.475868 | 0.000010 |
| 6 | 6 | 0 | -9.825243 | 0.182793 | 0.000017 |
| 7 | 6 | 0 | -7.298800 | -2.579948 | -0.000008 |
| 8 | 6 | 0 | -6.081323 | -1.879179 | -0.000004 |
| 9 | 6 | 0 | -6.109176 | -0.426884 | 0.000007 |
| 10 | 6 | 0 | -7.351247 | 0.227624 | 0.000014 |
| 11 | 6 | 0 | -4.833688 | -2.535529 | -0.000009 |
| 12 | 6 | 0 | -3.626284 | -1.832532 | -0.000005 |
| 13 | 6 | 0 | -3.654669 | -0.376603 | 0.000004 |
| 14 | 6 | 0 | -4.886656 | 0.277381 | 0.000011 |
| 15 | 6 | 0 | -2.371850 | -2.476815 | -0.000009 |
| 16 | 6 | 0 | -1.163380 | -1.770215 | -0.000005 |
| 17 | 6 | 0 | -1.192878 | -0.310978 | 0.000001 |
| 18 | 6 | 0 | -2.428682 | 0.330321 | 0.000007 |
| 19 | 6 | 0 | 0.074362 | -2.433954 | -0.000006 |
| 20 | 6 | 0 | 1.299792 | -1.747732 | -0.000002 |
| 21 | 6 | 0 | 1.302670 | -0.288189 | 0.000001 |
| 22 | 6 | 0 | 0.048453 | 0.410462 | 0.000002 |
| 23 | 6 | 0 | 2.520960 | -2.432099 | -0.000001 |
| 24 | 6 | 0 | 3.763429 | -1.765038 | 0.000000 |
| 25 | 6 | 0 | 3.765301 | -0.308786 | 0.000000 |
| 26 | 6 | 0 | 2.526524 | 0.375579 | 0.000000 |
| 27 | 6 | 0 | 4.983418 | -2.445977 | 0.000000 |
| 28 | 6 | 0 | 6.219012 | -1.767267 | 0.000000 |
| 29 | 6 | 0 | 6.220624 | -0.314711 | -0.000001 |
| 30 | 6 | 0 | 4.985428 | 0.367068 | -0.000001 |
| 31 | 6 | 0 | 7.448960 | -2.445927 | 0.000001 |
| 32 | 6 | 0 | 8.668580 | -1.765982 | 0.000000 |

| | | | | | |
|---|---|---|---|---|---|
| 33 | 6 | 0 | 8.669785 | -0.319522 | -0.000001 |
| 34 | 6 | 0 | 7.450732 | 0.362018 | -0.000001 |
| 35 | 6 | 0 | 9.923357 | -2.449001 | 0.000001 |
| 36 | 6 | 0 | 11.102250 | -1.756704 | 0.000001 |
| 37 | 6 | 0 | 11.103317 | -0.331915 | -0.000001 |
| 38 | 6 | 0 | 9.925198 | 0.361845 | -0.000001 |
| 39 | 6 | 0 | 0.034986 | 1.816555 | 0.000005 |
| 40 | 6 | 0 | 0.026802 | 3.033441 | 0.000007 |
| 41 | 6 | 0 | 0.003540 | 4.432731 | 0.000010 |
| 42 | 6 | 0 | 1.065408 | 5.316984 | 0.000069 |
| 43 | 6 | 0 | 0.665588 | 6.676318 | 0.000052 |
| 44 | 6 | 0 | -0.693286 | 6.833626 | -0.000020 |
| 45 | 16 | 0 | -1.519816 | 5.314308 | -0.000069 |
| 46 | 1 | 0 | -11.945071 | -0.017889 | 0.000018 |
| 47 | 1 | 0 | -11.898404 | -2.506208 | -0.000002 |
| 48 | 1 | 0 | -9.752128 | -3.712413 | -0.000014 |
| 49 | 1 | 0 | -9.845007 | 1.267625 | 0.000025 |
| 50 | 1 | 0 | -7.279642 | -3.665497 | -0.000016 |
| 51 | 1 | 0 | -7.372512 | 1.313116 | 0.000022 |
| 52 | 1 | 0 | -4.812786 | -3.620906 | -0.000017 |
| 53 | 1 | 0 | -4.907853 | 1.362650 | 0.000018 |
| 54 | 1 | 0 | -2.341181 | -3.561840 | -0.000015 |
| 55 | 1 | 0 | -2.459865 | 1.413419 | 0.000014 |
| 56 | 1 | 0 | 0.084280 | -3.519230 | -0.000009 |
| 57 | 1 | 0 | 2.510156 | -3.517499 | -0.000003 |
| 58 | 1 | 0 | 2.536781 | 1.459099 | -0.000001 |
| 59 | 1 | 0 | 4.982142 | -3.531551 | 0.000001 |
| 60 | 1 | 0 | 4.987268 | 1.452594 | -0.000002 |
| 61 | 1 | 0 | 7.449362 | -3.531640 | 0.000002 |
| 62 | 1 | 0 | 7.452603 | 1.447749 | -0.000002 |
| 63 | 1 | 0 | 9.922292 | -3.534011 | 0.000002 |
| 64 | 1 | 0 | 12.046506 | -2.289345 | 0.000001 |
| 65 | 1 | 0 | 12.048299 | 0.199409 | -0.000001 |
| 66 | 1 | 0 | 9.925486 | 1.446869 | -0.000002 |
| 67 | 1 | 0 | 2.093924 | 4.983571 | 0.000124 |
| 68 | 1 | 0 | 1.358256 | 7.507300 | 0.000092 |
| 69 | 1 | 0 | -1.260488 | 7.751683 | -0.000047 |

# Radical

R=Mt

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 0.000000 | 3.853088 | 0.000017 |
| 2 | 6 | 0 | 0.000000 | 2.598975 | 0.000013 |
| 3 | 6 | 0 | 0.000000 | 5.178102 | 0.000022 |
| 4 | 6 | 0 | 11.055996 | 0.311765 | -0.000020 |
| 5 | 6 | 0 | 11.034834 | -1.113686 | -0.000014 |
| 6 | 6 | 0 | 9.847465 | -1.789360 | -0.000007 |
| 7 | 6 | 0 | 8.601268 | -1.088447 | -0.000006 |
| 8 | 6 | 0 | 8.623185 | 0.358007 | -0.000012 |
| 9 | 6 | 0 | 9.888457 | 1.021852 | -0.000019 |
| 10 | 6 | 0 | 7.373645 | -1.750766 | 0.000001 |
| 11 | 6 | 0 | 6.153114 | -1.053716 | 0.000002 |
| 12 | 6 | 0 | 6.176652 | 0.397099 | -0.000005 |
| 13 | 6 | 0 | 7.414307 | 1.056525 | -0.000011 |
| 14 | 6 | 0 | 4.907340 | -1.714196 | 0.000008 |
| 15 | 6 | 0 | 3.700665 | -1.013144 | 0.000009 |
| 16 | 6 | 0 | 3.727593 | 0.439571 | 0.000003 |
| 17 | 6 | 0 | 4.948059 | 1.097590 | -0.000004 |
| 18 | 6 | 0 | 2.442517 | -1.656441 | 0.000014 |
| 19 | 6 | 0 | 1.237592 | -0.949162 | 0.000014 |
| 20 | 6 | 0 | 1.271530 | 0.508315 | 0.000009 |
| 21 | 6 | 0 | 2.486753 | 1.144328 | 0.000003 |
| 22 | 6 | 0 | 0.000000 | -1.619218 | 0.000018 |
| 23 | 6 | 0 | -1.237592 | -0.949162 | 0.000015 |
| 24 | 6 | 0 | -1.271530 | 0.508315 | 0.000009 |
| 25 | 6 | 0 | 0.000000 | 1.253915 | 0.000010 |
| 26 | 6 | 0 | -2.442517 | -1.656441 | 0.000016 |
| 27 | 6 | 0 | -3.700665 | -1.013144 | 0.000010 |
| 28 | 6 | 0 | -3.727593 | 0.439571 | 0.000002 |
| 29 | 6 | 0 | -2.486753 | 1.144328 | 0.000002 |
| 30 | 6 | 0 | -4.907340 | -1.714196 | 0.000010 |
| 31 | 6 | 0 | -6.153114 | -1.053716 | 0.000003 |
| 32 | 6 | 0 | -6.176652 | 0.397099 | -0.000005 |
| 33 | 6 | 0 | -4.948059 | 1.097590 | -0.000005 |
| 34 | 6 | 0 | -7.373645 | -1.750766 | 0.000002 |
| 35 | 6 | 0 | -8.601268 | -1.088447 | -0.000005 |
| 36 | 6 | 0 | -8.623185 | 0.358007 | -0.000013 |
| 37 | 6 | 0 | -7.414307 | 1.056525 | -0.000013 |
| 38 | 6 | 0 | -9.847465 | -1.789360 | -0.000006 |
| 39 | 6 | 0 | -11.034834 | -1.113686 | -0.000013 |
| 40 | 6 | 0 | -11.055996 | 0.311765 | -0.000021 |
| 41 | 6 | 0 | -9.888457 | 1.021852 | -0.000021 |
| 42 | 1 | 0 | -0.926533 | 5.741995 | 0.000024 |
| 43 | 1 | 0 | 0.926534 | 5.741995 | 0.000024 |
| 44 | 1 | 0 | 12.008526 | 0.829409 | -0.000026 |
| 45 | 1 | 0 | 11.971777 | -1.659117 | -0.000015 |
| 46 | 1 | 0 | 9.831107 | -2.874225 | -0.000003 |
| 47 | 1 | 0 | 9.903853 | 2.106749 | -0.000024 |
| 48 | 1 | 0 | 7.358238 | -2.836346 | 0.000005 |
| 49 | 1 | 0 | 7.431351 | 2.142121 | -0.000016 |
| 50 | 1 | 0 | 4.889285 | -2.799594 | 0.000013 |
| 51 | 1 | 0 | 4.965782 | 2.183020 | -0.000008 |
| 52 | 1 | 0 | 2.410767 | -2.741410 | 0.000018 |
| 53 | 1 | 0 | 2.517177 | 2.228241 | -0.000001 |
| 54 | 1 | 0 | 0.000000 | -2.704478 | 0.000022 |
| 55 | 1 | 0 | -2.410767 | -2.741410 | 0.000020 |
| 56 | 1 | 0 | -2.517177 | 2.228241 | -0.000003 |
| 57 | 1 | 0 | -4.889285 | -2.799594 | 0.000015 |
| 58 | 1 | 0 | -4.965782 | 2.183020 | -0.000011 |
| 59 | 1 | 0 | -7.358238 | -2.836346 | 0.000008 |
| 60 | 1 | 0 | -7.431351 | 2.142121 | -0.000019 |
| 61 | 1 | 0 | -9.831107 | -2.874225 | 0.000000 |
| 62 | 1 | 0 | -11.971777 | -1.659117 | -0.000014 |
| 63 | 1 | 0 | -12.008526 | 0.829409 | -0.000027 |
| 64 | 1 | 0 | -9.903853 | 2.106749 | -0.000027 |

R=DCM

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 11.037813 | -0.136797 | -0.000126 |
| 2 | 6 | 0 | 11.031069 | -1.562484 | -0.000079 |
| 3 | 6 | 0 | 9.851799 | -2.252267 | -0.000031 |
| 4 | 6 | 0 | 8.598597 | -1.564794 | -0.000027 |
| 5 | 6 | 0 | 8.605980 | -0.117725 | -0.000073 |
| 6 | 6 | 0 | 9.863423 | 0.561158 | -0.000123 |
| 7 | 6 | 0 | 7.378640 | -2.241881 | 0.000018 |
| 8 | 6 | 0 | 6.150903 | -1.558863 | 0.000020 |
| 9 | 6 | 0 | 6.160704 | -0.107149 | -0.000024 |
| 10 | 6 | 0 | 7.390936 | 0.568018 | -0.000070 |
| 11 | 6 | 0 | 4.912680 | -2.233939 | 0.000060 |
| 12 | 6 | 0 | 3.698438 | -1.546664 | 0.000057 |
| 13 | 6 | 0 | 3.713988 | -0.092928 | 0.000016 |
| 14 | 6 | 0 | 4.928620 | 0.581457 | -0.000023 |
| 15 | 6 | 0 | 2.446790 | -2.202256 | 0.000088 |
| 16 | 6 | 0 | 1.234778 | -1.506739 | 0.000077 |
| 17 | 6 | 0 | 1.260817 | -0.048366 | 0.000041 |
| 18 | 6 | 0 | 2.474876 | 0.602438 | 0.000014 |
| 19 | 6 | 0 | -0.000005 | -2.180088 | 0.000099 |
| 20 | 6 | 0 | -1.234786 | -1.506738 | 0.000077 |
| 21 | 6 | 0 | -1.260824 | -0.048364 | 0.000041 |
| 22 | 6 | 0 | -0.000004 | 0.686552 | 0.000039 |
| 23 | 6 | 0 | -2.446800 | -2.202253 | 0.000085 |
| 24 | 6 | 0 | -3.698446 | -1.546659 | 0.000053 |
| 25 | 6 | 0 | -3.713996 | -0.092923 | 0.000012 |
| 26 | 6 | 0 | -2.474883 | 0.602442 | 0.000011 |
| 27 | 6 | 0 | -4.912690 | -2.233933 | 0.000056 |
| 28 | 6 | 0 | -6.150911 | -1.558856 | 0.000016 |
| 29 | 6 | 0 | -6.160712 | -0.107143 | -0.000028 |
| 30 | 6 | 0 | -4.928627 | 0.581463 | -0.000027 |
| 31 | 6 | 0 | -7.378649 | -2.241873 | 0.000016 |
| 32 | 6 | 0 | -8.598605 | -1.564786 | -0.000027 |
| 33 | 6 | 0 | -8.605987 | -0.117717 | -0.000074 |
| 34 | 6 | 0 | -7.390943 | 0.568025 | -0.000072 |
| 35 | 6 | 0 | -9.851808 | -2.252259 | -0.000029 |
| 36 | 6 | 0 | -11.031077 | -1.562475 | -0.000074 |
| 37 | 6 | 0 | -11.037821 | -0.136788 | -0.000121 |
| 38 | 6 | 0 | -9.863430 | 0.561167 | -0.000120 |
| 39 | 6 | 0 | -0.000001 | 2.047605 | 0.000036 |
| 40 | 6 | 0 | 0.000007 | 3.284433 | 0.000039 |
| 41 | 6 | 0 | 0.000020 | 4.643219 | 0.000045 |
| 42 | 6 | 0 | -1.227257 | 5.362677 | 0.000047 |
| 43 | 6 | 0 | 1.227314 | 5.362651 | 0.000047 |
| 44 | 7 | 0 | 2.237455 | 5.927882 | 0.000049 |
| 45 | 7 | 0 | -2.237383 | 5.927935 | 0.000050 |
| 46 | 1 | 0 | 11.984936 | 0.390248 | -0.000164 |
| 47 | 1 | 0 | 11.973883 | -2.097517 | -0.000082 |
| 48 | 1 | 0 | 9.848007 | -3.337047 | 0.000005 |
| 49 | 1 | 0 | 9.866493 | 1.645890 | -0.000158 |
| 50 | 1 | 0 | 7.376296 | -3.327356 | 0.000054 |
| 51 | 1 | 0 | 7.394548 | 1.653429 | -0.000102 |
| 52 | 1 | 0 | 4.907488 | -3.319252 | 0.000094 |
| 53 | 1 | 0 | 4.932940 | 1.666768 | -0.000051 |
| 54 | 1 | 0 | 2.425676 | -3.287233 | 0.000120 |
| 55 | 1 | 0 | 2.498767 | 1.686362 | -0.000012 |
| 56 | 1 | 0 | -0.000005 | -3.264970 | 0.000129 |
| 57 | 1 | 0 | -2.425687 | -3.287230 | 0.000114 |
| 58 | 1 | 0 | -2.498770 | 1.686366 | -0.000017 |
| 59 | 1 | 0 | -4.907498 | -3.319246 | 0.000087 |
| 60 | 1 | 0 | -4.932946 | 1.666774 | -0.000058 |
| 61 | 1 | 0 | -7.376305 | -3.327349 | 0.000050 |
| 62 | 1 | 0 | -7.394555 | 1.653436 | -0.000106 |
| 63 | 1 | 0 | -9.848016 | -3.337038 | 0.000006 |
| 64 | 1 | 0 | -11.973892 | -2.097507 | -0.000075 |
| 65 | 1 | 0 | -11.984943 | 0.390258 | -0.000157 |
| 66 | 1 | 0 | -9.866500 | 1.645899 | -0.000155 |

R=DPM

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 11.054384 | -1.206479 | -0.113936 |
| 2 | 6 | 0 | 11.034598 | -2.631322 | -0.073716 |
| 3 | 6 | 0 | 9.847713 | -3.307344 | -0.042107 |
| 4 | 6 | 0 | 8.601044 | -2.607568 | -0.048378 |
| 5 | 6 | 0 | 8.621471 | -1.161630 | -0.088793 |
| 6 | 6 | 0 | 9.886163 | -0.497425 | -0.121212 |
| 7 | 6 | 0 | 7.373884 | -3.270349 | -0.017499 |
| 8 | 6 | 0 | 6.152840 | -2.574499 | -0.024026 |
| 9 | 6 | 0 | 6.174603 | -1.123919 | -0.063238 |
| 10 | 6 | 0 | 7.412024 | -0.464166 | -0.094950 |
| 11 | 6 | 0 | 4.907747 | -3.235714 | 0.004448 |
| 12 | 6 | 0 | 3.700212 | -2.536084 | -0.002300 |
| 13 | 6 | 0 | 3.725053 | -1.083245 | -0.037022 |
| 14 | 6 | 0 | 4.945983 | -0.424475 | -0.068401 |
| 15 | 6 | 0 | 2.443190 | -3.181003 | 0.014772 |
| 16 | 6 | 0 | 1.237023 | -2.475502 | 0.007672 |
| 17 | 6 | 0 | 1.267968 | -1.017289 | -0.005938 |
| 18 | 6 | 0 | 2.485343 | -0.379621 | -0.039892 |
| 19 | 6 | 0 | -0.000001 | -3.145995 | -0.000043 |
| 20 | 6 | 0 | -1.237025 | -2.475502 | -0.007733 |
| 21 | 6 | 0 | -1.267969 | -1.017289 | 0.005922 |
| 22 | 6 | 0 | -0.000001 | -0.279910 | -0.000007 |
| 23 | 6 | 0 | -2.443192 | -3.181002 | -0.014846 |
| 24 | 6 | 0 | -3.700214 | -2.536083 | 0.002259 |
| 25 | 6 | 0 | -3.725054 | -1.083245 | 0.037032 |
| 26 | 6 | 0 | -2.485343 | -0.379621 | 0.039912 |
| 27 | 6 | 0 | -4.907749 | -3.235712 | -0.004501 |
| 28 | 6 | 0 | -6.152841 | -2.574498 | 0.024009 |
| 29 | 6 | 0 | -6.174603 | -1.123919 | 0.063274 |
| 30 | 6 | 0 | -4.945983 | -0.424475 | 0.068449 |
| 31 | 6 | 0 | -7.373886 | -3.270346 | 0.017470 |
| 32 | 6 | 0 | -8.601045 | -2.607566 | 0.048386 |
| 33 | 6 | 0 | -8.621471 | -1.161629 | 0.088854 |
| 34 | 6 | 0 | -7.412024 | -0.464166 | 0.095023 |
| 35 | 6 | 0 | -9.847715 | -3.307341 | 0.042102 |
| 36 | 6 | 0 | -11.034598 | -2.631321 | 0.073749 |
| 37 | 6 | 0 | -11.054384 | -1.206479 | 0.114021 |
| 38 | 6 | 0 | -9.886163 | -0.497425 | 0.121310 |
| 39 | 6 | 0 | -0.000001 | 1.075366 | -0.000008 |
| 40 | 6 | 0 | -0.000002 | 2.320039 | -0.000010 |
| 41 | 6 | 0 | -0.000002 | 3.670661 | -0.000010 |
| 42 | 6 | 0 | -1.278609 | 4.396009 | -0.162871 |
| 43 | 6 | 0 | 1.278609 | 4.396005 | 0.162851 |

| | | | | | |
|---|---|---|---|---|---|
| 44 | 6 | 0 | 1.513524 | 5.616184 | -0.495313 |
| 45 | 6 | 0 | 2.734110 | 6.270460 | -0.368338 |
| 46 | 6 | 0 | 3.745943 | 5.728779 | 0.422633 |
| 47 | 6 | 0 | 3.526593 | 4.521257 | 1.085051 |
| 48 | 6 | 0 | 2.309824 | 3.862146 | 0.956484 |
| 49 | 6 | 0 | -1.513501 | 5.616213 | 0.495256 |
| 50 | 6 | 0 | -2.734084 | 6.270495 | 0.368283 |
| 51 | 6 | 0 | -3.745937 | 5.728796 | -0.422649 |
| 52 | 6 | 0 | -3.526611 | 4.521249 | -1.085030 |
| 53 | 6 | 0 | -2.309845 | 3.862133 | -0.956466 |
| 54 | 1 | 0 | 12.006365 | -0.688384 | -0.138976 |
| 55 | 1 | 0 | 11.971946 | -3.176046 | -0.068583 |
| 56 | 1 | 0 | 9.832307 | -4.391821 | -0.011730 |
| 57 | 1 | 0 | 9.900590 | 0.587071 | -0.152151 |
| 58 | 1 | 0 | 7.359493 | -4.355569 | 0.012058 |
| 59 | 1 | 0 | 7.427968 | 0.621013 | -0.126030 |
| 60 | 1 | 0 | 4.890863 | -4.320851 | 0.030551 |
| 61 | 1 | 0 | 4.961979 | 0.660579 | -0.097962 |
| 62 | 1 | 0 | 2.413015 | -4.265982 | 0.027818 |
| 63 | 1 | 0 | 2.516050 | 0.703420 | -0.078225 |
| 64 | 1 | 0 | -0.000001 | -4.231319 | -0.000061 |
| 65 | 1 | 0 | -2.413018 | -4.265980 | -0.027927 |
| 66 | 1 | 0 | -2.516049 | 0.703418 | 0.078282 |
| 67 | 1 | 0 | -4.890866 | -4.320848 | -0.030643 |
| 68 | 1 | 0 | -4.961978 | 0.660577 | 0.098048 |
| 69 | 1 | 0 | -7.359496 | -4.355565 | -0.012127 |
| 70 | 1 | 0 | -7.427967 | 0.621011 | 0.126142 |
| 71 | 1 | 0 | -9.832309 | -4.391817 | 0.011686 |
| 72 | 1 | 0 | -11.971947 | -3.176044 | 0.068606 |
| 73 | 1 | 0 | -12.006364 | -0.688384 | 0.139089 |
| 74 | 1 | 0 | -9.900588 | 0.587069 | 0.152289 |
| 75 | 1 | 0 | 0.741399 | 6.039014 | -1.126158 |
| 76 | 1 | 0 | 2.897718 | 7.204295 | -0.894652 |
| 77 | 1 | 0 | 4.694383 | 6.243734 | 0.524633 |
| 78 | 1 | 0 | 4.302160 | 4.097357 | 1.713365 |
| 79 | 1 | 0 | 2.137054 | 2.933890 | 1.488280 |
| 80 | 1 | 0 | -0.741360 | 6.039058 | 1.126072 |
| 81 | 1 | 0 | -2.897674 | 7.204349 | 0.894568 |
| 82 | 1 | 0 | -4.694375 | 6.243755 | -0.524647 |
| 83 | 1 | 0 | -4.302193 | 4.097334 | -1.713315 |
| 84 | 1 | 0 | -2.137093 | 2.933857 | -1.488234 |

R=Flu

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -11.052841 | -1.297374 | -0.000011 |
| 2 | 6 | 0 | -11.033044 | -2.722778 | -0.000002 |
| 3 | 6 | 0 | -9.846334 | -3.399825 | 0.000001 |
| 4 | 6 | 0 | -8.599655 | -2.700207 | -0.000004 |
| 5 | 6 | 0 | -8.620125 | -1.253659 | -0.000014 |
| 6 | 6 | 0 | -9.884644 | -0.588375 | -0.000017 |
| 7 | 6 | 0 | -7.372606 | -3.364018 | 0.000001 |
| 8 | 6 | 0 | -6.151476 | -2.668513 | -0.000003 |
| 9 | 6 | 0 | -6.173403 | -1.217352 | -0.000014 |
| 10 | 6 | 0 | -7.410705 | -0.556405 | -0.000019 |
| 11 | 6 | 0 | -4.906532 | -3.330461 | 0.000006 |
| 12 | 6 | 0 | -3.698820 | -2.631139 | 0.000004 |
| 13 | 6 | 0 | -3.723566 | -1.177889 | -0.000008 |
| 14 | 6 | 0 | -4.945045 | -0.518426 | -0.000018 |
| 15 | 6 | 0 | -2.442111 | -3.275810 | 0.000014 |
| 16 | 6 | 0 | -1.235758 | -2.570509 | 0.000013 |
| 17 | 6 | 0 | -1.265783 | -1.111989 | 0.000002 |
| 18 | 6 | 0 | -2.484798 | -0.475160 | -0.000010 |
| 19 | 6 | 0 | 0.000001 | -3.241748 | 0.000022 |
| 20 | 6 | 0 | 1.235758 | -2.570510 | 0.000017 |
| 21 | 6 | 0 | 1.265784 | -1.111990 | 0.000007 |
| 22 | 6 | 0 | 0.000001 | -0.373385 | 0.000004 |
| 23 | 6 | 0 | 2.442114 | -3.275810 | 0.000022 |
| 24 | 6 | 0 | 3.698822 | -2.631139 | 0.000014 |
| 25 | 6 | 0 | 3.723568 | -1.177889 | 0.000004 |
| 26 | 6 | 0 | 2.484799 | -0.475161 | 0.000004 |
| 27 | 6 | 0 | 4.906536 | -3.330461 | 0.000016 |
| 28 | 6 | 0 | 6.151480 | -2.668512 | 0.000007 |
| 29 | 6 | 0 | 6.173406 | -1.217350 | -0.000004 |
| 30 | 6 | 0 | 4.945046 | -0.518426 | -0.000003 |
| 31 | 6 | 0 | 7.372610 | -3.364016 | 0.000007 |
| 32 | 6 | 0 | 8.599660 | -2.700204 | -0.000003 |
| 33 | 6 | 0 | 8.620128 | -1.253656 | -0.000014 |
| 34 | 6 | 0 | 7.410707 | -0.556403 | -0.000013 |
| 35 | 6 | 0 | 9.846339 | -3.399821 | -0.000004 |
| 36 | 6 | 0 | 11.033049 | -2.722772 | -0.000014 |
| 37 | 6 | 0 | 11.052844 | -1.297368 | -0.000023 |
| 38 | 6 | 0 | 9.884646 | -0.588371 | -0.000023 |
| 39 | 6 | 0 | 0.000001 | 0.985555 | 0.000000 |
| 40 | 6 | 0 | 0.000002 | 2.228380 | 0.000003 |
| 41 | 6 | 0 | -0.000001 | 3.577514 | 0.000006 |
| 42 | 6 | 0 | 1.173774 | 4.455886 | 0.000006 |
| 43 | 6 | 0 | -1.173779 | 4.455882 | 0.000006 |
| 44 | 6 | 0 | -0.733189 | 5.803803 | 0.000002 |
| 45 | 6 | 0 | -1.657888 | 6.842339 | 0.000002 |
| 46 | 6 | 0 | -3.020146 | 6.535719 | 0.000005 |
| 47 | 6 | 0 | -3.453995 | 5.206453 | 0.000011 |
| 48 | 6 | 0 | -2.534803 | 4.158594 | 0.000013 |
| 49 | 6 | 0 | 2.534799 | 4.158603 | 0.000004 |
| 50 | 6 | 0 | 3.453987 | 5.206465 | 0.000002 |
| 51 | 6 | 0 | 3.020134 | 6.535730 | 0.000001 |
| 52 | 6 | 0 | 1.657875 | 6.842345 | -0.000001 |
| 53 | 6 | 0 | 0.733180 | 5.803806 | 0.000002 |
| 54 | 1 | 0 | -12.004857 | -0.778848 | -0.000013 |
| 55 | 1 | 0 | -11.970519 | -3.267244 | 0.000002 |
| 56 | 1 | 0 | -9.831182 | -4.484675 | 0.000007 |
| 57 | 1 | 0 | -9.898951 | 0.496502 | -0.000024 |
| 58 | 1 | 0 | -7.358527 | -4.449581 | 0.000008 |
| 59 | 1 | 0 | -7.426612 | 0.529170 | -0.000028 |
| 60 | 1 | 0 | -4.889819 | -4.415842 | 0.000015 |
| 61 | 1 | 0 | -4.962317 | 0.566938 | -0.000028 |
| 62 | 1 | 0 | -2.411622 | -4.360767 | 0.000023 |
| 63 | 1 | 0 | -2.514262 | 0.608200 | -0.000021 |
| 64 | 1 | 0 | 0.000002 | -4.326949 | 0.000031 |
| 65 | 1 | 0 | 2.411626 | -4.360768 | 0.000031 |
| 66 | 1 | 0 | 2.514262 | 0.608199 | 0.000004 |
| 67 | 1 | 0 | 4.889824 | -4.415842 | 0.000024 |
| 68 | 1 | 0 | 4.962318 | 0.566939 | -0.000010 |
| 69 | 1 | 0 | 7.358532 | -4.449579 | 0.000014 |
| 70 | 1 | 0 | 7.426613 | 0.529172 | -0.000021 |
| 71 | 1 | 0 | 9.831188 | -4.484671 | 0.000002 |
| 72 | 1 | 0 | 11.970525 | -3.267238 | -0.000015 |
| 73 | 1 | 0 | 12.004860 | -0.778842 | -0.000030 |
| 74 | 1 | 0 | 9.898952 | 0.496506 | -0.000031 |
| 75 | 1 | 0 | -1.332615 | 7.876952 | -0.000001 |
| 76 | 1 | 0 | -3.750364 | 7.337075 | 0.000005 |
| 77 | 1 | 0 | -4.516315 | 4.990129 | 0.000014 |
| 78 | 1 | 0 | -2.873535 | 3.128849 | 0.000017 |
| 79 | 1 | 0 | 2.873535 | 3.128860 | 0.000001 |
| 80 | 1 | 0 | 4.516308 | 4.990144 | 0.000001 |
| 81 | 1 | 0 | 3.750350 | 7.337088 | 0.000001 |
| 82 | 1 | 0 | 1.332597 | 7.876957 | -0.000002 |

R=PhO

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -11.046295 | -0.617675 | -0.000047 |
| 2 | 6 | 0 | -11.032116 | -2.043065 | 0.000007 |
| 3 | 6 | 0 | -9.848391 | -2.725553 | 0.000037 |
| 4 | 6 | 0 | -8.599139 | -2.031082 | 0.000016 |
| 5 | 6 | 0 | -8.613927 | -0.584335 | -0.000038 |
| 6 | 6 | 0 | -9.875351 | 0.086711 | -0.000068 |
| 7 | 6 | 0 | -7.374887 | -2.700613 | 0.000045 |
| 8 | 6 | 0 | -6.150875 | -2.010583 | 0.000024 |
| 9 | 6 | 0 | -6.167274 | -0.558925 | -0.000028 |
| 10 | 6 | 0 | -7.401934 | 0.107997 | -0.000058 |
| 11 | 6 | 0 | -4.909096 | -2.678266 | 0.000051 |
| 12 | 6 | 0 | -3.697678 | -1.984626 | 0.000031 |
| 13 | 6 | 0 | -3.717315 | -0.530676 | -0.000017 |
| 14 | 6 | 0 | -4.937593 | 0.135033 | -0.000046 |
| 15 | 6 | 0 | -2.444599 | -2.635235 | 0.000049 |
| 16 | 6 | 0 | -1.234636 | -1.934971 | 0.000029 |
| 17 | 6 | 0 | -1.260224 | -0.476500 | 0.000000 |
| 18 | 6 | 0 | -2.479930 | 0.168124 | -0.000028 |
| 19 | 6 | 0 | 0.000000 | -2.607593 | 0.000028 |
| 20 | 6 | 0 | 1.234636 | -1.934971 | 0.000010 |
| 21 | 6 | 0 | 1.260224 | -0.476500 | 0.000006 |
| 22 | 6 | 0 | 0.000000 | 0.255729 | 0.000000 |
| 23 | 6 | 0 | 2.444598 | -2.635236 | 0.000001 |
| 24 | 6 | 0 | 3.697677 | -1.984626 | -0.000003 |
| 25 | 6 | 0 | 3.717314 | -0.530676 | 0.000007 |
| 26 | 6 | 0 | 2.479930 | 0.168124 | 0.000011 |
| 27 | 6 | 0 | 4.909095 | -2.678266 | -0.000014 |
| 28 | 6 | 0 | 6.150875 | -2.010583 | -0.000011 |
| 29 | 6 | 0 | 6.167274 | -0.558925 | 0.000004 |
| 30 | 6 | 0 | 4.937592 | 0.135032 | 0.000012 |
| 31 | 6 | 0 | 7.374886 | -2.700613 | -0.000022 |
| 32 | 6 | 0 | 8.599139 | -2.031083 | -0.000018 |
| 33 | 6 | 0 | 8.613927 | -0.584336 | -0.000002 |
| 34 | 6 | 0 | 7.401933 | 0.107997 | 0.000009 |
| 35 | 6 | 0 | 9.848391 | -2.725553 | -0.000030 |
| 36 | 6 | 0 | 11.032115 | -2.043066 | -0.000025 |
| 37 | 6 | 0 | 11.046295 | -0.617676 | -0.000008 |
| 38 | 6 | 0 | 9.875351 | 0.086711 | 0.000003 |
| 39 | 6 | 0 | 0.000000 | 1.624551 | -0.000003 |
| 40 | 6 | 0 | 0.000000 | 2.859707 | 0.000000 |
| 41 | 6 | 0 | 0.000000 | 4.229578 | 0.000005 |
| 42 | 6 | 0 | -1.236250 | 4.970869 | 0.000012 |
| 43 | 6 | 0 | -1.242778 | 6.326338 | 0.000017 |
| 44 | 6 | 0 | 0.000001 | 7.106997 | 0.000016 |
| 45 | 6 | 0 | 1.242780 | 6.326337 | 0.000009 |
| 46 | 6 | 0 | 1.236251 | 4.970868 | 0.000004 |
| 47 | 8 | 0 | 0.000002 | 8.339931 | 0.000022 |
| 48 | 1 | 0 | -11.996197 | -0.095469 | -0.000070 |
| 49 | 1 | 0 | -11.971842 | -2.583536 | 0.000024 |
| 50 | 1 | 0 | -9.838064 | -3.810375 | 0.000078 |
| 51 | 1 | 0 | -9.885053 | 1.171540 | -0.000109 |
| 52 | 1 | 0 | -7.365859 | -3.786143 | 0.000086 |
| 53 | 1 | 0 | -7.412909 | 1.193538 | -0.000098 |
| 54 | 1 | 0 | -4.897550 | -3.763624 | 0.000089 |
| 55 | 1 | 0 | -4.949351 | 1.220419 | -0.000084 |
| 56 | 1 | 0 | -2.419190 | -3.720224 | 0.000076 |
| 57 | 1 | 0 | -2.504954 | 1.251705 | -0.000059 |

| | | | | | |
|---|---|---|---|---|---|
| 58 | 1 | 0 | 0.000000 | -3.692689 | 0.000041 |
| 59 | 1 | 0 | 2.419189 | -3.720224 | 0.000000 |
| 60 | 1 | 0 | 2.504953 | 1.251705 | 0.000015 |
| 61 | 1 | 0 | 4.897550 | -3.763624 | -0.000023 |
| 62 | 1 | 0 | 4.949351 | 1.220418 | 0.000021 |
| 63 | 1 | 0 | 7.365858 | -3.786143 | -0.000035 |
| 64 | 1 | 0 | 7.412909 | 1.193537 | 0.000020 |
| 65 | 1 | 0 | 9.838064 | -3.810376 | -0.000042 |
| 66 | 1 | 0 | 11.971841 | -2.583537 | -0.000033 |
| 67 | 1 | 0 | 11.996197 | -0.095470 | -0.000004 |
| 68 | 1 | 0 | 9.885053 | 1.171539 | 0.000016 |
| 69 | 1 | 0 | -2.165680 | 4.412244 | 0.000014 |
| 70 | 1 | 0 | -2.167460 | 6.891856 | 0.000023 |
| 71 | 1 | 0 | 2.167462 | 6.891854 | 0.000008 |
| 72 | 1 | 0 | 2.165681 | 4.412243 | -0.000002 |

