Table S1. Optimized cartesian coordinates for the studied oligofurans calculated using the selected theoretical methods (exchange-correlation DFT functionals) and CC2 with the def2-TZVPP basis set.

Part 1.

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| **2O/BP** | **Ground state** | | | **Excited state** | | |
| C | -2.8300959 | 0.4365768 | 0.0000000 | -2.8224440 | 0.4476766 | 0.0000000 |
| C | -2.8079253 | -0.9290084 | 0.0000000 | -2.7928955 | -0.9427104 | 0.0000000 |
| C | -1.4317100 | -1.3123968 | 0.0000000 | -1.4462633 | -1.3356537 | 0.0000000 |
| C | -0.7027945 | -0.1446012 | 0.0000000 | -0.6845698 | -0.1335271 | 0.0000000 |
| C | 0.7027945 | 0.1446012 | 0.0000000 | 0.6845698 | 0.1335271 | 0.0000000 |
| C | 1.4317100 | 1.3123968 | 0.0000000 | 1.4462633 | 1.3356537 | 0.0000000 |
| C | 2.8079253 | 0.9290084 | 0.0000000 | 2.7928955 | 0.9427104 | 0.0000000 |
| C | 2.8300959 | -0.4365768 | 0.0000000 | 2.8224440 | -0.4476766 | 0.0000000 |
| O | -1.5540498 | 0.9365544 | 0.0000000 | -1.5473754 | 0.9759807 | 0.0000000 |
| O | 1.5540498 | -0.9365544 | 0.0000000 | 1.5473754 | -0.9759807 | 0.0000000 |
| H | -3.6215146 | 1.1757085 | 0.0000000 | -3.6291854 | 1.1715651 | 0.0000000 |
| H | -3.6715531 | -1.5848992 | 0.0000000 | -3.6657851 | -1.5873117 | 0.0000000 |
| H | -1.0235539 | -2.3162402 | 0.0000000 | -1.0336319 | -2.3375854 | 0.0000000 |
| H | 1.0235539 | 2.3162402 | 0.0000000 | 1.0336319 | 2.3375854 | 0.0000000 |
| H | 3.6715531 | 1.5848992 | 0.0000000 | 3.6657851 | 1.5873117 | 0.0000000 |
| H | 3.6215146 | -1.1757085 | 0.0000000 | 3.6291854 | -1.1715651 | 0.0000000 |
|  |  |  |  |  |  |  |
| **3O/BP** | **Ground state** | | | **Excited state** | | |
| O | 3.4893371 | 0.0000000 | 0.8468783 | 3.4949827 | 0.0000000 | 0.8618028 |
| C | 4.5905360 | 0.0000000 | 0.0313440 | 4.5801514 | 0.0000000 | 0.0181425 |
| C | 4.2131964 | 0.0000000 | -1.2816386 | 4.1764241 | 0.0000000 | -1.3001209 |
| C | 2.7854336 | 0.0000000 | -1.2938134 | 2.7641562 | 0.0000000 | -1.3015294 |
| C | 2.3848704 | 0.0000000 | 0.0247082 | 2.3682678 | 0.0000000 | 0.0472240 |
| C | 1.1067417 | 0.0000000 | 0.6699482 | 1.1123126 | 0.0000000 | 0.6759543 |
| O | 0.0000000 | 0.0000000 | -0.1489916 | 0.0000000 | 0.0000000 | -0.1642063 |
| C | -1.1067417 | 0.0000000 | 0.6699482 | -1.1123126 | 0.0000000 | 0.6759543 |
| C | -0.7102443 | 0.0000000 | 1.9907970 | -0.6993405 | 0.0000000 | 2.0230545 |
| C | 0.7102443 | 0.0000000 | 1.9907970 | 0.6993405 | 0.0000000 | 2.0230545 |
| C | -2.3848704 | 0.0000000 | 0.0247082 | -2.3682678 | 0.0000000 | 0.0472240 |
| O | -3.4893371 | 0.0000000 | 0.8468783 | -3.4949827 | 0.0000000 | 0.8618028 |
| C | -4.5905360 | 0.0000000 | 0.0313440 | -4.5801514 | 0.0000000 | 0.0181425 |
| C | -4.2131964 | 0.0000000 | -1.2816386 | -4.1764241 | 0.0000000 | -1.3001209 |
| C | -2.7854336 | 0.0000000 | -1.2938134 | -2.7641562 | 0.0000000 | -1.3015294 |
| H | 5.5474170 | 0.0000000 | 0.5383374 | 5.5496609 | 0.0000000 | 0.5018140 |
| H | 4.8763602 | 0.0000000 | -2.1396881 | 4.8338507 | 0.0000000 | -2.1632994 |
| H | 2.1307170 | 0.0000000 | -2.1572215 | 2.0952029 | 0.0000000 | -2.1542637 |
| H | -2.1307170 | 0.0000000 | -2.1572215 | -2.0952029 | 0.0000000 | -2.1542637 |
| H | -5.5474170 | 0.0000000 | 0.5383374 | -5.5496609 | 0.0000000 | 0.5018140 |
| H | -4.8763602 | 0.0000000 | -2.1396881 | -4.8338507 | 0.0000000 | -2.1632994 |
| H | 1.3709898 | 0.0000000 | 2.8498467 | 1.3650126 | 0.0000000 | 2.8783268 |
| H | -1.3709898 | 0.0000000 | 2.8498467 | -1.3650126 | 0.0000000 | 2.8783268 |
|  |  |  |  |  |  |  |
| **4O/BP** | **Ground state** | | | **Excited state** | | |
| O | -1.7785469 | 0.3587455 | 0.0000000 | -1.7791961 | 0.3793094 | 0.0000000 |
| C | -2.8173427 | -0.5446709 | 0.0000000 | -2.8196837 | -0.5396912 | 0.0000000 |
| C | -2.3181112 | -1.8309539 | 0.0000000 | -2.3038268 | -1.8413363 | 0.0000000 |
| C | -0.9031682 | -1.7203703 | 0.0000000 | -0.9059014 | -1.7305322 | 0.0000000 |
| C | -0.6100044 | -0.3710587 | 0.0000000 | -0.6042575 | -0.3601624 | 0.0000000 |
| C | 0.6100044 | 0.3710587 | 0.0000000 | 0.6042575 | 0.3601624 | 0.0000000 |
| O | 1.7785469 | -0.3587455 | 0.0000000 | 1.7791961 | -0.3793094 | 0.0000000 |
| C | 2.8173427 | 0.5446709 | 0.0000000 | 2.8196837 | 0.5396912 | 0.0000000 |
| C | 2.3181112 | 1.8309539 | 0.0000000 | 2.3038268 | 1.8413363 | 0.0000000 |
| C | 0.9031682 | 1.7203703 | 0.0000000 | 0.9059014 | 1.7305322 | 0.0000000 |
| C | 4.1420467 | 0.0029759 | 0.0000000 | 4.1292217 | 0.0158639 | 0.0000000 |
| O | 5.1781125 | 0.9100662 | 0.0000000 | 5.1763784 | 0.9241844 | 0.0000000 |
| C | 6.3402278 | 0.1841341 | 0.0000000 | 6.3333711 | 0.1864035 | 0.0000000 |
| C | 6.0679739 | -1.1547040 | 0.0000000 | 6.0515427 | -1.1591208 | 0.0000000 |
| C | 4.6458754 | -1.2799287 | 0.0000000 | 4.6408129 | -1.2844687 | 0.0000000 |
| H | -2.9098310 | -2.7389447 | 0.0000000 | -2.8971320 | -2.7484101 | 0.0000000 |
| H | -0.1780123 | -2.5256989 | 0.0000000 | -0.1757460 | -2.5315761 | 0.0000000 |
| H | 4.0616357 | -2.1925004 | 0.0000000 | 4.0528188 | -2.1947798 | 0.0000000 |
| H | 7.2540659 | 0.7651467 | 0.0000000 | 7.2535853 | 0.7579792 | 0.0000000 |
| H | 6.7970019 | -1.9575359 | 0.0000000 | 6.7816266 | -1.9616056 | 0.0000000 |
| H | 0.1780123 | 2.5256989 | 0.0000000 | 0.1757460 | 2.5315761 | 0.0000000 |
| H | 2.9098310 | 2.7389447 | 0.0000000 | 2.8971320 | 2.7484101 | 0.0000000 |
| C | -4.1420467 | -0.0029759 | 0.0000000 | -4.1292217 | -0.0158639 | 0.0000000 |
| O | -5.1781125 | -0.9100662 | 0.0000000 | -5.1763784 | -0.9241844 | 0.0000000 |
| C | -6.3402278 | -0.1841341 | 0.0000000 | -6.3333711 | -0.1864035 | 0.0000000 |
| C | -6.0679739 | 1.1547040 | 0.0000000 | -6.0515427 | 1.1591208 | 0.0000000 |
| C | -4.6458754 | 1.2799287 | 0.0000000 | -4.6408129 | 1.2844687 | 0.0000000 |
| H | -4.0616357 | 2.1925004 | 0.0000000 | -4.0528188 | 2.1947798 | 0.0000000 |
| H | -7.2540659 | -0.7651467 | 0.0000000 | -7.2535853 | -0.7579792 | 0.0000000 |
| H | -6.7970019 | 1.9575359 | 0.0000000 | -6.7816266 | 1.9616056 | 0.0000000 |
|  |  |  |  |  |  |  |
| **5O/BP** | **Ground state** | | | **Excited state** | | |
| O | 3.4891881 | 0.0000000 | 0.2790949 | 3.4885593 | 0.0000000 | 0.3023461 |
| C | 4.5960688 | 0.0000000 | -0.5393788 | 4.5959260 | 0.0000000 | -0.5293016 |
| C | 4.2000867 | 0.0000000 | -1.8613207 | 4.1834120 | 0.0000000 | -1.8633945 |
| C | 2.7811622 | 0.0000000 | -1.8631617 | 2.7796553 | 0.0000000 | -1.8605168 |
| C | 2.3818733 | 0.0000000 | -0.5409943 | 2.3744713 | 0.0000000 | -0.5211837 |
| C | 1.1074582 | 0.0000000 | 0.1016384 | 1.1110319 | 0.0000000 | 0.1041543 |
| O | 0.0000000 | 0.0000000 | -0.7177990 | 0.0000000 | 0.0000000 | -0.7250302 |
| C | -1.1074582 | 0.0000000 | 0.1016384 | -1.1110319 | 0.0000000 | 0.1041543 |
| C | -0.7089569 | 0.0000000 | 1.4244841 | -0.7023845 | 0.0000000 | 1.4413089 |
| C | 0.7089569 | 0.0000000 | 1.4244841 | 0.7023845 | 0.0000000 | 1.4413089 |
| C | -2.3818733 | 0.0000000 | -0.5409943 | -2.3744713 | 0.0000000 | -0.5211837 |
| O | -3.4891881 | 0.0000000 | 0.2790949 | -3.4885593 | 0.0000000 | 0.3023461 |
| C | -4.5960688 | 0.0000000 | -0.5393788 | -4.5959260 | 0.0000000 | -0.5293016 |
| C | -4.2000867 | 0.0000000 | -1.8613207 | -4.1834120 | 0.0000000 | -1.8633945 |
| C | -2.7811622 | 0.0000000 | -1.8631617 | -2.7796553 | 0.0000000 | -1.8605168 |
| C | 5.8738210 | 0.0000000 | 0.1049865 | 5.8652768 | 0.0000000 | 0.0930487 |
| O | 6.9781829 | 0.0000000 | -0.7176350 | 6.9736315 | 0.0000000 | -0.7362722 |
| C | 8.0793919 | 0.0000000 | 0.0976371 | 8.0750730 | 0.0000000 | 0.0804499 |
| C | 7.7024751 | 0.0000000 | 1.4108994 | 7.6986801 | 0.0000000 | 1.4004254 |
| C | 6.2750051 | 0.0000000 | 1.4236704 | 6.2802090 | 0.0000000 | 1.4227767 |
| C | -5.8738210 | 0.0000000 | 0.1049865 | -5.8652768 | 0.0000000 | 0.0930487 |
| O | -6.9781829 | 0.0000000 | -0.7176350 | -6.9736315 | 0.0000000 | -0.7362722 |
| H | -4.8618489 | 0.0000000 | -2.7196034 | -4.8438754 | 0.0000000 | -2.7228881 |
| H | -2.1220997 | 0.0000000 | -2.7234201 | -2.1147036 | 0.0000000 | -2.7165082 |
| H | -1.3690953 | 0.0000000 | 2.2839360 | -1.3651843 | 0.0000000 | 2.2987701 |
| H | 1.3690953 | 0.0000000 | 2.2839360 | 1.3651843 | 0.0000000 | 2.2987701 |
| H | 2.1220997 | 0.0000000 | -2.7234201 | 2.1147036 | 0.0000000 | -2.7165082 |
| H | 4.8618489 | 0.0000000 | -2.7196034 | 4.8438754 | 0.0000000 | -2.7228881 |
| H | 5.6206829 | 0.0000000 | 2.2873754 | 5.6290259 | 0.0000000 | 2.2889010 |
| H | 8.3659827 | 0.0000000 | 2.2686700 | 8.3682297 | 0.0000000 | 2.2539395 |
| C | -8.0793919 | 0.0000000 | 0.0976371 | -8.0750730 | 0.0000000 | 0.0804499 |
| C | -7.7024751 | 0.0000000 | 1.4108994 | -7.6986801 | 0.0000000 | 1.4004254 |
| C | -6.2750051 | 0.0000000 | 1.4236704 | -6.2802090 | 0.0000000 | 1.4227767 |
| H | -5.6206829 | 0.0000000 | 2.2873754 | -5.6290259 | 0.0000000 | 2.2889010 |
| H | -9.0362001 | 0.0000000 | -0.4095103 | -9.0330422 | 0.0000000 | -0.4250721 |
| H | -8.3659827 | 0.0000000 | 2.2686700 | -8.3682297 | 0.0000000 | 2.2539395 |
| H | 9.0362001 | 0.0000000 | -0.4095103 | 9.0330422 | 0.0000000 | -0.4250721 |
|  |  |  |  |  |  |  |
| **6O/BP** | **Ground state** | | | **Excited state** | | |
| O | 1.8144441 | -0.0058103 | 0.0000000 | 1.8174727 | 0.0050666 | 0.0000000 |
| C | 0.5226866 | -0.4853221 | 0.0000000 | 0.5202788 | -0.4775213 | 0.0000000 |
| C | 0.5381572 | -1.8671772 | 0.0000000 | 0.5374649 | -1.8731743 | 0.0000000 |
| C | 1.8999293 | -2.2609314 | 0.0000000 | 1.8866074 | -2.2673611 | 0.0000000 |
| C | 2.6504714 | -1.1007336 | 0.0000000 | 2.6526298 | -1.0999436 | 0.0000000 |
| C | 4.0531634 | -0.8379807 | 0.0000000 | 4.0414268 | -0.8534460 | 0.0000000 |
| O | 4.8887239 | -1.9337264 | 0.0000000 | 4.8804739 | -1.9545379 | 0.0000000 |
| C | 6.1795192 | -1.4554076 | 0.0000000 | 6.1752427 | -1.4688930 | 0.0000000 |
| C | 6.1668590 | -0.0754144 | 0.0000000 | 6.1541360 | -0.0748859 | 0.0000000 |
| C | 4.8045382 | 0.3210050 | 0.0000000 | 4.8052504 | 0.3167286 | 0.0000000 |
| H | 7.0412530 | 0.5649050 | 0.0000000 | 7.0290302 | 0.5651122 | 0.0000000 |
| H | 2.2953414 | -3.2699357 | 0.0000000 | 2.2814509 | -3.2766243 | 0.0000000 |
| H | -0.3347158 | -2.5094677 | 0.0000000 | -0.3387679 | -2.5110667 | 0.0000000 |
| C | 7.2276699 | -2.4296342 | 0.0000000 | 7.2214438 | -2.4232609 | 0.0000000 |
| O | 8.5172213 | -1.9465368 | 0.0000000 | 8.5154943 | -1.9353032 | 0.0000000 |
| C | 9.3482587 | -3.0358545 | 0.0000000 | 9.3470135 | -3.0249796 | 0.0000000 |
| C | 8.6210347 | -4.1925384 | 0.0000000 | 8.6196057 | -4.1873308 | 0.0000000 |
| C | 7.2463405 | -3.8078845 | 0.0000000 | 7.2494914 | -3.8130562 | 0.0000000 |
| H | 6.3776698 | -4.4556005 | 0.0000000 | 6.3833214 | -4.4640931 | 0.0000000 |
| H | 10.4083599 | -2.8147906 | 0.0000000 | 10.4074775 | -2.8047002 | 0.0000000 |
| H | 9.0198570 | -5.2009758 | 0.0000000 | 9.0246968 | -5.1935647 | 0.0000000 |
| C | -0.5226866 | 0.4853221 | 0.0000000 | -0.5202788 | 0.4775213 | 0.0000000 |
| O | -1.8144441 | 0.0058103 | 0.0000000 | -1.8174727 | -0.0050666 | 0.0000000 |
| C | -2.6504714 | 1.1007336 | 0.0000000 | -2.6526298 | 1.0999436 | 0.0000000 |
| C | -1.8999293 | 2.2609314 | 0.0000000 | -1.8866074 | 2.2673611 | 0.0000000 |
| C | -0.5381572 | 1.8671772 | 0.0000000 | -0.5374649 | 1.8731743 | 0.0000000 |
| H | -2.2953414 | 3.2699357 | 0.0000000 | -2.2814509 | 3.2766243 | 0.0000000 |
| H | 0.3347158 | 2.5094677 | 0.0000000 | 0.3387679 | 2.5110667 | 0.0000000 |
| H | 4.4107932 | 1.3306459 | 0.0000000 | 4.4082911 | 1.3253119 | 0.0000000 |
| C | -4.0531634 | 0.8379807 | 0.0000000 | -4.0414268 | 0.8534460 | 0.0000000 |
| C | -4.8045382 | -0.3210050 | 0.0000000 | -4.8052504 | -0.3167286 | 0.0000000 |
| C | -6.1668590 | 0.0754144 | 0.0000000 | -6.1541360 | 0.0748859 | 0.0000000 |
| C | -6.1795192 | 1.4554076 | 0.0000000 | -6.1752427 | 1.4688930 | 0.0000000 |
| O | -4.8887239 | 1.9337264 | 0.0000000 | -4.8804739 | 1.9545379 | 0.0000000 |
| H | -7.0412530 | -0.5649050 | 0.0000000 | -7.0290302 | -0.5651122 | 0.0000000 |
| H | -4.4107932 | -1.3306459 | 0.0000000 | -4.4082911 | -1.3253119 | 0.0000000 |
| C | -7.2276699 | 2.4296342 | 0.0000000 | -7.2214438 | 2.4232609 | 0.0000000 |
| C | -7.2463405 | 3.8078845 | 0.0000000 | -7.2494914 | 3.8130562 | 0.0000000 |
| C | -8.6210347 | 4.1925384 | 0.0000000 | -8.6196057 | 4.1873308 | 0.0000000 |
| C | -9.3482587 | 3.0358545 | 0.0000000 | -9.3470135 | 3.0249796 | 0.0000000 |
| O | -8.5172213 | 1.9465368 | 0.0000000 | -8.5154943 | 1.9353032 | 0.0000000 |
| H | -9.0198570 | 5.2009758 | 0.0000000 | -9.0246968 | 5.1935647 | 0.0000000 |
| H | -10.408359 | 2.8147906 | 0.0000000 | -10.407477 | 2.8047002 | 0.0000000 |
| H | -6.3776698 | 4.4556005 | 0.0000000 | -6.3833214 | 4.4640931 | 0.0000000 |
|  |  |  |  |  |  |  |
| **7O/BP** | **Ground state** | | | **Excited state** | | |
| C | -9.7639698 | 0.0000000 | -1.4990653 | -9.7675455 | 0.0000000 | -1.5027171 |
| C | -9.3626496 | 0.0000000 | -0.1804034 | -9.3554743 | 0.0000000 | -0.1773665 |
| O | -10.466916 | 0.0000000 | 0.6423464 | -10.461958 | 0.0000000 | 0.6506286 |
| C | -11.568147 | 0.0000000 | -0.1728036 | -11.563899 | 0.0000000 | -0.1640661 |
| C | -11.191391 | 0.0000000 | -1.4861377 | -11.188993 | 0.0000000 | -1.4819771 |
| C | -8.0849004 | 0.0000000 | 0.4638409 | -8.0840956 | 0.0000000 | 0.4509105 |
| O | -6.9780591 | 0.0000000 | -0.3545556 | -6.9752063 | 0.0000000 | -0.3730026 |
| C | -5.8707487 | 0.0000000 | 0.4656494 | -5.8638633 | 0.0000000 | 0.4514860 |
| C | -6.2702206 | 0.0000000 | 1.7878776 | -6.2734078 | 0.0000000 | 1.7861728 |
