Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics


# Electronic structure and absorption spectra of supramolecular complexes of a fullerene crown ether with a π-extended TTF derivative

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## Supplementary material

- Table 1s: Absolute Energies and Complexation Energies of the **T**, **A**, **B**, benzene$_2$, $C_{60}$-benzene, **AT**, and **BT** systems at B3LYP, CAM-B3LYP, M06-HF, and M06-2X/6-31G(d,p) level of theory.
- The coordinates of all the **AT** and **BT** optimized structures are given at B3LYP, CAM-B3LYP, and M06-2X/6-31G(d,p) levels of theory.

**Table 1S.** Complexation Energies CE(eV) in the gas phase and in $CHCl_3$ solvent, $CE_{sol}$, of the **T**, **A**, **B**, **AT** and **BT** complexes at B3LYP, CAM-B3LYP and M06-2X/6-31G(d,p) level of theory.

| Structure | -E | $CE_u$[a] | CE[b] | $CE_{sol}$ | -E | $CE_u$[a] | CE[b] | $CE_{sol}$ | -E | $CE_u$[a] | CE[b] | $CE_{sol}$ | -E | $CE_u$[a] | CE[b] |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | B3LYP | | | | CAM-B3LYP | | | | M06-2X | | | | M06-HF | | |
| **T** | 3034.725652 | | | | 3033.857384 | | | | 3033.983934 | | | | | | |
| **A** | 3686.143418 | | | | 3684.245643 | | | | 3684.864325 | | | | | | |
| **B** | 3686.143040 | | | | 3684.245212 | | | | 3684.863844 | | | | | | |
| **AT1** | 6720.921803 | 1.43 | 1.08 | 0.40 | 6718.168868 | 1.79 | 1.39 | 0.66 | 6718.936345 | 2.40 | 2.02 | 1.27 | | | |
| **AT2** | 6720.914743 | 1.24 | 0.87 | 0.15 | 6718.162683 | 1.62 | 1.20 | 0.42 | 6718.937291 | 2.42 | 2.00 | 1.19 | | | |
| **AT3** | | | | | | | | | 6718.937229 | 2.42 | 1.93 | 1.16 | | | |
| **AT4** | | | | | 6718.157795 | 1.49 | 1.06 | 0.35 | 6718.931805 | 2.27 | 1.84 | 1.09 | | | |
| **AT5** | | | | | | | | | 6718.929992 | 2.22 | 1.79 | 1.06 | | | |
| **BT1** | | | | | | | | | 6718.940289 | 2.50 | 1.99 | 1.18 | | | |
| **BT2** | 6720.915626 | 1.27 | 0.92 | 0.20 | 6718.162890 | 1.63 | 1.25 | 0.48 | 6718.935089 | 2.36 | 1.97 | 1.19 | | | |
| **Benzene** | 232.2582123 | | | | 232.113833 | | | | 232.1441867 | | | | 232.187774 | | |
| **C60** | 2286.174104 | | | | 2284.944970 | | | | 2285.456457 | | | | 2285.889422 | | |
| **$Benzene_2$** | 464.517379 | 0.03 | 0 | | 464.228679 | 0.03 | -0.01 | | 464.293563 | 0.14 | 0.06 | 0.02 | 464.380786 | 0.14 | 0.04 |
| **C60-Benzene** | 2518.432774 | 0.01 | -0.03 | | 2517.060472 | 0.05 | -0.02 | | 2517.608354 | 0.21 | 0.12 | 0.05 | 2518.085776 | 0.23 | 0.12 |

**AT1: B3LYP/6-31G(d,p)**

Standard orientation:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 9.660522 | 0.380760 | 1.046873 |
| 2 | 6 | 0 | 10.691191 | -0.549417 | 1.057911 |
| 3 | 6 | 0 | 10.584359 | -1.772106 | 0.376120 |
| 4 | 6 | 0 | 9.396276 | -2.045598 | -0.359581 |
| 5 | 6 | 0 | 8.377227 | -1.092761 | -0.388088 |
| 6 | 6 | 0 | 8.484372 | 0.120515 | 0.319855 |
| 7 | 6 | 0 | 11.662314 | -2.779109 | 0.338605 |
| 8 | 6 | 0 | 9.325988 | -3.327281 | -1.096446 |
| 9 | 6 | 0 | 10.615635 | -3.721134 | -1.708315 |
| 10 | 6 | 0 | 11.801370 | -3.443750 | -0.978961 |
| 11 | 6 | 0 | 13.041087 | -3.755352 | -1.554055 |
| 12 | 1 | 0 | 13.955542 | -3.492279 | -1.033352 |
| 13 | 6 | 0 | 13.122413 | -4.357960 | -2.808927 |
| 14 | 6 | 0 | 11.957965 | -4.632027 | -3.523598 |
| 15 | 6 | 0 | 10.717364 | -4.300883 | -2.980127 |
| 16 | 1 | 0 | 9.767505 | 1.321899 | 1.575441 |
| 17 | 1 | 0 | 11.611908 | -0.303372 | 1.575064 |
| 18 | 1 | 0 | 7.492104 | -1.263057 | -0.990046 |
| 19 | 1 | 0 | 14.094652 | -4.588159 | -3.233578 |
| 20 | 1 | 0 | 12.011934 | -5.078957 | -4.511495 |
| 21 | 1 | 0 | 9.820516 | -4.463064 | -3.568623 |
| 22 | 16 | 0 | 6.675177 | -3.710000 | -0.296736 |
| 23 | 6 | 0 | 6.608545 | -6.204018 | -1.209643 |
| 24 | 6 | 0 | 5.942524 | -5.298232 | -0.487739 |
| 25 | 1 | 0 | 6.265251 | -7.209984 | -1.418366 |
| 26 | 1 | 0 | 4.977972 | -5.457186 | -0.021414 |
| 27 | 6 | 0 | 12.401982 | -3.127627 | 1.435487 |
| 28 | 16 | 0 | 13.616588 | -4.439290 | 1.434206 |
| 29 | 6 | 0 | 13.197279 | -3.575171 | 3.910706 |
| 30 | 6 | 0 | 13.844066 | -4.484584 | 3.175699 |
| 31 | 1 | 0 | 13.261684 | -3.479540 | 4.987615 |
| 32 | 1 | 0 | 14.514111 | -5.240873 | 3.565987 |
| 33 | 16 | 0 | 8.152983 | -5.726618 | -1.900269 |
| 34 | 16 | 0 | 12.178992 | -2.420125 | 3.062986 |
| 35 | 6 | 0 | 8.210559 | -4.112907 | -1.126914 |
| 36 | 6 | 0 | 7.433189 | 1.075926 | 0.272418 |
| 37 | 6 | 0 | 6.533303 | 1.895235 | 0.229774 |
| 38 | 6 | 0 | 5.485549 | 2.850914 | 0.180383 |
| 39 | 6 | 0 | 4.342159 | 2.632601 | -0.618059 |
| 40 | 6 | 0 | 5.567069 | 4.052761 | 0.915663 |
| 41 | 6 | 0 | 3.317433 | 3.570521 | -0.664760 |
| 42 | 1 | 0 | 4.279677 | 1.724955 | -1.208980 |
| 43 | 6 | 0 | 4.537970 | 4.984664 | 0.862075 |
| 44 | 1 | 0 | 6.449360 | 4.246332 | 1.515888 |
| 45 | 6 | 0 | 3.389469 | 4.753108 | 0.088141 |
| 46 | 1 | 0 | 2.456562 | 3.400382 | -1.304131 |
| 47 | 1 | 0 | 4.637926 | 5.913286 | 1.418859 |
| 48 | 1 | 0 | -0.378372 | 3.433687 | 5.978641 |
| 49 | 6 | 0 | -0.380322 | 4.313921 | 5.343502 |
| 50 | 6 | 0 | 0.590081 | 4.453454 | 4.350300 |
| 51 | 6 | 0 | -1.340667 | 5.308858 | 5.525728 |
| 52 | 6 | 0 | 0.614936 | 5.593158 | 3.538624 |
| 53 | 1 | 0 | 1.338484 | 3.677643 | 4.213858 |
| 54 | 6 | 0 | -1.326564 | 6.446560 | 4.715263 |
| 55 | 1 | 0 | -2.092988 | 5.203948 | 6.301224 |
| 56 | 6 | 0 | 1.703178 | 5.755667 | 2.507202 |
| 57 | 6 | 0 | -0.350380 | 6.592219 | 3.731468 |
| 58 | 1 | 0 | -2.066638 | 7.227297 | 4.861772 |
| 59 | 7 | 0 | 1.206052 | 5.612539 | 1.088712 |
| 60 | 1 | 0 | 2.163715 | 6.746929 | 2.564356 |
| 61 | 1 | 0 | 2.487008 | 5.010187 | 2.642011 |
| 62 | 1 | 0 | -0.342887 | 7.482394 | 3.108181 |
| 63 | 6 | 0 | 2.282510 | 5.771103 | 0.021055 |
| 64 | 1 | 0 | 0.495353 | 6.345378 | 0.908580 |
| 65 | 1 | 0 | 0.704799 | 4.707696 | 0.978982 |
| 66 | 1 | 0 | 1.747197 | 5.732993 | -0.929660 |
| 67 | 1 | 0 | 2.677202 | 6.780829 | 0.159482 |
| 68 | 1 | 0 | -3.637144 | 1.100047 | 5.958874 |
| 69 | 6 | 0 | -2.790374 | 0.827822 | 5.302452 |
| 70 | 7 | 0 | -3.217226 | 0.134310 | 4.092783 |
| 71 | 1 | 0 | -2.113350 | 0.182381 | 5.869610 |
| 72 | 1 | 0 | -2.253596 | 1.742063 | 5.038291 |
| 73 | 6 | 0 | -3.937403 | -1.098932 | 4.377424 |
| 74 | 6 | 0 | -4.123817 | 0.902534 | 3.243254 |
| 75 | 6 | 0 | -4.511525 | -1.553510 | 3.005410 |
| 76 | 1 | 0 | -3.274254 | -1.849736 | 4.816416 |
| 77 | 1 | 0 | -4.771880 | -0.929929 | 5.083726 |
| 78 | 6 | 0 | -4.628760 | -0.169843 | 2.188072 |
| 79 | 1 | 0 | -5.017327 | 1.223950 | 3.813243 |
| 80 | 6 | 0 | -3.491607 | 2.133082 | 2.631655 |
| 81 | 6 | 0 | -5.827943 | -2.326680 | 3.135553 |
| 82 | 6 | 0 | -3.639264 | -2.620176 | 2.328403 |
| 83 | 6 | 0 | -3.848655 | -0.159733 | 0.865827 |
| 84 | 6 | 0 | -6.035383 | 0.145143 | 1.669424 |
| 85 | 6 | 0 | -2.170831 | 2.098759 | 2.163007 |
| 86 | 6 | 0 | -4.225329 | 3.306626 | 2.460504 |
| 87 | 6 | 0 | -7.062948 | -1.804999 | 2.816376 |
| 88 | 6 | 0 | -5.594727 | -3.735668 | 2.973926 |
| 89 | 6 | 0 | -2.811888 | -2.381782 | 1.254647 |
| 90 | 6 | 0 | -4.243361 | -3.916964 | 2.476539 |
| 91 | 6 | 0 | -4.616192 | 0.501017 | -0.155790 |
| 92 | 6 | 0 | -2.924424 | -1.113994 | 0.498914 |
| 93 | 6 | 0 | -5.966781 | 0.689420 | 0.340276 |
| 94 | 6 | 0 | -7.168572 | -0.536504 | 2.059471 |
| 95 | 6 | 0 | -1.621813 | 3.187535 | 1.500743 |
| 96 | 1 | 0 | -1.577825 | 1.203684 | 2.315348 |
| 97 | 6 | 0 | -3.675716 | 4.417744 | 1.815213 |
| 98 | 1 | 0 | -5.246665 | 3.362049 | 2.825625 |
| 99 | 6 | 0 | -8.123907 | -2.675290 | 2.357887 |
| 100 | 6 | 0 | -6.615326 | -4.597521 | 2.558487 |
| 101 | 6 | 0 | -2.529888 | -3.433298 | 0.301640 |
| 102 | 6 | 0 | -3.961592 | -4.956305 | 1.582592 |
| 103 | 6 | 0 | -4.399120 | 0.241916 | -1.513925 |
| 104 | 6 | 0 | -2.702231 | -1.418301 | -0.899383 |
| 105 | 6 | 0 | -7.051770 | 0.602184 | -0.539072 |
| 106 | 6 | 0 | -8.293307 | -0.659644 | 1.156857 |
| 107 | 8 | 0 | -0.317354 | 3.141899 | 1.014321 |
| 108 | 6 | 0 | -2.373267 | 4.363383 | 1.314344 |
| 109 | 1 | 0 | -4.276106 | 5.311169 | 1.696274 |
| 110 | 6 | 0 | -8.883030 | -1.973628 | 1.338536 |
| 111 | 6 | 0 | -7.913254 | -4.053408 | 2.241851 |
| 112 | 6 | 0 | -6.324938 | -5.665564 | 1.615034 |
| 113 | 6 | 0 | -3.083053 | -4.708082 | 0.465667 |
| 114 | 6 | 0 | -2.459352 | -2.844217 | -1.023396 |
| 115 | 6 | 0 | -5.026985 | -5.840586 | 1.137631 |
| 116 | 6 | 0 | -3.416499 | -0.743432 | -1.896653 |
| 117 | 6 | 0 | -5.528571 | 0.137770 | -2.424815 |
| 118 | 6 | 0 | -8.246190 | -0.089122 | -0.119924 |
| 119 | 6 | 0 | -6.826551 | 0.312321 | -1.946436 |
| 120 | 6 | 0 | -0.095864 | 2.177702 | -0.039627 |
| 121 | 8 | 0 | -1.750591 | 5.378248 | 0.635991 |
| 122 | 6 | 0 | -9.398754 | -2.668433 | 0.244845 |
| 123 | 6 | 0 | -8.437624 | -4.776216 | 1.097557 |
| 124 | 6 | 0 | -7.454768 | -5.774744 | 0.708956 |
| 125 | 6 | 0 | -3.598199 | -5.431417 | -0.682450 |
| 126 | 6 | 0 | -2.942378 | -3.542977 | -2.130144 |
| 127 | 6 | 0 | -4.801501 | -6.133998 | -0.266754 |
| 128 | 6 | 0 | -3.929932 | -1.470738 | -3.043372 |
| 129 | 6 | 0 | -5.237712 | -0.925403 | -3.371023 |
| 130 | 6 | 0 | -8.770967 | -0.815484 | -1.262041 |
| 131 | 6 | 0 | -7.892407 | -0.566641 | -2.393836 |
| 132 | 6 | 0 | -0.651625 | 2.624589 | -1.377347 |
| 133 | 1 | 0 | 0.986461 | 2.046354 | -0.091798 |
| 134 | 1 | 0 | -0.551732 | 1.221503 | 0.234595 |
| 135 | 6 | 0 | -2.490420 | 6.574242 | 0.389663 |
| 136 | 6 | 0 | -9.333701 | -2.080681 | -1.083867 |
| 137 | 6 | 0 | -9.165152 | -4.098066 | 0.117844 |
| 138 | 6 | 0 | -7.240055 | -6.053790 | -0.641980 |
| 139 | 6 | 0 | -3.529064 | -4.861992 | -1.955643 |
| 140 | 6 | 0 | -3.699915 | -2.843547 | -3.156401 |
| 141 | 6 | 0 | -5.886014 | -6.236406 | -1.139703 |
| 142 | 6 | 0 | -6.260243 | -1.775532 | -3.797298 |
| 143 | 6 | 0 | -7.613890 | -1.592257 | -3.299596 |
| 144 | 1 | 0 | -1.705363 | 2.919235 | -1.265694 |
| 145 | 1 | 0 | -0.622243 | 1.768162 | -2.069904 |
| 146 | 8 | 0 | 0.122133 | 3.702030 | -1.893846 |
| 147 | 6 | 0 | -1.607344 | 7.520278 | -0.391829 |
| 148 | 1 | 0 | -2.794234 | 7.034743 | 1.337956 |
| 149 | 1 | 0 | -3.390270 | 6.350100 | -0.198972 |
| 150 | 6 | 0 | -9.048509 | -3.143534 | -2.027725 |
| 151 | 6 | 0 | -8.944649 | -4.390992 | -1.284776 |
| 152 | 6 | 0 | -8.000263 | -5.349215 | -1.658793 |
| 153 | 6 | 0 | -4.654650 | -4.971795 | -2.863010 |
| 154 | 6 | 0 | -4.759519 | -3.724426 | -3.606341 |
| 155 | 6 | 0 | -5.811102 | -5.644541 | -2.463704 |
| 156 | 6 | 0 | -6.016301 | -3.201869 | -3.919134 |
| 157 | 6 | 0 | -8.204887 | -2.905592 | -3.114275 |
| 158 | 6 | 0 | -0.387396 | 4.172802 | -3.134861 |
| 159 | 8 | 0 | -0.514035 | 7.938847 | 0.445109 |
| 160 | 1 | 0 | -1.223700 | 7.051804 | -1.302425 |
| 161 | 1 | 0 | -2.204333 | 8.393345 | -0.681996 |
| 162 | 6 | 0 | -7.117961 | -5.096638 | -2.785703 |
| 163 | 6 | 0 | -7.218679 | -3.901181 | -3.498633 |
| 164 | 1 | 0 | -0.585601 | 3.323533 | -3.807310 |
| 165 | 1 | 0 | -1.336106 | 4.709140 | -2.984958 |
| 166 | 6 | 0 | 0.614892 | 5.071533 | -3.825722 |
| 167 | 6 | 0 | 0.003190 | 9.243325 | 0.161326 |
| 168 | 1 | 0 | 0.274950 | 5.242303 | -4.855403 |
| 169 | 1 | 0 | 1.593124 | 4.574551 | -3.862171 |
| 170 | 8 | 0 | 0.709116 | 6.318968 | -3.136211 |
| 171 | 1 | 0 | -0.827838 | 9.919969 | -0.074868 |
| 172 | 1 | 0 | 0.477951 | 9.598411 | 1.082144 |
| 173 | 6 | 0 | 1.026388 | 9.271334 | -0.959837 |
| 174 | 6 | 0 | 1.387902 | 7.333300 | -3.772678 |
| 175 | 1 | 0 | 1.390968 | 10.302735 | -1.072553 |
| 176 | 1 | 0 | 1.891533 | 8.641553 | -0.712850 |
| 177 | 8 | 0 | 0.403642 | 8.801314 | -2.150758 |
| 178 | 6 | 0 | 1.242594 | 8.628912 | -3.237031 |
| 179 | 6 | 0 | 2.198639 | 7.151814 | -4.897894 |
| 180 | 6 | 0 | 1.894965 | 9.707467 | -3.828199 |
| 181 | 6 | 0 | 2.855215 | 8.240566 | -5.477717 |
| 182 | 1 | 0 | 2.334622 | 6.165789 | -5.324513 |
| 183 | 6 | 0 | 2.706894 | 9.518968 | -4.948026 |
| 184 | 1 | 0 | 1.746012 | 10.700461 | -3.415481 |
| 185 | 1 | 0 | 3.481464 | 8.077862 | -6.348889 |
| 186 | 1 | 0 | 3.207751 | 10.366601 | -5.403402 |