R=NO

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -11.034804 | -0.014311 | 0.000008 |
| 2 | 6 | 0 | -11.016338 | -1.439337 | 0.000009 |
| 3 | 6 | 0 | -9.829723 | -2.117425 | 0.000007 |
| 4 | 6 | 0 | -8.582865 | -1.419013 | 0.000004 |
| 5 | 6 | 0 | -8.601905 | 0.027359 | 0.000003 |
| 6 | 6 | 0 | -9.865556 | 0.693690 | 0.000005 |
| 7 | 6 | 0 | -7.355716 | -2.083988 | 0.000002 |
| 8 | 6 | 0 | -6.134209 | -1.389596 | -0.000001 |
| 9 | 6 | 0 | -6.154432 | 0.062045 | -0.000002 |
| 10 | 6 | 0 | -7.391589 | 0.723994 | 0.000000 |
| 11 | 6 | 0 | -4.889952 | -2.052848 | -0.000002 |
| 12 | 6 | 0 | -3.680531 | -1.354873 | -0.000004 |
| 13 | 6 | 0 | -3.703235 | 0.099357 | -0.000005 |
| 14 | 6 | 0 | -4.926702 | 0.760615 | -0.000004 |
| 15 | 6 | 0 | -2.426535 | -2.003382 | -0.000004 |
| 16 | 6 | 0 | -1.217500 | -1.300453 | -0.000005 |
| 17 | 6 | 0 | -1.245730 | 0.157464 | -0.000006 |
| 18 | 6 | 0 | -2.468575 | 0.802545 | -0.000006 |
| 19 | 6 | 0 | 0.018915 | -1.970522 | -0.000004 |
| 20 | 6 | 0 | 1.252589 | -1.295252 | -0.000005 |
| 21 | 6 | 0 | 1.274421 | 0.163174 | -0.000006 |
| 22 | 6 | 0 | 0.013913 | 0.882977 | -0.000007 |
| 23 | 6 | 0 | 2.464912 | -1.992339 | -0.000004 |
| 24 | 6 | 0 | 3.716514 | -1.339305 | -0.000004 |
| 25 | 6 | 0 | 3.734414 | 0.115208 | -0.000005 |
| 26 | 6 | 0 | 2.495392 | 0.810774 | -0.000007 |
| 27 | 6 | 0 | 4.928644 | -2.032648 | -0.000002 |
| 28 | 6 | 0 | 6.170879 | -1.365824 | -0.000001 |
| 29 | 6 | 0 | 6.186865 | 0.085849 | -0.000002 |
| 30 | 6 | 0 | 4.956284 | 0.779385 | -0.000004 |
| 31 | 6 | 0 | 7.394549 | -2.056485 | 0.000002 |
| 32 | 6 | 0 | 8.619814 | -1.388159 | 0.000004 |
| 33 | 6 | 0 | 8.634762 | 0.058262 | 0.000003 |
| 34 | 6 | 0 | 7.422269 | 0.751085 | 0.000000 |
| 35 | 6 | 0 | 9.868618 | -2.083127 | 0.000007 |
| 36 | 6 | 0 | 11.053393 | -1.401889 | 0.000009 |
| 37 | 6 | 0 | 11.067842 | 0.023184 | 0.000008 |
| 38 | 6 | 0 | 9.896643 | 0.727943 | 0.000005 |
| 39 | 6 | 0 | -0.007347 | 2.258096 | -0.000005 |
| 40 | 6 | 0 | -0.086751 | 3.483630 | -0.000002 |
| 41 | 7 | 0 | -0.241095 | 4.788992 | 0.000003 |
| 42 | 8 | 0 | -1.395585 | 5.344792 | 0.000005 |
| 43 | 6 | 0 | 0.930525 | 5.684305 | 0.000003 |
| 44 | 1 | 0 | -11.986243 | 0.505320 | 0.000010 |
| 45 | 1 | 0 | -11.954203 | -1.983188 | 0.000011 |
| 46 | 1 | 0 | -9.815536 | -3.202334 | 0.000007 |
| 47 | 1 | 0 | -9.878707 | 1.778569 | 0.000005 |
| 48 | 1 | 0 | -7.342659 | -3.169618 | 0.000003 |
| 49 | 1 | 0 | -7.406121 | 1.809514 | -0.000001 |
| 50 | 1 | 0 | -4.874452 | -3.138309 | -0.000001 |
| 51 | 1 | 0 | -4.941045 | 1.845901 | -0.000005 |
| 52 | 1 | 0 | -2.398975 | -3.088480 | -0.000003 |
| 53 | 1 | 0 | -2.500245 | 1.886393 | -0.000007 |
| 54 | 1 | 0 | 0.021474 | -3.055746 | -0.000003 |
| 55 | 1 | 0 | 2.442183 | -3.077503 | -0.000003 |
| 56 | 1 | 0 | 2.519747 | 1.894770 | -0.000008 |
| 57 | 1 | 0 | 4.916627 | -3.118110 | -0.000001 |
| 58 | 1 | 0 | 4.969141 | 1.864981 | -0.000005 |
| 59 | 1 | 0 | 7.384531 | -3.142115 | 0.000003 |
| 60 | 1 | 0 | 7.434487 | 1.836782 | -0.000001 |
| 61 | 1 | 0 | 9.857354 | -3.168046 | 0.000008 |
| 62 | 1 | 0 | 11.992733 | -1.943124 | 0.000012 |
| 63 | 1 | 0 | 12.017852 | 0.545423 | 0.000010 |
| 64 | 1 | 0 | 9.907163 | 1.812909 | 0.000004 |
| 65 | 1 | 0 | 1.849110 | 5.099527 | 0.000012 |
| 66 | 1 | 0 | 0.872585 | 6.312098 | -0.889873 |
| 67 | 1 | 0 | 0.872574 | 6.312109 | 0.889870 |

R=Allyl

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 0.000000 | 3.510900 | -0.000002 |
| 2 | 6 | 0 | 0.000000 | 2.296064 | -0.000002 |
| 3 | 6 | 0 | -0.000001 | 4.938735 | -0.000003 |
| 4 | 6 | 0 | 1.220695 | 5.618420 | -0.000167 |
| 5 | 6 | 0 | 11.047480 | 0.043532 | 0.000016 |
| 6 | 6 | 0 | 11.033539 | -1.381166 | 0.000008 |
| 7 | 6 | 0 | 9.848460 | -2.062819 | 0.000001 |
| 8 | 6 | 0 | 8.599910 | -1.368480 | 0.000002 |
| 9 | 6 | 0 | 8.614205 | 0.077854 | 0.000011 |
| 10 | 6 | 0 | 9.875653 | 0.747899 | 0.000018 |
| 11 | 6 | 0 | 7.374180 | -2.037402 | -0.000004 |
| 12 | 6 | 0 | 6.150468 | -1.347621 | -0.000003 |
| 13 | 6 | 0 | 6.165288 | 0.104765 | 0.000005 |
| 14 | 6 | 0 | 7.401281 | 0.770398 | 0.000012 |
| 15 | 6 | 0 | 4.908678 | -2.015127 | -0.000009 |
| 16 | 6 | 0 | 3.695065 | -1.323074 | -0.000007 |
| 17 | 6 | 0 | 3.710206 | 0.132978 | 0.000000 |
| 18 | 6 | 0 | 4.936101 | 0.797761 | 0.000006 |
| 19 | 6 | 0 | 2.446320 | -1.978580 | -0.000010 |
| 20 | 6 | 0 | 1.231766 | -1.282770 | -0.000008 |
| 21 | 6 | 0 | 1.247588 | 0.176821 | -0.000004 |
| 22 | 6 | 0 | 2.477412 | 0.828757 | 0.000001 |
| 23 | 6 | 0 | 0.000000 | -1.957733 | -0.000006 |
| 24 | 6 | 0 | -1.231766 | -1.282770 | -0.000002 |
| 25 | 6 | 0 | -1.247588 | 0.176821 | -0.000002 |
| 26 | 6 | 0 | 0.000000 | 0.888069 | -0.000003 |
| 27 | 6 | 0 | -2.446320 | -1.978580 | -0.000001 |
| 28 | 6 | 0 | -3.695065 | -1.323074 | 0.000000 |
| 29 | 6 | 0 | -3.710206 | 0.132978 | -0.000002 |
| 30 | 6 | 0 | -2.477412 | 0.828757 | -0.000003 |
| 31 | 6 | 0 | -4.908677 | -2.015127 | 0.000002 |
| 32 | 6 | 0 | -6.150468 | -1.347621 | 0.000001 |
| 33 | 6 | 0 | -6.165288 | 0.104765 | -0.000001 |
| 34 | 6 | 0 | -4.936101 | 0.797760 | -0.000003 |
| 35 | 6 | 0 | -7.374179 | -2.037403 | 0.000003 |
| 36 | 6 | 0 | -8.599909 | -1.368481 | 0.000001 |
| 37 | 6 | 0 | -8.614205 | 0.077854 | -0.000001 |
| 38 | 6 | 0 | -7.401281 | 0.770398 | -0.000003 |
| 39 | 6 | 0 | -9.848460 | -2.062819 | 0.000003 |
| 40 | 6 | 0 | -11.033538 | -1.381167 | 0.000001 |
| 41 | 6 | 0 | -11.047479 | 0.043532 | -0.000001 |
| 42 | 6 | 0 | -9.875653 | 0.747899 | -0.000003 |
| 43 | 6 | 0 | -1.220699 | 5.618419 | 0.000158 |
| 44 | 1 | 0 | 2.161815 | 5.086690 | -0.000298 |
| 45 | 1 | 0 | 1.242783 | 6.701039 | -0.000169 |
| 46 | 1 | 0 | 11.997211 | 0.566310 | 0.000022 |
| 47 | 1 | 0 | 11.972952 | -1.922306 | 0.000007 |
| 48 | 1 | 0 | 9.837611 | -3.147774 | -0.000005 |
| 49 | 1 | 0 | 9.885710 | 1.832871 | 0.000024 |
| 50 | 1 | 0 | 7.364777 | -3.123074 | -0.000010 |
| 51 | 1 | 0 | 7.412930 | 1.856063 | 0.000018 |
| 52 | 1 | 0 | 4.897559 | -3.100645 | -0.000014 |
| 53 | 1 | 0 | 4.947833 | 1.883218 | 0.000013 |
| 54 | 1 | 0 | 2.425439 | -3.063843 | -0.000013 |
| 55 | 1 | 0 | 2.496630 | 1.912031 | 0.000009 |
| 56 | 1 | 0 | 0.000000 | -3.043086 | -0.000008 |
| 57 | 1 | 0 | -2.425438 | -3.063843 | 0.000000 |
| 58 | 1 | 0 | -2.496629 | 1.912031 | -0.000007 |
| 59 | 1 | 0 | -4.897558 | -3.100646 | 0.000004 |
| 60 | 1 | 0 | -4.947833 | 1.883218 | -0.000005 |
| 61 | 1 | 0 | -7.364777 | -3.123075 | 0.000005 |
| 62 | 1 | 0 | -7.412930 | 1.856063 | -0.000005 |
| 63 | 1 | 0 | -9.837610 | -3.147774 | 0.000005 |
| 64 | 1 | 0 | -11.972951 | -1.922306 | 0.000002 |
| 65 | 1 | 0 | -11.997211 | 0.566309 | -0.000003 |
| 66 | 1 | 0 | -9.885710 | 1.832871 | -0.000005 |
| 67 | 1 | 0 | -1.242788 | 6.701037 | 0.000157 |
| 68 | 1 | 0 | -2.161818 | 5.086687 | 0.000291 |

R=IN

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -11.276279 | -0.623363 | 0.000495 |
| 2 | 6 | 0 | -11.324186 | -2.047369 | 0.008030 |
| 3 | 6 | 0 | -10.169990 | -2.780053 | 0.011838 |
| 4 | 6 | 0 | -8.892367 | -2.140734 | 0.008367 |
| 5 | 6 | 0 | -8.843903 | -0.695058 | 0.000697 |
| 6 | 6 | 0 | -10.075003 | 0.029355 | -0.003042 |
| 7 | 6 | 0 | -7.697023 | -2.862482 | 0.012106 |
| 8 | 6 | 0 | -6.444380 | -2.226613 | 0.008596 |
| 9 | 6 | 0 | -6.396365 | -0.774873 | 0.000847 |
| 10 | 6 | 0 | -7.602274 | -0.055815 | -0.002820 |
| 11 | 6 | 0 | -5.232927 | -2.947547 | 0.012283 |
| 12 | 6 | 0 | -3.990142 | -2.309038 | 0.008625 |
| 13 | 6 | 0 | -3.943113 | -0.853289 | 0.000819 |
| 14 | 6 | 0 | -5.139013 | -0.135300 | -0.002779 |
| 15 | 6 | 0 | -2.771403 | -3.019215 | 0.012054 |
| 16 | 6 | 0 | -1.527889 | -2.376524 | 0.008045 |
| 17 | 6 | 0 | -1.484192 | -0.917997 | 0.000312 |
| 18 | 6 | 0 | -2.682797 | -0.209911 | -0.002899 |
| 19 | 6 | 0 | -0.323141 | -3.100117 | 0.010932 |
| 20 | 6 | 0 | 0.936731 | -2.477741 | 0.006159 |
| 21 | 6 | 0 | 1.012248 | -1.020714 | -0.001140 |
| 22 | 6 | 0 | -0.207934 | -0.265457 | -0.003152 |
| 23 | 6 | 0 | 2.123502 | -3.220381 | 0.007821 |
| 24 | 6 | 0 | 3.395864 | -2.611293 | 0.001931 |

| | | | | | |
|---|---|---|---|---|---|
| 25 | 6 | 0 | 3.466263 | -1.156739 | -0.006084 |
| 26 | 6 | 0 | 2.264127 | -0.410300 | -0.007259 |
| 27 | 6 | 0 | 4.583214 | -3.347751 | 0.003037 |
| 28 | 6 | 0 | 5.848435 | -2.725642 | -0.003658 |
| 29 | 6 | 0 | 5.916841 | -1.274604 | -0.011917 |
| 30 | 6 | 0 | 4.715246 | -0.535473 | -0.012781 |
| 31 | 6 | 0 | 7.046131 | -3.459736 | -0.002835 |
| 32 | 6 | 0 | 8.295445 | -2.835925 | -0.009799 |
| 33 | 6 | 0 | 8.362899 | -1.391037 | -0.018103 |
| 34 | 6 | 0 | 7.176409 | -0.654370 | -0.018902 |
| 35 | 6 | 0 | 9.517778 | -3.575451 | -0.009118 |
| 36 | 6 | 0 | 10.726971 | -2.937549 | -0.016149 |
| 37 | 6 | 0 | 10.793265 | -1.514310 | -0.024346 |
| 38 | 6 | 0 | 9.648022 | -0.767547 | -0.025280 |
| 39 | 6 | 0 | -0.133842 | 1.136888 | -0.009010 |
| 40 | 6 | 0 | -0.023931 | 2.344795 | -0.012908 |
| 41 | 6 | 0 | 0.196837 | 3.735799 | -0.025219 |
| 42 | 7 | 0 | 1.522272 | 4.218037 | -0.031568 |
| 43 | 6 | 0 | 1.492584 | 5.699792 | 0.198826 |
| 44 | 6 | 0 | -0.016590 | 5.979227 | -0.169827 |
| 45 | 7 | 0 | -0.701843 | 4.666412 | -0.029784 |
| 46 | 6 | 0 | -0.712516 | 7.002403 | 0.733374 |
| 47 | 6 | 0 | -0.209022 | 6.395661 | -1.642093 |
| 48 | 6 | 0 | 2.552982 | 6.374495 | -0.669844 |
| 49 | 6 | 0 | 1.825686 | 5.913642 | 1.686323 |
| 50 | 8 | 0 | 2.575562 | 3.522580 | -0.007980 |
| 51 | 1 | 0 | -12.202416 | -0.059874 | -0.002422 |
| 52 | 1 | 0 | -12.286255 | -2.547125 | 0.010732 |
| 53 | 1 | 0 | -10.206461 | -3.864425 | 0.017577 |
| 54 | 1 | 0 | -10.037663 | 1.113684 | -0.008780 |
| 55 | 1 | 0 | -7.734999 | -3.947504 | 0.017872 |
| 56 | 1 | 0 | -7.566191 | 1.029227 | -0.008579 |
| 57 | 1 | 0 | -5.269142 | -4.032488 | 0.018063 |
| 58 | 1 | 0 | -5.102419 | 0.949468 | -0.008549 |
| 59 | 1 | 0 | -2.798369 | -4.104297 | 0.017803 |
| 60 | 1 | 0 | -2.655235 | 0.873784 | -0.008635 |
| 61 | 1 | 0 | -0.367924 | -4.184618 | 0.016556 |
| 62 | 1 | 0 | 2.061623 | -4.304068 | 0.013407 |
| 63 | 1 | 0 | 2.329734 | 0.672186 | -0.013783 |
| 64 | 1 | 0 | 4.532724 | -4.432156 | 0.009027 |
| 65 | 1 | 0 | 4.762228 | 0.548775 | -0.019059 |
| 66 | 1 | 0 | 6.997275 | -4.544345 | 0.003316 |
| 67 | 1 | 0 | 7.226561 | 0.430048 | -0.025226 |
| 68 | 1 | 0 | 9.467352 | -4.659276 | -0.002908 |
| 69 | 1 | 0 | 11.645924 | -3.512790 | -0.015556 |
| 70 | 1 | 0 | 11.761545 | -1.026779 | -0.029888 |
| 71 | 1 | 0 | 9.697435 | 0.316295 | -0.031570 |
| 72 | 1 | 0 | -1.752071 | 7.106091 | 0.416801 |
| 73 | 1 | 0 | -0.713816 | 6.691203 | 1.777806 |
| 74 | 1 | 0 | -0.231869 | 7.982341 | 0.660458 |
| 75 | 1 | 0 | 0.205501 | 7.388991 | -1.831385 |
| 76 | 1 | 0 | 0.258729 | 5.684370 | -2.325735 |
| 77 | 1 | 0 | -1.277359 | 6.417458 | -1.863678 |
| 78 | 1 | 0 | 3.538635 | 5.998397 | -0.390179 |
| 79 | 1 | 0 | 2.406856 | 6.174632 | -1.730805 |
| 80 | 1 | 0 | 2.538661 | 7.455571 | -0.511704 |
| 81 | 1 | 0 | 1.848124 | 6.977179 | 1.931680 |
| 82 | 1 | 0 | 1.101497 | 5.421024 | 2.337659 |
| 83 | 1 | 0 | 2.810755 | 5.488799 | 1.889674 |

R=Phen

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -11.047628 | -1.546009 | 0.000148 |
| 2 | 6 | 0 | -11.033385 | -2.970717 | 0.000121 |
| 3 | 6 | 0 | -9.848149 | -3.652086 | 0.000090 |
| 4 | 6 | 0 | -8.599743 | -2.957482 | 0.000084 |
| 5 | 6 | 0 | -8.614331 | -1.511125 | 0.000111 |
| 6 | 6 | 0 | -9.875965 | -0.841391 | 0.000143 |
| 7 | 6 | 0 | -7.373886 | -3.626122 | 0.000054 |
| 8 | 6 | 0 | -6.150289 | -2.936104 | 0.000048 |
| 9 | 6 | 0 | -6.165354 | -1.483681 | 0.000074 |
| 10 | 6 | 0 | -7.401579 | -0.818360 | 0.000105 |
| 11 | 6 | 0 | -4.908427 | -3.603358 | 0.000021 |
| 12 | 6 | 0 | -3.694894 | -2.911094 | 0.000017 |
| 13 | 6 | 0 | -3.710200 | -1.455016 | 0.000039 |
| 14 | 6 | 0 | -4.936359 | -0.790527 | 0.000068 |
| 15 | 6 | 0 | -2.446138 | -3.566382 | 0.000000 |
| 16 | 6 | 0 | -1.231633 | -2.870397 | -0.000001 |
| 17 | 6 | 0 | -1.247583 | -1.410842 | 0.000006 |
| 18 | 6 | 0 | -2.477592 | -0.759147 | 0.000033 |
| 19 | 6 | 0 | 0.000000 | -3.545419 | -0.000001 |
| 20 | 6 | 0 | 1.231634 | -2.870397 | -0.000001 |
| 21 | 6 | 0 | 1.247583 | -1.410842 | -0.000007 |
| 22 | 6 | 0 | 0.000000 | -0.699334 | 0.000000 |
| 23 | 6 | 0 | 2.446138 | -3.566382 | -0.000002 |
| 24 | 6 | 0 | 3.694895 | -2.911094 | -0.000019 |
| 25 | 6 | 0 | 3.710201 | -1.455016 | -0.000039 |
| 26 | 6 | 0 | 2.477593 | -0.759147 | -0.000032 |
| 27 | 6 | 0 | 4.908427 | -3.603357 | -0.000023 |
| 28 | 6 | 0 | 6.150289 | -2.936104 | -0.000049 |
| 29 | 6 | 0 | 6.165355 | -1.483680 | -0.000073 |
| 30 | 6 | 0 | 4.936360 | -0.790526 | -0.000067 |
| 31 | 6 | 0 | 7.373887 | -3.626121 | -0.000055 |
| 32 | 6 | 0 | 8.599744 | -2.957481 | -0.000084 |
| 33 | 6 | 0 | 8.614332 | -1.511124 | -0.000109 |
| 34 | 6 | 0 | 7.401579 | -0.818359 | -0.000102 |
| 35 | 6 | 0 | 9.848150 | -3.652085 | -0.000091 |
| 36 | 6 | 0 | 11.033386 | -2.970716 | -0.000121 |
| 37 | 6 | 0 | 11.047629 | -1.546008 | -0.000145 |
| 38 | 6 | 0 | 9.875965 | -0.841390 | -0.000140 |
| 39 | 6 | 0 | 0.000000 | 0.707813 | 0.000000 |
| 40 | 6 | 0 | 0.000000 | 1.923588 | 0.000000 |
| 41 | 6 | 0 | 0.000000 | 3.342302 | 0.000000 |
| 42 | 6 | 0 | 1.212580 | 4.052707 | 0.000611 |
| 43 | 6 | 0 | 1.236467 | 5.463974 | 0.000625 |
| 44 | 6 | 0 | -0.000001 | 6.181022 | 0.000000 |
| 45 | 6 | 0 | -1.236469 | 5.463973 | -0.000626 |
| 46 | 6 | 0 | -1.212581 | 4.052706 | -0.000611 |
| 47 | 6 | 0 | 2.449905 | 6.197109 | 0.001244 |
| 48 | 6 | 0 | 2.440464 | 7.586740 | 0.001241 |
| 49 | 6 | 0 | 1.241964 | 8.290746 | 0.000632 |
| 50 | 6 | 0 | -0.000001 | 7.608231 | 0.000000 |
| 51 | 6 | 0 | -1.241967 | 8.290745 | -0.000632 |
| 52 | 6 | 0 | -2.440466 | 7.586738 | -0.001242 |
| 53 | 6 | 0 | -2.449907 | 6.197108 | -0.001245 |
| 54 | 1 | 0 | -11.997480 | -1.023444 | 0.000173 |
| 55 | 1 | 0 | -11.972677 | -3.512063 | 0.000126 |
| 56 | 1 | 0 | -9.837049 | -4.737038 | 0.000070 |
| 57 | 1 | 0 | -9.886292 | 0.243584 | 0.000164 |
| 58 | 1 | 0 | -7.364245 | -4.711791 | 0.000034 |
| 59 | 1 | 0 | -7.413507 | 0.267309 | 0.000126 |
| 60 | 1 | 0 | -4.897095 | -4.688872 | 0.000004 |
| 61 | 1 | 0 | -4.948298 | 0.294933 | 0.000089 |
| 62 | 1 | 0 | -2.425060 | -4.651637 | -0.000008 |
| 63 | 1 | 0 | -2.497074 | 0.324124 | 0.000058 |
| 64 | 1 | 0 | 0.000001 | -4.630763 | -0.000002 |
| 65 | 1 | 0 | 2.425061 | -4.651637 | 0.000004 |
| 66 | 1 | 0 | 2.497075 | 0.324125 | -0.000056 |
| 67 | 1 | 0 | 4.897096 | -4.688871 | -0.000008 |
| 68 | 1 | 0 | 4.948299 | 0.294933 | -0.000086 |
| 69 | 1 | 0 | 7.364246 | -4.711790 | -0.000037 |
| 70 | 1 | 0 | 7.413507 | 0.267310 | -0.000122 |
| 71 | 1 | 0 | 9.837050 | -4.737037 | -0.000072 |
| 72 | 1 | 0 | 11.972678 | -3.512062 | -0.000126 |
| 73 | 1 | 0 | 11.997480 | -1.023443 | -0.000169 |
| 74 | 1 | 0 | 9.886292 | 0.243586 | -0.000159 |
| 75 | 1 | 0 | 2.148209 | 3.506518 | 0.001095 |
| 76 | 1 | 0 | -2.148209 | 3.506517 | -0.001095 |
| 77 | 1 | 0 | 3.390195 | 5.657010 | 0.001723 |
| 78 | 1 | 0 | 3.379842 | 8.128331 | 0.001721 |
| 79 | 1 | 0 | 1.245534 | 9.375178 | 0.000634 |
| 80 | 1 | 0 | -1.245537 | 9.375178 | -0.000635 |
| 81 | 1 | 0 | -3.379845 | 8.128330 | -0.001722 |
| 82 | 1 | 0 | -3.390197 | 5.657009 | -0.001724 |

R=Ver

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -11.044981 | -2.147949 | 0.092142 |
| 2 | 6 | 0 | -11.033750 | -3.571987 | 0.047121 |
| 3 | 6 | 0 | -9.850143 | -4.255361 | 0.014017 |
| 4 | 6 | 0 | -8.600292 | -3.563430 | 0.023519 |
| 5 | 6 | 0 | -8.611841 | -2.117728 | 0.068833 |
| 6 | 6 | 0 | -9.871889 | -1.445852 | 0.102616 |
| 7 | 6 | 0 | -7.376020 | -4.234222 | -0.008780 |
| 8 | 6 | 0 | -6.150986 | -3.546835 | 0.001013 |
| 9 | 6 | 0 | -6.163147 | -2.095038 | 0.045292 |
| 10 | 6 | 0 | -7.397770 | -1.427466 | 0.078317 |
| 11 | 6 | 0 | -4.910679 | -4.216357 | -0.029297 |
| 12 | 6 | 0 | -3.695666 | -3.526709 | -0.018787 |
| 13 | 6 | 0 | -3.708793 | -2.071037 | 0.022491 |
| 14 | 6 | 0 | -4.933234 | -1.403875 | 0.054064 |
| 15 | 6 | 0 | -2.448357 | -4.184792 | -0.044204 |
| 16 | 6 | 0 | -1.232699 | -3.490979 | -0.031424 |
| 17 | 6 | 0 | -1.248607 | -2.032230 | 0.004232 |
| 18 | 6 | 0 | -2.476098 | -1.375825 | 0.030539 |
| 19 | 6 | 0 | -0.000007 | -4.164860 | -0.050896 |
| 20 | 6 | 0 | 1.232687 | -3.490981 | -0.031423 |
| 21 | 6 | 0 | 1.248597 | -2.032232 | 0.004234 |
| 22 | 6 | 0 | -0.000005 | -1.325586 | 0.012833 |
| 23 | 6 | 0 | 2.448343 | -4.184796 | -0.044201 |
| 24 | 6 | 0 | 3.695654 | -3.526715 | -0.018782 |
| 25 | 6 | 0 | 3.708783 | -2.071043 | 0.022496 |
| 26 | 6 | 0 | 2.476089 | -1.375829 | 0.030542 |
| 27 | 6 | 0 | 4.910665 | -4.216365 | -0.029289 |
| 28 | 6 | 0 | 6.150973 | -3.546845 | 0.001022 |
| 29 | 6 | 0 | 6.163137 | -2.095048 | 0.045299 |
| 30 | 6 | 0 | 4.933224 | -1.403883 | 0.054069 |
| 31 | 6 | 0 | 7.376006 | -4.234234 | -0.008768 |
| 32 | 6 | 0 | 8.600279 | -3.563444 | 0.023531 |
| 33 | 6 | 0 | 8.611831 | -2.117743 | 0.068844 |
| 34 | 6 | 0 | 7.397760 | -1.427478 | 0.078325 |
| 35 | 6 | 0 | 9.850128 | -4.255377 | 0.014032 |
| 36 | 6 | 0 | 11.033737 | -3.572005 | 0.047137 |
| 37 | 6 | 0 | 11.044970 | -2.147967 | 0.092157 |
| 38 | 6 | 0 | 9.871880 | -1.445868 | 0.102628 |
| 39 | 6 | 0 | -0.000003 | 0.080022 | 0.027026 |

| | | | | | |
|---|---|---|---|---|---|
| 40 | 6 | 0 | -0.000001 | 1.292705 | 0.033411 |
| 41 | 6 | 0 | 0.000003 | 2.713118 | 0.042475 |
| 42 | 7 | 0 | 1.196215 | 3.307677 | 0.053666 |
| 43 | 7 | 0 | 1.173323 | 4.671205 | 0.064797 |
| 44 | 6 | 0 | 0.000013 | 5.443098 | 0.029813 |
| 45 | 7 | 0 | -1.173303 | 4.671214 | 0.064813 |
| 46 | 7 | 0 | -1.196203 | 3.307686 | 0.053685 |
| 47 | 8 | 0 | 0.000018 | 6.650861 | -0.023655 |
| 48 | 6 | 0 | -2.467373 | 5.292858 | -0.018708 |
| 49 | 6 | 0 | -2.753599 | 6.476509 | 0.665383 |
| 50 | 6 | 0 | -4.031056 | 7.021504 | 0.579712 |
| 51 | 6 | 0 | -5.021545 | 6.398577 | -0.175696 |
| 52 | 6 | 0 | -4.728564 | 5.215058 | -0.849899 |
| 53 | 6 | 0 | -3.456493 | 4.659373 | -0.774811 |
| 54 | 6 | 0 | 2.467397 | 5.292842 | -0.018740 |
| 55 | 6 | 0 | 2.753642 | 6.476481 | 0.665363 |
| 56 | 6 | 0 | 4.031100 | 7.021470 | 0.579677 |
| 57 | 6 | 0 | 5.021571 | 6.398547 | -0.175758 |
| 58 | 6 | 0 | 4.728571 | 5.215039 | -0.849974 |
| 59 | 6 | 0 | 3.456498 | 4.659362 | -0.774869 |
| 60 | 1 | 0 | -11.993672 | -1.623966 | 0.118314 |
| 61 | 1 | 0 | -11.974179 | -4.111292 | 0.039494 |
| 62 | 1 | 0 | -9.841502 | -5.339786 | -0.020012 |
| 63 | 1 | 0 | -9.879704 | -0.361435 | 0.137267 |
| 64 | 1 | 0 | -7.368880 | -5.319387 | -0.042036 |
| 65 | 1 | 0 | -7.406836 | -0.342384 | 0.112989 |
| 66 | 1 | 0 | -4.901845 | -5.301430 | -0.060633 |
| 67 | 1 | 0 | -4.941535 | -0.319018 | 0.087887 |
| 68 | 1 | 0 | -2.429805 | -5.269700 | -0.072496 |
| 69 | 1 | 0 | -2.494433 | -0.292547 | 0.061563 |
| 70 | 1 | 0 | -0.000008 | -5.249883 | -0.078586 |
| 71 | 1 | 0 | 2.429790 | -5.269704 | -0.072492 |
| 72 | 1 | 0 | 2.494426 | -0.292551 | 0.061565 |
| 73 | 1 | 0 | 4.901829 | -5.301438 | -0.060625 |
| 74 | 1 | 0 | 4.941527 | -0.319026 | 0.087892 |
| 75 | 1 | 0 | 7.368864 | -5.319399 | -0.042024 |
| 76 | 1 | 0 | 7.406828 | -0.342396 | 0.112997 |
| 77 | 1 | 0 | 9.841486 | -5.339802 | -0.019995 |
| 78 | 1 | 0 | 11.974165 | -4.111312 | 0.039512 |
| 79 | 1 | 0 | 11.993662 | -1.623986 | 0.118331 |
| 80 | 1 | 0 | 9.879696 | -0.361451 | 0.137279 |
| 81 | 1 | 0 | -1.989641 | 6.969756 | 1.246172 |
| 82 | 1 | 0 | -4.249647 | 7.939830 | 1.112256 |
| 83 | 1 | 0 | -6.013210 | 6.831416 | -0.238055 |
| 84 | 1 | 0 | -5.490347 | 4.721550 | -1.442387 |
| 85 | 1 | 0 | -3.221120 | 3.735994 | -1.285379 |
| 86 | 1 | 0 | 1.989697 | 6.969725 | 1.246173 |
| 87 | 1 | 0 | 4.249707 | 7.939786 | 1.112229 |
| 88 | 1 | 0 | 6.013238 | 6.831380 | -0.238129 |
| 89 | 1 | 0 | 5.490340 | 4.721535 | -1.442482 |
| 90 | 1 | 0 | 3.221110 | 3.735991 | -1.285447 |

R=NN

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -11.041805 | -1.188309 | -0.014500 |
| 2 | 6 | 0 | -11.034710 | -2.612554 | -0.015033 |
| 3 | 6 | 0 | -9.852864 | -3.300225 | -0.013152 |
| 4 | 6 | 0 | -8.601591 | -2.612022 | -0.010633 |
| 5 | 6 | 0 | -8.608905 | -1.166726 | -0.010073 |
| 6 | 6 | 0 | -9.866309 | -0.489926 | -0.012087 |
| 7 | 6 | 0 | -7.377876 | -3.287115 | -0.008799 |
| 8 | 6 | 0 | -6.154126 | -2.603490 | -0.006501 |
| 9 | 6 | 0 | -6.162057 | -1.152884 | -0.005878 |
| 10 | 6 | 0 | -7.391606 | -0.480347 | -0.007669 |
| 11 | 6 | 0 | -4.910903 | -3.277384 | -0.004959 |
| 12 | 6 | 0 | -3.700710 | -2.592742 | -0.003067 |
| 13 | 6 | 0 | -3.710201 | -1.136100 | -0.002337 |
| 14 | 6 | 0 | -4.926357 | -0.464842 | -0.003667 |
| 15 | 6 | 0 | -2.448221 | -3.255482 | -0.002023 |
| 16 | 6 | 0 | -1.235703 | -2.567987 | -0.000734 |
| 17 | 6 | 0 | -1.250241 | -1.104363 | -0.000093 |
| 18 | 6 | 0 | -2.470920 | -0.442793 | -0.000720 |
| 19 | 6 | 0 | 0.000001 | -3.240789 | -0.000008 |
| 20 | 6 | 0 | 1.235704 | -2.567987 | 0.000723 |
| 21 | 6 | 0 | 1.250242 | -1.104363 | 0.000089 |
| 22 | 6 | 0 | 0.000000 | -0.405811 | 0.000000 |
| 23 | 6 | 0 | 2.448222 | -3.255482 | 0.002009 |
| 24 | 6 | 0 | 3.700712 | -2.592742 | 0.003058 |
| 25 | 6 | 0 | 3.710202 | -1.136099 | 0.002336 |
| 26 | 6 | 0 | 2.470921 | -0.442793 | 0.000720 |
| 27 | 6 | 0 | 4.910904 | -3.277383 | 0.004948 |
| 28 | 6 | 0 | 6.154127 | -2.603489 | 0.006496 |
| 29 | 6 | 0 | 6.162058 | -1.152883 | 0.005882 |
| 30 | 6 | 0 | 4.926357 | -0.464842 | 0.003671 |
| 31 | 6 | 0 | 7.377877 | -3.287113 | 0.008793 |
| 32 | 6 | 0 | 8.601592 | -2.612021 | 0.010636 |
| 33 | 6 | 0 | 8.608906 | -1.166725 | 0.010085 |
| 34 | 6 | 0 | 7.391607 | -0.480346 | 0.007681 |
| 35 | 6 | 0 | 9.852865 | -3.300223 | 0.013154 |
| 36 | 6 | 0 | 11.034711 | -2.612552 | 0.015044 |
| 37 | 6 | 0 | 11.041806 | -1.188307 | 0.014520 |
| 38 | 6 | 0 | 9.866309 | -0.489925 | 0.012107 |
| 39 | 6 | 0 | 0.000001 | 1.001398 | 0.000001 |
| 40 | 6 | 0 | 0.000000 | 2.213140 | 0.000001 |
| 41 | 6 | 0 | -0.000001 | 3.607204 | 0.000001 |
| 42 | 7 | 0 | -1.115156 | 4.382430 | 0.003862 |
| 43 | 6 | 0 | -0.757825 | 5.836629 | 0.204164 |
| 44 | 6 | 0 | 0.757822 | 5.836627 | -0.204171 |
| 45 | 7 | 0 | 1.115153 | 4.382430 | -0.003863 |
| 46 | 6 | 0 | 1.009910 | 6.130220 | -1.692877 |
| 47 | 6 | 0 | 1.673651 | 6.701884 | 0.658892 |
| 48 | 6 | 0 | -1.009911 | 6.130228 | 1.692870 |
| 49 | 6 | 0 | -1.673656 | 6.701884 | -0.658900 |
| 50 | 8 | 0 | 2.315060 | 3.976859 | -0.020383 |
| 51 | 8 | 0 | -2.315062 | 3.976859 | 0.020386 |
| 52 | 1 | 0 | -11.988901 | -0.660784 | -0.016047 |
| 53 | 1 | 0 | -11.976709 | -3.149226 | -0.016970 |
| 54 | 1 | 0 | -9.847518 | -4.385223 | -0.013583 |
| 55 | 1 | 0 | -9.870430 | 0.595048 | -0.011710 |
| 56 | 1 | 0 | -7.374094 | -4.372852 | -0.009276 |
| 57 | 1 | 0 | -7.396509 | 0.605271 | -0.007300 |
| 58 | 1 | 0 | -4.905856 | -4.363023 | -0.005456 |
| 59 | 1 | 0 | -4.929828 | 0.620522 | -0.003273 |
| 60 | 1 | 0 | -2.434322 | -4.340920 | -0.002445 |
| 61 | 1 | 0 | -2.488779 | 0.641650 | -0.000186 |
| 62 | 1 | 0 | 0.000001 | -4.326200 | -0.000010 |
| 63 | 1 | 0 | 2.434324 | -4.340919 | 0.002425 |
| 64 | 1 | 0 | 2.488780 | 0.641651 | 0.000192 |
| 65 | 1 | 0 | 4.905858 | -4.363022 | 0.005439 |
| 66 | 1 | 0 | 4.929828 | 0.620522 | 0.003283 |
| 67 | 1 | 0 | 7.374095 | -4.372851 | 0.009264 |
| 68 | 1 | 0 | 7.396510 | 0.605272 | 0.007318 |
| 69 | 1 | 0 | 9.847520 | -4.385222 | 0.013577 |
| 70 | 1 | 0 | 11.976710 | -3.149224 | 0.016980 |
| 71 | 1 | 0 | 11.988901 | -0.660782 | 0.016073 |
| 72 | 1 | 0 | 9.870430 | 0.595049 | 0.011737 |
| 73 | 1 | 0 | 0.823467 | 7.181560 | -1.920020 |
| 74 | 1 | 0 | 2.053491 | 5.903823 | -1.916262 |
| 75 | 1 | 0 | 0.381924 | 5.515129 | -2.340008 |
| 76 | 1 | 0 | 2.706692 | 6.535775 | 0.353594 |
| 77 | 1 | 0 | 1.433288 | 7.758570 | 0.519475 |
| 78 | 1 | 0 | 1.595213 | 6.459721 | 1.717935 |
| 79 | 1 | 0 | -0.823473 | 7.181571 | 1.920005 |
| 80 | 1 | 0 | -2.053490 | 5.903826 | 1.916258 |
| 81 | 1 | 0 | -0.381919 | 5.515144 | 2.340002 |
| 82 | 1 | 0 | -2.706696 | 6.535770 | -0.353603 |
| 83 | 1 | 0 | -1.433296 | 7.758570 | -0.519481 |
| 84 | 1 | 0 | -1.595215 | 6.459724 | -1.717943 |