| C | -7.6890015 | 0.0000000 | 1.7859162 | -7.6789091 | 0.0000000 | 1.7829916 |
| C | -4.5964807 | 0.0000000 | -0.1767396 | -4.5977651 | 0.0000000 | -0.1709043 |
| O | -3.4889524 | 0.0000000 | 0.6424465 | -3.4880701 | 0.0000000 | 0.6566229 |
| C | -2.3814866 | 0.0000000 | -0.1774619 | -2.3766200 | 0.0000000 | -0.1665088 |
| C | -2.7807860 | 0.0000000 | -1.5005597 | -2.7816084 | 0.0000000 | -1.5014543 |
| C | -4.1982337 | 0.0000000 | -1.4999909 | -4.1867431 | 0.0000000 | -1.5046451 |
| C | -1.1075419 | 0.0000000 | 0.4639884 | -1.1102991 | 0.0000000 | 0.4604624 |
| O | 0.0000000 | 0.0000000 | -0.3556499 | 0.0000000 | 0.0000000 | -0.3648840 |
| C | 1.1075419 | 0.0000000 | 0.4639884 | 1.1102991 | 0.0000000 | 0.4604624 |
| C | 0.7085952 | 0.0000000 | 1.7873419 | 0.7035160 | 0.0000000 | 1.7937882 |
| C | -0.7085952 | 0.0000000 | 1.7873419 | -0.7035160 | 0.0000000 | 1.7937882 |
| C | 2.3814866 | 0.0000000 | -0.1774619 | 2.3766200 | 0.0000000 | -0.1665088 |
| O | 3.4889524 | 0.0000000 | 0.6424465 | 3.4880701 | 0.0000000 | 0.6566229 |
| C | 4.5964807 | 0.0000000 | -0.1767396 | 4.5977651 | 0.0000000 | -0.1709043 |
| C | 4.1982337 | 0.0000000 | -1.4999909 | 4.1867431 | 0.0000000 | -1.5046451 |
| C | 2.7807860 | 0.0000000 | -1.5005597 | 2.7816084 | 0.0000000 | -1.5014543 |
| C | 5.8707487 | 0.0000000 | 0.4656494 | 5.8638633 | 0.0000000 | 0.4514860 |
| O | 6.9780591 | 0.0000000 | -0.3545556 | 6.9752063 | 0.0000000 | -0.3730026 |
| C | 8.0849004 | 0.0000000 | 0.4638409 | 8.0840956 | 0.0000000 | 0.4509105 |
| C | 7.6890015 | 0.0000000 | 1.7859162 | 7.6789091 | 0.0000000 | 1.7829916 |
| C | 6.2702206 | 0.0000000 | 1.7878776 | 6.2734078 | 0.0000000 | 1.7861728 |
| C | 9.3626496 | 0.0000000 | -0.1804034 | 9.3554743 | 0.0000000 | -0.1773665 |
| C | 9.7639698 | 0.0000000 | -1.4990653 | 9.7675455 | 0.0000000 | -1.5027171 |
| C | 11.1913910 | 0.0000000 | -1.4861377 | 11.1889937 | 0.0000000 | -1.4819771 |
| C | 11.5681477 | 0.0000000 | -0.1728036 | 11.5638996 | 0.0000000 | -0.1640661 |
| O | 10.4669167 | 0.0000000 | 0.6423464 | 10.4619586 | 0.0000000 | 0.6506286 |
| H | -1.3686883 | 0.0000000 | 2.6468317 | -1.3652130 | 0.0000000 | 2.6521076 |
| H | 2.1210394 | 0.0000000 | -2.3603167 | 2.1179238 | 0.0000000 | -2.3583681 |
| H | 4.8587085 | 0.0000000 | -2.3591822 | 4.8464219 | 0.0000000 | -2.3645440 |
| H | -2.1210394 | 0.0000000 | -2.3603167 | -2.1179238 | 0.0000000 | -2.3583681 |
| H | -4.8587085 | 0.0000000 | -2.3591822 | -4.8464219 | 0.0000000 | -2.3645440 |
| H | 8.3508522 | 0.0000000 | 2.6441256 | 8.3423191 | 0.0000000 | 2.6402907 |
| H | 5.6112709 | 0.0000000 | 2.6482253 | 5.6133264 | 0.0000000 | 2.6458265 |
| H | 1.3686883 | 0.0000000 | 2.6468317 | 1.3652130 | 0.0000000 | 2.6521076 |
| H | 11.8549982 | 0.0000000 | -2.3438247 | 11.8574301 | 0.0000000 | -2.3361782 |
| H | 9.1097630 | 0.0000000 | -2.3628592 | 9.1165512 | 0.0000000 | -2.3688871 |
| H | -5.6112709 | 0.0000000 | 2.6482253 | -5.6133264 | 0.0000000 | 2.6458265 |
| H | -8.3508522 | 0.0000000 | 2.6441256 | -8.3423191 | 0.0000000 | 2.6402907 |
| H | -9.1097630 | 0.0000000 | -2.3628592 | -9.1165512 | 0.0000000 | -2.3688871 |
| H | -11.854998 | 0.0000000 | -2.3438247 | -11.857430 | 0.0000000 | -2.3361782 |
| H | -12.524913 | 0.0000000 | 0.3344288 | -12.520885 | 0.0000000 | 0.3430667 |
| H | 12.5249135 | 0.0000000 | 0.3344288 | 12.5208850 | 0.0000000 | 0.3430667 |
|  |  |  |  |  |  |  |
| **8O/BP** | **Ground state** | | | **Excited state** | | |
| O | -11.9493588 | 2.5647623 | 0.0000000 | -11.945986 | 2.5577313 | 0.0000000 |
| C | -10.6746677 | 3.0857915 | 0.0000000 | -10.668491 | 3.0826894 | 0.0000000 |
| C | -10.7340802 | 4.4628900 | 0.0000000 | -10.735492 | 4.4673015 | 0.0000000 |
| C | -12.1195241 | 4.8067166 | 0.0000000 | -12.117858 | 4.8033367 | 0.0000000 |
| C | -12.8122125 | 3.6290109 | 0.0000000 | -12.809659 | 3.6214771 | 0.0000000 |
| C | -9.5982033 | 2.1429721 | 0.0000000 | -9.5939216 | 2.1544629 | 0.0000000 |
| C | -9.5448983 | 0.7639049 | 0.0000000 | -9.5358081 | 0.7649811 | 0.0000000 |
| C | -8.1715439 | 0.4078201 | 0.0000000 | -8.1748201 | 0.4095330 | 0.0000000 |
| C | -7.4546279 | 1.5884621 | 0.0000000 | -7.4450903 | 1.5982721 | 0.0000000 |
| O | -8.3221193 | 2.6591311 | 0.0000000 | -8.3149142 | 2.6738773 | 0.0000000 |
| C | -6.0603645 | 1.8924365 | 0.0000000 | -6.0631910 | 1.8850820 | 0.0000000 |
| O | -5.1923381 | 0.8227923 | 0.0000000 | -5.1945700 | 0.8081320 | 0.0000000 |
| C | -3.9152848 | 1.3404060 | 0.0000000 | -3.9131548 | 1.3276928 | 0.0000000 |
| C | -3.9717855 | 2.7213128 | 0.0000000 | -3.9734098 | 2.7213892 | 0.0000000 |
| C | -5.3444867 | 3.0744740 | 0.0000000 | -5.3331236 | 3.0739239 | 0.0000000 |
| C | -2.8417429 | 0.4013992 | 0.0000000 | -2.8426265 | 0.4060787 | 0.0000000 |
| O | -1.5647153 | 0.9186454 | 0.0000000 | -1.5617746 | 0.9284299 | 0.0000000 |
| C | -0.6967728 | -0.1515369 | 0.0000000 | -0.6919690 | -0.1460501 | 0.0000000 |
| C | -1.4135252 | -1.3334725 | 0.0000000 | -1.4168655 | -1.3355828 | 0.0000000 |
| C | -2.7857448 | -0.9797336 | 0.0000000 | -2.7797971 | -0.9861836 | 0.0000000 |
| C | 0.6967728 | 0.1515369 | 0.0000000 | 0.6919690 | 0.1460501 | 0.0000000 |
| O | 1.5647153 | -0.9186454 | 0.0000000 | 1.5617746 | -0.9284299 | 0.0000000 |
| C | 2.8417429 | -0.4013992 | 0.0000000 | 2.8426265 | -0.4060787 | 0.0000000 |
| C | 2.7857448 | 0.9797336 | 0.0000000 | 2.7797971 | 0.9861836 | 0.0000000 |
| C | 1.4135252 | 1.3334725 | 0.0000000 | 1.4168655 | 1.3355828 | 0.0000000 |
| C | 3.9152848 | -1.3404060 | 0.0000000 | 3.9131548 | -1.3276928 | 0.0000000 |
| O | 5.1923381 | -0.8227923 | 0.0000000 | 5.1945700 | -0.8081320 | 0.0000000 |
| C | 6.0603645 | -1.8924365 | 0.0000000 | 6.0631910 | -1.8850820 | 0.0000000 |
| C | 5.3444867 | -3.0744740 | 0.0000000 | 5.3331236 | -3.0739239 | 0.0000000 |
| C | 3.9717855 | -2.7213128 | 0.0000000 | 3.9734098 | -2.7213892 | 0.0000000 |
| H | 3.6395061 | 1.6472173 | 0.0000000 | 3.6337308 | 1.6535270 | 0.0000000 |
| H | -0.9888915 | -2.3305362 | 0.0000000 | -0.9894216 | -2.3315460 | 0.0000000 |
| H | -3.6395061 | -1.6472173 | 0.0000000 | -3.6337308 | -1.6535270 | 0.0000000 |
| H | 3.1183649 | -3.3892384 | 0.0000000 | 3.1175824 | -3.3864812 | 0.0000000 |
| C | 7.4546279 | -1.5884621 | 0.0000000 | 7.4450903 | -1.5982721 | 0.0000000 |
| H | 5.7696639 | -4.0712976 | 0.0000000 | 5.7577766 | -4.0711082 | 0.0000000 |
| H | -5.7696639 | 4.0712976 | 0.0000000 | -5.7577766 | 4.0711082 | 0.0000000 |
| H | -3.1183649 | 3.3892384 | 0.0000000 | -3.1175824 | 3.3864812 | 0.0000000 |
| H | 0.9888915 | 2.3305362 | 0.0000000 | 0.9894216 | 2.3315460 | 0.0000000 |
| H | -10.4000470 | 0.0981059 | 0.0000000 | -10.392664 | 0.1010028 | 0.0000000 |
| H | -7.7482430 | -0.5897929 | 0.0000000 | -7.7513965 | -0.5881284 | 0.0000000 |
| H | -12.5480098 | 5.8029086 | 0.0000000 | -12.551145 | 5.7976320 | 0.0000000 |
| H | -13.8653146 | 3.3766959 | 0.0000000 | -13.862850 | 3.3690411 | 0.0000000 |
| H | -9.8849489 | 5.1360198 | 0.0000000 | -9.8886256 | 5.1432019 | 0.0000000 |
| O | 8.3221193 | -2.6591311 | 0.0000000 | 8.3149142 | -2.6738773 | 0.0000000 |
| C | 9.5982033 | -2.1429721 | 0.0000000 | 9.5939216 | -2.1544629 | 0.0000000 |
| C | 9.5448983 | -0.7639049 | 0.0000000 | 9.5358081 | -0.7649811 | 0.0000000 |
| C | 8.1715439 | -0.4078201 | 0.0000000 | 8.1748201 | -0.4095330 | 0.0000000 |
| H | 7.7482430 | 0.5897929 | 0.0000000 | 7.7513965 | 0.5881284 | 0.0000000 |
| H | 10.4000470 | -0.0981059 | 0.0000000 | 10.3926647 | -0.1010028 | 0.0000000 |
| C | 10.6746677 | -3.0857915 | 0.0000000 | 10.6684916 | -3.0826894 | 0.0000000 |
| O | 11.9493588 | -2.5647623 | 0.0000000 | 11.9459867 | -2.5577313 | 0.0000000 |
| C | 12.8122125 | -3.6290109 | 0.0000000 | 12.8096595 | -3.6214771 | 0.0000000 |
| C | 12.1195241 | -4.8067166 | 0.0000000 | 12.1178584 | -4.8033367 | 0.0000000 |
| C | 10.7340802 | -4.4628900 | 0.0000000 | 10.7354929 | -4.4673015 | 0.0000000 |
| H | 9.8849489 | -5.1360198 | 0.0000000 | 9.8886256 | -5.1432019 | 0.0000000 |
| H | 12.5480098 | -5.8029086 | 0.0000000 | 12.5511452 | -5.7976320 | 0.0000000 |
| H | 13.8653146 | -3.3766959 | 0.0000000 | 13.8628503 | -3.3690411 | 0.0000000 |
|  |  |  |  |  |  |  |
| **9O/BP** | **Ground state** | | | **Excited state** | | |
| C | -13.2528363 | 0.0000000 | -1.5354357 | -13.254085 | 0.0000000 | -1.5391724 |
| C | -12.8514250 | 0.0000000 | -0.2168026 | -12.844958 | 0.0000000 | -0.2161265 |
| O | -13.9556198 | 0.0000000 | 0.6060341 | -13.950593 | 0.0000000 | 0.6104383 |
| C | -15.0568884 | 0.0000000 | -0.2090272 | -15.052364 | 0.0000000 | -0.2039517 |
| C | -14.6802414 | 0.0000000 | -1.5224021 | -14.677406 | 0.0000000 | -1.5204645 |
| C | -11.5736461 | 0.0000000 | 0.4273678 | -11.571904 | 0.0000000 | 0.4164978 |
| O | -10.4668510 | 0.0000000 | -0.3910352 | -10.463219 | 0.0000000 | -0.4046309 |
| C | -9.3595296 | 0.0000000 | 0.4291635 | -9.3528978 | 0.0000000 | 0.4195647 |
| C | -9.7589848 | 0.0000000 | 1.7514017 | -9.7625000 | 0.0000000 | 1.7515329 |
| C | -11.1777375 | 0.0000000 | 1.7494658 | -11.170367 | 0.0000000 | 1.7464176 |
| C | -8.0853048 | 0.0000000 | -0.2132556 | -8.0857985 | 0.0000000 | -0.2040412 |
| O | -6.9777423 | 0.0000000 | 0.6058072 | -6.9757950 | 0.0000000 | 0.6208413 |
| C | -5.8703463 | 0.0000000 | -0.2142411 | -5.8648103 | 0.0000000 | -0.2021112 |
| C | -6.2698099 | 0.0000000 | -1.5373193 | -6.2720465 | 0.0000000 | -1.5363218 |
| C | -7.6871965 | 0.0000000 | -1.5366027 | -7.6766371 | 0.0000000 | -1.5370485 |
| C | -4.5964111 | 0.0000000 | 0.4270519 | -4.5980775 | 0.0000000 | 0.4218090 |
| O | -3.4888988 | 0.0000000 | -0.3925168 | -3.4880815 | 0.0000000 | -0.4034736 |
| C | -2.3813386 | 0.0000000 | 0.4272372 | -2.3775730 | 0.0000000 | 0.4191367 |
| C | -2.7804845 | 0.0000000 | 1.7506607 | -2.7826046 | 0.0000000 | 1.7519698 |
| C | -4.1975190 | 0.0000000 | 1.7505482 | -4.1889250 | 0.0000000 | 1.7542264 |
| C | -1.1075512 | 0.0000000 | -0.2139450 | -1.1100014 | 0.0000000 | -0.2084973 |
| O | 0.0000000 | 0.0000000 | 0.6057147 | 0.0000000 | 0.0000000 | 0.6152514 |
| C | 1.1075512 | 0.0000000 | -0.2139450 | 1.1100014 | 0.0000000 | -0.2084973 |
| C | 0.7084848 | 0.0000000 | -1.5374580 | 0.7038785 | 0.0000000 | -1.5402198 |
| C | -0.7084848 | 0.0000000 | -1.5374580 | -0.7038785 | 0.0000000 | -1.5402198 |
| C | 2.3813386 | 0.0000000 | 0.4272372 | 2.3775730 | 0.0000000 | 0.4191367 |
| O | 3.4888988 | 0.0000000 | -0.3925168 | 3.4880815 | 0.0000000 | -0.4034736 |
| C | 4.5964111 | 0.0000000 | 0.4270519 | 4.5980775 | 0.0000000 | 0.4218090 |
| C | 4.1975190 | 0.0000000 | 1.7505482 | 4.1889250 | 0.0000000 | 1.7542264 |
| C | 2.7804845 | 0.0000000 | 1.7506607 | 2.7826046 | 0.0000000 | 1.7519698 |
| C | 5.8703463 | 0.0000000 | -0.2142411 | 5.8648103 | 0.0000000 | -0.2021112 |
| C | 6.2698099 | 0.0000000 | -1.5373193 | 6.2720465 | 0.0000000 | -1.5363218 |
| C | 7.6871965 | 0.0000000 | -1.5366027 | 7.6766371 | 0.0000000 | -1.5370485 |
| C | 8.0853048 | 0.0000000 | -0.2132556 | 8.0857985 | 0.0000000 | -0.2040412 |
| O | 6.9777423 | 0.0000000 | 0.6058072 | 6.9757950 | 0.0000000 | 0.6208413 |
| C | 9.3595296 | 0.0000000 | 0.4291635 | 9.3528978 | 0.0000000 | 0.4195647 |
| O | 10.4668510 | 0.0000000 | -0.3910352 | 10.4632194 | 0.0000000 | -0.4046309 |
| C | 11.5736461 | 0.0000000 | 0.4273678 | 11.5719048 | 0.0000000 | 0.4164978 |
| C | 11.1777375 | 0.0000000 | 1.7494658 | 11.1703677 | 0.0000000 | 1.7464176 |
| C | 9.7589848 | 0.0000000 | 1.7514017 | 9.7625000 | 0.0000000 | 1.7515329 |
| H | -4.8576949 | 0.0000000 | 2.6099700 | -4.8488221 | 0.0000000 | 2.6139630 |
| H | -1.3685747 | 0.0000000 | -2.3969507 | -1.3650879 | 0.0000000 | -2.3989364 |
| H | 1.3685747 | 0.0000000 | -2.3969507 | 1.3650879 | 0.0000000 | -2.3989364 |
| H | -5.6101754 | 0.0000000 | -2.3971657 | -5.6101710 | 0.0000000 | -2.3946189 |
| H | -8.3477658 | 0.0000000 | -2.3957174 | -8.3372817 | 0.0000000 | -2.3963136 |
| H | 4.8576949 | 0.0000000 | 2.6099700 | 4.8488221 | 0.0000000 | 2.6139630 |
| H | 2.1204892 | 0.0000000 | 2.6102296 | 2.1200195 | 0.0000000 | 2.6096964 |
| H | -2.1204892 | 0.0000000 | 2.6102296 | -2.1200195 | 0.0000000 | 2.6096964 |
| H | 8.3477658 | 0.0000000 | -2.3957174 | 8.3372817 | 0.0000000 | -2.3963136 |
| H | 5.6101754 | 0.0000000 | -2.3971657 | 5.6101710 | 0.0000000 | -2.3946189 |
| H | 11.8395799 | 0.0000000 | 2.6076786 | 11.8346081 | 0.0000000 | 2.6030520 |
| C | 12.8514250 | 0.0000000 | -0.2168026 | 12.8449582 | 0.0000000 | -0.2161265 |
| H | 9.1000355 | 0.0000000 | 2.6117514 | 9.1040057 | 0.0000000 | 2.6123031 |
| H | -9.1000355 | 0.0000000 | 2.6117514 | -9.1040057 | 0.0000000 | 2.6123031 |
| H | -11.839579 | 0.0000000 | 2.6076786 | -11.834608 | 0.0000000 | 2.6030520 |
| H | -12.5987036 | 0.0000000 | -2.3992869 | -12.602384 | 0.0000000 | -2.4047981 |
| H | -15.3439155 | 0.0000000 | -2.3800346 | -15.344583 | 0.0000000 | -2.3755378 |
| H | -16.0136204 | 0.0000000 | 0.2982712 | -16.009123 | 0.0000000 | 0.3034890 |
| O | 13.9556198 | 0.0000000 | 0.6060341 | 13.9505935 | 0.0000000 | 0.6104383 |
| C | 15.0568884 | 0.0000000 | -0.2090272 | 15.0523644 | 0.0000000 | -0.2039517 |
| C | 14.6802414 | 0.0000000 | -1.5224021 | 14.6774063 | 0.0000000 | -1.5204645 |
| C | 13.2528363 | 0.0000000 | -1.5354357 | 13.2540855 | 0.0000000 | -1.5391724 |
| H | 12.5987036 | 0.0000000 | -2.3992869 | 12.6023846 | 0.0000000 | -2.4047981 |
| H | 15.3439155 | 0.0000000 | -2.3800346 | 15.3445835 | 0.0000000 | -2.3755378 |
| H | 16.0136204 | 0.0000000 | 0.2982712 | 16.0091233 | 0.0000000 | 0.3034890 |

Part 2.