**AT2: B3LYP/6-31G(d,p)**

Standard orientation:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 10.025693 | -2.957974 | 0.133586 |
| 2 | 6 | 0 | 11.230479 | -3.638086 | 0.016063 |
| 3 | 6 | 0 | 12.452336 | -3.027577 | 0.339804 |
| 4 | 6 | 0 | 12.443803 | -1.687188 | 0.819552 |
| 5 | 6 | 0 | 11.225978 | -1.018505 | 0.954110 |
| 6 | 6 | 0 | 10.007158 | -1.632357 | 0.604564 |
| 7 | 6 | 0 | 13.752874 | -3.720581 | 0.259637 |
| 8 | 6 | 0 | 13.743205 | -1.086626 | 1.196347 |
| 9 | 6 | 0 | 14.661556 | -2.045563 | 1.852872 |
| 10 | 6 | 0 | 14.668371 | -3.382083 | 1.375003 |
| 11 | 6 | 0 | 15.487313 | -4.326429 | 2.009111 |
| 12 | 1 | 0 | 15.455455 | -5.363430 | 1.692560 |
| 13 | 6 | 0 | 16.311057 | -3.965611 | 3.074747 |
| 14 | 6 | 0 | 16.304693 | -2.653148 | 3.543099 |
| 15 | 6 | 0 | 15.474008 | -1.707358 | 2.943468 |
| 16 | 1 | 0 | 9.092322 | -3.452812 | -0.112852 |
| 17 | 1 | 0 | 11.217069 | -4.676695 | -0.295386 |
| 18 | 1 | 0 | 11.199519 | -0.018049 | 1.370289 |
| 19 | 1 | 0 | 16.935038 | -4.715636 | 3.550843 |
| 20 | 1 | 0 | 16.923940 | -2.368383 | 4.388081 |
| 21 | 1 | 0 | 15.431151 | -0.703685 | 3.352959 |
| 22 | 16 | 0 | 13.043332 | 1.338764 | -0.004733 |
| 23 | 6 | 0 | 15.491016 | 2.338818 | 0.252819 |
| 24 | 6 | 0 | 14.292270 | 2.542448 | -0.300935 |
| 25 | 1 | 0 | 16.339601 | 3.006404 | 0.165399 |
| 26 | 1 | 0 | 14.020932 | 3.399218 | -0.905380 |
| 27 | 6 | 0 | 14.109318 | -4.528008 | -0.785104 |
| 28 | 16 | 0 | 15.728012 | -5.266702 | -0.958436 |
| 29 | 6 | 0 | 14.304057 | -5.638718 | -3.170090 |
| 30 | 6 | 0 | 15.504369 | -5.819097 | -2.611251 |
| 31 | 1 | 0 | 14.026687 | -5.947025 | -4.170596 |
| 32 | 1 | 0 | 16.350554 | -6.296260 | -3.090387 |
| 33 | 16 | 0 | 15.710261 | 0.890001 | 1.223246 |
| 34 | 16 | 0 | 13.062373 | -4.863690 | -2.196242 |
| 35 | 6 | 0 | 14.094807 | 0.195124 | 0.887431 |
| 36 | 6 | 0 | 8.778101 | -0.933248 | 0.755439 |
| 37 | 6 | 0 | 7.724364 | -0.337083 | 0.885503 |
| 38 | 6 | 0 | 6.492364 | 0.353582 | 1.033962 |
| 39 | 6 | 0 | 6.465264 | 1.738606 | 1.302132 |
| 40 | 6 | 0 | 5.263302 | -0.331365 | 0.920698 |
| 41 | 6 | 0 | 5.255419 | 2.405820 | 1.446286 |
| 42 | 1 | 0 | 7.401729 | 2.276060 | 1.401208 |
| 43 | 6 | 0 | 4.058167 | 0.347523 | 1.060882 |
| 44 | 1 | 0 | 5.270787 | -1.400390 | 0.735599 |
| 45 | 6 | 0 | 4.034774 | 1.724800 | 1.319639 |
| 46 | 1 | 0 | 5.257751 | 3.469680 | 1.670998 |
| 47 | 1 | 0 | 3.124493 | -0.197112 | 0.963720 |
| 48 | 1 | 0 | 4.072655 | 7.654808 | 1.925670 |
| 49 | 6 | 0 | 3.180431 | 7.067548 | 2.120824 |
| 50 | 6 | 0 | 2.805595 | 6.063071 | 1.229004 |
| 51 | 6 | 0 | 2.409608 | 7.325928 | 3.256445 |
| 52 | 6 | 0 | 1.656906 | 5.292530 | 1.470341 |
| 53 | 1 | 0 | 3.416008 | 5.872735 | 0.350811 |
| 54 | 6 | 0 | 1.264988 | 6.568176 | 3.502148 |
| 55 | 1 | 0 | 2.701132 | 8.112551 | 3.945307 |
| 56 | 6 | 0 | 1.193363 | 4.223245 | 0.508816 |
| 57 | 6 | 0 | 0.896001 | 5.553804 | 2.617271 |
| 58 | 1 | 0 | 0.661208 | 6.760695 | 4.383448 |
| 59 | 7 | 0 | 2.226226 | 3.140199 | 0.251442 |
| 60 | 1 | 0 | 0.312707 | 3.712762 | 0.894007 |
| 61 | 1 | 0 | 0.961335 | 4.620431 | -0.480704 |
| 62 | 1 | 0 | 0.004498 | 4.964357 | 2.815187 |
| 63 | 6 | 0 | 2.738742 | 2.465010 | 1.512940 |
| 64 | 1 | 0 | 2.995313 | 3.548188 | -0.304277 |
| 65 | 1 | 0 | 1.805545 | 2.420243 | -0.359370 |
| 66 | 1 | 0 | 2.857536 | 3.261103 | 2.248627 |
| 67 | 1 | 0 | 1.927822 | 1.811842 | 1.839628 |
| 68 | 1 | 0 | -6.342403 | 1.579428 | 4.428337 |
| 69 | 6 | 0 | -5.253280 | 1.707562 | 4.349925 |
| 70 | 7 | 0 | -4.665244 | 1.180214 | 3.114802 |
| 71 | 1 | 0 | -4.788284 | 1.208974 | 5.204738 |
| 72 | 1 | 0 | -5.026454 | 2.774575 | 4.427226 |
| 73 | 6 | 0 | -4.794259 | -0.256087 | 2.930831 |
| 74 | 6 | 0 | -5.142090 | 1.807674 | 1.885899 |
| 75 | 6 | 0 | -6.095536 | -0.535883 | 2.091729 |
| 76 | 1 | 0 | -3.941944 | -0.634443 | 2.354341 |
| 77 | 1 | 0 | -4.801851 | -0.777986 | 3.890173 |
| 78 | 6 | 0 | -6.301903 | 0.841762 | 1.290890 |
| 79 | 1 | 0 | -5.614635 | 2.762003 | 2.135329 |
| 80 | 6 | 0 | -4.006325 | 2.115136 | 0.909801 |
| 81 | 6 | 0 | -7.298419 | -0.964856 | 2.944703 |
| 82 | 6 | 0 | -5.938582 | -1.777624 | 1.212881 |
| 83 | 6 | 0 | -6.311329 | 0.676442 | -0.233627 |
| 84 | 6 | 0 | -7.686186 | 1.478816 | 1.491574 |
| 85 | 6 | 0 | -2.714243 | 1.619733 | 1.108261 |
| 86 | 6 | 0 | -4.217324 | 2.958857 | -0.185864 |
| 87 | 6 | 0 | -8.389226 | -0.165942 | 3.208598 |
| 88 | 6 | 0 | -7.483696 | -2.390043 | 2.855668 |
| 89 | 6 | 0 | -5.724858 | -1.735950 | -0.147663 |
| 90 | 6 | 0 | -6.640300 | -2.891755 | 1.787132 |
| 91 | 6 | 0 | -7.332761 | 1.504722 | -0.820570 |
| 92 | 6 | 0 | -5.926807 | -0.473021 | -0.891559 |
| 93 | 6 | 0 | -8.178906 | 2.005081 | 0.246496 |
| 94 | 6 | 0 | -8.588117 | 1.093875 | 2.459389 |
| 95 | 6 | 0 | -1.684136 | 1.905561 | 0.216911 |
| 96 | 1 | 0 | -2.492003 | 1.033712 | 1.992788 |
| 97 | 6 | 0 | -3.190237 | 3.270630 | -1.077193 |
| 98 | 1 | 0 | -5.197175 | 3.393690 | -0.354944 |
| 99 | 6 | 0 | -9.693458 | -0.751059 | 3.432301 |
| 100 | 6 | 0 | -8.731136 | -2.978675 | 3.091767 |
| 101 | 6 | 0 | -6.186819 | -2.819815 | -0.988233 |
| 102 | 6 | 0 | -7.069632 | -3.962270 | 0.995034 |
| 103 | 6 | 0 | -7.886974 | 1.207763 | -2.070252 |
| 104 | 6 | 0 | -6.506479 | -0.814015 | -2.174160 |
| 105 | 6 | 0 | -9.548702 | 2.187371 | 0.024789 |
| 106 | 6 | 0 | -10.010065 | 1.252563 | 2.241627 |
| 107 | 8 | 0 | -0.404666 | 1.420174 | 0.467528 |
| 108 | 6 | 0 | -1.911712 | 2.732174 | -0.898302 |
| 109 | 1 | 0 | -3.400358 | 3.930687 | -1.909781 |
| 110 | 6 | 0 | -10.692336 | 0.119527 | 2.839227 |
| 111 | 6 | 0 | -9.865718 | -2.138379 | 3.388590 |
| 112 | 6 | 0 | -9.185814 | -4.079207 | 2.255881 |
| 113 | 6 | 0 | -6.838607 | -3.924453 | -0.428671 |
| 114 | 6 | 0 | -6.666909 | -2.255663 | -2.236649 |
| 115 | 6 | 0 | -8.373167 | -4.561558 | 1.231180 |
| 116 | 6 | 0 | -7.462382 | 0.017661 | -2.766811 |
| 117 | 6 | 0 | -9.312853 | 1.383203 | -2.294772 |
| 118 | 6 | 0 | -10.489216 | 1.803641 | 1.048820 |
| 119 | 6 | 0 | -10.126068 | 1.862781 | -1.269430 |
| 120 | 6 | 0 | -0.184640 | 0.046682 | 0.113003 |
| 121 | 8 | 0 | -0.843534 | 2.957007 | -1.730737 |
| 122 | 6 | 0 | -11.819882 | -0.424037 | 2.224108 |
| 123 | 6 | 0 | -11.031466 | -2.706653 | 2.736906 |
| 124 | 6 | 0 | -10.611391 | -3.909463 | 2.035881 |
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| 126 | 6 | 0 | -7.774011 | -2.811524 | -2.878151 |
| 127 | 6 | 0 | -8.948982 | -4.891287 | -0.060582 |
| 128 | 6 | 0 | -8.621172 | -0.557475 | -3.425206 |
| 129 | 6 | 0 | -9.767652 | 0.288299 | -3.134067 |
| 130 | 6 | 0 | -11.655069 | 1.232078 | 0.399857 |
| 131 | 6 | 0 | -11.431473 | 1.269464 | -1.036453 |
| 132 | 6 | 0 | 0.358121 | -0.101287 | -1.293829 |
| 133 | 1 | 0 | 0.539189 | -0.348217 | 0.832967 |
| 134 | 1 | 0 | -1.114991 | -0.523558 | 0.210197 |
| 135 | 6 | 0 | -1.030202 | 3.859638 | -2.820217 |
| 136 | 6 | 0 | -12.306485 | 0.139189 | 0.974598 |
| 137 | 6 | 0 | -11.989826 | -1.867191 | 2.165564 |
| 138 | 6 | 0 | -11.166630 | -4.223581 | 0.794173 |
| 139 | 6 | 0 | -8.457908 | -3.951340 | -2.288599 |
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| 141 | 6 | 0 | -10.318167 | -4.724039 | -0.275772 |
| 142 | 6 | 0 | -11.019445 | -0.287346 | -2.907743 |
| 143 | 6 | 0 | -11.868028 | 0.213275 | -1.838198 |
| 144 | 1 | 0 | -0.312736 | 0.381658 | -2.016158 |
| 145 | 1 | 0 | 0.420456 | -1.172561 | -1.541760 |
| 146 | 8 | 0 | 1.658461 | 0.485793 | -1.352916 |
| 147 | 6 | 0 | 0.265039 | 3.965888 | -3.595285 |
| 148 | 1 | 0 | -1.323810 | 4.849637 | -2.448359 |
| 149 | 1 | 0 | -1.817001 | 3.492286 | -3.492615 |
| 150 | 6 | 0 | -12.764226 | -0.955050 | 0.140953 |
| 151 | 6 | 0 | -12.568326 | -2.195541 | 0.876915 |
| 152 | 6 | 0 | -12.165061 | -3.350127 | 0.203141 |
| 153 | 6 | 0 | -9.880307 | -3.781701 | -2.513356 |
| 154 | 6 | 0 | -10.076484 | -2.540876 | -3.249106 |
| 155 | 6 | 0 | -10.792881 | -4.158974 | -1.526266 |
| 156 | 6 | 0 | -11.177411 | -1.729502 | -2.967565 |
| 157 | 6 | 0 | -12.549249 | -0.920318 | -1.238310 |
| 158 | 6 | 0 | 2.248282 | 0.341188 | -2.639488 |
| 159 | 8 | 0 | 1.254352 | 4.589628 | -2.794488 |
| 160 | 1 | 0 | 0.596692 | 2.966816 | -3.916538 |
| 161 | 1 | 0 | 0.069631 | 4.560465 | -4.501744 |
| 162 | 6 | 0 | -11.935209 | -3.310517 | -1.231055 |
| 163 | 6 | 0 | -12.123564 | -2.121360 | -1.936507 |
| 164 | 1 | 0 | 2.176466 | -0.705897 | -2.970812 |
| 165 | 1 | 0 | 1.718434 | 0.962063 | -3.376759 |
| 166 | 6 | 0 | 3.714096 | 0.711394 | -2.601592 |
| 167 | 6 | 0 | 2.432091 | 4.914692 | -3.519885 |
| 168 | 1 | 0 | 4.149481 | 0.490450 | -3.585164 |
| 169 | 1 | 0 | 4.239465 | 0.122779 | -1.840880 |
| 170 | 8 | 0 | 3.829798 | 2.103815 | -2.309212 |
| 171 | 1 | 0 | 2.879246 | 4.014449 | -3.963886 |
| 172 | 1 | 0 | 2.194203 | 5.615490 | -4.336896 |
| 173 | 6 | 0 | 3.417442 | 5.587769 | -2.583979 |
| 174 | 6 | 0 | 5.083243 | 2.660282 | -2.330621 |
| 175 | 1 | 0 | 4.221853 | 6.051109 | -3.163997 |
| 176 | 1 | 0 | 2.904731 | 6.364131 | -2.009254 |
| 177 | 8 | 0 | 3.990245 | 4.684776 | -1.613034 |
| 178 | 6 | 0 | 5.154698 | 4.026355 | -2.002209 |
| 179 | 6 | 0 | 6.261044 | 1.975841 | -2.644390 |
| 180 | 6 | 0 | 6.376235 | 4.691497 | -1.998795 |
| 181 | 6 | 0 | 7.483515 | 2.652638 | -2.645800 |
| 182 | 1 | 0 | 6.240167 | 0.919573 | -2.881460 |
| 183 | 6 | 0 | 7.547823 | 4.007456 | -2.329269 |
| 184 | 1 | 0 | 6.399374 | 5.741674 | -1.723826 |
| 185 | 1 | 0 | 8.388082 | 2.105517 | -2.890397 |
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**BT2: B3LYP/6-31G(d,p)**

Standard orientation:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -7.711408 | -2.318735 | 1.981849 |
| 2 | 6 | 0 | -8.604018 | -3.371699 | 1.831699 |
| 3 | 6 | 0 | -9.558053 | -3.384907 | 0.801682 |
| 4 | 6 | 0 | -9.589787 | -2.297384 | -0.116567 |
| 5 | 6 | 0 | -8.669065 | -1.258324 | 0.024068 |
| 6 | 6 | 0 | -7.729919 | -1.244110 | 1.073936 |
| 7 | 6 | 0 | -10.506057 | -4.494689 | 0.584155 |
| 8 | 6 | 0 | -10.586103 | -2.351992 | -1.210048 |
| 9 | 6 | 0 | -10.776195 | -3.713794 | -1.759208 |
| 10 | 6 | 0 | -10.734464 | -4.801538 | -0.847949 |
| 11 | 6 | 0 | -10.854822 | -6.107257 | -1.343319 |
| 12 | 1 | 0 | -10.763227 | -6.948960 | -0.665257 |
| 13 | 6 | 0 | -11.046151 | -6.347543 | -2.703512 |
| 14 | 6 | 0 | -11.090980 | -5.279192 | -3.597103 |
| 15 | 6 | 0 | -10.941706 | -3.975342 | -3.126018 |
| 16 | 1 | 0 | -6.978578 | -2.332721 | 2.781438 |
| 17 | 1 | 0 | -8.531559 | -4.217983 | 2.505697 |
| 18 | 1 | 0 | -8.645965 | -0.453340 | -0.701390 |
| 19 | 1 | 0 | -11.135578 | -7.368207 | -3.062521 |
| 20 | 1 | 0 | -11.216993 | -5.457289 | -4.660623 |
| 21 | 1 | 0 | -10.918504 | -3.154675 | -3.835221 |
| 22 | 16 | 0 | -11.189553 | 0.355472 | -0.870464 |
| 23 | 6 | 0 | -13.284546 | 0.242267 | -2.500385 |
| 24 | 6 | 0 | -12.640645 | 1.011751 | -1.618086 |
| 25 | 1 | 0 | -14.177903 | 0.528045 | -3.042245 |
| 26 | 1 | 0 | -12.931747 | 2.015714 | -1.334476 |
| 27 | 6 | 0 | -11.175866 | -5.120298 | 1.599842 |
| 28 | 16 | 0 | -12.424092 | -6.373150 | 1.338486 |
| 29 | 6 | 0 | -12.365915 | -5.649668 | 3.893642 |
| 30 | 6 | 0 | -13.005118 | -6.405819 | 2.996282 |
| 31 | 1 | 0 | -12.607678 | -5.589481 | 4.947660 |
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| 33 | 16 | 0 | -12.623689 | -1.352855 | -2.831711 |
| 34 | 16 | 0 | -11.004497 | -4.692681 | 3.327819 |
| 35 | 6 | 0 | -11.323101 | -1.273161 | -1.604154 |
| 36 | 6 | 0 | -6.795813 | -0.178532 | 1.188423 |
| 37 | 6 | 0 | -5.991421 | 0.730847 | 1.281156 |
| 38 | 6 | 0 | -5.044451 | 1.783919 | 1.379229 |
| 39 | 6 | 0 | -4.947150 | 2.764996 | 0.367841 |
| 40 | 6 | 0 | -4.181147 | 1.882847 | 2.489315 |
| 41 | 6 | 0 | -4.011362 | 3.787338 | 0.458386 |
| 42 | 1 | 0 | -5.624089 | 2.715235 | -0.478663 |
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| 44 | 1 | 0 | -4.257076 | 1.150171 | 3.285300 |
| 45 | 6 | 0 | -3.135443 | 3.868179 | 1.552887 |
| 46 | 1 | 0 | -3.955351 | 4.531626 | -0.331194 |
| 47 | 1 | 0 | -2.611789 | 2.981973 | 3.447731 |
| 48 | 1 | 0 | 0.861179 | 2.751089 | 5.546459 |
| 49 | 6 | 0 | 1.139766 | 3.330223 | 4.671656 |
| 50 | 6 | 0 | 0.418278 | 3.186210 | 3.485413 |
| 51 | 6 | 0 | 2.224391 | 4.205228 | 4.726558 |
| 52 | 6 | 0 | 0.767158 | 3.919573 | 2.344355 |
| 53 | 1 | 0 | -0.405331 | 2.480151 | 3.438938 |
| 54 | 6 | 0 | 2.593543 | 4.925752 | 3.588129 |
| 55 | 1 | 0 | 2.790280 | 4.313695 | 5.646562 |
| 56 | 6 | 0 | 0.019017 | 3.738783 | 1.047473 |
| 57 | 6 | 0 | 1.873550 | 4.780264 | 2.403196 |
| 58 | 1 | 0 | 3.454626 | 5.586721 | 3.620415 |
| 59 | 1 | 0 | 2.175832 | 5.323207 | 1.511846 |
| 60 | 1 | 0 | -0.457573 | 5.772815 | 0.740400 |
| 61 | 6 | 0 | 3.688261 | -0.624165 | 1.378550 |
| 62 | 6 | 0 | 3.106558 | -1.896099 | 1.388518 |
| 63 | 6 | 0 | 4.726972 | -0.299120 | 2.339438 |
| 64 | 6 | 0 | 3.998628 | 0.034931 | 0.126863 |
| 65 | 6 | 0 | 3.553433 | -2.894695 | 2.342910 |
| 66 | 6 | 0 | 2.847013 | -2.559332 | 0.133755 |
| 67 | 6 | 0 | 5.150435 | -1.252979 | 3.265269 |
| 68 | 6 | 0 | 5.693843 | 0.565318 | 1.687997 |
| 69 | 6 | 0 | 5.260875 | 0.782346 | 0.324413 |
| 70 | 6 | 0 | 3.729617 | -0.584905 | -1.075791 |
| 71 | 6 | 0 | 4.556901 | -2.580563 | 3.261937 |
| 72 | 6 | 0 | 3.565204 | -4.183726 | 1.669780 |
| 73 | 6 | 0 | 3.126345 | -3.976770 | 0.300763 |
| 74 | 6 | 0 | 3.180026 | -1.915912 | -1.062895 |
| 75 | 6 | 0 | 6.566119 | -1.391453 | 3.568835 |
| 76 | 6 | 0 | 7.054632 | 0.438367 | 1.989593 |
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| 78 | 6 | 0 | 4.530141 | -0.352654 | -2.364672 |
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| 80 | 6 | 0 | 4.578831 | -5.104120 | 1.943680 |
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| 84 | 6 | 0 | 7.499007 | -0.562048 | 2.942695 |
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| 91 | 6 | 0 | 5.189732 | -5.857867 | 0.860227 |
| 92 | 6 | 0 | 4.762713 | -5.661273 | -0.454208 |
| 93 | 6 | 0 | 4.043872 | -4.035665 | -1.987899 |
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| 96 | 6 | 0 | 9.080510 | -0.456168 | 1.207439 |
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| 98 | 6 | 0 | 5.703471 | 1.731668 | -3.031848 |
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| 101 | 7 | 0 | 4.744655 | 1.425939 | -4.080475 |
| 102 | 6 | 0 | 2.479940 | 1.163710 | -3.059423 |
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| 110 | 6 | 0 | 9.663139 | -1.178429 | 0.166996 |
| 111 | 6 | 0 | 7.177662 | -1.582164 | -3.076996 |
| 112 | 1 | 0 | 5.308869 | 2.523169 | -2.383659 |
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| 114 | 6 | 0 | 9.218559 | -0.973975 | -1.203255 |
| 115 | 6 | 0 | 6.209519 | -3.736638 | -3.095048 |
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| 117 | 6 | 0 | 1.325907 | 0.393160 | -2.883739 |
| 118 | 6 | 0 | 2.418219 | 2.541707 | -2.821765 |
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| 139 | 8 | 0 | 1.096295 | 4.482317 | -2.106744 |
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| 175 | 1 | 0 | -0.851645 | 9.273345 | 3.612406 |
| 176 | 6 | 0 | -3.576074 | 10.220347 | 1.810967 |
| 177 | 1 | 0 | -4.123886 | 9.439004 | -0.112202 |
| 178 | 1 | 0 | -2.808962 | 10.819726 | 3.734905 |
| 179 | 1 | 0 | -4.438853 | 10.877059 | 1.853970 |
| 180 | 1 | 0 | -1.271353 | 4.727075 | -0.243753 |
| 181 | 7 | 0 | -0.949307 | 4.863975 | 0.727248 |
| 182 | 6 | 0 | -2.145770 | 4.998709 | 1.654672 |
| 183 | 1 | 0 | -0.571121 | 2.822382 | 1.036214 |
| 184 | 1 | 0 | 0.702399 | 3.719614 | 0.200472 |
| 185 | 1 | 0 | -1.736025 | 5.093004 | 2.660987 |
| 186 | 1 | 0 | -2.603606 | 5.949169 | 1.380586 |

**AT1: CAM-B3LYP/6-31G(d,p)**

Standard orientation:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 9.496080 | 0.551241 | 1.015341 |
| 2 | 6 | 0 | 10.538553 | -0.360617 | 1.034928 |
| 3 | 6 | 0 | 10.443564 | -1.582355 | 0.367425 |
| 4 | 6 | 0 | 9.267501 | -1.878166 | -0.358034 |
| 5 | 6 | 0 | 8.236664 | -0.947584 | -0.394833 |
| 6 | 6 | 0 | 8.331407 | 0.266155 | 0.297456 |
| 7 | 6 | 0 | 11.534575 | -2.577648 | 0.331494 |
| 8 | 6 | 0 | 9.222887 | -3.165655 | -1.086191 |
| 9 | 6 | 0 | 10.515453 | -3.525479 | -1.712074 |
| 10 | 6 | 0 | 11.689901 | -3.227665 | -0.990617 |
| 11 | 6 | 0 | 12.929144 | -3.504165 | -1.566191 |
| 12 | 1 | 0 | 13.838017 | -3.230517 | -1.042385 |
| 13 | 6 | 0 | 13.017618 | -4.091787 | -2.822463 |
| 14 | 6 | 0 | 11.861741 | -4.385501 | -3.531445 |
| 15 | 6 | 0 | 10.619934 | -4.090151 | -2.982072 |
| 16 | 1 | 0 | 9.587807 | 1.497703 | 1.535732 |
| 17 | 1 | 0 | 11.454506 | -0.101721 | 1.553009 |
| 18 | 1 | 0 | 7.351078 | -1.140590 | -0.988427 |
| 19 | 1 | 0 | 13.991865 | -4.298222 | -3.252500 |
| 20 | 1 | 0 | 11.922401 | -4.824510 | -4.521545 |
| 21 | 1 | 0 | 9.723356 | -4.274371 | -3.563342 |
| 22 | 16 | 0 | 6.616314 | -3.611388 | -0.246717 |
| 23 | 6 | 0 | 6.602669 | -6.098329 | -1.147403 |
| 24 | 6 | 0 | 5.926515 | -5.213008 | -0.422915 |
| 25 | 1 | 0 | 6.281643 | -7.113001 | -1.344614 |
| 26 | 1 | 0 | 4.974865 | -5.399949 | 0.057250 |
| 27 | 6 | 0 | 12.256011 | -2.928739 | 1.423404 |
| 28 | 16 | 0 | 13.483934 | -4.215477 | 1.419373 |
| 29 | 6 | 0 | 13.029626 | -3.382824 | 3.888610 |
| 30 | 6 | 0 | 13.692662 | -4.271888 | 3.156608 |
| 31 | 1 | 0 | 13.082610 | -3.299999 | 4.966321 |
| 32 | 1 | 0 | 14.366466 | -5.021682 | 3.550538 |
| 33 | 16 | 0 | 8.118615 | -5.585008 | -1.858097 |
| 34 | 16 | 0 | 12.007993 | -2.237738 | 3.044317 |
| 35 | 6 | 0 | 8.141099 | -3.977651 | -1.092245 |
| 36 | 6 | 0 | 7.262514 | 1.209639 | 0.244722 |
| 37 | 6 | 0 | 6.358426 | 2.011169 | 0.198958 |
| 38 | 6 | 0 | 5.295470 | 2.957941 | 0.148076 |
| 39 | 6 | 0 | 4.165490 | 2.725865 | -0.648959 |
| 40 | 6 | 0 | 5.364237 | 4.149122 | 0.883840 |
| 41 | 6 | 0 | 3.132675 | 3.648805 | -0.696372 |
| 42 | 1 | 0 | 4.115822 | 1.817952 | -1.239408 |
| 43 | 6 | 0 | 4.328190 | 5.067009 | 0.830559 |
| 44 | 1 | 0 | 6.242081 | 4.348568 | 1.487325 |
| 45 | 6 | 0 | 3.191812 | 4.824139 | 0.055575 |
| 46 | 1 | 0 | 2.270946 | 3.469014 | -1.331058 |
| 47 | 1 | 0 | 4.413549 | 5.993854 | 1.391248 |
| 48 | 1 | 0 | -0.574065 | 3.384493 | 5.878132 |
| 49 | 6 | 0 | -0.593751 | 4.261659 | 5.240317 |
| 50 | 6 | 0 | 0.393060 | 4.436341 | 4.276702 |
| 51 | 6 | 0 | -1.593969 | 5.213320 | 5.391126 |
| 52 | 6 | 0 | 0.393725 | 5.568199 | 3.465579 |
| 53 | 1 | 0 | 1.172492 | 3.689528 | 4.159943 |
| 54 | 6 | 0 | -1.603121 | 6.343870 | 4.579724 |
| 55 | 1 | 0 | -2.362757 | 5.080065 | 6.144681 |
| 56 | 6 | 0 | 1.490934 | 5.763685 | 2.454695 |
| 57 | 6 | 0 | -0.611048 | 6.524563 | 3.626027 |
| 58 | 1 | 0 | -2.377864 | 7.093419 | 4.702208 |
| 59 | 7 | 0 | 1.007187 | 5.632993 | 1.043253 |
| 60 | 1 | 0 | 1.935714 | 6.759733 | 2.535122 |
| 61 | 1 | 0 | 2.283108 | 5.028471 | 2.591221 |
| 62 | 1 | 0 | -0.623495 | 7.409754 | 2.996720 |
| 63 | 6 | 0 | 2.073001 | 5.826162 | -0.005903 |
| 64 | 1 | 0 | 0.282136 | 6.353488 | 0.871324 |
| 65 | 1 | 0 | 0.523213 | 4.719985 | 0.927545 |
| 66 | 1 | 0 | 1.548927 | 5.795075 | -0.962614 |
| 67 | 1 | 0 | 2.457714 | 6.836827 | 0.147400 |
| 68 | 1 | 0 | -3.716534 | 0.987009 | 6.017690 |
| 69 | 6 | 0 | -2.842507 | 0.757386 | 5.383781 |
| 70 | 7 | 0 | -3.211369 | 0.064101 | 4.163350 |
| 71 | 1 | 0 | -2.154715 | 0.136139 | 5.962460 |
| 72 | 1 | 0 | -2.338452 | 1.694956 | 5.141599 |
| 73 | 6 | 0 | -3.894812 | -1.190268 | 4.415632 |
| 74 | 6 | 0 | -4.122675 | 0.805872 | 3.309336 |
| 75 | 6 | 0 | -4.417391 | -1.640809 | 3.031035 |
| 76 | 1 | 0 | -3.221001 | -1.924961 | 4.862903 |
| 77 | 1 | 0 | -4.749349 | -1.051443 | 5.101865 |
| 78 | 6 | 0 | -4.560066 | -0.259666 | 2.237265 |
| 79 | 1 | 0 | -5.035140 | 1.089540 | 3.867205 |
| 80 | 6 | 0 | -3.525706 | 2.056274 | 2.715287 |
| 81 | 6 | 0 | -5.704690 | -2.458246 | 3.112084 |
| 82 | 6 | 0 | -3.493457 | -2.662210 | 2.364993 |
| 83 | 6 | 0 | -3.746320 | -0.200728 | 0.942712 |
| 84 | 6 | 0 | -5.955415 | 0.016098 | 1.684427 |
| 85 | 6 | 0 | -2.201100 | 2.064752 | 2.275305 |
| 86 | 6 | 0 | -4.300795 | 3.187857 | 2.504918 |
| 87 | 6 | 0 | -6.940025 | -1.978142 | 2.769004 |
| 88 | 6 | 0 | -5.419652 | -3.852442 | 2.937381 |
| 89 | 6 | 0 | -2.647801 | -2.381127 | 1.328266 |
| 90 | 6 | 0 | -4.052350 | -3.978477 | 2.476928 |
| 91 | 6 | 0 | -4.501913 | 0.452671 | -0.086921 |
| 92 | 6 | 0 | -2.783467 | -1.106871 | 0.589985 |
| 93 | 6 | 0 | -5.868672 | 0.586954 | 0.371666 |
| 94 | 6 | 0 | -7.068449 | -0.702426 | 2.029588 |
| 95 | 6 | 0 | -1.691770 | 3.151165 | 1.592598 |
| 96 | 1 | 0 | -1.576471 | 1.197464 | 2.456469 |
| 97 | 6 | 0 | -3.788554 | 4.300561 | 1.841616 |
| 98 | 1 | 0 | -5.330396 | 3.206419 | 2.847937 |
| 99 | 6 | 0 | -7.952717 | -2.872885 | 2.266292 |
| 100 | 6 | 0 | -6.390587 | -4.734008 | 2.479488 |
| 101 | 6 | 0 | -2.305055 | -3.401913 | 0.369880 |
| 102 | 6 | 0 | -3.712334 | -4.983833 | 1.579899 |
| 103 | 6 | 0 | -4.238528 | 0.225561 | -1.432333 |
| 104 | 6 | 0 | -2.511975 | -1.378885 | -0.800865 |
| 105 | 6 | 0 | -6.916999 | 0.476725 | -0.533318 |
| 106 | 6 | 0 | -8.157127 | -0.849358 | 1.095498 |
| 107 | 8 | 0 | -0.391070 | 3.136707 | 1.111555 |
| 108 | 6 | 0 | -2.484595 | 4.283248 | 1.361462 |
| 109 | 1 | 0 | -4.422458 | 5.164152 | 1.688754 |
| 110 | 6 | 0 | -8.705240 | -2.182215 | 1.239262 |
| 111 | 6 | 0 | -7.692942 | -4.231367 | 2.135358 |
| 112 | 6 | 0 | -6.037344 | -5.772933 | 1.529850 |
| 113 | 6 | 0 | -2.814237 | -4.688469 | 0.496692 |
| 114 | 6 | 0 | -2.216342 | -2.789993 | -0.940015 |
| 115 | 6 | 0 | -4.730754 | -5.894926 | 1.091118 |
| 116 | 6 | 0 | -3.214705 | -0.715881 | -1.801024 |
| 117 | 6 | 0 | -5.335276 | 0.097732 | -2.375034 |
| 118 | 6 | 0 | -8.094311 | -0.259595 | -0.161249 |
| 119 | 6 | 0 | -6.642068 | 0.218604 | -1.935094 |
| 120 | 6 | 0 | -0.154041 | 2.171131 | 0.074965 |
| 121 | 8 | 0 | -1.899066 | 5.295151 | 0.657642 |
| 122 | 6 | 0 | -9.160577 | -2.870535 | 0.127811 |
| 123 | 6 | 0 | -8.158117 | -4.950222 | 0.967021 |
| 124 | 6 | 0 | -7.133556 | -5.905293 | 0.592313 |
| 125 | 6 | 0 | -3.270156 | -5.407428 | -0.675178 |
| 126 | 6 | 0 | -2.641014 | -3.480711 | -2.062714 |
| 127 | 6 | 0 | -4.455974 | -6.156190 | -0.307011 |
| 128 | 6 | 0 | -3.669433 | -1.440212 | -2.970494 |
| 129 | 6 | 0 | -4.981769 | -0.936054 | -3.326129 |
| 130 | 6 | 0 | -8.559145 | -0.983268 | -1.326938 |
| 131 | 6 | 0 | -7.660609 | -0.686510 | -2.425697 |
| 132 | 6 | 0 | -0.753034 | 2.583867 | -1.247767 |
| 133 | 1 | 0 | 0.930104 | 2.079372 | -0.000990 |
| 134 | 1 | 0 | -0.567816 | 1.202781 | 0.369786 |
| 135 | 6 | 0 | -2.674406 | 6.453729 | 0.390968 |
| 136 | 6 | 0 | -9.078517 | -2.260091 | -1.185763 |
| 137 | 6 | 0 | -8.875292 | -4.285609 | -0.014888 |
| 138 | 6 | 0 | -6.872855 | -6.152130 | -0.746581 |
| 139 | 6 | 0 | -3.184894 | -4.818627 | -1.927091 |
| 140 | 6 | 0 | -3.390506 | -2.792254 | -3.097100 |
| 141 | 6 | 0 | -5.503547 | -6.280056 | -1.206417 |
| 142 | 6 | 0 | -5.954674 | -1.807247 | -3.792801 |
| 143 | 6 | 0 | -7.323772 | -1.679274 | -3.333247 |
| 144 | 1 | 0 | -1.817786 | 2.822480 | -1.118555 |
| 145 | 1 | 0 | -0.690095 | 1.733353 | -1.942723 |
| 146 | 8 | 0 | -0.049103 | 3.697128 | -1.768627 |
| 147 | 6 | 0 | -1.820863 | 7.414058 | -0.395116 |
| 148 | 1 | 0 | -2.997329 | 6.916704 | 1.330625 |
| 149 | 1 | 0 | -3.562403 | 6.191051 | -0.197532 |
| 150 | 6 | 0 | -8.731253 | -3.294231 | -2.135563 |
| 151 | 6 | 0 | -8.605456 | -4.546002 | -1.411861 |
| 152 | 6 | 0 | -7.625820 | -5.458522 | -1.771044 |
| 153 | 6 | 0 | -4.276717 | -4.951257 | -2.866640 |
| 154 | 6 | 0 | -4.403227 | -3.699365 | -3.590422 |
| 155 | 6 | 0 | -5.411563 | -5.665101 | -2.514729 |
| 156 | 6 | 0 | -5.658619 | -3.218433 | -3.929432 |
| 157 | 6 | 0 | -7.872813 | -3.011580 | -3.186488 |
| 158 | 6 | 0 | -0.609221 | 4.150627 | -2.985209 |
| 159 | 8 | 0 | -0.749161 | 7.865265 | 0.439491 |
| 160 | 1 | 0 | -1.419176 | 6.948147 | -1.298192 |
| 161 | 1 | 0 | -2.436836 | 8.267893 | -0.697039 |
| 162 | 6 | 0 | -6.723648 | -5.158147 | -2.865311 |
| 163 | 6 | 0 | -6.844621 | -3.963913 | -3.556853 |
| 164 | 1 | 0 | -0.819662 | 3.294912 | -3.642955 |
| 165 | 1 | 0 | -1.558124 | 4.673426 | -2.801723 |
| 166 | 6 | 0 | 0.350859 | 5.055227 | -3.714455 |
| 167 | 6 | 0 | -0.283697 | 9.184576 | 0.178147 |
| 168 | 1 | 0 | -0.020835 | 5.211035 | -4.734190 |
| 169 | 1 | 0 | 1.333568 | 4.571956 | -3.774360 |
| 170 | 8 | 0 | 0.445566 | 6.304136 | -3.044581 |
| 171 | 1 | 0 | -1.139521 | 9.835873 | -0.034078 |
| 172 | 1 | 0 | 0.192902 | 9.538767 | 1.096853 |
| 173 | 6 | 0 | 0.710838 | 9.258227 | -0.957710 |
| 174 | 6 | 0 | 1.079671 | 7.317838 | -3.716060 |
| 175 | 1 | 0 | 1.049776 | 10.297514 | -1.064793 |
| 176 | 1 | 0 | 1.592622 | 8.643154 | -0.740794 |
| 177 | 8 | 0 | 0.071968 | 8.795120 | -2.133022 |
| 178 | 6 | 0 | 0.896890 | 8.616921 | -3.221137 |
| 179 | 6 | 0 | 1.879527 | 7.128348 | -4.839387 |
| 180 | 6 | 0 | 1.504058 | 9.694230 | -3.846312 |
| 181 | 6 | 0 | 2.491161 | 8.216573 | -5.455914 |
| 182 | 1 | 0 | 2.041834 | 6.135628 | -5.238598 |
| 183 | 6 | 0 | 2.307318 | 9.499540 | -4.964807 |
| 184 | 1 | 0 | 1.325018 | 10.691738 | -3.459022 |
| 185 | 1 | 0 | 3.112477 | 8.049233 | -6.328693 |
| 186 | 1 | 0 | 2.775542 | 10.347846 | -5.450587 |