# Sat-Radical

R=Sat-H

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -11.048445 | 0.427181 | 0.014969 |
| 2 | 6 | 0 | -11.028792 | -0.994378 | 0.105350 |
| 3 | 6 | 0 | -9.840771 | -1.670957 | 0.129281 |
| 4 | 6 | 0 | -8.595433 | -0.974393 | 0.064689 |
| 5 | 6 | 0 | -8.615445 | 0.468904 | -0.027102 |
| 6 | 6 | 0 | -9.879404 | 1.133631 | -0.049068 |
| 7 | 6 | 0 | -7.366749 | -1.638247 | 0.087213 |
| 8 | 6 | 0 | -6.146073 | -0.946521 | 0.023443 |
| 9 | 6 | 0 | -6.166295 | 0.503311 | -0.068743 |
| 10 | 6 | 0 | -7.405300 | 1.163687 | -0.091006 |
| 11 | 6 | 0 | -4.901616 | -1.608706 | 0.046129 |
| 12 | 6 | 0 | -3.690842 | -0.914297 | -0.017187 |
| 13 | 6 | 0 | -3.709834 | 0.538326 | -0.111111 |
| 14 | 6 | 0 | -4.940582 | 1.198174 | -0.133092 |
| 15 | 6 | 0 | -2.439421 | -1.560981 | 0.009161 |
| 16 | 6 | 0 | -1.227341 | -0.862586 | -0.051437 |
| 17 | 6 | 0 | -1.234674 | 0.597813 | -0.157964 |
| 18 | 6 | 0 | -2.482754 | 1.236670 | -0.178263 |
| 19 | 6 | 0 | 0.000002 | -1.538777 | -0.008700 |
| 20 | 6 | 0 | 1.227344 | -0.862585 | -0.051437 |
| 21 | 6 | 0 | 1.234676 | 0.597814 | -0.157964 |
| 22 | 6 | 0 | 0.000000 | 1.305244 | -0.229654 |
| 23 | 6 | 0 | 2.439424 | -1.560980 | 0.009162 |
| 24 | 6 | 0 | 3.690845 | -0.914295 | -0.017185 |
| 25 | 6 | 0 | 3.709837 | 0.538327 | -0.111110 |
| 26 | 6 | 0 | 2.482757 | 1.236671 | -0.178262 |
| 27 | 6 | 0 | 4.901620 | -1.608705 | 0.046131 |
| 28 | 6 | 0 | 6.146076 | -0.946520 | 0.023444 |
| 29 | 6 | 0 | 6.166298 | 0.503313 | -0.068742 |
| 30 | 6 | 0 | 4.940585 | 1.198175 | -0.133092 |
| 31 | 6 | 0 | 7.366752 | -1.638245 | 0.087215 |
| 32 | 6 | 0 | 8.595437 | -0.974391 | 0.064690 |
| 33 | 6 | 0 | 8.615448 | 0.468906 | -0.027102 |
| 34 | 6 | 0 | 7.405303 | 1.163689 | -0.091006 |
| 35 | 6 | 0 | 9.840775 | -1.670955 | 0.129282 |
| 36 | 6 | 0 | 11.028795 | -0.994376 | 0.105350 |
| 37 | 6 | 0 | 11.048448 | 0.427184 | 0.014968 |
| 38 | 6 | 0 | 9.879407 | 1.133633 | -0.049069 |
| 39 | 6 | 0 | -0.000004 | 2.814912 | -0.345827 |
| 40 | 6 | 0 | -0.000039 | 3.536455 | 1.015864 |
| 41 | 1 | 0 | -12.000103 | 0.946186 | -0.002732 |
| 42 | 1 | 0 | -11.965807 | -1.537395 | 0.155164 |
| 43 | 1 | 0 | -9.825488 | -2.753701 | 0.198102 |
| 44 | 1 | 0 | -9.893921 | 2.216395 | -0.117925 |
| 45 | 1 | 0 | -7.353026 | -2.721713 | 0.156107 |
| 46 | 1 | 0 | -7.421525 | 2.247143 | -0.159941 |
| 47 | 1 | 0 | -4.885743 | -2.691966 | 0.115661 |
| 48 | 1 | 0 | -4.957590 | 2.281521 | -0.202821 |
| 49 | 1 | 0 | -2.412045 | -2.643711 | 0.083261 |
| 50 | 1 | 0 | -2.536213 | 2.315544 | -0.242618 |
| 51 | 1 | 0 | 0.000002 | -2.621434 | 0.068696 |
| 52 | 1 | 0 | 2.412048 | -2.643710 | 0.083262 |
| 53 | 1 | 0 | 2.536217 | 2.315545 | -0.242616 |
| 54 | 1 | 0 | 4.885747 | -2.691964 | 0.115663 |
| 55 | 1 | 0 | 4.957592 | 2.281522 | -0.202821 |
| 56 | 1 | 0 | 7.353030 | -2.721711 | 0.156110 |
| 57 | 1 | 0 | 7.421527 | 2.247145 | -0.159941 |
| 58 | 1 | 0 | 9.825492 | -2.753699 | 0.198104 |
| 59 | 1 | 0 | 11.965811 | -1.537392 | 0.155164 |
| 60 | 1 | 0 | 12.000106 | 0.946189 | -0.002733 |
| 61 | 1 | 0 | 9.893924 | 2.216397 | -0.117927 |
| 62 | 1 | 0 | 0.865655 | 3.139952 | -0.926302 |
| 63 | 1 | 0 | -0.865640 | 3.139942 | -0.926342 |
| 64 | 1 | 0 | -0.000038 | 4.621697 | 0.879399 |
| 65 | 1 | 0 | -0.881387 | 3.268233 | 1.603340 |
| 66 | 1 | 0 | 0.881282 | 3.268237 | 1.603383 |

R=Sat-Mt

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 1.228915 | 0.460817 | -0.201247 |
| 2 | 6 | 0 | 1.221366 | -0.995339 | -0.028438 |
| 3 | 6 | 0 | -0.000001 | -1.670654 | 0.045789 |
| 4 | 6 | 0 | -1.221368 | -0.995339 | -0.028437 |
| 5 | 6 | 0 | -1.228916 | 0.460817 | -0.201245 |
| 6 | 6 | 0 | -0.000001 | 1.164662 | -0.303903 |
| 7 | 6 | 0 | 2.483591 | 1.098440 | -0.251461 |
| 8 | 6 | 0 | 3.694340 | 0.403207 | -0.153622 |
| 9 | 6 | 0 | 3.674853 | -1.047453 | 0.007118 |
| 10 | 6 | 0 | 2.438831 | -1.692209 | 0.063589 |
| 11 | 6 | 0 | -2.438833 | -1.692208 | 0.063591 |
| 12 | 6 | 0 | -3.674855 | -1.047452 | 0.007120 |
| 13 | 6 | 0 | -3.694341 | 0.403208 | -0.153619 |
| 14 | 6 | 0 | -2.483592 | 1.098442 | -0.251457 |
| 15 | 6 | 0 | 0.000000 | 2.665157 | -0.478953 |
| 16 | 6 | 0 | 0.000015 | 3.443283 | 0.882042 |
| 17 | 6 | 0 | 0.000013 | 4.920137 | 0.709637 |
| 18 | 6 | 0 | -4.898958 | -1.740913 | 0.102276 |
| 19 | 6 | 0 | -6.124299 | -1.082803 | 0.047917 |
| 20 | 6 | 0 | -6.145670 | 0.369094 | -0.112166 |
| 21 | 6 | 0 | -4.940365 | 1.060296 | -0.206705 |
| 22 | 6 | 0 | 4.940364 | 1.060294 | -0.206709 |
| 23 | 6 | 0 | 6.145668 | 0.369092 | -0.112168 |
| 24 | 6 | 0 | 6.124297 | -1.082805 | 0.047916 |
| 25 | 6 | 0 | 4.898956 | -1.740915 | 0.102274 |
| 26 | 6 | 0 | -7.360055 | -1.772597 | 0.142938 |
| 27 | 6 | 0 | -8.573693 | -1.113344 | 0.088359 |
| 28 | 6 | 0 | -8.595081 | 0.335276 | -0.071567 |
| 29 | 6 | 0 | -7.401302 | 1.025986 | -0.166010 |
| 30 | 6 | 0 | 7.401301 | 1.025985 | -0.166012 |
| 31 | 6 | 0 | 8.595079 | 0.335275 | -0.071568 |
| 32 | 6 | 0 | 8.573691 | -1.113345 | 0.088360 |
| 33 | 6 | 0 | 7.360053 | -1.772598 | 0.142938 |
| 34 | 6 | 0 | 9.870115 | 0.995631 | -0.125315 |
| 35 | 6 | 0 | 11.030613 | 0.292111 | -0.029927 |
| 36 | 6 | 0 | 11.009593 | -1.133510 | 0.127410 |
| 37 | 6 | 0 | 9.828770 | -1.806624 | 0.184006 |
| 38 | 6 | 0 | -9.828772 | -1.806623 | 0.184004 |
| 39 | 6 | 0 | -11.009595 | -1.133508 | 0.127407 |
| 40 | 6 | 0 | -11.030615 | 0.292113 | -0.029929 |
| 41 | 6 | 0 | -9.870117 | 0.995632 | -0.125315 |
| 42 | 1 | 0 | -0.000001 | -2.748582 | 0.171725 |
| 43 | 1 | 0 | 2.537828 | 2.172994 | -0.365624 |
| 44 | 1 | 0 | 2.410717 | -2.770330 | 0.187053 |
| 45 | 1 | 0 | -2.410719 | -2.770329 | 0.187054 |
| 46 | 1 | 0 | -2.537830 | 2.172995 | -0.365620 |
| 47 | 1 | 0 | 0.866957 | 2.980864 | -1.061170 |
| 48 | 1 | 0 | -0.866966 | 2.980868 | -1.061155 |
| 49 | 1 | 0 | -0.879022 | 3.123792 | 1.451199 |
| 50 | 1 | 0 | 0.879067 | 3.123793 | 1.451176 |
| 51 | 1 | 0 | -0.926108 | 5.466824 | 0.575740 |
| 52 | 1 | 0 | 0.926126 | 5.466810 | 0.575632 |
| 53 | 1 | 0 | -4.881333 | -2.819665 | 0.222094 |
| 54 | 1 | 0 | -4.958338 | 2.139176 | -0.326193 |
| 55 | 1 | 0 | 4.958337 | 2.139174 | -0.326197 |
| 56 | 1 | 0 | 4.881331 | -2.819666 | 0.222093 |
| 57 | 1 | 0 | -7.344819 | -2.851627 | 0.261977 |
| 58 | 1 | 0 | -7.418491 | 2.104992 | -0.285112 |
| 59 | 1 | 0 | 7.418489 | 2.104990 | -0.285114 |
| 60 | 1 | 0 | 7.344817 | -2.851628 | 0.261978 |
| 61 | 1 | 0 | 9.886164 | 2.073961 | -0.244318 |
| 62 | 1 | 0 | 11.984745 | 0.805139 | -0.072228 |
| 63 | 1 | 0 | 11.948215 | -1.671014 | 0.201032 |
| 64 | 1 | 0 | 9.812811 | -2.884955 | 0.302995 |
| 65 | 1 | 0 | -9.812813 | -2.884954 | 0.302992 |
| 66 | 1 | 0 | -11.948217 | -1.671013 | 0.201028 |
| 67 | 1 | 0 | -11.984747 | 0.805140 | -0.072230 |
| 68 | 1 | 0 | -9.886166 | 2.073962 | -0.244318 |

R=Sat-DCM

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -11.045268 | -0.191002 | -0.042855 |
| 2 | 6 | 0 | -11.024824 | -1.600999 | 0.163003 |
| 3 | 6 | 0 | -9.837252 | -2.273363 | 0.240416 |
| 4 | 6 | 0 | -8.592068 | -1.583522 | 0.117480 |
| 5 | 6 | 0 | -8.612954 | -0.151876 | -0.091728 |
| 6 | 6 | 0 | -9.877443 | 0.508753 | -0.165909 |
| 7 | 6 | 0 | -7.364121 | -2.242906 | 0.192494 |
| 8 | 6 | 0 | -6.143428 | -1.557393 | 0.070554 |
| 9 | 6 | 0 | -6.164701 | -0.119543 | -0.140033 |
| 10 | 6 | 0 | -7.404544 | 0.536562 | -0.214040 |
| 11 | 6 | 0 | -4.900097 | -2.214794 | 0.145876 |
| 12 | 6 | 0 | -3.689449 | -1.526011 | 0.024207 |
| 13 | 6 | 0 | -3.709889 | -0.085921 | -0.189487 |
| 14 | 6 | 0 | -4.941457 | 0.569643 | -0.263603 |
| 15 | 6 | 0 | -2.439084 | -2.167621 | 0.102407 |
| 16 | 6 | 0 | -1.227624 | -1.474622 | -0.015849 |
| 17 | 6 | 0 | -1.236368 | -0.028546 | -0.244903 |
| 18 | 6 | 0 | -2.484935 | 0.606202 | -0.317378 |
| 19 | 6 | 0 | -0.000002 | -2.143022 | 0.084621 |
| 20 | 6 | 0 | 1.227621 | -1.474622 | -0.015849 |
| 21 | 6 | 0 | 1.236365 | -0.028547 | -0.244904 |
| 22 | 6 | 0 | -0.000001 | 0.665065 | -0.375808 |
| 23 | 6 | 0 | 2.439080 | -2.167622 | 0.102407 |
| 24 | 6 | 0 | 3.689446 | -1.526013 | 0.024207 |
| 25 | 6 | 0 | 3.709886 | -0.085922 | -0.189487 |
| 26 | 6 | 0 | 2.484932 | 0.606201 | -0.317379 |
| 27 | 6 | 0 | 4.900094 | -2.214796 | 0.145877 |
| 28 | 6 | 0 | 6.143424 | -1.557395 | 0.070554 |
| 29 | 6 | 0 | 6.164698 | -0.119545 | -0.140033 |
| 30 | 6 | 0 | 4.941454 | 0.569641 | -0.263604 |
| 31 | 6 | 0 | 7.364118 | -2.242908 | 0.192495 |
| 32 | 6 | 0 | 8.592064 | -1.583524 | 0.117482 |
| 33 | 6 | 0 | 8.612951 | -0.151879 | -0.091728 |
| 34 | 6 | 0 | 7.404541 | 0.536560 | -0.214041 |
| 35 | 6 | 0 | 9.837248 | -2.273366 | 0.240418 |
| 36 | 6 | 0 | 11.024820 | -1.601003 | 0.163006 |
| 37 | 6 | 0 | 11.045265 | -0.191006 | -0.042853 |
| 38 | 6 | 0 | 9.877440 | 0.508750 | -0.165909 |
| 39 | 6 | 0 | -0.000001 | 2.156450 | -0.621614 |

| | | | | | |
|---|---|---|---|---|---|
| 40 | 6 | 0 | 0.000002 | 2.972772 | 0.706242 |
| 41 | 6 | 0 | 0.000008 | 4.460149 | 0.455527 |
| 42 | 6 | 0 | -1.208933 | 5.147840 | 0.293773 |
| 43 | 6 | 0 | 1.208957 | 5.147822 | 0.293748 |
| 44 | 7 | 0 | 2.239646 | 5.672585 | 0.168455 |
| 45 | 7 | 0 | -2.239616 | 5.672620 | 0.168502 |
| 46 | 1 | 0 | -11.997320 | 0.324093 | -0.101245 |
| 47 | 1 | 0 | -11.961724 | -2.138003 | 0.258120 |
| 48 | 1 | 0 | -9.821486 | -3.346807 | 0.397188 |
| 49 | 1 | 0 | -9.892548 | 1.582169 | -0.322495 |
| 50 | 1 | 0 | -7.349483 | -3.317021 | 0.349655 |
| 51 | 1 | 0 | -7.421318 | 1.610613 | -0.370773 |
| 52 | 1 | 0 | -4.882764 | -3.288581 | 0.304038 |
| 53 | 1 | 0 | -4.959689 | 1.643488 | -0.421350 |
| 54 | 1 | 0 | -2.410160 | -3.240771 | 0.263109 |
| 55 | 1 | 0 | -2.544491 | 1.675185 | -0.476096 |
| 56 | 1 | 0 | -0.000002 | -3.214961 | 0.255090 |
| 57 | 1 | 0 | 2.410155 | -3.240772 | 0.263109 |
| 58 | 1 | 0 | 2.544489 | 1.675183 | -0.476098 |
| 59 | 1 | 0 | 4.882760 | -3.288583 | 0.304039 |
| 60 | 1 | 0 | 4.959687 | 1.643486 | -0.421351 |
| 61 | 1 | 0 | 7.349479 | -3.317023 | 0.349657 |
| 62 | 1 | 0 | 7.421315 | 1.610611 | -0.370774 |
| 63 | 1 | 0 | 9.821482 | -3.346810 | 0.397192 |
| 64 | 1 | 0 | 11.961720 | -2.138006 | 0.258124 |
| 65 | 1 | 0 | 11.997317 | 0.324089 | -0.101244 |
| 66 | 1 | 0 | 9.892545 | 1.582166 | -0.322495 |
| 67 | 1 | 0 | 0.868784 | 2.446916 | -1.213703 |
| 68 | 1 | 0 | -0.868786 | 2.446917 | -1.213701 |
| 69 | 1 | 0 | -0.882081 | 2.708641 | 1.293253 |
| 70 | 1 | 0 | 0.882083 | 2.708634 | 1.293254 |

R=Sat-DPM

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 1.159391 | -0.995258 | -0.192685 |
| 2 | 6 | 0 | 1.138891 | -2.426825 | 0.113575 |
| 3 | 6 | 0 | -0.094515 | -3.079847 | 0.244572 |
| 4 | 6 | 0 | -1.315399 | -2.409373 | 0.087174 |
| 5 | 6 | 0 | -1.310465 | -0.977324 | -0.221299 |
| 6 | 6 | 0 | -0.069184 | -0.290296 | -0.353238 |
| 7 | 6 | 0 | 2.413294 | -0.379300 | -0.314738 |
| 8 | 6 | 0 | 3.633539 | -1.075820 | -0.159849 |
| 9 | 6 | 0 | 3.601738 | -2.498342 | 0.147106 |
| 10 | 6 | 0 | 2.344410 | -3.121404 | 0.272189 |
| 11 | 6 | 0 | -2.533020 | -3.087722 | 0.222169 |
| 12 | 6 | 0 | -3.779723 | -2.449937 | 0.069617 |
| 13 | 6 | 0 | -3.787460 | -1.028409 | -0.243278 |
| 14 | 6 | 0 | -2.555127 | -0.348949 | -0.373973 |
| 15 | 6 | 0 | -0.046856 | 1.199639 | -0.617955 |
| 16 | 6 | 0 | 0.022084 | 2.044755 | 0.689783 |
| 17 | 6 | 0 | 0.119002 | 3.528758 | 0.427275 |
| 18 | 6 | 0 | -1.039376 | 4.376615 | 0.560453 |
| 19 | 6 | 0 | 1.415989 | 4.051031 | -0.019084 |
| 20 | 6 | 0 | -0.925897 | 5.788502 | 0.687545 |
| 21 | 6 | 0 | -2.040859 | 6.595899 | 0.844297 |
| 22 | 6 | 0 | -3.322698 | 6.042334 | 0.884369 |
| 23 | 6 | 0 | -3.465162 | 4.657809 | 0.779177 |
| 24 | 6 | 0 | -2.354361 | 3.842067 | 0.627928 |
| 25 | 6 | 0 | 1.510958 | 4.994660 | -1.066138 |
| 26 | 6 | 0 | 2.741448 | 5.458354 | -1.514275 |
| 27 | 6 | 0 | 3.923814 | 5.004472 | -0.930240 |
| 28 | 6 | 0 | 3.856535 | 4.071601 | 0.103733 |
| 29 | 6 | 0 | 2.627231 | 3.595281 | 0.545212 |
| 30 | 6 | 0 | 4.806544 | -3.188665 | 0.303090 |
| 31 | 6 | 0 | 6.056690 | -2.550704 | 0.169872 |
| 32 | 6 | 0 | 6.089410 | -1.131611 | -0.140494 |
| 33 | 6 | 0 | 4.869980 | -0.439994 | -0.294943 |
| 34 | 6 | 0 | -5.013263 | -0.378831 | -0.406844 |
| 35 | 6 | 0 | -6.244227 | -1.054421 | -0.275040 |
| 36 | 6 | 0 | -6.235189 | -2.472537 | 0.041125 |
| 37 | 6 | 0 | -4.995849 | -3.124907 | 0.202671 |
| 38 | 6 | 0 | -7.461212 | -3.144779 | 0.173304 |
| 39 | 6 | 0 | -8.684794 | -2.491338 | 0.009533 |
| 40 | 6 | 0 | -8.693652 | -1.079891 | -0.306182 |
| 41 | 6 | 0 | -7.478139 | -0.404535 | -0.438982 |
| 42 | 6 | 0 | 7.334405 | -0.496470 | -0.276808 |
| 43 | 6 | 0 | 8.538584 | -1.187045 | -0.121610 |
| 44 | 6 | 0 | 8.506059 | -2.599368 | 0.188833 |
| 45 | 6 | 0 | 7.271566 | -3.238336 | 0.324889 |
| 46 | 6 | 0 | 9.808463 | -0.547835 | -0.258839 |
| 47 | 6 | 0 | 10.971449 | -1.249488 | -0.101094 |
| 48 | 6 | 0 | 10.939461 | -2.640440 | 0.205038 |
| 49 | 6 | 0 | 9.745492 | -3.292012 | 0.344902 |
| 50 | 6 | 0 | -9.935478 | -3.168293 | 0.142391 |
| 51 | 6 | 0 | -11.118267 | -2.502654 | -0.024028 |
| 52 | 6 | 0 | -11.126926 | -1.112534 | -0.335199 |
| 53 | 6 | 0 | -9.952429 | -0.425631 | -0.471392 |
| 54 | 1 | 0 | -0.104785 | -4.140430 | 0.475167 |
| 55 | 1 | 0 | 2.479149 | 0.676713 | -0.540472 |
| 56 | 1 | 0 | 2.306692 | -4.182420 | 0.498843 |
| 57 | 1 | 0 | -2.513356 | -4.148526 | 0.451995 |
| 58 | 1 | 0 | -2.602758 | 0.705032 | -0.612970 |
| 59 | 1 | 0 | -0.924131 | 1.502640 | -1.190709 |
| 60 | 1 | 0 | 0.806215 | 1.459599 | -1.246553 |
| 61 | 1 | 0 | 0.895716 | 1.710071 | 1.255754 |
| 62 | 1 | 0 | -0.840980 | 1.812269 | 1.315373 |
| 63 | 1 | 0 | 0.057174 | 6.240189 | 0.696573 |
| 64 | 1 | 0 | -1.910904 | 7.667434 | 0.950855 |
| 65 | 1 | 0 | -4.192597 | 6.676957 | 1.006853 |
| 66 | 1 | 0 | -4.452750 | 4.211009 | 0.817639 |
| 67 | 1 | 0 | -2.504354 | 2.773367 | 0.550028 |
| 68 | 1 | 0 | 0.604241 | 5.340406 | -1.547103 |
| 69 | 1 | 0 | 2.778377 | 6.171599 | -2.330438 |
| 70 | 1 | 0 | 4.883076 | 5.370931 | -1.277205 |
| 71 | 1 | 0 | 4.766376 | 3.718329 | 0.576865 |
| 72 | 1 | 0 | 2.604409 | 2.886709 | 1.364174 |
| 73 | 1 | 0 | 4.781389 | -4.249496 | 0.532338 |
| 74 | 1 | 0 | 4.894560 | 0.619839 | -0.528779 |
| 75 | 1 | 0 | -5.021880 | 0.680272 | -0.645673 |
| 76 | 1 | 0 | -4.988285 | -4.185054 | 0.436189 |
| 77 | 1 | 0 | -7.455884 | -4.204463 | 0.409621 |
| 78 | 1 | 0 | -7.486049 | 0.654901 | -0.676520 |
| 79 | 1 | 0 | 7.359874 | 0.563417 | -0.511022 |
| 80 | 1 | 0 | 7.248500 | -4.298736 | 0.556952 |
| 81 | 1 | 0 | 9.832434 | 0.511540 | -0.492297 |
| 82 | 1 | 0 | 11.927701 | -0.750110 | -0.208486 |
| 83 | 1 | 0 | 11.871840 | -3.180124 | 0.326461 |
| 84 | 1 | 0 | 9.720828 | -4.351465 | 0.577811 |
| 85 | 1 | 0 | -9.928587 | -4.227127 | 0.379258 |
| 86 | 1 | 0 | -12.059483 | -3.030486 | 0.080041 |
| 87 | 1 | 0 | -12.074567 | -0.601867 | -0.463681 |
| 88 | 1 | 0 | -9.958597 | 0.633151 | -0.708583 |

R=Sat-Flu

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -1.235151 | -1.069590 | 0.206330 |
| 2 | 6 | 0 | -1.227425 | -2.507937 | -0.068485 |
| 3 | 6 | 0 | 0.000023 | -3.172883 | -0.196243 |
| 4 | 6 | 0 | 1.227467 | -2.507931 | -0.068489 |
| 5 | 6 | 0 | 1.235186 | -1.069584 | 0.206329 |
| 6 | 6 | 0 | 0.000017 | -0.372216 | 0.340493 |
| 7 | 6 | 0 | -2.484218 | -0.442844 | 0.324429 |
| 8 | 6 | 0 | -3.710895 | -1.132645 | 0.194314 |
| 9 | 6 | 0 | -3.691203 | -2.561875 | -0.081200 |
| 10 | 6 | 0 | -2.439344 | -3.196619 | -0.201755 |
| 11 | 6 | 0 | 2.439390 | -3.196606 | -0.201765 |
| 12 | 6 | 0 | 3.691245 | -2.561856 | -0.081212 |
| 13 | 6 | 0 | 3.710930 | -1.132627 | 0.194309 |
| 14 | 6 | 0 | 2.484250 | -0.442833 | 0.324430 |
| 15 | 6 | 0 | 0.000014 | 1.121750 | 0.579393 |
| 16 | 6 | 0 | 0.000018 | 1.943175 | -0.746522 |
| 17 | 6 | 0 | -0.000014 | 3.417380 | -0.508528 |
| 18 | 6 | 0 | 1.158638 | 4.252761 | -0.334980 |
| 19 | 6 | 0 | 0.732501 | 5.585962 | -0.044149 |
| 20 | 6 | 0 | -0.732644 | 5.585936 | -0.044205 |
| 21 | 6 | 0 | -1.158710 | 4.252719 | -0.335069 |
| 22 | 6 | 0 | -1.664086 | 6.590409 | 0.165929 |
| 23 | 6 | 0 | -3.027821 | 6.281444 | 0.085263 |
| 24 | 6 | 0 | -3.451972 | 4.980889 | -0.207217 |
| 25 | 6 | 0 | -2.526864 | 3.960765 | -0.419190 |
| 26 | 6 | 0 | 2.526809 | 3.960858 | -0.418993 |
| 27 | 6 | 0 | 3.451864 | 4.981014 | -0.206945 |
| 28 | 6 | 0 | 3.027642 | 6.281553 | 0.085504 |
| 29 | 6 | 0 | 1.663890 | 6.590468 | 0.166062 |
| 30 | 6 | 0 | 4.942228 | -0.485899 | 0.324203 |
| 31 | 6 | 0 | 6.167621 | -1.171757 | 0.193914 |
| 32 | 6 | 0 | 6.146724 | -2.597584 | -0.084627 |
| 33 | 6 | 0 | 4.901921 | -3.246917 | -0.212621 |
| 34 | 6 | 0 | -4.901876 | -3.246944 | -0.212602 |
| 35 | 6 | 0 | -6.146681 | -2.597617 | -0.084606 |
| 36 | 6 | 0 | -6.167585 | -1.171789 | 0.193928 |
| 37 | 6 | 0 | -4.942195 | -0.485924 | 0.324208 |
| 38 | 6 | 0 | 7.407035 | -0.524805 | 0.324608 |
| 39 | 6 | 0 | 8.616961 | -1.210413 | 0.193860 |
| 40 | 6 | 0 | 8.596327 | -2.629599 | -0.084480 |
| 41 | 6 | 0 | 7.367260 | -3.280117 | -0.215114 |
| 42 | 6 | 0 | -7.367214 | -3.280157 | -0.215086 |
| 43 | 6 | 0 | -8.596284 | -2.629645 | -0.084449 |
| 44 | 6 | 0 | -8.616925 | -1.210458 | 0.193885 |
| 45 | 6 | 0 | -7.407001 | -0.524843 | 0.324624 |
| 46 | 6 | 0 | -9.881260 | -0.559283 | 0.325561 |
| 47 | 6 | 0 | -11.050083 | -1.256304 | 0.192369 |
| 48 | 6 | 0 | -11.029826 | -2.654062 | -0.081972 |
| 49 | 6 | 0 | -9.841449 | -3.317070 | -0.215598 |
| 50 | 6 | 0 | 9.841495 | -3.317017 | -0.215638 |
| 51 | 6 | 0 | 11.029868 | -2.654003 | -0.082015 |
| 52 | 6 | 0 | 11.050120 | -1.256246 | 0.192331 |
| 53 | 6 | 0 | 9.881293 | -0.559232 | 0.325533 |
| 54 | 1 | 0 | 0.000025 | -4.238511 | -0.402421 |
| 55 | 1 | 0 | -2.539722 | 0.617806 | 0.531158 |
| 56 | 1 | 0 | -2.411206 | -4.262583 | -0.405230 |
| 57 | 1 | 0 | 2.411256 | -4.262570 | -0.405242 |
| 58 | 1 | 0 | 2.539749 | 0.617817 | 0.531164 |
| 59 | 1 | 0 | -0.865692 | 1.414599 | 1.174467 |
| 60 | 1 | 0 | 0.865711 | 1.414603 | 1.174478 |
| 61 | 1 | 0 | 0.876262 | 1.656369 | -1.335362 |

| | | | | | |
|---|---|---|---|---|---|
| 62 | 1 | 0 | -0.876198 | 1.656338 | -1.335387 |
| 63 | 1 | 0 | -1.350419 | 7.604823 | 0.388014 |
| 64 | 1 | 0 | -3.763868 | 7.060771 | 0.246859 |
| 65 | 1 | 0 | -4.512775 | 4.767174 | -0.273447 |
| 66 | 1 | 0 | -2.867022 | 2.959102 | -0.659028 |
| 67 | 1 | 0 | 2.867024 | 2.959207 | -0.658802 |
| 68 | 1 | 0 | 4.512680 | 4.767337 | -0.273092 |
| 69 | 1 | 0 | 3.763649 | 7.060906 | 0.247161 |
| 70 | 1 | 0 | 1.350168 | 7.604871 | 0.388126 |
| 71 | 1 | 0 | 4.959648 | 0.578907 | 0.535541 |
| 72 | 1 | 0 | 4.885615 | -4.312726 | -0.418204 |
| 73 | 1 | 0 | -4.885564 | -4.312754 | -0.418180 |
| 74 | 1 | 0 | -4.959621 | 0.578883 | 0.535541 |
| 75 | 1 | 0 | 7.423734 | 0.540430 | 0.533985 |
| 76 | 1 | 0 | 7.353114 | -4.345590 | -0.423313 |
| 77 | 1 | 0 | -7.353063 | -4.345631 | -0.423280 |
| 78 | 1 | 0 | -7.423705 | 0.540393 | 0.533996 |
| 79 | 1 | 0 | -9.896254 | 0.505301 | 0.534653 |
| 80 | 1 | 0 | -12.002083 | -0.747947 | 0.295119 |
| 81 | 1 | 0 | -11.966746 | -3.189819 | -0.184216 |
| 82 | 1 | 0 | -9.825767 | -4.381691 | -0.424388 |
| 83 | 1 | 0 | 9.825817 | -4.381636 | -0.424432 |
| 84 | 1 | 0 | 11.966790 | -3.189754 | -0.184265 |
| 85 | 1 | 0 | 12.002117 | -0.747884 | 0.295078 |
| 86 | 1 | 0 | 9.896283 | 0.505351 | 0.534628 |