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| **2O/**  **TPSSh** | **Ground state** | | | **Excited state** | | |
| C | -2.8183862 | 0.4334075 | 0.0000000 | -2.8084512 | 0.4449548 | 0.0000000 |
| C | -2.7980694 | -0.9242583 | 0.0000000 | -2.7800261 | -0.9384330 | 0.0000000 |
| C | -1.4245153 | -1.3069473 | 0.0000000 | -1.4404738 | -1.3321118 | 0.0000000 |
| C | -0.7018155 | -0.1455675 | 0.0000000 | -0.6797095 | -0.1326912 | 0.0000000 |
| C | 0.7018155 | 0.1455675 | 0.0000000 | 0.6797095 | 0.1326912 | 0.0000000 |
| C | 1.4245153 | 1.3069473 | 0.0000000 | 1.4404738 | 1.3321118 | 0.0000000 |
| C | 2.7980694 | 0.9242583 | 0.0000000 | 2.7800261 | 0.9384330 | 0.0000000 |
| C | 2.8183862 | -0.4334075 | 0.0000000 | 2.8084512 | -0.4449548 | 0.0000000 |
| O | -1.5481839 | 0.9292588 | 0.0000000 | -1.5409844 | 0.9687817 | 0.0000000 |
| O | 1.5481839 | -0.9292588 | 0.0000000 | 1.5409844 | -0.9687817 | 0.0000000 |
| H | -3.6035178 | 1.1692253 | 0.0000000 | -3.6100628 | 1.1643397 | 0.0000000 |
| H | -3.6569230 | -1.5756293 | 0.0000000 | -3.6492779 | -1.5770079 | 0.0000000 |
| H | -1.0181188 | -2.3044725 | 0.0000000 | -1.0298963 | -2.3278064 | 0.0000000 |
| H | 1.0181188 | 2.3044725 | 0.0000000 | 1.0298963 | 2.3278064 | 0.0000000 |
| H | 3.6569230 | 1.5756293 | 0.0000000 | 3.6492779 | 1.5770079 | 0.0000000 |
| H | 3.6035178 | -1.1692253 | 0.0000000 | 3.6100628 | -1.1643397 | 0.0000000 |
|  |  |  |  |  |  |  |
| **3O/**  **TPSSh** | **Ground state** | | | **Excited state** | | |
| O | 3.4749960 | 0.0000000 | 0.8393779 | 3.4786274 | 0.0000000 | 0.8556377 |
| C | 4.5709333 | 0.0000000 | 0.0284136 | 4.5590116 | 0.0000000 | 0.0192121 |
| C | 4.1962749 | 0.0000000 | -1.2770268 | 4.1605691 | 0.0000000 | -1.2923799 |
| C | 2.7711738 | 0.0000000 | -1.2878112 | 2.7525260 | 0.0000000 | -1.2965567 |
| C | 2.3762803 | 0.0000000 | 0.0231454 | 2.3573282 | 0.0000000 | 0.0462034 |
| C | 1.1009696 | 0.0000000 | 0.6709683 | 1.1078560 | 0.0000000 | 0.6694023 |
| O | 0.0000000 | 0.0000000 | -0.1426157 | 0.0000000 | 0.0000000 | -0.1654335 |
| C | -1.1009696 | 0.0000000 | 0.6709683 | -1.1078560 | 0.0000000 | 0.6694023 |
| C | -0.7091193 | 0.0000000 | 1.9838914 | -0.6939836 | 0.0000000 | 2.0141465 |
| C | 0.7091193 | 0.0000000 | 1.9838914 | 0.6939836 | 0.0000000 | 2.0141465 |
| C | -2.3762803 | 0.0000000 | 0.0231454 | -2.3573282 | 0.0000000 | 0.0462034 |
| O | -3.4749960 | 0.0000000 | 0.8393779 | -3.4786274 | 0.0000000 | 0.8556377 |
| C | -4.5709333 | 0.0000000 | 0.0284136 | -4.5590116 | 0.0000000 | 0.0192121 |
| C | -4.1962749 | 0.0000000 | -1.2770268 | -4.1605691 | 0.0000000 | -1.2923799 |
| C | -2.7711738 | 0.0000000 | -1.2878112 | -2.7525260 | 0.0000000 | -1.2965567 |
| H | 5.5213076 | 0.0000000 | 0.5330248 | 5.5214519 | 0.0000000 | 0.5017625 |
| H | 4.8552345 | 0.0000000 | -2.1300596 | 4.8163561 | 0.0000000 | -2.1485825 |
| H | 2.1188255 | 0.0000000 | -2.1448858 | 2.0877986 | 0.0000000 | -2.1443771 |
| H | -2.1188255 | 0.0000000 | -2.1448858 | -2.0877986 | 0.0000000 | -2.1443771 |
| H | -5.5213076 | 0.0000000 | 0.5330248 | -5.5214519 | 0.0000000 | 0.5017625 |
| H | -4.8552345 | 0.0000000 | -2.1300596 | -4.8163561 | 0.0000000 | -2.1485825 |
| H | 1.3665026 | 0.0000000 | 2.8372721 | 1.3570699 | 0.0000000 | 2.8632508 |
| H | -1.3665026 | 0.0000000 | 2.8372721 | -1.3570699 | 0.0000000 | 2.8632508 |
|  |  |  |  |  |  |  |
| **4O/**  **TPSSh** | **Ground state** | | | **Excited state** | | |
| O | -1.7709338 | 0.3518479 | 0.0000000 | -1.7715972 | 0.3791061 | 0.0000000 |
| C | -2.8041099 | -0.5460791 | 0.0000000 | -2.8067382 | -0.5341768 | 0.0000000 |
| C | -2.3097151 | -1.8245799 | 0.0000000 | -2.2927166 | -1.8316138 | 0.0000000 |
| C | -0.8969509 | -1.7135527 | 0.0000000 | -0.9039843 | -1.7244158 | 0.0000000 |
| C | -0.6084336 | -0.3725493 | 0.0000000 | -0.6002125 | -0.3556400 | 0.0000000 |
| C | 0.6084336 | 0.3725493 | 0.0000000 | 0.6002125 | 0.3556400 | 0.0000000 |
| O | 1.7709338 | -0.3518479 | 0.0000000 | 1.7715972 | -0.3791061 | 0.0000000 |
| C | 2.8041099 | 0.5460791 | 0.0000000 | 2.8067382 | 0.5341768 | 0.0000000 |
| C | 2.3097151 | 1.8245799 | 0.0000000 | 2.2927166 | 1.8316138 | 0.0000000 |
| C | 0.8969509 | 1.7135527 | 0.0000000 | 0.9039843 | 1.7244158 | 0.0000000 |
| C | 4.1263916 | 0.0018573 | 0.0000000 | 4.1116515 | 0.0133113 | 0.0000000 |
| O | 5.1569339 | 0.9028178 | 0.0000000 | 5.1527267 | 0.9162443 | 0.0000000 |
| C | 6.3136398 | 0.1813444 | 0.0000000 | 6.3049242 | 0.1856361 | 0.0000000 |
| C | 6.0438038 | -1.1498225 | 0.0000000 | 6.0282183 | -1.1523946 | 0.0000000 |
| C | 4.6242583 | -1.2737866 | 0.0000000 | 4.6206861 | -1.2794994 | 0.0000000 |
| H | -2.8981604 | -2.7268823 | 0.0000000 | -2.8850828 | -2.7316406 | 0.0000000 |
| H | -0.1751811 | -2.5131712 | 0.0000000 | -0.1780623 | -2.5205402 | 0.0000000 |
| H | 4.0420985 | -2.1799972 | 0.0000000 | 4.0364415 | -2.1845334 | 0.0000000 |
| H | 7.2210124 | 0.7597305 | 0.0000000 | 7.2177463 | 0.7561530 | 0.0000000 |
| H | 6.7684185 | -1.9478262 | 0.0000000 | 6.7556550 | -1.9484229 | 0.0000000 |
| H | 0.1751811 | 2.5131712 | 0.0000000 | 0.1780623 | 2.5205402 | 0.0000000 |
| H | 2.8981604 | 2.7268823 | 0.0000000 | 2.8850828 | 2.7316406 | 0.0000000 |
| C | -4.1263916 | -0.0018573 | 0.0000000 | -4.1116515 | -0.0133113 | 0.0000000 |
| O | -5.1569339 | -0.9028178 | 0.0000000 | -5.1527267 | -0.9162443 | 0.0000000 |
| C | -6.3136398 | -0.1813444 | 0.0000000 | -6.3049242 | -0.1856361 | 0.0000000 |
| C | -6.0438038 | 1.1498225 | 0.0000000 | -6.0282183 | 1.1523946 | 0.0000000 |
| C | -4.6242583 | 1.2737866 | 0.0000000 | -4.6206861 | 1.2794994 | 0.0000000 |
| H | -4.0420985 | 2.1799972 | 0.0000000 | -4.0364415 | 2.1845334 | 0.0000000 |
| H | -7.2210124 | -0.7597305 | 0.0000000 | -7.2177463 | -0.7561530 | 0.0000000 |
| H | -6.7684185 | 1.9478262 | 0.0000000 | -6.7556550 | 1.9484229 | 0.0000000 |
|  |  |  |  |  |  |  |
| **5O/**  **TPSSh** | **Ground state** | | | **Excited state** | | |
| O | 3.4748873 | 0.0000000 | 0.2726931 | 3.4728369 | 0.0000000 | 0.2988335 |
| C | 4.5758134 | 0.0000000 | -0.5406406 | 4.5746371 | 0.0000000 | -0.5261926 |
| C | 4.1841723 | 0.0000000 | -1.8544522 | 4.1664975 | 0.0000000 | -1.8544192 |
| C | 2.7673449 | 0.0000000 | -1.8557792 | 2.7697183 | 0.0000000 | -1.8557289 |
| C | 2.3732802 | 0.0000000 | -0.5416140 | 2.3628453 | 0.0000000 | -0.5200704 |
| C | 1.1016006 | 0.0000000 | 0.1041228 | 1.1070073 | 0.0000000 | 0.0970978 |
| O | 0.0000000 | 0.0000000 | -0.7097659 | 0.0000000 | 0.0000000 | -0.7277878 |
| C | -1.1016006 | 0.0000000 | 0.1041228 | -1.1070073 | 0.0000000 | 0.0970978 |
| C | -0.7079593 | 0.0000000 | 1.4188296 | -0.6966661 | 0.0000000 | 1.4326193 |
| C | 0.7079593 | 0.0000000 | 1.4188296 | 0.6966661 | 0.0000000 | 1.4326193 |
| C | -2.3732802 | 0.0000000 | -0.5416140 | -2.3628453 | 0.0000000 | -0.5200704 |
| O | -3.4748873 | 0.0000000 | 0.2726931 | -3.4728369 | 0.0000000 | 0.2988335 |
| C | -4.5758134 | 0.0000000 | -0.5406406 | -4.5746371 | 0.0000000 | -0.5261926 |
| C | -4.1841723 | 0.0000000 | -1.8544522 | -4.1664975 | 0.0000000 | -1.8544192 |
| C | -2.7673449 | 0.0000000 | -1.8557792 | -2.7697183 | 0.0000000 | -1.8557289 |
| C | 5.8509313 | 0.0000000 | 0.1061624 | 5.8402979 | 0.0000000 | 0.0964854 |
| O | 6.9493116 | 0.0000000 | -0.7107598 | 6.9425202 | 0.0000000 | -0.7266292 |
| C | 8.0454709 | 0.0000000 | 0.0996527 | 8.0390457 | 0.0000000 | 0.0838231 |
| C | 7.6715538 | 0.0000000 | 1.4054448 | 7.6667857 | 0.0000000 | 1.3960565 |
| C | 6.2467140 | 0.0000000 | 1.4171332 | 6.2506992 | 0.0000000 | 1.4180759 |
| C | -5.8509313 | 0.0000000 | 0.1061624 | -5.8402979 | 0.0000000 | 0.0964854 |
| O | -6.9493116 | 0.0000000 | -0.7107598 | -6.9425202 | 0.0000000 | -0.7266292 |
| H | -4.8422850 | 0.0000000 | -2.7072717 | -4.8260643 | 0.0000000 | -2.7064868 |
| H | -2.1112568 | 0.0000000 | -2.7101144 | -2.1095225 | 0.0000000 | -2.7071545 |
| H | -1.3648079 | 0.0000000 | 2.2725889 | -1.3568613 | 0.0000000 | 2.2840008 |
| H | 1.3648079 | 0.0000000 | 2.2725889 | 1.3568613 | 0.0000000 | 2.2840008 |
| H | 2.1112568 | 0.0000000 | -2.7101144 | 2.1095225 | 0.0000000 | -2.7071545 |
| H | 4.8422850 | 0.0000000 | -2.7072717 | 4.8260643 | 0.0000000 | -2.7064868 |
| H | 5.5949554 | 0.0000000 | 2.2746548 | 5.6024943 | 0.0000000 | 2.2783599 |
| H | 8.3310443 | 0.0000000 | 2.2580504 | 8.3328056 | 0.0000000 | 2.2439941 |
| C | -8.0454709 | 0.0000000 | 0.0996527 | -8.0390457 | 0.0000000 | 0.0838231 |
| C | -7.6715538 | 0.0000000 | 1.4054448 | -7.6667857 | 0.0000000 | 1.3960565 |
| C | -6.2467140 | 0.0000000 | 1.4171332 | -6.2506992 | 0.0000000 | 1.4180759 |
| H | -5.5949554 | 0.0000000 | 2.2746548 | -5.6024943 | 0.0000000 | 2.2783599 |
| H | -8.9956433 | 0.0000000 | -0.4053494 | -8.9900111 | 0.0000000 | -0.4203023 |
| H | -8.3310443 | 0.0000000 | 2.2580504 | -8.3328056 | 0.0000000 | 2.2439941 |
| H | 8.9956433 | 0.0000000 | -0.4053494 | 8.9900111 | 0.0000000 | -0.4203023 |
|  |  |  |  |  |  |  |
| **6O/**  **TPSSh** | **Ground state** | | | **Excited state** | | |
| O | 1.8055465 | -0.0102666 | 0.0000000 | 1.8102479 | 0.0090146 | 0.0000000 |
| C | 0.5210946 | -0.4863451 | 0.0000000 | 0.5178960 | -0.4712815 | 0.0000000 |
| C | 0.5344173 | -1.8589609 | 0.0000000 | 0.5387195 | -1.8661524 | 0.0000000 |
| C | 1.8943841 | -2.2519014 | 0.0000000 | 1.8786255 | -2.2546018 | 0.0000000 |
| C | 2.6377269 | -1.0980407 | 0.0000000 | 2.6428584 | -1.0896051 | 0.0000000 |
| C | 4.0386660 | -0.8313770 | 0.0000000 | 4.0241375 | -0.8458709 | 0.0000000 |
| O | 4.8702988 | -1.9200085 | 0.0000000 | 4.8603181 | -1.9404755 | 0.0000000 |
| C | 6.1539838 | -1.4450774 | 0.0000000 | 6.1475449 | -1.4597129 | 0.0000000 |
| C | 6.1433059 | -0.0741101 | 0.0000000 | 6.1294112 | -0.0741374 | 0.0000000 |
| C | 4.7828547 | 0.3213107 | 0.0000000 | 4.7860269 | 0.3191951 | 0.0000000 |
| H | 7.0126496 | 0.5620109 | 0.0000000 | 7.0008108 | 0.5596729 | 0.0000000 |
| H | 2.2883579 | -3.2544584 | 0.0000000 | 2.2741665 | -3.2567412 | 0.0000000 |
| H | -0.3335432 | -2.4969283 | 0.0000000 | -0.3321420 | -2.5004449 | 0.0000000 |
| C | 7.1987360 | -2.4211459 | 0.0000000 | 7.1902354 | -2.4154408 | 0.0000000 |
| O | 8.4811043 | -1.9422563 | 0.0000000 | 8.4765453 | -1.9322065 | 0.0000000 |
| C | 9.3083119 | -3.0257740 | 0.0000000 | 9.3047176 | -3.0149862 | 0.0000000 |
| C | 8.5856765 | -4.1758784 | 0.0000000 | 8.5828221 | -4.1705963 | 0.0000000 |
| C | 7.2139404 | -3.7904856 | 0.0000000 | 7.2150841 | -3.7955259 | 0.0000000 |
| H | 6.3492871 | -4.4327522 | 0.0000000 | 6.3530577 | -4.4413337 | 0.0000000 |
| H | 10.3615258 | -2.8053021 | 0.0000000 | 10.3581559 | -2.7945502 | 0.0000000 |
| H | 8.9817070 | -5.1783781 | 0.0000000 | 8.9852497 | -5.1708139 | 0.0000000 |
| C | -0.5210946 | 0.4863451 | 0.0000000 | -0.5178960 | 0.4712815 | 0.0000000 |
| O | -1.8055465 | 0.0102666 | 0.0000000 | -1.8102479 | -0.0090146 | 0.0000000 |
| C | -2.6377269 | 1.0980407 | 0.0000000 | -2.6428584 | 1.0896051 | 0.0000000 |
| C | -1.8943841 | 2.2519014 | 0.0000000 | -1.8786255 | 2.2546018 | 0.0000000 |
| C | -0.5344173 | 1.8589609 | 0.0000000 | -0.5387195 | 1.8661524 | 0.0000000 |
| H | -2.2883579 | 3.2544584 | 0.0000000 | -2.2741665 | 3.2567412 | 0.0000000 |
| H | 0.3335432 | 2.4969283 | 0.0000000 | 0.3321420 | 2.5004449 | 0.0000000 |
| H | 4.3904514 | 1.3244830 | 0.0000000 | 4.3920984 | 1.3219428 | 0.0000000 |
| C | -4.0386660 | 0.8313770 | 0.0000000 | -4.0241375 | 0.8458709 | 0.0000000 |
| C | -4.7828547 | -0.3213107 | 0.0000000 | -4.7860269 | -0.3191951 | 0.0000000 |
| C | -6.1433059 | 0.0741101 | 0.0000000 | -6.1294112 | 0.0741374 | 0.0000000 |
| C | -6.1539838 | 1.4450774 | 0.0000000 | -6.1475449 | 1.4597129 | 0.0000000 |
| O | -4.8702988 | 1.9200085 | 0.0000000 | -4.8603181 | 1.9404755 | 0.0000000 |
| H | -7.0126496 | -0.5620109 | 0.0000000 | -7.0008108 | -0.5596729 | 0.0000000 |
| H | -4.3904514 | -1.3244830 | 0.0000000 | -4.3920984 | -1.3219428 | 0.0000000 |
| C | -7.1987360 | 2.4211459 | 0.0000000 | -7.1902354 | 2.4154408 | 0.0000000 |
| C | -7.2139404 | 3.7904856 | 0.0000000 | -7.2150841 | 3.7955259 | 0.0000000 |
| C | -8.5856765 | 4.1758784 | 0.0000000 | -8.5828221 | 4.1705963 | 0.0000000 |
| C | -9.3083119 | 3.0257740 | 0.0000000 | -9.3047176 | 3.0149862 | 0.0000000 |
| O | -8.4811043 | 1.9422563 | 0.0000000 | -8.4765453 | 1.9322065 | 0.0000000 |
| H | -8.9817070 | 5.1783781 | 0.0000000 | -8.9852497 | 5.1708139 | 0.0000000 |
| H | -10.3615258 | 2.8053021 | 0.0000000 | -10.358155 | 2.7945502 | 0.0000000 |
| H | -6.3492871 | 4.4327522 | 0.0000000 | -6.3530577 | 4.4413337 | 0.0000000 |
|  |  |  |  |  |  |  |
| **7O/**  **TPSSh** | **Ground state** | | | **Excited state** | | |
| C | -9.7217870 | 0.0000000 | -1.4912276 | 9.720856 | 0.0000000 | 1.540989 |
| C | -9.3254584 | 0.0000000 | -0.1804120 | 9.315849 | 0.0000000 | 0.224011 |
| O | -10.4234747 | 0.0000000 | 0.6369888 | 10.416584 | 0.0000000 | -0.596579 |
| C | -11.5199246 | 0.0000000 | -0.1729510 | 11.512904 | 0.0000000 | 0.213288 |
| C | -11.1465844 | 0.0000000 | -1.4789295 | 11.140391 | 0.0000000 | 1.522915 |