**AT2: CAM-B3LYP/6-31G(d,p)**

Standard orientation:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 10.137139 | -2.966587 | 0.705480 |
| 2 | 6 | 0 | 11.376986 | -3.576032 | 0.603898 |
| 3 | 6 | 0 | 12.554806 | -2.828506 | 0.633171 |
| 4 | 6 | 0 | 12.473377 | -1.426576 | 0.790062 |
| 5 | 6 | 0 | 11.227477 | -0.824957 | 0.915684 |
| 6 | 6 | 0 | 10.049447 | -1.580782 | 0.863744 |
| 7 | 6 | 0 | 13.902764 | -3.428802 | 0.562585 |
| 8 | 6 | 0 | 13.746432 | -0.675542 | 0.861504 |
| 9 | 6 | 0 | 14.797606 | -1.384330 | 1.626455 |
| 10 | 6 | 0 | 14.877913 | -2.783659 | 1.472371 |
| 11 | 6 | 0 | 15.820136 | -3.495564 | 2.213134 |
| 12 | 1 | 0 | 15.854698 | -4.576774 | 2.141821 |
| 13 | 6 | 0 | 16.692587 | -2.841563 | 3.074771 |
| 14 | 6 | 0 | 16.613415 | -1.464604 | 3.225554 |
| 15 | 6 | 0 | 15.661178 | -0.744808 | 2.513983 |
| 16 | 1 | 0 | 9.232098 | -3.563036 | 0.688594 |
| 17 | 1 | 0 | 11.428521 | -4.656321 | 0.534552 |
| 18 | 1 | 0 | 11.154269 | 0.242237 | 1.088246 |
| 19 | 1 | 0 | 17.417759 | -3.414276 | 3.642916 |
| 20 | 1 | 0 | 17.276123 | -0.949270 | 3.912486 |
| 21 | 1 | 0 | 15.570356 | 0.323365 | 2.676587 |
| 22 | 16 | 0 | 12.741365 | 1.298889 | -0.809771 |
| 23 | 6 | 0 | 15.100749 | 2.463198 | -1.082272 |
| 24 | 6 | 0 | 13.850979 | 2.447449 | -1.533424 |
| 25 | 1 | 0 | 15.877575 | 3.130725 | -1.432289 |
| 26 | 1 | 0 | 13.461178 | 3.098805 | -2.304719 |
| 27 | 6 | 0 | 14.235632 | -4.407230 | -0.313341 |
| 28 | 16 | 0 | 15.885063 | -5.048284 | -0.492349 |
| 29 | 6 | 0 | 14.314830 | -5.999983 | -2.396623 |
| 30 | 6 | 0 | 15.565077 | -5.967202 | -1.947564 |
| 31 | 1 | 0 | 13.981802 | -6.541963 | -3.272098 |
| 32 | 1 | 0 | 16.402220 | -6.479096 | -2.404263 |
| 33 | 16 | 0 | 15.525121 | 1.337179 | 0.189649 |
| 34 | 16 | 0 | 13.103958 | -5.118486 | -1.488274 |
| 35 | 6 | 0 | 13.958690 | 0.490481 | 0.210491 |
| 36 | 6 | 0 | 8.779748 | -0.943576 | 0.999369 |
| 37 | 6 | 0 | 7.704597 | -0.402790 | 1.116408 |
| 38 | 6 | 0 | 6.436653 | 0.236197 | 1.240732 |
| 39 | 6 | 0 | 6.351021 | 1.617812 | 1.460227 |
| 40 | 6 | 0 | 5.250770 | -0.504019 | 1.135919 |
| 41 | 6 | 0 | 5.115624 | 2.235398 | 1.557383 |
| 42 | 1 | 0 | 7.262168 | 2.196921 | 1.551674 |
| 43 | 6 | 0 | 4.018242 | 0.124415 | 1.225433 |
| 44 | 1 | 0 | 5.309319 | -1.576524 | 0.987296 |
| 45 | 6 | 0 | 3.934699 | 1.500995 | 1.428812 |
| 46 | 1 | 0 | 5.066100 | 3.305395 | 1.740755 |
| 47 | 1 | 0 | 3.110143 | -0.460061 | 1.124682 |
| 48 | 1 | 0 | 4.137034 | 7.275764 | 1.896450 |
| 49 | 6 | 0 | 3.206174 | 6.743029 | 2.060430 |
| 50 | 6 | 0 | 2.827769 | 5.732357 | 1.185854 |
| 51 | 6 | 0 | 2.394103 | 7.078921 | 3.138811 |
| 52 | 6 | 0 | 1.633243 | 5.035040 | 1.387751 |
| 53 | 1 | 0 | 3.473541 | 5.479049 | 0.350469 |
| 54 | 6 | 0 | 1.204204 | 6.393145 | 3.344324 |
| 55 | 1 | 0 | 2.690172 | 7.871998 | 3.816931 |
| 56 | 6 | 0 | 1.169885 | 3.956227 | 0.442404 |
| 57 | 6 | 0 | 0.830701 | 5.372937 | 2.476481 |
| 58 | 1 | 0 | 0.566309 | 6.646744 | 4.184139 |
| 59 | 7 | 0 | 2.170540 | 2.847195 | 0.255294 |
| 60 | 1 | 0 | 0.259894 | 3.488701 | 0.812037 |
| 61 | 1 | 0 | 0.983199 | 4.336170 | -0.562146 |
| 62 | 1 | 0 | -0.098559 | 4.836206 | 2.644201 |
| 63 | 6 | 0 | 2.608886 | 2.197954 | 1.542732 |
| 64 | 1 | 0 | 2.974578 | 3.216027 | -0.279832 |
| 65 | 1 | 0 | 1.753474 | 2.121154 | -0.349684 |
| 66 | 1 | 0 | 2.662266 | 2.995016 | 2.283781 |
| 67 | 1 | 0 | 1.800954 | 1.522409 | 1.823482 |
| 68 | 1 | 0 | -6.413398 | 1.869169 | 4.216098 |
| 69 | 6 | 0 | -5.318499 | 1.944545 | 4.181064 |
| 70 | 7 | 0 | -4.707543 | 1.307466 | 3.018543 |
| 71 | 1 | 0 | -4.916009 | 1.489540 | 5.088681 |
| 72 | 1 | 0 | -5.046820 | 3.002542 | 4.195161 |
| 73 | 6 | 0 | -4.900371 | -0.125605 | 2.933551 |
| 74 | 6 | 0 | -5.117445 | 1.856960 | 1.735652 |
| 75 | 6 | 0 | -6.184413 | -0.397780 | 2.088614 |
| 76 | 1 | 0 | -4.054221 | -0.581573 | 2.408249 |
| 77 | 1 | 0 | -4.953983 | -0.576482 | 3.925993 |
| 78 | 6 | 0 | -6.293425 | 0.913981 | 1.184299 |
| 79 | 1 | 0 | -5.543663 | 2.850046 | 1.898669 |
| 80 | 6 | 0 | -3.942935 | 2.033450 | 0.781627 |
| 81 | 6 | 0 | -7.428351 | -0.694427 | 2.931051 |
| 82 | 6 | 0 | -6.072108 | -1.707060 | 1.316734 |
| 83 | 6 | 0 | -6.269288 | 0.629940 | -0.318474 |
| 84 | 6 | 0 | -7.643577 | 1.630549 | 1.288196 |
| 85 | 6 | 0 | -2.685507 | 1.510985 | 1.069875 |
| 86 | 6 | 0 | -4.081666 | 2.785299 | -0.382151 |
| 87 | 6 | 0 | -8.474340 | 0.171857 | 3.097892 |
| 88 | 6 | 0 | -7.686229 | -2.107121 | 2.949016 |
| 89 | 6 | 0 | -5.817119 | -1.785422 | -0.025211 |
| 90 | 6 | 0 | -6.843622 | -2.733202 | 1.952145 |
| 91 | 6 | 0 | -7.224172 | 1.459172 | -0.999484 |
| 92 | 6 | 0 | -5.930125 | -0.576821 | -0.869988 |
| 93 | 6 | 0 | -8.069700 | 2.083925 | -0.004564 |
| 94 | 6 | 0 | -8.584546 | 1.376356 | 2.247969 |
| 95 | 6 | 0 | -1.619162 | 1.687718 | 0.202673 |
| 96 | 1 | 0 | -2.519247 | 0.990656 | 2.005724 |
| 97 | 6 | 0 | -3.016060 | 2.987290 | -1.251416 |
| 98 | 1 | 0 | -5.037782 | 3.237041 | -0.623559 |
| 99 | 6 | 0 | -9.809366 | -0.324557 | 3.321445 |
| 100 | 6 | 0 | -8.961103 | -2.605900 | 3.186448 |
| 101 | 6 | 0 | -6.312673 | -2.902288 | -0.791097 |
| 102 | 6 | 0 | -7.305142 | -3.830540 | 1.236000 |
| 103 | 6 | 0 | -7.754915 | 1.094346 | -2.230143 |
| 104 | 6 | 0 | -6.490759 | -0.987459 | -2.134791 |
| 105 | 6 | 0 | -9.411708 | 2.316036 | -0.280979 |
| 106 | 6 | 0 | -9.984339 | 1.587868 | 1.973594 |
| 107 | 8 | 0 | -0.374843 | 1.179701 | 0.536458 |
| 108 | 6 | 0 | -1.771475 | 2.427306 | -0.975745 |
| 109 | 1 | 0 | -3.170725 | 3.582677 | -2.141688 |
| 110 | 6 | 0 | -10.741427 | 0.544879 | 2.634019 |
| 111 | 6 | 0 | -10.053144 | -1.690560 | 3.380326 |
| 112 | 6 | 0 | -9.449763 | -3.741807 | 2.426167 |
| 113 | 6 | 0 | -7.033206 | -3.917515 | -0.173458 |
| 114 | 6 | 0 | -6.725246 | -2.415988 | -2.091261 |
| 115 | 6 | 0 | -8.642081 | -4.340736 | 1.475374 |
| 116 | 6 | 0 | -7.376729 | -0.163190 | -2.816444 |
| 117 | 6 | 0 | -9.159349 | 1.324403 | -2.512808 |
| 118 | 6 | 0 | -10.396738 | 2.063834 | 0.735753 |
| 119 | 6 | 0 | -9.968026 | 1.920695 | -1.561352 |
| 120 | 6 | 0 | -0.190490 | -0.208290 | 0.264773 |
| 121 | 8 | 0 | -0.665918 | 2.556892 | -1.770604 |
| 122 | 6 | 0 | -11.869800 | 0.016628 | 2.030055 |
| 123 | 6 | 0 | -11.226649 | -2.246052 | 2.738272 |
| 124 | 6 | 0 | -10.853578 | -3.516991 | 2.148490 |
| 125 | 6 | 0 | -8.200981 | -4.477716 | -0.822288 |
| 126 | 6 | 0 | -7.834429 | -2.958750 | -2.718285 |
| 127 | 6 | 0 | -9.196838 | -4.740809 | 0.198478 |
| 128 | 6 | 0 | -8.543502 | -0.727195 | -3.463487 |
| 129 | 6 | 0 | -9.647300 | 0.194295 | -3.276399 |
| 130 | 6 | 0 | -11.570285 | 1.504146 | 0.097239 |
| 131 | 6 | 0 | -11.305718 | 1.416555 | -1.325730 |
| 132 | 6 | 0 | 0.366947 | -0.439065 | -1.118338 |
| 133 | 1 | 0 | 0.513760 | -0.582262 | 1.013168 |
| 134 | 1 | 0 | -1.136610 | -0.746432 | 0.380899 |
| 135 | 6 | 0 | -0.776210 | 3.394329 | -2.910832 |
| 136 | 6 | 0 | -12.289989 | 0.502577 | 0.729252 |
| 137 | 6 | 0 | -12.115066 | -1.412180 | 2.078028 |
| 138 | 6 | 0 | -11.386063 | -3.896800 | 0.926286 |
| 139 | 6 | 0 | -8.593184 | -4.009675 | -2.066564 |
| 140 | 6 | 0 | -8.768328 | -2.094026 | -3.414071 |
| 141 | 6 | 0 | -10.538975 | -4.521784 | -0.070986 |
| 142 | 6 | 0 | -10.925002 | -0.293188 | -3.048601 |
| 143 | 6 | 0 | -11.772738 | 0.331756 | -2.051603 |
| 144 | 1 | 0 | -0.285650 | 0.013861 | -1.874468 |
| 145 | 1 | 0 | 0.422064 | -1.520781 | -1.309003 |
| 146 | 8 | 0 | 1.665334 | 0.130169 | -1.182052 |
| 147 | 6 | 0 | 0.554035 | 3.433823 | -3.617873 |
| 148 | 1 | 0 | -1.064414 | 4.408508 | -2.609728 |
| 149 | 1 | 0 | -1.535942 | 3.006365 | -3.600546 |
| 150 | 6 | 0 | -12.781478 | -0.626748 | -0.029398 |
| 151 | 6 | 0 | -12.673370 | -1.810190 | 0.804035 |
| 152 | 6 | 0 | -12.317030 | -3.024886 | 0.239593 |
| 153 | 6 | 0 | -9.994341 | -3.786240 | -2.348916 |
| 154 | 6 | 0 | -10.102328 | -2.602470 | -3.181996 |
| 155 | 6 | 0 | -10.946575 | -4.034994 | -1.372742 |
| 156 | 6 | 0 | -11.157740 | -1.722003 | -3.001901 |
| 157 | 6 | 0 | -12.528482 | -0.711566 | -1.389710 |
| 158 | 6 | 0 | 2.277373 | -0.083604 | -2.439080 |
| 159 | 8 | 0 | 1.510462 | 4.059513 | -2.792929 |
| 160 | 1 | 0 | 0.874101 | 2.416249 | -3.881913 |
| 161 | 1 | 0 | 0.424818 | 3.996712 | -4.554108 |
| 162 | 6 | 0 | -12.046890 | -3.110625 | -1.181974 |
| 163 | 6 | 0 | -12.150124 | -1.981311 | -1.977528 |
| 164 | 1 | 0 | 2.178890 | -1.138540 | -2.731563 |
| 165 | 1 | 0 | 1.787612 | 0.524775 | -3.211154 |
| 166 | 6 | 0 | 3.746523 | 0.240574 | -2.371156 |
| 167 | 6 | 0 | 2.717741 | 4.349571 | -3.468337 |
| 168 | 1 | 0 | 4.206491 | -0.023612 | -3.331415 |
| 169 | 1 | 0 | 4.226604 | -0.339801 | -1.576727 |
| 170 | 8 | 0 | 3.896523 | 1.628234 | -2.116293 |
| 171 | 1 | 0 | 3.182731 | 3.429704 | -3.845058 |
| 172 | 1 | 0 | 2.524386 | 5.013036 | -4.325004 |
| 173 | 6 | 0 | 3.648054 | 5.058022 | -2.512782 |
| 174 | 6 | 0 | 5.167547 | 2.124996 | -2.060540 |
| 175 | 1 | 0 | 4.499287 | 5.474941 | -3.058622 |
| 176 | 1 | 0 | 3.112101 | 5.872536 | -2.019258 |
| 177 | 8 | 0 | 4.129363 | 4.204968 | -1.465172 |
| 178 | 6 | 0 | 5.280970 | 3.485206 | -1.751297 |
| 179 | 6 | 0 | 6.324552 | 1.383331 | -2.277283 |
| 180 | 6 | 0 | 6.522550 | 4.090622 | -1.664033 |
| 181 | 6 | 0 | 7.570818 | 1.997951 | -2.190710 |
| 182 | 1 | 0 | 6.270742 | 0.326070 | -2.500701 |
| 183 | 6 | 0 | 7.676952 | 3.347777 | -1.889568 |
| 184 | 1 | 0 | 6.572947 | 5.143109 | -1.404673 |
| 185 | 1 | 0 | 8.463130 | 1.403574 | -2.352500 |
| 186 | 1 | 0 | 8.649488 | 3.820630 | -1.817281 |