R=Sat-PhO

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 1.239263 | -0.454800 | -0.232638 |
| 2 | 6 | 0 | 1.230543 | -1.904870 | 0.004579 |
| 3 | 6 | 0 | -0.000008 | -2.571365 | 0.108167 |
| 4 | 6 | 0 | -1.230557 | -1.904868 | 0.004578 |
| 5 | 6 | 0 | -1.239274 | -0.454798 | -0.232639 |
| 6 | 6 | 0 | -0.000006 | 0.242361 | -0.365171 |
| 7 | 6 | 0 | 2.480316 | 0.175293 | -0.314708 |
| 8 | 6 | 0 | 3.715692 | -0.515173 | -0.188318 |
| 9 | 6 | 0 | 3.695904 | -1.952498 | 0.039150 |
| 10 | 6 | 0 | 2.436459 | -2.592659 | 0.126621 |
| 11 | 6 | 0 | -2.436473 | -2.592654 | 0.126619 |
| 12 | 6 | 0 | -3.695917 | -1.952490 | 0.039149 |
| 13 | 6 | 0 | -3.715702 | -0.515166 | -0.188318 |
| 14 | 6 | 0 | -2.480325 | 0.175298 | -0.314708 |
| 15 | 6 | 0 | -0.000005 | 1.733542 | -0.582076 |
| 16 | 6 | 0 | -0.000031 | 2.535378 | 0.763054 |
| 17 | 6 | 0 | -0.000003 | 4.019147 | 0.541476 |
| 18 | 6 | 0 | 1.216791 | 4.730021 | 0.410010 |
| 19 | 6 | 0 | 1.233411 | 6.078900 | 0.159125 |
| 20 | 6 | 0 | 0.000055 | 6.832192 | 0.015530 |
| 21 | 6 | 0 | -1.233334 | 6.078906 | 0.158886 |
| 22 | 6 | 0 | -1.216770 | 4.730029 | 0.409778 |
| 23 | 8 | 0 | 0.000080 | 8.060838 | -0.213782 |
| 24 | 6 | 0 | 4.938112 | 0.138379 | -0.277925 |
| 25 | 6 | 0 | 6.168821 | -0.548120 | -0.154731 |
| 26 | 6 | 0 | 6.148520 | -1.980636 | 0.072612 |
| 27 | 6 | 0 | 4.899443 | -2.637331 | 0.161900 |
| 28 | 6 | 0 | -4.899456 | -2.637320 | 0.161899 |
| 29 | 6 | 0 | -6.148532 | -1.980623 | 0.072614 |
| 30 | 6 | 0 | -6.168829 | -0.548107 | -0.154726 |
| 31 | 6 | 0 | -4.938120 | 0.138389 | -0.277921 |
| 32 | 6 | 0 | 7.403995 | 0.107444 | -0.245259 |
| 33 | 6 | 0 | 8.615325 | -0.578591 | -0.122457 |
| 34 | 6 | 0 | 8.595552 | -2.005824 | 0.104525 |
| 35 | 6 | 0 | 7.366192 | -2.664089 | 0.195234 |
| 36 | 6 | 0 | -7.366204 | -2.664073 | 0.195237 |
| 37 | 6 | 0 | -8.595563 | -2.005806 | 0.104531 |
| 38 | 6 | 0 | -8.615333 | -0.578572 | -0.122448 |
| 39 | 6 | 0 | -7.404002 | 0.107460 | -0.245250 |
| 40 | 6 | 0 | -9.840675 | -2.694202 | 0.228078 |
| 41 | 6 | 0 | -11.028212 | -2.023157 | 0.134490 |
| 42 | 6 | 0 | -11.047551 | -0.616684 | -0.089261 |
| 43 | 6 | 0 | -9.878441 | 0.081232 | -0.213439 |
| 44 | 6 | 0 | 9.878434 | 0.081210 | -0.213453 |
| 45 | 6 | 0 | 11.047543 | -0.616709 | -0.089275 |
| 46 | 6 | 0 | 11.028201 | -2.023181 | 0.134480 |
| 47 | 6 | 0 | 9.840662 | -2.694223 | 0.228071 |
| 48 | 1 | 0 | -0.000008 | -3.642561 | 0.282989 |
| 49 | 1 | 0 | 2.537046 | 1.242445 | -0.485398 |
| 50 | 1 | 0 | 2.409209 | -3.664125 | 0.298749 |
| 51 | 1 | 0 | -2.409227 | -3.664120 | 0.298747 |
| 52 | 1 | 0 | -2.537051 | 1.242448 | -0.485399 |
| 53 | 1 | 0 | 0.866984 | 2.037308 | -1.169787 |
| 54 | 1 | 0 | -0.866976 | 2.037304 | -1.169817 |
| 55 | 1 | 0 | -0.879980 | 2.240122 | 1.340874 |
| 56 | 1 | 0 | 0.879877 | 2.240097 | 1.340925 |
| 57 | 1 | 0 | 2.151924 | 4.189479 | 0.522592 |
| 58 | 1 | 0 | 2.159801 | 6.633537 | 0.065208 |
| 59 | 1 | 0 | -2.159702 | 6.633548 | 0.064790 |
| 60 | 1 | 0 | -2.151927 | 4.189494 | 0.522184 |
| 61 | 1 | 0 | 4.955521 | 1.210335 | -0.449770 |
| 62 | 1 | 0 | 4.884092 | -3.709534 | 0.331083 |
| 63 | 1 | 0 | -4.884107 | -3.709524 | 0.331081 |
| 64 | 1 | 0 | -4.955527 | 1.210345 | -0.449764 |
| 65 | 1 | 0 | 7.419603 | 1.179555 | -0.415990 |
| 66 | 1 | 0 | 7.352797 | -3.736282 | 0.365334 |
| 67 | 1 | 0 | -7.352811 | -3.736267 | 0.365334 |
| 68 | 1 | 0 | -7.419607 | 1.179570 | -0.415978 |
| 69 | 1 | 0 | -9.825849 | -3.765606 | 0.398412 |
| 70 | 1 | 0 | -11.965504 | -2.559398 | 0.230295 |
| 71 | 1 | 0 | -11.999121 | -0.102291 | -0.160611 |
| 72 | 1 | 0 | -9.892462 | 1.152626 | -0.383956 |
| 73 | 1 | 0 | 9.892457 | 1.152603 | -0.383973 |
| 74 | 1 | 0 | 11.999114 | -0.102318 | -0.160628 |
| 75 | 1 | 0 | 11.965492 | -2.559424 | 0.230284 |
| 76 | 1 | 0 | 9.825835 | -3.765626 | 0.398408 |

R=Sat-NO

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 1.286055 | 0.159980 | -0.229702 |
| 2 | 6 | 0 | 1.285953 | -1.297473 | -0.038356 |
| 3 | 6 | 0 | 0.059381 | -1.975915 | 0.039881 |
| 4 | 6 | 0 | -1.176522 | -1.315269 | -0.039171 |
| 5 | 6 | 0 | -1.194626 | 0.140768 | -0.227997 |
| 6 | 6 | 0 | 0.040886 | 0.847536 | -0.349506 |
| 7 | 6 | 0 | 2.522755 | 0.801369 | -0.280565 |
| 8 | 6 | 0 | 3.762941 | 0.116409 | -0.168499 |
| 9 | 6 | 0 | 3.751834 | -1.328452 | 0.008339 |
| 10 | 6 | 0 | 2.496291 | -1.980120 | 0.066352 |
| 11 | 6 | 0 | -2.378353 | -2.013560 | 0.060962 |
| 12 | 6 | 0 | -3.640787 | -1.375009 | 0.002653 |
| 13 | 6 | 0 | -3.667354 | 0.070196 | -0.166583 |
| 14 | 6 | 0 | -2.436443 | 0.773111 | -0.277496 |
| 15 | 6 | 0 | 0.005764 | 2.336612 | -0.560751 |
| 16 | 6 | 0 | -0.168938 | 3.125673 | 0.765929 |
| 17 | 7 | 0 | -0.530840 | 4.520483 | 0.517428 |
| 18 | 6 | 0 | 0.501896 | 5.542179 | 0.355750 |
| 19 | 8 | 0 | -1.670748 | 4.739951 | -0.019110 |
| 20 | 6 | 0 | -4.840799 | -2.069335 | 0.105383 |
| 21 | 6 | 0 | -6.092681 | -1.413872 | 0.052559 |
| 22 | 6 | 0 | -6.119008 | 0.026945 | -0.113037 |
| 23 | 6 | 0 | -4.891741 | 0.723363 | -0.217600 |
| 24 | 6 | 0 | 4.981714 | 0.780184 | -0.224627 |
| 25 | 6 | 0 | 6.216664 | 0.098085 | -0.116134 |
| 26 | 6 | 0 | 6.204617 | -1.341786 | 0.059519 |
| 27 | 6 | 0 | 4.959135 | -2.009109 | 0.115616 |
| 28 | 6 | 0 | -7.356756 | 0.681686 | -0.164617 |
| 29 | 6 | 0 | -8.565007 | -0.013148 | -0.061396 |
| 30 | 6 | 0 | -8.539277 | -1.448779 | 0.103331 |
| 31 | 6 | 0 | -7.307263 | -2.106212 | 0.155516 |
| 32 | 6 | 0 | 7.425901 | -2.021326 | 0.167318 |
| 33 | 6 | 0 | 8.651722 | -1.352696 | 0.110310 |
| 34 | 6 | 0 | 8.663513 | 0.081791 | -0.065136 |
| 35 | 6 | 0 | 7.448316 | 0.763860 | -0.173050 |
| 36 | 6 | 0 | -9.781490 | -2.145770 | 0.207263 |
| 37 | 6 | 0 | -10.971784 | -1.475246 | 0.152863 |
| 38 | 6 | 0 | -10.996996 | -0.060432 | -0.009395 |
| 39 | 6 | 0 | -9.830808 | 0.645794 | -0.112972 |
| 40 | 6 | 0 | 9.923076 | 0.752092 | -0.122108 |
| 41 | 6 | 0 | 11.096055 | 0.057832 | -0.013547 |
| 42 | 6 | 0 | 11.084520 | -1.355813 | 0.159447 |
| 43 | 6 | 0 | 9.900492 | -2.036988 | 0.219177 |
| 44 | 1 | 0 | 0.067615 | -3.052524 | 0.178092 |
| 45 | 1 | 0 | 2.572012 | 1.875096 | -0.409614 |
| 46 | 1 | 0 | 2.476190 | -3.056938 | 0.202701 |
| 47 | 1 | 0 | -2.345970 | -3.090645 | 0.193115 |
| 48 | 1 | 0 | -2.499792 | 1.848060 | -0.392631 |
| 49 | 1 | 0 | 0.905250 | 2.680985 | -1.072429 |
| 50 | 1 | 0 | -0.833385 | 2.611170 | -1.201839 |
| 51 | 1 | 0 | -0.982229 | 2.689265 | 1.347714 |
| 52 | 1 | 0 | 0.743131 | 3.094258 | 1.365758 |
| 53 | 1 | 0 | 0.023546 | 6.513079 | 0.475124 |
| 54 | 1 | 0 | 1.278872 | 5.413642 | 1.111388 |
| 55 | 1 | 0 | 0.953962 | 5.491774 | -0.642949 |
| 56 | 1 | 0 | -4.820568 | -3.147535 | 0.230855 |
| 57 | 1 | 0 | -4.911308 | 1.801574 | -0.341747 |
| 58 | 1 | 0 | 4.993265 | 1.857787 | -0.358020 |
| 59 | 1 | 0 | 4.949719 | -3.086754 | 0.246732 |
| 60 | 1 | 0 | -7.376180 | 1.760093 | -0.288375 |
| 61 | 1 | 0 | -7.289235 | -3.184731 | 0.279363 |
| 62 | 1 | 0 | 7.418144 | -3.099065 | 0.298722 |
| 63 | 1 | 0 | 7.458302 | 1.841573 | -0.305182 |
| 64 | 1 | 0 | -9.762121 | -3.223563 | 0.330827 |
| 65 | 1 | 0 | -11.906697 | -2.018263 | 0.233156 |
| 66 | 1 | 0 | -11.950576 | 0.453668 | -0.050306 |
| 67 | 1 | 0 | -9.848992 | 1.723558 | -0.236605 |
| 68 | 1 | 0 | 9.931371 | 1.829064 | -0.254073 |
| 69 | 1 | 0 | 12.044658 | 0.580740 | -0.058762 |
| 70 | 1 | 0 | 12.024537 | -1.889316 | 0.243548 |
| 71 | 1 | 0 | 9.891276 | -3.113962 | 0.350793 |

R=Sat-Allyl

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 1.234936 | 0.172257 | -0.215061 |
| 2 | 6 | 0 | 1.227413 | -1.273661 | 0.016130 |

| | | | | | |
|---|---|---|---|---|---|
| 3 | 6 | 0 | -0.000003 | -1.943102 | 0.119252 |
| 4 | 6 | 0 | -1.227419 | -1.273660 | 0.016129 |
| 5 | 6 | 0 | -1.234941 | 0.172257 | -0.215063 |
| 6 | 6 | 0 | -0.000002 | 0.872000 | -0.340532 |
| 7 | 6 | 0 | 2.483370 | 0.805180 | -0.299032 |
| 8 | 6 | 0 | 3.710353 | 0.113923 | -0.178447 |
| 9 | 6 | 0 | 3.691036 | -1.324515 | 0.044418 |
| 10 | 6 | 0 | 2.439378 | -1.965046 | 0.133329 |
| 11 | 6 | 0 | -2.439385 | -1.965044 | 0.133327 |
| 12 | 6 | 0 | -3.691042 | -1.324513 | 0.044416 |
| 13 | 6 | 0 | -3.710358 | 0.113925 | -0.178449 |
| 14 | 6 | 0 | -2.483374 | 0.805181 | -0.299036 |
| 15 | 6 | 0 | -0.000001 | 2.367794 | -0.566609 |
| 16 | 6 | 0 | -0.000004 | 3.185160 | 0.751373 |
| 17 | 6 | 0 | 0.000026 | 4.684471 | 0.499604 |
| 18 | 6 | 0 | 1.211255 | 5.350282 | 0.373858 |
| 19 | 6 | 0 | -1.211176 | 5.350298 | 0.373665 |
| 20 | 6 | 0 | -4.901770 | -2.011875 | 0.162306 |
| 21 | 6 | 0 | -6.146450 | -1.355882 | 0.072384 |
| 22 | 6 | 0 | -6.166997 | 0.079726 | -0.150096 |
| 23 | 6 | 0 | -4.941358 | 0.767529 | -0.268200 |
| 24 | 6 | 0 | 4.941353 | 0.767526 | -0.268199 |
| 25 | 6 | 0 | 6.166991 | 0.079721 | -0.150096 |
| 26 | 6 | 0 | 6.146444 | -1.355886 | 0.072384 |
| 27 | 6 | 0 | 4.901763 | -2.011878 | 0.162307 |
| 28 | 6 | 0 | -7.367110 | -2.040575 | 0.189834 |
| 29 | 6 | 0 | -8.596003 | -1.382991 | 0.098914 |
| 30 | 6 | 0 | -8.616292 | 0.046112 | -0.122871 |
| 31 | 6 | 0 | -7.406199 | 0.733861 | -0.240571 |
| 32 | 6 | 0 | 7.406194 | 0.733855 | -0.240573 |
| 33 | 6 | 0 | 8.616286 | 0.046105 | -0.122876 |
| 34 | 6 | 0 | 8.595996 | -1.382998 | 0.098910 |
| 35 | 6 | 0 | 7.367102 | -2.040580 | 0.189833 |
| 36 | 6 | 0 | 9.841320 | -2.072505 | 0.217161 |
| 37 | 6 | 0 | 11.029531 | -1.402348 | 0.123664 |
| 38 | 6 | 0 | 11.049443 | 0.005226 | -0.094802 |
| 39 | 6 | 0 | 9.880447 | 0.704545 | -0.213870 |
| 40 | 6 | 0 | -9.880452 | 0.704553 | -0.213864 |
| 41 | 6 | 0 | -11.049449 | 0.005235 | -0.094793 |
| 42 | 6 | 0 | -11.029538 | -1.402339 | 0.123673 |
| 43 | 6 | 0 | -9.841327 | -2.072497 | 0.217167 |
| 44 | 1 | 0 | -0.000004 | -3.014941 | 0.290359 |
| 45 | 1 | 0 | 2.537420 | 1.873424 | -0.462622 |
| 46 | 1 | 0 | 2.411647 | -3.037192 | 0.301407 |
| 47 | 1 | 0 | -2.411655 | -3.037191 | 0.301406 |
| 48 | 1 | 0 | -2.537424 | 1.873425 | -0.462627 |
| 49 | 1 | 0 | 0.865660 | 2.661121 | -1.163155 |
| 50 | 1 | 0 | -0.865659 | 2.661121 | -1.163161 |
| 51 | 1 | 0 | -0.876654 | 2.908354 | 1.343143 |
| 52 | 1 | 0 | 0.876621 | 2.908324 | 1.343164 |
| 53 | 1 | 0 | 1.247768 | 6.412580 | 0.162301 |
| 54 | 1 | 0 | 2.156030 | 4.834520 | 0.497198 |
| 55 | 1 | 0 | -2.155977 | 4.834548 | 0.496858 |
| 56 | 1 | 0 | -1.247642 | 6.412595 | 0.162101 |
| 57 | 1 | 0 | -4.885659 | -3.084600 | 0.328184 |
| 58 | 1 | 0 | -4.958767 | 1.840093 | -0.435804 |
| 59 | 1 | 0 | 4.958762 | 1.840089 | -0.435803 |
| 60 | 1 | 0 | 4.885652 | -3.084604 | 0.328185 |
| 61 | 1 | 0 | -7.353204 | -3.113415 | 0.356065 |
| 62 | 1 | 0 | -7.422643 | 1.806643 | -0.407143 |
| 63 | 1 | 0 | 7.422638 | 1.806638 | -0.407145 |
| 64 | 1 | 0 | 7.353196 | -3.113421 | 0.356063 |
| 65 | 1 | 0 | 9.825882 | -3.144598 | 0.383487 |
| 66 | 1 | 0 | 11.966543 | -1.939851 | 0.215489 |
| 67 | 1 | 0 | 12.001280 | 0.519254 | -0.166178 |
| 68 | 1 | 0 | 9.895157 | 1.776644 | -0.380292 |
| 69 | 1 | 0 | -9.895162 | 1.776652 | -0.380285 |
| 70 | 1 | 0 | -12.001285 | 0.519264 | -0.166167 |
| 71 | 1 | 0 | -11.966549 | -1.939841 | 0.215499 |
| 72 | 1 | 0 | -9.825889 | -3.144590 | 0.383492 |

R=Sat-IN

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 1.448195 | -0.870346 | -0.236066 |
| 2 | 6 | 0 | 1.492522 | -2.321477 | -0.042769 |
| 3 | 6 | 0 | 0.289690 | -3.038336 | 0.035413 |
| 4 | 6 | 0 | -0.962123 | -2.411335 | -0.045575 |
| 5 | 6 | 0 | -1.021575 | -0.961636 | -0.237420 |
| 6 | 6 | 0 | 0.188249 | -0.219631 | -0.358471 |
| 7 | 6 | 0 | 2.671339 | -0.186087 | -0.284423 |
| 8 | 6 | 0 | 3.922446 | -0.833311 | -0.168360 |
| 9 | 6 | 0 | 3.956105 | -2.278210 | 0.007482 |
| 10 | 6 | 0 | 2.729329 | -2.969039 | 0.064110 |
| 11 | 6 | 0 | -2.149633 | -3.146158 | 0.057222 |
| 12 | 6 | 0 | -3.421814 | -2.542456 | 0.000353 |
| 13 | 6 | 0 | -3.488762 | -1.098314 | -0.170179 |
| 14 | 6 | 0 | -2.287957 | -0.360961 | -0.285592 |
| 15 | 6 | 0 | 0.119743 | 1.272336 | -0.592949 |
| 16 | 6 | 0 | 0.013307 | 2.086294 | 0.724256 |
| 17 | 6 | 0 | -0.178866 | 3.544814 | 0.466869 |
| 18 | 7 | 0 | -1.420502 | 4.003308 | 0.000831 |
| 19 | 6 | 0 | -1.435931 | 5.502442 | 0.023637 |
| 20 | 6 | 0 | 0.120492 | 5.760018 | 0.126631 |
| 21 | 7 | 0 | 0.693785 | 4.472886 | 0.612762 |
| 22 | 6 | 0 | 0.779448 | 6.026299 | -1.240153 |
| 23 | 6 | 0 | 0.516702 | 6.877940 | 1.096275 |
| 24 | 6 | 0 | -2.228694 | 5.908519 | 1.278824 |
| 25 | 6 | 0 | -2.144957 | 6.028778 | -1.223539 |
| 26 | 8 | 0 | -2.447189 | 3.289755 | -0.208956 |
| 27 | 6 | 0 | -4.739204 | -0.477895 | -0.215393 |
| 28 | 6 | 0 | -5.941075 | -1.207870 | -0.106089 |
| 29 | 6 | 0 | -5.874220 | -2.649907 | 0.059263 |
| 30 | 6 | 0 | -4.609317 | -3.270948 | 0.107683 |
| 31 | 6 | 0 | 5.191170 | -2.922152 | 0.117509 |
| 32 | 6 | 0 | 6.410529 | -2.216266 | 0.065619 |
| 33 | 6 | 0 | 6.377921 | -0.774029 | -0.107051 |
| 34 | 6 | 0 | 5.128093 | -0.129964 | -0.218289 |
| 35 | 6 | 0 | 7.591809 | -0.069999 | -0.157895 |
| 36 | 6 | 0 | 8.826240 | -0.714461 | -0.047772 |
| 37 | 6 | 0 | 8.858847 | -2.150190 | 0.124020 |
| 38 | 6 | 0 | 7.655351 | -2.857238 | 0.175689 |
| 39 | 6 | 0 | -7.072076 | -3.375420 | 0.167080 |
| 40 | 6 | 0 | -8.321234 | -2.752323 | 0.120362 |
| 41 | 6 | 0 | -8.387557 | -1.316797 | -0.043867 |
| 42 | 6 | 0 | -7.200532 | -0.588558 | -0.152000 |
| 43 | 6 | 0 | -9.672119 | -0.693992 | -0.089642 |
| 44 | 6 | 0 | -10.817874 | -1.432420 | 0.018823 |
| 45 | 6 | 0 | -10.752607 | -2.846323 | 0.180554 |
| 46 | 6 | 0 | -9.543621 | -3.483265 | 0.229454 |
| 47 | 6 | 0 | 10.128522 | -2.794999 | 0.235130 |
| 48 | 6 | 0 | 11.290925 | -2.076873 | 0.181039 |
| 49 | 6 | 0 | 11.258757 | -0.662773 | 0.011859 |
| 50 | 6 | 0 | 10.064909 | -0.005204 | -0.098674 |
| 51 | 1 | 0 | 0.329365 | -4.114106 | 0.174759 |
| 52 | 1 | 0 | 2.685892 | 0.889150 | -0.408020 |
| 53 | 1 | 0 | 2.741925 | -4.045898 | 0.201148 |
| 54 | 1 | 0 | -2.086156 | -4.221582 | 0.191722 |
| 55 | 1 | 0 | -2.380672 | 0.711849 | -0.399370 |
| 56 | 1 | 0 | 0.996378 | 1.613162 | -1.145586 |
| 57 | 1 | 0 | -0.740269 | 1.506745 | -1.220583 |
| 58 | 1 | 0 | -0.833856 | 1.715355 | 1.306873 |
| 59 | 1 | 0 | 0.919797 | 1.967742 | 1.318500 |
| 60 | 1 | 0 | 1.862956 | 6.043306 | -1.109739 |
| 61 | 1 | 0 | 0.543311 | 5.241234 | -1.961412 |
| 62 | 1 | 0 | 0.465301 | 6.987420 | -1.654691 |
| 63 | 1 | 0 | 0.110078 | 7.841440 | 0.775514 |
| 64 | 1 | 0 | 0.177630 | 6.677571 | 2.112512 |
| 65 | 1 | 0 | 1.605255 | 6.956881 | 1.120304 |
| 66 | 1 | 0 | -3.237195 | 5.496386 | 1.205294 |
| 67 | 1 | 0 | -1.769153 | 5.522573 | 2.190467 |
| 68 | 1 | 0 | -2.302212 | 6.994692 | 1.359358 |
| 69 | 1 | 0 | -2.162219 | 7.121243 | -1.216485 |
| 70 | 1 | 0 | -1.667496 | 5.693978 | -2.143890 |
| 71 | 1 | 0 | -3.175250 | 5.668393 | -1.229719 |
| 72 | 1 | 0 | -4.786758 | 0.599581 | -0.337731 |
| 73 | 1 | 0 | -4.558904 | -4.348059 | 0.233970 |
| 74 | 1 | 0 | 5.214752 | -3.999643 | 0.247964 |
| 75 | 1 | 0 | 5.105315 | 0.947760 | -0.347473 |
| 76 | 1 | 0 | 7.568367 | 1.007851 | -0.286580 |
| 77 | 1 | 0 | 7.681132 | -3.934982 | 0.304786 |
| 78 | 1 | 0 | -7.023783 | -4.453070 | 0.290621 |
| 79 | 1 | 0 | -7.250530 | 0.488933 | -0.275470 |
| 80 | 1 | 0 | -9.721064 | 0.382927 | -0.212928 |
| 81 | 1 | 0 | -11.785602 | -0.945030 | -0.017782 |
| 82 | 1 | 0 | -11.671635 | -3.415277 | 0.264808 |
| 83 | 1 | 0 | -9.493715 | -4.560167 | 0.352606 |
| 84 | 1 | 0 | 10.152723 | -3.872097 | 0.364016 |
| 85 | 1 | 0 | 12.246919 | -2.580937 | 0.266893 |
| 86 | 1 | 0 | 12.190678 | -0.110289 | -0.028660 |
| 87 | 1 | 0 | 10.039872 | 1.071895 | -0.227431 |

R=Sat-Phen

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 1.235078 | -1.336508 | -0.208461 |
| 2 | 6 | 0 | 1.227442 | -2.785408 | 0.003315 |
| 3 | 6 | 0 | 0.000020 | -3.456038 | 0.097898 |
| 4 | 6 | 0 | -1.227406 | -2.785416 | 0.003315 |
| 5 | 6 | 0 | -1.235051 | -1.336515 | -0.208461 |
| 6 | 6 | 0 | 0.000012 | -0.634995 | -0.323176 |
| 7 | 6 | 0 | 2.483655 | -0.703017 | -0.285426 |
| 8 | 6 | 0 | 3.710607 | -1.396132 | -0.175282 |
| 9 | 6 | 0 | 3.691059 | -2.837202 | 0.029633 |
| 10 | 6 | 0 | 2.439301 | -3.478477 | 0.111074 |
| 11 | 6 | 0 | -2.439261 | -3.478492 | 0.111073 |
| 12 | 6 | 0 | -3.691023 | -2.837224 | 0.029631 |
| 13 | 6 | 0 | -3.710579 | -1.396154 | -0.175283 |
| 14 | 6 | 0 | -2.483631 | -0.703032 | -0.285426 |
| 15 | 6 | 0 | 0.000007 | 0.864327 | -0.522552 |
| 16 | 6 | 0 | 0.000001 | 1.656343 | 0.813394 |
| 17 | 6 | 0 | -0.000015 | 3.153807 | 0.600213 |
| 18 | 6 | 0 | 1.201650 | 3.853151 | 0.483557 |
| 19 | 6 | 0 | 1.234165 | 5.248157 | 0.244572 |
| 20 | 6 | 0 | -0.000047 | 5.955203 | 0.121685 |
| 21 | 6 | 0 | -1.234244 | 5.248136 | 0.244617 |
| 22 | 6 | 0 | -1.201696 | 3.853131 | 0.483600 |
| 23 | 6 | 0 | -0.000064 | 7.363541 | -0.117306 |

| | | | | | |
|---|---|---|---|---|---|
| 24 | 6 | 0 | -1.242026 | 8.035609 | -0.230290 |
| 25 | 6 | 0 | -2.439693 | 7.340593 | -0.108257 |
| 26 | 6 | 0 | -2.447502 | 5.970524 | 0.126446 |
| 27 | 6 | 0 | 2.447407 | 5.970565 | 0.126356 |
| 28 | 6 | 0 | 2.439567 | 7.340634 | -0.108347 |
| 29 | 6 | 0 | 1.241883 | 8.035630 | -0.230336 |
| 30 | 6 | 0 | -4.941701 | -0.741998 | -0.258813 |
| 31 | 6 | 0 | -6.167252 | -1.431593 | -0.150626 |
| 32 | 6 | 0 | -6.146420 | -2.869727 | 0.054784 |
| 33 | 6 | 0 | -4.901623 | -3.526356 | 0.137994 |
| 34 | 6 | 0 | 4.901663 | -3.526327 | 0.137997 |
| 35 | 6 | 0 | 6.146457 | -2.869691 | 0.054787 |
| 36 | 6 | 0 | 6.167280 | -1.431556 | -0.150622 |
| 37 | 6 | 0 | 4.941726 | -0.741969 | -0.258810 |
| 38 | 6 | 0 | 7.366984 | -3.556166 | 0.162771 |
| 39 | 6 | 0 | 8.596009 | -2.898002 | 0.078175 |
| 40 | 6 | 0 | 8.616592 | -1.466420 | -0.126943 |
| 41 | 6 | 0 | 7.406620 | -0.776892 | -0.235043 |
| 42 | 6 | 0 | -7.406595 | -0.776937 | -0.235048 |
| 43 | 6 | 0 | -8.616564 | -1.466472 | -0.126950 |
| 44 | 6 | 0 | -8.595972 | -2.898053 | 0.078168 |
| 45 | 6 | 0 | -7.366943 | -3.556210 | 0.162766 |
| 46 | 6 | 0 | -9.880869 | -0.807513 | -0.211893 |
| 47 | 6 | 0 | -11.049714 | -1.508635 | -0.102387 |
| 48 | 6 | 0 | -11.029501 | -2.918638 | 0.099772 |
| 49 | 6 | 0 | -9.841148 | -3.589386 | 0.186906 |
| 50 | 6 | 0 | 9.841189 | -3.589327 | 0.186914 |
| 51 | 6 | 0 | 11.029538 | -2.918572 | 0.099783 |
| 52 | 6 | 0 | 11.049742 | -1.508569 | -0.102376 |
| 53 | 6 | 0 | 9.880894 | -0.807454 | -0.211883 |
| 54 | 1 | 0 | 0.000023 | -4.530008 | 0.255013 |
| 55 | 1 | 0 | 2.538090 | 0.367056 | -0.436449 |
| 56 | 1 | 0 | 2.411380 | -4.552700 | 0.265225 |
| 57 | 1 | 0 | -2.411334 | -4.552714 | 0.265224 |
| 58 | 1 | 0 | -2.538073 | 0.367041 | -0.436449 |
| 59 | 1 | 0 | 0.865522 | 1.169534 | -1.113118 |
| 60 | 1 | 0 | -0.865507 | 1.169528 | -1.113121 |
| 61 | 1 | 0 | -0.876564 | 1.364488 | 1.398591 |
| 62 | 1 | 0 | 0.876574 | 1.364505 | 1.398589 |
| 63 | 1 | 0 | 2.143370 | 3.322640 | 0.588156 |
| 64 | 1 | 0 | -2.143403 | 3.322604 | 0.588233 |
| 65 | 1 | 0 | -1.246892 | 9.104700 | -0.412556 |
| 66 | 1 | 0 | -3.379757 | 7.874013 | -0.196407 |
| 67 | 1 | 0 | -3.387944 | 5.438628 | 0.221560 |
| 68 | 1 | 0 | 3.387862 | 5.438685 | 0.221435 |
| 69 | 1 | 0 | 3.379618 | 7.874069 | -0.196532 |
| 70 | 1 | 0 | 1.246725 | 9.104721 | -0.412602 |
| 71 | 1 | 0 | -4.959334 | 0.332459 | -0.413835 |
| 72 | 1 | 0 | -4.885309 | -4.601027 | 0.290681 |
| 73 | 1 | 0 | 4.885355 | -4.600998 | 0.290683 |
| 74 | 1 | 0 | 4.959352 | 0.332489 | -0.413832 |
| 75 | 1 | 0 | 7.352861 | -4.630884 | 0.316324 |
| 76 | 1 | 0 | 7.423325 | 0.297744 | -0.389195 |
| 77 | 1 | 0 | -7.423307 | 0.297700 | -0.389201 |
| 78 | 1 | 0 | -7.352814 | -4.630928 | 0.316319 |
| 79 | 1 | 0 | -9.895839 | 0.266428 | -0.365948 |
| 80 | 1 | 0 | -12.001674 | -0.994207 | -0.169009 |
| 81 | 1 | 0 | -11.966408 | -3.457521 | 0.184212 |
| 82 | 1 | 0 | -9.825480 | -4.663330 | 0.340765 |
| 83 | 1 | 0 | 9.825527 | -4.663271 | 0.340774 |
| 84 | 1 | 0 | 11.966448 | -3.457449 | 0.184223 |
| 85 | 1 | 0 | 12.001700 | -0.994135 | -0.168997 |
| 86 | 1 | 0 | 9.895858 | 0.266488 | -0.365938 |

R=Sat-Ver

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 1.235451 | -1.923950 | -0.239950 |
| 2 | 6 | 0 | 1.227947 | -3.376270 | -0.054744 |
| 3 | 6 | 0 | -0.000051 | -4.048745 | 0.023780 |
| 4 | 6 | 0 | -1.228048 | -3.376259 | -0.054662 |
| 5 | 6 | 0 | -1.235553 | -1.923938 | -0.239865 |
| 6 | 6 | 0 | -0.000052 | -1.224717 | -0.352376 |
| 7 | 6 | 0 | 2.482099 | -1.283900 | -0.292763 |
| 8 | 6 | 0 | 3.709236 | -1.977360 | -0.187385 |
| 9 | 6 | 0 | 3.691402 | -3.422956 | -0.016029 |
| 10 | 6 | 0 | 2.440675 | -4.069102 | 0.044342 |
| 11 | 6 | 0 | -2.440776 | -4.069081 | 0.044505 |
| 12 | 6 | 0 | -3.691502 | -3.422924 | -0.015779 |
| 13 | 6 | 0 | -3.709335 | -1.977326 | -0.187130 |
| 14 | 6 | 0 | -2.482198 | -1.283877 | -0.292590 |
| 15 | 6 | 0 | -0.000050 | 0.272926 | -0.556877 |
| 16 | 6 | 0 | 0.000018 | 1.066415 | 0.774196 |
| 17 | 6 | 0 | 0.000043 | 2.553146 | 0.532135 |
| 18 | 7 | 0 | -1.186347 | 3.132865 | 0.406500 |
| 19 | 7 | 0 | -1.171669 | 4.473773 | 0.132329 |
| 20 | 6 | 0 | 0.000091 | 5.238713 | 0.021242 |
| 21 | 7 | 0 | 1.171817 | 4.473693 | 0.132115 |
| 22 | 7 | 0 | 1.186451 | 3.132784 | 0.406286 |
| 23 | 6 | 0 | 2.467847 | 5.091967 | 0.088865 |
| 24 | 6 | 0 | 3.470110 | 4.585470 | 0.921046 |
| 25 | 6 | 0 | 4.745947 | 5.135918 | 0.880337 |
| 26 | 6 | 0 | 5.032246 | 6.189366 | 0.014692 |
| 27 | 6 | 0 | 4.029914 | 6.686201 | -0.814798 |
| 28 | 6 | 0 | 2.748298 | 6.145043 | -0.786185 |
| 29 | 6 | 0 | -2.467664 | 5.092139 | 0.089318 |
| 30 | 6 | 0 | -3.469809 | 4.585712 | 0.921685 |
| 31 | 6 | 0 | -4.745614 | 5.136253 | 0.881215 |
| 32 | 6 | 0 | -5.031998 | 6.189723 | 0.015627 |
| 33 | 6 | 0 | -4.029785 | 6.686488 | -0.814049 |
| 34 | 6 | 0 | -2.748202 | 6.145236 | -0.785678 |
| 35 | 8 | 0 | 0.000116 | 6.435829 | -0.154733 |
| 36 | 6 | 0 | -4.939083 | -1.317669 | -0.244331 |
| 37 | 6 | 0 | -6.165307 | -2.007104 | -0.143078 |
| 38 | 6 | 0 | -6.146702 | -3.449854 | 0.027422 |
| 39 | 6 | 0 | -4.903062 | -4.111480 | 0.085477 |
| 40 | 6 | 0 | 4.902963 | -4.111523 | 0.085148 |
| 41 | 6 | 0 | 6.146604 | -3.449908 | 0.027006 |
| 42 | 6 | 0 | 6.165210 | -2.007159 | -0.143501 |
| 43 | 6 | 0 | 4.938985 | -1.317714 | -0.244673 |
| 44 | 6 | 0 | 7.368104 | -4.135739 | 0.128019 |
| 45 | 6 | 0 | 8.595976 | -3.472636 | 0.068818 |
| 46 | 6 | 0 | 8.614326 | -2.036498 | -0.101893 |
| 47 | 6 | 0 | 7.403418 | -1.347513 | -0.202704 |
| 48 | 6 | 0 | -7.403514 | -1.347447 | -0.202195 |
| 49 | 6 | 0 | -8.614420 | -2.036423 | -0.101305 |
| 50 | 6 | 0 | -8.596071 | -3.472561 | 0.069398 |
| 51 | 6 | 0 | -7.368201 | -4.135675 | 0.128514 |
| 52 | 6 | 0 | -9.877616 | -1.372529 | -0.160894 |
| 53 | 6 | 0 | -11.047489 | -2.073107 | -0.059065 |
| 54 | 6 | 0 | -11.029465 | -3.487570 | 0.109415 |
| 55 | 6 | 0 | -9.842253 | -4.163144 | 0.171321 |
| 56 | 6 | 0 | 9.842159 | -4.163229 | 0.170660 |
| 57 | 6 | 0 | 11.029373 | -3.487665 | 0.108672 |
| 58 | 6 | 0 | 11.047398 | -2.073202 | -0.059817 |
| 59 | 6 | 0 | 9.877523 | -1.372616 | -0.161570 |
| 60 | 1 | 0 | -0.000051 | -5.125721 | 0.159042 |
| 61 | 1 | 0 | 2.535630 | -0.209344 | -0.411034 |
| 62 | 1 | 0 | 2.414622 | -5.146302 | 0.176606 |
| 63 | 1 | 0 | -2.414724 | -5.146281 | 0.176766 |
| 64 | 1 | 0 | -2.535727 | -0.209319 | -0.410856 |
| 65 | 1 | 0 | 0.868720 | 0.574960 | -1.143910 |
| 66 | 1 | 0 | -0.868868 | 0.574976 | -1.143831 |
| 67 | 1 | 0 | -0.883754 | 0.804862 | 1.358514 |
| 68 | 1 | 0 | 0.883825 | 0.804822 | 1.358443 |
| 69 | 1 | 0 | 3.241193 | 3.761618 | 1.582124 |
| 70 | 1 | 0 | 5.516107 | 4.740967 | 1.532923 |
| 71 | 1 | 0 | 6.026882 | 6.618976 | -0.013109 |
| 72 | 1 | 0 | 4.242077 | 7.502508 | -1.495557 |
| 73 | 1 | 0 | 1.976144 | 6.543025 | -1.425728 |
| 74 | 1 | 0 | -3.240829 | 3.761841 | 1.582718 |
| 75 | 1 | 0 | -5.515680 | 4.741355 | 1.533943 |
| 76 | 1 | 0 | -6.026607 | 6.619405 | -0.011988 |
| 77 | 1 | 0 | -4.242016 | 7.502812 | -1.494767 |
| 78 | 1 | 0 | -1.976139 | 6.543165 | -1.425363 |
| 79 | 1 | 0 | -4.953970 | -0.239728 | -0.372491 |
| 80 | 1 | 0 | -4.888544 | -5.189465 | 0.213050 |
| 81 | 1 | 0 | 4.888443 | -5.189507 | 0.212726 |
| 82 | 1 | 0 | 4.953872 | -0.239774 | -0.372838 |
| 83 | 1 | 0 | 7.355735 | -5.213885 | 0.255603 |
| 84 | 1 | 0 | 7.418016 | -0.269524 | -0.331362 |
| 85 | 1 | 0 | -7.418111 | -0.269458 | -0.330847 |
| 86 | 1 | 0 | -7.355832 | -5.213821 | 0.256092 |
| 87 | 1 | 0 | -9.890782 | -0.295223 | -0.289570 |
| 88 | 1 | 0 | -11.998575 | -1.554905 | -0.106280 |
| 89 | 1 | 0 | -11.967125 | -4.026016 | 0.188230 |
| 90 | 1 | 0 | -9.828292 | -5.240503 | 0.299381 |
| 91 | 1 | 0 | 9.828198 | -5.240588 | 0.298726 |
| 92 | 1 | 0 | 11.967034 | -4.026118 | 0.187427 |
| 93 | 1 | 0 | 11.998485 | -1.555008 | -0.107097 |
| 94 | 1 | 0 | 9.890690 | -0.295310 | -0.290252 |