| C | -8.0501239 | 0.0000000 | 0.4658754 | 8.047364 | 0.0000000 | -0.408355 |
| O | -6.9494986 | 0.0000000 | -0.3477352 | 6.944121 | 0.0000000 | 0.408173 |
| C | -5.8476422 | 0.0000000 | 0.4663153 | 5.838257 | 0.0000000 | -0.410884 |
| C | -6.2414331 | 0.0000000 | 1.7806467 | 6.246165 | 0.0000000 | -1.738456 |
| C | -7.6581411 | 0.0000000 | 1.7796756 | 7.648454 | 0.0000000 | -1.732472 |
| C | -4.5762936 | 0.0000000 | -0.1796529 | 4.577071 | 0.0000000 | 0.209296 |
| O | -3.4743915 | 0.0000000 | 0.6336442 | 3.472502 | 0.0000000 | -0.612620 |
| C | -2.3730510 | 0.0000000 | -0.1809844 | 2.364907 | 0.0000000 | 0.206013 |
| C | -2.7677759 | 0.0000000 | -1.4957588 | 2.771717 | 0.0000000 | 1.538176 |
| C | -4.1833009 | 0.0000000 | -1.4948313 | 4.168425 | 0.0000000 | 1.538333 |
| C | -1.1016387 | 0.0000000 | 0.4634719 | 1.106417 | 0.0000000 | -0.412137 |
| O | 0.0000000 | 0.0000000 | -0.3505933 | 0.000000 | 0.0000000 | 0.409062 |
| C | 1.1016387 | 0.0000000 | 0.4634719 | -1.106417 | 0.0000000 | -0.412137 |
| C | 0.7076388 | 0.0000000 | 1.7786009 | -0.697847 | 0.0000000 | -1.743834 |
| C | -0.7076388 | 0.0000000 | 1.7786009 | 0.697847 | 0.0000000 | -1.743834 |
| C | 2.3730510 | 0.0000000 | -0.1809844 | -2.364907 | 0.0000000 | 0.206013 |
| O | 3.4743915 | 0.0000000 | 0.6336442 | -3.472502 | 0.0000000 | -0.612620 |
| C | 4.5762936 | 0.0000000 | -0.1796529 | -4.577071 | 0.0000000 | 0.209296 |
| C | 4.1833009 | 0.0000000 | -1.4948313 | -4.168425 | 0.0000000 | 1.538333 |
| C | 2.7677759 | 0.0000000 | -1.4957588 | -2.771717 | 0.0000000 | 1.538176 |
| C | 5.8476422 | 0.0000000 | 0.4663153 | -5.838257 | 0.0000000 | -0.410884 |
| O | 6.9494986 | 0.0000000 | -0.3477352 | -6.944121 | 0.0000000 | 0.408173 |
| C | 8.0501239 | 0.0000000 | 0.4658754 | -8.047364 | 0.0000000 | -0.408355 |
| C | 7.6581411 | 0.0000000 | 1.7796756 | -7.648454 | 0.0000000 | -1.732472 |
| C | 6.2414331 | 0.0000000 | 1.7806467 | -6.246165 | 0.0000000 | -1.738456 |
| C | 9.3254584 | 0.0000000 | -0.1804120 | -9.315849 | 0.0000000 | 0.224011 |
| C | 9.7217870 | 0.0000000 | -1.4912276 | -9.720856 | 0.0000000 | 1.540989 |
| C | 11.1465844 | 0.0000000 | -1.4789295 | -11.140391 | 0.0000000 | 1.522915 |
| C | 11.5199246 | 0.0000000 | -0.1729510 | -11.512904 | 0.0000000 | 0.213288 |
| O | 10.4234747 | 0.0000000 | 0.6369888 | -10.416584 | 0.0000000 | -0.596579 |
| H | -1.3644498 | 0.0000000 | 2.6323869 | 1.356825 | 0.0000000 | -2.596159 |
| H | 2.1115464 | 0.0000000 | -2.3499996 | -2.112278 | 0.0000000 | 2.390147 |
| H | 4.8406940 | 0.0000000 | -2.3481643 | -4.826602 | 0.0000000 | 2.391334 |
| H | -2.1115464 | 0.0000000 | -2.3499996 | 2.112278 | 0.0000000 | 2.390147 |
| H | -4.8406940 | 0.0000000 | -2.3481643 | 4.826602 | 0.0000000 | 2.391334 |
| H | 8.3160484 | 0.0000000 | 2.6326473 | -8.310003 | 0.0000000 | -2.582974 |
| H | 5.5851711 | 0.0000000 | 2.6348519 | -5.590705 | 0.0000000 | -2.593417 |
| H | 1.3644498 | 0.0000000 | 2.6323869 | -1.356825 | 0.0000000 | -2.596159 |
| H | 11.8064358 | 0.0000000 | -2.3312492 | -11.803862 | 0.0000000 | 2.372657 |
| H | 9.0704225 | 0.0000000 | -2.3490501 | -9.071727 | 0.0000000 | 2.400490 |
| H | -5.5851711 | 0.0000000 | 2.6348519 | 5.590705 | 0.0000000 | -2.593417 |
| H | -8.3160484 | 0.0000000 | 2.6326473 | 8.310003 | 0.0000000 | -2.582974 |
| H | -9.0704225 | 0.0000000 | -2.3490501 | 9.071727 | 0.0000000 | 2.400490 |
| H | -11.8064358 | 0.0000000 | -2.3312492 | 11.803862 | 0.0000000 | 2.372657 |
| H | -12.4698968 | 0.0000000 | 0.3324309 | 12.463420 | 0.0000000 | -0.291412 |
| H | 12.4698968 | 0.0000000 | 0.3324309 | -12.463420 | 0.0000000 | -0.291412 |
|  |  |  |  |  |  |  |
| **8O/**  **TPSSh** | **Ground state** | | | **Excited state** | | |
| O | 5.057667 | 11.070292 | 0.000000 | 4.935522 | 11.117223 | 0.000000 |
| C | 5.289589 | 9.721227 | 0.000000 | 5.183935 | 9.767806 | 0.000000 |
| C | 6.637844 | 9.481362 | 0.000000 | 6.542175 | 9.547264 | 0.000000 |
| C | 7.271735 | 10.757418 | 0.000000 | 7.155670 | 10.828697 | 0.000000 |
| C | 6.276147 | 11.681426 | 0.000000 | 6.146802 | 11.742001 | 0.000000 |
| C | 4.136127 | 8.876427 | 0.000000 | 4.052405 | 8.910348 | 0.000000 |
| C | 2.787116 | 9.121263 | 0.000000 | 2.690886 | 9.139757 | 0.000000 |
| C | 2.145296 | 7.858293 | 0.000000 | 2.063752 | 7.883040 | 0.000000 |
| C | 3.139247 | 6.912452 | 0.000000 | 3.072067 | 6.931879 | 0.000000 |
| O | 4.363721 | 7.526810 | 0.000000 | 4.295114 | 7.560513 | 0.000000 |
| C | 3.140330 | 5.486425 | 0.000000 | 3.072067 | 5.523875 | 0.000000 |
| O | 1.916691 | 4.871378 | 0.000000 | 1.848118 | 4.896284 | 0.000000 |
| C | 2.145296 | 3.520698 | 0.000000 | 2.091790 | 3.541750 | 0.000000 |
| C | 3.496489 | 3.278271 | 0.000000 | 3.464568 | 3.317725 | 0.000000 |
| C | 4.135700 | 4.541192 | 0.000000 | 4.082487 | 4.572130 | 0.000000 |
| C | 0.995705 | 2.678002 | 0.000000 | 0.979098 | 2.685975 | 0.000000 |
| O | 1.223907 | 1.327415 | 0.000000 | 1.225815 | 1.331212 | 0.000000 |
| C | -0.000211 | 0.712627 | 0.000000 | 0.001305 | 0.701421 | 0.000000 |
| C | -0.995254 | 1.658621 | 0.000000 | -1.012006 | 1.655809 | 0.000000 |
| C | -0.355577 | 2.920993 | 0.000000 | -0.394189 | 2.908241 | 0.000000 |
| C | 0.000211 | -0.712627 | 0.000000 | -0.001305 | -0.701421 | 0.000000 |
| O | -1.223907 | -1.327415 | 0.000000 | -1.225815 | -1.331212 | 0.000000 |
| C | -0.995705 | -2.678002 | 0.000000 | -0.979098 | -2.685975 | 0.000000 |
| C | 0.355577 | -2.920993 | 0.000000 | 0.394189 | -2.908241 | 0.000000 |
| C | 0.995254 | -1.658621 | 0.000000 | 1.012006 | -1.655809 | 0.000000 |
| C | -2.145296 | -3.520698 | 0.000000 | -2.091790 | -3.541750 | 0.000000 |
| O | -1.916691 | -4.871378 | 0.000000 | -1.848118 | -4.896284 | 0.000000 |
| C | -3.140330 | -5.486425 | 0.000000 | -3.072067 | -5.523875 | 0.000000 |
| C | -4.135700 | -4.541192 | 0.000000 | -4.082487 | -4.572130 | 0.000000 |
| C | -3.496489 | -3.278271 | 0.000000 | -3.464568 | -3.317725 | 0.000000 |
| H | 0.820351 | -3.892759 | 0.000000 | 0.867685 | -3.875995 | 0.000000 |
| H | -2.053746 | 1.458761 | 0.000000 | -2.067944 | 1.442048 | 0.000000 |
| H | -0.820351 | 3.892759 | 0.000000 | -0.867685 | 3.875995 | 0.000000 |
| H | -3.961765 | -2.306735 | 0.000000 | -3.937986 | -2.349975 | 0.000000 |
| C | -3.139247 | -6.912452 | 0.000000 | -3.072067 | -6.931879 | 0.000000 |
| H | -5.194073 | -4.741628 | 0.000000 | -5.138626 | -4.785216 | 0.000000 |
| H | 5.194073 | 4.741628 | 0.000000 | 5.138626 | 4.785216 | 0.000000 |
| H | 3.961765 | 2.306735 | 0.000000 | 3.937986 | 2.349975 | 0.000000 |
| H | 2.053746 | -1.458761 | 0.000000 | 2.067944 | -1.442048 | 0.000000 |
| H | 2.324015 | 10.093855 | 0.000000 | 2.220962 | 10.109344 | 0.000000 |
| H | 1.086589 | 7.659594 | 0.000000 | 1.006892 | 7.674368 | 0.000000 |
| H | 8.330413 | 10.960009 | 0.000000 | 8.211417 | 11.046739 | 0.000000 |
| H | 6.255471 | 12.757267 | 0.000000 | 6.114599 | 12.817682 | 0.000000 |
| H | 7.108039 | 8.512317 | 0.000000 | 7.025268 | 8.584606 | 0.000000 |
| O | -4.363721 | -7.526810 | 0.000000 | -4.295114 | -7.560513 | 0.000000 |
| C | -4.136127 | -8.876427 | 0.000000 | -4.052405 | -8.910348 | 0.000000 |
| C | -2.787116 | -9.121263 | 0.000000 | -2.690886 | -9.139757 | 0.000000 |
| C | -2.145296 | -7.858293 | 0.000000 | -2.063752 | -7.883040 | 0.000000 |
| H | -1.086589 | -7.659594 | 0.000000 | -1.006892 | -7.674368 | 0.000000 |
| H | -2.324015 | -10.093855 | 0.000000 | -2.220962 | -10.109344 | 0.000000 |
| C | -5.289589 | -9.721227 | 0.000000 | -5.183935 | -9.767806 | 0.000000 |
| O | -5.057667 | -11.070292 | 0.000000 | -4.935522 | -11.117223 | 0.000000 |
| C | -6.276147 | -11.681426 | 0.000000 | -6.146802 | -11.742001 | 0.000000 |
| C | -7.271735 | -10.757418 | 0.000000 | -7.155670 | -10.828697 | 0.000000 |
| C | -6.637844 | -9.481362 | 0.000000 | -6.542175 | -9.547264 | 0.000000 |
| H | -7.108039 | -8.512317 | 0.000000 | -7.025268 | -8.584606 | 0.000000 |
| H | -8.330413 | -10.960009 | 0.000000 | -8.211417 | -11.046739 | 0.000000 |
| H | -6.255471 | -12.757267 | 0.000000 | -6.114599 | -12.817682 | 0.000000 |
|  |  |  |  |  |  |  |
| **9O/BP** | **Ground state** | | | **Excited state** | | |
| C | 0.000000 | 13.194603 | -1.558878 | -0.000000 | 13.192354 | -1.562677 |
| C | 0.000000 | 12.799487 | -0.247690 | -0.000000 | 12.790675 | -0.248019 |
| O | 0.000000 | 13.898239 | 0.568697 | -0.000000 | 13.890530 | 0.571198 |
| C | 0.000000 | 14.993929 | -0.242250 | -0.000000 | 14.986664 | -0.238699 |
| C | 0.000000 | 14.619379 | -1.547896 | -0.000000 | 14.613791 | -1.546931 |
| C | 0.000000 | 11.524683 | 0.399630 | -0.000000 | 11.520110 | 0.389608 |
| O | 0.000000 | 10.423514 | -0.413186 | -0.000000 | 10.417230 | -0.424367 |
| C | 0.000000 | 9.322212 | 0.401612 | -0.000000 | 9.313040 | 0.393850 |
| C | 0.000000 | 9.716920 | 1.715676 | -0.000000 | 9.718533 | 1.716984 |
| C | 0.000000 | 11.133605 | 1.713731 | -0.000000 | 11.124936 | 1.710733 |
| C | 0.000000 | 8.050553 | -0.243695 | -0.000000 | 8.049102 | -0.231982 |
| O | 0.000000 | 6.948957 | 0.569941 | -0.000000 | 6.944944 | 0.586371 |
| C | 0.000000 | 5.847358 | -0.244368 | -0.000000 | 5.838728 | -0.231061 |
| C | 0.000000 | 6.241695 | -1.559284 | -0.000000 | 6.244771 | -1.559444 |
| C | 0.000000 | 7.657146 | -1.558802 | -0.000000 | 7.644803 | -1.557699 |
| C | 0.000000 | 4.576114 | 0.400285 | -0.000000 | 4.577789 | 0.389543 |
| O | 0.000000 | 3.474442 | -0.413607 | -0.000000 | 3.472461 | -0.430382 |
| C | 0.000000 | 2.372835 | 0.400595 | -0.000000 | 2.365984 | 0.387951 |
| C | 0.000000 | 2.767088 | 1.715747 | -0.000000 | 2.772799 | 1.718062 |
| C | 0.000000 | 4.182245 | 1.715565 | -0.000000 | 4.170256 | 1.717951 |
| C | 0.000000 | 1.101647 | -0.243846 | -0.000000 | 1.106085 | -0.231035 |
| O | 0.000000 | 0.000000 | 0.570200 | -0.000000 | 0.000000 | 0.588508 |
| C | 0.000000 | -1.101647 | -0.243846 | -0.000000 | -1.106085 | -0.231035 |
| C | 0.000000 | -0.707550 | -1.559104 | 0.000000 | -0.698451 | -1.560850 |
| C | 0.000000 | 0.707550 | -1.559104 | 0.000000 | 0.698451 | -1.560850 |
| C | 0.000000 | -2.372835 | 0.400595 | -0.000000 | -2.365984 | 0.387951 |
| O | 0.000000 | -3.474442 | -0.413607 | -0.000000 | -3.472461 | -0.430382 |
| C | 0.000000 | -4.576114 | 0.400285 | -0.000000 | -4.577789 | 0.389543 |
| C | 0.000000 | -4.182245 | 1.715565 | -0.000000 | -4.170256 | 1.717951 |
| C | 0.000000 | -2.767088 | 1.715747 | -0.000000 | -2.772799 | 1.718062 |
| C | 0.000000 | -5.847358 | -0.244368 | -0.000000 | -5.838728 | -0.231061 |
| C | 0.000000 | -6.241695 | -1.559284 | -0.000000 | -6.244771 | -1.559444 |
| C | 0.000000 | -7.657146 | -1.558802 | -0.000000 | -7.644803 | -1.557699 |
| C | 0.000000 | -8.050553 | -0.243695 | -0.000000 | -8.049102 | -0.231982 |
| O | 0.000000 | -6.948957 | 0.569941 | -0.000000 | -6.944944 | 0.586371 |
| C | 0.000000 | -9.322212 | 0.401612 | -0.000000 | -9.313040 | 0.393850 |
| O | 0.000000 | -10.423514 | -0.413186 | -0.000000 | -10.417230 | -0.424367 |
| C | 0.000000 | -11.524683 | 0.399630 | -0.000000 | -11.520110 | 0.389608 |
| C | 0.000000 | -11.133605 | 1.713731 | -0.000000 | -11.124936 | 1.710733 |
| C | 0.000000 | -9.716920 | 1.715676 | -0.000000 | -9.718533 | 1.716984 |
| H | 0.000000 | 4.839117 | 2.569297 | -0.000000 | 4.828376 | 2.570986 |
| H | 0.000000 | 1.364296 | -2.412938 | 0.000000 | 1.356917 | -2.413577 |
| H | 0.000000 | -1.364296 | -2.412938 | -0.000000 | -1.356917 | -2.413577 |
| H | 0.000000 | 5.585258 | -2.413366 | -0.000000 | 5.587188 | -2.412784 |
| H | 0.000000 | 8.314236 | -2.412362 | -0.000000 | 8.303456 | -2.410352 |
| H | 0.000000 | -4.839117 | 2.569297 | -0.000000 | -4.828376 | 2.570986 |
| H | 0.000000 | -2.110483 | 2.569695 | -0.000000 | -2.114187 | 2.570652 |
| H | 0.000000 | 2.110483 | 2.569695 | 0.000000 | 2.114187 | 2.570652 |
| H | 0.000000 | -8.314236 | -2.412362 | -0.000000 | -8.303456 | -2.410352 |
| H | 0.000000 | -5.585258 | -2.413366 | -0.000000 | -5.587188 | -2.412784 |
| H | 0.000000 | -11.792041 | 2.566290 | 0.000000 | -11.786373 | 2.561233 |
| C | 0.000000 | -12.799487 | -0.247690 | -0.000000 | -12.790675 | -0.248019 |
| H | 0.000000 | -9.061320 | 2.570390 | 0.000000 | -9.064068 | 2.572625 |
| H | 0.000000 | 9.061320 | 2.570390 | 0.000000 | 9.064068 | 2.572625 |
| H | 0.000000 | 11.792041 | 2.566290 | 0.000000 | 11.786373 | 2.561233 |
| H | 0.000000 | 12.542504 | -2.416141 | -0.000000 | 12.542378 | -2.421523 |
| H | 0.000000 | 15.278418 | -2.400839 | -0.000000 | 15.275808 | -2.397698 |
| H | 0.000000 | 15.944381 | 0.262233 | -0.000000 | 15.937035 | 0.266139 |
| O | 0.000000 | -13.898239 | 0.568697 | -0.000000 | -13.890530 | 0.571198 |
| C | 0.000000 | -14.993929 | -0.242250 | -0.000000 | -14.986664 | -0.238699 |
| C | 0.000000 | -14.619379 | -1.547896 | -0.000000 | -14.613791 | -1.546931 |
| C | 0.000000 | -13.194603 | -1.558878 | -0.000000 | -13.192354 | -1.562677 |
| H | 0.000000 | -12.542504 | -2.416141 | -0.000000 | -12.542378 | -2.421523 |
| H | 0.000000 | -15.278418 | -2.400839 | -0.000000 | -15.275808 | -2.397698 |
| H | 0.000000 | -15.944381 | 0.262233 | -0.000000 | -15.937035 | 0.266139 |

Part 3.