**AT4: CAM-B3LYP/6-31G(d,p)**

Standard orientation:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -6.565724 | -1.582378 | -3.108495 |
| 2 | 6 | 0 | -7.395543 | -2.671397 | -2.893537 |
| 3 | 6 | 0 | -8.130732 | -2.801232 | -1.714518 |
| 4 | 6 | 0 | -8.038180 | -1.787015 | -0.734988 |
| 5 | 6 | 0 | -7.222172 | -0.688263 | -0.966831 |
| 6 | 6 | 0 | -6.469731 | -0.577516 | -2.143277 |
| 7 | 6 | 0 | -9.053217 | -3.923347 | -1.446934 |
| 8 | 6 | 0 | -8.868527 | -1.934111 | 0.480981 |
| 9 | 6 | 0 | -10.212416 | -2.490510 | 0.203159 |
| 10 | 6 | 0 | -10.304262 | -3.503370 | -0.773878 |
| 11 | 6 | 0 | -11.557638 | -4.019041 | -1.100297 |
| 12 | 1 | 0 | -11.645576 | -4.759648 | -1.887021 |
| 13 | 6 | 0 | -12.704836 | -3.567625 | -0.458904 |
| 14 | 6 | 0 | -12.613698 | -2.570667 | 0.501636 |
| 15 | 6 | 0 | -11.374274 | -2.027923 | 0.818411 |
| 16 | 1 | 0 | -6.006227 | -1.495605 | -4.032852 |
| 17 | 1 | 0 | -7.496765 | -3.417023 | -3.673405 |
| 18 | 1 | 0 | -7.182989 | 0.121843 | -0.248318 |
| 19 | 1 | 0 | -13.670361 | -3.981614 | -0.729108 |
| 20 | 1 | 0 | -13.506827 | -2.197075 | 0.990847 |
| 21 | 1 | 0 | -11.317396 | -1.212237 | 1.530564 |
| 22 | 16 | 0 | -6.761341 | -1.111468 | 2.093247 |
| 23 | 6 | 0 | -8.028217 | -1.780497 | 4.317372 |
| 24 | 6 | 0 | -6.855929 | -1.399647 | 3.821321 |
| 25 | 1 | 0 | -8.223290 | -1.976799 | 5.363845 |
| 26 | 1 | 0 | -5.957242 | -1.242647 | 4.403459 |
| 27 | 6 | 0 | -8.744149 | -5.217274 | -1.705273 |
| 28 | 16 | 0 | -9.793432 | -6.585511 | -1.270501 |
| 29 | 6 | 0 | -7.449796 | -7.458800 | -2.131223 |
| 30 | 6 | 0 | -8.616170 | -7.833970 | -1.616750 |
| 31 | 1 | 0 | -6.645490 | -8.129125 | -2.404825 |
| 32 | 1 | 0 | -8.902874 | -8.856622 | -1.408530 |
| 33 | 16 | 0 | -9.368355 | -1.960715 | 3.205002 |
| 34 | 16 | 0 | -7.201077 | -5.748264 | -2.413637 |
| 35 | 6 | 0 | -8.414586 | -1.674307 | 1.727698 |
| 36 | 6 | 0 | -5.642199 | 0.568289 | -2.337266 |
| 37 | 6 | 0 | -4.955489 | 1.556292 | -2.454205 |
| 38 | 6 | 0 | -4.159397 | 2.737627 | -2.496215 |
| 39 | 6 | 0 | -3.994547 | 3.492288 | -1.327255 |
| 40 | 6 | 0 | -3.531807 | 3.169888 | -3.671283 |
| 41 | 6 | 0 | -3.228479 | 4.642667 | -1.326798 |
| 42 | 1 | 0 | -4.488537 | 3.171287 | -0.419770 |
| 43 | 6 | 0 | -2.779352 | 4.334989 | -3.669394 |
| 44 | 1 | 0 | -3.651538 | 2.596720 | -4.583347 |
| 45 | 6 | 0 | -2.623678 | 5.085557 | -2.502429 |
| 46 | 1 | 0 | -3.089822 | 5.177654 | -0.393877 |
| 47 | 1 | 0 | -2.319243 | 4.672059 | -4.593953 |
| 48 | 1 | 0 | 4.892777 | 7.023545 | -1.666796 |
| 49 | 6 | 0 | 3.965073 | 7.443376 | -1.293845 |
| 50 | 6 | 0 | 2.771544 | 7.179642 | -1.954335 |
| 51 | 6 | 0 | 3.968761 | 8.251635 | -0.163947 |
| 52 | 6 | 0 | 1.573066 | 7.719542 | -1.490216 |
| 53 | 1 | 0 | 2.773681 | 6.558093 | -2.845014 |
| 54 | 6 | 0 | 2.776961 | 8.794349 | 0.306378 |
| 55 | 1 | 0 | 4.901385 | 8.468373 | 0.345877 |
| 56 | 6 | 0 | 0.302998 | 7.503035 | -2.262992 |
| 57 | 6 | 0 | 1.584697 | 8.531982 | -0.355915 |
| 58 | 1 | 0 | 2.779644 | 9.438018 | 1.179739 |
| 59 | 7 | 0 | -0.599309 | 6.412796 | -1.750273 |
| 60 | 1 | 0 | -0.304149 | 8.411579 | -2.270387 |
| 61 | 1 | 0 | 0.527377 | 7.244322 | -3.299451 |
| 62 | 1 | 0 | 0.656904 | 8.961825 | 0.009435 |
| 63 | 6 | 0 | -1.872638 | 6.383833 | -2.554040 |
| 64 | 1 | 0 | -0.818343 | 6.581002 | -0.748418 |
| 65 | 1 | 0 | -0.126563 | 5.483386 | -1.772567 |
| 66 | 1 | 0 | -2.478206 | 7.217159 | -2.187133 |
| 67 | 1 | 0 | -1.595107 | 6.609097 | -3.585097 |
| 68 | 1 | 0 | 6.896747 | 4.266839 | -2.589130 |
| 69 | 6 | 0 | 5.975014 | 3.838271 | -3.020144 |
| 70 | 7 | 0 | 5.641797 | 2.548429 | -2.446350 |
| 71 | 1 | 0 | 6.119937 | 3.732136 | -4.097765 |
| 72 | 1 | 0 | 5.157234 | 4.542568 | -2.853847 |
| 73 | 6 | 0 | 6.683655 | 1.560094 | -2.646196 |
| 74 | 6 | 0 | 5.429167 | 2.569039 | -1.008594 |
| 75 | 6 | 0 | 6.261773 | 0.358827 | -1.768569 |
| 76 | 1 | 0 | 6.775549 | 1.289978 | -3.700974 |
| 77 | 1 | 0 | 7.665224 | 1.935153 | -2.305188 |
| 78 | 6 | 0 | 5.372067 | 1.042848 | -0.628089 |
| 79 | 1 | 0 | 6.310326 | 2.992978 | -0.490873 |
| 80 | 6 | 0 | 4.212419 | 3.356541 | -0.591268 |
| 81 | 6 | 0 | 7.452813 | -0.441668 | -1.248390 |
| 82 | 6 | 0 | 5.539505 | -0.725387 | -2.570147 |
| 83 | 6 | 0 | 3.950252 | 0.485521 | -0.531204 |
| 84 | 6 | 0 | 5.855783 | 0.779814 | 0.796221 |
| 85 | 6 | 0 | 3.046873 | 3.309590 | -1.360964 |
| 86 | 6 | 0 | 4.198189 | 4.081251 | 0.592636 |
| 87 | 6 | 0 | 7.898906 | -0.398341 | 0.044749 |
| 88 | 6 | 0 | 7.610242 | -1.647615 | -2.007187 |
| 89 | 6 | 0 | 4.192079 | -0.952448 | -2.526786 |
| 90 | 6 | 0 | 6.427638 | -1.822786 | -2.824407 |
| 91 | 6 | 0 | 3.562577 | 0.355557 | 0.843984 |
| 92 | 6 | 0 | 3.371065 | -0.327619 | -1.466897 |
| 93 | 6 | 0 | 4.740984 | 0.536729 | 1.665408 |
| 94 | 6 | 0 | 7.072153 | 0.228855 | 1.100026 |
| 95 | 6 | 0 | 1.897908 | 3.937957 | -0.926927 |
| 96 | 1 | 0 | 3.048374 | 2.760564 | -2.295732 |
| 97 | 6 | 0 | 3.046516 | 4.734328 | 1.030136 |
| 98 | 1 | 0 | 5.097080 | 4.136210 | 1.198804 |
| 99 | 6 | 0 | 8.546908 | -1.546890 | 0.627325 |
| 100 | 6 | 0 | 8.255250 | -2.755058 | -1.471616 |
| 101 | 6 | 0 | 3.668213 | -2.276041 | -2.755583 |
| 102 | 6 | 0 | 5.941159 | -3.099866 | -3.075115 |
| 103 | 6 | 0 | 2.572979 | -0.538680 | 1.234878 |
| 104 | 6 | 0 | 2.361130 | -1.282255 | -1.079274 |
| 105 | 6 | 0 | 4.886071 | -0.192332 | 2.839178 |
| 106 | 6 | 0 | 7.237406 | -0.551985 | 2.301159 |
| 107 | 8 | 0 | 0.721500 | 3.884537 | -1.654517 |
| 108 | 6 | 0 | 1.882861 | 4.654492 | 0.277877 |
| 109 | 1 | 0 | 3.069863 | 5.297241 | 1.954515 |
| 110 | 6 | 0 | 8.145092 | -1.643891 | 2.015244 |
| 111 | 6 | 0 | 8.738180 | -2.703611 | -0.118297 |
| 112 | 6 | 0 | 7.736681 | -4.087066 | -1.721076 |
| 113 | 6 | 0 | 4.523030 | -3.333829 | -3.040263 |
| 114 | 6 | 0 | 2.540337 | -2.482127 | -1.870460 |
| 115 | 6 | 0 | 6.607840 | -4.255244 | -2.503526 |
| 116 | 6 | 0 | 1.954142 | -1.381380 | 0.246494 |
| 117 | 6 | 0 | 2.731903 | -1.309486 | 2.454988 |
| 118 | 6 | 0 | 6.169475 | -0.750477 | 3.167768 |
| 119 | 6 | 0 | 3.861597 | -1.140968 | 3.236645 |
| 120 | 6 | 0 | 0.116775 | 2.577680 | -1.744510 |
| 121 | 8 | 0 | 0.691486 | 5.226040 | 0.598948 |
| 122 | 6 | 0 | 7.947496 | -2.884012 | 2.597841 |
| 123 | 6 | 0 | 8.519280 | -4.001580 | 0.486353 |
| 124 | 6 | 0 | 7.900242 | -4.858713 | -0.506039 |
| 125 | 6 | 0 | 4.295854 | -4.632656 | -2.440708 |
| 126 | 6 | 0 | 2.315312 | -3.726368 | -1.305705 |
| 127 | 6 | 0 | 5.586697 | -5.204269 | -2.109705 |
| 128 | 6 | 0 | 1.728885 | -2.682863 | 0.841633 |
| 129 | 6 | 0 | 2.210204 | -2.638153 | 2.208741 |
| 130 | 6 | 0 | 5.954045 | -2.050986 | 3.768891 |
| 131 | 6 | 0 | 4.524998 | -2.292502 | 3.812065 |
| 132 | 6 | 0 | -0.167463 | 1.932947 | -0.407051 |
| 133 | 1 | 0 | -0.809660 | 2.725315 | -2.300607 |
| 134 | 1 | 0 | 0.776882 | 1.919423 | -2.318776 |
| 135 | 6 | 0 | 0.567570 | 5.913149 | 1.833009 |
| 136 | 6 | 0 | 6.822043 | -3.094254 | 3.488935 |
| 137 | 6 | 0 | 8.132974 | -4.090654 | 1.814268 |
| 138 | 6 | 0 | 6.922519 | -5.764752 | -0.125663 |
| 139 | 6 | 0 | 3.216203 | -4.826143 | -1.593415 |
| 140 | 6 | 0 | 1.907775 | -3.829221 | 0.082956 |
| 141 | 6 | 0 | 5.739572 | -5.941031 | -0.945613 |
| 142 | 6 | 0 | 2.846591 | -3.742429 | 2.755349 |
| 143 | 6 | 0 | 4.029411 | -3.565631 | 3.574872 |
| 144 | 1 | 0 | 0.738858 | 1.935917 | 0.214002 |
| 145 | 1 | 0 | -0.422821 | 0.878637 | -0.594885 |
| 146 | 8 | 0 | -1.231440 | 2.593656 | 0.239860 |
| 147 | 6 | 0 | -0.891365 | 6.235515 | 2.018835 |
| 148 | 1 | 0 | 1.183517 | 6.819104 | 1.823578 |
| 149 | 1 | 0 | 0.890497 | 5.272230 | 2.662816 |
| 150 | 6 | 0 | 6.305403 | -4.423470 | 3.246694 |
| 151 | 6 | 0 | 7.115408 | -5.038902 | 2.211426 |
| 152 | 6 | 0 | 6.522268 | -5.857622 | 1.263109 |
| 153 | 6 | 0 | 3.375151 | -5.598620 | -0.380710 |
| 154 | 6 | 0 | 2.565928 | -4.982881 | 0.655241 |
| 155 | 6 | 0 | 4.609311 | -6.143467 | -0.062583 |
| 156 | 6 | 0 | 3.026902 | -4.940877 | 1.962094 |
| 157 | 6 | 0 | 4.939414 | -4.655277 | 3.287892 |
| 158 | 6 | 0 | -1.457022 | 2.121645 | 1.550484 |
| 159 | 8 | 0 | -1.325562 | 7.135149 | 0.984880 |
| 160 | 1 | 0 | -1.494900 | 5.327549 | 1.996039 |
| 161 | 1 | 0 | -1.027067 | 6.714448 | 2.994441 |
| 162 | 6 | 0 | 5.092509 | -6.092948 | 1.303107 |
| 163 | 6 | 0 | 4.319707 | -5.507172 | 2.292216 |
| 164 | 1 | 0 | -1.221942 | 1.050454 | 1.625103 |
| 165 | 1 | 0 | -0.816967 | 2.653685 | 2.269007 |
| 166 | 6 | 0 | -2.912487 | 2.286078 | 1.915263 |
| 167 | 6 | 0 | -2.390859 | 8.001836 | 1.359723 |
| 168 | 1 | 0 | -3.104623 | 1.803017 | 2.882125 |
| 169 | 1 | 0 | -3.524697 | 1.793542 | 1.151716 |
| 170 | 8 | 0 | -3.223590 | 3.667333 | 1.990301 |
| 171 | 1 | 0 | -2.193127 | 8.400824 | 2.361824 |
| 172 | 1 | 0 | -2.381944 | 8.838840 | 0.654928 |
| 173 | 6 | 0 | -3.760455 | 7.350385 | 1.337545 |
| 174 | 6 | 0 | -4.526645 | 4.018735 | 2.199743 |
| 175 | 1 | 0 | -4.500188 | 8.095943 | 1.658464 |
| 176 | 1 | 0 | -4.029283 | 7.024570 | 0.324629 |
| 177 | 8 | 0 | -3.709674 | 6.241001 | 2.210757 |
| 178 | 6 | 0 | -4.793566 | 5.397478 | 2.265062 |
| 179 | 6 | 0 | -5.578587 | 3.117747 | 2.327855 |
| 180 | 6 | 0 | -6.091292 | 5.849399 | 2.432252 |
| 181 | 6 | 0 | -6.882296 | 3.583229 | 2.493869 |
| 182 | 1 | 0 | -5.402780 | 2.050062 | 2.292130 |
| 183 | 6 | 0 | -7.143029 | 4.942082 | 2.540109 |
| 184 | 1 | 0 | -6.281050 | 6.915345 | 2.494326 |
| 185 | 1 | 0 | -7.689497 | 2.865008 | 2.585780 |
| 186 | 1 | 0 | -8.156269 | 5.304568 | 2.670085 |

**BT2: CAM-B3LYP/6-31G(d,p)**

Standard orientation:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -7.832727 | -2.202816 | 2.139192 |
| 2 | 6 | 0 | -8.707838 | -3.272938 | 2.050348 |
| 3 | 6 | 0 | -9.526658 | -3.447518 | 0.933988 |
| 4 | 6 | 0 | -9.440441 | -2.522612 | -0.130728 |
| 5 | 6 | 0 | -8.541298 | -1.466924 | -0.045935 |
| 6 | 6 | 0 | -7.739522 | -1.286646 | 1.088098 |
| 7 | 6 | 0 | -10.454919 | -4.585615 | 0.774591 |
| 8 | 6 | 0 | -10.295896 | -2.764917 | -1.313807 |
| 9 | 6 | 0 | -10.408400 | -4.198215 | -1.667001 |
| 10 | 6 | 0 | -10.489723 | -5.123090 | -0.605437 |
| 11 | 6 | 0 | -10.545245 | -6.485736 | -0.894671 |
| 12 | 1 | 0 | -10.554950 | -7.206755 | -0.085129 |
| 13 | 6 | 0 | -10.549888 | -6.937219 | -2.208998 |
| 14 | 6 | 0 | -10.471422 | -6.026836 | -3.253035 |
| 15 | 6 | 0 | -10.387512 | -4.666939 | -2.979482 |
| 16 | 1 | 0 | -7.201278 | -2.084036 | 3.012210 |
| 17 | 1 | 0 | -8.729818 | -4.002322 | 2.851550 |
| 18 | 1 | 0 | -8.430327 | -0.779879 | -0.876272 |
| 19 | 1 | 0 | -10.593576 | -8.001926 | -2.412061 |
| 20 | 1 | 0 | -10.453789 | -6.371883 | -4.281343 |
| 21 | 1 | 0 | -10.274480 | -3.965293 | -3.798386 |
| 22 | 16 | 0 | -10.949474 | -0.072675 | -1.457551 |
| 23 | 6 | 0 | -12.819070 | -0.479134 | -3.284039 |
| 24 | 6 | 0 | -12.296582 | 0.424991 | -2.462202 |
| 25 | 1 | 0 | -13.641700 | -0.297695 | -3.963628 |
| 26 | 1 | 0 | -12.630822 | 1.450395 | -2.372670 |
| 27 | 6 | 0 | -11.263446 | -5.029513 | 1.767183 |
| 28 | 16 | 0 | -12.473357 | -6.315082 | 1.550585 |
| 29 | 6 | 0 | -12.749970 | -5.179139 | 3.923242 |
| 30 | 6 | 0 | -13.269987 | -6.075134 | 3.090978 |
| 31 | 1 | 0 | -13.134734 | -4.946880 | 4.907688 |
| 32 | 1 | 0 | -14.142364 | -6.681537 | 3.297376 |
| 33 | 16 | 0 | -12.114915 | -2.082747 | -3.287631 |
| 34 | 16 | 0 | -11.315577 | -4.321790 | 3.398863 |
| 35 | 6 | 0 | -10.984760 | -1.786021 | -1.944037 |
| 36 | 6 | 0 | -6.819109 | -0.198117 | 1.151696 |
| 37 | 6 | 0 | -6.036661 | 0.722167 | 1.202839 |
| 38 | 6 | 0 | -5.110074 | 1.803473 | 1.253552 |
| 39 | 6 | 0 | -4.965837 | 2.671038 | 0.160346 |
| 40 | 6 | 0 | -4.332388 | 2.030378 | 2.395844 |
| 41 | 6 | 0 | -4.061087 | 3.717895 | 0.206750 |
| 42 | 1 | 0 | -5.584273 | 2.517972 | -0.717135 |
| 43 | 6 | 0 | -3.427569 | 3.080772 | 2.432969 |
| 44 | 1 | 0 | -4.451039 | 1.379919 | 3.254642 |
| 45 | 6 | 0 | -3.266497 | 3.927130 | 1.336680 |
| 46 | 1 | 0 | -3.969015 | 4.389083 | -0.641982 |
| 47 | 1 | 0 | -2.851351 | 3.256230 | 3.335632 |
| 48 | 1 | 0 | 0.363371 | 3.030080 | 5.682168 |
| 49 | 6 | 0 | 0.670128 | 3.601495 | 4.812766 |
| 50 | 6 | 0 | 0.077582 | 3.354874 | 3.578848 |
| 51 | 6 | 0 | 1.659589 | 4.569098 | 4.927125 |
| 52 | 6 | 0 | 0.463890 | 4.074757 | 2.449928 |
| 53 | 1 | 0 | -0.676813 | 2.579954 | 3.488899 |
| 54 | 6 | 0 | 2.064364 | 5.280465 | 3.801694 |
| 55 | 1 | 0 | 2.125867 | 4.759618 | 5.887788 |
| 56 | 6 | 0 | -0.141043 | 3.777580 | 1.104415 |
| 57 | 6 | 0 | 1.474626 | 5.031090 | 2.569672 |
| 58 | 1 | 0 | 2.854777 | 6.019631 | 3.883439 |
| 59 | 1 | 0 | 1.804604 | 5.574154 | 1.688837 |
| 60 | 1 | 0 | -0.540840 | 5.757983 | 0.538790 |
| 61 | 6 | 0 | 3.467456 | -1.136562 | 1.298984 |
| 62 | 6 | 0 | 3.032317 | -2.418527 | 0.989867 |
| 63 | 6 | 0 | 4.334621 | -0.926569 | 2.439911 |
| 64 | 6 | 0 | 3.855502 | -0.220133 | 0.253889 |
| 65 | 6 | 0 | 3.461669 | -3.545529 | 1.792165 |
| 66 | 6 | 0 | 3.002990 | -2.834781 | -0.386427 |
| 67 | 6 | 0 | 4.737956 | -2.001301 | 3.214723 |
| 68 | 6 | 0 | 5.273862 | 0.123854 | 2.106432 |
| 69 | 6 | 0 | 4.993444 | 0.573721 | 0.765487 |
| 70 | 6 | 0 | 3.807118 | -0.603369 | -1.060056 |
| 71 | 6 | 0 | 4.296968 | -3.341995 | 2.879316 |
| 72 | 6 | 0 | 3.694531 | -4.665372 | 0.901038 |
| 73 | 6 | 0 | 3.409542 | -4.226134 | -0.449695 |
| 74 | 6 | 0 | 3.406329 | -1.946440 | -1.374932 |
| 75 | 6 | 0 | 6.108207 | -2.082142 | 3.684378 |
| 76 | 6 | 0 | 6.583059 | 0.051407 | 2.567509 |
| 77 | 6 | 0 | 6.020118 | 0.913762 | -0.072053 |
| 78 | 6 | 0 | 4.725044 | -0.051865 | -2.153018 |
| 79 | 6 | 0 | 5.397060 | -4.247333 | 3.128955 |
| 80 | 6 | 0 | 4.752149 | -5.530028 | 1.137387 |
| 81 | 6 | 0 | 4.187816 | -4.672285 | -1.503181 |
| 82 | 6 | 0 | 4.219153 | -2.413471 | -2.477545 |
| 83 | 6 | 0 | 6.516601 | -3.468793 | 3.626278 |
| 84 | 6 | 0 | 7.009870 | -1.078267 | 3.367630 |
| 85 | 6 | 0 | 7.661102 | 0.403885 | 1.683371 |
| 86 | 6 | 0 | 5.958435 | 0.792347 | -1.589829 |
| 87 | 6 | 0 | 7.373281 | 0.808869 | 0.386101 |
| 88 | 6 | 0 | 5.129521 | -1.363674 | -2.833952 |
| 89 | 6 | 0 | 4.039212 | 0.936440 | -3.216724 |
| 90 | 6 | 0 | 5.621184 | -5.317224 | 2.276442 |
| 91 | 6 | 0 | 5.567521 | -5.997972 | 0.033166 |
| 92 | 6 | 0 | 5.290031 | -5.580179 | -1.259092 |
| 93 | 6 | 0 | 4.597100 | -3.748982 | -2.544735 |
| 94 | 6 | 0 | 7.809463 | -3.795303 | 3.247803 |
| 95 | 6 | 0 | 8.363331 | -1.419105 | 2.973983 |
| 96 | 6 | 0 | 8.768640 | -0.500008 | 1.930273 |
| 97 | 6 | 0 | 7.331698 | 0.171182 | -1.860849 |
| 98 | 6 | 0 | 5.753809 | 2.186325 | -2.259664 |
| 99 | 6 | 0 | 8.185412 | 0.345404 | -0.719029 |
| 100 | 6 | 0 | 6.407906 | -1.685935 | -3.198523 |
| 101 | 7 | 0 | 4.998624 | 1.997799 | -3.481741 |
| 102 | 6 | 0 | 2.673843 | 1.475433 | -2.803250 |
| 103 | 1 | 0 | 3.882283 | 0.367927 | -4.136747 |
| 104 | 6 | 0 | 6.973526 | -5.654682 | 1.878132 |
| 105 | 6 | 0 | 6.939625 | -6.073789 | 0.491003 |
| 106 | 6 | 0 | 6.373247 | -5.215649 | -2.151337 |
| 107 | 6 | 0 | 5.936627 | -4.085238 | -2.944877 |
| 108 | 6 | 0 | 8.041887 | -4.911103 | 2.352150 |
| 109 | 6 | 0 | 8.752712 | -2.748182 | 2.913570 |
| 110 | 6 | 0 | 9.544787 | -0.946101 | 0.874889 |
| 111 | 6 | 0 | 7.548511 | -0.892673 | -2.693412 |
| 112 | 1 | 0 | 5.179793 | 2.807858 | -1.563550 |
| 113 | 1 | 0 | 6.699501 | 2.695118 | -2.454689 |
| 114 | 6 | 0 | 9.254101 | -0.509427 | -0.478783 |
| 115 | 6 | 0 | 6.827262 | -3.064663 | -3.251300 |
| 116 | 6 | 0 | 5.806587 | 1.805535 | -4.682616 |
| 117 | 6 | 0 | 1.571971 | 0.625147 | -2.746376 |
| 118 | 6 | 0 | 2.496751 | 2.830251 | -2.529309 |
| 119 | 6 | 0 | 7.974736 | -5.725437 | -0.362682 |
| 120 | 6 | 0 | 7.685105 | -5.285137 | -1.709772 |
| 121 | 6 | 0 | 9.128013 | -4.551228 | 1.462374 |
| 122 | 6 | 0 | 9.567968 | -3.215442 | 1.809163 |
| 123 | 6 | 0 | 9.957213 | -2.333392 | 0.812992 |
| 124 | 6 | 0 | 8.637215 | -1.805854 | -2.448854 |
| 125 | 6 | 0 | 9.488660 | -1.614604 | -1.368470 |
| 126 | 6 | 0 | 8.198714 | -3.142551 | -2.793142 |
| 127 | 1 | 0 | 5.149189 | 1.752067 | -5.553299 |
| 128 | 1 | 0 | 6.432900 | 0.903936 | -4.666611 |
| 129 | 1 | 0 | 6.458939 | 2.671376 | -4.815490 |
| 130 | 6 | 0 | 0.324296 | 1.114457 | -2.385227 |
| 131 | 1 | 0 | 1.681132 | -0.427828 | -2.979095 |
| 132 | 6 | 0 | 1.247620 | 3.328056 | -2.172046 |
| 133 | 1 | 0 | 3.349943 | 3.483231 | -2.648640 |
| 134 | 6 | 0 | 9.094231 | -4.946532 | 0.134302 |
| 135 | 6 | 0 | 8.620557 | -4.227812 | -2.043887 |
| 136 | 6 | 0 | 9.920851 | -2.747509 | -0.576187 |
| 137 | 6 | 0 | 0.155346 | 2.458590 | -2.094124 |
| 138 | 1 | 0 | -0.533541 | 0.453640 | -2.317220 |
| 139 | 8 | 0 | 0.995175 | 4.642932 | -1.873427 |
| 140 | 6 | 0 | 9.496477 | -4.024906 | -0.905603 |
| 141 | 8 | 0 | -1.074291 | 2.941422 | -1.686684 |
| 142 | 6 | 0 | 2.095851 | 5.536668 | -1.888095 |
| 143 | 6 | 0 | -2.054649 | 3.084112 | -2.716231 |
| 144 | 6 | 0 | 1.605990 | 6.926092 | -1.576875 |
| 145 | 1 | 0 | 2.847632 | 5.228260 | -1.151538 |
| 146 | 1 | 0 | 2.567435 | 5.547998 | -2.878157 |
| 147 | 6 | 0 | -2.033509 | 4.475033 | -3.301997 |
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| 149 | 1 | 0 | -1.883225 | 2.346798 | -3.506105 |
| 150 | 1 | 0 | 0.809260 | 7.211763 | -2.277055 |
| 151 | 1 | 0 | 2.445829 | 7.619875 | -1.724074 |
| 152 | 8 | 0 | 1.141475 | 7.005828 | -0.243401 |
| 153 | 8 | 0 | -2.406299 | 5.401541 | -2.293925 |
| 154 | 1 | 0 | -1.030480 | 4.710884 | -3.680914 |
| 155 | 1 | 0 | -2.740977 | 4.526941 | -4.142654 |
| 156 | 6 | 0 | 0.921818 | 8.349654 | 0.158688 |
| 157 | 6 | 0 | -2.389571 | 6.732117 | -2.768310 |
| 158 | 1 | 0 | 1.862805 | 8.916291 | 0.103980 |
| 159 | 1 | 0 | 0.191741 | 8.828452 | -0.506444 |
| 160 | 6 | 0 | 0.415038 | 8.357461 | 1.580206 |
| 161 | 1 | 0 | -1.357871 | 7.060620 | -2.954943 |
| 162 | 1 | 0 | -2.939087 | 6.801743 | -3.718060 |
| 163 | 6 | 0 | -3.057156 | 7.655817 | -1.783521 |
| 164 | 1 | 0 | 0.355367 | 9.387317 | 1.945465 |
| 165 | 1 | 0 | 1.092620 | 7.796330 | 2.226334 |
| 166 | 8 | 0 | -0.858915 | 7.721407 | 1.679471 |
| 167 | 1 | 0 | -3.146322 | 8.648160 | -2.242459 |
| 168 | 1 | 0 | -4.064391 | 7.290455 | -1.549827 |
| 169 | 8 | 0 | -2.272020 | 7.726566 | -0.603986 |
| 170 | 6 | 0 | -1.952973 | 8.557991 | 1.574037 |
| 171 | 6 | 0 | -2.711698 | 8.553942 | 0.395515 |
| 172 | 6 | 0 | -2.327543 | 9.355103 | 2.643806 |
| 173 | 6 | 0 | -3.845417 | 9.357575 | 0.315364 |
| 174 | 6 | 0 | -3.453130 | 10.167099 | 2.556123 |
| 175 | 1 | 0 | -1.730762 | 9.319616 | 3.549264 |
| 176 | 6 | 0 | -4.206492 | 10.162962 | 1.392320 |
| 177 | 1 | 0 | -4.453755 | 9.368441 | -0.579457 |
| 178 | 1 | 0 | -3.741324 | 10.788062 | 3.396364 |
| 179 | 1 | 0 | -5.090643 | 10.785570 | 1.312350 |
| 180 | 1 | 0 | -1.280918 | 4.618924 | -0.388213 |
| 181 | 7 | 0 | -1.048002 | 4.860613 | 0.587959 |
| 182 | 6 | 0 | -2.308983 | 5.084994 | 1.380769 |
| 183 | 1 | 0 | -0.734270 | 2.863756 | 1.118493 |
| 184 | 1 | 0 | 0.631992 | 3.668884 | 0.346613 |
| 185 | 1 | 0 | -1.993475 | 5.319648 | 2.396756 |
| 186 | 1 | 0 | -2.755196 | 5.976107 | 0.946095 |