R=Sat-NN

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -11.064470 | -1.114267 | 0.075252 |
| 2 | 6 | 0 | -11.054946 | -2.533608 | 0.197050 |
| 3 | 6 | 0 | -9.872255 | -3.219639 | 0.216666 |
| 4 | 6 | 0 | -8.622391 | -2.535500 | 0.116081 |
| 5 | 6 | 0 | -8.632117 | -1.094471 | -0.007746 |
| 6 | 6 | 0 | -9.890810 | -0.419589 | -0.023736 |
| 7 | 6 | 0 | -7.398982 | -3.209199 | 0.133779 |
| 8 | 6 | 0 | -6.173904 | -2.529497 | 0.034458 |
| 9 | 6 | 0 | -6.183924 | -1.082013 | -0.090790 |
| 10 | 6 | 0 | -7.417638 | -0.411575 | -0.107194 |
| 11 | 6 | 0 | -4.934578 | -3.201517 | 0.054548 |
| 12 | 6 | 0 | -3.719502 | -2.518857 | -0.044253 |
| 13 | 6 | 0 | -3.729496 | -1.068969 | -0.176759 |
| 14 | 6 | 0 | -4.954417 | -0.398341 | -0.192230 |
| 15 | 6 | 0 | -2.472663 | -3.175130 | -0.011669 |
| 16 | 6 | 0 | -1.256435 | -2.487791 | -0.104973 |
| 17 | 6 | 0 | -1.258368 | -1.032827 | -0.266296 |
| 18 | 6 | 0 | -2.499608 | -0.380630 | -0.286211 |
| 19 | 6 | 0 | -0.030357 | -3.166529 | -0.042639 |
| 20 | 6 | 0 | 1.200879 | -2.496896 | -0.101635 |
| 21 | 6 | 0 | 1.213796 | -1.042145 | -0.263380 |
| 22 | 6 | 0 | -0.019616 | -0.341942 | -0.384893 |
| 23 | 6 | 0 | 2.411839 | -3.193070 | -0.005078 |

```
   24         6          0       3.663406   -2.545635   -0.034629
   25         6          0       3.683947   -1.095944   -0.167667
   26         6          0       2.459515   -0.398414   -0.280888
   27         6          0       4.873438   -3.236725    0.067609
   28         6          0       6.117416   -2.573234    0.050592
   29         6          0       6.137809   -1.125866   -0.074985
   30         6          0       4.913405   -0.433626   -0.179988
   31         6          0       7.337518   -3.261355    0.153366
   32         6          0       8.565589   -2.596129    0.138823
   33         6          0       8.585627   -1.155221    0.014733
   34         6          0       7.376178   -0.463983   -0.088160
   35         6          0       9.810433   -3.288862    0.242920
   36         6          0      10.997888   -2.611035    0.226373
   37         6          0      11.017566   -1.191811    0.104325
   38         6          0       9.849006   -0.489069    0.002022
   39         6          0      -0.012110    1.148745   -0.620186
   40         6          0      -0.001876    1.972913    0.697515
   41         6          0       0.034098    3.426962    0.425365
   42         7          0      -1.052266    4.209040    0.287095
   43         6          0      -0.669767    5.667331    0.168960
   44         6          0       0.849582    5.549388   -0.222490
   45         7          0       1.157621    4.137569    0.222452
   46         8          0       2.346215    3.679421    0.231113
   47         8          0      -2.264091    3.834471    0.394718
   48         6          0       1.118201    5.581321   -1.735875
   49         6          0       1.794367    6.515637    0.490025
   50         6          0      -0.922813    6.282564    1.555085
   51         6          0      -1.569817    6.339367   -0.866195
   52         1          0     -12.012001   -0.587594    0.061686
   53         1          0     -11.995427   -3.067397    0.274419
   54         1          0      -9.864765   -4.300699    0.309550
   55         1          0      -9.897286    0.661480   -0.116358
   56         1          0      -7.393056   -4.290915    0.227402
   57         1          0      -7.425354    0.670140   -0.199727
   58         1          0      -4.926367   -4.282727    0.152214
   59         1          0      -4.961392    0.683231   -0.284320
   60         1          0      -2.452935   -4.255023    0.098156
   61         1          0      -2.547973    0.698186   -0.367665
   62         1          0      -0.034568   -4.246034    0.071183
   63         1          0       2.384054   -4.272780    0.104852
   64         1          0       2.516394    0.680026   -0.363052
   65         1          0       4.857537   -4.317823    0.165624
   66         1          0       4.927498    0.647857   -0.272076
   67         1          0       7.323885   -4.342985    0.247219
   68         1          0       7.391528    0.617628   -0.180920
   69         1          0       9.795224   -4.369826    0.335993
   70         1          0      11.934442   -3.151303    0.306387
   71         1          0      11.968754   -0.671710    0.093221
   72         1          0       9.863195    0.591912   -0.090799
   73         1          0       0.859931    1.429679   -1.212068
   74         1          0      -0.883737    1.441228   -1.207065
   75         1          0      -0.897988    1.755278    1.280988
   76         1          0       0.880530    1.715223    1.286134
   77         1          0       0.957030    6.582417   -2.140035
   78         1          0       2.157558    5.297877   -1.906982
   79         1          0       0.481001    4.879481   -2.277062
   80         1          0       2.821299    6.255784    0.232721
   81         1          0       1.601309    7.540974    0.165844
   82         1          0       1.698797    6.466144    1.573939
   83         1          0      -0.711143    7.353475    1.551780
   84         1          0      -1.973129    6.134578    1.810424
   85         1          0      -0.315284    5.808194    2.327826
   86         1          0      -2.605907    6.255988   -0.538059
   87         1          0      -1.315641    7.398096   -0.956602
   88         1          0      -1.492324    5.874631   -1.848258
--------------------------------------------------------------------
```

# 5-6. Triangulenes(**Tri**)

## Non-Radical

R=$NO_2$

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -0.859661 | -3.688050 | -0.000011 |
| 2 | 6 | 0 | 0.522128 | -3.686570 | -0.000008 |
| 3 | 6 | 0 | 1.244440 | -2.466494 | -0.000004 |
| 4 | 6 | 0 | 0.523079 | -1.235932 | -0.000002 |
| 5 | 6 | 0 | -0.905625 | -1.251331 | -0.000005 |
| 6 | 6 | 0 | -1.572550 | -2.487851 | -0.000009 |
| 7 | 6 | 0 | 1.236821 | 0.000000 | 0.000001 |
| 8 | 6 | 0 | 0.523076 | 1.235932 | -0.000001 |
| 9 | 6 | 0 | -0.905627 | 1.251329 | -0.000005 |
| 10 | 6 | 0 | -1.620645 | -0.000003 | -0.000003 |
| 11 | 6 | 0 | 1.244436 | 2.466495 | -0.000002 |
| 12 | 6 | 0 | 0.522121 | 3.686570 | -0.000007 |
| 13 | 6 | 0 | -0.859667 | 3.688047 | -0.000013 |
| 14 | 6 | 0 | -1.572554 | 2.487846 | -0.000011 |
| 15 | 6 | 0 | 2.650430 | 0.000002 | 0.000005 |
| 16 | 6 | 0 | 3.371964 | 1.242557 | 0.000007 |
| 17 | 6 | 0 | 2.656393 | 2.440732 | 0.000004 |
| 18 | 6 | 0 | 2.656396 | -2.440729 | -0.000002 |
| 19 | 6 | 0 | 3.371965 | -1.242553 | 0.000003 |
| 20 | 6 | 0 | 4.797530 | -1.208485 | 0.000004 |
| 21 | 6 | 0 | 5.481814 | 0.000002 | 0.000009 |
| 22 | 6 | 0 | 4.797527 | 1.208489 | 0.000012 |
| 23 | 6 | 0 | -3.017837 | -0.000005 | 0.000002 |
| 24 | 6 | 0 | -4.230003 | -0.000001 | 0.000007 |
| 25 | 7 | 0 | -5.609681 | 0.000000 | 0.000010 |
| 26 | 8 | 0 | -6.171489 | 1.097262 | -0.000002 |
| 27 | 8 | 0 | -6.171490 | -1.097261 | 0.000022 |
| 28 | 1 | 0 | -1.400476 | -4.627190 | -0.000014 |
| 29 | 1 | 0 | 1.072175 | -4.621074 | -0.000010 |
| 30 | 1 | 0 | -2.655262 | -2.504761 | -0.000010 |
| 31 | 1 | 0 | 1.072168 | 4.621074 | -0.000008 |
| 32 | 1 | 0 | -1.400485 | 4.627185 | -0.000019 |
| 33 | 1 | 0 | -2.655266 | 2.504755 | -0.000016 |
| 34 | 1 | 0 | 3.196927 | 3.381513 | 0.000013 |
| 35 | 1 | 0 | 3.196931 | -3.381509 | -0.000005 |
| 36 | 1 | 0 | 5.341564 | -2.146122 | -0.000003 |
| 37 | 1 | 0 | 6.566033 | 0.000003 | 0.000011 |
| 38 | 1 | 0 | 5.341561 | 2.146126 | 0.000018 |

R=CN

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -1.197169 | 3.689689 | 0.000000 |
| 2 | 6 | 0 | 0.184059 | 3.687985 | -0.000001 |
| 3 | 6 | 0 | 0.904715 | 2.466667 | 0.000003 |
| 4 | 6 | 0 | 0.182870 | 1.236077 | 0.000007 |
| 5 | 6 | 0 | -1.246460 | 1.251862 | 0.000006 |
| 6 | 6 | 0 | -1.910637 | 2.489502 | 0.000004 |
| 7 | 6 | 0 | 0.896810 | 0.000000 | 0.000008 |
| 8 | 6 | 0 | 0.182869 | -1.236079 | 0.000007 |
| 9 | 6 | 0 | -1.246460 | -1.251866 | 0.000005 |
| 10 | 6 | 0 | -1.961432 | -0.000001 | 0.000005 |
| 11 | 6 | 0 | 0.904715 | -2.466669 | 0.000002 |
| 12 | 6 | 0 | 0.184059 | -3.687986 | -0.000001 |
| 13 | 6 | 0 | -1.197167 | -3.689690 | 0.000001 |
| 14 | 6 | 0 | -1.910635 | -2.489505 | 0.000003 |
| 15 | 6 | 0 | 2.316708 | 2.440333 | 0.000002 |
| 16 | 6 | 0 | 3.031962 | 1.242375 | 0.000001 |
| 17 | 6 | 0 | 2.310387 | 0.000000 | 0.000004 |
| 18 | 6 | 0 | 3.031963 | -1.242373 | -0.000001 |
| 19 | 6 | 0 | 2.316710 | -2.440333 | 0.000002 |
| 20 | 6 | 0 | 4.457693 | 1.208406 | -0.000006 |
| 21 | 6 | 0 | 5.142094 | 0.000002 | -0.000009 |
| 22 | 6 | 0 | 4.457692 | -1.208402 | -0.000008 |
| 23 | 6 | 0 | -3.359850 | 0.000000 | -0.000002 |
| 24 | 6 | 0 | -4.578458 | 0.000002 | -0.000005 |
| 25 | 6 | 0 | -5.938474 | 0.000004 | -0.000007 |
| 26 | 7 | 0 | -7.100616 | 0.000000 | -0.000010 |
| 27 | 1 | 0 | -1.737594 | 4.629209 | -0.000004 |
| 28 | 1 | 0 | 0.735119 | 4.621841 | -0.000009 |
| 29 | 1 | 0 | -2.993099 | 2.509126 | 0.000006 |
| 30 | 1 | 0 | 0.735124 | -4.621839 | 0.000007 |
| 31 | 1 | 0 | -1.737594 | -4.629210 | 0.000003 |
| 32 | 1 | 0 | -2.993098 | -2.509129 | -0.000006 |
| 33 | 1 | 0 | 2.857270 | 3.381133 | -0.000009 |
| 34 | 1 | 0 | 2.857275 | -3.381132 | -0.000016 |
| 35 | 1 | 0 | 5.001586 | 2.146162 | -0.000014 |
| 36 | 1 | 0 | 6.226356 | 0.000003 | -0.000010 |
| 37 | 1 | 0 | 5.001583 | -2.146160 | -0.000003 |

R=Cl

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 1.078102 | -3.687166 | -0.000004 |
| 2 | 6 | 0 | -0.303307 | -3.688070 | 0.000000 |
| 3 | 6 | 0 | -1.024588 | -2.466572 | 0.000003 |
| 4 | 6 | 0 | -0.303329 | -1.235442 | 0.000000 |
| 5 | 6 | 0 | 1.127613 | -1.247734 | -0.000001 |
| 6 | 6 | 0 | 1.791322 | -2.486941 | -0.000004 |
| 7 | 6 | 0 | -1.017951 | 0.000000 | 0.000000 |
| 8 | 6 | 0 | -0.303336 | 1.235445 | 0.000000 |
| 9 | 6 | 0 | 1.127608 | 1.247743 | 0.000002 |
| 10 | 6 | 0 | 1.842000 | 0.000007 | 0.000000 |
| 11 | 6 | 0 | -1.024600 | 2.466571 | -0.000003 |
| 12 | 6 | 0 | -0.303324 | 3.688075 | 0.000000 |
| 13 | 6 | 0 | 1.078085 | 3.687177 | 0.000004 |
| 14 | 6 | 0 | 1.791311 | 2.486954 | 0.000004 |
| 15 | 6 | 0 | -2.436839 | -2.440049 | 0.000005 |
| 16 | 6 | 0 | -3.152592 | -1.242395 | 0.000004 |
| 17 | 6 | 0 | -2.431928 | -0.000003 | 0.000000 |
| 18 | 6 | 0 | -3.152598 | 1.242385 | -0.000004 |
| 19 | 6 | 0 | -2.436851 | 2.440042 | -0.000005 |
| 20 | 6 | 0 | -4.578678 | -1.208531 | 0.000005 |
| 21 | 6 | 0 | -5.263070 | -0.000010 | 0.000000 |
| 22 | 6 | 0 | -4.578685 | 1.208513 | -0.000005 |
| 23 | 6 | 0 | 3.252192 | 0.000009 | 0.000001 |
| 24 | 6 | 0 | 4.461838 | 0.000002 | 0.000000 |
| 25 | 17 | 0 | 6.108193 | -0.000002 | 0.000000 |
| 26 | 1 | 0 | 1.619107 | -4.626744 | -0.000008 |
| 27 | 1 | 0 | -0.853778 | -4.622354 | -0.000002 |
| 28 | 1 | 0 | 2.873685 | -2.502912 | -0.000006 |
| 29 | 1 | 0 | -0.853798 | 4.622356 | 0.000003 |
| 30 | 1 | 0 | 1.619085 | 4.626758 | 0.000008 |
| 31 | 1 | 0 | 2.873674 | 2.502930 | 0.000006 |
| 32 | 1 | 0 | -2.977432 | -3.381016 | 0.000005 |
| 33 | 1 | 0 | -2.977448 | 3.381006 | -0.000009 |
| 34 | 1 | 0 | -5.122617 | -2.146399 | 0.000007 |
| 35 | 1 | 0 | -6.347494 | -0.000012 | 0.000001 |
| 36 | 1 | 0 | -5.122630 | 2.146378 | -0.000007 |

R=H

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -1.708374 | -3.686824 | 0.000000 |
| 2 | 6 | 0 | -0.326883 | -3.687879 | -0.000001 |
| 3 | 6 | 0 | 0.394501 | -2.466437 | -0.000002 |
| 4 | 6 | 0 | -0.326737 | -1.235355 | 0.000000 |
| 5 | 6 | 0 | -1.757881 | -1.247468 | 0.000000 |
| 6 | 6 | 0 | -2.421887 | -2.486807 | 0.000001 |
| 7 | 6 | 0 | 0.387897 | 0.000000 | -0.000001 |
| 8 | 6 | 0 | -0.326732 | 1.235360 | 0.000000 |
| 9 | 6 | 0 | -1.757878 | 1.247474 | -0.000001 |
| 10 | 6 | 0 | -2.471718 | 0.000003 | -0.000001 |
| 11 | 6 | 0 | 0.394508 | 2.466440 | 0.000000 |
| 12 | 6 | 0 | -0.326874 | 3.687882 | -0.000001 |
| 13 | 6 | 0 | -1.708366 | 3.686831 | -0.000003 |
| 14 | 6 | 0 | -2.421881 | 2.486815 | -0.000003 |
| 15 | 6 | 0 | 1.801996 | -0.000002 | 0.000000 |
| 16 | 6 | 0 | 2.522611 | 1.242379 | 0.000002 |
| 17 | 6 | 0 | 1.806774 | 2.439982 | 0.000001 |
| 18 | 6 | 0 | 1.806765 | -2.439986 | -0.000004 |
| 19 | 6 | 0 | 2.522606 | -1.242384 | -0.000001 |
| 20 | 6 | 0 | 3.948745 | -1.208538 | -0.000001 |
| 21 | 6 | 0 | 4.633125 | -0.000008 | 0.000003 |
| 22 | 6 | 0 | 3.948749 | 1.208527 | 0.000004 |
| 23 | 6 | 0 | -3.883990 | 0.000004 | -0.000001 |
| 24 | 6 | 0 | -5.092857 | -0.000006 | 0.000007 |
| 25 | 1 | 0 | -2.249261 | -4.626513 | 0.000002 |
| 26 | 1 | 0 | 0.223582 | -4.622192 | 0.000001 |
| 27 | 1 | 0 | -3.504203 | -2.501356 | 0.000000 |
| 28 | 1 | 0 | 0.223590 | 4.622196 | -0.000003 |
| 29 | 1 | 0 | -2.249248 | 4.626523 | -0.000005 |
| 30 | 1 | 0 | -3.504197 | 2.501366 | -0.000003 |
| 31 | 1 | 0 | 2.347343 | 3.380982 | 0.000001 |
| 32 | 1 | 0 | 2.347332 | -3.380988 | -0.000006 |
| 33 | 1 | 0 | 4.492680 | -2.146419 | 0.000000 |
| 34 | 1 | 0 | 5.717563 | -0.000008 | 0.000004 |
| 35 | 1 | 0 | 4.492692 | 2.146403 | 0.000004 |
| 36 | 1 | 0 | -6.155184 | -0.000009 | 0.000013 |

R=CHO

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -1.412988 | -3.527040 | 0.000003 |
| 2 | 6 | 0 | -0.036114 | -3.631916 | 0.000001 |
| 3 | 6 | 0 | 0.777234 | -2.468986 | 0.000000 |
| 4 | 6 | 0 | 0.152064 | -1.186707 | 0.000000 |
| 5 | 6 | 0 | -1.274363 | -1.092138 | 0.000002 |
| 6 | 6 | 0 | -2.032517 | -2.275119 | 0.000003 |
| 7 | 6 | 0 | 0.958586 | -0.009832 | 0.000000 |
| 8 | 6 | 0 | 0.340853 | 1.278182 | 0.000001 |
| 9 | 6 | 0 | -1.082380 | 1.402421 | 0.000001 |
| 10 | 6 | 0 | -1.894340 | 0.209521 | 0.000002 |
| 11 | 6 | 0 | 1.155347 | 2.449993 | 0.000000 |

| | | | | | |
|---|---|---|---|---|---|
| 12 | 6 | 0 | 0.530196 | 3.721528 | 0.000000 |
| 13 | 6 | 0 | -0.847522 | 3.828413 | 0.000000 |
| 14 | 6 | 0 | -1.650120 | 2.686415 | 0.000000 |
| 15 | 6 | 0 | 2.185853 | -2.551606 | -0.000002 |
| 16 | 6 | 0 | 2.991451 | -1.412071 | -0.000001 |
| 17 | 6 | 0 | 2.367820 | -0.118456 | -0.000001 |
| 18 | 6 | 0 | 3.183280 | 1.065485 | 0.000000 |
| 19 | 6 | 0 | 2.562247 | 2.315011 | 0.000000 |
| 20 | 6 | 0 | 4.416084 | -1.489004 | -0.000002 |
| 21 | 6 | 0 | 5.190930 | -0.337470 | -0.000001 |
| 22 | 6 | 0 | 4.601121 | 0.920824 | 0.000000 |
| 23 | 6 | 0 | -3.288882 | 0.303850 | 0.000001 |
| 24 | 6 | 0 | -4.506947 | 0.336405 | 0.000001 |
| 25 | 6 | 0 | -5.937442 | 0.334016 | -0.000002 |
| 26 | 8 | 0 | -6.613071 | -0.677745 | -0.000006 |
| 27 | 1 | 0 | -2.024821 | -4.421661 | 0.000004 |
| 28 | 1 | 0 | 0.441719 | -4.605372 | 0.000000 |
| 29 | 1 | 0 | -3.113140 | -2.207986 | 0.000005 |
| 30 | 1 | 0 | 1.150597 | 4.610910 | 0.000001 |
| 31 | 1 | 0 | -1.313955 | 4.806937 | 0.000000 |
| 32 | 1 | 0 | -2.728303 | 2.783935 | 0.000001 |
| 33 | 1 | 0 | 2.652751 | -3.531146 | -0.000002 |
| 34 | 1 | 0 | 3.173586 | 3.211456 | 0.000001 |
| 35 | 1 | 0 | 4.885633 | -2.466119 | -0.000004 |
| 36 | 1 | 0 | 6.272046 | -0.420479 | -0.000002 |
| 37 | 1 | 0 | 5.216275 | 1.813528 | 0.000001 |
| 38 | 1 | 0 | -6.404516 | 1.337642 | 0.000003 |

R=$SiMe_3$

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 0.189787 | -3.691531 | -0.000007 |
| 2 | 6 | 0 | -1.191503 | -3.689700 | -0.000004 |
| 3 | 6 | 0 | -1.910050 | -2.466667 | -0.000001 |
| 4 | 6 | 0 | -1.186024 | -1.236954 | -0.000002 |
| 5 | 6 | 0 | 0.244697 | -1.252312 | -0.000004 |
| 6 | 6 | 0 | 0.905564 | -2.492600 | -0.000007 |
| 7 | 6 | 0 | -1.898572 | -0.000080 | 0.000000 |
| 8 | 6 | 0 | -1.181276 | 1.234058 | -0.000001 |
| 9 | 6 | 0 | 0.249438 | 1.243873 | -0.000003 |
| 10 | 6 | 0 | 0.964069 | -0.005625 | -0.000002 |
| 11 | 6 | 0 | -1.900522 | 2.466567 | -0.000002 |
| 12 | 6 | 0 | -1.177206 | 3.686773 | -0.000004 |
| 13 | 6 | 0 | 0.204092 | 3.683235 | -0.000006 |
| 14 | 6 | 0 | 0.915267 | 2.481544 | -0.000005 |
| 15 | 6 | 0 | -3.322247 | -2.437363 | 0.000002 |
| 16 | 6 | 0 | -4.035651 | -1.238369 | 0.000004 |
| 17 | 6 | 0 | -3.312365 | 0.002651 | 0.000002 |
| 18 | 6 | 0 | -4.030856 | 1.246470 | 0.000002 |
| 19 | 6 | 0 | -3.312836 | 2.442709 | 0.000000 |
| 20 | 6 | 0 | -5.461620 | -1.201721 | 0.000007 |
| 21 | 6 | 0 | -6.143697 | 0.008115 | 0.000006 |
| 22 | 6 | 0 | -5.456943 | 1.215318 | 0.000003 |
| 23 | 6 | 0 | 2.372174 | -0.007492 | 0.000001 |
| 24 | 6 | 0 | 3.593348 | -0.006814 | 0.000003 |
| 25 | 14 | 0 | 5.435526 | -0.000271 | 0.000004 |
| 26 | 6 | 0 | 6.043701 | -0.890675 | -1.546792 |
| 27 | 6 | 0 | 6.043700 | -0.890272 | 1.547032 |
| 28 | 6 | 0 | 6.024941 | 1.790546 | -0.000229 |
| 29 | 1 | 0 | 0.728752 | -4.632368 | -0.000010 |
| 30 | 1 | 0 | -1.744126 | -4.622760 | -0.000006 |
| 31 | 1 | 0 | 1.987865 | -2.508290 | -0.000009 |
| 32 | 1 | 0 | -1.726196 | 4.621980 | -0.000002 |
| 33 | 1 | 0 | 0.746769 | 4.621932 | -0.000008 |
| 34 | 1 | 0 | 1.997642 | 2.493195 | -0.000008 |
| 35 | 1 | 0 | -3.864708 | -3.377291 | 0.000002 |
| 36 | 1 | 0 | -3.851673 | 3.384720 | 0.000001 |
| 37 | 1 | 0 | -6.007366 | -2.138564 | 0.000009 |
| 38 | 1 | 0 | -7.228145 | 0.010213 | 0.000008 |
| 39 | 1 | 0 | -5.999074 | 2.154258 | 0.000003 |
| 40 | 1 | 0 | 5.685953 | -0.396104 | -2.453804 |
| 41 | 1 | 0 | 7.137815 | -0.905284 | -1.579940 |
| 42 | 1 | 0 | 5.693575 | -1.926233 | -1.571445 |
| 43 | 1 | 0 | 5.685919 | -0.395487 | 2.453914 |
| 44 | 1 | 0 | 7.137814 | -0.904838 | 1.580203 |
| 45 | 1 | 0 | 5.693605 | -1.925834 | 1.571935 |
| 46 | 1 | 0 | 5.666636 | 2.325027 | -0.884279 |
| 47 | 1 | 0 | 5.666610 | 2.325267 | 0.883665 |
| 48 | 1 | 0 | 7.118497 | 1.838133 | -0.000219 |

R=OMe

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -0.807630 | 3.812038 | 0.000000 |
| 2 | 6 | 0 | 0.570349 | 3.717461 | 0.000001 |
| 3 | 6 | 0 | 1.203767 | 2.448172 | 0.000001 |
| 4 | 6 | 0 | 0.398175 | 1.269872 | 0.000000 |
| 5 | 6 | 0 | -1.028714 | 1.381224 | 0.000000 |
| 6 | 6 | 0 | -1.602988 | 2.664355 | 0.000000 |
| 7 | 6 | 0 | 1.026098 | -0.012041 | 0.000000 |
| 8 | 6 | 0 | 0.226343 | -1.194417 | 0.000000 |
| 9 | 6 | 0 | -1.202672 | -1.106182 | 0.000000 |
| 10 | 6 | 0 | -1.831234 | 0.187243 | -0.000001 |
| 11 | 6 | 0 | 0.860860 | -2.473278 | 0.000000 |
| 12 | 6 | 0 | 0.057358 | -3.642649 | 0.000001 |
| 13 | 6 | 0 | -1.320315 | -3.544912 | 0.000001 |
| 14 | 6 | 0 | -1.948422 | -2.297862 | 0.000000 |
| 15 | 6 | 0 | 2.610870 | 2.323112 | 0.000001 |
| 16 | 6 | 0 | 3.241851 | 1.078795 | 0.000000 |
| 17 | 6 | 0 | 2.436608 | -0.110414 | -0.000001 |
| 18 | 6 | 0 | 3.068986 | -1.399737 | -0.000001 |
| 19 | 6 | 0 | 2.271596 | -2.544581 | 0.000000 |
| 20 | 6 | 0 | 4.662122 | 0.946210 | 0.000000 |
| 21 | 6 | 0 | 5.260980 | -0.307002 | 0.000000 |
| 22 | 6 | 0 | 4.494053 | -1.464972 | 0.000000 |
| 23 | 6 | 0 | -3.238272 | 0.289971 | -0.000001 |
| 24 | 6 | 0 | -4.443860 | 0.397250 | -0.000001 |
| 25 | 8 | 0 | -5.729293 | 0.568019 | -0.000002 |
| 26 | 6 | 0 | -6.523239 | -0.643790 | 0.000001 |
| 27 | 1 | 0 | -1.282227 | 4.787061 | 0.000000 |
| 28 | 1 | 0 | 1.185051 | 4.610859 | 0.000000 |
| 29 | 1 | 0 | -2.681495 | 2.755930 | 0.000001 |
| 30 | 1 | 0 | 0.542084 | -4.612696 | 0.000002 |
| 31 | 1 | 0 | -1.925075 | -4.445188 | 0.000002 |
| 32 | 1 | 0 | -3.029136 | -2.238302 | 0.000000 |
| 33 | 1 | 0 | 3.215602 | 3.224333 | 0.000002 |
| 34 | 1 | 0 | 2.745538 | -3.520931 | -0.000001 |
| 35 | 1 | 0 | 5.269835 | 1.844170 | -0.000001 |
| 36 | 1 | 0 | 6.342883 | -0.382443 | 0.000000 |
| 37 | 1 | 0 | 4.971506 | -2.438482 | 0.000001 |
| 38 | 1 | 0 | -7.559603 | -0.314512 | 0.000007 |
| 39 | 1 | 0 | -6.308325 | -1.228588 | -0.896688 |
| 40 | 1 | 0 | -6.308315 | -1.228590 | 0.896687 |

R=$NH_2$

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 1.384782 | -3.688294 | -0.016550 |
| 2 | 6 | 0 | 0.003844 | -3.689878 | -0.009134 |
| 3 | 6 | 0 | -0.715794 | -2.467254 | -0.003821 |
| 4 | 6 | 0 | 0.006331 | -1.235469 | -0.005711 |
| 5 | 6 | 0 | 1.437412 | -1.247758 | -0.011410 |
| 6 | 6 | 0 | 2.098489 | -2.487918 | -0.017619 |
| 7 | 6 | 0 | -0.709469 | 0.000001 | -0.001950 |
| 8 | 6 | 0 | 0.006327 | 1.235467 | -0.005711 |
| 9 | 6 | 0 | 1.437413 | 1.247759 | -0.011411 |
| 10 | 6 | 0 | 2.155407 | 0.000005 | -0.009987 |
| 11 | 6 | 0 | -0.715801 | 2.467251 | -0.003820 |
| 12 | 6 | 0 | 0.003839 | 3.689882 | -0.009133 |
| 13 | 6 | 0 | 1.384774 | 3.688299 | -0.016553 |
| 14 | 6 | 0 | 2.098486 | 2.487923 | -0.017623 |
| 15 | 6 | 0 | -2.123128 | 0.000000 | 0.004224 |
| 16 | 6 | 0 | -2.843804 | 1.242274 | 0.007103 |
| 17 | 6 | 0 | -2.128121 | 2.439851 | 0.002909 |
| 18 | 6 | 0 | -2.128121 | -2.439855 | 0.002906 |
| 19 | 6 | 0 | -2.843805 | -1.242279 | 0.007101 |
| 20 | 6 | 0 | -4.269793 | -1.208495 | 0.013653 |
| 21 | 6 | 0 | -4.954430 | -0.000001 | 0.016888 |
| 22 | 6 | 0 | -4.269797 | 1.208489 | 0.013655 |
| 23 | 6 | 0 | 3.561711 | 0.000003 | -0.005627 |
| 24 | 6 | 0 | 4.775409 | 0.000002 | 0.021270 |
| 25 | 7 | 0 | 6.116551 | -0.000001 | -0.025740 |
| 26 | 1 | 0 | 1.925687 | -4.628305 | -0.022331 |
| 27 | 1 | 0 | -0.547530 | -4.623671 | -0.008159 |
| 28 | 1 | 0 | 3.180827 | -2.505130 | -0.025823 |
| 29 | 1 | 0 | -0.547538 | 4.623673 | -0.008156 |
| 30 | 1 | 0 | 1.925678 | 4.628311 | -0.022335 |
| 31 | 1 | 0 | 3.180824 | 2.505138 | -0.025830 |
| 32 | 1 | 0 | -2.668963 | 3.380830 | 0.004523 |
| 33 | 1 | 0 | -2.668960 | -3.380835 | 0.004521 |
| 34 | 1 | 0 | -4.813659 | -2.146546 | 0.015865 |
| 35 | 1 | 0 | -6.038982 | -0.000003 | 0.021779 |
| 36 | 1 | 0 | -4.813662 | 2.146540 | 0.015869 |
| 37 | 1 | 0 | 6.578720 | -0.843981 | 0.284181 |
| 38 | 1 | 0 | 6.578725 | 0.843971 | 0.284194 |

R=Ph

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 0.066298 | -3.689113 | 0.000021 |
| 2 | 6 | 0 | -1.314504 | -3.689177 | 0.000014 |
| 3 | 6 | 0 | -2.033943 | -2.466936 | 0.000006 |
| 4 | 6 | 0 | -1.311340 | -1.235866 | 0.000002 |
| 5 | 6 | 0 | 0.118798 | -1.249510 | 0.000003 |
| 6 | 6 | 0 | 0.779752 | -2.488445 | 0.000016 |
| 7 | 6 | 0 | -2.026675 | 0.000000 | -0.000001 |
| 8 | 6 | 0 | -1.311342 | 1.235864 | -0.000007 |
| 9 | 6 | 0 | 0.118800 | 1.249508 | -0.000013 |
| 10 | 6 | 0 | 0.839577 | 0.000001 | -0.000004 |
| 11 | 6 | 0 | -2.033944 | 2.466934 | -0.000009 |
| 12 | 6 | 0 | -1.314503 | 3.689178 | -0.000022 |
| 13 | 6 | 0 | 0.066297 | 3.689114 | -0.000036 |
| 14 | 6 | 0 | 0.779752 | 2.488445 | -0.000032 |
| 15 | 6 | 0 | -3.446149 | -2.440035 | 0.000005 |

| | | | | | |
|---|---|---|---|---|---|
| 16 | 6 | 0 | -4.161474 | -1.242382 | 0.000004 |
| 17 | 6 | 0 | -3.439959 | 0.000000 | 0.000002 |
| 18 | 6 | 0 | -4.161472 | 1.242381 | 0.000003 |
| 19 | 6 | 0 | -3.446146 | 2.440034 | -0.000001 |
| 20 | 6 | 0 | -5.587277 | -1.208442 | 0.000006 |
| 21 | 6 | 0 | -6.271824 | 0.000002 | 0.000008 |
| 22 | 6 | 0 | -5.587278 | 1.208444 | 0.000007 |
| 23 | 6 | 0 | 2.241218 | 0.000000 | -0.000002 |
| 24 | 6 | 0 | 3.458698 | 0.000000 | 0.000000 |
| 25 | 6 | 0 | 4.876128 | 0.000000 | 0.000002 |
| 26 | 6 | 0 | 5.596196 | -1.211842 | -0.000090 |
| 27 | 6 | 0 | 6.984546 | -1.206290 | -0.000087 |
| 28 | 6 | 0 | 7.685211 | 0.000001 | 0.000007 |
| 29 | 6 | 0 | 6.984546 | 1.206290 | 0.000098 |
| 30 | 6 | 0 | 5.596195 | 1.211843 | 0.000096 |
| 31 | 1 | 0 | 0.606966 | -4.628981 | 0.000033 |
| 32 | 1 | 0 | -1.866208 | -4.622770 | 0.000023 |
| 33 | 1 | 0 | 1.861929 | -2.503999 | 0.000019 |
| 34 | 1 | 0 | -1.866208 | 4.622771 | -0.000031 |
| 35 | 1 | 0 | 0.606965 | 4.628981 | -0.000053 |
| 36 | 1 | 0 | 1.861928 | 2.504000 | -0.000039 |
| 37 | 1 | 0 | -3.986926 | -3.380931 | 0.000004 |
| 38 | 1 | 0 | -3.986923 | 3.380929 | -0.000004 |
| 39 | 1 | 0 | -6.131146 | -2.146388 | 0.000016 |
| 40 | 1 | 0 | -7.356276 | 0.000002 | 0.000010 |
| 41 | 1 | 0 | -6.131145 | 2.146391 | -0.000001 |
| 42 | 1 | 0 | 5.052619 | -2.148794 | -0.000166 |
| 43 | 1 | 0 | 7.523819 | -2.146832 | -0.000159 |
| 44 | 1 | 0 | 8.769086 | 0.000001 | 0.000009 |
| 45 | 1 | 0 | 7.523818 | 2.146833 | 0.000172 |
| 46 | 1 | 0 | 5.052618 | 2.148793 | 0.000171 |