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| **2O/**  **B3LYP** | **Ground state** | | | **Excited state** | | |
| C | -2.8190940 | 0.4341628 | 0.0000000 | -2.8081144 | 0.4456540 | 0.0000000 |
| C | -2.7982727 | -0.9215637 | 0.0000000 | -2.7787890 | -0.9358735 | 0.0000000 |
| C | -1.4230031 | -1.3034771 | 0.0000000 | -1.4399029 | -1.3295354 | 0.0000000 |
| C | -0.7029923 | -0.1431515 | 0.0000000 | -0.6784797 | -0.1295999 | 0.0000000 |
| C | 0.7029923 | 0.1431515 | 0.0000000 | 0.6784797 | 0.1295999 | 0.0000000 |
| C | 1.4230031 | 1.3034771 | 0.0000000 | 1.4399029 | 1.3295354 | 0.0000000 |
| C | 2.7982727 | 0.9215637 | 0.0000000 | 2.7787890 | 0.9358735 | 0.0000000 |
| C | 2.8190940 | -0.4341628 | 0.0000000 | 2.8081144 | -0.4456540 | 0.0000000 |
| O | -1.5496748 | 0.9282192 | 0.0000000 | -1.5423451 | 0.9671495 | 0.0000000 |
| O | 1.5496748 | -0.9282192 | 0.0000000 | 1.5423451 | -0.9671495 | 0.0000000 |
| H | -3.6075069 | 1.1649149 | 0.0000000 | -3.6127580 | 1.1598791 | 0.0000000 |
| H | -3.6556326 | -1.5727312 | 0.0000000 | -3.6464983 | -1.5744265 | 0.0000000 |
| H | -1.0164377 | -2.2995183 | 0.0000000 | -1.0309084 | -2.3243734 | 0.0000000 |
| H | 1.0164377 | 2.2995183 | 0.0000000 | 1.0309084 | 2.3243734 | 0.0000000 |
| H | 3.6556326 | 1.5727312 | 0.0000000 | 3.6464983 | 1.5744265 | 0.0000000 |
| H | 3.6075069 | -1.1649149 | 0.0000000 | 3.6127580 | -1.1598791 | 0.0000000 |
|  |  |  |  |  |  |  |
| **3O/**  **B3LYP** | **Ground state** | | | **Excited state** | | |
| O | 3.4775663 | 0.0000000 | 0.8384332 | 3.4787911 | 0.0000000 | 0.8555899 |
| C | 4.5735628 | 0.0000000 | 0.0298076 | 4.5608832 | 0.0000000 | 0.0248102 |
| C | 4.1993641 | 0.0000000 | -1.2736859 | 4.1664147 | 0.0000000 | -1.2857471 |
| C | 2.7727129 | 0.0000000 | -1.2836711 | 2.7577923 | 0.0000000 | -1.2936817 |
| C | 2.3797687 | 0.0000000 | 0.0253420 | 2.3593977 | 0.0000000 | 0.0472835 |
| C | 1.1005172 | 0.0000000 | 0.6688564 | 1.1082590 | 0.0000000 | 0.6613023 |
| O | 0.0000000 | 0.0000000 | -0.1418624 | 0.0000000 | 0.0000000 | -0.1702929 |
| C | -1.1005172 | 0.0000000 | 0.6688564 | -1.1082590 | 0.0000000 | 0.6613023 |
| C | -0.7101102 | 0.0000000 | 1.9793499 | -0.6925231 | 0.0000000 | 2.0067728 |
| C | 0.7101102 | 0.0000000 | 1.9793499 | 0.6925231 | 0.0000000 | 2.0067728 |
| H | 1.3664370 | 0.0000000 | 2.8318808 | 1.3541078 | 0.0000000 | 2.8554274 |
| H | -1.3664370 | 0.0000000 | 2.8318808 | -1.3541078 | 0.0000000 | 2.8554274 |
| H | 2.1209240 | 0.0000000 | -2.1394969 | 2.0968036 | 0.0000000 | -2.1426473 |
| H | 5.5255620 | 0.0000000 | 0.5290851 | 5.5235283 | 0.0000000 | 0.5045041 |
| H | 4.8570748 | 0.0000000 | -2.1260224 | 4.8232493 | 0.0000000 | -2.1395203 |
| C | -2.3797687 | 0.0000000 | 0.0253420 | -2.3593977 | 0.0000000 | 0.0472835 |
| O | -3.4775663 | 0.0000000 | 0.8384332 | -3.4787911 | 0.0000000 | 0.8555899 |
| C | -4.5735628 | 0.0000000 | 0.0298076 | -4.5608832 | 0.0000000 | 0.0248102 |
| C | -4.1993641 | 0.0000000 | -1.2736859 | -4.1664147 | 0.0000000 | -1.2857471 |
| C | -2.7727129 | 0.0000000 | -1.2836711 | -2.7577923 | 0.0000000 | -1.2936817 |
| H | -2.1209240 | 0.0000000 | -2.1394969 | -2.0968036 | 0.0000000 | -2.1426473 |
| H | -5.5255620 | 0.0000000 | 0.5290851 | -5.5235283 | 0.0000000 | 0.5045041 |
| H | -4.8570748 | 0.0000000 | -2.1260224 | -4.8232493 | 0.0000000 | -2.1395203 |
|  |  |  |  |  |  |  |
| **4O/**  **B3LYP** | **Ground state** | | | **Excited state** | | |
| O | -1.5236148 | 0.9711279 | 0.0000000 | -1.5126462 | 0.9996816 | 0.0000000 |
| C | -2.8112942 | 0.5128477 | 0.0000000 | -2.8078149 | 0.5285364 | 0.0000000 |
| C | -2.8161982 | -0.8550739 | 0.0000000 | -2.8006710 | -0.8667632 | 0.0000000 |
| C | -1.4576380 | -1.2657473 | 0.0000000 | -1.4706860 | -1.2731669 | 0.0000000 |
| C | -0.7036363 | -0.1233262 | 0.0000000 | -0.6869517 | -0.1083646 | 0.0000000 |
| C | 0.7036363 | 0.1233262 | 0.0000000 | 0.6869517 | 0.1083646 | 0.0000000 |
| O | 1.5236148 | -0.9711279 | 0.0000000 | 1.5126462 | -0.9996816 | 0.0000000 |
| C | 2.8112942 | -0.5128477 | 0.0000000 | 2.8078149 | -0.5285364 | 0.0000000 |
| C | 2.8161982 | 0.8550739 | 0.0000000 | 2.8006710 | 0.8667632 | 0.0000000 |
| C | 1.4576380 | 1.2657473 | 0.0000000 | 1.4706860 | 1.2731669 | 0.0000000 |
| H | 1.0765223 | 2.2718360 | 0.0000000 | 1.0860779 | 2.2781268 | 0.0000000 |
| H | 3.6911369 | 1.4812311 | 0.0000000 | 3.6790594 | 1.4886421 | 0.0000000 |
| H | -1.0765223 | -2.2718360 | 0.0000000 | -1.0860779 | -2.2781268 | 0.0000000 |
| H | -3.6911369 | -1.4812311 | 0.0000000 | -3.6790594 | -1.4886421 | 0.0000000 |
| C | 3.8501140 | -1.4977865 | 0.0000000 | 3.8383841 | -1.4823601 | 0.0000000 |
| O | 5.1359941 | -1.0361984 | 0.0000000 | 5.1345333 | -1.0219489 | 0.0000000 |
| C | 5.9517306 | -2.1268172 | 0.0000000 | 5.9439690 | -2.1179023 | 0.0000000 |
| C | 5.2171317 | -3.2668616 | 0.0000000 | 5.2021786 | -3.2625796 | 0.0000000 |
| C | 3.8484718 | -2.8646799 | 0.0000000 | 3.8432401 | -2.8698182 | 0.0000000 |
| H | 2.9774001 | -3.4959332 | 0.0000000 | 2.9718422 | -3.5008152 | 0.0000000 |
| H | 7.0073628 | -1.9237593 | 0.0000000 | 7.0014700 | -1.9226646 | 0.0000000 |
| H | 5.6008424 | -4.2727455 | 0.0000000 | 5.5904265 | -4.2671992 | 0.0000000 |
| C | -3.8501140 | 1.4977865 | 0.0000000 | -3.8383841 | 1.4823601 | 0.0000000 |
| O | -5.1359941 | 1.0361984 | 0.0000000 | -5.1345333 | 1.0219489 | 0.0000000 |
| C | -5.9517306 | 2.1268172 | 0.0000000 | -5.9439690 | 2.1179023 | 0.0000000 |
| C | -5.2171317 | 3.2668616 | 0.0000000 | -5.2021786 | 3.2625796 | 0.0000000 |
| C | -3.8484718 | 2.8646799 | 0.0000000 | -3.8432401 | 2.8698182 | 0.0000000 |
| H | -7.0073628 | 1.9237593 | 0.0000000 | -7.0014700 | 1.9226646 | 0.0000000 |
| H | -5.6008424 | 4.2727455 | 0.0000000 | -5.5904265 | 4.2671992 | 0.0000000 |
| H | -2.9774001 | 3.4959332 | 0.0000000 | -2.9718422 | 3.5008152 | 0.0000000 |
|  |  |  |  |  |  |  |
| **5O/**  **B3LYP** | **Ground state** | | | **Excited state** | | |
| O | 6.9559344 | 0.0000000 | 0.7035637 | 6.9465007 | 0.0000000 | 0.7186730 |
| C | 8.0504797 | 0.0000000 | -0.1068254 | 8.0420281 | 0.0000000 | -0.0902842 |
| C | 7.6742720 | 0.0000000 | -1.4098516 | 7.6689115 | 0.0000000 | -1.3997698 |
| C | 6.2478414 | 0.0000000 | -1.4177071 | 6.2511260 | 0.0000000 | -1.4193380 |
| C | 5.8568253 | 0.0000000 | -0.1078932 | 5.8441214 | 0.0000000 | -0.0994274 |
| C | 4.5788012 | 0.0000000 | 0.5368190 | 4.5761588 | 0.0000000 | 0.5197813 |
| O | 3.4774361 | 0.0000000 | -0.2724227 | 3.4739420 | 0.0000000 | -0.3003125 |
| C | 2.3771881 | 0.0000000 | 0.5400038 | 2.3641547 | 0.0000000 | 0.5169278 |
| C | 2.7709891 | 0.0000000 | 1.8511819 | 2.7746010 | 0.0000000 | 1.8521627 |
| C | 4.1900329 | 0.0000000 | 1.8484861 | 4.1706354 | 0.0000000 | 1.8471762 |
| C | 1.1010492 | 0.0000000 | -0.1011576 | 1.1075615 | 0.0000000 | -0.0902460 |
| O | 0.0000000 | 0.0000000 | 0.7098091 | 0.0000000 | 0.0000000 | 0.7320178 |
| C | -1.1010492 | 0.0000000 | -0.1011576 | -1.1075615 | 0.0000000 | -0.0902460 |
| C | -0.7090883 | 0.0000000 | -1.4132524 | -0.6950020 | 0.0000000 | -1.4270688 |
| C | 0.7090883 | 0.0000000 | -1.4132524 | 0.6950020 | 0.0000000 | -1.4270688 |
| C | -2.3771881 | 0.0000000 | 0.5400038 | -2.3641547 | 0.0000000 | 0.5169278 |
| O | -3.4774361 | 0.0000000 | -0.2724227 | -3.4739420 | 0.0000000 | -0.3003125 |
| C | -4.5788012 | 0.0000000 | 0.5368190 | -4.5761588 | 0.0000000 | 0.5197813 |
| C | -4.1900329 | 0.0000000 | 1.8484861 | -4.1706354 | 0.0000000 | 1.8471762 |
| C | -2.7709891 | 0.0000000 | 1.8511819 | -2.7746010 | 0.0000000 | 1.8521627 |
| C | -5.8568253 | 0.0000000 | -0.1078932 | -5.8441214 | 0.0000000 | -0.0994274 |
| O | -6.9559344 | 0.0000000 | 0.7035637 | -6.9465007 | 0.0000000 | 0.7186730 |
| C | -8.0504797 | 0.0000000 | -0.1068254 | -8.0420281 | 0.0000000 | -0.0902842 |
| C | -7.6742720 | 0.0000000 | -1.4098516 | -7.6689115 | 0.0000000 | -1.3997698 |
| C | -6.2478414 | 0.0000000 | -1.4177071 | -6.2511260 | 0.0000000 | -1.4193380 |
| H | 9.0033318 | 0.0000000 | 0.3908211 | 8.9950589 | 0.0000000 | 0.4076213 |
| H | 8.3307028 | 0.0000000 | -2.2631568 | 8.3325239 | 0.0000000 | -2.2479160 |
| H | 5.5947629 | 0.0000000 | -2.2725444 | 5.6027659 | 0.0000000 | -2.2778131 |
| H | 4.8479222 | 0.0000000 | 2.6998226 | 4.8308821 | 0.0000000 | 2.6971459 |
| H | 2.1167456 | 0.0000000 | 2.7052446 | 2.1176686 | 0.0000000 | 2.7043960 |
| H | 1.3650427 | 0.0000000 | -2.2660360 | 1.3540588 | 0.0000000 | -2.2777172 |
| H | -1.3650427 | 0.0000000 | -2.2660360 | -1.3540588 | 0.0000000 | -2.2777172 |
| H | -2.1167456 | 0.0000000 | 2.7052446 | -2.1176686 | 0.0000000 | 2.7043960 |
| H | -4.8479222 | 0.0000000 | 2.6998226 | -4.8308821 | 0.0000000 | 2.6971459 |
| H | -5.5947629 | 0.0000000 | -2.2725444 | -5.6027659 | 0.0000000 | -2.2778131 |
| H | -9.0033318 | 0.0000000 | 0.3908211 | -8.9950589 | 0.0000000 | 0.4076213 |
| H | -8.3307028 | 0.0000000 | -2.2631568 | -8.3325239 | 0.0000000 | -2.2479160 |
|  |  |  |  |  |  |  |
| **6O/**  **B3LYP** | **Ground state** | | | **Excited state** | | |
| O | 1.8067172 | 0.0016196 | 0.0000000 | 1.8116201 | 0.0257952 | 0.0000000 |
| C | 0.5271621 | -0.4812338 | 0.0000000 | 0.5230121 | -0.4621603 | 0.0000000 |
| C | 0.5497113 | -1.8506904 | 0.0000000 | 0.5572329 | -1.8588275 | 0.0000000 |
| C | 1.9148421 | -2.2342040 | 0.0000000 | 1.8979479 | -2.2346249 | 0.0000000 |
| C | 2.6472430 | -1.0769420 | 0.0000000 | 2.6538590 | -1.0633485 | 0.0000000 |
| C | 4.0490464 | -0.8044948 | 0.0000000 | 4.0324587 | -0.8168063 | 0.0000000 |
| O | 4.8893948 | -1.8835869 | 0.0000000 | 4.8778738 | -1.9022694 | 0.0000000 |
| C | 6.1681491 | -1.4013038 | 0.0000000 | 6.1598686 | -1.4153759 | 0.0000000 |
| C | 6.1475571 | -0.0333321 | 0.0000000 | 6.1325677 | -0.0324252 | 0.0000000 |
| C | 4.7819053 | 0.3519394 | 0.0000000 | 4.7862116 | 0.3526153 | 0.0000000 |
| H | 7.0107211 | 0.6089465 | 0.0000000 | 6.9985242 | 0.6066599 | 0.0000000 |
| H | 2.3157233 | -3.2326043 | 0.0000000 | 2.3014471 | -3.2322453 | 0.0000000 |
| H | -0.3124449 | -2.4942652 | 0.0000000 | -0.3069000 | -2.5000644 | 0.0000000 |
| C | 7.2252908 | -2.3663672 | 0.0000000 | 7.2140947 | -2.3604990 | 0.0000000 |
| O | 8.5022336 | -1.8806123 | 0.0000000 | 8.4949258 | -1.8712704 | 0.0000000 |
| C | 9.3383015 | -2.9556243 | 0.0000000 | 9.3316399 | -2.9454535 | 0.0000000 |
| C | 8.6253377 | -4.1093692 | 0.0000000 | 8.6193319 | -4.1041542 | 0.0000000 |
| C | 7.2494151 | -3.7330916 | 0.0000000 | 7.2473754 | -3.7374363 | 0.0000000 |
| H | 6.3903972 | -4.3806500 | 0.0000000 | 6.3909116 | -4.3883917 | 0.0000000 |
| H | 10.3899335 | -2.7327664 | 0.0000000 | 10.3835013 | -2.7227003 | 0.0000000 |
| H | 9.0279758 | -5.1078174 | 0.0000000 | 9.0277193 | -5.1005245 | 0.0000000 |
| C | -0.5271621 | 0.4812338 | 0.0000000 | -0.5230121 | 0.4621603 | 0.0000000 |
| O | -1.8067172 | -0.0016196 | 0.0000000 | -1.8116201 | -0.0257952 | 0.0000000 |
| C | -2.6472430 | 1.0769420 | 0.0000000 | -2.6538590 | 1.0633485 | 0.0000000 |
| C | -1.9148421 | 2.2342040 | 0.0000000 | -1.8979479 | 2.2346249 | 0.0000000 |
| C | -0.5497113 | 1.8506904 | 0.0000000 | -0.5572329 | 1.8588275 | 0.0000000 |
| H | -2.3157233 | 3.2326043 | 0.0000000 | -2.3014471 | 3.2322453 | 0.0000000 |
| H | 0.3124449 | 2.4942652 | 0.0000000 | 0.3069000 | 2.5000644 | 0.0000000 |
| H | 4.3821459 | 1.3507685 | 0.0000000 | 4.3866636 | 1.3516819 | 0.0000000 |
| C | -4.0490464 | 0.8044948 | 0.0000000 | -4.0324587 | 0.8168063 | 0.0000000 |
| C | -4.7819053 | -0.3519394 | 0.0000000 | -4.7862116 | -0.3526153 | 0.0000000 |
| C | -6.1475571 | 0.0333321 | 0.0000000 | -6.1325677 | 0.0324252 | 0.0000000 |
| C | -6.1681491 | 1.4013038 | 0.0000000 | -6.1598686 | 1.4153759 | 0.0000000 |
| O | -4.8893948 | 1.8835869 | 0.0000000 | -4.8778738 | 1.9022694 | 0.0000000 |
| H | -7.0107211 | -0.6089465 | 0.0000000 | -6.9985242 | -0.6066599 | 0.0000000 |
| H | -4.3821459 | -1.3507685 | 0.0000000 | -4.3866636 | -1.3516819 | 0.0000000 |
| C | -7.2252908 | 2.3663672 | 0.0000000 | -7.2140947 | 2.3604990 | 0.0000000 |
| C | -7.2494151 | 3.7330916 | 0.0000000 | -7.2473754 | 3.7374363 | 0.0000000 |
| C | -8.6253377 | 4.1093692 | 0.0000000 | -8.6193319 | 4.1041542 | 0.0000000 |
| C | -9.3383015 | 2.9556243 | 0.0000000 | -9.3316399 | 2.9454535 | 0.0000000 |
| O | -8.5022336 | 1.8806123 | 0.0000000 | -8.4949258 | 1.8712704 | 0.0000000 |
| H | -9.0279758 | 5.1078174 | 0.0000000 | -9.0277193 | 5.1005245 | 0.0000000 |
| H | -10.3899335 | 2.7327664 | 0.0000000 | -10.383501 | 2.7227003 | 0.0000000 |
| H | -6.3903972 | 4.3806500 | 0.0000000 | -6.3909116 | 4.3883917 | 0.0000000 |
|  |  |  |  |  |  |  |
| **7O/**  **B3LYP** | **Ground state** | | | **Excited state** | | |
| C | -9.7272152 | 0.0000000 | -1.4887993 | -9.7242204 | 0.0000000 | -1.4936583 |
| C | -9.3341612 | 0.0000000 | -0.1795247 | -9.3220984 | 0.0000000 | -0.1790129 |
| O | -10.4320487 | 0.0000000 | 0.6336557 | -10.422019 | 0.0000000 | 0.6376150 |
| C | -11.5278003 | 0.0000000 | -0.1750216 | -11.518155 | 0.0000000 | -0.1699831 |
| C | -11.1536268 | 0.0000000 | -1.4786918 | -11.145783 | 0.0000000 | -1.4771687 |
| C | -8.0554316 | 0.0000000 | 0.4636535 | -8.0498432 | 0.0000000 | 0.4501606 |
| O | -6.9548985 | 0.0000000 | -0.3465832 | -6.9473329 | 0.0000000 | -0.3626887 |
| C | -5.8539816 | 0.0000000 | 0.4649276 | -5.8415501 | 0.0000000 | 0.4530980 |
| C | -6.2466181 | 0.0000000 | 1.7766021 | -6.2492095 | 0.0000000 | 1.7788173 |
| C | -7.6655632 | 0.0000000 | 1.7751289 | -7.6529940 | 0.0000000 | 1.7717708 |