**AT1: M06-2X/6-31G(d,p)**

Standard orientation:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 8.927793 | 1.250167 | 0.885455 |
| 2 | 6 | 0 | 9.994154 | 0.364857 | 0.940181 |
| 3 | 6 | 0 | 9.950278 | -0.861114 | 0.270156 |
| 4 | 6 | 0 | 8.807629 | -1.186020 | -0.499459 |
| 5 | 6 | 0 | 7.753111 | -0.281276 | -0.573679 |
| 6 | 6 | 0 | 7.794607 | 0.932518 | 0.127030 |
| 7 | 6 | 0 | 11.059502 | -1.834963 | 0.286710 |
| 8 | 6 | 0 | 8.817001 | -2.476811 | -1.221101 |
| 9 | 6 | 0 | 10.139553 | -2.835665 | -1.780259 |
| 10 | 6 | 0 | 11.278774 | -2.511440 | -1.011940 |
| 11 | 6 | 0 | 12.547539 | -2.793872 | -1.521565 |
| 12 | 1 | 0 | 13.429223 | -2.493513 | -0.964110 |
| 13 | 6 | 0 | 12.697011 | -3.416566 | -2.757370 |
| 14 | 6 | 0 | 11.574860 | -3.736146 | -3.513382 |
| 15 | 6 | 0 | 10.305204 | -3.431953 | -3.031682 |
| 16 | 1 | 0 | 8.974059 | 2.199424 | 1.407720 |
| 17 | 1 | 0 | 10.889052 | 0.647606 | 1.484598 |
| 18 | 1 | 0 | 6.894495 | -0.494985 | -1.202101 |
| 19 | 1 | 0 | 13.691199 | -3.627212 | -3.137156 |
| 20 | 1 | 0 | 11.685282 | -4.199095 | -4.488294 |
| 21 | 1 | 0 | 9.435797 | -3.630295 | -3.650895 |
| 22 | 16 | 0 | 6.185850 | -2.953248 | -0.484339 |
| 23 | 6 | 0 | 6.258321 | -5.455938 | -1.342470 |
| 24 | 6 | 0 | 5.537888 | -4.572418 | -0.655169 |
| 25 | 1 | 0 | 5.965862 | -6.480374 | -1.535154 |
| 26 | 1 | 0 | 4.573495 | -4.770968 | -0.205444 |
| 27 | 6 | 0 | 11.740912 | -2.159346 | 1.415754 |
| 28 | 16 | 0 | 12.975838 | -3.434805 | 1.481384 |
| 29 | 6 | 0 | 12.386926 | -2.582730 | 3.917021 |
| 30 | 6 | 0 | 13.091317 | -3.477631 | 3.227391 |
| 31 | 1 | 0 | 12.384461 | -2.489234 | 4.995325 |
| 32 | 1 | 0 | 13.747869 | -4.220365 | 3.662310 |
| 33 | 16 | 0 | 7.785528 | -4.919668 | -2.010907 |
| 34 | 16 | 0 | 11.411714 | -1.446441 | 3.009852 |
| 35 | 6 | 0 | 7.744810 | -3.305142 | -1.266066 |
| 36 | 6 | 0 | 6.699265 | 1.846735 | 0.049854 |
| 37 | 6 | 0 | 5.770649 | 2.623836 | -0.005570 |
| 38 | 6 | 0 | 4.670904 | 3.531431 | -0.051397 |
| 39 | 6 | 0 | 3.548731 | 3.256420 | -0.849484 |
| 40 | 6 | 0 | 4.693833 | 4.716235 | 0.701269 |
| 41 | 6 | 0 | 2.470566 | 4.130478 | -0.873494 |
| 42 | 1 | 0 | 3.540737 | 2.354682 | -1.452277 |
| 43 | 6 | 0 | 3.611685 | 5.583927 | 0.671973 |
| 44 | 1 | 0 | 5.567458 | 4.945535 | 1.301082 |
| 45 | 6 | 0 | 2.480493 | 5.292894 | -0.096588 |
| 46 | 1 | 0 | 1.605811 | 3.917523 | -1.496406 |
| 47 | 1 | 0 | 3.648121 | 6.503624 | 1.251666 |
| 48 | 1 | 0 | -0.622044 | 2.891980 | 5.571299 |
| 49 | 6 | 0 | -0.868179 | 3.783258 | 5.003121 |
| 50 | 6 | 0 | 0.044252 | 4.284344 | 4.079701 |
| 51 | 6 | 0 | -2.089152 | 4.423814 | 5.193345 |
| 52 | 6 | 0 | -0.250626 | 5.437387 | 3.353699 |
| 53 | 1 | 0 | 0.988213 | 3.772345 | 3.915394 |
| 54 | 6 | 0 | -2.385970 | 5.580372 | 4.473803 |
| 55 | 1 | 0 | -2.806790 | 4.028304 | 5.905389 |
| 56 | 6 | 0 | 0.751567 | 5.959608 | 2.359032 |
| 57 | 6 | 0 | -1.466078 | 6.093675 | 3.564812 |
| 58 | 1 | 0 | -3.333933 | 6.086084 | 4.628377 |
| 59 | 7 | 0 | 0.268829 | 5.832793 | 0.946383 |
| 60 | 1 | 0 | 0.964750 | 7.023170 | 2.513404 |
| 61 | 1 | 0 | 1.688222 | 5.404217 | 2.429410 |
| 62 | 1 | 0 | -1.700251 | 6.994943 | 3.002995 |
| 63 | 6 | 0 | 1.291119 | 6.212338 | -0.089645 |
| 64 | 1 | 0 | -0.555974 | 6.451809 | 0.830509 |
| 65 | 1 | 0 | -0.084464 | 4.868938 | 0.791712 |
| 66 | 1 | 0 | 0.758368 | 6.210876 | -1.044051 |
| 67 | 1 | 0 | 1.595304 | 7.236948 | 0.145804 |
| 68 | 1 | 0 | -3.664679 | 0.454090 | 6.210006 |
| 69 | 6 | 0 | -2.745872 | 0.411177 | 5.599197 |
| 70 | 7 | 0 | -2.954509 | -0.292897 | 4.345617 |
| 71 | 1 | 0 | -1.966761 | -0.091904 | 6.177062 |
| 72 | 1 | 0 | -2.422224 | 1.433611 | 5.387950 |
| 73 | 6 | 0 | -3.457133 | -1.643016 | 4.537447 |
| 74 | 6 | 0 | -3.961194 | 0.328611 | 3.505119 |
| 75 | 6 | 0 | -3.849650 | -2.109749 | 3.112576 |
| 76 | 1 | 0 | -2.701696 | -2.289838 | 4.991651 |
| 77 | 1 | 0 | -4.355332 | -1.648426 | 5.182520 |
| 78 | 6 | 0 | -4.170634 | -0.735236 | 2.368497 |
| 79 | 1 | 0 | -4.924759 | 0.418029 | 4.046404 |
| 80 | 6 | 0 | -3.579189 | 1.676742 | 2.958755 |
| 81 | 6 | 0 | -4.996112 | -3.117708 | 3.087959 |
| 82 | 6 | 0 | -2.743315 | -2.940515 | 2.461449 |
| 83 | 6 | 0 | -3.306157 | -0.480202 | 1.132585 |
| 84 | 6 | 0 | -5.557674 | -0.642012 | 1.747067 |
| 85 | 6 | 0 | -2.277254 | 1.895693 | 2.500000 |
| 86 | 6 | 0 | -4.540809 | 2.652854 | 2.732706 |
| 87 | 6 | 0 | -6.274082 | -2.816154 | 2.689825 |
| 88 | 6 | 0 | -4.486840 | -4.442963 | 2.868621 |
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| 90 | 6 | 0 | -3.092772 | -4.333159 | 2.484880 |
| 91 | 6 | 0 | -4.095661 | 0.112744 | 0.089228 |
| 92 | 6 | 0 | -2.190074 | -1.203307 | 0.801625 |
| 93 | 6 | 0 | -5.491426 | 0.009923 | 0.469117 |
| 94 | 6 | 0 | -6.563965 | -1.538415 | 1.997177 |
| 95 | 6 | 0 | -1.971073 | 3.030110 | 1.773743 |
| 96 | 1 | 0 | -1.510420 | 1.145798 | 2.674419 |
| 97 | 6 | 0 | -4.230623 | 3.822666 | 2.037748 |
| 98 | 1 | 0 | -5.558723 | 2.495400 | 3.078446 |
| 99 | 6 | 0 | -7.106124 | -3.830170 | 2.086857 |
| 100 | 6 | 0 | -5.282951 | -5.439973 | 2.314403 |
| 101 | 6 | 0 | -1.343679 | -3.383251 | 0.512636 |
| 102 | 6 | 0 | -2.549765 | -5.227589 | 1.566821 |
| 103 | 6 | 0 | -3.727529 | -0.000594 | -1.248739 |
| 104 | 6 | 0 | -1.805183 | -1.355730 | -0.582339 |
| 105 | 6 | 0 | -6.461697 | -0.212888 | -0.502904 |
| 106 | 6 | 0 | -7.564968 | -1.801305 | 0.991384 |
| 107 | 8 | 0 | -0.705731 | 3.181266 | 1.232575 |
| 108 | 6 | 0 | -2.946404 | 4.010985 | 1.532796 |
| 109 | 1 | 0 | -5.005300 | 4.561368 | 1.875554 |
| 110 | 6 | 0 | -7.902944 | -3.210239 | 1.044743 |
| 111 | 6 | 0 | -6.629657 | -5.125745 | 1.913208 |
| 112 | 6 | 0 | -4.720237 | -6.361925 | 1.342315 |
| 113 | 6 | 0 | -1.651953 | -4.739808 | 0.552837 |
| 114 | 6 | 0 | -1.283405 | -2.696098 | -0.763777 |
| 115 | 6 | 0 | -3.386820 | -6.259191 | 0.978273 |
| 116 | 6 | 0 | -2.548822 | -0.754712 | -1.595371 |
| 117 | 6 | 0 | -4.740744 | -0.246641 | -2.262500 |
| 118 | 6 | 0 | -7.527986 | -1.142658 | -0.234288 |
| 119 | 6 | 0 | -6.074505 | -0.352117 | -1.897003 |
| 120 | 6 | 0 | -0.472072 | 2.313155 | 0.114714 |
| 121 | 8 | 0 | -2.551449 | 5.092262 | 0.796315 |
| 122 | 6 | 0 | -8.185150 | -3.902736 | -0.122787 |
| 123 | 6 | 0 | -6.912854 | -5.845426 | 0.686582 |
| 124 | 6 | 0 | -5.731810 | -6.611717 | 0.333283 |
| 125 | 6 | 0 | -1.928033 | -5.458418 | -0.675923 |
| 126 | 6 | 0 | -1.535621 | -3.385568 | -1.940562 |
| 127 | 6 | 0 | -3.000824 | -6.400781 | -0.412707 |
| 128 | 6 | 0 | -2.822232 | -1.479208 | -2.821786 |
| 129 | 6 | 0 | -4.178753 | -1.164992 | -3.234428 |
| 130 | 6 | 0 | -7.810505 | -1.868759 | -1.457222 |
| 131 | 6 | 0 | -6.911783 | -1.378841 | -2.486863 |
| 132 | 6 | 0 | -1.238545 | 2.768618 | -1.102916 |
| 133 | 1 | 0 | 0.605509 | 2.342668 | -0.063640 |
| 134 | 1 | 0 | -0.767044 | 1.287622 | 0.367956 |
| 135 | 6 | 0 | -3.503891 | 6.134462 | 0.641841 |
| 136 | 6 | 0 | -8.130407 | -3.218141 | -1.402910 |
| 137 | 6 | 0 | -7.673386 | -5.248529 | -0.308830 |
| 138 | 6 | 0 | -5.364628 | -6.746078 | -0.998683 |
| 139 | 6 | 0 | -1.869711 | -4.798134 | -1.895600 |
| 140 | 6 | 0 | -2.328495 | -2.766344 | -2.988949 |
| 141 | 6 | 0 | -3.968142 | -6.636425 | -1.379844 |
| 142 | 6 | 0 | -4.977995 | -2.152152 | -3.796357 |
| 143 | 6 | 0 | -6.374089 | -2.260835 | -3.414963 |
| 144 | 1 | 0 | -2.311833 | 2.834609 | -0.866662 |
| 145 | 1 | 0 | -1.118366 | 2.022803 | -1.903133 |
| 146 | 8 | 0 | -0.746014 | 4.030278 | -1.526925 |
| 147 | 6 | 0 | -2.841423 | 7.274440 | -0.090078 |
| 148 | 1 | 0 | -3.847789 | 6.471816 | 1.628906 |
| 149 | 1 | 0 | -4.368450 | 5.778443 | 0.065770 |
| 150 | 6 | 0 | -7.574294 | -4.136457 | -2.374961 |
| 151 | 6 | 0 | -7.292808 | -5.391504 | -1.698672 |
| 152 | 6 | 0 | -6.162274 | -6.122817 | -2.036832 |
| 153 | 6 | 0 | -2.876460 | -5.047630 | -2.905464 |
| 154 | 6 | 0 | -3.159487 | -3.792797 | -3.582141 |
| 155 | 6 | 0 | -3.903936 | -5.946397 | -2.653843 |
| 156 | 6 | 0 | -4.456614 | -3.493520 | -3.975948 |
| 157 | 6 | 0 | -6.715063 | -3.669663 | -3.360192 |
| 158 | 6 | 0 | -1.494746 | 4.511075 | -2.626586 |
| 159 | 8 | 0 | -1.799917 | 7.781421 | 0.745916 |
| 160 | 1 | 0 | -2.426386 | 6.954140 | -1.051012 |
| 161 | 1 | 0 | -3.581162 | 8.060970 | -0.280218 |
| 162 | 6 | 0 | -5.260202 | -5.628829 | -3.060506 |
| 163 | 6 | 0 | -5.530501 | -4.432201 | -3.707795 |
| 164 | 1 | 0 | -1.715116 | 3.680004 | -3.312289 |
| 165 | 1 | 0 | -2.453622 | 4.927642 | -2.284215 |
| 166 | 6 | 0 | -0.720998 | 5.543292 | -3.411578 |
| 167 | 6 | 0 | -1.470183 | 9.151325 | 0.565419 |
| 168 | 1 | 0 | -1.195641 | 5.666212 | -4.392795 |
| 169 | 1 | 0 | 0.308533 | 5.190843 | -3.563299 |
| 170 | 8 | 0 | -0.729381 | 6.790585 | -2.730401 |
| 171 | 1 | 0 | -2.388105 | 9.752773 | 0.549834 |
| 172 | 1 | 0 | -0.879902 | 9.440461 | 1.440230 |
| 173 | 6 | 0 | -0.673741 | 9.403009 | -0.693115 |
| 174 | 6 | 0 | -0.419056 | 7.890244 | -3.492121 |
| 175 | 1 | 0 | -0.291765 | 10.433693 | -0.696346 |
| 176 | 1 | 0 | 0.185631 | 8.719779 | -0.738597 |
| 177 | 8 | 0 | -1.524415 | 9.182678 | -1.805575 |
| 178 | 6 | 0 | -0.839436 | 9.134316 | -2.999573 |
| 179 | 6 | 0 | 0.266504 | 7.835466 | -4.703743 |
| 180 | 6 | 0 | -0.579438 | 10.296774 | -3.708387 |
| 181 | 6 | 0 | 0.523770 | 9.010010 | -5.411208 |
| 182 | 1 | 0 | 0.610224 | 6.887855 | -5.101192 |
| 183 | 6 | 0 | 0.101597 | 10.239494 | -4.922687 |
| 184 | 1 | 0 | -0.936557 | 11.237575 | -3.301340 |
| 185 | 1 | 0 | 1.057995 | 8.951745 | -6.353207 |
| 186 | 1 | 0 | 0.297124 | 11.148774 | -5.479395 |

**AT2: M06-2X/6-31G(d,p)**

Standard orientation:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -10.639932 | -2.288995 | -2.343584 |
| 2 | 6 | 0 | -11.938832 | -2.725070 | -2.121016 |
| 3 | 6 | 0 | -12.791919 | -2.046179 | -1.245940 |
| 4 | 6 | 0 | -12.323589 | -0.878598 | -0.598300 |
| 5 | 6 | 0 | -11.032850 | -0.427070 | -0.852502 |
| 6 | 6 | 0 | -10.176431 | -1.130761 | -1.711576 |
| 7 | 6 | 0 | -14.187009 | -2.454430 | -0.988580 |
| 8 | 6 | 0 | -13.263665 | -0.171625 | 0.298262 |
| 9 | 6 | 0 | -14.658273 | -0.156569 | -0.196926 |
| 10 | 6 | 0 | -15.126053 | -1.317620 | -0.849326 |
| 11 | 6 | 0 | -16.420359 | -1.328064 | -1.372832 |
| 12 | 1 | 0 | -16.767270 | -2.192743 | -1.929803 |
| 13 | 6 | 0 | -17.256826 | -0.225071 | -1.229739 |
| 14 | 6 | 0 | -16.795514 | 0.917310 | -0.585713 |
| 15 | 6 | 0 | -15.497072 | 0.953692 | -0.086374 |
| 16 | 1 | 0 | -9.990909 | -2.823196 | -3.028695 |
| 17 | 1 | 0 | -12.306212 | -3.587515 | -2.667483 |
| 18 | 1 | 0 | -10.680552 | 0.502497 | -0.415004 |
| 19 | 1 | 0 | -18.258862 | -0.252982 | -1.644561 |
| 20 | 1 | 0 | -17.433948 | 1.789524 | -0.493303 |
| 21 | 1 | 0 | -15.120792 | 1.868316 | 0.361814 |
| 22 | 16 | 0 | -11.254504 | 0.197452 | 2.173681 |
| 23 | 6 | 0 | -12.955997 | 1.018095 | 4.026172 |
| 24 | 6 | 0 | -11.698019 | 0.638751 | 3.812420 |
| 25 | 1 | 0 | -13.353712 | 1.330391 | 4.983533 |
| 26 | 1 | 0 | -10.923849 | 0.592514 | 4.567471 |
| 27 | 6 | 0 | -14.556280 | -3.747389 | -0.794448 |
| 28 | 16 | 0 | -16.203273 | -4.236516 | -0.346662 |
| 29 | 6 | 0 | -14.547674 | -6.295022 | -0.190641 |
| 30 | 6 | 0 | -15.798299 | -5.897060 | 0.032139 |
| 31 | 1 | 0 | -14.172224 | -7.295729 | -0.019791 |
| 32 | 1 | 0 | -16.592439 | -6.527138 | 0.411784 |
| 33 | 16 | 0 | -14.048733 | 1.042567 | 2.658107 |
| 34 | 16 | 0 | -13.426190 | -5.117587 | -0.840512 |
| 35 | 6 | 0 | -12.901762 | 0.318438 | 1.508210 |
| 36 | 6 | 0 | -8.854421 | -0.632159 | -1.931652 |
| 37 | 6 | 0 | -7.743646 | -0.164240 | -2.056514 |
| 38 | 6 | 0 | -6.441542 | 0.422350 | -2.102345 |
| 39 | 6 | 0 | -6.300566 | 1.816133 | -2.068892 |
| 40 | 6 | 0 | -5.290260 | -0.380338 | -2.116319 |
| 41 | 6 | 0 | -5.036950 | 2.388427 | -2.015305 |
| 42 | 1 | 0 | -7.189640 | 2.436996 | -2.067998 |
| 43 | 6 | 0 | -4.030714 | 0.199583 | -2.057894 |
| 44 | 1 | 0 | -5.400754 | -1.459216 | -2.162121 |
| 45 | 6 | 0 | -3.893023 | 1.587238 | -1.988284 |
| 46 | 1 | 0 | -4.934780 | 3.471124 | -1.986924 |
| 47 | 1 | 0 | -3.142883 | -0.425433 | -2.038278 |
| 48 | 1 | 0 | -4.577784 | 6.877562 | -1.226826 |
| 49 | 6 | 0 | -3.545120 | 6.569366 | -1.354870 |
| 50 | 6 | 0 | -3.102939 | 5.383308 | -0.776370 |
| 51 | 6 | 0 | -2.667850 | 7.361032 | -2.092589 |
| 52 | 6 | 0 | -1.777108 | 4.969878 | -0.941203 |
| 53 | 1 | 0 | -3.803724 | 4.770063 | -0.215580 |
| 54 | 6 | 0 | -1.347816 | 6.955424 | -2.259502 |
| 55 | 1 | 0 | -3.014684 | 8.286984 | -2.538816 |
| 56 | 6 | 0 | -1.243352 | 3.709262 | -0.306529 |
| 57 | 6 | 0 | -0.908321 | 5.761483 | -1.693231 |
| 58 | 1 | 0 | -0.660465 | 7.562195 | -2.839393 |
| 59 | 7 | 0 | -2.149305 | 2.522596 | -0.464673 |
| 60 | 1 | 0 | -0.289527 | 3.434825 | -0.758785 |
| 61 | 1 | 0 | -1.104710 | 3.822304 | 0.770918 |
| 62 | 1 | 0 | 0.120445 | 5.441328 | -1.836022 |
| 63 | 6 | 0 | -2.538184 | 2.231413 | -1.893037 |
| 64 | 1 | 0 | -2.994465 | 2.642805 | 0.122993 |
| 65 | 1 | 0 | -1.663439 | 1.692232 | -0.083371 |
| 66 | 1 | 0 | -2.534396 | 3.187661 | -2.418869 |
| 67 | 1 | 0 | -1.744245 | 1.607583 | -2.302898 |
| 68 | 1 | 0 | 6.924937 | 2.949575 | -3.353065 |
| 69 | 6 | 0 | 5.847125 | 3.055005 | -3.535135 |
| 70 | 7 | 0 | 5.016950 | 2.140909 | -2.751160 |
| 71 | 1 | 0 | 5.657592 | 2.879485 | -4.596392 |
| 72 | 1 | 0 | 5.555783 | 4.082871 | -3.307030 |
| 73 | 6 | 0 | 5.264661 | 0.738584 | -3.023452 |
| 74 | 6 | 0 | 5.172668 | 2.290810 | -1.312837 |
| 75 | 6 | 0 | 6.439937 | 0.268238 | -2.105749 |
| 76 | 1 | 0 | 4.379693 | 0.151980 | -2.747971 |
| 77 | 1 | 0 | 5.470887 | 0.567652 | -4.082661 |
| 78 | 6 | 0 | 6.328473 | 1.266409 | -0.866836 |
| 79 | 1 | 0 | 5.522981 | 3.305003 | -1.094042 |
| 80 | 6 | 0 | 3.853629 | 2.102028 | -0.576271 |
| 81 | 6 | 0 | 7.808038 | 0.258713 | -2.794707 |
| 82 | 6 | 0 | 6.306855 | -1.209759 | -1.761871 |
| 83 | 6 | 0 | 6.107447 | 0.562640 | 0.470836 |
| 84 | 6 | 0 | 7.623866 | 2.020944 | -0.553231 |
| 85 | 6 | 0 | 2.692981 | 1.722289 | -1.246191 |
| 86 | 6 | 0 | 3.758080 | 2.377453 | 0.787710 |
| 87 | 6 | 0 | 8.808192 | 1.162608 | -2.545234 |
| 88 | 6 | 0 | 8.164291 | -1.083859 | -3.167863 |
| 89 | 6 | 0 | 5.861930 | -1.678652 | -0.553125 |
| 90 | 6 | 0 | 7.231126 | -1.992131 | -2.531113 |
| 91 | 6 | 0 | 6.892191 | 1.187809 | 1.501141 |
| 92 | 6 | 0 | 5.768519 | -0.759876 | 0.603745 |
| 93 | 6 | 0 | 7.826210 | 2.096809 | 0.867386 |
| 94 | 6 | 0 | 8.711053 | 2.077207 | -1.385479 |
| 95 | 6 | 0 | 1.491938 | 1.570026 | -0.566073 |
| 96 | 1 | 0 | 2.709072 | 1.582036 | -2.322673 |
| 97 | 6 | 0 | 2.558491 | 2.239132 | 1.478321 |
| 98 | 1 | 0 | 4.633094 | 2.716405 | 1.334185 |
| 99 | 6 | 0 | 10.193942 | 0.784695 | -2.684927 |
| 100 | 6 | 0 | 9.493774 | -1.461917 | -3.330588 |
| 101 | 6 | 0 | 6.319592 | -2.956782 | -0.061897 |
| 102 | 6 | 0 | 7.659205 | -3.239245 | -2.086529 |
| 103 | 6 | 0 | 7.260915 | 0.498864 | 2.651488 |
| 104 | 6 | 0 | 6.168594 | -1.502260 | 1.776954 |
| 105 | 6 | 0 | 9.096627 | 2.272974 | 1.408010 |
| 106 | 6 | 0 | 10.039329 | 2.236387 | -0.843218 |
| 107 | 8 | 0 | 0.351145 | 1.224389 | -1.265493 |
| 108 | 6 | 0 | 1.408035 | 1.815519 | 0.810532 |
| 109 | 1 | 0 | 2.540416 | 2.463737 | 2.536761 |
| 110 | 6 | 0 | 10.954570 | 1.444546 | -1.641532 |
| 111 | 6 | 0 | 10.538384 | -0.501944 | -3.084994 |
| 112 | 6 | 0 | 9.945143 | -2.757391 | -2.850776 |
| 113 | 6 | 0 | 7.192182 | -3.734270 | -0.817689 |
| 114 | 6 | 0 | 6.505799 | -2.853413 | 1.372638 |
| 115 | 6 | 0 | 9.050660 | -3.625333 | -2.244733 |
| 116 | 6 | 0 | 6.888542 | -0.885006 | 2.794542 |
| 117 | 6 | 0 | 8.591957 | 0.673356 | 3.206786 |
| 118 | 6 | 0 | 10.234750 | 2.348020 | 0.529403 |
| 119 | 6 | 0 | 9.487490 | 1.539175 | 2.599195 |
| 120 | 6 | 0 | 0.265676 | -0.162844 | -1.586125 |
| 121 | 8 | 0 | 0.183526 | 1.637766 | 1.407486 |
| 122 | 6 | 0 | 12.019237 | 0.792844 | -1.037880 |
| 123 | 6 | 0 | 11.643329 | -1.189786 | -2.445223 |
| 124 | 6 | 0 | 11.277148 | -2.587289 | -2.301701 |
| 125 | 6 | 0 | 8.291168 | -4.428049 | -0.174427 |
| 126 | 6 | 0 | 7.549996 | -3.525397 | 1.990951 |
| 127 | 6 | 0 | 9.441352 | -4.361972 | -1.058148 |
| 128 | 6 | 0 | 7.986972 | -1.582153 | 3.435241 |
| 129 | 6 | 0 | 9.041685 | -0.617527 | 3.690896 |
| 130 | 6 | 0 | 11.340193 | 1.656732 | 1.163815 |
| 131 | 6 | 0 | 10.878672 | 1.157573 | 2.446424 |
| 132 | 6 | 0 | -0.251850 | -0.939236 | -0.401018 |
| 133 | 1 | 0 | -0.434235 | -0.246091 | -2.423533 |
| 134 | 1 | 0 | 1.243156 | -0.542931 | -1.903632 |
| 135 | 6 | 0 | 0.112415 | 2.035017 | 2.770852 |
| 136 | 6 | 0 | 12.212264 | 0.895559 | 0.398109 |
| 137 | 6 | 0 | 12.367484 | -0.557228 | -1.444458 |
| 138 | 6 | 0 | 11.652092 | -3.288806 | -1.164020 |
| 139 | 6 | 0 | 8.466298 | -4.326819 | 1.198963 |
| 140 | 6 | 0 | 8.311487 | -2.872922 | 3.041197 |
| 141 | 6 | 0 | 10.713645 | -4.195941 | -0.527952 |
| 142 | 6 | 0 | 10.371432 | -0.987087 | 3.540779 |
| 143 | 6 | 0 | 11.310014 | -0.079999 | 2.904465 |
| 144 | 1 | 0 | 0.399069 | -0.776690 | 0.470654 |
| 145 | 1 | 0 | -0.270166 | -2.015108 | -0.627980 |
| 146 | 8 | 0 | -1.561093 | -0.472699 | -0.130180 |
| 147 | 6 | 0 | -1.298379 | 1.897403 | 3.282710 |
| 148 | 1 | 0 | 0.425416 | 3.083066 | 2.866359 |
| 149 | 1 | 0 | 0.778687 | 1.412159 | 3.381444 |
| 150 | 6 | 0 | 12.666723 | -0.392547 | 0.878822 |
| 151 | 6 | 0 | 12.762200 | -1.290765 | -0.259848 |
| 152 | 6 | 0 | 12.412084 | -2.626782 | -0.121207 |
| 153 | 6 | 0 | 9.793999 | -4.158452 | 1.751869 |
| 154 | 6 | 0 | 9.698835 | -3.260270 | 2.890594 |
| 155 | 6 | 0 | 10.893689 | -4.092665 | 0.907235 |
| 156 | 6 | 0 | 10.707322 | -2.337410 | 3.132759 |
| 157 | 6 | 0 | 12.225206 | -0.871146 | 2.104803 |
| 158 | 6 | 0 | -2.083344 | -1.048206 | 1.047917 |
| 159 | 8 | 0 | -2.144604 | 2.766676 | 2.570285 |
| 160 | 1 | 0 | -1.661289 | 0.864069 | 3.204160 |
| 161 | 1 | 0 | -1.283661 | 2.163481 | 4.350762 |
| 162 | 6 | 0 | 11.944315 | -3.123930 | 1.159220 |
| 163 | 6 | 0 | 11.853937 | -2.267003 | 2.246321 |
| 164 | 1 | 0 | -1.904137 | -2.133831 | 1.051986 |
| 165 | 1 | 0 | -1.574890 | -0.623369 | 1.923096 |
| 166 | 6 | 0 | -3.575463 | -0.842806 | 1.110464 |
| 167 | 6 | 0 | -3.392030 | 2.929819 | 3.214550 |
| 168 | 1 | 0 | -3.964539 | -1.350348 | 2.003644 |
| 169 | 1 | 0 | -4.040038 | -1.287024 | 0.221981 |
| 170 | 8 | 0 | -3.879567 | 0.542007 | 1.164673 |
| 171 | 1 | 0 | -3.877789 | 1.954142 | 3.364504 |
| 172 | 1 | 0 | -3.256400 | 3.405973 | 4.197104 |
| 173 | 6 | 0 | -4.247135 | 3.807360 | 2.335253 |
| 174 | 6 | 0 | -5.217288 | 0.846584 | 1.174772 |
| 175 | 1 | 0 | -5.177191 | 4.079565 | 2.845398 |
| 176 | 1 | 0 | -3.699543 | 4.717842 | 2.072192 |
| 177 | 8 | 0 | -4.543705 | 3.153799 | 1.098318 |
| 178 | 6 | 0 | -5.553595 | 2.206800 | 1.174245 |
| 179 | 6 | 0 | -6.247047 | -0.095824 | 1.191731 |
| 180 | 6 | 0 | -6.878584 | 2.614432 | 1.187916 |
| 181 | 6 | 0 | -7.578194 | 0.318864 | 1.202598 |
| 182 | 1 | 0 | -6.030521 | -1.156343 | 1.178220 |
| 183 | 6 | 0 | -7.901775 | 1.670184 | 1.202647 |
| 184 | 1 | 0 | -7.091309 | 3.679312 | 1.163764 |
| 185 | 1 | 0 | -8.366220 | -0.428050 | 1.188900 |
| 186 | 1 | 0 | -8.940245 | 1.983964 | 1.208697 |