R=BzTh

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -0.958929 | -3.644824 | 0.000002 |
| 2 | 6 | 0 | -2.339369 | -3.660987 | 0.000001 |
| 3 | 6 | 0 | -3.073362 | -2.447563 | 0.000001 |
| 4 | 6 | 0 | -2.365632 | -1.207838 | 0.000001 |
| 5 | 6 | 0 | -0.936117 | -1.205441 | 0.000002 |
| 6 | 6 | 0 | -0.259986 | -2.435345 | 0.000002 |
| 7 | 6 | 0 | -3.095939 | 0.019603 | 0.000000 |
| 8 | 6 | 0 | -2.395868 | 1.264587 | 0.000001 |
| 9 | 6 | 0 | -0.966648 | 1.297071 | 0.000003 |
| 10 | 6 | 0 | -0.230371 | 0.054639 | 0.000003 |
| 11 | 6 | 0 | -3.133793 | 2.486664 | 0.000001 |
| 12 | 6 | 0 | -2.429641 | 3.717627 | 0.000001 |
| 13 | 6 | 0 | -1.049195 | 3.735102 | 0.000003 |
| 14 | 6 | 0 | -0.320829 | 2.543113 | 0.000004 |
| 15 | 6 | 0 | -4.485712 | -2.437795 | -0.000001 |
| 16 | 6 | 0 | -5.215364 | -1.248860 | -0.000002 |
| 17 | 6 | 0 | -4.508718 | 0.002319 | -0.000001 |
| 18 | 6 | 0 | -5.245799 | 1.235844 | -0.000002 |
| 19 | 6 | 0 | -4.545526 | 2.442315 | -0.000001 |
| 20 | 6 | 0 | -6.641305 | -1.232379 | -0.000003 |
| 21 | 6 | 0 | -7.340620 | -0.032459 | -0.000004 |
| 22 | 6 | 0 | -6.670886 | 1.184263 | -0.000004 |
| 23 | 6 | 0 | 1.165993 | 0.070755 | 0.000003 |
| 24 | 6 | 0 | 2.385957 | 0.089770 | 0.000003 |
| 25 | 6 | 0 | 3.781319 | 0.088093 | 0.000001 |
| 26 | 6 | 0 | 4.636470 | 1.163723 | 0.000000 |
| 27 | 6 | 0 | 6.017384 | 0.801146 | -0.000001 |
| 28 | 6 | 0 | 6.204182 | -0.604345 | -0.000001 |
| 29 | 16 | 0 | 4.669731 | -1.452342 | 0.000001 |
| 30 | 6 | 0 | 7.152675 | 1.634175 | -0.000002 |
| 31 | 6 | 0 | 8.415997 | 1.069742 | -0.000003 |
| 32 | 6 | 0 | 8.579401 | -0.326171 | -0.000004 |
| 33 | 6 | 0 | 7.478736 | -1.172269 | -0.000003 |
| 34 | 1 | 0 | -0.406530 | -4.577695 | 0.000003 |
| 35 | 1 | 0 | -2.879950 | -4.601052 | 0.000001 |
| 36 | 1 | 0 | 0.822441 | -2.440533 | 0.000003 |
| 37 | 1 | 0 | -2.992986 | 4.644226 | 0.000001 |
| 38 | 1 | 0 | -0.520222 | 4.681536 | 0.000003 |
| 39 | 1 | 0 | 0.761180 | 2.573354 | 0.000005 |
| 40 | 1 | 0 | -5.015028 | -3.385150 | -0.000001 |
| 41 | 1 | 0 | -5.097904 | 3.376409 | -0.000003 |
| 42 | 1 | 0 | -7.173609 | -2.176913 | -0.000004 |
| 43 | 1 | 0 | -8.424962 | -0.045726 | -0.000006 |
| 44 | 1 | 0 | -7.226245 | 2.115436 | -0.000005 |
| 45 | 1 | 0 | 4.280526 | 2.185144 | 0.000000 |
| 46 | 1 | 0 | 7.029233 | 2.711485 | -0.000002 |
| 47 | 1 | 0 | 9.291420 | 1.708765 | -0.000004 |
| 48 | 1 | 0 | 9.577164 | -0.749438 | -0.000005 |
| 49 | 1 | 0 | 7.608738 | -2.248033 | -0.000003 |

R=Th

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 0.099405 | 3.768103 | -0.000003 |
| 2 | 6 | 0 | 1.478838 | 3.712512 | -0.000001 |
| 3 | 6 | 0 | 2.148465 | 2.462361 | -0.000001 |
| 4 | 6 | 0 | 1.376880 | 1.261191 | -0.000002 |
| 5 | 6 | 0 | -0.051032 | 1.333171 | -0.000003 |
| 6 | 6 | 0 | -0.661888 | 2.596842 | -0.000004 |
| 7 | 6 | 0 | 2.042146 | -0.002756 | -0.000001 |
| 8 | 6 | 0 | 1.277882 | -1.209390 | -0.000002 |
| 9 | 6 | 0 | -0.151196 | -1.166955 | -0.000003 |
| 10 | 6 | 0 | -0.821510 | 0.111971 | -0.000004 |
| 11 | 6 | 0 | 1.950842 | -2.468401 | -0.000001 |
| 12 | 6 | 0 | 1.183421 | -3.661059 | -0.000002 |
| 13 | 6 | 0 | -0.196013 | -3.606241 | -0.000003 |
| 14 | 6 | 0 | -0.861102 | -2.377803 | -0.000004 |
| 15 | 6 | 0 | 3.558445 | 2.378671 | 0.000001 |
| 16 | 6 | 0 | 4.224934 | 1.153225 | 0.000002 |
| 17 | 6 | 0 | 3.453934 | -0.059332 | 0.000001 |
| 18 | 6 | 0 | 4.125409 | -1.329664 | 0.000002 |
| 19 | 6 | 0 | 3.362948 | -2.497822 | 0.000001 |
| 20 | 6 | 0 | 5.648076 | 1.062068 | 0.000004 |
| 21 | 6 | 0 | 6.283724 | -0.172820 | 0.000005 |
| 22 | 6 | 0 | 5.551298 | -1.352842 | 0.000004 |
| 23 | 6 | 0 | -2.217654 | 0.167524 | -0.000006 |
| 24 | 6 | 0 | -3.436403 | 0.220198 | -0.000005 |
| 25 | 6 | 0 | -4.831684 | 0.267550 | -0.000001 |
| 26 | 6 | 0 | -5.662460 | 1.374375 | 0.000003 |
| 27 | 6 | 0 | -7.039160 | 1.043933 | 0.000007 |
| 28 | 6 | 0 | -7.265881 | -0.305788 | 0.000007 |
| 29 | 16 | 0 | -5.791199 | -1.209902 | 0.000002 |
| 30 | 1 | 0 | -0.403142 | 4.728878 | -0.000004 |
| 31 | 1 | 0 | 2.067721 | 4.623102 | -0.000001 |
| 32 | 1 | 0 | -1.742650 | 2.657072 | -0.000006 |
| 33 | 1 | 0 | 1.697655 | -4.615797 | -0.000001 |
| 34 | 1 | 0 | -0.774141 | -4.523458 | -0.000004 |
| 35 | 1 | 0 | -1.943249 | -2.352687 | -0.000005 |
| 36 | 1 | 0 | 4.136615 | 3.297052 | 0.000003 |
| 37 | 1 | 0 | 3.865744 | -3.459539 | 0.000001 |
| 38 | 1 | 0 | 6.229113 | 1.977459 | 0.000005 |
| 39 | 1 | 0 | 7.367301 | -0.216236 | 0.000007 |
| 40 | 1 | 0 | 6.057147 | -2.311825 | 0.000005 |
| 41 | 1 | 0 | -5.276919 | 2.384500 | 0.000002 |
| 42 | 1 | 0 | -7.834002 | 1.777825 | 0.000010 |
| 43 | 1 | 0 | -8.211988 | -0.824864 | 0.000010 |

## Radical

R=Mt

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 4.820698 | 0.000000 | -0.000029 |
| 2 | 6 | 0 | 3.565902 | 0.000002 | -0.000010 |
| 3 | 6 | 0 | 6.144973 | 0.000000 | -0.000051 |
| 4 | 6 | 0 | 1.411733 | -3.701930 | 0.000024 |
| 5 | 6 | 0 | 0.033843 | -3.696024 | 0.000016 |
| 6 | 6 | 0 | -0.680178 | -2.472247 | 0.000007 |
| 7 | 6 | 0 | 0.049403 | -1.240086 | 0.000006 |
| 8 | 6 | 0 | 1.471060 | -1.266231 | 0.000012 |
| 9 | 6 | 0 | 2.126181 | -2.497788 | 0.000021 |
| 10 | 6 | 0 | -0.667854 | 0.000000 | 0.000001 |
| 11 | 6 | 0 | 0.049401 | 1.240087 | 0.000006 |
| 12 | 6 | 0 | 1.471058 | 1.266233 | 0.000012 |
| 13 | 6 | 0 | 2.222071 | 0.000001 | 0.000005 |
| 14 | 6 | 0 | -0.680181 | 2.472247 | 0.000006 |
| 15 | 6 | 0 | 0.033839 | 3.696024 | 0.000016 |
| 16 | 6 | 0 | 1.411728 | 3.701932 | 0.000025 |
| 17 | 6 | 0 | 2.126178 | 2.497791 | 0.000023 |
| 18 | 6 | 0 | -2.090167 | -2.443520 | -0.000001 |
| 19 | 6 | 0 | -2.803716 | -1.242408 | -0.000008 |
| 20 | 6 | 0 | -2.076986 | -0.000001 | -0.000006 |
| 21 | 6 | 0 | -2.803717 | 1.242406 | -0.000009 |
| 22 | 6 | 0 | -2.090170 | 2.443518 | -0.000003 |
| 23 | 6 | 0 | -4.225036 | -1.208065 | -0.000016 |
| 24 | 6 | 0 | -4.910763 | -0.000002 | -0.000021 |
| 25 | 6 | 0 | -4.225036 | 1.208061 | -0.000018 |
| 26 | 1 | 0 | 6.708833 | 0.926608 | -0.000061 |
| 27 | 1 | 0 | 6.708831 | -0.926609 | -0.000061 |
| 28 | 1 | 0 | 1.951866 | -4.641891 | 0.000032 |
| 29 | 1 | 0 | -0.522611 | -4.626971 | 0.000017 |
| 30 | 1 | 0 | 3.208941 | -2.516307 | 0.000027 |
| 31 | 1 | 0 | -0.522616 | 4.626971 | 0.000016 |
| 32 | 1 | 0 | 1.951861 | 4.641894 | 0.000034 |
| 33 | 1 | 0 | 3.208938 | 2.516311 | 0.000029 |
| 34 | 1 | 0 | -2.633213 | -3.383052 | -0.000001 |
| 35 | 1 | 0 | -2.633216 | 3.383048 | -0.000003 |
| 36 | 1 | 0 | -4.769023 | -2.146039 | -0.000019 |
| 37 | 1 | 0 | -5.995137 | -0.000003 | -0.000028 |
| 38 | 1 | 0 | -4.769025 | 2.146035 | -0.000022 |

R=DCM

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 0.492367 | -3.694359 | -0.000011 |
| 2 | 6 | 0 | -0.888137 | -3.687802 | -0.000009 |
| 3 | 6 | 0 | -1.607866 | -2.468260 | -0.000005 |
| 4 | 6 | 0 | -0.882082 | -1.235827 | -0.000005 |
| 5 | 6 | 0 | 0.540316 | -1.259575 | -0.000008 |
| 6 | 6 | 0 | 1.203734 | -2.491709 | -0.000010 |
| 7 | 6 | 0 | -1.598361 | 0.000000 | -0.000002 |
| 8 | 6 | 0 | -0.882084 | 1.235828 | -0.000004 |
| 9 | 6 | 0 | 0.540314 | 1.259579 | -0.000010 |
| 10 | 6 | 0 | 1.279644 | 0.000003 | -0.000008 |
| 11 | 6 | 0 | -1.607870 | 2.468260 | -0.000001 |
| 12 | 6 | 0 | -0.888144 | 3.687803 | -0.000005 |
| 13 | 6 | 0 | 0.492360 | 3.694363 | -0.000014 |
| 14 | 6 | 0 | 1.203729 | 2.491715 | -0.000016 |
| 15 | 6 | 0 | -3.009319 | -0.000001 | 0.000003 |
| 16 | 6 | 0 | -3.734300 | 1.242367 | 0.000008 |
| 17 | 6 | 0 | -3.018019 | 2.443291 | 0.000006 |
| 18 | 6 | 0 | -3.018015 | -2.443294 | -0.000001 |
| 19 | 6 | 0 | -3.734298 | -1.242371 | 0.000004 |
| 20 | 6 | 0 | -5.155481 | -1.208262 | 0.000008 |
| 21 | 6 | 0 | -5.840713 | -0.000004 | 0.000014 |
| 22 | 6 | 0 | -5.155484 | 1.208255 | 0.000014 |
| 23 | 6 | 0 | 2.637588 | 0.000004 | -0.000005 |
| 24 | 6 | 0 | 3.875998 | 0.000000 | 0.000000 |
| 25 | 6 | 0 | 5.232031 | 0.000000 | 0.000007 |
| 26 | 6 | 0 | 5.954437 | -1.226619 | 0.000013 |
| 27 | 6 | 0 | 5.954436 | 1.226619 | 0.000008 |
| 28 | 7 | 0 | 6.526042 | 2.232705 | 0.000008 |
| 29 | 7 | 0 | 6.526042 | -2.232706 | 0.000020 |
| 30 | 1 | 0 | 1.032846 | -4.633334 | -0.000014 |
| 31 | 1 | 0 | -1.440676 | -4.620993 | -0.000011 |
| 32 | 1 | 0 | 2.286350 | -2.511444 | -0.000012 |
| 33 | 1 | 0 | -1.440685 | 4.620993 | -0.000002 |
| 34 | 1 | 0 | 1.032836 | 4.633339 | -0.000018 |
| 35 | 1 | 0 | 2.286345 | 2.511452 | -0.000023 |
| 36 | 1 | 0 | -3.558939 | 3.383696 | 0.000010 |
| 37 | 1 | 0 | -3.558933 | -3.383699 | -0.000003 |
| 38 | 1 | 0 | -5.699811 | -2.145753 | 0.000007 |
| 39 | 1 | 0 | -6.924777 | -0.000005 | 0.000018 |
| 40 | 1 | 0 | -5.699816 | 2.145745 | 0.000019 |

R=DPM

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 1.093807 | 3.692192 | -0.242234 |
| 2 | 6 | 0 | 2.472339 | 3.688838 | -0.224165 |
| 3 | 6 | 0 | 3.186966 | 2.467995 | -0.143229 |
| 4 | 6 | 0 | 2.458057 | 1.237402 | -0.070686 |
| 5 | 6 | 0 | 1.035114 | 1.260678 | -0.079008 |
| 6 | 6 | 0 | 0.379100 | 2.491112 | -0.174495 |
| 7 | 6 | 0 | 3.174883 | 0.000000 | 0.000000 |
| 8 | 6 | 0 | 2.458056 | -1.237402 | 0.070685 |
| 9 | 6 | 0 | 1.035114 | -1.260678 | 0.079005 |
| 10 | 6 | 0 | 0.291270 | 0.000000 | -0.000002 |
| 11 | 6 | 0 | 3.186966 | -2.467995 | 0.143228 |
| 12 | 6 | 0 | 2.472338 | -3.688838 | 0.224165 |
| 13 | 6 | 0 | 1.093806 | -3.692192 | 0.242232 |
| 14 | 6 | 0 | 0.379099 | -2.491111 | 0.174492 |
| 15 | 6 | 0 | 4.596779 | 2.439587 | -0.138075 |
| 16 | 6 | 0 | 5.311037 | 1.240181 | -0.068746 |
| 17 | 6 | 0 | 4.585266 | 0.000000 | 0.000000 |
| 18 | 6 | 0 | 5.311037 | -1.240181 | 0.068747 |
| 19 | 6 | 0 | 4.596778 | -2.439587 | 0.138076 |
| 20 | 6 | 0 | 6.732270 | 1.206261 | -0.066503 |
| 21 | 6 | 0 | 7.418033 | -0.000001 | 0.000002 |
| 22 | 6 | 0 | 6.732270 | -1.206262 | 0.066506 |
| 23 | 6 | 0 | -1.062280 | 0.000000 | -0.000002 |
| 24 | 6 | 0 | -2.308066 | 0.000000 | -0.000002 |
| 25 | 6 | 0 | -3.657378 | 0.000000 | -0.000001 |
| 26 | 6 | 0 | -4.384287 | -1.287293 | -0.065280 |
| 27 | 6 | 0 | -5.603816 | -1.469776 | 0.610194 |
| 28 | 6 | 0 | -5.603818 | 1.469776 | -0.610190 |
| 29 | 6 | 0 | -4.384287 | 1.287294 | 0.065280 |
| 30 | 6 | 0 | -3.852554 | -2.376623 | -0.778104 |
| 31 | 6 | 0 | -4.512630 | -3.599134 | -0.812007 |
| 32 | 6 | 0 | -5.719793 | -3.765747 | -0.134072 |
| 33 | 6 | 0 | -6.259703 | -2.695693 | 0.577424 |
| 34 | 6 | 0 | -6.259705 | 2.695693 | -0.577419 |
| 35 | 6 | 0 | -5.719793 | 3.765748 | 0.134074 |
| 36 | 6 | 0 | -4.512627 | 3.599135 | 0.812005 |
| 37 | 6 | 0 | -3.852552 | 2.376624 | 0.778101 |
| 38 | 1 | 0 | 0.553396 | 4.629314 | -0.314263 |
| 39 | 1 | 0 | 3.028016 | 4.618612 | -0.278770 |
| 40 | 1 | 0 | -0.703064 | 2.509786 | -0.205472 |
| 41 | 1 | 0 | 3.028015 | -4.618612 | 0.278770 |
| 42 | 1 | 0 | 0.553395 | -4.629314 | 0.314261 |
| 43 | 1 | 0 | -0.703065 | -2.509786 | 0.205468 |
| 44 | 1 | 0 | 5.139777 | 3.377578 | -0.192780 |
| 45 | 1 | 0 | 5.139776 | -3.377578 | 0.192781 |
| 46 | 1 | 0 | 7.276238 | 2.142834 | -0.118406 |
| 47 | 1 | 0 | 8.502436 | -0.000001 | 0.000003 |
| 48 | 1 | 0 | 7.276237 | -2.142836 | 0.118410 |
| 49 | 1 | 0 | -6.025196 | -0.651088 | 1.180389 |
| 50 | 1 | 0 | -6.025200 | 0.651087 | -1.180383 |
| 51 | 1 | 0 | -2.924077 | -2.246412 | -1.321557 |
| 52 | 1 | 0 | -4.088971 | -4.421968 | -1.377114 |
| 53 | 1 | 0 | -6.235352 | -4.718919 | -0.162139 |
| 54 | 1 | 0 | -7.193279 | -2.817393 | 1.115474 |
| 55 | 1 | 0 | -7.193283 | 2.817392 | -1.115466 |
| 56 | 1 | 0 | -6.235351 | 4.718919 | 0.162142 |
| 57 | 1 | 0 | -4.088967 | 4.421970 | 1.377110 |
| 58 | 1 | 0 | -2.924073 | 2.246413 | 1.321551 |

R=Flu

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -1.226662 | -3.698794 | 0.000003 |
| 2 | 6 | 0 | -2.605796 | -3.693869 | 0.000001 |
| 3 | 6 | 0 | -3.320669 | -2.470883 | 0.000000 |
| 4 | 6 | 0 | -2.592136 | -1.238098 | 0.000001 |
| 5 | 6 | 0 | -1.168934 | -1.261244 | 0.000002 |
| 6 | 6 | 0 | -0.513598 | -2.495993 | 0.000003 |
| 7 | 6 | 0 | -3.309071 | 0.000000 | 0.000000 |
| 8 | 6 | 0 | -2.592136 | 1.238098 | 0.000000 |
| 9 | 6 | 0 | -1.168934 | 1.261243 | 0.000001 |
| 10 | 6 | 0 | -0.424627 | 0.000000 | 0.000002 |
| 11 | 6 | 0 | -3.320669 | 2.470883 | 0.000000 |
| 12 | 6 | 0 | -2.605795 | 3.693868 | 0.000000 |
| 13 | 6 | 0 | -1.226661 | 3.698793 | 0.000001 |
| 14 | 6 | 0 | -0.513597 | 2.495993 | 0.000002 |
| 15 | 6 | 0 | -4.730462 | -2.443155 | -0.000001 |
| 16 | 6 | 0 | -5.445417 | -1.241916 | -0.000001 |
| 17 | 6 | 0 | -4.719892 | 0.000000 | -0.000001 |
| 18 | 6 | 0 | -5.445417 | 1.241916 | -0.000002 |
| 19 | 6 | 0 | -4.730462 | 2.443155 | -0.000002 |
| 20 | 6 | 0 | -6.866556 | -1.208085 | -0.000002 |
| 21 | 6 | 0 | -7.552272 | 0.000000 | -0.000003 |
| 22 | 6 | 0 | -6.866555 | 1.208085 | -0.000003 |
| 23 | 6 | 0 | 0.932311 | -0.000001 | 0.000003 |
| 24 | 6 | 0 | 2.176153 | 0.000000 | 0.000004 |
| 25 | 6 | 0 | 3.523782 | 0.000000 | 0.000003 |
| 26 | 6 | 0 | 4.402721 | 1.174286 | 0.000001 |
| 27 | 6 | 0 | 5.750231 | 0.733278 | -0.000002 |
| 28 | 6 | 0 | 5.750231 | -0.733278 | -0.000003 |
| 29 | 6 | 0 | 4.402721 | -1.174286 | 0.000001 |
| 30 | 6 | 0 | 4.105440 | 2.535195 | 0.000004 |
| 31 | 6 | 0 | 5.153547 | 3.454229 | 0.000002 |

| | | | | | |
|---|---|---|---|---|---|
| 32 | 6 | 0 | 6.482679 | 3.020050 | -0.000002 |
| 33 | 6 | 0 | 6.789070 | 1.657795 | -0.000004 |
| 34 | 6 | 0 | 6.789070 | -1.657794 | -0.000005 |
| 35 | 6 | 0 | 6.482680 | -3.020049 | -0.000004 |
| 36 | 6 | 0 | 5.153549 | -3.454229 | 0.000000 |
| 37 | 6 | 0 | 4.105441 | -2.535196 | 0.000002 |
| 38 | 1 | 0 | -0.686620 | -4.638750 | 0.000003 |
| 39 | 1 | 0 | -3.161060 | -4.625426 | 0.000001 |
| 40 | 1 | 0 | 0.568586 | -2.514051 | 0.000004 |
| 41 | 1 | 0 | -3.161059 | 4.625426 | -0.000001 |
| 42 | 1 | 0 | -0.686619 | 4.638749 | 0.000001 |
| 43 | 1 | 0 | 0.568587 | 2.514050 | 0.000003 |
| 44 | 1 | 0 | -5.272820 | -3.383016 | 0.000000 |
| 45 | 1 | 0 | -5.272819 | 3.383016 | -0.000002 |
| 46 | 1 | 0 | -7.410517 | -2.146031 | -0.000002 |
| 47 | 1 | 0 | -8.636598 | 0.000001 | -0.000004 |
| 48 | 1 | 0 | -7.410517 | 2.146032 | -0.000003 |
| 49 | 1 | 0 | 3.076053 | 2.875063 | 0.000008 |
| 50 | 1 | 0 | 4.936968 | 4.516473 | 0.000005 |
| 51 | 1 | 0 | 7.284182 | 3.750131 | -0.000003 |
| 52 | 1 | 0 | 7.823602 | 1.332243 | -0.000008 |
| 53 | 1 | 0 | 7.823603 | -1.332241 | -0.000008 |
| 54 | 1 | 0 | 7.284184 | -3.750130 | -0.000005 |
| 55 | 1 | 0 | 4.936970 | -4.516473 | 0.000001 |
| 56 | 1 | 0 | 3.076055 | -2.875064 | 0.000005 |

R=PhO

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 0.237111 | -3.694894 | 0.000024 |
| 2 | 6 | 0 | 1.617919 | -3.690551 | 0.000015 |
| 3 | 6 | 0 | 2.336029 | -2.469580 | 0.000007 |
| 4 | 6 | 0 | 1.609136 | -1.236243 | 0.000009 |
| 5 | 6 | 0 | 0.185521 | -1.257333 | 0.000017 |
| 6 | 6 | 0 | -0.474721 | -2.493189 | 0.000024 |
| 7 | 6 | 0 | 2.325312 | 0.000000 | 0.000003 |
| 8 | 6 | 0 | 1.609134 | 1.236242 | 0.000009 |
| 9 | 6 | 0 | 0.185520 | 1.257330 | 0.000019 |
| 10 | 6 | 0 | -0.552370 | -0.000002 | 0.000017 |
| 11 | 6 | 0 | 2.336026 | 2.469581 | 0.000004 |
| 12 | 6 | 0 | 1.617914 | 3.690550 | 0.000013 |
| 13 | 6 | 0 | 0.237107 | 3.694891 | 0.000027 |
| 14 | 6 | 0 | -0.474725 | 2.493185 | 0.000030 |
| 15 | 6 | 0 | 3.745387 | -2.443491 | -0.000005 |
| 16 | 6 | 0 | 4.462070 | -1.241589 | -0.000013 |
| 17 | 6 | 0 | 3.737813 | 0.000001 | -0.000008 |
| 18 | 6 | 0 | 4.462068 | 1.241592 | -0.000014 |
| 19 | 6 | 0 | 3.745383 | 2.443493 | -0.000008 |
| 20 | 6 | 0 | 5.882700 | -1.208167 | -0.000025 |
| 21 | 6 | 0 | 6.568324 | 0.000003 | -0.000032 |
| 22 | 6 | 0 | 5.882699 | 1.208172 | -0.000026 |
| 23 | 6 | 0 | -1.918209 | -0.000003 | 0.000012 |
| 24 | 6 | 0 | -3.154777 | -0.000003 | 0.000003 |
| 25 | 6 | 0 | -4.522254 | -0.000001 | -0.000002 |
| 26 | 6 | 0 | -5.263961 | -1.237453 | -0.000006 |
| 27 | 6 | 0 | -6.618661 | -1.243637 | -0.000014 |
| 28 | 6 | 0 | -7.399391 | 0.000001 | -0.000020 |
| 29 | 6 | 0 | -6.618659 | 1.243638 | -0.000015 |
| 30 | 6 | 0 | -5.263958 | 1.237452 | -0.000006 |
| 31 | 8 | 0 | -8.631538 | 0.000002 | -0.000028 |
| 32 | 1 | 0 | -0.302754 | -4.634704 | 0.000030 |
| 33 | 1 | 0 | 2.170950 | -4.623390 | 0.000015 |
| 34 | 1 | 0 | -1.557046 | -2.510052 | 0.000030 |
| 35 | 1 | 0 | 2.170944 | 4.623390 | 0.000008 |
| 36 | 1 | 0 | -0.302760 | 4.634700 | 0.000035 |
| 37 | 1 | 0 | -1.557050 | 2.510047 | 0.000042 |
| 38 | 1 | 0 | 4.287124 | -3.383573 | -0.000008 |
| 39 | 1 | 0 | 4.287120 | 3.383576 | -0.000011 |
| 40 | 1 | 0 | 6.426831 | -2.145909 | -0.000028 |
| 41 | 1 | 0 | 7.652518 | 0.000004 | -0.000041 |
| 42 | 1 | 0 | 6.426828 | 2.145915 | -0.000032 |
| 43 | 1 | 0 | -4.705122 | -2.166739 | -0.000002 |
| 44 | 1 | 0 | -7.184540 | -2.168075 | -0.000018 |
| 45 | 1 | 0 | -7.184536 | 2.168077 | -0.000019 |
| 46 | 1 | 0 | -4.705118 | 2.166737 | -0.000004 |

R=NO

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -0.859208 | 3.663502 | -0.000003 |
| 2 | 6 | 0 | 0.521851 | 3.680374 | 0.000000 |
| 3 | 6 | 0 | 1.257400 | 2.468814 | 0.000000 |
| 4 | 6 | 0 | 0.547600 | 1.224610 | -0.000001 |
| 5 | 6 | 0 | -0.876813 | 1.225636 | -0.000003 |
| 6 | 6 | 0 | -1.556917 | 2.453608 | -0.000004 |
| 7 | 6 | 0 | 1.280180 | -0.002398 | -0.000001 |
| 8 | 6 | 0 | 0.581588 | -1.249033 | -0.000001 |
| 9 | 6 | 0 | -0.842491 | -1.287928 | -0.000001 |
| 10 | 6 | 0 | -1.589176 | -0.042294 | -0.000002 |
| 11 | 6 | 0 | 1.325012 | -2.473610 | -0.000001 |
| 12 | 6 | 0 | 0.623141 | -3.705065 | -0.000001 |
| 13 | 6 | 0 | -0.757941 | -3.726123 | -0.000001 |
| 14 | 6 | 0 | -1.486308 | -2.534689 | -0.000001 |
| 15 | 6 | 0 | 2.666246 | 2.460540 | 0.000001 |
| 16 | 6 | 0 | 3.399917 | 1.267482 | 0.000002 |
| 17 | 6 | 0 | 2.693803 | 0.016600 | 0.000001 |
| 18 | 6 | 0 | 3.433863 | -1.214576 | 0.000000 |
| 19 | 6 | 0 | 2.733129 | -2.427328 | 0.000000 |
| 20 | 6 | 0 | 4.820398 | 1.253804 | 0.000003 |
| 21 | 6 | 0 | 5.522764 | 0.055135 | 0.000002 |
| 22 | 6 | 0 | 4.853395 | -1.162347 | 0.000001 |
| 23 | 6 | 0 | -2.961047 | -0.044665 | -0.000002 |
| 24 | 6 | 0 | -4.189621 | 0.007231 | 0.000000 |
| 25 | 7 | 0 | -5.496474 | 0.126320 | 0.000002 |
| 26 | 8 | 0 | -6.087038 | 1.263019 | 0.000004 |
| 27 | 6 | 0 | -6.357941 | -1.071222 | 0.000003 |
| 28 | 1 | 0 | -1.413217 | 4.595229 | -0.000003 |
| 29 | 1 | 0 | 1.061704 | 4.620933 | 0.000001 |
| 30 | 1 | 0 | -2.639938 | 2.459801 | -0.000006 |
| 31 | 1 | 0 | 1.188440 | -4.630507 | -0.000002 |
| 32 | 1 | 0 | -1.285109 | -4.673522 | -0.000001 |
| 33 | 1 | 0 | -2.568684 | -2.567693 | 0.000000 |
| 34 | 1 | 0 | 3.196006 | 3.407599 | 0.000001 |
| 35 | 1 | 0 | 3.288451 | -3.359620 | -0.000001 |
| 36 | 1 | 0 | 5.351654 | 2.199057 | 0.000004 |
| 37 | 1 | 0 | 6.607010 | 0.069953 | 0.000003 |
| 38 | 1 | 0 | 5.410211 | -2.092782 | 0.000000 |
| 39 | 1 | 0 | -5.747723 | -1.973130 | 0.000000 |
| 40 | 1 | 0 | -6.987054 | -1.030032 | 0.889803 |
| 41 | 1 | 0 | -6.987059 | -1.030030 | -0.889793 |

R=Allyl

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 4.250111 | 0.000000 | -0.000002 |
| 2 | 6 | 0 | 3.038421 | 0.000000 | -0.000003 |
| 3 | 6 | 0 | 5.687656 | 0.000000 | 0.000002 |
| 4 | 6 | 0 | 6.360124 | 0.716827 | 0.987920 |
| 5 | 6 | 0 | 6.360131 | -0.716826 | -0.987912 |
| 6 | 6 | 0 | 0.870221 | 3.683651 | -0.072122 |
| 7 | 6 | 0 | -0.516135 | 3.687113 | -0.070632 |
| 8 | 6 | 0 | -1.241137 | 2.468695 | -0.046540 |
| 9 | 6 | 0 | -0.518193 | 1.231679 | -0.022996 |
| 10 | 6 | 0 | 0.910541 | 1.241321 | -0.023544 |
| 11 | 6 | 0 | 1.580680 | 2.487703 | -0.049355 |
| 12 | 6 | 0 | -1.231997 | 0.000000 | -0.000001 |
| 13 | 6 | 0 | -0.518193 | -1.231679 | 0.022995 |
| 14 | 6 | 0 | 0.910541 | -1.241320 | 0.023541 |
| 15 | 6 | 0 | 1.622025 | 0.000000 | -0.000002 |
| 16 | 6 | 0 | -1.241137 | -2.468695 | 0.046539 |
| 17 | 6 | 0 | -0.516135 | -3.687113 | 0.070631 |
| 18 | 6 | 0 | 0.870222 | -3.683651 | 0.072119 |
| 19 | 6 | 0 | 1.580681 | -2.487703 | 0.049351 |
| 20 | 6 | 0 | -2.648295 | 2.443862 | -0.045754 |
| 21 | 6 | 0 | -3.371038 | 1.239043 | -0.023087 |
| 22 | 6 | 0 | -2.653048 | 0.000000 | 0.000000 |
| 23 | 6 | 0 | -3.371038 | -1.239043 | 0.023088 |
| 24 | 6 | 0 | -2.648295 | -2.443862 | 0.045755 |
| 25 | 6 | 0 | -4.790296 | 1.208125 | -0.022489 |
| 26 | 6 | 0 | -5.476420 | 0.000000 | 0.000002 |
| 27 | 6 | 0 | -4.790296 | -1.208125 | 0.022492 |
| 28 | 1 | 0 | 5.822927 | 1.259419 | 1.753220 |
| 29 | 1 | 0 | 7.442893 | 0.737513 | 1.006111 |
| 30 | 1 | 0 | 7.442900 | -0.737512 | -1.006096 |
| 31 | 1 | 0 | 5.822940 | -1.259419 | -1.753215 |
| 32 | 1 | 0 | 1.410632 | 4.623505 | -0.091833 |
| 33 | 1 | 0 | -1.063795 | 4.622907 | -0.088508 |
| 34 | 1 | 0 | 2.662992 | 2.498217 | -0.052639 |
| 35 | 1 | 0 | -1.063794 | -4.622907 | 0.088508 |
| 36 | 1 | 0 | 1.410633 | -4.623505 | 0.091830 |
| 37 | 1 | 0 | 2.662993 | -2.498217 | 0.052634 |
| 38 | 1 | 0 | -3.190016 | 3.384026 | -0.063407 |
| 39 | 1 | 0 | -3.190015 | -3.384026 | 0.063409 |
| 40 | 1 | 0 | -5.334355 | 2.145968 | -0.039979 |
| 41 | 1 | 0 | -6.560805 | 0.000000 | 0.000003 |
| 42 | 1 | 0 | -5.334355 | -2.145968 | 0.039984 |