| C | -4.5784733 | 0.0000000 | -0.1769608 | -4.5783752 | 0.0000000 | -0.1614684 |
| O | -3.4773774 | 0.0000000 | 0.6337311 | -3.4737661 | 0.0000000 | 0.6567677 |
| C | -2.3763245 | 0.0000000 | -0.1775127 | -2.3657733 | 0.0000000 | -0.1595849 |
| C | -2.7688496 | 0.0000000 | -1.4898335 | -2.7752448 | 0.0000000 | -1.4921941 |
| C | -4.1867309 | 0.0000000 | -1.4894195 | -4.1704530 | 0.0000000 | -1.4902054 |
| C | -1.1011023 | 0.0000000 | 0.4637143 | -1.1069898 | 0.0000000 | 0.4488417 |
| O | 0.0000000 | 0.0000000 | -0.3473177 | 0.0000000 | 0.0000000 | -0.3698296 |
| C | 1.1011023 | 0.0000000 | 0.4637143 | 1.1069898 | 0.0000000 | 0.4488417 |
| C | 0.7088438 | 0.0000000 | 1.7762324 | 0.6962327 | 0.0000000 | 1.7819429 |
| C | -0.7088438 | 0.0000000 | 1.7762324 | -0.6962327 | 0.0000000 | 1.7819429 |
| C | 2.3763245 | 0.0000000 | -0.1775127 | 2.3657733 | 0.0000000 | -0.1595849 |
| O | 3.4773774 | 0.0000000 | 0.6337311 | 3.4737661 | 0.0000000 | 0.6567677 |
| C | 4.5784733 | 0.0000000 | -0.1769608 | 4.5783752 | 0.0000000 | -0.1614684 |
| C | 4.1867309 | 0.0000000 | -1.4894195 | 4.1704530 | 0.0000000 | -1.4902054 |
| C | 2.7688496 | 0.0000000 | -1.4898335 | 2.7752448 | 0.0000000 | -1.4921941 |
| C | 5.8539816 | 0.0000000 | 0.4649276 | 5.8415501 | 0.0000000 | 0.4530980 |
| O | 6.9548985 | 0.0000000 | -0.3465832 | 6.9473329 | 0.0000000 | -0.3626887 |
| C | 8.0554316 | 0.0000000 | 0.4636535 | 8.0498432 | 0.0000000 | 0.4501606 |
| C | 7.6655632 | 0.0000000 | 1.7751289 | 7.6529940 | 0.0000000 | 1.7717708 |
| C | 6.2466181 | 0.0000000 | 1.7766021 | 6.2492095 | 0.0000000 | 1.7788173 |
| C | 9.3341612 | 0.0000000 | -0.1795247 | 9.3220984 | 0.0000000 | -0.1790129 |
| C | 9.7272152 | 0.0000000 | -1.4887993 | 9.7242204 | 0.0000000 | -1.4936583 |
| C | 11.1536268 | 0.0000000 | -1.4786918 | 11.1457831 | 0.0000000 | -1.4771687 |
| C | 11.5278003 | 0.0000000 | -0.1750216 | 11.5181551 | 0.0000000 | -0.1699831 |
| O | 10.4320487 | 0.0000000 | 0.6336557 | 10.4220192 | 0.0000000 | 0.6376150 |
| H | -1.3644407 | 0.0000000 | 2.6292835 | -1.3540347 | 0.0000000 | 2.6335766 |
| H | 2.1135020 | 0.0000000 | -2.3430814 | 2.1181532 | 0.0000000 | -2.3443148 |
| H | 4.8426283 | 0.0000000 | -2.3422323 | 4.8284386 | 0.0000000 | -2.3417708 |
| H | -2.1135020 | 0.0000000 | -2.3430814 | -2.1181532 | 0.0000000 | -2.3443148 |
| H | -4.8426283 | 0.0000000 | -2.3422323 | -4.8284386 | 0.0000000 | -2.3417708 |
| H | 8.3226746 | 0.0000000 | 2.6270695 | 8.3138044 | 0.0000000 | 2.6212268 |
| H | 5.5918519 | 0.0000000 | 2.6302891 | 5.5956574 | 0.0000000 | 2.6335597 |
| H | 1.3644407 | 0.0000000 | 2.6292835 | 1.3540347 | 0.0000000 | 2.6335766 |
| H | 11.8113759 | 0.0000000 | -2.3309925 | 11.8074364 | 0.0000000 | -2.3266697 |
| H | 9.0756938 | 0.0000000 | -2.3448504 | 9.0754983 | 0.0000000 | -2.3518313 |
| H | -5.5918519 | 0.0000000 | 2.6302891 | -5.5956574 | 0.0000000 | 2.6335597 |
| H | -8.3226746 | 0.0000000 | 2.6270695 | -8.3138044 | 0.0000000 | 2.6212268 |
| H | -9.0756938 | 0.0000000 | -2.3448504 | -9.0754983 | 0.0000000 | -2.3518313 |
| H | -11.8113759 | 0.0000000 | -2.3309925 | -11.807436 | 0.0000000 | -2.3266697 |
| H | -12.4798565 | 0.0000000 | 0.3241678 | -12.470290 | 0.0000000 | 0.3293818 |
| H | 12.4798565 | 0.0000000 | 0.3241678 | 12.4702902 | 0.0000000 | 0.3293818 |
|  |  |  |  |  |  |  |
| **8O/**  **B3LYP** | **Ground state** | | | **Excited state** | | |
| O | -11.9080393 | 2.5620270 | 0.0000000 | -11.898616 | 2.5562592 | 0.0000000 |
| C | -10.6419639 | 3.0755120 | 0.0000000 | -10.630510 | 3.0722554 | 0.0000000 |
| C | -10.6958567 | 4.4414491 | 0.0000000 | -10.690566 | 4.4438303 | 0.0000000 |
| C | -12.0796568 | 4.7876146 | 0.0000000 | -12.072077 | 4.7839349 | 0.0000000 |
| C | -12.7673135 | 3.6185556 | 0.0000000 | -12.758667 | 3.6117098 | 0.0000000 |
| C | -9.5641963 | 2.1335764 | 0.0000000 | -9.5548219 | 2.1422481 | 0.0000000 |
| C | -9.5139647 | 0.7662900 | 0.0000000 | -9.5017287 | 0.7658870 | 0.0000000 |
| C | -8.1402932 | 0.4107554 | 0.0000000 | -8.1412258 | 0.4085151 | 0.0000000 |
| C | -7.4327366 | 1.5829408 | 0.0000000 | -7.4185477 | 1.5882435 | 0.0000000 |
| O | -8.2962977 | 2.6435211 | 0.0000000 | -8.2849984 | 2.6531541 | 0.0000000 |
| C | -6.0374104 | 1.8862303 | 0.0000000 | -6.0388455 | 1.8719169 | 0.0000000 |
| O | -5.1734326 | 0.8264610 | 0.0000000 | -5.1731079 | 0.8063129 | 0.0000000 |
| C | -3.9047849 | 1.3373492 | 0.0000000 | -3.8976973 | 1.3198164 | 0.0000000 |
| C | -3.9574771 | 2.7061092 | 0.0000000 | -3.9614357 | 2.7092631 | 0.0000000 |
| C | -5.3305933 | 3.0594653 | 0.0000000 | -5.3160834 | 3.0551142 | 0.0000000 |
| C | -2.8299000 | 0.3982548 | 0.0000000 | -2.8291241 | 0.4137489 | 0.0000000 |
| O | -1.5612832 | 0.9088368 | 0.0000000 | -1.5540473 | 0.9298704 | 0.0000000 |
| C | -0.6973858 | -0.1513381 | 0.0000000 | -0.6855796 | -0.1375161 | 0.0000000 |
| C | -1.4048442 | -1.3244644 | 0.0000000 | -1.4149407 | -1.3254078 | 0.0000000 |
| C | -2.7776069 | -0.9706826 | 0.0000000 | -2.7645209 | -0.9769786 | 0.0000000 |
| C | 0.6973858 | 0.1513381 | 0.0000000 | 0.6855796 | 0.1375161 | 0.0000000 |
| O | 1.5612832 | -0.9088368 | 0.0000000 | 1.5540473 | -0.9298704 | 0.0000000 |
| C | 2.8299000 | -0.3982548 | 0.0000000 | 2.8291241 | -0.4137489 | 0.0000000 |
| C | 2.7776069 | 0.9706826 | 0.0000000 | 2.7645209 | 0.9769786 | 0.0000000 |
| C | 1.4048442 | 1.3244644 | 0.0000000 | 1.4149407 | 1.3254078 | 0.0000000 |
| C | 3.9047849 | -1.3373492 | 0.0000000 | 3.8976973 | -1.3198164 | 0.0000000 |
| O | 5.1734326 | -0.8264610 | 0.0000000 | 5.1731079 | -0.8063129 | 0.0000000 |
| C | 6.0374104 | -1.8862303 | 0.0000000 | 6.0388455 | -1.8719169 | 0.0000000 |
| C | 5.3305933 | -3.0594653 | 0.0000000 | 5.3160834 | -3.0551142 | 0.0000000 |
| C | 3.9574771 | -2.7061092 | 0.0000000 | 3.9614357 | -2.7092631 | 0.0000000 |
| H | 3.6253557 | 1.6331176 | 0.0000000 | 3.6138222 | 1.6378312 | 0.0000000 |
| H | -0.9829075 | -2.3141495 | 0.0000000 | -0.9909289 | -2.3144186 | 0.0000000 |
| H | -3.6253557 | -1.6331176 | 0.0000000 | -3.6138222 | -1.6378312 | 0.0000000 |
| H | 3.1099806 | -3.3688807 | 0.0000000 | 3.1134056 | -3.3715770 | 0.0000000 |
| C | 7.4327366 | -1.5829408 | 0.0000000 | 7.4185477 | -1.5882435 | 0.0000000 |
| H | 5.7529667 | -4.0489539 | 0.0000000 | 5.7410771 | -4.0437919 | 0.0000000 |
| H | -5.7529667 | 4.0489539 | 0.0000000 | -5.7410771 | 4.0437919 | 0.0000000 |
| H | -3.1099806 | 3.3688807 | 0.0000000 | -3.1134056 | 3.3715770 | 0.0000000 |
| H | 0.9829075 | 2.3141495 | 0.0000000 | 0.9909289 | 2.3144186 | 0.0000000 |
| H | -10.3628957 | 0.1052970 | 0.0000000 | -10.353289 | 0.1078713 | 0.0000000 |
| H | -7.7193014 | -0.5793295 | 0.0000000 | -7.7219266 | -0.5823603 | 0.0000000 |
| H | -12.5039084 | 5.7770885 | 0.0000000 | -12.500061 | 5.7719446 | 0.0000000 |
| H | -13.8138214 | 3.3727447 | 0.0000000 | -13.805186 | 3.3654397 | 0.0000000 |
| H | -9.8513291 | 5.1078410 | 0.0000000 | -9.8479439 | 5.1126170 | 0.0000000 |
| O | 8.2962977 | -2.6435211 | 0.0000000 | 8.2849984 | -2.6531541 | 0.0000000 |
| C | 9.5641963 | -2.1335764 | 0.0000000 | 9.5548219 | -2.1422481 | 0.0000000 |
| C | 9.5139647 | -0.7662900 | 0.0000000 | 9.5017287 | -0.7658870 | 0.0000000 |
| C | 8.1402932 | -0.4107554 | 0.0000000 | 8.1412258 | -0.4085151 | 0.0000000 |
| H | 7.7193014 | 0.5793295 | 0.0000000 | 7.7219266 | 0.5823603 | 0.0000000 |
| H | 10.3628957 | -0.1052970 | 0.0000000 | 10.3532891 | -0.1078713 | 0.0000000 |
| C | 10.6419639 | -3.0755120 | 0.0000000 | 10.6305106 | -3.0722554 | 0.0000000 |
| O | 11.9080393 | -2.5620270 | 0.0000000 | 11.8986164 | -2.5562592 | 0.0000000 |
| C | 12.7673135 | -3.6185556 | 0.0000000 | 12.7586672 | -3.6117098 | 0.0000000 |
| C | 12.0796568 | -4.7876146 | 0.0000000 | 12.0720774 | -4.7839349 | 0.0000000 |
| C | 10.6958567 | -4.4414491 | 0.0000000 | 10.6905663 | -4.4438303 | 0.0000000 |
| H | 9.8513291 | -5.1078410 | 0.0000000 | 9.8479439 | -5.1126170 | 0.0000000 |
| H | 12.5039084 | -5.7770885 | 0.0000000 | 12.5000618 | -5.7719446 | 0.0000000 |
| H | 13.8138214 | -3.3727447 | 0.0000000 | 13.8051864 | -3.3654397 | 0.0000000 |
|  |  |  |  |  |  |  |
| **9O/**  **B3LYP** | **Ground state** | | | **Excited state** | | |
| C | -13.2044812 | 0.0000000 | -1.5252232 | -13.198212 | 0.0000000 | -1.5288123 |
| C | -12.8113756 | 0.0000000 | -0.2159653 | -12.799422 | 0.0000000 | -0.2165507 |
| O | -13.9092169 | 0.0000000 | 0.5972666 | -13.898323 | 0.0000000 | 0.5989124 |
| C | -15.0049909 | 0.0000000 | -0.2113594 | -14.994405 | 0.0000000 | -0.2087278 |
| C | -14.6308813 | 0.0000000 | -1.5150530 | -14.621718 | 0.0000000 | -1.5145848 |
| C | -11.5326271 | 0.0000000 | 0.4271662 | -11.524674 | 0.0000000 | 0.4181110 |
| O | -10.4321211 | 0.0000000 | -0.3830645 | -10.422709 | 0.0000000 | -0.3926209 |
| C | -9.3312050 | 0.0000000 | 0.4284529 | -9.3188522 | 0.0000000 | 0.4219438 |
| C | -9.7238384 | 0.0000000 | 1.7401266 | -9.7224203 | 0.0000000 | 1.7423190 |
| C | -11.1427649 | 0.0000000 | 1.7386608 | -11.131392 | 0.0000000 | 1.7361474 |
| C | -8.0557183 | 0.0000000 | -0.2134502 | -8.0517211 | 0.0000000 | -0.2007502 |
| O | -6.9546086 | 0.0000000 | 0.5971573 | -6.9479619 | 0.0000000 | 0.6135609 |
| C | -5.8536049 | 0.0000000 | -0.2141828 | -5.8418909 | 0.0000000 | -0.2011882 |
| C | -6.2462298 | 0.0000000 | -1.5264803 | -6.2487411 | 0.0000000 | -1.5280914 |
| C | -7.6640731 | 0.0000000 | -1.5259731 | -7.6496018 | 0.0000000 | -1.5246098 |
| C | -4.5783869 | 0.0000000 | 0.4269595 | -4.5791993 | 0.0000000 | 0.4127956 |
| O | -3.4773102 | 0.0000000 | -0.3839979 | -3.4738399 | 0.0000000 | -0.4038607 |
| C | -2.3762124 | 0.0000000 | 0.4271246 | -2.3668796 | 0.0000000 | 0.4120311 |
| C | -2.7686086 | 0.0000000 | 1.7396658 | -2.7759153 | 0.0000000 | 1.7426938 |
| C | -4.1861977 | 0.0000000 | 1.7395800 | -4.1716755 | 0.0000000 | 1.7411751 |
| C | -1.1010943 | 0.0000000 | -0.2139509 | -1.1066009 | 0.0000000 | -0.1975658 |
| O | 0.0000000 | 0.0000000 | 0.5970791 | 0.0000000 | 0.0000000 | 0.6194097 |
| C | 1.1010943 | 0.0000000 | -0.2139509 | 1.1066009 | 0.0000000 | -0.1975658 |
| C | 0.7087735 | 0.0000000 | -1.5265664 | 0.6970098 | 0.0000000 | -1.5285707 |
| C | -0.7087735 | 0.0000000 | -1.5265664 | -0.6970098 | 0.0000000 | -1.5285707 |
| C | 2.3762124 | 0.0000000 | 0.4271246 | 2.3668796 | 0.0000000 | 0.4120311 |
| O | 3.4773102 | 0.0000000 | -0.3839979 | 3.4738399 | 0.0000000 | -0.4038607 |
| C | 4.5783869 | 0.0000000 | 0.4269595 | 4.5791993 | 0.0000000 | 0.4127956 |
| C | 4.1861977 | 0.0000000 | 1.7395800 | 4.1716755 | 0.0000000 | 1.7411751 |
| C | 2.7686086 | 0.0000000 | 1.7396658 | 2.7759153 | 0.0000000 | 1.7426938 |
| C | 5.8536049 | 0.0000000 | -0.2141828 | 5.8418909 | 0.0000000 | -0.2011882 |
| C | 6.2462298 | 0.0000000 | -1.5264803 | 6.2487411 | 0.0000000 | -1.5280914 |
| C | 7.6640731 | 0.0000000 | -1.5259731 | 7.6496018 | 0.0000000 | -1.5246098 |
| C | 8.0557183 | 0.0000000 | -0.2134502 | 8.0517211 | 0.0000000 | -0.2007502 |
| O | 6.9546086 | 0.0000000 | 0.5971573 | 6.9479619 | 0.0000000 | 0.6135609 |
| C | 9.3312050 | 0.0000000 | 0.4284529 | 9.3188522 | 0.0000000 | 0.4219438 |
| O | 10.4321211 | 0.0000000 | -0.3830645 | 10.4227090 | 0.0000000 | -0.3926209 |
| C | 11.5326271 | 0.0000000 | 0.4271662 | 11.5246747 | 0.0000000 | 0.4181110 |
| C | 11.1427649 | 0.0000000 | 1.7386608 | 11.1313924 | 0.0000000 | 1.7361474 |
| C | 9.7238384 | 0.0000000 | 1.7401266 | 9.7224203 | 0.0000000 | 1.7423190 |
| H | -4.8418595 | 0.0000000 | 2.5925752 | -4.8292720 | 0.0000000 | 2.5930161 |
| H | -1.3643620 | 0.0000000 | -2.3796229 | -1.3543181 | 0.0000000 | -2.3805834 |
| H | 1.3643620 | 0.0000000 | -2.3796229 | 1.3543181 | 0.0000000 | -2.3805834 |
| H | -5.5909608 | 0.0000000 | -2.3797921 | -5.5934400 | 0.0000000 | -2.3815145 |
| H | -8.3200310 | 0.0000000 | -2.3787352 | -8.3078341 | 0.0000000 | -2.3759556 |
| H | 4.8418595 | 0.0000000 | 2.5925752 | 4.8292720 | 0.0000000 | 2.5930161 |
| H | 2.1130988 | 0.0000000 | 2.5927882 | 2.1192292 | 0.0000000 | 2.5951226 |
| H | -2.1130988 | 0.0000000 | 2.5927882 | -2.1192292 | 0.0000000 | 2.5951226 |
| H | 8.3200310 | 0.0000000 | -2.3787352 | 8.3078341 | 0.0000000 | -2.3759556 |
| H | 5.5909608 | 0.0000000 | -2.3797921 | 5.5934400 | 0.0000000 | -2.3815145 |
| H | 11.7998782 | 0.0000000 | 2.5905971 | 11.7915062 | 0.0000000 | 2.5860234 |
| C | 12.8113756 | 0.0000000 | -0.2159653 | 12.7994221 | 0.0000000 | -0.2165507 |
| H | 9.0690812 | 0.0000000 | 2.5938221 | 9.0692829 | 0.0000000 | 2.5973099 |
| H | -9.0690812 | 0.0000000 | 2.5938221 | -9.0692829 | 0.0000000 | 2.5973099 |
| H | -11.7998782 | 0.0000000 | 2.5905971 | -11.791506 | 0.0000000 | 2.5860234 |
| H | -12.5530072 | 0.0000000 | -2.3813112 | -12.548646 | 0.0000000 | -2.3863355 |
| H | -15.2886668 | 0.0000000 | -2.3673236 | -15.281994 | 0.0000000 | -2.3650521 |
| H | -15.9570270 | 0.0000000 | 0.2878688 | -15.946383 | 0.0000000 | 0.2908068 |
| O | 13.9092169 | 0.0000000 | 0.5972666 | 13.8983238 | 0.0000000 | 0.5989124 |
| C | 15.0049909 | 0.0000000 | -0.2113594 | 14.9944052 | 0.0000000 | -0.2087278 |
| C | 14.6308813 | 0.0000000 | -1.5150530 | 14.6217188 | 0.0000000 | -1.5145848 |
| C | 13.2044812 | 0.0000000 | -1.5252232 | 13.1982129 | 0.0000000 | -1.5288123 |
| H | 12.5530072 | 0.0000000 | -2.3813112 | 12.5486461 | 0.0000000 | -2.3863355 |
| H | 15.2886668 | 0.0000000 | -2.3673236 | 15.2819944 | 0.0000000 | -2.3650521 |
| H | 15.9570270 | 0.0000000 | 0.2878688 | 15.9463830 | 0.0000000 | 0.2908068 |

Part 4.