**AT3: M06-2X/6-31G(d,p)**

Standard orientation:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -1.240255 | 5.467852 | 3.331802 |
| 2 | 6 | 0 | -0.157038 | 6.275588 | 3.009759 |
| 3 | 6 | 0 | 0.249428 | 6.454293 | 1.683068 |
| 4 | 6 | 0 | -0.487584 | 5.828339 | 0.650391 |
| 5 | 6 | 0 | -1.595129 | 5.056918 | 0.977368 |
| 6 | 6 | 0 | -1.966921 | 4.845597 | 2.312326 |
| 7 | 6 | 0 | 1.390090 | 7.300098 | 1.282379 |
| 8 | 6 | 0 | -0.058299 | 6.054802 | -0.746514 |
| 9 | 6 | 0 | 0.429322 | 7.429214 | -1.000443 |
| 10 | 6 | 0 | 1.161048 | 8.058828 | 0.030648 |
| 11 | 6 | 0 | 1.592895 | 9.374508 | -0.149013 |
| 12 | 1 | 0 | 2.099966 | 9.888515 | 0.661180 |
| 13 | 6 | 0 | 1.339989 | 10.054042 | -1.336670 |
| 14 | 6 | 0 | 0.619915 | 9.433420 | -2.351078 |
| 15 | 6 | 0 | 0.154771 | 8.134028 | -2.174105 |
| 16 | 1 | 0 | -1.535888 | 5.331356 | 4.366084 |
| 17 | 1 | 0 | 0.364347 | 6.798780 | 3.804578 |
| 18 | 1 | 0 | -2.209185 | 4.619429 | 0.196660 |
| 19 | 1 | 0 | 1.684838 | 11.075686 | -1.455353 |
| 20 | 1 | 0 | 0.396912 | 9.965398 | -3.269733 |
| 21 | 1 | 0 | -0.459606 | 7.677917 | -2.944188 |
| 22 | 16 | 0 | -0.491096 | 3.375216 | -1.333995 |
| 23 | 6 | 0 | 0.560178 | 3.588181 | -3.753981 |
| 24 | 6 | 0 | 0.075522 | 2.727892 | -2.860715 |
| 25 | 1 | 0 | 0.936029 | 3.317136 | -4.732557 |
| 26 | 1 | 0 | 0.004745 | 1.656159 | -3.007026 |
| 27 | 6 | 0 | 2.579479 | 7.298829 | 1.939850 |
| 28 | 16 | 0 | 4.003141 | 8.204804 | 1.388082 |
| 29 | 6 | 0 | 4.642686 | 6.600207 | 3.392179 |
| 30 | 6 | 0 | 5.130575 | 7.458405 | 2.499018 |
| 31 | 1 | 0 | 5.225007 | 6.086990 | 4.146564 |
| 32 | 1 | 0 | 6.170840 | 7.746774 | 2.418148 |
| 33 | 16 | 0 | 0.574512 | 5.286755 | -3.331423 |
| 34 | 16 | 0 | 2.918449 | 6.300148 | 3.369227 |
| 35 | 6 | 0 | -0.034107 | 5.066825 | -1.674318 |
| 36 | 6 | 0 | -3.068795 | 3.971038 | 2.558260 |
| 37 | 6 | 0 | -3.980484 | 3.175814 | 2.635211 |
| 38 | 6 | 0 | -4.967002 | 2.147849 | 2.542139 |
| 39 | 6 | 0 | -5.290261 | 1.671529 | 1.262772 |
| 40 | 6 | 0 | -5.552187 | 1.543138 | 3.663182 |
| 41 | 6 | 0 | -6.138265 | 0.590077 | 1.095867 |
| 42 | 1 | 0 | -4.842962 | 2.147243 | 0.402223 |
| 43 | 6 | 0 | -6.412392 | 0.464933 | 3.493427 |
| 44 | 1 | 0 | -5.312379 | 1.905957 | 4.656406 |
| 45 | 6 | 0 | -6.703394 | -0.024488 | 2.216863 |
| 46 | 1 | 0 | -6.309604 | 0.209675 | 0.089625 |
| 47 | 1 | 0 | -6.852555 | -0.010037 | 4.366116 |
| 48 | 1 | 0 | -4.043107 | -6.985589 | 1.551812 |
| 49 | 6 | 0 | -4.870649 | -6.494527 | 1.050688 |
| 50 | 6 | 0 | -5.545863 | -5.452238 | 1.679757 |
| 51 | 6 | 0 | -5.261277 | -6.908573 | -0.219107 |
| 52 | 6 | 0 | -6.613533 | -4.819821 | 1.039770 |
| 53 | 1 | 0 | -5.242880 | -5.130585 | 2.673662 |
| 54 | 6 | 0 | -6.320861 | -6.274867 | -0.866335 |
| 55 | 1 | 0 | -4.739738 | -7.725555 | -0.706949 |
| 56 | 6 | 0 | -7.358382 | -3.709085 | 1.726100 |
| 57 | 6 | 0 | -6.995473 | -5.233578 | -0.237122 |
| 58 | 1 | 0 | -6.630585 | -6.601973 | -1.853771 |
| 59 | 7 | 0 | -6.811818 | -2.353780 | 1.391639 |
| 60 | 1 | 0 | -8.413126 | -3.696294 | 1.436428 |
| 61 | 1 | 0 | -7.300025 | -3.808640 | 2.812924 |
| 62 | 1 | 0 | -7.823893 | -4.737123 | -0.737979 |
| 63 | 6 | 0 | -7.567344 | -1.242986 | 2.059256 |
| 64 | 1 | 0 | -6.856900 | -2.209913 | 0.364517 |
| 65 | 1 | 0 | -5.795778 | -2.295016 | 1.616617 |
| 66 | 1 | 0 | -8.452631 | -1.057531 | 1.441390 |
| 67 | 1 | 0 | -7.902631 | -1.608753 | 3.032674 |
| 68 | 1 | 0 | -0.832620 | -7.377089 | 2.538635 |
| 69 | 6 | 0 | -0.978948 | -6.382890 | 2.996258 |
| 70 | 7 | 0 | -0.086154 | -5.384086 | 2.433493 |
| 71 | 1 | 0 | -0.799596 | -6.465992 | 4.070717 |
| 72 | 1 | 0 | -2.017095 | -6.076363 | 2.842761 |
| 73 | 6 | 0 | 1.313554 | -5.708115 | 2.639322 |
| 74 | 6 | 0 | -0.201992 | -5.248863 | 0.990998 |
| 75 | 6 | 0 | 2.073788 | -4.675465 | 1.772286 |
| 76 | 1 | 0 | 1.588016 | -5.643866 | 3.695719 |
| 77 | 1 | 0 | 1.546809 | -6.727489 | 2.278780 |
| 78 | 6 | 0 | 1.020718 | -4.332853 | 0.621823 |
| 79 | 1 | 0 | -0.035577 | -6.224980 | 0.492321 |
| 80 | 6 | 0 | -1.523217 | -4.687045 | 0.540104 |
| 81 | 6 | 0 | 3.414686 | -5.198127 | 1.268466 |
| 82 | 6 | 0 | 2.539197 | -3.466365 | 2.584151 |
| 83 | 6 | 0 | 0.658780 | -2.848926 | 0.526520 |
| 84 | 6 | 0 | 1.520811 | -4.579339 | -0.796616 |
| 85 | 6 | 0 | -2.179533 | -3.746885 | 1.340287 |
| 86 | 6 | 0 | -2.054197 | -5.003952 | -0.704405 |
| 87 | 6 | 0 | 3.646784 | -5.591528 | -0.023976 |
| 88 | 6 | 0 | 4.487591 | -4.641273 | 2.041696 |
| 89 | 6 | 0 | 1.954495 | -2.228542 | 2.540382 |
| 90 | 6 | 0 | 3.945865 | -3.570719 | 2.856383 |
| 91 | 6 | 0 | 0.552684 | -2.453969 | -0.851027 |
| 92 | 6 | 0 | 0.981330 | -1.907791 | 1.470065 |
| 93 | 6 | 0 | 1.088171 | -3.524620 | -1.670242 |
| 94 | 6 | 0 | 2.670628 | -5.267647 | -1.090671 |
| 95 | 6 | 0 | -3.326908 | -3.127622 | 0.885833 |
| 96 | 1 | 0 | -1.766218 | -3.492929 | 2.312623 |
| 97 | 6 | 0 | -3.219792 | -4.387982 | -1.165817 |
| 98 | 1 | 0 | -1.551872 | -5.734247 | -1.333105 |
| 99 | 6 | 0 | 4.967810 | -5.467677 | -0.592526 |
| 100 | 6 | 0 | 5.772784 | -4.539505 | 1.519835 |
| 101 | 6 | 0 | 2.742164 | -1.042486 | 2.779371 |
| 102 | 6 | 0 | 4.715170 | -2.441459 | 3.118132 |
| 103 | 6 | 0 | 0.729119 | -1.127431 | -1.237849 |
| 104 | 6 | 0 | 1.194193 | -0.531000 | 1.086281 |
| 105 | 6 | 0 | 1.783947 | -3.226711 | -2.838690 |
| 106 | 6 | 0 | 3.419020 | -4.955565 | -2.284920 |
| 107 | 8 | 0 | -3.990027 | -2.190277 | 1.651342 |
| 108 | 6 | 0 | -3.858755 | -3.438882 | -0.376412 |
| 109 | 1 | 0 | -3.632268 | -4.664837 | -2.129390 |
| 110 | 6 | 0 | 4.832466 | -5.078853 | -1.983226 |
| 111 | 6 | 0 | 6.019787 | -4.964335 | 0.166740 |
| 112 | 6 | 0 | 6.567840 | -3.352076 | 1.779825 |
| 113 | 6 | 0 | 4.097774 | -1.141784 | 3.078789 |
| 114 | 6 | 0 | 2.275549 | 0.004644 | 1.890562 |
| 115 | 6 | 0 | 6.052151 | -2.329177 | 2.559781 |
| 116 | 6 | 0 | 1.057735 | -0.136553 | -0.243011 |
| 117 | 6 | 0 | 1.469693 | -0.817696 | -2.450981 |
| 118 | 6 | 0 | 2.979898 | -3.962654 | -3.155380 |
| 119 | 6 | 0 | 1.984934 | -1.841761 | -3.231021 |
| 120 | 6 | 0 | -3.236434 | -1.009225 | 1.973862 |
| 121 | 8 | 0 | -5.001844 | -2.786940 | -0.713286 |
| 122 | 6 | 0 | 5.745701 | -4.206623 | -2.555470 |
| 123 | 6 | 0 | 6.968229 | -4.042150 | -0.426915 |
| 124 | 6 | 0 | 7.309259 | -3.044300 | 0.572197 |
| 125 | 6 | 0 | 5.042434 | -0.212586 | 2.489282 |
| 126 | 6 | 0 | 3.177455 | 0.900783 | 1.334953 |
| 127 | 6 | 0 | 6.253802 | -0.946733 | 2.170323 |
| 128 | 6 | 0 | 2.009241 | 0.789201 | -0.826609 |
| 129 | 6 | 0 | 2.264320 | 0.367730 | -2.191935 |
| 130 | 6 | 0 | 3.932929 | -3.041753 | -3.745517 |
| 131 | 6 | 0 | 3.316565 | -1.728320 | -3.793347 |
| 132 | 6 | 0 | -2.555984 | -0.394303 | 0.762037 |
| 133 | 1 | 0 | -3.963492 | -0.327716 | 2.414897 |
| 134 | 1 | 0 | -2.472867 | -1.243137 | 2.725757 |
| 135 | 6 | 0 | -5.427646 | -2.810575 | -2.063485 |
| 136 | 6 | 0 | 5.284020 | -3.159772 | -3.450409 |
| 137 | 6 | 0 | 6.834566 | -3.670964 | -1.757464 |
| 138 | 6 | 0 | 7.499589 | -1.721891 | 0.195567 |
| 139 | 6 | 0 | 4.593423 | 0.787224 | 1.637886 |
| 140 | 6 | 0 | 3.045020 | 1.297556 | -0.055659 |
| 141 | 6 | 0 | 6.960031 | -0.649572 | 1.012364 |
| 142 | 6 | 0 | 3.540112 | 0.478015 | -2.727743 |
| 143 | 6 | 0 | 4.078350 | -0.594116 | -3.544329 |
| 144 | 1 | 0 | -1.684571 | -1.000539 | 0.470745 |
| 145 | 1 | 0 | -2.192014 | 0.606316 | 1.049870 |
| 146 | 8 | 0 | -3.475645 | -0.335696 | -0.304991 |
| 147 | 6 | 0 | -6.331928 | -1.618078 | -2.243806 |
| 148 | 1 | 0 | -5.940305 | -3.756560 | -2.281109 |
| 149 | 1 | 0 | -4.569135 | -2.705282 | -2.739163 |
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| 151 | 6 | 0 | 7.037297 | -2.292015 | -2.149918 |
| 152 | 6 | 0 | 7.361353 | -1.337936 | -1.195729 |
| 153 | 6 | 0 | 5.332675 | 1.099789 | 0.432334 |
| 154 | 6 | 0 | 4.375922 | 1.414995 | -0.614902 |
| 155 | 6 | 0 | 6.489312 | 0.396155 | 0.124734 |
| 156 | 6 | 0 | 4.619534 | 1.013865 | -1.921256 |
| 157 | 6 | 0 | 5.491087 | -0.720000 | -3.242914 |
| 158 | 6 | 0 | -2.930236 | 0.176887 | -1.504751 |
| 159 | 8 | 0 | -7.441270 | -1.740530 | -1.340502 |
| 160 | 1 | 0 | -5.779511 | -0.697822 | -2.039451 |
| 161 | 1 | 0 | -6.703267 | -1.585468 | -3.275402 |
| 162 | 6 | 0 | 6.738972 | -0.027521 | -1.240567 |
| 163 | 6 | 0 | 5.826142 | 0.274418 | -2.240331 |
| 164 | 1 | 0 | -1.832476 | 0.215266 | -1.459493 |
| 165 | 1 | 0 | -3.212254 | -0.499197 | -2.322022 |
| 166 | 6 | 0 | -3.479893 | 1.560477 | -1.786314 |
| 167 | 6 | 0 | -8.613362 | -1.037509 | -1.733463 |
| 168 | 1 | 0 | -3.013961 | 2.000083 | -2.679435 |
| 169 | 1 | 0 | -3.267698 | 2.221237 | -0.934475 |
| 170 | 8 | 0 | -4.875711 | 1.405308 | -1.971988 |
| 171 | 1 | 0 | -8.777563 | -1.186820 | -2.808129 |
| 172 | 1 | 0 | -9.451667 | -1.489814 | -1.193520 |
| 173 | 6 | 0 | -8.565938 | 0.453064 | -1.437448 |
| 174 | 6 | 0 | -5.668533 | 2.512378 | -1.907734 |
| 175 | 1 | 0 | -9.483542 | 0.912738 | -1.830080 |
| 176 | 1 | 0 | -8.514063 | 0.654055 | -0.356866 |
| 177 | 8 | 0 | -7.409561 | 0.946105 | -2.074526 |
| 178 | 6 | 0 | -7.053699 | 2.256784 | -1.889905 |
| 179 | 6 | 0 | -5.207223 | 3.819095 | -1.811132 |
| 180 | 6 | 0 | -7.951466 | 3.297876 | -1.724142 |
| 181 | 6 | 0 | -6.121053 | 4.865841 | -1.655748 |
| 182 | 1 | 0 | -4.143520 | 4.029255 | -1.852021 |
| 183 | 6 | 0 | -7.481451 | 4.608344 | -1.599537 |
| 184 | 1 | 0 | -9.017074 | 3.096878 | -1.700523 |
| 185 | 1 | 0 | -5.752584 | 5.882184 | -1.573528 |
| 186 | 1 | 0 | -8.188913 | 5.419255 | -1.469533 |