R=IN

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -1.277105 | 3.847144 | 0.037640 |
| 2 | 6 | 0 | -2.659577 | 3.742892 | 0.044735 |
| 3 | 6 | 0 | -3.289240 | 2.472589 | 0.031944 |
| 4 | 6 | 0 | -2.473311 | 1.295390 | 0.011312 |
| 5 | 6 | 0 | -1.050879 | 1.417081 | 0.004396 |
| 6 | 6 | 0 | -0.476204 | 2.709495 | 0.017986 |
| 7 | 6 | 0 | -3.088715 | 0.010948 | -0.002120 |
| 8 | 6 | 0 | -2.282555 | -1.163168 | -0.023355 |
| 9 | 6 | 0 | -0.858226 | -1.064876 | -0.030710 |
| 10 | 6 | 0 | -0.248457 | 0.231669 | -0.015502 |
| 11 | 6 | 0 | -2.907686 | -2.451921 | -0.037357 |
| 12 | 6 | 0 | -2.089541 | -3.609705 | -0.059131 |
| 13 | 6 | 0 | -0.707629 | -3.499427 | -0.067125 |
| 14 | 6 | 0 | -0.089205 | -2.252688 | -0.053332 |

| | | | | | |
|---|---|---|---|---|---|
| 15 | 6 | 0 | -4.690262 | 2.338977 | 0.039010 |
| 16 | 6 | 0 | -5.317106 | 1.081513 | 0.026336 |
| 17 | 6 | 0 | -4.505218 | -0.098718 | 0.005327 |
| 18 | 6 | 0 | -5.125607 | -1.389956 | -0.008207 |
| 19 | 6 | 0 | -4.312521 | -2.535688 | -0.029259 |
| 20 | 6 | 0 | -6.729657 | 0.940879 | 0.033560 |
| 21 | 6 | 0 | -7.320197 | -0.316849 | 0.020524 |
| 22 | 6 | 0 | -6.543014 | -1.468473 | -0.000048 |
| 23 | 6 | 0 | 1.156079 | 0.329586 | -0.019538 |
| 24 | 6 | 0 | 2.366199 | 0.383624 | -0.022183 |
| 25 | 6 | 0 | 3.779331 | 0.370766 | -0.028229 |
| 26 | 7 | 0 | 4.446183 | -0.875796 | -0.063109 |
| 27 | 6 | 0 | 5.905575 | -0.637841 | 0.187474 |
| 28 | 6 | 0 | 5.966628 | 0.905175 | -0.141965 |
| 29 | 7 | 0 | 4.566364 | 1.389217 | -0.001685 |
| 30 | 6 | 0 | 6.870218 | 1.717701 | 0.790778 |
| 31 | 6 | 0 | 6.365829 | 1.192091 | -1.603301 |
| 32 | 6 | 0 | 6.735730 | -1.567496 | -0.696097 |
| 33 | 6 | 0 | 6.149259 | -0.973973 | 1.669887 |
| 34 | 8 | 0 | 3.908282 | -2.017272 | -0.071046 |
| 35 | 1 | 0 | -0.810636 | 4.825749 | 0.047495 |
| 36 | 1 | 0 | -3.277458 | 4.633924 | 0.060181 |
| 37 | 1 | 0 | 0.602334 | 2.804159 | 0.012757 |
| 38 | 1 | 0 | -2.562968 | -4.585331 | -0.069757 |
| 39 | 1 | 0 | -0.095420 | -4.393925 | -0.084474 |
| 40 | 1 | 0 | 0.991950 | -2.184192 | -0.060703 |
| 41 | 1 | 0 | -5.303281 | 3.234253 | 0.054743 |
| 42 | 1 | 0 | -4.780377 | -3.514759 | -0.039704 |
| 43 | 1 | 0 | -7.344569 | 1.833836 | 0.049482 |
| 44 | 1 | 0 | -8.401287 | -0.400691 | 0.026413 |
| 45 | 1 | 0 | -7.013151 | -2.445520 | -0.010200 |
| 46 | 1 | 0 | 6.824030 | 2.769296 | 0.501429 |
| 47 | 1 | 0 | 6.552928 | 1.646492 | 1.830953 |
| 48 | 1 | 0 | 7.910420 | 1.386867 | 0.718059 |
| 49 | 1 | 0 | 7.410456 | 0.930256 | -1.789877 |
| 50 | 1 | 0 | 5.736060 | 0.644001 | -2.307037 |
| 51 | 1 | 0 | 6.234689 | 2.257583 | -1.799462 |
| 52 | 1 | 0 | 6.504281 | -2.604019 | -0.444453 |
| 53 | 1 | 0 | 6.527264 | -1.425427 | -1.755959 |
| 54 | 1 | 0 | 7.801609 | -1.400211 | -0.523326 |
| 55 | 1 | 0 | 7.202094 | -0.848786 | 1.930033 |
| 56 | 1 | 0 | 5.550081 | -0.344840 | 2.330609 |
| 57 | 1 | 0 | 5.869253 | -2.014913 | 1.844026 |

R=Phen

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -1.614785 | -3.672174 | 0.311575 |
| 2 | 6 | 0 | -3.000814 | -3.675404 | 0.306942 |
| 3 | 6 | 0 | -3.724744 | -2.460694 | 0.203597 |
| 4 | 6 | 0 | -3.001211 | -1.227906 | 0.101212 |
| 5 | 6 | 0 | -1.572798 | -1.238079 | 0.103600 |
| 6 | 6 | 0 | -0.904325 | -2.479925 | 0.212959 |
| 7 | 6 | 0 | -3.715281 | 0.000000 | -0.000001 |
| 8 | 6 | 0 | -3.001209 | 1.227905 | -0.101218 |
| 9 | 6 | 0 | -1.572797 | 1.238075 | -0.103611 |
| 10 | 6 | 0 | -0.858926 | -0.000003 | -0.000004 |
| 11 | 6 | 0 | -3.724740 | 2.460694 | -0.203601 |
| 12 | 6 | 0 | -3.000808 | 3.675402 | -0.306951 |
| 13 | 6 | 0 | -1.614779 | 3.672170 | -0.311590 |
| 14 | 6 | 0 | -0.904321 | 2.479919 | -0.212975 |
| 15 | 6 | 0 | -5.131954 | -2.435837 | 0.200728 |
| 16 | 6 | 0 | -5.854395 | -1.235060 | 0.101460 |
| 17 | 6 | 0 | -5.136016 | 0.000001 | 0.000002 |
| 18 | 6 | 0 | -5.854393 | 1.235064 | -0.101453 |
| 19 | 6 | 0 | -5.131950 | 2.435839 | -0.200726 |
| 20 | 6 | 0 | -7.273684 | -1.204220 | 0.098883 |
| 21 | 6 | 0 | -7.959863 | 0.000004 | 0.000010 |
| 22 | 6 | 0 | -7.273682 | 1.204227 | -0.098867 |
| 23 | 6 | 0 | 0.553134 | -0.000003 | -0.000001 |
| 24 | 6 | 0 | 1.766889 | -0.000002 | 0.000001 |
| 25 | 6 | 0 | 3.191152 | -0.000001 | 0.000003 |
| 26 | 6 | 0 | 3.898709 | 1.172575 | 0.304344 |
| 27 | 6 | 0 | 5.309622 | 1.196304 | 0.310230 |
| 28 | 6 | 0 | 6.026352 | 0.000000 | 0.000002 |
| 29 | 6 | 0 | 5.309624 | -1.196304 | -0.310226 |
| 30 | 6 | 0 | 3.898710 | -1.172576 | -0.304340 |
| 31 | 6 | 0 | 7.454604 | 0.000001 | 0.000002 |
| 32 | 6 | 0 | 8.136371 | -1.201800 | -0.312286 |
| 33 | 6 | 0 | 7.431777 | -2.362315 | -0.613977 |
| 34 | 6 | 0 | 6.043014 | -2.371700 | -0.616140 |
| 35 | 6 | 0 | 6.043012 | 2.371701 | 0.616144 |
| 36 | 6 | 0 | 7.431775 | 2.362317 | 0.613981 |
| 37 | 6 | 0 | 8.136371 | 1.201802 | 0.312290 |
| 38 | 1 | 0 | -1.074646 | -4.608758 | 0.394208 |
| 39 | 1 | 0 | -3.549112 | -4.607780 | 0.384265 |
| 40 | 1 | 0 | 0.177747 | -2.490390 | 0.222634 |
| 41 | 1 | 0 | -3.549104 | 4.607780 | -0.384273 |
| 42 | 1 | 0 | -1.074639 | 4.608752 | -0.394229 |
| 43 | 1 | 0 | 0.177751 | 2.490382 | -0.222656 |
| 44 | 1 | 0 | -5.673669 | -3.372950 | 0.278360 |
| 45 | 1 | 0 | -5.673665 | 3.372954 | -0.278355 |
| 46 | 1 | 0 | -7.817661 | -2.139116 | 0.175712 |
| 47 | 1 | 0 | -9.044242 | 0.000005 | 0.000013 |
| 48 | 1 | 0 | -7.817657 | 2.139124 | -0.175694 |
| 49 | 1 | 0 | 3.351621 | 2.076291 | 0.544915 |
| 50 | 1 | 0 | 3.351623 | -2.076292 | -0.544909 |
| 51 | 1 | 0 | 9.220809 | -1.205716 | -0.313407 |
| 52 | 1 | 0 | 7.973597 | -3.271302 | -0.850532 |
| 53 | 1 | 0 | 5.502492 | -3.281392 | -0.852984 |
| 54 | 1 | 0 | 5.502489 | 3.281392 | 0.852988 |
| 55 | 1 | 0 | 7.973594 | 3.271304 | 0.850535 |
| 56 | 1 | 0 | 9.220808 | 1.205720 | 0.313411 |

R=Ver

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -2.431587 | -3.684524 | 0.056258 |
| 2 | 6 | 0 | -3.817974 | -3.687696 | 0.041303 |
| 3 | 6 | 0 | -4.543438 | -2.469514 | 0.031136 |
| 4 | 6 | 0 | -3.820670 | -1.232492 | 0.035999 |
| 5 | 6 | 0 | -2.392645 | -1.243288 | 0.048710 |
| 6 | 6 | 0 | -1.720639 | -2.488664 | 0.059727 |
| 7 | 6 | 0 | -4.533879 | -0.000001 | 0.028458 |
| 8 | 6 | 0 | -3.820668 | 1.232489 | 0.036018 |
| 9 | 6 | 0 | -2.392643 | 1.243283 | 0.048729 |
| 10 | 6 | 0 | -1.683434 | -0.000003 | 0.050809 |
| 11 | 6 | 0 | -4.543434 | 2.469512 | 0.031173 |
| 12 | 6 | 0 | -3.817968 | 3.687693 | 0.041358 |
| 13 | 6 | 0 | -2.431581 | 3.684518 | 0.056312 |
| 14 | 6 | 0 | -1.720634 | 2.488658 | 0.059764 |
| 15 | 6 | 0 | -5.950498 | -2.444592 | 0.017084 |
| 16 | 6 | 0 | -6.672901 | -1.239345 | 0.008767 |
| 17 | 6 | 0 | -5.954843 | 0.000001 | 0.015175 |
| 18 | 6 | 0 | -6.672899 | 1.239347 | 0.008785 |
| 19 | 6 | 0 | -5.950494 | 2.444593 | 0.017120 |
| 20 | 6 | 0 | -8.092055 | -1.208348 | -0.005037 |
| 21 | 6 | 0 | -8.778050 | 0.000003 | -0.011847 |
| 22 | 6 | 0 | -8.092053 | 1.208353 | -0.005019 |
| 23 | 6 | 0 | -0.271940 | -0.000004 | 0.053252 |
| 24 | 6 | 0 | 0.938476 | -0.000004 | 0.052658 |
| 25 | 6 | 0 | 2.365524 | -0.000002 | 0.056174 |
| 26 | 7 | 0 | 2.956972 | 1.193955 | 0.065611 |
| 27 | 7 | 0 | 4.320745 | 1.173117 | 0.069257 |
| 28 | 6 | 0 | 5.092911 | 0.000002 | 0.027240 |
| 29 | 7 | 0 | 4.320749 | -1.173115 | 0.069265 |
| 30 | 7 | 0 | 2.956975 | -1.193956 | 0.065616 |
| 31 | 8 | 0 | 6.300451 | 0.000004 | -0.036821 |
| 32 | 6 | 0 | 4.939728 | -2.468358 | -0.011470 |
| 33 | 6 | 0 | 4.939722 | 2.468360 | -0.011490 |
| 34 | 6 | 0 | 4.288928 | -3.466275 | -0.741396 |
| 35 | 6 | 0 | 4.840838 | -4.740090 | -0.811938 |
| 36 | 6 | 0 | 6.037718 | -5.027018 | -0.159068 |
| 37 | 6 | 0 | 6.677794 | -4.028218 | 0.570576 |
| 38 | 6 | 0 | 6.137195 | -2.748648 | 0.651481 |
| 39 | 6 | 0 | 6.137188 | 2.748659 | 0.651458 |
| 40 | 6 | 0 | 6.677784 | 4.028229 | 0.570540 |
| 41 | 6 | 0 | 6.037707 | 5.027021 | -0.159113 |
| 42 | 6 | 0 | 4.840827 | 4.740085 | -0.811980 |
| 43 | 6 | 0 | 4.288919 | 3.466269 | -0.741426 |
| 44 | 1 | 0 | -1.891148 | -4.624368 | 0.066283 |
| 45 | 1 | 0 | -4.365365 | -4.623798 | 0.038352 |
| 46 | 1 | 0 | -0.638248 | -2.500152 | 0.073705 |
| 47 | 1 | 0 | -4.365357 | 4.623796 | 0.038422 |
| 48 | 1 | 0 | -1.891141 | 4.624362 | 0.066351 |
| 49 | 1 | 0 | -0.638244 | 2.500144 | 0.073740 |
| 50 | 1 | 0 | -6.492380 | -3.384766 | 0.013044 |
| 51 | 1 | 0 | -6.492374 | 3.384768 | 0.013095 |
| 52 | 1 | 0 | -8.636127 | -2.146286 | -0.009987 |
| 53 | 1 | 0 | -9.862347 | 0.000004 | -0.022331 |
| 54 | 1 | 0 | -8.636123 | 2.146292 | -0.009954 |
| 55 | 1 | 0 | 3.354902 | -3.236150 | -1.234410 |
| 56 | 1 | 0 | 4.332938 | -5.508553 | -1.383199 |
| 57 | 1 | 0 | 6.467182 | -6.020379 | -0.217548 |
| 58 | 1 | 0 | 7.606523 | -4.241806 | 1.086880 |
| 59 | 1 | 0 | 6.644054 | -1.978956 | 1.212323 |
| 60 | 1 | 0 | 6.644050 | 1.978973 | 1.212306 |
| 61 | 1 | 0 | 7.606513 | 4.241823 | 1.086842 |
| 62 | 1 | 0 | 6.467168 | 6.020383 | -0.217603 |
| 63 | 1 | 0 | 4.332926 | 5.508541 | -1.383249 |
| 64 | 1 | 0 | 3.354894 | 3.236138 | -1.234437 |

R=NN

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 1.143463 | -3.683283 | -0.051280 |
| 2 | 6 | 0 | 2.530542 | -3.686965 | -0.050921 |
| 3 | 6 | 0 | 3.257872 | -2.469884 | -0.033975 |
| 4 | 6 | 0 | 2.535848 | -1.232801 | -0.016911 |
| 5 | 6 | 0 | 1.108184 | -1.244223 | -0.017039 |
| 6 | 6 | 0 | 0.431680 | -2.488270 | -0.034857 |
| 7 | 6 | 0 | 3.248403 | 0.000000 | -0.000002 |
| 8 | 6 | 0 | 2.535845 | 1.232799 | 0.016903 |
| 9 | 6 | 0 | 1.108180 | 1.244217 | 0.017022 |
| 10 | 6 | 0 | 0.403294 | -0.000004 | -0.000010 |
| 11 | 6 | 0 | 3.257865 | 2.469884 | 0.033971 |

| | | | | | |
|---|---|---|---|---|---|
| 12 | 6 | 0 | 2.530532 | 3.686964 | 0.050912 |
| 13 | 6 | 0 | 1.143454 | 3.683278 | 0.051262 |
| 14 | 6 | 0 | 0.431673 | 2.488263 | 0.034836 |
| 15 | 6 | 0 | 4.669908 | 0.000002 | 0.000003 |
| 16 | 6 | 0 | 5.387557 | 1.239317 | 0.016985 |
| 17 | 6 | 0 | 4.664933 | 2.444883 | 0.033559 |
| 18 | 6 | 0 | 4.664939 | -2.444879 | -0.033554 |
| 19 | 6 | 0 | 5.387560 | -1.239311 | -0.016973 |
| 20 | 6 | 0 | 6.806738 | -1.208310 | -0.016537 |
| 21 | 6 | 0 | 7.492683 | 0.000006 | 0.000014 |
| 22 | 6 | 0 | 6.806735 | 1.208320 | 0.016559 |
| 23 | 6 | 0 | -1.005269 | -0.000005 | -0.000012 |
| 24 | 6 | 0 | -2.216615 | -0.000005 | -0.000011 |
| 25 | 6 | 0 | -3.611633 | -0.000003 | -0.000004 |
| 26 | 7 | 0 | -4.386180 | 1.114816 | 0.028979 |
| 27 | 6 | 0 | -5.840964 | 0.763824 | -0.180282 |
| 28 | 6 | 0 | -5.840966 | -0.763822 | 0.180294 |
| 29 | 7 | 0 | -4.386184 | -1.114818 | -0.028982 |
| 30 | 6 | 0 | -6.136135 | 1.063108 | -1.659888 |
| 31 | 6 | 0 | -6.704457 | 1.652809 | 0.712165 |
| 32 | 6 | 0 | -6.136122 | -1.063104 | 1.659904 |
| 33 | 6 | 0 | -6.704470 | -1.652804 | -0.712143 |
| 34 | 8 | 0 | -3.980631 | -2.314337 | -0.047509 |
| 35 | 8 | 0 | -3.980622 | 2.314333 | 0.047504 |
| 36 | 1 | 0 | 0.602219 | -4.622494 | -0.064669 |
| 37 | 1 | 0 | 3.077009 | -4.623577 | -0.063840 |
| 38 | 1 | 0 | -0.651551 | -2.501372 | -0.036000 |
| 39 | 1 | 0 | 3.076996 | 4.623577 | 0.063834 |
| 40 | 1 | 0 | 0.602206 | 4.622487 | 0.064647 |
| 41 | 1 | 0 | -0.651557 | 2.501362 | 0.035973 |
| 42 | 1 | 0 | 5.207071 | 3.384843 | 0.046482 |
| 43 | 1 | 0 | 5.207081 | -3.384838 | -0.046472 |
| 44 | 1 | 0 | 7.350906 | -2.146126 | -0.029380 |
| 45 | 1 | 0 | 8.577051 | 0.000007 | 0.000018 |
| 46 | 1 | 0 | 7.350900 | 2.146137 | 0.029406 |
| 47 | 1 | 0 | -7.187714 | 0.883954 | -1.891712 |
| 48 | 1 | 0 | -5.909915 | 2.113285 | -1.850016 |
| 49 | 1 | 0 | -5.521739 | 0.456083 | -2.327375 |
| 50 | 1 | 0 | -6.536432 | 2.694835 | 0.440240 |
| 51 | 1 | 0 | -7.761609 | 1.418955 | 0.565381 |
| 52 | 1 | 0 | -6.462241 | 1.539838 | 1.768079 |
| 53 | 1 | 0 | -7.187698 | -0.883946 | 1.891739 |
| 54 | 1 | 0 | -5.909905 | -2.113282 | 1.850029 |
| 55 | 1 | 0 | -5.521717 | -0.456083 | 2.327384 |
| 56 | 1 | 0 | -6.536445 | -2.694830 | -0.440220 |
| 57 | 1 | 0 | -7.761620 | -1.418947 | -0.565347 |
| 58 | 1 | 0 | -6.462266 | -1.539833 | -1.768060 |

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# Sat-Radical

R=Sat-H

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -3.890600 | -0.000009 | -0.338750 |
| 2 | 6 | 0 | -4.602470 | 0.000013 | 1.028808 |
| 3 | 6 | 0 | -1.604542 | 3.687852 | -0.124473 |
| 4 | 6 | 0 | -0.224942 | 3.687468 | -0.062844 |
| 5 | 6 | 0 | 0.489986 | 2.462542 | -0.043116 |
| 6 | 6 | 0 | -0.232856 | 1.232614 | -0.090424 |
| 7 | 6 | 0 | -1.668060 | 1.236461 | -0.169409 |
| 8 | 6 | 0 | -2.319468 | 2.491077 | -0.177451 |
| 9 | 6 | 0 | 0.482151 | -0.000002 | -0.057674 |
| 10 | 6 | 0 | -0.232850 | -1.232617 | -0.090427 |
| 11 | 6 | 0 | -1.668056 | -1.236469 | -0.169405 |
| 12 | 6 | 0 | -2.382352 | -0.000009 | -0.234449 |
| 13 | 6 | 0 | 0.489999 | -2.462541 | -0.043122 |
| 14 | 6 | 0 | -0.224928 | -3.687477 | -0.062841 |
| 15 | 6 | 0 | -1.604528 | -3.687865 | -0.124457 |
| 16 | 6 | 0 | -2.319460 | -2.491090 | -0.177434 |
| 17 | 6 | 0 | 1.897328 | 0.000002 | 0.015402 |
| 18 | 6 | 0 | 2.616665 | 1.240572 | 0.053753 |
| 19 | 6 | 0 | 4.041702 | 1.208052 | 0.123577 |
| 20 | 6 | 0 | 4.725927 | 0.000010 | 0.156396 |
| 21 | 6 | 0 | 4.041711 | -1.208033 | 0.123571 |
| 22 | 6 | 0 | 2.616671 | -1.240562 | 0.053745 |
| 23 | 6 | 0 | 1.900281 | -2.436951 | 0.024896 |
| 24 | 6 | 0 | 1.900272 | 2.436956 | 0.024914 |
| 25 | 1 | 0 | -4.220372 | -0.866284 | -0.915971 |
| 26 | 1 | 0 | -4.220374 | 0.866250 | -0.915995 |
| 27 | 1 | 0 | -5.688701 | 0.000007 | 0.900278 |
| 28 | 1 | 0 | -4.329470 | 0.881499 | 1.613945 |
| 29 | 1 | 0 | -4.329463 | -0.881446 | 1.613980 |
| 30 | 1 | 0 | -2.144559 | 4.628267 | -0.132603 |
| 31 | 1 | 0 | 0.327401 | 4.619832 | -0.025543 |
| 32 | 1 | 0 | -3.398532 | 2.538222 | -0.219733 |
| 33 | 1 | 0 | 0.327419 | -4.619838 | -0.025548 |
| 34 | 1 | 0 | -2.144541 | -4.628282 | -0.132579 |
| 35 | 1 | 0 | -3.398524 | -2.538239 | -0.219702 |
| 36 | 1 | 0 | 4.583981 | 2.146532 | 0.151397 |
| 37 | 1 | 0 | 5.809127 | 0.000013 | 0.209406 |
| 38 | 1 | 0 | 4.583998 | -2.146509 | 0.151387 |
| 39 | 1 | 0 | 2.438569 | -3.378783 | 0.057265 |
| 40 | 1 | 0 | 2.438555 | 3.378790 | 0.057295 |

R=Sat-Mt

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -3.606722 | -0.000002 | -0.489657 |
| 2 | 6 | 0 | -4.350342 | 0.000002 | 0.898812 |
| 3 | 6 | 0 | -5.827981 | 0.000000 | 0.767778 |
| 4 | 6 | 0 | -1.342002 | 3.687633 | -0.208409 |
| 5 | 6 | 0 | 0.039062 | 3.688205 | -0.102535 |
| 6 | 6 | 0 | 0.755586 | 2.465660 | -0.061931 |
| 7 | 6 | 0 | 0.032032 | 1.229757 | -0.134004 |
| 8 | 6 | 0 | -1.396403 | 1.233151 | -0.259691 |
| 9 | 6 | 0 | -2.052127 | 2.494251 | -0.286635 |
| 10 | 6 | 0 | 0.744936 | 0.000000 | -0.078571 |
| 11 | 6 | 0 | 0.032033 | -1.229758 | -0.134004 |
| 12 | 6 | 0 | -1.396402 | -1.233153 | -0.259690 |
| 13 | 6 | 0 | -2.106770 | -0.000001 | -0.351433 |
| 14 | 6 | 0 | 0.755588 | -2.465660 | -0.061931 |
| 15 | 6 | 0 | 0.039065 | -3.688206 | -0.102535 |
| 16 | 6 | 0 | -1.341999 | -3.687635 | -0.208409 |
| 17 | 6 | 0 | -2.052124 | -2.494253 | -0.286634 |
| 18 | 6 | 0 | 2.163186 | 0.000001 | 0.040647 |
| 19 | 6 | 0 | 2.879358 | 1.237457 | 0.101911 |
| 20 | 6 | 0 | 4.294037 | 1.207722 | 0.216544 |
| 21 | 6 | 0 | 4.978809 | 0.000002 | 0.271204 |
| 22 | 6 | 0 | 4.294038 | -1.207719 | 0.216544 |
| 23 | 6 | 0 | 2.879359 | -1.237455 | 0.101910 |
| 24 | 6 | 0 | 2.157721 | -2.441511 | 0.050325 |
| 25 | 6 | 0 | 2.157719 | 2.441512 | 0.050326 |
| 26 | 1 | 0 | -3.939716 | -0.867786 | -1.059978 |
| 27 | 1 | 0 | -3.939716 | 0.867780 | -1.059982 |
| 28 | 1 | 0 | -4.012107 | 0.879932 | 1.455394 |
| 29 | 1 | 0 | -4.012105 | -0.879921 | 1.455403 |
| 30 | 1 | 0 | -6.376167 | 0.925806 | 0.636851 |
| 31 | 1 | 0 | -6.376170 | -0.925811 | 0.636897 |
| 32 | 1 | 0 | -1.880886 | 4.628439 | -0.231992 |
| 33 | 1 | 0 | 0.587999 | 4.621647 | -0.046357 |
| 34 | 1 | 0 | -3.129147 | 2.539494 | -0.365349 |
| 35 | 1 | 0 | 0.588004 | -4.621647 | -0.046357 |
| 36 | 1 | 0 | -1.880882 | -4.628441 | -0.231991 |
| 37 | 1 | 0 | -3.129144 | -2.539497 | -0.365348 |
| 38 | 1 | 0 | 4.835234 | 2.146341 | 0.261880 |
| 39 | 1 | 0 | 6.059675 | 0.000002 | 0.358719 |
| 40 | 1 | 0 | 4.835236 | -2.146337 | 0.261879 |
| 41 | 1 | 0 | 2.695979 | -3.382551 | 0.100368 |
| 42 | 1 | 0 | 2.695975 | 3.382552 | 0.100368 |

R=Sat-DCM

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 2.718883 | 0.000002 | 0.673609 |
| 2 | 6 | 0 | 3.486728 | 0.000001 | -0.708628 |
| 3 | 6 | 0 | 4.971354 | -0.000001 | -0.522509 |
| 4 | 6 | 0 | 0.479551 | 3.687217 | 0.293371 |
| 5 | 6 | 0 | -0.896488 | 3.685317 | 0.137903 |
| 6 | 6 | 0 | -1.612470 | 2.464344 | 0.076254 |
| 7 | 6 | 0 | -0.893236 | 1.229687 | 0.178818 |
| 8 | 6 | 0 | 0.528321 | 1.235196 | 0.358640 |
| 9 | 6 | 0 | 1.185087 | 2.493347 | 0.404170 |
| 10 | 6 | 0 | -1.603183 | 0.000000 | 0.097988 |
| 11 | 6 | 0 | -0.893234 | -1.229686 | 0.178814 |
| 12 | 6 | 0 | 0.528323 | -1.235193 | 0.358636 |
| 13 | 6 | 0 | 1.233348 | 0.000002 | 0.484888 |
| 14 | 6 | 0 | -1.612466 | -2.464344 | 0.076247 |
| 15 | 6 | 0 | -0.896483 | -3.685315 | 0.137893 |
| 16 | 6 | 0 | 0.479556 | -3.687214 | 0.293361 |
| 17 | 6 | 0 | 1.185091 | -2.493343 | 0.404163 |
| 18 | 6 | 0 | -3.014758 | -0.000001 | -0.074422 |
| 19 | 6 | 0 | -3.728985 | 1.238021 | -0.162935 |
| 20 | 6 | 0 | -5.138783 | 1.207764 | -0.329266 |
| 21 | 6 | 0 | -5.820690 | -0.000002 | -0.408653 |
| 22 | 6 | 0 | -5.138782 | -1.207768 | -0.329269 |
| 23 | 6 | 0 | -3.728984 | -1.238023 | -0.162938 |
| 24 | 6 | 0 | -3.010178 | -2.441401 | -0.086895 |
| 25 | 6 | 0 | -3.010181 | 2.441400 | -0.086889 |
| 26 | 6 | 0 | 5.658865 | 1.210853 | -0.366055 |
| 27 | 6 | 0 | 5.658857 | -1.210856 | -0.366023 |
| 28 | 7 | 0 | 6.180709 | 2.243406 | -0.244753 |
| 29 | 7 | 0 | 6.180693 | -2.243409 | -0.244697 |
| 30 | 1 | 0 | 3.042678 | -0.870599 | 1.242571 |
| 31 | 1 | 0 | 3.042678 | 0.870605 | 1.242569 |
| 32 | 1 | 0 | 3.185042 | 0.884444 | -1.273119 |
| 33 | 1 | 0 | 3.185041 | -0.884444 | -1.273116 |
| 34 | 1 | 0 | 1.018071 | 4.627087 | 0.331652 |
| 35 | 1 | 0 | -1.442012 | 4.618929 | 0.057781 |
| 36 | 1 | 0 | 2.258259 | 2.542773 | 0.523740 |
| 37 | 1 | 0 | -1.442005 | -4.618928 | 0.057767 |
| 38 | 1 | 0 | 1.018078 | -4.627084 | 0.331639 |
| 39 | 1 | 0 | 2.258262 | -2.542769 | 0.523735 |
| 40 | 1 | 0 | -5.678086 | 2.146039 | -0.394771 |
| 41 | 1 | 0 | -6.897401 | -0.000003 | -0.535600 |
| 42 | 1 | 0 | -5.678082 | -2.146043 | -0.394779 |
| 43 | 1 | 0 | -3.545348 | -3.382577 | -0.157790 |
| 44 | 1 | 0 | -3.545353 | 3.382575 | -0.157780 |

R=Sat-DPM

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -1.225226 | 0.012176 | -0.749183 |
| 2 | 6 | 0 | -2.014189 | -0.063847 | 0.603122 |
| 3 | 6 | 0 | -3.506925 | -0.028672 | 0.414694 |
| 4 | 6 | 0 | -4.286658 | -1.240713 | 0.502462 |
| 5 | 6 | 0 | -4.115863 | 1.259250 | 0.065198 |
| 6 | 6 | 0 | -5.690049 | -1.213166 | 0.725914 |
| 7 | 6 | 0 | -6.430247 | -2.378904 | 0.842114 |
| 8 | 6 | 0 | -5.813626 | -3.628046 | 0.741682 |
| 9 | 6 | 0 | -4.434387 | -3.687145 | 0.537633 |
| 10 | 6 | 0 | -3.685364 | -2.525169 | 0.427697 |
| 11 | 6 | 0 | -5.128613 | 1.355580 | -0.915419 |
| 12 | 6 | 0 | -5.675006 | 2.581145 | -1.274848 |
| 13 | 6 | 0 | -5.236940 | 3.756919 | -0.666126 |
| 14 | 6 | 0 | -4.236107 | 3.688837 | 0.302155 |
| 15 | 6 | 0 | -3.678875 | 2.465521 | 0.655297 |
| 16 | 6 | 0 | 0.978046 | 3.648148 | 0.055016 |
| 17 | 6 | 0 | 2.347452 | 3.643171 | 0.262295 |
| 18 | 6 | 0 | 3.075789 | 2.428100 | 0.210421 |
| 19 | 6 | 0 | 2.376257 | 1.205790 | -0.059815 |
| 20 | 6 | 0 | 0.959286 | 1.215492 | -0.278344 |
| 21 | 6 | 0 | 0.290194 | 2.468170 | -0.208693 |
| 22 | 6 | 0 | 3.101363 | -0.016941 | -0.107729 |
| 23 | 6 | 0 | 2.412592 | -1.233204 | -0.372004 |
| 24 | 6 | 0 | 0.994880 | -1.230215 | -0.593371 |
| 25 | 6 | 0 | 0.270224 | -0.002325 | -0.555556 |
| 26 | 6 | 0 | 3.150122 | -2.462591 | -0.412970 |
| 27 | 6 | 0 | 2.460831 | -3.673888 | -0.671428 |
| 28 | 6 | 0 | 1.092260 | -3.668343 | -0.883829 |
| 29 | 6 | 0 | 0.368659 | -2.481247 | -0.848125 |
| 30 | 6 | 0 | 4.508203 | -0.022996 | 0.109412 |
| 31 | 6 | 0 | 5.200005 | 1.201198 | 0.374951 |
| 32 | 6 | 0 | 6.603456 | 1.165778 | 0.585965 |
| 33 | 6 | 0 | 7.300803 | -0.034956 | 0.537823 |
| 34 | 6 | 0 | 6.639856 | -1.230041 | 0.282122 |
| 35 | 6 | 0 | 5.237400 | -1.253296 | 0.063352 |
| 36 | 6 | 0 | 4.540027 | -2.444540 | -0.196224 |
| 37 | 6 | 0 | 4.466622 | 2.398348 | 0.419240 |
| 38 | 1 | 0 | -1.542023 | -0.813689 | -1.386076 |
| 39 | 1 | 0 | -1.533674 | 0.916516 | -1.275872 |
| 40 | 1 | 0 | -1.691747 | 0.781986 | 1.216538 |
| 41 | 1 | 0 | -1.707484 | -0.959203 | 1.145627 |

| | | | | | |
|---|---|---|---|---|---|
| 42 | 1 | 0 | -6.186989 | -0.259207 | 0.843138 |
| 43 | 1 | 0 | -7.497284 | -2.315460 | 1.026112 |
| 44 | 1 | 0 | -6.395794 | -4.537803 | 0.830850 |
| 45 | 1 | 0 | -3.938866 | -4.649076 | 0.463162 |
| 46 | 1 | 0 | -2.618596 | -2.610684 | 0.268398 |
| 47 | 1 | 0 | -5.463600 | 0.455985 | -1.416678 |
| 48 | 1 | 0 | -6.440635 | 2.620043 | -2.042016 |
| 49 | 1 | 0 | -5.666370 | 4.712276 | -0.944901 |
| 50 | 1 | 0 | -3.891194 | 4.593781 | 0.790437 |
| 51 | 1 | 0 | -2.917204 | 2.440443 | 1.425087 |
| 52 | 1 | 0 | 0.429944 | 4.583024 | 0.096186 |
| 53 | 1 | 0 | 2.878593 | 4.566257 | 0.466418 |
| 54 | 1 | 0 | -0.777540 | 2.519900 | -0.367114 |
| 55 | 1 | 0 | 3.020804 | -4.601926 | -0.701359 |
| 56 | 1 | 0 | 0.573895 | -4.599747 | -1.083433 |
| 57 | 1 | 0 | -0.695596 | -2.523935 | -1.029289 |
| 58 | 1 | 0 | 7.126014 | 2.094563 | 0.786590 |
| 59 | 1 | 0 | 8.372699 | -0.039472 | 0.701961 |
| 60 | 1 | 0 | 7.190615 | -2.163499 | 0.246558 |
| 61 | 1 | 0 | 5.087964 | -3.380658 | -0.230957 |
| 62 | 1 | 0 | 4.986561 | 3.329292 | 0.621204 |