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| **2O/**  **PBE0** | **Ground state** | | | **Excited state** | | |
| C | -2.8019400 | 0.4335265 | 0.0000000 | -2.7896848 | 0.4449416 | 0.0000000 |
| C | -2.7873208 | -0.9201693 | 0.0000000 | -2.7670467 | -0.9340221 | 0.0000000 |
| C | -1.4168361 | -1.3022381 | 0.0000000 | -1.4324512 | -1.3281350 | 0.0000000 |
| C | -0.7020601 | -0.1421696 | 0.0000000 | -0.6772813 | -0.1278106 | 0.0000000 |
| C | 0.7020601 | 0.1421696 | 0.0000000 | 0.6772813 | 0.1278106 | 0.0000000 |
| C | 1.4168361 | 1.3022381 | 0.0000000 | 1.4324512 | 1.3281350 | 0.0000000 |
| C | 2.7873208 | 0.9201693 | 0.0000000 | 2.7670467 | 0.9340221 | 0.0000000 |
| C | 2.8019400 | -0.4335265 | 0.0000000 | 2.7896848 | -0.4449416 | 0.0000000 |
| O | -1.5409886 | 0.9215955 | 0.0000000 | -1.5326338 | 0.9606364 | 0.0000000 |
| O | 1.5409886 | -0.9215955 | 0.0000000 | 1.5326338 | -0.9606364 | 0.0000000 |
| H | -3.5905478 | 1.1662342 | 0.0000000 | -3.5949874 | 1.1608028 | 0.0000000 |
| H | -3.6481223 | -1.5684999 | 0.0000000 | -3.6383551 | -1.5695130 | 0.0000000 |
| H | -1.0068822 | -2.2981827 | 0.0000000 | -1.0203277 | -2.3230511 | 0.0000000 |
| H | 1.0068822 | 2.2981827 | 0.0000000 | 1.0203277 | 2.3230511 | 0.0000000 |
| H | 3.6481223 | 1.5684999 | 0.0000000 | 3.6383551 | 1.5695130 | 0.0000000 |
| H | 3.5905478 | -1.1662342 | 0.0000000 | 3.5949874 | -1.1608028 | 0.0000000 |
|  |  |  |  |  |  |  |
| **3O/**  **PBE0** | **Ground state** | | | **Excited state** | | |
| O | 3.4583749 | 0.0000000 | 0.8315297 | 3.4593820 | 0.0000000 | 0.8487667 |
| C | 4.5464821 | 0.0000000 | 0.0291529 | 4.5327317 | 0.0000000 | 0.0233276 |
| C | 4.1767175 | 0.0000000 | -1.2734029 | 4.1420904 | 0.0000000 | -1.2857617 |
| C | 2.7545994 | 0.0000000 | -1.2824632 | 2.7374186 | 0.0000000 | -1.2916707 |
| C | 2.3688621 | 0.0000000 | 0.0254887 | 2.3479072 | 0.0000000 | 0.0485762 |
| C | 1.0917222 | 0.0000000 | 0.6685318 | 1.0990937 | 0.0000000 | 0.6606933 |
| O | 0.0000000 | 0.0000000 | -0.1357129 | 0.0000000 | 0.0000000 | -0.1645660 |
| C | -1.0917222 | 0.0000000 | 0.6685318 | -1.0990937 | 0.0000000 | 0.6606933 |
| C | -0.7081531 | 0.0000000 | 1.9778930 | -0.6902602 | 0.0000000 | 2.0055916 |
| C | 0.7081531 | 0.0000000 | 1.9778930 | 0.6902602 | 0.0000000 | 2.0055916 |
| C | -2.3688621 | 0.0000000 | 0.0254887 | -2.3479072 | 0.0000000 | 0.0485762 |
| O | -3.4583749 | 0.0000000 | 0.8315297 | -3.4593820 | 0.0000000 | 0.8487667 |
| C | -4.5464821 | 0.0000000 | 0.0291529 | -4.5327317 | 0.0000000 | 0.0233276 |
| C | -4.1767175 | 0.0000000 | -1.2734029 | -4.1420904 | 0.0000000 | -1.2857617 |
| C | -2.7545994 | 0.0000000 | -1.2824632 | -2.7374186 | 0.0000000 | -1.2916707 |
| H | 5.4999988 | 0.0000000 | 0.5287181 | 5.4974306 | 0.0000000 | 0.5023639 |
| H | 4.8371374 | 0.0000000 | -2.1249508 | 4.8010727 | 0.0000000 | -2.1392026 |
| H | 2.0982346 | 0.0000000 | -2.1363103 | 2.0711290 | 0.0000000 | -2.1381007 |
| H | -2.0982346 | 0.0000000 | -2.1363103 | -2.0711290 | 0.0000000 | -2.1381007 |
| H | -5.4999988 | 0.0000000 | 0.5287181 | -5.4974306 | 0.0000000 | 0.5023639 |
| H | -4.8371374 | 0.0000000 | -2.1249508 | -4.8010727 | 0.0000000 | -2.1392026 |
| H | 1.3686750 | 0.0000000 | 2.8286717 | 1.3558620 | 0.0000000 | 2.8527016 |
| H | -1.3686750 | 0.0000000 | 2.8286717 | -1.3558620 | 0.0000000 | 2.8527016 |
|  |  |  |  |  |  |  |
| **4O/**  **PBE0** | **Ground state** | | | **Excited state** | | |
| O | -1.7622633 | 0.3445737 | 0.0000000 | -1.7624997 | 0.3765569 | 0.0000000 |
| C | -2.7865876 | -0.5437700 | 0.0000000 | -2.7886039 | -0.5267268 | 0.0000000 |
| C | -2.3002088 | -1.8190298 | 0.0000000 | -2.2810910 | -1.8233623 | 0.0000000 |
| C | -0.8892151 | -1.7073449 | 0.0000000 | -0.8987537 | -1.7185898 | 0.0000000 |
| C | -0.6095548 | -0.3706287 | 0.0000000 | -0.5993055 | -0.3492399 | 0.0000000 |
| C | 0.6095548 | 0.3706287 | 0.0000000 | 0.5993055 | 0.3492399 | 0.0000000 |
| O | 1.7622633 | -0.3445737 | 0.0000000 | 1.7624997 | -0.3765569 | 0.0000000 |
| C | 2.7865876 | 0.5437700 | 0.0000000 | 2.7886039 | 0.5267268 | 0.0000000 |
| C | 2.3002088 | 1.8190298 | 0.0000000 | 2.2810910 | 1.8233623 | 0.0000000 |
| C | 0.8892151 | 1.7073449 | 0.0000000 | 0.8987537 | 1.7185898 | 0.0000000 |
| C | 4.1106133 | 0.0048969 | 0.0000000 | 4.0938335 | 0.0152246 | 0.0000000 |
| O | 5.1324032 | 0.8953566 | 0.0000000 | 5.1253866 | 0.9081513 | 0.0000000 |
| C | 6.2809267 | 0.1822915 | 0.0000000 | 6.2699099 | 0.1878785 | 0.0000000 |
| C | 6.0162735 | -1.1456929 | 0.0000000 | 6.0006633 | -1.1467823 | 0.0000000 |
| C | 4.5995683 | -1.2682416 | 0.0000000 | 4.5958602 | -1.2745290 | 0.0000000 |
| H | -2.8914673 | -2.7193248 | 0.0000000 | -2.8772166 | -2.7209188 | 0.0000000 |
| H | -0.1641650 | -2.5037929 | 0.0000000 | -0.1710844 | -2.5129758 | 0.0000000 |
| H | 4.0135256 | -2.1718045 | 0.0000000 | 4.0094160 | -2.1780096 | 0.0000000 |
| H | 7.1916005 | 0.7562634 | 0.0000000 | 7.1851746 | 0.7553153 | 0.0000000 |
| H | 6.7425350 | -1.9418185 | 0.0000000 | 6.7307437 | -1.9400145 | 0.0000000 |
| H | 0.1641650 | 2.5037929 | 0.0000000 | 0.1710844 | 2.5129758 | 0.0000000 |
| H | 2.8914673 | 2.7193248 | 0.0000000 | 2.8772166 | 2.7209188 | 0.0000000 |
| C | -4.1106133 | -0.0048969 | 0.0000000 | -4.0938335 | -0.0152246 | 0.0000000 |
| O | -5.1324032 | -0.8953566 | 0.0000000 | -5.1253866 | -0.9081513 | 0.0000000 |
| C | -6.2809267 | -0.1822915 | 0.0000000 | -6.2699099 | -0.1878785 | 0.0000000 |
| C | -6.0162735 | 1.1456929 | 0.0000000 | -6.0006633 | 1.1467823 | 0.0000000 |
| C | -4.5995683 | 1.2682416 | 0.0000000 | -4.5958602 | 1.2745290 | 0.0000000 |
| H | -4.0135256 | 2.1718045 | 0.0000000 | -4.0094160 | 2.1780096 | 0.0000000 |
| H | -7.1916005 | -0.7562634 | 0.0000000 | -7.1851746 | -0.7553153 | 0.0000000 |
| H | -6.7425350 | 1.9418185 | 0.0000000 | -6.7307437 | 1.9400145 | 0.0000000 |
|  |  |  |  |  |  |  |
| **5O/**  **PBE0** | **Ground state** | | | **Excited state** | | |
| O | 3.4583005 | 0.0000000 | 0.2652565 | 3.4543768 | 0.0000000 | 0.2929201 |
| C | 4.5501069 | 0.0000000 | -0.5385886 | 4.5471257 | 0.0000000 | -0.5211871 |
| C | 4.1669640 | 0.0000000 | -1.8487095 | 4.1483471 | 0.0000000 | -1.8472249 |
| C | 2.7517755 | 0.0000000 | -1.8500085 | 2.7562470 | 0.0000000 | -1.8521886 |
| C | 2.3662147 | 0.0000000 | -0.5396974 | 2.3529960 | 0.0000000 | -0.5174478 |
| C | 1.0922158 | 0.0000000 | 0.1015676 | 1.0987271 | 0.0000000 | 0.0868404 |
| O | 0.0000000 | 0.0000000 | -0.7028729 | 0.0000000 | 0.0000000 | -0.7292294 |
| C | -1.0922158 | 0.0000000 | 0.1015676 | -1.0987271 | 0.0000000 | 0.0868404 |
| C | -0.7072225 | 0.0000000 | 1.4123810 | -0.6926181 | 0.0000000 | 1.4233685 |
| C | 0.7072225 | 0.0000000 | 1.4123810 | 0.6926181 | 0.0000000 | 1.4233685 |
| C | -2.3662147 | 0.0000000 | -0.5396974 | -2.3529960 | 0.0000000 | -0.5174478 |
| O | -3.4583005 | 0.0000000 | 0.2652565 | -3.4543768 | 0.0000000 | 0.2929201 |
| C | -4.5501069 | 0.0000000 | -0.5385886 | -4.5471257 | 0.0000000 | -0.5211871 |
| C | -4.1669640 | 0.0000000 | -1.8487095 | -4.1483471 | 0.0000000 | -1.8472249 |
| C | -2.7517755 | 0.0000000 | -1.8500085 | -2.7562470 | 0.0000000 | -1.8521886 |
| C | 5.8269940 | 0.0000000 | 0.1038728 | 5.8139210 | 0.0000000 | 0.0960875 |
| O | 6.9163603 | 0.0000000 | -0.7025186 | 6.9069941 | 0.0000000 | -0.7158090 |
| C | 8.0044856 | 0.0000000 | 0.0996127 | 7.9953687 | 0.0000000 | 0.0857856 |
| C | 7.6350868 | 0.0000000 | 1.4023811 | 7.6282736 | 0.0000000 | 1.3944502 |
| C | 6.2131717 | 0.0000000 | 1.4118920 | 6.2144567 | 0.0000000 | 1.4142219 |
| C | -5.8269940 | 0.0000000 | 0.1038728 | -5.8139210 | 0.0000000 | 0.0960875 |
| O | -6.9163603 | 0.0000000 | -0.7025186 | -6.9069941 | 0.0000000 | -0.7158090 |
| H | -4.8281761 | 0.0000000 | -2.6989487 | -4.8126001 | 0.0000000 | -2.6956153 |
| H | -2.0926711 | 0.0000000 | -2.7018386 | -2.0952148 | 0.0000000 | -2.7028007 |
| H | -1.3670992 | 0.0000000 | 2.2636133 | -1.3555884 | 0.0000000 | 2.2725483 |
| H | 1.3670992 | 0.0000000 | 2.2636133 | 1.3555884 | 0.0000000 | 2.2725483 |
| H | 2.0926711 | 0.0000000 | -2.7018386 | 2.0952148 | 0.0000000 | -2.7028007 |
| H | 4.8281761 | 0.0000000 | -2.6989487 | 4.8126001 | 0.0000000 | -2.6956153 |
| H | 5.5571609 | 0.0000000 | 2.2660142 | 5.5623367 | 0.0000000 | 2.2714134 |
| H | 8.2957556 | 0.0000000 | 2.2537217 | 8.2953342 | 0.0000000 | 2.2412042 |
| C | -8.0044856 | 0.0000000 | 0.0996127 | -7.9953687 | 0.0000000 | 0.0857856 |
| C | -7.6350868 | 0.0000000 | 1.4023811 | -7.6282736 | 0.0000000 | 1.3944502 |
| C | -6.2131717 | 0.0000000 | 1.4118920 | -6.2144567 | 0.0000000 | 1.4142219 |
| H | -5.5571609 | 0.0000000 | 2.2660142 | -5.5623367 | 0.0000000 | 2.2714134 |
| H | -8.9579331 | 0.0000000 | -0.4000981 | -8.9493910 | 0.0000000 | -0.4134834 |
| H | -8.2957556 | 0.0000000 | 2.2537217 | -8.2953342 | 0.0000000 | 2.2412042 |
| H | 8.9579331 | 0.0000000 | -0.4000981 | 8.9493910 | 0.0000000 | -0.4134834 |
|  |  |  |  |  |  |  |
| **6O/**  **PBE0** | **Ground state** | | | **Excited state** | | |
| O | 1.7955626 | -0.0149158 | 0.0000000 | 1.8010614 | 0.0107363 | 0.0000000 |
| C | 0.5228434 | -0.4846099 | 0.0000000 | 0.5189176 | -0.4640284 | 0.0000000 |
| C | 0.5289798 | -1.8509896 | 0.0000000 | 0.5367796 | -1.8588996 | 0.0000000 |
| C | 1.8876446 | -2.2434744 | 0.0000000 | 1.8703641 | -2.2430171 | 0.0000000 |
| C | 2.6214534 | -1.0909223 | 0.0000000 | 2.6283164 | -1.0761262 | 0.0000000 |
| C | 4.0233469 | -0.8288035 | 0.0000000 | 4.0062217 | -0.8415852 | 0.0000000 |
| O | 4.8488455 | -1.9054686 | 0.0000000 | 4.8368694 | -1.9245862 | 0.0000000 |
| C | 6.1209359 | -1.4365705 | 0.0000000 | 6.1119001 | -1.4510332 | 0.0000000 |
| C | 6.1168473 | -0.0715334 | 0.0000000 | 6.1016474 | -0.0713445 | 0.0000000 |
| C | 4.7577793 | 0.3228426 | 0.0000000 | 4.7617294 | 0.3230847 | 0.0000000 |
| H | 6.9882408 | 0.5615365 | 0.0000000 | 6.9759140 | 0.5583922 | 0.0000000 |
| H | 2.2853325 | -3.2444087 | 0.0000000 | 2.2707048 | -3.2432385 | 0.0000000 |
| H | -0.3411772 | -2.4857093 | 0.0000000 | -0.3352893 | -2.4913968 | 0.0000000 |
| C | 7.1691173 | -2.4084049 | 0.0000000 | 7.1579709 | -2.4027583 | 0.0000000 |
| O | 8.4395904 | -1.9363041 | 0.0000000 | 8.4319325 | -1.9269912 | 0.0000000 |
| C | 9.2620775 | -3.0090971 | 0.0000000 | 9.2553676 | -2.9986725 | 0.0000000 |
| C | 8.5453696 | -4.1580201 | 0.0000000 | 8.5398867 | -4.1525963 | 0.0000000 |
| C | 7.1767839 | -3.7722205 | 0.0000000 | 7.1746801 | -3.7763538 | 0.0000000 |
| H | 6.3093609 | -4.4105425 | 0.0000000 | 6.3098987 | -4.4183072 | 0.0000000 |
| H | 10.3168102 | -2.7938853 | 0.0000000 | 10.3102626 | -2.7831493 | 0.0000000 |
| H | 8.9435779 | -5.1593631 | 0.0000000 | 8.9440304 | -5.1518124 | 0.0000000 |
| C | -0.5228434 | 0.4846099 | 0.0000000 | -0.5189176 | 0.4640284 | 0.0000000 |
| O | -1.7955626 | 0.0149158 | 0.0000000 | -1.8010614 | -0.0107363 | 0.0000000 |
| C | -2.6214534 | 1.0909223 | 0.0000000 | -2.6283164 | 1.0761262 | 0.0000000 |
| C | -1.8876446 | 2.2434744 | 0.0000000 | -1.8703641 | 2.2430171 | 0.0000000 |
| C | -0.5289798 | 1.8509896 | 0.0000000 | -0.5367796 | 1.8588996 | 0.0000000 |
| H | -2.2853325 | 3.2444087 | 0.0000000 | -2.2707048 | 3.2432385 | 0.0000000 |
| H | 0.3411772 | 2.4857093 | 0.0000000 | 0.3352893 | 2.4913968 | 0.0000000 |