**AT4: M06-2X/6-31G(d,p)**

Standard orientation:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -6.283072 | -0.900301 | -3.269618 |
| 2 | 6 | 0 | -7.097165 | -1.996994 | -3.023500 |
| 3 | 6 | 0 | -7.603093 | -2.251018 | -1.744509 |
| 4 | 6 | 0 | -7.296497 | -1.356107 | -0.692251 |
| 5 | 6 | 0 | -6.503438 | -0.243257 | -0.950554 |
| 6 | 6 | 0 | -5.979868 | -0.013039 | -2.232070 |
| 7 | 6 | 0 | -8.484222 | -3.391107 | -1.429877 |
| 8 | 6 | 0 | -7.875698 | -1.637914 | 0.638820 |
| 9 | 6 | 0 | -9.252592 | -2.177949 | 0.589212 |
| 10 | 6 | 0 | -9.557524 | -3.071005 | -0.462353 |
| 11 | 6 | 0 | -10.855631 | -3.574614 | -0.570175 |
| 12 | 1 | 0 | -11.116278 | -4.208610 | -1.411960 |
| 13 | 6 | 0 | -11.832459 | -3.236086 | 0.361774 |
| 14 | 6 | 0 | -11.529910 | -2.360586 | 1.398780 |
| 15 | 6 | 0 | -10.249739 | -1.822891 | 1.499539 |
| 16 | 1 | 0 | -5.901309 | -0.709657 | -4.266526 |
| 17 | 1 | 0 | -7.376193 | -2.643979 | -3.848738 |
| 18 | 1 | 0 | -6.311505 | 0.488601 | -0.170576 |
| 19 | 1 | 0 | -12.834620 | -3.639023 | 0.261092 |
| 20 | 1 | 0 | -12.293593 | -2.074478 | 2.114164 |
| 21 | 1 | 0 | -10.036189 | -1.090989 | 2.272725 |
| 22 | 16 | 0 | -5.442297 | -1.054242 | 1.833273 |
| 23 | 6 | 0 | -6.241772 | -1.938092 | 4.197017 |
| 24 | 6 | 0 | -5.181909 | -1.532801 | 3.500511 |
| 25 | 1 | 0 | -6.219385 | -2.245501 | 5.234969 |
| 26 | 1 | 0 | -4.173275 | -1.464008 | 3.887759 |
| 27 | 6 | 0 | -8.260882 | -4.648454 | -1.898347 |
| 28 | 16 | 0 | -9.217394 | -6.059622 | -1.406695 |
| 29 | 6 | 0 | -7.102933 | -6.811346 | -2.807637 |
| 30 | 6 | 0 | -8.145362 | -7.252136 | -2.106133 |
| 31 | 1 | 0 | -6.377998 | -7.441199 | -3.307005 |
| 32 | 1 | 0 | -8.391197 | -8.294642 | -1.948920 |
| 33 | 16 | 0 | -7.795951 | -1.948611 | 3.390023 |
| 34 | 16 | 0 | -6.905011 | -5.078498 | -2.960774 |
| 35 | 6 | 0 | -7.162135 | -1.520878 | 1.785638 |
| 36 | 6 | 0 | -5.175295 | 1.148589 | -2.443541 |
| 37 | 6 | 0 | -4.511544 | 2.156004 | -2.560900 |
| 38 | 6 | 0 | -3.727345 | 3.349203 | -2.516072 |
| 39 | 6 | 0 | -3.364787 | 3.835378 | -1.252232 |
| 40 | 6 | 0 | -3.312427 | 4.042224 | -3.661219 |
| 41 | 6 | 0 | -2.603705 | 4.984302 | -1.118421 |
| 42 | 1 | 0 | -3.697431 | 3.295475 | -0.377489 |
| 43 | 6 | 0 | -2.570306 | 5.209644 | -3.525168 |
| 44 | 1 | 0 | -3.581178 | 3.669856 | -4.643541 |
| 45 | 6 | 0 | -2.221492 | 5.692590 | -2.260611 |
| 46 | 1 | 0 | -2.297228 | 5.297614 | -0.119755 |
| 47 | 1 | 0 | -2.264402 | 5.756386 | -4.413072 |
| 48 | 1 | 0 | 5.274735 | 6.500850 | -1.504266 |
| 49 | 6 | 0 | 4.444149 | 6.966860 | -0.984410 |
| 50 | 6 | 0 | 3.213893 | 7.108618 | -1.620649 |
| 51 | 6 | 0 | 4.608594 | 7.430298 | 0.318094 |
| 52 | 6 | 0 | 2.141475 | 7.703093 | -0.951604 |
| 53 | 1 | 0 | 3.082261 | 6.750525 | -2.639399 |
| 54 | 6 | 0 | 3.539145 | 8.014054 | 0.993607 |
| 55 | 1 | 0 | 5.570052 | 7.329875 | 0.811232 |
| 56 | 6 | 0 | 0.818869 | 7.879896 | -1.643870 |
| 57 | 6 | 0 | 2.306754 | 8.147972 | 0.359695 |
| 58 | 1 | 0 | 3.668972 | 8.377788 | 2.008367 |
| 59 | 7 | 0 | -0.150928 | 6.767393 | -1.379942 |
| 60 | 1 | 0 | 0.326907 | 8.803036 | -1.322153 |
| 61 | 1 | 0 | 0.949629 | 7.916854 | -2.728543 |
| 62 | 1 | 0 | 1.467323 | 8.604256 | 0.880864 |
| 63 | 6 | 0 | -1.428496 | 6.962947 | -2.143335 |
| 64 | 1 | 0 | -0.373735 | 6.719858 | -0.365694 |
| 65 | 1 | 0 | 0.261382 | 5.833059 | -1.602673 |
| 66 | 1 | 0 | -1.983380 | 7.744203 | -1.611747 |
| 67 | 1 | 0 | -1.161873 | 7.344768 | -3.131968 |
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| 70 | 7 | 0 | 5.566139 | 2.143617 | -2.707092 |
| 71 | 1 | 0 | 6.189482 | 3.177053 | -4.413260 |
| 72 | 1 | 0 | 5.319977 | 4.156900 | -3.218774 |
| 73 | 6 | 0 | 6.486405 | 1.028404 | -2.855831 |
| 74 | 6 | 0 | 5.427073 | 2.269222 | -1.267372 |
| 75 | 6 | 0 | 5.912864 | -0.063448 | -1.917211 |
| 76 | 1 | 0 | 6.547369 | 0.692533 | -3.894626 |
| 77 | 1 | 0 | 7.501419 | 1.303634 | -2.512774 |
| 78 | 6 | 0 | 5.142116 | 0.788710 | -0.811667 |
| 79 | 1 | 0 | 6.389868 | 2.567477 | -0.804417 |
| 80 | 6 | 0 | 4.345239 | 3.213935 | -0.818797 |
| 81 | 6 | 0 | 6.977820 | -1.002663 | -1.358632 |
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| 83 | 6 | 0 | 3.649300 | 0.468765 | -0.698372 |
| 84 | 6 | 0 | 5.581973 | 0.533584 | 0.624045 |
| 85 | 6 | 0 | 3.202360 | 3.393396 | -1.609491 |
| 86 | 6 | 0 | 4.367685 | 3.727797 | 0.470708 |
| 87 | 6 | 0 | 7.430178 | -0.965301 | -0.064088 |
| 88 | 6 | 0 | 6.951973 | -2.255355 | -2.059985 |
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| 90 | 6 | 0 | 5.751152 | -2.290571 | -2.872876 |
| 91 | 6 | 0 | 3.248092 | 0.467958 | 0.681864 |
| 92 | 6 | 0 | 2.946298 | -0.286266 | -1.602572 |
| 93 | 6 | 0 | 4.444294 | 0.508887 | 1.500862 |
| 94 | 6 | 0 | 6.708883 | -0.172461 | 0.960350 |
| 95 | 6 | 0 | 2.103459 | 4.050813 | -1.090964 |
| 96 | 1 | 0 | 3.171738 | 2.967971 | -2.609572 |
| 97 | 6 | 0 | 3.260462 | 4.393902 | 1.000143 |
| 98 | 1 | 0 | 5.248101 | 3.580632 | 1.091173 |
| 99 | 6 | 0 | 7.900898 | -2.171037 | 0.575492 |
| 100 | 6 | 0 | 7.428211 | -3.422099 | -1.469685 |
| 101 | 6 | 0 | 2.952718 | -2.323147 | -2.795882 |
| 102 | 6 | 0 | 5.078767 | -3.493351 | -3.066270 |
| 103 | 6 | 0 | 2.135750 | -0.253790 | 1.110985 |
| 104 | 6 | 0 | 1.809196 | -1.066708 | -1.171023 |
| 105 | 6 | 0 | 4.482185 | -0.179681 | 2.710301 |
| 106 | 6 | 0 | 6.757519 | -0.912777 | 2.198592 |
| 107 | 8 | 0 | 0.939019 | 4.212525 | -1.817425 |
| 108 | 6 | 0 | 2.115646 | 4.541028 | 0.226367 |
| 109 | 1 | 0 | 3.301835 | 4.790507 | 2.007596 |
| 110 | 6 | 0 | 7.491356 | -2.142157 | 1.966750 |
| 111 | 6 | 0 | 7.916007 | -3.378960 | -0.115416 |
| 112 | 6 | 0 | 6.712995 | -4.673134 | -1.656647 |
| 113 | 6 | 0 | 3.640241 | -3.510858 | -3.026613 |
| 114 | 6 | 0 | 1.807099 | -2.317149 | -1.905558 |
| 115 | 6 | 0 | 5.568370 | -4.708594 | -2.437374 |
| 116 | 6 | 0 | 1.395439 | -1.042916 | 0.159077 |
| 117 | 6 | 0 | 2.180567 | -0.982848 | 2.367372 |
| 118 | 6 | 0 | 5.670716 | -0.909057 | 3.068894 |
| 119 | 6 | 0 | 3.326722 | -0.947161 | 3.146736 |
| 120 | 6 | 0 | 0.227645 | 2.989192 | -2.108948 |
| 121 | 8 | 0 | 0.961398 | 5.132461 | 0.633846 |
| 122 | 6 | 0 | 7.110756 | -3.311438 | 2.606674 |
| 123 | 6 | 0 | 7.506797 | -4.601626 | 0.549246 |
| 124 | 6 | 0 | 6.762483 | -5.403649 | -0.405358 |
| 125 | 6 | 0 | 3.223016 | -4.732400 | -2.366021 |
| 126 | 6 | 0 | 1.399385 | -3.487990 | -1.283288 |
| 127 | 6 | 0 | 4.416417 | -5.476253 | -2.003883 |
| 128 | 6 | 0 | 0.979743 | -2.268112 | 0.813695 |
| 129 | 6 | 0 | 1.464309 | -2.230909 | 2.182168 |
| 130 | 6 | 0 | 5.263904 | -2.134164 | 3.729862 |
| 131 | 6 | 0 | 3.813092 | -2.158367 | 3.778675 |
| 132 | 6 | 0 | 0.025323 | 2.087363 | -0.910952 |
| 133 | 1 | 0 | -0.737446 | 3.310351 | -2.510802 |
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| 135 | 6 | 0 | 0.839445 | 5.488321 | 2.000111 |
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| 139 | 6 | 0 | 2.126177 | -4.724007 | -1.514997 |
| 140 | 6 | 0 | 0.984224 | -3.464278 | 0.108276 |
| 141 | 6 | 0 | 4.460495 | -6.173837 | -0.804107 |
| 142 | 6 | 0 | 1.933042 | -3.392899 | 2.782070 |
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| 145 | 1 | 0 | -0.400493 | 1.140498 | -1.277428 |
| 146 | 8 | 0 | -0.848133 | 2.694891 | 0.013814 |
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| 154 | 6 | 0 | 1.465515 | -4.676349 | 0.737441 |
| 155 | 6 | 0 | 3.313445 | -6.163761 | 0.083163 |
| 156 | 6 | 0 | 1.931505 | -4.642318 | 2.044694 |
| 157 | 6 | 0 | 3.870442 | -4.582952 | 3.366972 |
| 158 | 6 | 0 | -1.008470 | 1.953563 | 1.204779 |
| 159 | 8 | 0 | -0.932702 | 6.969835 | 1.368556 |
| 160 | 1 | 0 | -1.229224 | 4.985696 | 1.935713 |
| 161 | 1 | 0 | -0.797201 | 6.099288 | 3.251380 |
| 162 | 6 | 0 | 3.803319 | -6.121089 | 1.449247 |
| 163 | 6 | 0 | 3.127599 | -5.379508 | 2.407491 |
| 164 | 1 | 0 | -0.739583 | 0.897279 | 1.054079 |
| 165 | 1 | 0 | -0.358191 | 2.359022 | 1.995631 |
| 166 | 6 | 0 | -2.467834 | 2.009567 | 1.609755 |
| 167 | 6 | 0 | -2.011793 | 7.771659 | 1.832784 |
| 168 | 1 | 0 | -2.657866 | 1.398281 | 2.502998 |
| 169 | 1 | 0 | -3.069908 | 1.612151 | 0.778699 |
| 170 | 8 | 0 | -2.803802 | 3.363955 | 1.856340 |
| 171 | 1 | 0 | -1.871573 | 7.975820 | 2.902281 |
| 172 | 1 | 0 | -1.952949 | 8.719684 | 1.288836 |
| 173 | 6 | 0 | -3.382877 | 7.144185 | 1.618939 |
| 174 | 6 | 0 | -4.127435 | 3.676745 | 1.999881 |
| 175 | 1 | 0 | -4.142661 | 7.811270 | 2.048783 |
| 176 | 1 | 0 | -3.605320 | 7.007664 | 0.550904 |
| 177 | 8 | 0 | -3.352560 | 5.890943 | 2.271190 |
| 178 | 6 | 0 | -4.426357 | 5.045641 | 2.137548 |
| 179 | 6 | 0 | -5.163049 | 2.749165 | 1.965735 |
| 180 | 6 | 0 | -5.745445 | 5.468456 | 2.195498 |
| 181 | 6 | 0 | -6.488725 | 3.183856 | 2.035729 |
| 182 | 1 | 0 | -4.960900 | 1.686457 | 1.889703 |
| 183 | 6 | 0 | -6.782787 | 4.535677 | 2.134380 |
| 184 | 1 | 0 | -5.962432 | 6.526122 | 2.305045 |
| 185 | 1 | 0 | -7.284007 | 2.445492 | 2.009995 |
| 186 | 1 | 0 | -7.811767 | 4.873561 | 2.180192 |

**AT5: M06-2X/6-31G(d,p)**

Standard orientation:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -6.127581 | -1.856408 | -2.452312 |
| 2 | 6 | 0 | -6.868496 | -3.008964 | -2.235955 |
| 3 | 6 | 0 | -7.977856 | -3.007563 | -1.384657 |
| 4 | 6 | 0 | -8.368391 | -1.796871 | -0.763469 |
| 5 | 6 | 0 | -7.640701 | -0.637207 | -1.012078 |
| 6 | 6 | 0 | -6.508284 | -0.657650 | -1.838725 |
| 7 | 6 | 0 | -8.802068 | -4.203855 | -1.124870 |
| 8 | 6 | 0 | -9.567634 | -1.829016 | 0.101113 |
| 9 | 6 | 0 | -10.640965 | -2.713808 | -0.404953 |
| 10 | 6 | 0 | -10.252137 | -3.919863 | -1.026785 |
| 11 | 6 | 0 | -11.232834 | -4.758310 | -1.560614 |
| 12 | 1 | 0 | -10.939541 | -5.655794 | -2.096032 |
| 13 | 6 | 0 | -12.582093 | -4.433964 | -1.456456 |
| 14 | 6 | 0 | -12.964460 | -3.245768 | -0.844272 |
| 15 | 6 | 0 | -11.995952 | -2.384868 | -0.337124 |
| 16 | 1 | 0 | -5.268814 | -1.870244 | -3.114275 |
| 17 | 1 | 0 | -6.600447 | -3.916698 | -2.766322 |
| 18 | 1 | 0 | -7.962686 | 0.311674 | -0.593898 |
| 19 | 1 | 0 | -13.328865 | -5.098936 | -1.877130 |
| 20 | 1 | 0 | -14.012828 | -2.973739 | -0.782773 |
| 21 | 1 | 0 | -12.297245 | -1.430620 | 0.083571 |
| 22 | 16 | 0 | -8.320306 | -0.202055 | 1.970217 |
| 23 | 6 | 0 | -10.222991 | -0.572281 | 3.768502 |
| 24 | 6 | 0 | -9.012070 | -0.055097 | 3.573738 |
| 25 | 1 | 0 | -10.768590 | -0.536061 | 4.702880 |
| 26 | 1 | 0 | -8.427795 | 0.463890 | 4.322412 |
| 27 | 6 | 0 | -8.270648 | -5.431408 | -0.888445 |
| 28 | 16 | 0 | -9.243833 | -6.844494 | -0.431618 |
| 29 | 6 | 0 | -6.662449 | -7.371965 | -0.183131 |
| 30 | 6 | 0 | -7.886941 | -7.854016 | 0.017304 |
| 31 | 1 | 0 | -5.742447 | -7.899673 | 0.032744 |
| 32 | 1 | 0 | -8.109413 | -8.832983 | 0.422462 |
| 33 | 16 | 0 | -11.012536 | -1.346064 | 2.411133 |
| 34 | 16 | 0 | -6.526637 | -5.771393 | -0.880243 |
| 35 | 6 | 0 | -9.636501 | -1.191876 | 1.295797 |
| 36 | 6 | 0 | -5.761037 | 0.541179 | -2.052072 |
| 37 | 6 | 0 | -5.123305 | 1.561204 | -2.204170 |
| 38 | 6 | 0 | -4.331315 | 2.744458 | -2.314246 |
| 39 | 6 | 0 | -4.813763 | 3.969793 | -1.833000 |
| 40 | 6 | 0 | -3.044158 | 2.683324 | -2.871993 |
| 41 | 6 | 0 | -4.000044 | 5.093652 | -1.863179 |
| 42 | 1 | 0 | -5.818065 | 4.030353 | -1.425712 |
| 43 | 6 | 0 | -2.251504 | 3.817997 | -2.920614 |
| 44 | 1 | 0 | -2.684899 | 1.738589 | -3.266576 |
| 45 | 6 | 0 | -2.711633 | 5.024652 | -2.388842 |
| 46 | 1 | 0 | -4.390196 | 6.038068 | -1.494954 |
| 47 | 1 | 0 | -1.262417 | 3.773562 | -3.372519 |
| 48 | 1 | 0 | 4.876954 | 6.960027 | -0.842992 |
| 49 | 6 | 0 | 3.885329 | 7.189498 | -0.466906 |
| 50 | 6 | 0 | 2.773656 | 7.013745 | -1.286471 |
| 51 | 6 | 0 | 3.720698 | 7.662113 | 0.831200 |
| 52 | 6 | 0 | 1.494995 | 7.315394 | -0.815871 |
| 53 | 1 | 0 | 2.901861 | 6.649639 | -2.302906 |
| 54 | 6 | 0 | 2.443866 | 7.946377 | 1.313231 |
| 55 | 1 | 0 | 4.585826 | 7.808078 | 1.469966 |
| 56 | 6 | 0 | 0.321232 | 7.234092 | -1.752061 |
| 57 | 6 | 0 | 1.334530 | 7.781270 | 0.491000 |
| 58 | 1 | 0 | 2.315343 | 8.319347 | 2.324551 |
| 59 | 7 | 0 | -0.676496 | 6.146988 | -1.459480 |
| 60 | 1 | 0 | -0.250993 | 8.166909 | -1.736808 |
| 61 | 1 | 0 | 0.660946 | 7.064325 | -2.776565 |
| 62 | 1 | 0 | 0.339419 | 8.007492 | 0.866334 |
| 63 | 6 | 0 | -1.826247 | 6.232934 | -2.427990 |
| 64 | 1 | 0 | -1.027385 | 6.233521 | -0.483728 |
| 65 | 1 | 0 | -0.230671 | 5.208484 | -1.502065 |
| 66 | 1 | 0 | -2.374914 | 7.145580 | -2.180980 |
| 67 | 1 | 0 | -1.378306 | 6.359480 | -3.417926 |
| 68 | 1 | 0 | 7.045872 | 4.809653 | -1.954258 |
| 69 | 6 | 0 | 6.244465 | 4.327209 | -2.541571 |
| 70 | 7 | 0 | 5.973642 | 2.973023 | -2.092034 |
| 71 | 1 | 0 | 6.545926 | 4.309919 | -3.591419 |
| 72 | 1 | 0 | 5.335860 | 4.929480 | -2.452973 |
| 73 | 6 | 0 | 7.131751 | 2.100655 | -2.196075 |
| 74 | 6 | 0 | 5.613110 | 2.891011 | -0.688779 |
| 75 | 6 | 0 | 6.695958 | 0.807220 | -1.461365 |
| 76 | 1 | 0 | 7.397494 | 1.913059 | -3.239764 |
| 77 | 1 | 0 | 8.010013 | 2.536036 | -1.683776 |
| 78 | 6 | 0 | 5.606586 | 1.342969 | -0.424466 |
| 79 | 1 | 0 | 6.409420 | 3.327219 | -0.052041 |
| 80 | 6 | 0 | 4.298342 | 3.532366 | -0.338935 |
| 81 | 6 | 0 | 7.848140 | 0.038416 | -0.819205 |
| 82 | 6 | 0 | 6.174810 | -0.248688 | -2.436164 |
| 83 | 6 | 0 | 4.222780 | 0.714034 | -0.592795 |
| 84 | 6 | 0 | 5.878942 | 1.005233 | 1.035012 |
| 85 | 6 | 0 | 3.219689 | 3.426543 | -1.225193 |
| 86 | 6 | 0 | 4.085164 | 4.060309 | 0.928834 |
| 87 | 6 | 0 | 8.086326 | 0.001735 | 0.531533 |
| 88 | 6 | 0 | 8.194490 | -1.099840 | -1.624206 |
| 89 | 6 | 0 | 4.851699 | -0.545102 | -2.625729 |
| 90 | 6 | 0 | 7.161084 | -1.274082 | -2.626506 |
| 91 | 6 | 0 | 3.631361 | 0.467862 | 0.693216 |
| 92 | 6 | 0 | 3.840663 | -0.047155 | -1.665809 |
| 93 | 6 | 0 | 4.658734 | 0.644733 | 1.701478 |
| 94 | 6 | 0 | 7.070265 | 0.501061 | 1.488442 |
| 95 | 6 | 0 | 1.958952 | 3.815172 | -0.820513 |
| 96 | 1 | 0 | 3.366803 | 2.982544 | -2.206014 |
| 97 | 6 | 0 | 2.817810 | 4.488484 | 1.332124 |
| 98 | 1 | 0 | 4.914972 | 4.126297 | 1.627576 |
| 99 | 6 | 0 | 8.708429 | -1.155898 | 1.128878 |
| 100 | 6 | 0 | 8.818726 | -2.213018 | -1.070505 |
| 101 | 6 | 0 | 4.453112 | -1.872973 | -3.024855 |
| 102 | 6 | 0 | 6.799026 | -2.552798 | -3.039823 |
| 103 | 6 | 0 | 2.649965 | -0.505506 | 0.861437 |
| 104 | 6 | 0 | 2.842951 | -1.079474 | -1.507332 |
| 105 | 6 | 0 | 4.669191 | -0.166069 | 2.832313 |
| 106 | 6 | 0 | 7.097734 | -0.362110 | 2.645337 |
| 107 | 8 | 0 | 0.847510 | 3.599186 | -1.618964 |
| 108 | 6 | 0 | 1.750925 | 4.368000 | 0.452756 |
| 109 | 1 | 0 | 2.674559 | 4.909647 | 2.320465 |
| 110 | 6 | 0 | 8.105736 | -1.381349 | 2.428933 |
| 111 | 6 | 0 | 9.084725 | -2.241536 | 0.343953 |
| 112 | 6 | 0 | 8.427002 | -3.548191 | -1.488587 |
| 113 | 6 | 0 | 5.407971 | -2.861456 | -3.244425 |
| 114 | 6 | 0 | 3.216860 | -2.204799 | -2.342337 |
| 115 | 6 | 0 | 7.441925 | -3.713905 | -2.449500 |
| 116 | 6 | 0 | 2.243164 | -1.301151 | -0.269730 |
| 117 | 6 | 0 | 2.669723 | -1.360452 | 2.036851 |
| 118 | 6 | 0 | 5.922353 | -0.681406 | 3.319490 |
| 119 | 6 | 0 | 3.656878 | -1.195428 | 2.997008 |
| 120 | 6 | 0 | 0.459921 | 2.208870 | -1.598048 |
| 121 | 8 | 0 | 0.467828 | 4.738822 | 0.700768 |
| 122 | 6 | 0 | 7.899052 | -2.673236 | 2.887312 |
| 123 | 6 | 0 | 8.856799 | -3.593442 | 0.817166 |
| 124 | 6 | 0 | 8.451327 | -4.403008 | -0.317562 |
| 125 | 6 | 0 | 5.173453 | -4.214283 | -2.777162 |
| 126 | 6 | 0 | 2.986689 | -3.500641 | -1.905524 |
| 127 | 6 | 0 | 6.433424 | -4.742801 | -2.286143 |
| 128 | 6 | 0 | 2.012421 | -2.656286 | 0.193022 |
| 129 | 6 | 0 | 2.276308 | -2.692637 | 1.620449 |
| 130 | 6 | 0 | 5.699176 | -2.035797 | 3.788162 |
| 131 | 6 | 0 | 4.296270 | -2.353621 | 3.589893 |
| 132 | 6 | 0 | -0.053755 | 1.705453 | -0.264995 |
| 133 | 1 | 0 | -0.318676 | 2.096430 | -2.352396 |
| 134 | 1 | 0 | 1.330191 | 1.605893 | -1.884821 |
| 135 | 6 | 0 | 0.079964 | 5.004363 | 2.037149 |
| 136 | 6 | 0 | 6.664894 | -3.009741 | 3.575508 |
| 137 | 6 | 0 | 8.277291 | -3.805384 | 2.060219 |
| 138 | 6 | 0 | 7.484903 | -5.387363 | -0.158032 |
| 139 | 6 | 0 | 3.989849 | -4.527840 | -2.123119 |
| 140 | 6 | 0 | 2.378675 | -3.731057 | -0.606447 |
| 141 | 6 | 0 | 6.453048 | -5.560424 | -1.164445 |
| 142 | 6 | 0 | 2.891958 | -3.803284 | 2.183052 |
| 143 | 6 | 0 | 3.923819 | -3.629947 | 3.188876 |
| 144 | 1 | 0 | 0.634012 | 1.983548 | 0.550295 |
| 145 | 1 | 0 | -0.044479 | 0.604674 | -0.323717 |
| 146 | 8 | 0 | -1.363014 | 2.166908 | -0.019122 |
| 147 | 6 | 0 | -1.402208 | 5.272198 | 1.983992 |
| 148 | 1 | 0 | 0.622979 | 5.874100 | 2.430189 |
| 149 | 1 | 0 | 0.290830 | 4.130172 | 2.668369 |
| 150 | 6 | 0 | 6.275284 | -4.342194 | 3.163640 |
| 151 | 6 | 0 | 7.272378 | -4.834038 | 2.227476 |
| 152 | 6 | 0 | 6.883142 | -5.608000 | 1.142758 |
| 153 | 6 | 0 | 4.010008 | -5.383515 | -0.955193 |
| 154 | 6 | 0 | 3.014125 | -4.891183 | -0.017913 |
| 155 | 6 | 0 | 5.214614 | -5.888224 | -0.484895 |
| 156 | 6 | 0 | 3.266484 | -4.927460 | 1.346714 |
| 157 | 6 | 0 | 4.934612 | -4.646997 | 2.973840 |
| 158 | 6 | 0 | -1.935993 | 1.512126 | 1.094957 |
| 159 | 8 | 0 | -1.610885 | 6.510202 | 1.282221 |
| 160 | 1 | 0 | -1.919596 | 4.462095 | 1.462330 |
| 161 | 1 | 0 | -1.811035 | 5.346531 | 2.996421 |
| 162 | 6 | 0 | 5.479849 | -5.918835 | 0.941330 |
| 163 | 6 | 0 | 4.528508 | -5.450622 | 1.835840 |
| 164 | 1 | 0 | -1.717930 | 0.434184 | 1.052622 |
| 165 | 1 | 0 | -1.516641 | 1.902490 | 2.036139 |
| 166 | 6 | 0 | -3.436336 | 1.682723 | 1.087706 |
| 167 | 6 | 0 | -2.625410 | 7.343630 | 1.821677 |
| 168 | 1 | 0 | -3.883835 | 0.990003 | 1.813473 |
| 169 | 1 | 0 | -3.828759 | 1.450920 | 0.089479 |
| 170 | 8 | 0 | -3.736966 | 3.021422 | 1.440679 |
| 171 | 1 | 0 | -2.541033 | 7.354029 | 2.915450 |
| 172 | 1 | 0 | -2.440274 | 8.357891 | 1.453993 |
| 173 | 6 | 0 | -4.021015 | 6.901761 | 1.418946 |
| 174 | 6 | 0 | -5.017988 | 3.441254 | 1.260173 |
| 175 | 1 | 0 | -4.761150 | 7.518085 | 1.948482 |
| 176 | 1 | 0 | -4.175631 | 7.031706 | 0.339281 |
| 177 | 8 | 0 | -4.115659 | 5.541964 | 1.763981 |
| 178 | 6 | 0 | -5.216336 | 4.833131 | 1.376178 |
| 179 | 6 | 0 | -6.095173 | 2.622278 | 0.946012 |
| 180 | 6 | 0 | -6.453946 | 5.390398 | 1.100897 |
| 181 | 6 | 0 | -7.350309 | 3.188965 | 0.693885 |
| 182 | 1 | 0 | -5.966788 | 1.548748 | 0.855213 |
| 183 | 6 | 0 | -7.527106 | 4.561904 | 0.751535 |
| 184 | 1 | 0 | -6.595920 | 6.463572 | 1.170542 |
| 185 | 1 | 0 | -8.184558 | 2.539305 | 0.451273 |
| 186 | 1 | 0 | -8.496615 | 5.001043 | 0.544879 |