R=Sat-Flu

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 1.111500 | 0.000023 | 0.711108 |
| 2 | 6 | 0 | 1.886906 | 0.000011 | -0.657581 |
| 3 | 6 | 0 | 3.362221 | 0.000005 | -0.475190 |
| 4 | 6 | 0 | 4.202652 | -1.158888 | -0.323607 |
| 5 | 6 | 0 | 5.545408 | -0.732493 | -0.082440 |
| 6 | 6 | 0 | 5.545412 | 0.732481 | -0.082417 |
| 7 | 6 | 0 | 4.202657 | 1.158890 | -0.323572 |
| 8 | 6 | 0 | 6.556840 | 1.663825 | 0.093705 |
| 9 | 6 | 0 | 6.244463 | 3.027543 | 0.031676 |
| 10 | 6 | 0 | 4.933342 | 3.452106 | -0.208167 |
| 11 | 6 | 0 | 3.906754 | 2.527135 | -0.387311 |
| 12 | 6 | 0 | 3.906742 | -2.527130 | -0.387390 |
| 13 | 6 | 0 | 4.933325 | -3.452111 | -0.208277 |
| 14 | 6 | 0 | 6.244449 | -3.027562 | 0.031579 |
| 15 | 6 | 0 | 6.556832 | -1.663847 | 0.093651 |
| 16 | 6 | 0 | -1.151211 | 3.689386 | 0.370110 |
| 17 | 6 | 0 | -2.519045 | 3.687936 | 0.183520 |
| 18 | 6 | 0 | -3.228030 | 2.462643 | 0.096771 |
| 19 | 6 | 0 | -2.511299 | 1.232903 | 0.205326 |
| 20 | 6 | 0 | -1.088654 | 1.237742 | 0.407392 |
| 21 | 6 | 0 | -0.442600 | 2.492272 | 0.480608 |
| 22 | 6 | 0 | -3.220382 | 0.000001 | 0.108409 |
| 23 | 6 | 0 | -2.511289 | -1.232894 | 0.205352 |
| 24 | 6 | 0 | -1.088644 | -1.237716 | 0.407417 |
| 25 | 6 | 0 | -0.380619 | 0.000017 | 0.528338 |
| 26 | 6 | 0 | -3.228009 | -2.462643 | 0.096825 |
| 27 | 6 | 0 | -2.519014 | -3.687927 | 0.183602 |
| 28 | 6 | 0 | -1.151180 | -3.689362 | 0.370189 |
| 29 | 6 | 0 | -0.442579 | -2.492239 | 0.480661 |
| 30 | 6 | 0 | -4.623316 | -0.000007 | -0.088803 |
| 31 | 6 | 0 | -5.337049 | 1.240506 | -0.189918 |
| 32 | 6 | 0 | -6.750068 | 1.207946 | -0.385616 |
| 33 | 6 | 0 | -7.428720 | -0.000023 | -0.479115 |
| 34 | 6 | 0 | -6.750058 | -1.207985 | -0.385592 |
| 35 | 6 | 0 | -5.337039 | -1.240529 | -0.189891 |
| 36 | 6 | 0 | -4.626570 | -2.437043 | -0.095937 |
| 37 | 6 | 0 | -4.626590 | 2.437028 | -0.095990 |
| 38 | 1 | 0 | 1.431689 | -0.867631 | 1.288182 |
| 39 | 1 | 0 | 1.431687 | 0.867686 | 1.288168 |
| 40 | 1 | 0 | 1.571903 | 0.878128 | -1.228473 |
| 41 | 1 | 0 | 1.571896 | -0.878111 | -1.228459 |
| 42 | 1 | 0 | 7.578895 | 1.349622 | 0.276690 |
| 43 | 1 | 0 | 7.028720 | 3.763419 | 0.168413 |
| 44 | 1 | 0 | 4.715624 | 4.513032 | -0.257196 |
| 45 | 1 | 0 | 2.895902 | 2.868128 | -0.583681 |
| 46 | 1 | 0 | 2.895888 | -2.868111 | -0.583770 |
| 47 | 1 | 0 | 4.715603 | -4.513034 | -0.257339 |
| 48 | 1 | 0 | 7.028702 | -3.763446 | 0.168292 |
| 49 | 1 | 0 | 7.578888 | -1.349656 | 0.276648 |
| 50 | 1 | 0 | -0.615492 | 4.629998 | 0.434558 |
| 51 | 1 | 0 | -3.066925 | 4.619925 | 0.100318 |
| 52 | 1 | 0 | 0.626502 | 2.541417 | 0.631653 |
| 53 | 1 | 0 | -3.066886 | -4.619923 | 0.100421 |
| 54 | 1 | 0 | -0.615453 | -4.629968 | 0.434659 |
| 55 | 1 | 0 | 0.626524 | -2.541371 | 0.631704 |
| 56 | 1 | 0 | -7.287771 | 2.146407 | -0.460943 |
| 57 | 1 | 0 | -8.502920 | -0.000029 | -0.627826 |
| 58 | 1 | 0 | -7.287754 | -2.146451 | -0.460899 |
| 59 | 1 | 0 | -5.160199 | -3.378799 | -0.173805 |
| 60 | 1 | 0 | -5.160227 | 3.378777 | -0.173882 |

R=Sat-PhO

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -2.038671 | 0.000026 | -0.649433 |
| 2 | 6 | 0 | -2.806745 | 0.000015 | 0.713635 |
| 3 | 6 | 0 | -4.296202 | 0.000007 | 0.528948 |
| 4 | 6 | 0 | -5.009747 | 1.217121 | 0.415448 |
| 5 | 6 | 0 | -6.364583 | 1.233660 | 0.199210 |
| 6 | 6 | 0 | -7.120865 | -0.000009 | 0.075724 |
| 7 | 6 | 0 | -6.364580 | -1.233669 | 0.199278 |
| 8 | 6 | 0 | -5.009745 | -1.217114 | 0.415520 |
| 9 | 8 | 0 | -8.355096 | -0.000016 | -0.121504 |
| 10 | 6 | 0 | 0.219357 | -3.688306 | -0.320380 |
| 11 | 6 | 0 | 1.594779 | -3.687935 | -0.156473 |
| 12 | 6 | 0 | 2.308199 | -2.465353 | -0.082454 |
| 13 | 6 | 0 | 1.587735 | -1.229683 | -0.180396 |
| 14 | 6 | 0 | 0.165141 | -1.233442 | -0.360813 |
| 15 | 6 | 0 | -0.487663 | -2.495050 | -0.421699 |
| 16 | 6 | 0 | 2.297326 | -0.000001 | -0.095302 |
| 17 | 6 | 0 | 1.587750 | 1.229690 | -0.180389 |
| 18 | 6 | 0 | 0.165157 | 1.233469 | -0.360805 |
| 19 | 6 | 0 | -0.541138 | 0.000018 | -0.471208 |
| 20 | 6 | 0 | 2.308230 | 2.465350 | -0.082440 |
| 21 | 6 | 0 | 1.594826 | 3.687942 | -0.156452 |
| 22 | 6 | 0 | 0.219405 | 3.688332 | -0.320358 |
| 23 | 6 | 0 | -0.487631 | 2.495085 | -0.421683 |
| 24 | 6 | 0 | 3.709854 | -0.000011 | 0.080282 |
| 25 | 6 | 0 | 4.423168 | -1.237362 | 0.169560 |
| 26 | 6 | 0 | 5.832010 | -1.207688 | 0.341357 |
| 27 | 6 | 0 | 6.513959 | -0.000030 | 0.423927 |
| 28 | 6 | 0 | 5.832026 | 1.207637 | 0.341362 |
| 29 | 6 | 0 | 4.423184 | 1.237331 | 0.169566 |
| 30 | 6 | 0 | 3.704593 | 2.441415 | 0.086888 |
| 31 | 6 | 0 | 3.704561 | -2.441437 | 0.086876 |
| 32 | 1 | 0 | -2.356731 | -0.866749 | -1.229931 |
| 33 | 1 | 0 | -2.356725 | 0.866815 | -1.229915 |
| 34 | 1 | 0 | -2.497863 | 0.879612 | 1.285013 |
| 35 | 1 | 0 | -2.497852 | -0.879584 | 1.285002 |
| 36 | 1 | 0 | -4.466281 | 2.152178 | 0.513048 |
| 37 | 1 | 0 | -6.921473 | 2.159931 | 0.118617 |
| 38 | 1 | 0 | -6.921468 | -2.159946 | 0.118738 |
| 39 | 1 | 0 | -4.466276 | -2.152164 | 0.513174 |
| 40 | 1 | 0 | -0.316745 | -4.629394 | -0.372792 |
| 41 | 1 | 0 | 2.141445 | -4.621295 | -0.081544 |
| 42 | 1 | 0 | -1.559686 | -2.542098 | -0.550872 |
| 43 | 1 | 0 | 2.141505 | 4.621295 | -0.081517 |
| 44 | 1 | 0 | -0.316686 | 4.629426 | -0.372764 |
| 45 | 1 | 0 | -1.559653 | 2.542148 | -0.550855 |
| 46 | 1 | 0 | 6.370960 | -2.146235 | 0.408049 |
| 47 | 1 | 0 | 7.590306 | -0.000037 | 0.555057 |
| 48 | 1 | 0 | 6.370988 | 2.146178 | 0.408059 |
| 49 | 1 | 0 | 4.240453 | 3.382440 | 0.156849 |
| 50 | 1 | 0 | 4.240409 | -3.382468 | 0.156831 |

R=Sat-NO

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 3.028030 | -0.187059 | -0.569806 |
| 2 | 6 | 0 | 3.791780 | -0.070109 | 0.776655 |
| 3 | 7 | 0 | 5.218786 | 0.172800 | 0.567656 |
| 4 | 6 | 0 | 6.152491 | -0.943748 | 0.432595 |
| 5 | 8 | 0 | 5.548067 | 1.288236 | 0.035579 |
| 6 | 6 | 0 | 0.598262 | -3.785884 | -0.240550 |
| 7 | 6 | 0 | -0.779683 | -3.719795 | -0.114514 |
| 8 | 6 | 0 | -1.435775 | -2.464107 | -0.063790 |
| 9 | 6 | 0 | -0.654949 | -1.264433 | -0.147103 |
| 10 | 6 | 0 | 0.770118 | -1.336713 | -0.293556 |
| 11 | 6 | 0 | 1.363642 | -2.628123 | -0.329153 |
| 12 | 6 | 0 | -1.307062 | -0.001669 | -0.082602 |
| 13 | 6 | 0 | -0.537686 | 1.193256 | -0.148862 |
| 14 | 6 | 0 | 0.886566 | 1.129278 | -0.294127 |
| 15 | 6 | 0 | 1.533805 | -0.137744 | -0.394824 |
| 16 | 6 | 0 | -1.199536 | 2.462385 | -0.069722 |
| 17 | 6 | 0 | -0.424179 | 3.648151 | -0.123767 |
| 18 | 6 | 0 | 0.953674 | 3.580891 | -0.247348 |
| 19 | 6 | 0 | 1.606733 | 2.355119 | -0.332524 |
| 20 | 6 | 0 | -2.721840 | 0.066393 | 0.056377 |
| 21 | 6 | 0 | -3.495602 | -1.135302 | 0.129434 |
| 22 | 6 | 0 | -4.905397 | -1.037863 | 0.264130 |
| 23 | 6 | 0 | -5.530527 | 0.201427 | 0.326620 |
| 24 | 6 | 0 | -4.789549 | 1.374863 | 0.260344 |
| 25 | 6 | 0 | -3.376801 | 1.337003 | 0.125754 |
| 26 | 6 | 0 | -2.599463 | 2.505383 | 0.061777 |
| 27 | 6 | 0 | -2.833358 | -2.372676 | 0.068978 |
| 28 | 1 | 0 | 3.368068 | 0.638233 | -1.197029 |
| 29 | 1 | 0 | 3.331792 | -1.101446 | -1.080944 |
| 30 | 1 | 0 | 3.667399 | -0.972859 | 1.378859 |
| 31 | 1 | 0 | 3.408111 | 0.779824 | 1.343339 |
| 32 | 1 | 0 | 7.157180 | -0.549549 | 0.577283 |
| 33 | 1 | 0 | 5.938772 | -1.705415 | 1.184592 |
| 34 | 1 | 0 | 6.089999 | -1.392346 | -0.567011 |
| 35 | 1 | 0 | 1.090442 | -4.751726 | -0.272260 |
| 36 | 1 | 0 | -1.371936 | -4.625785 | -0.050366 |
| 37 | 1 | 0 | 2.436185 | -2.726152 | -0.423643 |
| 38 | 1 | 0 | -0.926276 | 4.607335 | -0.062396 |
| 39 | 1 | 0 | 1.537688 | 4.493884 | -0.278988 |
| 40 | 1 | 0 | 2.685070 | 2.350450 | -0.416593 |
| 41 | 1 | 0 | -5.490288 | -1.949384 | 0.318401 |
| 42 | 1 | 0 | -6.608781 | 0.253393 | 0.429340 |
| 43 | 1 | 0 | -5.284607 | 2.338288 | 0.311689 |

| | | | | | |
|---|---|---|---|---|---|
| 44 | 1 | 0 | -3.091659 | 3.470985 | 0.117217 |
| 45 | 1 | 0 | -3.415348 | -3.286762 | 0.127800 |

R=Sat-Allyl

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -3.083696 | 0.000006 | -0.606316 |
| 2 | 6 | 0 | -3.856301 | 0.000012 | 0.738459 |
| 3 | 6 | 0 | -5.363311 | -0.000001 | 0.537910 |
| 4 | 6 | 0 | -6.032876 | 1.211280 | 0.434468 |
| 5 | 6 | 0 | -6.032870 | -1.211295 | 0.434581 |
| 6 | 6 | 0 | -0.818629 | 3.687428 | -0.295550 |
| 7 | 6 | 0 | 0.558830 | 3.687981 | -0.146195 |
| 8 | 6 | 0 | 1.273158 | 2.465461 | -0.077830 |
| 9 | 6 | 0 | 0.551628 | 1.229393 | -0.166807 |
| 10 | 6 | 0 | -0.873121 | 1.232293 | -0.331642 |
| 11 | 6 | 0 | -1.526817 | 2.494455 | -0.387451 |
| 12 | 6 | 0 | 1.262316 | 0.000000 | -0.088951 |
| 13 | 6 | 0 | 0.551625 | -1.229392 | -0.166812 |
| 14 | 6 | 0 | -0.873124 | -1.232287 | -0.331646 |
| 15 | 6 | 0 | -1.581458 | 0.000004 | -0.431554 |
| 16 | 6 | 0 | 1.273153 | -2.465461 | -0.077841 |
| 17 | 6 | 0 | 0.558822 | -3.687980 | -0.146210 |
| 18 | 6 | 0 | -0.818637 | -3.687423 | -0.295564 |
| 19 | 6 | 0 | -1.526823 | -2.494448 | -0.387459 |
| 20 | 6 | 0 | 2.677060 | -0.000002 | 0.071294 |
| 21 | 6 | 0 | 3.390948 | 1.237280 | 0.152816 |
| 22 | 6 | 0 | 4.801491 | 1.207697 | 0.309941 |
| 23 | 6 | 0 | 5.484309 | -0.000006 | 0.385480 |
| 24 | 6 | 0 | 4.801488 | -1.207707 | 0.309935 |
| 25 | 6 | 0 | 3.390946 | -1.237286 | 0.152809 |
| 26 | 6 | 0 | 2.671149 | -2.441449 | 0.077035 |
| 27 | 6 | 0 | 2.671155 | 2.441445 | 0.077046 |
| 28 | 1 | 0 | -3.397296 | -0.865739 | -1.192348 |
| 29 | 1 | 0 | -3.397293 | 0.865748 | -1.192355 |
| 30 | 1 | 0 | -3.559248 | 0.876616 | 1.320603 |
| 31 | 1 | 0 | -3.559234 | -0.876575 | 1.320619 |
| 32 | 1 | 0 | -7.101709 | 1.247693 | 0.258793 |
| 33 | 1 | 0 | -5.513107 | 2.156176 | 0.538675 |
| 34 | 1 | 0 | -7.101703 | -1.247728 | 0.258911 |
| 35 | 1 | 0 | -5.513093 | -2.156178 | 0.538874 |
| 36 | 1 | 0 | -1.355494 | 4.628508 | -0.342852 |
| 37 | 1 | 0 | 1.106206 | 4.621527 | -0.077981 |
| 38 | 1 | 0 | -2.600540 | 2.539448 | -0.501747 |
| 39 | 1 | 0 | 1.106196 | -4.621527 | -0.078002 |
| 40 | 1 | 0 | -1.355504 | -4.628501 | -0.342869 |
| 41 | 1 | 0 | -2.600546 | -2.539438 | -0.501752 |
| 42 | 1 | 0 | 5.341107 | 2.146336 | 0.370956 |
| 43 | 1 | 0 | 6.562050 | -0.000007 | 0.505457 |
| 44 | 1 | 0 | 5.341102 | -2.146347 | 0.370942 |
| 45 | 1 | 0 | 3.207802 | -3.382544 | 0.141194 |
| 46 | 1 | 0 | 3.207809 | 3.382538 | 0.141206 |

R=Sat-IN

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 1.319656 | 0.270951 | 0.595846 |
| 2 | 6 | 0 | 2.108335 | 0.304168 | -0.739846 |
| 3 | 6 | 0 | 3.586494 | 0.300782 | -0.524547 |
| 4 | 7 | 0 | 4.214690 | -0.872006 | -0.079167 |
| 5 | 6 | 0 | 5.637449 | -0.567522 | 0.283764 |
| 6 | 6 | 0 | 5.785091 | 0.823737 | -0.452835 |
| 7 | 7 | 0 | 4.388351 | 1.287979 | -0.687472 |
| 8 | 6 | 0 | 6.536053 | 1.891580 | 0.349028 |
| 9 | 6 | 0 | 6.427210 | 0.702813 | -1.848014 |
| 10 | 6 | 0 | 6.542545 | -1.703514 | -0.191632 |
| 11 | 6 | 0 | 5.685261 | -0.478674 | 1.819451 |
| 12 | 8 | 0 | 3.641975 | -1.973286 | 0.177180 |
| 13 | 6 | 0 | -1.171143 | 3.820624 | 0.326707 |
| 14 | 6 | 0 | -2.548248 | 3.734449 | 0.198836 |
| 15 | 6 | 0 | -3.183587 | 2.469774 | 0.115573 |
| 16 | 6 | 0 | -2.382454 | 1.281914 | 0.168958 |
| 17 | 6 | 0 | -0.959126 | 1.374768 | 0.320298 |
| 18 | 6 | 0 | -0.385701 | 2.674879 | 0.387917 |
| 19 | 6 | 0 | -3.011783 | 0.010272 | 0.070549 |
| 20 | 6 | 0 | -2.221071 | -1.171592 | 0.105898 |
| 21 | 6 | 0 | -0.797915 | -1.085744 | 0.256148 |
| 22 | 6 | 0 | -0.175723 | 0.188231 | 0.393271 |
| 23 | 6 | 0 | -2.859833 | -2.449845 | -0.009700 |
| 24 | 6 | 0 | -2.062771 | -3.622116 | 0.011402 |
| 25 | 6 | 0 | -0.685698 | -3.532759 | 0.137041 |
| 26 | 6 | 0 | -0.054265 | -2.299197 | 0.258092 |
| 27 | 6 | 0 | -4.425486 | -0.079037 | -0.072379 |
| 28 | 6 | 0 | -5.219873 | 1.110349 | -0.114554 |
| 29 | 6 | 0 | -6.627635 | 0.991637 | -0.253672 |
| 30 | 6 | 0 | -7.230602 | -0.256429 | -0.350169 |
| 31 | 6 | 0 | -6.468976 | -1.418019 | -0.314538 |
| 32 | 6 | 0 | -5.057311 | -1.358652 | -0.177021 |
| 33 | 6 | 0 | -4.258672 | -2.514306 | -0.144237 |
| 34 | 6 | 0 | -4.579234 | 2.357394 | -0.020901 |
| 35 | 1 | 0 | 1.661062 | -0.581432 | 1.183360 |
| 36 | 1 | 0 | 1.576063 | 1.158642 | 1.176069 |
| 37 | 1 | 0 | 1.854609 | 1.197942 | -1.310457 |
| 38 | 1 | 0 | 1.838944 | -0.571832 | -1.336040 |
| 39 | 1 | 0 | 6.555822 | 2.818425 | -0.227453 |
| 40 | 1 | 0 | 6.051339 | 2.105087 | 1.301644 |
| 41 | 1 | 0 | 7.568439 | 1.586526 | 0.543100 |
| 42 | 1 | 0 | 7.480566 | 0.419640 | -1.780050 |
| 43 | 1 | 0 | 5.907325 | -0.030103 | -2.468249 |
| 44 | 1 | 0 | 6.359936 | 1.669620 | -2.349952 |
| 45 | 1 | 0 | 6.243071 | -2.630584 | 0.300591 |
| 46 | 1 | 0 | 6.479355 | -1.860191 | -1.267950 |
| 47 | 1 | 0 | 7.582391 | -1.494248 | 0.070610 |
| 48 | 1 | 0 | 6.699301 | -0.271857 | 2.166784 |
| 49 | 1 | 0 | 5.022126 | 0.299692 | 2.201198 |
| 50 | 1 | 0 | 5.363378 | -1.434995 | 2.236760 |
| 51 | 1 | 0 | -0.694996 | 4.793491 | 0.379943 |
| 52 | 1 | 0 | -3.155524 | 4.631809 | 0.156397 |
| 53 | 1 | 0 | 0.685541 | 2.788387 | 0.479542 |
| 54 | 1 | 0 | -2.547240 | -4.588251 | -0.077729 |
| 55 | 1 | 0 | -0.085167 | -4.435676 | 0.140889 |
| 56 | 1 | 0 | 1.024290 | -2.277512 | 0.339092 |
| 57 | 1 | 0 | -7.228566 | 1.893811 | -0.284546 |
| 58 | 1 | 0 | -8.307717 | -0.324694 | -0.455807 |
| 59 | 1 | 0 | -6.946834 | -2.388351 | -0.392690 |
| 60 | 1 | 0 | -4.733336 | -3.486730 | -0.227503 |
| 61 | 1 | 0 | -5.177199 | 3.262361 | -0.056927 |

R=Sat-Phen

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 0.735010 | -0.000011 | -0.606747 |
| 2 | 6 | 0 | 1.501339 | 0.000000 | 0.744164 |
| 3 | 6 | 0 | 3.002586 | 0.000001 | 0.559742 |
| 4 | 6 | 0 | 3.703850 | -1.201734 | 0.455908 |
| 5 | 6 | 0 | 5.103046 | -1.234218 | 0.242780 |
| 6 | 6 | 0 | 5.812286 | 0.000001 | 0.133177 |
| 7 | 6 | 0 | 5.103050 | 1.234219 | 0.242804 |
| 8 | 6 | 0 | 3.703853 | 1.201734 | 0.455932 |
| 9 | 6 | 0 | 7.224788 | 0.000000 | -0.079842 |
| 10 | 6 | 0 | 7.898788 | 1.241978 | -0.180592 |
| 11 | 6 | 0 | 7.201568 | 2.439656 | -0.071826 |
| 12 | 6 | 0 | 5.827384 | 2.447518 | 0.137492 |
| 13 | 6 | 0 | 5.827376 | -2.447518 | 0.137442 |
| 14 | 6 | 0 | 7.201560 | -2.439656 | -0.071876 |
| 15 | 6 | 0 | 7.898784 | -1.241977 | -0.180617 |
| 16 | 6 | 0 | -1.530874 | -3.687594 | -0.304055 |
| 17 | 6 | 0 | -2.908327 | -3.688033 | -0.155029 |
| 18 | 6 | 0 | -3.622530 | -2.465450 | -0.086640 |
| 19 | 6 | 0 | -2.900895 | -1.229421 | -0.175115 |
| 20 | 6 | 0 | -1.476031 | -1.232392 | -0.339014 |
| 21 | 6 | 0 | -0.822554 | -2.494619 | -0.395100 |
| 22 | 6 | 0 | -3.611571 | 0.000000 | -0.097481 |
| 23 | 6 | 0 | -2.900890 | 1.229418 | -0.175125 |
| 24 | 6 | 0 | -1.476026 | 1.232383 | -0.339025 |
| 25 | 6 | 0 | -0.767602 | -0.000007 | -0.437708 |
| 26 | 6 | 0 | -3.622520 | 2.465451 | -0.086659 |
| 27 | 6 | 0 | -2.908313 | 3.688031 | -0.155057 |
| 28 | 6 | 0 | -1.530860 | 3.687585 | -0.304084 |
| 29 | 6 | 0 | -0.822545 | 2.494606 | -0.395121 |
| 30 | 6 | 0 | -5.026372 | 0.000004 | 0.062213 |
| 31 | 6 | 0 | -5.740327 | -1.237259 | 0.143435 |
| 32 | 6 | 0 | -7.150913 | -1.207682 | 0.300128 |
| 33 | 6 | 0 | -7.833756 | 0.000010 | 0.375486 |
| 34 | 6 | 0 | -7.150908 | 1.207699 | 0.300119 |
| 35 | 6 | 0 | -5.740322 | 1.237270 | 0.143426 |
| 36 | 6 | 0 | -5.020560 | 2.441433 | 0.067733 |
| 37 | 6 | 0 | -5.020570 | -2.441425 | 0.067750 |
| 38 | 1 | 0 | 1.051950 | 0.865571 | -1.191015 |
| 39 | 1 | 0 | 1.051947 | -0.865605 | -1.191000 |
| 40 | 1 | 0 | 1.197970 | -0.876523 | 1.323736 |
| 41 | 1 | 0 | 1.197968 | 0.876531 | 1.323722 |
| 42 | 1 | 0 | 3.171399 | -2.143504 | 0.549700 |
| 43 | 1 | 0 | 3.171405 | 2.143504 | 0.549744 |
| 44 | 1 | 0 | 8.971061 | 1.246838 | -0.343157 |
| 45 | 1 | 0 | 7.736438 | 3.379736 | -0.150587 |
| 46 | 1 | 0 | 5.293657 | 3.387934 | 0.221960 |
| 47 | 1 | 0 | 5.293647 | -3.387933 | 0.221891 |
| 48 | 1 | 0 | 7.736427 | -3.379735 | -0.150656 |
| 49 | 1 | 0 | 8.971057 | -1.246838 | -0.343183 |
| 50 | 1 | 0 | -0.994173 | -4.628729 | -0.351974 |
| 51 | 1 | 0 | -3.455830 | -4.621532 | -0.087368 |
| 52 | 1 | 0 | 0.251060 | -2.539877 | -0.510296 |
| 53 | 1 | 0 | -3.455812 | 4.621532 | -0.087401 |
| 54 | 1 | 0 | -0.994155 | 4.628717 | -0.352009 |
| 55 | 1 | 0 | 0.251069 | 2.539860 | -0.510319 |
| 56 | 1 | 0 | -7.690542 | -2.146317 | 0.360939 |
| 57 | 1 | 0 | -8.911522 | 0.000013 | 0.495145 |
| 58 | 1 | 0 | -7.690533 | 2.146338 | 0.360927 |
| 59 | 1 | 0 | -5.557249 | 3.382520 | 0.131542 |
| 60 | 1 | 0 | -5.557262 | -3.382510 | 0.131567 |

R=Sat-Ver

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -0.042716 | -0.000004 | -0.617991 |
| 2 | 6 | 0 | 0.733546 | -0.000015 | 0.725565 |
| 3 | 6 | 0 | 2.222980 | -0.000008 | 0.504395 |
| 4 | 7 | 0 | 2.804281 | 1.186478 | 0.385693 |
| 5 | 7 | 0 | 4.148837 | 1.171812 | 0.130187 |
| 6 | 6 | 0 | 4.915479 | 0.000006 | 0.032272 |
| 7 | 7 | 0 | 4.148850 | -1.171808 | 0.130198 |
| 8 | 7 | 0 | 2.804295 | -1.186488 | 0.385704 |
| 9 | 6 | 0 | 4.767282 | -2.468012 | 0.092121 |
| 10 | 6 | 0 | 5.835202 | -2.745375 | -0.765871 |
| 11 | 6 | 0 | 6.375888 | -4.027233 | -0.790982 |
| 12 | 6 | 0 | 5.863994 | -5.033066 | 0.024985 |
| 13 | 6 | 0 | 4.795812 | -4.749909 | 0.873346 |
| 14 | 6 | 0 | 4.245762 | -3.473835 | 0.910567 |
| 15 | 6 | 0 | 4.767252 | 2.468023 | 0.092096 |
| 16 | 6 | 0 | 4.245721 | 3.473848 | 0.910533 |
| 17 | 6 | 0 | 4.795756 | 4.749928 | 0.873298 |
| 18 | 6 | 0 | 5.863933 | 5.033090 | 0.024932 |
| 19 | 6 | 0 | 6.375839 | 4.027255 | -0.791025 |
| 20 | 6 | 0 | 5.835168 | 2.745390 | -0.765900 |
| 21 | 8 | 0 | 6.115391 | 0.000013 | -0.123865 |
| 22 | 6 | 0 | -2.307060 | 3.687553 | -0.279874 |
| 23 | 6 | 0 | -3.682385 | 3.687316 | -0.154783 |
| 24 | 6 | 0 | -4.396650 | 2.462833 | -0.103089 |
| 25 | 6 | 0 | -3.677367 | 1.232963 | -0.185652 |
| 26 | 6 | 0 | -2.247789 | 1.237406 | -0.332517 |
| 27 | 6 | 0 | -1.595032 | 2.490893 | -0.368421 |
| 28 | 6 | 0 | -4.389692 | -0.000004 | -0.119715 |
| 29 | 6 | 0 | -3.677370 | -1.232972 | -0.185675 |
| 30 | 6 | 0 | -2.247792 | -1.237416 | -0.332539 |
| 31 | 6 | 0 | -1.540286 | -0.000005 | -0.435341 |
| 32 | 6 | 0 | -4.396656 | -2.462841 | -0.103134 |
| 33 | 6 | 0 | -3.682394 | -3.687326 | -0.154850 |
| 34 | 6 | 0 | -2.307069 | -3.687564 | -0.279941 |
| 35 | 6 | 0 | -1.595038 | -2.490904 | -0.368466 |
| 36 | 6 | 0 | -5.799731 | -0.000004 | 0.020247 |
| 37 | 6 | 0 | -6.516396 | 1.240693 | 0.092788 |
| 38 | 6 | 0 | -7.936525 | 1.208072 | 0.229653 |
| 39 | 6 | 0 | -8.618388 | -0.000003 | 0.294593 |
| 40 | 6 | 0 | -7.936528 | -1.208078 | 0.229631 |
| 41 | 6 | 0 | -6.516399 | -1.240700 | 0.092765 |
| 42 | 6 | 0 | -5.802188 | -2.437245 | 0.030890 |
| 43 | 6 | 0 | -5.802183 | 2.437238 | 0.030935 |
| 44 | 1 | 0 | 0.268305 | 0.869570 | -1.199353 |
| 45 | 1 | 0 | 0.268304 | -0.869571 | -1.199366 |
| 46 | 1 | 0 | 0.463007 | -0.884126 | 1.305282 |
| 47 | 1 | 0 | 0.463000 | 0.884084 | 1.305298 |
| 48 | 1 | 0 | 6.244780 | -1.970757 | -1.394973 |
| 49 | 1 | 0 | 7.203659 | -4.236864 | -1.458571 |
| 50 | 1 | 0 | 6.292913 | -6.028061 | -0.000330 |
| 51 | 1 | 0 | 4.388230 | -5.523124 | 1.514419 |
| 52 | 1 | 0 | 3.410110 | -3.247613 | 1.557543 |
| 53 | 1 | 0 | 3.410073 | 3.247622 | 1.557513 |
| 54 | 1 | 0 | 4.388165 | 5.523145 | 1.514364 |
| 55 | 1 | 0 | 6.292840 | 6.028089 | -0.000393 |
| 56 | 1 | 0 | 7.203606 | 4.236889 | -1.458617 |
| 57 | 1 | 0 | 6.244755 | 1.970771 | -1.394994 |
| 58 | 1 | 0 | -1.767450 | 4.627606 | -0.311464 |
| 59 | 1 | 0 | -4.231916 | 4.619920 | -0.090995 |
| 60 | 1 | 0 | -0.518601 | 2.538937 | -0.458019 |
| 61 | 1 | 0 | -4.231927 | -4.619929 | -0.091079 |
| 62 | 1 | 0 | -1.767461 | -4.627617 | -0.311548 |
| 63 | 1 | 0 | -0.518607 | -2.538949 | -0.458064 |
| 64 | 1 | 0 | -8.476957 | 2.146492 | 0.283079 |
| 65 | 1 | 0 | -9.697877 | -0.000003 | 0.398524 |
| 66 | 1 | 0 | -8.476962 | -2.146499 | 0.283039 |
| 67 | 1 | 0 | -6.338431 | -3.378988 | 0.089010 |
| 68 | 1 | 0 | -6.338423 | 3.378980 | 0.089072 |

R=Sat-NN

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 1.166138 | 0.008923 | 0.631743 |
| 2 | 6 | 0 | 1.980491 | -0.011664 | -0.690133 |
| 3 | 6 | 0 | 3.438773 | -0.005055 | -0.432395 |
| 4 | 7 | 0 | 4.191032 | -1.107445 | -0.263417 |
| 5 | 6 | 0 | 5.661235 | -0.764182 | -0.179032 |
| 6 | 6 | 0 | 5.593234 | 0.772340 | 0.152363 |
| 7 | 7 | 0 | 4.184579 | 1.104357 | -0.286061 |
| 8 | 6 | 0 | 5.654636 | 1.100149 | 1.653085 |
| 9 | 6 | 0 | 6.576115 | 1.658986 | -0.610308 |
| 10 | 6 | 0 | 6.249316 | -1.090722 | -1.561550 |
| 11 | 6 | 0 | 6.320755 | -1.642260 | 0.882753 |
| 12 | 8 | 0 | 3.780336 | -2.311089 | -0.320850 |
| 13 | 6 | 0 | -1.076541 | 3.686931 | 0.168499 |
| 14 | 6 | 0 | -2.457311 | 3.686632 | 0.049817 |
| 15 | 6 | 0 | -3.176092 | 2.464811 | 0.022683 |
| 16 | 6 | 0 | -2.454746 | 1.230319 | 0.126225 |
| 17 | 6 | 0 | -1.028750 | 1.236739 | 0.275019 |
| 18 | 6 | 0 | -0.366573 | 2.496294 | 0.280539 |
| 19 | 6 | 0 | -3.165736 | -0.000847 | 0.081196 |
| 20 | 6 | 0 | -2.453752 | -1.229546 | 0.162860 |
| 21 | 6 | 0 | -1.027749 | -1.230353 | 0.311663 |
| 22 | 6 | 0 | -0.326757 | 0.005142 | 0.405001 |
| 23 | 6 | 0 | -3.174083 | -2.467169 | 0.096031 |
| 24 | 6 | 0 | -2.454312 | -3.687058 | 0.159434 |
| 25 | 6 | 0 | -1.073539 | -3.682697 | 0.277964 |
| 26 | 6 | 0 | -0.364579 | -2.488661 | 0.354528 |
| 27 | 6 | 0 | -4.582569 | -0.003500 | -0.057896 |
| 28 | 6 | 0 | -5.297596 | 1.232719 | -0.148225 |
| 29 | 6 | 0 | -6.710535 | 1.200314 | -0.281488 |
| 30 | 6 | 0 | -7.393864 | -0.008661 | -0.327183 |
| 31 | 6 | 0 | -6.709543 | -1.215181 | -0.245608 |
| 32 | 6 | 0 | -5.296583 | -1.242446 | -0.111439 |
| 33 | 6 | 0 | -4.574643 | -2.445620 | -0.034577 |
| 34 | 6 | 0 | -4.576640 | 2.438240 | -0.107167 |
| 35 | 8 | 0 | 3.762546 | 2.304595 | -0.339521 |
| 36 | 1 | 0 | 1.456457 | -0.853457 | 1.233265 |
| 37 | 1 | 0 | 1.456225 | 0.889724 | 1.206107 |
| 38 | 1 | 0 | 1.738033 | 0.869023 | -1.287761 |
| 39 | 1 | 0 | 1.738520 | -0.909545 | -1.261720 |
| 40 | 1 | 0 | 6.656441 | 0.926077 | 2.050131 |
| 41 | 1 | 0 | 5.403417 | 2.153343 | 1.785748 |
| 42 | 1 | 0 | 4.942720 | 0.505686 | 2.228641 |
| 43 | 1 | 0 | 6.349506 | 2.702582 | -0.391563 |
| 44 | 1 | 0 | 7.599942 | 1.448935 | -0.291925 |
| 45 | 1 | 0 | 6.508527 | 1.521451 | -1.688730 |
| 46 | 1 | 0 | 7.326008 | -0.911684 | -1.580590 |
| 47 | 1 | 0 | 6.066434 | -2.145400 | -1.772409 |
| 48 | 1 | 0 | 5.782384 | -0.500367 | -2.351952 |
| 49 | 1 | 0 | 6.200724 | -2.687606 | 0.598191 |
| 50 | 1 | 0 | 7.387982 | -1.417716 | 0.948519 |
| 51 | 1 | 0 | 5.873067 | -1.510880 | 1.867006 |
| 52 | 1 | 0 | -0.535998 | 4.626916 | 0.172849 |
| 53 | 1 | 0 | -3.003992 | 4.619680 | -0.031038 |
| 54 | 1 | 0 | 0.711859 | 2.544169 | 0.351328 |
| 55 | 1 | 0 | -3.000223 | -4.622545 | 0.106328 |
| 56 | 1 | 0 | -0.532210 | -4.621683 | 0.310188 |
| 57 | 1 | 0 | 0.713904 | -2.533525 | 0.426187 |
| 58 | 1 | 0 | -7.251592 | 2.137726 | -0.348664 |
| 59 | 1 | 0 | -8.473479 | -0.010620 | -0.429360 |
| 60 | 1 | 0 | -7.249827 | -2.154619 | -0.284921 |
| 61 | 1 | 0 | -5.111783 | -3.387553 | -0.080230 |
| 62 | 1 | 0 | -5.114557 | 3.377961 | -0.180733 |