**BT1: M06-2X/6-31G(d,p)**

Standard orientation:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -2.943964 | 2.937989 | 2.908438 |
| 2 | 6 | 0 | -4.324420 | 2.842811 | 2.805629 |
| 3 | 6 | 0 | -4.984046 | 3.158933 | 1.613474 |
| 4 | 6 | 0 | -4.227855 | 3.614171 | 0.508468 |
| 5 | 6 | 0 | -2.841305 | 3.684366 | 0.609813 |
| 6 | 6 | 0 | -2.188262 | 3.337832 | 1.800114 |
| 7 | 6 | 0 | -6.430813 | 2.952487 | 1.406829 |
| 8 | 6 | 0 | -4.955479 | 3.910439 | -0.745103 |
| 9 | 6 | 0 | -6.038713 | 2.947259 | -1.038085 |
| 10 | 6 | 0 | -6.767558 | 2.436599 | 0.059482 |
| 11 | 6 | 0 | -7.728796 | 1.448099 | -0.162276 |
| 12 | 1 | 0 | -8.244522 | 1.001949 | 0.682757 |
| 13 | 6 | 0 | -8.003379 | 0.995170 | -1.450480 |
| 14 | 6 | 0 | -7.299235 | 1.512691 | -2.532195 |
| 15 | 6 | 0 | -6.311644 | 2.471655 | -2.321944 |
| 16 | 1 | 0 | -2.438344 | 2.647633 | 3.823034 |
| 17 | 1 | 0 | -4.889794 | 2.450237 | 3.644797 |
| 18 | 1 | 0 | -2.243910 | 3.942991 | -0.259284 |
| 19 | 1 | 0 | -8.751184 | 0.223555 | -1.601308 |
| 20 | 1 | 0 | -7.491821 | 1.148967 | -3.536335 |
| 21 | 1 | 0 | -5.712869 | 2.814282 | -3.160527 |
| 22 | 16 | 0 | -3.465690 | 6.218554 | -1.091544 |
| 23 | 6 | 0 | -5.005221 | 7.078753 | -3.065334 |
| 24 | 6 | 0 | -4.016420 | 7.420315 | -2.241972 |
| 25 | 1 | 0 | -5.426056 | 7.720578 | -3.828759 |
| 26 | 1 | 0 | -3.515651 | 8.379922 | -2.236524 |
| 27 | 6 | 0 | -7.370999 | 3.287795 | 2.327213 |
| 28 | 16 | 0 | -9.117451 | 3.139906 | 2.043343 |
| 29 | 6 | 0 | -8.645967 | 4.448221 | 4.295596 |
| 30 | 6 | 0 | -9.601748 | 4.046336 | 3.460732 |
| 31 | 1 | 0 | -8.811818 | 4.997138 | 5.213578 |
| 32 | 1 | 0 | -10.660946 | 4.221652 | 3.599446 |
| 33 | 16 | 0 | -5.664315 | 5.462792 | -2.922098 |
| 34 | 16 | 0 | -6.992402 | 4.034137 | 3.893858 |
| 35 | 6 | 0 | -4.707192 | 5.011345 | -1.496062 |
| 36 | 6 | 0 | -0.761233 | 3.241799 | 1.812217 |
| 37 | 6 | 0 | 0.434815 | 3.059274 | 1.745527 |
| 38 | 6 | 0 | 1.843051 | 2.843921 | 1.631083 |
| 39 | 6 | 0 | 2.650659 | 3.778179 | 0.968747 |
| 40 | 6 | 0 | 2.432406 | 1.687168 | 2.162947 |
| 41 | 6 | 0 | 4.010086 | 3.546686 | 0.834082 |
| 42 | 1 | 0 | 2.199432 | 4.673114 | 0.554979 |
| 43 | 6 | 0 | 3.797432 | 1.466369 | 2.033133 |
| 44 | 1 | 0 | 1.800372 | 0.972133 | 2.678847 |
| 45 | 6 | 0 | 4.596480 | 2.390295 | 1.354149 |
| 46 | 1 | 0 | 4.624301 | 4.259361 | 0.289659 |
| 47 | 1 | 0 | 4.248629 | 0.573974 | 2.460232 |
| 48 | 1 | 0 | 5.675153 | 4.452034 | -3.172027 |
| 49 | 6 | 0 | 5.070092 | 3.633572 | -2.794354 |
| 50 | 6 | 0 | 5.667232 | 2.625152 | -2.043290 |
| 51 | 6 | 0 | 3.701020 | 3.593457 | -3.048612 |
| 52 | 6 | 0 | 4.898729 | 1.581093 | -1.529048 |
| 53 | 1 | 0 | 6.732880 | 2.673813 | -1.833740 |
| 54 | 6 | 0 | 2.933171 | 2.542293 | -2.551882 |
| 55 | 1 | 0 | 3.232791 | 4.381193 | -3.629377 |
| 56 | 6 | 0 | 5.515079 | 0.500368 | -0.682367 |
| 57 | 6 | 0 | 3.529312 | 1.542929 | -1.790197 |
| 58 | 1 | 0 | 1.864726 | 2.506494 | -2.738615 |
| 59 | 1 | 0 | 2.920619 | 0.745009 | -1.369877 |
| 60 | 1 | 0 | 6.714632 | 0.235351 | 0.975017 |
| 61 | 6 | 0 | 0.801422 | -1.621118 | -1.853098 |
| 62 | 6 | 0 | 0.572559 | -2.697098 | -2.705325 |
| 63 | 6 | 0 | -0.009323 | -0.423230 | -1.969772 |
| 64 | 6 | 0 | 1.097190 | -1.838396 | -0.454327 |
| 65 | 6 | 0 | -0.487030 | -2.631579 | -3.693415 |
| 66 | 6 | 0 | 0.603855 | -4.033983 | -2.172040 |
| 67 | 6 | 0 | -1.018930 | -0.356463 | -2.921026 |
| 68 | 6 | 0 | -0.225753 | 0.109446 | -0.637002 |
| 69 | 6 | 0 | 0.452306 | -0.746658 | 0.310379 |
| 70 | 6 | 0 | 1.140770 | -3.113080 | 0.053463 |
| 71 | 6 | 0 | -1.266580 | -1.488122 | -3.797862 |
| 72 | 6 | 0 | -1.107810 | -3.941992 | -3.771924 |
| 73 | 6 | 0 | -0.431293 | -4.812170 | -2.829542 |
| 74 | 6 | 0 | 0.860458 | -4.221376 | -0.817909 |
| 75 | 6 | 0 | -2.300126 | 0.237680 | -2.582336 |
| 76 | 6 | 0 | -1.453432 | 0.682386 | -0.318490 |
| 77 | 6 | 0 | -0.126626 | -1.017951 | 1.523565 |
| 78 | 6 | 0 | 0.808842 | -3.478396 | 1.500631 |
| 79 | 6 | 0 | -2.697748 | -1.599767 | -3.989847 |
| 80 | 6 | 0 | -2.480599 | -4.049063 | -3.949869 |
| 81 | 6 | 0 | -1.152862 | -5.752361 | -2.110364 |
| 82 | 6 | 0 | 0.109305 | -5.208018 | -0.066731 |
| 83 | 6 | 0 | -3.337721 | -0.533541 | -3.238855 |
| 84 | 6 | 0 | -2.511648 | 0.744547 | -1.308076 |
| 85 | 6 | 0 | -2.057741 | 0.389759 | 0.955234 |
| 86 | 6 | 0 | 0.101393 | -2.301993 | 2.310653 |
| 87 | 6 | 0 | -1.402582 | -0.448214 | 1.849412 |
| 88 | 6 | 0 | -0.082062 | -4.699845 | 1.263315 |
| 89 | 6 | 0 | 2.067831 | -3.869767 | 2.422742 |
| 90 | 6 | 0 | -3.292530 | -2.852512 | -4.062635 |
| 91 | 6 | 0 | -3.236405 | -5.035156 | -3.197348 |
| 92 | 6 | 0 | -2.586226 | -5.870179 | -2.299149 |
| 93 | 6 | 0 | -0.873832 | -5.961547 | -0.700268 |
| 94 | 6 | 0 | -4.542661 | -0.769780 | -2.590623 |
| 95 | 6 | 0 | -3.773684 | 0.497083 | -0.631727 |
| 96 | 6 | 0 | -3.492006 | 0.281420 | 0.772374 |
| 97 | 6 | 0 | -1.334117 | -2.605671 | 2.750854 |
| 98 | 6 | 0 | 1.100445 | -2.057836 | 3.487090 |
| 99 | 6 | 0 | -2.153508 | -1.432013 | 2.604950 |
| 100 | 6 | 0 | -1.275118 | -4.925425 | 1.898621 |
| 101 | 7 | 0 | 1.821919 | -3.290991 | 3.734256 |
| 102 | 6 | 0 | 3.400483 | -3.430306 | 1.839239 |
| 103 | 1 | 0 | 2.092807 | -4.960765 | 2.510718 |
| 104 | 6 | 0 | -4.550716 | -3.098024 | -3.382531 |
| 105 | 6 | 0 | -4.514569 | -4.446427 | -2.846063 |
| 106 | 6 | 0 | -3.185394 | -6.152270 | -1.006447 |
| 107 | 6 | 0 | -2.120298 | -6.210502 | -0.024160 |
| 108 | 6 | 0 | -5.161369 | -2.080526 | -2.663232 |
| 109 | 6 | 0 | -4.762793 | -0.244607 | -1.257551 |
| 110 | 6 | 0 | -4.213863 | -0.654634 | 1.495250 |
| 111 | 6 | 0 | -1.925389 | -3.840453 | 2.667369 |
| 112 | 1 | 0 | 1.806468 | -1.287320 | 3.154237 |
| 113 | 1 | 0 | 0.601770 | -1.697447 | 4.390198 |
| 114 | 6 | 0 | -3.532396 | -1.527847 | 2.436001 |
| 115 | 6 | 0 | -2.316871 | -5.684540 | 1.248283 |
| 116 | 6 | 0 | 1.141637 | -4.200753 | 4.656321 |
| 117 | 6 | 0 | 3.899133 | -4.049248 | 0.694165 |
| 118 | 6 | 0 | 4.159311 | -2.416728 | 2.422741 |
| 119 | 6 | 0 | -5.085362 | -4.715283 | -1.609694 |
| 120 | 6 | 0 | -4.406046 | -5.583550 | -0.670926 |
| 121 | 6 | 0 | -5.765709 | -2.361820 | -1.372976 |
| 122 | 6 | 0 | -5.521704 | -1.225834 | -0.505191 |
| 123 | 6 | 0 | -5.253514 | -1.425931 | 0.842734 |
| 124 | 6 | 0 | -3.349343 | -3.962326 | 2.467768 |
| 125 | 6 | 0 | -4.147557 | -2.828076 | 2.367044 |
| 126 | 6 | 0 | -3.595200 | -5.096948 | 1.598152 |
| 127 | 1 | 0 | 1.786823 | -5.061648 | 4.846176 |
| 128 | 1 | 0 | 0.172172 | -4.564700 | 4.289844 |
| 129 | 1 | 0 | 0.981207 | -3.685818 | 5.605948 |
| 130 | 6 | 0 | 5.093295 | -3.643890 | 0.105976 |
| 131 | 1 | 0 | 3.345005 | -4.863726 | 0.236509 |
| 132 | 6 | 0 | 5.346717 | -1.997913 | 1.840998 |
| 133 | 1 | 0 | 3.835946 | -1.954589 | 3.350162 |
| 134 | 6 | 0 | -5.725497 | -3.649757 | -0.855916 |
| 135 | 6 | 0 | -4.618412 | -5.050113 | 0.663605 |
| 136 | 6 | 0 | -5.210270 | -2.772925 | 1.381160 |
| 137 | 6 | 0 | 5.822525 | -2.597802 | 0.668025 |
| 138 | 1 | 0 | 5.436919 | -4.148786 | -0.787947 |
| 139 | 8 | 0 | 6.031939 | -0.922968 | 2.376652 |
| 140 | 6 | 0 | -5.441169 | -3.859232 | 0.548533 |
| 141 | 8 | 0 | 6.983384 | -2.088562 | 0.148487 |
| 142 | 6 | 0 | 7.001214 | -1.210367 | 3.394529 |
| 143 | 6 | 0 | 7.441572 | -2.680867 | -1.056271 |
| 144 | 6 | 0 | 8.392785 | -1.105416 | 2.812925 |
| 145 | 1 | 0 | 6.868973 | -0.454345 | 4.173433 |
| 146 | 1 | 0 | 6.819834 | -2.203020 | 3.817347 |
| 147 | 6 | 0 | 8.708255 | -1.984802 | -1.477999 |
| 148 | 1 | 0 | 6.681653 | -2.573504 | -1.841820 |
| 149 | 1 | 0 | 7.643613 | -3.748510 | -0.902896 |
| 150 | 1 | 0 | 8.504356 | -1.817301 | 1.984681 |
| 151 | 1 | 0 | 9.144412 | -1.331192 | 3.583252 |
| 152 | 8 | 0 | 8.540180 | 0.224526 | 2.350026 |
| 153 | 8 | 0 | 8.412539 | -0.638726 | -1.786214 |
| 154 | 1 | 0 | 9.461204 | -2.037376 | -0.676224 |
| 155 | 1 | 0 | 9.111224 | -2.502623 | -2.360552 |
| 156 | 6 | 0 | 9.634063 | 0.396318 | 1.470137 |
| 157 | 6 | 0 | 9.486857 | -0.007526 | -2.451497 |
| 158 | 1 | 0 | 10.493601 | -0.210657 | 1.790401 |
| 159 | 1 | 0 | 9.343013 | 0.086302 | 0.453761 |
| 160 | 6 | 0 | 10.044185 | 1.853466 | 1.485558 |
| 161 | 1 | 0 | 10.411550 | -0.112132 | -1.863200 |
| 162 | 1 | 0 | 9.650814 | -0.459172 | -3.440165 |
| 163 | 6 | 0 | 9.162253 | 1.457873 | -2.601900 |
| 164 | 1 | 0 | 10.822954 | 2.024193 | 0.734587 |
| 165 | 1 | 0 | 10.434142 | 2.122814 | 2.472879 |
| 166 | 8 | 0 | 8.900812 | 2.669760 | 1.225279 |
| 167 | 1 | 0 | 9.993835 | 1.968408 | -3.100643 |
| 168 | 1 | 0 | 8.243549 | 1.604098 | -3.185522 |
| 169 | 8 | 0 | 8.987683 | 1.955949 | -1.284517 |
| 170 | 6 | 0 | 9.046056 | 3.665110 | 0.290279 |
| 171 | 6 | 0 | 9.063775 | 3.306568 | -1.066087 |
| 172 | 6 | 0 | 9.074364 | 5.000469 | 0.656319 |
| 173 | 6 | 0 | 9.106796 | 4.283821 | -2.051938 |
| 174 | 6 | 0 | 9.128378 | 5.987184 | -0.329931 |
| 175 | 1 | 0 | 9.048093 | 5.249064 | 1.711953 |
| 176 | 6 | 0 | 9.146514 | 5.628079 | -1.671446 |
| 177 | 1 | 0 | 9.097884 | 4.014933 | -3.102566 |
| 178 | 1 | 0 | 9.154401 | 7.032711 | -0.044851 |
| 179 | 1 | 0 | 9.185646 | 6.393284 | -2.439005 |
| 180 | 1 | 0 | 7.387736 | 1.249861 | -0.129150 |
| 181 | 7 | 0 | 6.495253 | 1.015189 | 0.332655 |
| 182 | 6 | 0 | 6.079523 | 2.204461 | 1.186779 |
| 183 | 1 | 0 | 6.085245 | -0.214009 | -1.281093 |
| 184 | 1 | 0 | 4.739811 | -0.036261 | -0.129841 |
| 185 | 1 | 0 | 6.602006 | 2.054117 | 2.133571 |
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**BT2: M06-2X/6-31G(d,p)**

Standard orientation:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 7.275680 | -1.647219 | -1.994161 |
| 2 | 6 | 0 | 8.325598 | -2.547360 | -1.885597 |
| 3 | 6 | 0 | 9.257765 | -2.449055 | -0.848481 |
| 4 | 6 | 0 | 9.106254 | -1.428256 | 0.119468 |
| 5 | 6 | 0 | 8.035008 | -0.545635 | 0.020704 |
| 6 | 6 | 0 | 7.121674 | -0.635275 | -1.038975 |
| 7 | 6 | 0 | 10.381519 | -3.390566 | -0.675863 |
| 8 | 6 | 0 | 10.090359 | -1.383258 | 1.222879 |
| 9 | 6 | 0 | 10.505077 | -2.720471 | 1.702923 |
| 10 | 6 | 0 | 10.655430 | -3.739227 | 0.736652 |
| 11 | 6 | 0 | 11.003837 | -5.026065 | 1.151378 |
| 12 | 1 | 0 | 11.063579 | -5.827422 | 0.421626 |
| 13 | 6 | 0 | 11.233645 | -5.304694 | 2.495489 |
| 14 | 6 | 0 | 11.086269 | -4.301328 | 3.446416 |
| 15 | 6 | 0 | 10.708713 | -3.021467 | 3.050780 |
| 16 | 1 | 0 | 6.556703 | -1.735668 | -2.801061 |
| 17 | 1 | 0 | 8.400573 | -3.361566 | -2.598864 |
| 18 | 1 | 0 | 7.875497 | 0.206646 | 0.786121 |
| 19 | 1 | 0 | 11.504273 | -6.310801 | 2.797902 |
| 20 | 1 | 0 | 11.241612 | -4.516383 | 4.498370 |
| 21 | 1 | 0 | 10.538543 | -2.257808 | 3.803237 |
| 22 | 16 | 0 | 10.253721 | 1.376954 | 1.013691 |
| 23 | 6 | 0 | 12.331631 | 1.512304 | 2.647439 |
| 24 | 6 | 0 | 11.581342 | 2.209645 | 1.797172 |
| 25 | 1 | 0 | 13.170010 | 1.910587 | 3.204699 |
| 26 | 1 | 0 | 11.720370 | 3.256801 | 1.561092 |
| 27 | 6 | 0 | 11.156596 | -3.812461 | -1.708214 |
| 28 | 16 | 0 | 12.594251 | -4.835284 | -1.499620 |
| 29 | 6 | 0 | 12.436599 | -3.947944 | -3.987630 |
| 30 | 6 | 0 | 13.189333 | -4.637868 | -3.133404 |
| 31 | 1 | 0 | 12.679353 | -3.767295 | -5.026917 |
| 32 | 1 | 0 | 14.136567 | -5.102951 | -3.375139 |
| 33 | 16 | 0 | 11.923526 | -0.170598 | 2.905174 |
| 34 | 16 | 0 | 10.920068 | -3.303624 | -3.394158 |
| 35 | 6 | 0 | 10.642530 | -0.229836 | 1.672699 |
| 36 | 6 | 0 | 6.025618 | 0.278071 | -1.122423 |
| 37 | 6 | 0 | 5.093783 | 1.049840 | -1.193476 |
| 38 | 6 | 0 | 3.991822 | 1.953483 | -1.275634 |
| 39 | 6 | 0 | 3.825248 | 2.965386 | -0.315142 |
| 40 | 6 | 0 | 3.066388 | 1.855947 | -2.324497 |
| 41 | 6 | 0 | 2.750106 | 3.836683 | -0.395107 |
| 42 | 1 | 0 | 4.559890 | 3.062652 | 0.477684 |
| 43 | 6 | 0 | 1.990261 | 2.731777 | -2.393773 |
| 44 | 1 | 0 | 3.205206 | 1.093280 | -3.082541 |
| 45 | 6 | 0 | 1.809242 | 3.716472 | -1.421743 |
| 46 | 1 | 0 | 2.636262 | 4.633791 | 0.336488 |
| 47 | 1 | 0 | 1.294160 | 2.663741 | -3.224691 |
| 48 | 1 | 0 | -2.102282 | 1.501571 | -4.765985 |
| 49 | 6 | 0 | -2.398895 | 2.110853 | -3.918662 |
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| 51 | 6 | 0 | -3.630648 | 2.757393 | -3.920738 |
| 52 | 6 | 0 | -1.933231 | 2.981335 | -1.709106 |
| 53 | 1 | 0 | -0.617023 | 1.672197 | -2.791835 |
| 54 | 6 | 0 | -4.022421 | 3.506467 | -2.812006 |
| 55 | 1 | 0 | -4.294114 | 2.662084 | -4.773981 |
| 56 | 6 | 0 | -1.054364 | 3.089033 | -0.491777 |
| 57 | 6 | 0 | -3.178639 | 3.615286 | -1.711844 |
| 58 | 1 | 0 | -4.996233 | 3.986615 | -2.797685 |
| 59 | 1 | 0 | -3.484818 | 4.188660 | -0.839262 |
| 60 | 1 | 0 | -1.054205 | 5.185400 | -0.415770 |
| 61 | 6 | 0 | -2.554031 | -0.562502 | -0.733928 |
| 62 | 6 | 0 | -1.850303 | -1.763179 | -0.717895 |
| 63 | 6 | 0 | -3.427374 | -0.256369 | -1.850167 |
| 64 | 6 | 0 | -3.159199 | -0.046123 | 0.472259 |
| 65 | 6 | 0 | -2.000375 | -2.710646 | -1.805491 |
| 66 | 6 | 0 | -1.759555 | -2.507719 | 0.511528 |
| 67 | 6 | 0 | -3.562046 | -1.154546 | -2.898501 |
| 68 | 6 | 0 | -4.583652 | 0.455542 | -1.342967 |
| 69 | 6 | 0 | -4.437891 | 0.596061 | 0.087402 |
| 70 | 6 | 0 | -3.070010 | -0.754723 | 1.643550 |
| 71 | 6 | 0 | -2.838791 | -2.413438 | -2.871277 |
| 72 | 6 | 0 | -1.997171 | -4.047773 | -1.239458 |
| 73 | 6 | 0 | -1.846054 | -3.923227 | 0.197583 |
| 74 | 6 | 0 | -2.377843 | -2.012514 | 1.654326 |
| 75 | 6 | 0 | -4.869814 | -1.396410 | -3.480587 |
| 76 | 6 | 0 | -5.835270 | 0.230292 | -1.909778 |
| 77 | 6 | 0 | -5.534545 | 0.475308 | 0.901733 |
| 78 | 6 | 0 | -4.106667 | -0.706873 | 2.764303 |
| 79 | 6 | 0 | -3.703535 | -3.434860 | -3.424400 |
| 80 | 6 | 0 | -2.830587 | -5.025586 | -1.765270 |
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| 83 | 6 | 0 | -4.959279 | -2.806726 | -3.800137 |
| 84 | 6 | 0 | -5.981151 | -0.719408 | -2.995983 |
| 85 | 6 | 0 | -6.985228 | 0.105693 | -1.051501 |
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| 88 | 6 | 0 | -4.218780 | -2.199827 | 3.081036 |
| 89 | 6 | 0 | -3.639305 | 0.133634 | 4.054985 |
| 90 | 6 | 0 | -3.701356 | -4.712661 | -2.881713 |
| 91 | 6 | 0 | -3.544915 | -5.925025 | -0.876568 |
| 92 | 6 | 0 | -3.395697 | -5.806360 | 0.498561 |
| 93 | 6 | 0 | -3.157808 | -4.265917 | 2.251275 |
| 94 | 6 | 0 | -6.156010 | -3.485832 | -3.615734 |
| 95 | 6 | 0 | -7.233985 | -1.429041 | -2.806127 |
| 96 | 6 | 0 | -7.858304 | -0.917096 | -1.600974 |
| 97 | 6 | 0 | -6.685801 | -0.966177 | 2.343116 |
| 98 | 6 | 0 | -5.614765 | 1.166084 | 3.350269 |
| 99 | 6 | 0 | -7.534375 | -0.684142 | 1.216716 |
| 100 | 6 | 0 | -5.402054 | -2.869732 | 3.254488 |
| 101 | 7 | 0 | -4.800884 | 0.877717 | 4.517877 |
| 102 | 6 | 0 | -2.442103 | 1.001724 | 3.716973 |
| 103 | 1 | 0 | -3.333252 | -0.576025 | 4.829849 |
| 104 | 6 | 0 | -4.953703 | -5.419262 | -2.685488 |
| 105 | 6 | 0 | -4.856775 | -6.166991 | -1.444998 |
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| 108 | 6 | 0 | -6.152194 | -4.819591 | -3.043583 |
| 109 | 6 | 0 | -7.317418 | -2.782089 | -3.106505 |
| 110 | 6 | 0 | -8.537469 | -1.775882 | -0.750823 |
| 111 | 6 | 0 | -6.680991 | -2.230653 | 2.871770 |
| 112 | 1 | 0 | -5.253571 | 2.067215 | 2.844147 |
| 113 | 1 | 0 | -6.655120 | 1.341943 | 3.634213 |
| 114 | 6 | 0 | -8.381342 | -1.653566 | 0.688955 |
| 115 | 6 | 0 | -5.502725 | -4.272914 | 2.929119 |
| 116 | 6 | 0 | -5.540270 | 0.174424 | 5.568437 |
| 117 | 6 | 0 | -1.184412 | 0.411850 | 3.601700 |
| 118 | 6 | 0 | -2.601235 | 2.347375 | 3.388849 |
| 119 | 6 | 0 | -5.963376 | -6.276725 | -0.614674 |
| 120 | 6 | 0 | -5.808798 | -6.149312 | 0.819594 |
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| 130 | 6 | 0 | -0.118938 | 1.133773 | 3.075769 |
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| 137 | 6 | 0 | -0.300896 | 2.446525 | 2.667240 |
| 138 | 1 | 0 | 0.856121 | 0.678506 | 2.932985 |
| 139 | 8 | 0 | -1.645208 | 4.366666 | 2.403357 |
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| 154 | 1 | 0 | 0.338107 | 5.220921 | 3.654775 |
| 155 | 1 | 0 | 2.073664 | 5.621538 | 3.800334 |
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| 157 | 6 | 0 | 0.962606 | 7.209782 | 2.073391 |
| 158 | 1 | 0 | -4.001555 | 7.711618 | -0.067146 |
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| 160 | 6 | 0 | -2.834213 | 7.055179 | -1.746174 |
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| 163 | 6 | 0 | 1.177046 | 7.945519 | 0.776568 |
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| 177 | 1 | 0 | 1.881462 | 9.502091 | -1.043754 |
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| 184 | 1 | 0 | -1.654359 | 2.992286 | 0.413634 |
| 185 | 1 | 0 | 0.108012 | 4.614804 | -2.426460 |
| 186 | 1 | 0 | 0.984012 | 5.697855 | -1.329134 |