| H | 4.3612956 | 1.3242611 | 0.0000000 | 4.3656934 | 1.3248581 | 0.0000000 |
| C | -4.0233469 | 0.8288035 | 0.0000000 | -4.0062217 | 0.8415852 | 0.0000000 |
| C | -4.7577793 | -0.3228426 | 0.0000000 | -4.7617294 | -0.3230847 | 0.0000000 |
| C | -6.1168473 | 0.0715334 | 0.0000000 | -6.1016474 | 0.0713445 | 0.0000000 |
| C | -6.1209359 | 1.4365705 | 0.0000000 | -6.1119001 | 1.4510332 | 0.0000000 |
| O | -4.8488455 | 1.9054686 | 0.0000000 | -4.8368694 | 1.9245862 | 0.0000000 |
| H | -6.9882408 | -0.5615365 | 0.0000000 | -6.9759140 | -0.5583922 | 0.0000000 |
| H | -4.3612956 | -1.3242611 | 0.0000000 | -4.3656934 | -1.3248581 | 0.0000000 |
| C | -7.1691173 | 2.4084049 | 0.0000000 | -7.1579709 | 2.4027583 | 0.0000000 |
| C | -7.1767839 | 3.7722205 | 0.0000000 | -7.1746801 | 3.7763538 | 0.0000000 |
| C | -8.5453696 | 4.1580201 | 0.0000000 | -8.5398867 | 4.1525963 | 0.0000000 |
| C | -9.2620775 | 3.0090971 | 0.0000000 | -9.2553676 | 2.9986725 | 0.0000000 |
| O | -8.4395904 | 1.9363041 | 0.0000000 | -8.4319325 | 1.9269912 | 0.0000000 |
| H | -8.9435779 | 5.1593631 | 0.0000000 | -8.9440304 | 5.1518124 | 0.0000000 |
| H | -10.3168102 | 2.7938853 | 0.0000000 | -10.310262 | 2.7831493 | 0.0000000 |
| H | -6.3093609 | 4.4105425 | 0.0000000 | -6.3098987 | 4.4183072 | 0.0000000 |
|  |  |  |  |  |  |  |
| **7O/**  **PBE0** | **Ground state** | | | **Excited state** | | |
| C | -9.6712412 | 0.0000000 | -1.4872084 | -9.6677781 | 0.0000000 | -1.4920121 |
| C | -9.2849801 | 0.0000000 | -0.1792117 | -9.2729820 | 0.0000000 | -0.1790145 |
| O | -10.3742669 | 0.0000000 | 0.6272762 | -10.364066 | 0.0000000 | 0.6307268 |
| C | -11.4624095 | 0.0000000 | -0.1747739 | -11.452588 | 0.0000000 | -0.1702014 |
| C | -11.0931253 | 0.0000000 | -1.4775906 | -11.085265 | 0.0000000 | -1.4763211 |
| C | -8.0080858 | 0.0000000 | 0.4631824 | -8.0021054 | 0.0000000 | 0.4496456 |
| O | -6.9162984 | 0.0000000 | -0.3405735 | -6.9085222 | 0.0000000 | -0.3564801 |
| C | -5.8242552 | 0.0000000 | 0.4644872 | -5.8117039 | 0.0000000 | 0.4528345 |
| C | -6.2099431 | 0.0000000 | 1.7748038 | -6.2123700 | 0.0000000 | 1.7770326 |
| C | -7.6250512 | 0.0000000 | 1.7734022 | -7.6128339 | 0.0000000 | 1.7696872 |
| C | -4.5503255 | 0.0000000 | -0.1766369 | -4.5499584 | 0.0000000 | -0.1598922 |
| O | -3.4580822 | 0.0000000 | 0.6275829 | -3.4543454 | 0.0000000 | 0.6518710 |
| C | -2.3659096 | 0.0000000 | -0.1771889 | -2.3550350 | 0.0000000 | -0.1582010 |
| C | -2.7514112 | 0.0000000 | -1.4881161 | -2.7581410 | 0.0000000 | -1.4901223 |
| C | -4.1655714 | 0.0000000 | -1.4877249 | -4.1492222 | 0.0000000 | -1.4875694 |
| C | -1.0922263 | 0.0000000 | 0.4633387 | -1.0982494 | 0.0000000 | 0.4468739 |
| O | 0.0000000 | 0.0000000 | -0.3412158 | 0.0000000 | 0.0000000 | -0.3656048 |
| C | 1.0922263 | 0.0000000 | 0.4633387 | 1.0982494 | 0.0000000 | 0.4468739 |
| C | 0.7069957 | 0.0000000 | 1.7744589 | 0.6938825 | 0.0000000 | 1.7795672 |
| C | -0.7069957 | 0.0000000 | 1.7744589 | -0.6938825 | 0.0000000 | 1.7795672 |
| C | 2.3659096 | 0.0000000 | -0.1771889 | 2.3550350 | 0.0000000 | -0.1582010 |
| O | 3.4580822 | 0.0000000 | 0.6275829 | 3.4543454 | 0.0000000 | 0.6518710 |
| C | 4.5503255 | 0.0000000 | -0.1766369 | 4.5499584 | 0.0000000 | -0.1598922 |
| C | 4.1655714 | 0.0000000 | -1.4877249 | 4.1492222 | 0.0000000 | -1.4875694 |
| C | 2.7514112 | 0.0000000 | -1.4881161 | 2.7581410 | 0.0000000 | -1.4901223 |
| C | 5.8242552 | 0.0000000 | 0.4644872 | 5.8117039 | 0.0000000 | 0.4528345 |
| O | 6.9162984 | 0.0000000 | -0.3405735 | 6.9085222 | 0.0000000 | -0.3564801 |
| C | 8.0080858 | 0.0000000 | 0.4631824 | 8.0021054 | 0.0000000 | 0.4496456 |
| C | 7.6250512 | 0.0000000 | 1.7734022 | 7.6128339 | 0.0000000 | 1.7696872 |
| C | 6.2099431 | 0.0000000 | 1.7748038 | 6.2123700 | 0.0000000 | 1.7770326 |
| C | 9.2849801 | 0.0000000 | -0.1792117 | 9.2729820 | 0.0000000 | -0.1790145 |
| C | 9.6712412 | 0.0000000 | -1.4872084 | 9.6677781 | 0.0000000 | -1.4920121 |
| C | 11.0931253 | 0.0000000 | -1.4775906 | 11.0852654 | 0.0000000 | -1.4763211 |
| C | 11.4624095 | 0.0000000 | -0.1747739 | 11.4525882 | 0.0000000 | -0.1702014 |
| O | 10.3742669 | 0.0000000 | 0.6272762 | 10.3640663 | 0.0000000 | 0.6307268 |
| H | -1.3667800 | 0.0000000 | 2.6257631 | -1.3557994 | 0.0000000 | 2.6295588 |
| H | 2.0918709 | 0.0000000 | -2.3396160 | 2.0972167 | 0.0000000 | -2.3408025 |
| H | 4.8256537 | 0.0000000 | -2.3387886 | 4.8116050 | 0.0000000 | -2.3372666 |
| H | -2.0918709 | 0.0000000 | -2.3396160 | -2.0972167 | 0.0000000 | -2.3408025 |
| H | -4.8256537 | 0.0000000 | -2.3387886 | -4.8116050 | 0.0000000 | -2.3372666 |
| H | 8.2863233 | 0.0000000 | 2.6235891 | 8.2779744 | 0.0000000 | 2.6172557 |
| H | 5.5509594 | 0.0000000 | 2.6267325 | 5.5548980 | 0.0000000 | 2.6302750 |
| H | 1.3667800 | 0.0000000 | 2.6257631 | 1.3557994 | 0.0000000 | 2.6295588 |
| H | 11.7538577 | 0.0000000 | -2.3288764 | 11.7497664 | 0.0000000 | -2.3248865 |
| H | 9.0153193 | 0.0000000 | -2.3414009 | 9.0145809 | 0.0000000 | -2.3483078 |
| H | -5.5509594 | 0.0000000 | 2.6267325 | -5.5548980 | 0.0000000 | 2.6302750 |
| H | -8.2863233 | 0.0000000 | 2.6235891 | -8.2779744 | 0.0000000 | 2.6172557 |
| H | -9.0153193 | 0.0000000 | -2.3414009 | -9.0145809 | 0.0000000 | -2.3483078 |
| H | -11.7538577 | 0.0000000 | -2.3288764 | -11.749766 | 0.0000000 | -2.3248865 |
| H | -12.4158311 | 0.0000000 | 0.3249908 | -12.406048 | 0.0000000 | 0.3298446 |
| H | 12.4158311 | 0.0000000 | 0.3249908 | 12.4060488 | 0.0000000 | 0.3298446 |
|  |  |  |  |  |  |  |
| **8O/**  **PBE0** | **Ground state** | | | **Excited state** | | |
| O | -11.8415162 | 2.5496746 | 0.0000000 | -11.831959 | 2.5442751 | 0.0000000 |
| C | -10.5854893 | 3.0589560 | 0.0000000 | -10.574135 | 3.0558845 | 0.0000000 |
| C | -10.6332663 | 4.4219533 | 0.0000000 | -10.627597 | 4.4240663 | 0.0000000 |
| C | -12.0125923 | 4.7673226 | 0.0000000 | -12.004928 | 4.7638358 | 0.0000000 |
| C | -12.6951827 | 3.5977976 | 0.0000000 | -12.686359 | 3.5913418 | 0.0000000 |
| C | -9.5092063 | 2.1183479 | 0.0000000 | -9.4996275 | 2.1266798 | 0.0000000 |
| C | -9.4650962 | 0.7539887 | 0.0000000 | -9.4532436 | 0.7537807 | 0.0000000 |
| C | -8.0950735 | 0.3996651 | 0.0000000 | -8.0958104 | 0.3972633 | 0.0000000 |
| C | -7.3947414 | 1.5723614 | 0.0000000 | -7.3806891 | 1.5772294 | 0.0000000 |
| O | -8.2514613 | 2.6243641 | 0.0000000 | -8.2401575 | 2.6334631 | 0.0000000 |
| C | -6.0011796 | 1.8755282 | 0.0000000 | -6.0025478 | 1.8602896 | 0.0000000 |
| O | -5.1439969 | 0.8243672 | 0.0000000 | -5.1437089 | 0.8034953 | 0.0000000 |
| C | -3.8856438 | 1.3313974 | 0.0000000 | -3.8784816 | 1.3132578 | 0.0000000 |
| C | -3.9320895 | 2.6970435 | 0.0000000 | -3.9363221 | 2.7000030 | 0.0000000 |
| C | -5.3016520 | 3.0492849 | 0.0000000 | -5.2875737 | 3.0441745 | 0.0000000 |
| C | -2.8119405 | 0.3935064 | 0.0000000 | -2.8107831 | 0.4103992 | 0.0000000 |
| O | -1.5536156 | 0.9002273 | 0.0000000 | -1.5459340 | 0.9228343 | 0.0000000 |
| C | -0.6965372 | -0.1513221 | 0.0000000 | -0.6841363 | -0.1362253 | 0.0000000 |
| C | -1.3966414 | -1.3249510 | 0.0000000 | -1.4070676 | -1.3253555 | 0.0000000 |
| C | -2.7658911 | -0.9723106 | 0.0000000 | -2.7522962 | -0.9779861 | 0.0000000 |
| C | 0.6965372 | 0.1513221 | 0.0000000 | 0.6841363 | 0.1362253 | 0.0000000 |
| O | 1.5536156 | -0.9002273 | 0.0000000 | 1.5459340 | -0.9228343 | 0.0000000 |
| C | 2.8119405 | -0.3935064 | 0.0000000 | 2.8107831 | -0.4103992 | 0.0000000 |
| C | 2.7658911 | 0.9723106 | 0.0000000 | 2.7522962 | 0.9779861 | 0.0000000 |
| C | 1.3966414 | 1.3249510 | 0.0000000 | 1.4070676 | 1.3253555 | 0.0000000 |
| C | 3.8856438 | -1.3313974 | 0.0000000 | 3.8784816 | -1.3132578 | 0.0000000 |
| O | 5.1439969 | -0.8243672 | 0.0000000 | 5.1437089 | -0.8034953 | 0.0000000 |
| C | 6.0011796 | -1.8755282 | 0.0000000 | 6.0025478 | -1.8602896 | 0.0000000 |
| C | 5.3016520 | -3.0492849 | 0.0000000 | 5.2875737 | -3.0441745 | 0.0000000 |
| C | 3.9320895 | -2.6970435 | 0.0000000 | 3.9363221 | -2.7000030 | 0.0000000 |
| H | 3.6171649 | 1.6321302 | 0.0000000 | 3.6051690 | 1.6362231 | 0.0000000 |
| H | -0.9700427 | -2.3139167 | 0.0000000 | -0.9786541 | -2.3137896 | 0.0000000 |
| H | -3.6171649 | -1.6321302 | 0.0000000 | -3.6051690 | -1.6362231 | 0.0000000 |
| H | 3.0810560 | -3.3571896 | 0.0000000 | 3.0850682 | -3.3601254 | 0.0000000 |
| C | 7.3947414 | -1.5723614 | 0.0000000 | 7.3806891 | -1.5772294 | 0.0000000 |
| H | 5.7286890 | -4.0380487 | 0.0000000 | 5.7174695 | -4.0320464 | 0.0000000 |
| H | -5.7286890 | 4.0380487 | 0.0000000 | -5.7174695 | 4.0320464 | 0.0000000 |
| H | -3.0810560 | 3.3571896 | 0.0000000 | -3.0850682 | 3.3601254 | 0.0000000 |
| H | 0.9700427 | 2.3139167 | 0.0000000 | 0.9786541 | 2.3137896 | 0.0000000 |
| H | -10.3175431 | 0.0956337 | 0.0000000 | -10.308368 | 0.0984795 | 0.0000000 |
| H | -7.6694113 | -0.5897069 | 0.0000000 | -7.6721230 | -0.5930425 | 0.0000000 |
| H | -12.4401107 | 5.7565046 | 0.0000000 | -12.435940 | 5.7516374 | 0.0000000 |
| H | -13.7431278 | 3.3516447 | 0.0000000 | -13.734319 | 3.3447085 | 0.0000000 |
| H | -9.7850017 | 5.0855254 | 0.0000000 | -9.7811439 | 5.0899543 | 0.0000000 |
| O | 8.2514613 | -2.6243641 | 0.0000000 | 8.2401575 | -2.6334631 | 0.0000000 |
| C | 9.5092063 | -2.1183479 | 0.0000000 | 9.4996275 | -2.1266798 | 0.0000000 |
| C | 9.4650962 | -0.7539887 | 0.0000000 | 9.4532436 | -0.7537807 | 0.0000000 |
| C | 8.0950735 | -0.3996651 | 0.0000000 | 8.0958104 | -0.3972633 | 0.0000000 |
| H | 7.6694113 | 0.5897069 | 0.0000000 | 7.6721230 | 0.5930425 | 0.0000000 |
| H | 10.3175431 | -0.0956337 | 0.0000000 | 10.3083683 | -0.0984795 | 0.0000000 |
| C | 10.5854893 | -3.0589560 | 0.0000000 | 10.5741351 | -3.0558845 | 0.0000000 |
| O | 11.8415162 | -2.5496746 | 0.0000000 | 11.8319598 | -2.5442751 | 0.0000000 |
| C | 12.6951827 | -3.5977976 | 0.0000000 | 12.6863594 | -3.5913418 | 0.0000000 |
| C | 12.0125923 | -4.7673226 | 0.0000000 | 12.0049287 | -4.7638358 | 0.0000000 |
| C | 10.6332663 | -4.4219533 | 0.0000000 | 10.6275970 | -4.4240663 | 0.0000000 |
| H | 9.7850017 | -5.0855254 | 0.0000000 | 9.7811439 | -5.0899543 | 0.0000000 |
| H | 12.4401107 | -5.7565046 | 0.0000000 | 12.4359403 | -5.7516374 | 0.0000000 |
| H | 13.7431278 | -3.3516447 | 0.0000000 | 13.7343198 | -3.3447085 | 0.0000000 |
|  |  |  |  |  |  |  |
| **9O/**  **PBE0** | **Ground state** | | | **Excited state** | | |
| C | -13.1291733 | 0.0000000 | -1.5237444 | -13.122630 | 0.0000000 | -1.5269235 |
| C | -12.7428928 | 0.0000000 | -0.2157564 | -12.731110 | 0.0000000 | -0.2162461 |
| O | -13.8321544 | 0.0000000 | 0.5907582 | -13.821229 | 0.0000000 | 0.5923546 |
| C | -14.9202976 | 0.0000000 | -0.2112673 | -14.909698 | 0.0000000 | -0.2086599 |
| C | -14.5510474 | 0.0000000 | -1.5140995 | -14.541951 | 0.0000000 | -1.5134874 |
| C | -11.4659972 | 0.0000000 | 0.4266312 | -11.457788 | 0.0000000 | 0.4180933 |
| O | -10.3742153 | 0.0000000 | -0.3770918 | -10.364731 | 0.0000000 | -0.3860067 |
| C | -9.2821949 | 0.0000000 | 0.4280045 | -9.2699050 | 0.0000000 | 0.4219714 |
| C | -9.6679106 | 0.0000000 | 1.7383080 | -9.6660698 | 0.0000000 | 1.7405585 |
| C | -11.0830027 | 0.0000000 | 1.7368787 | -11.071904 | 0.0000000 | 1.7344621 |
| C | -8.0082710 | 0.0000000 | -0.2131139 | -8.0039688 | 0.0000000 | -0.2000775 |
| O | -6.9160305 | 0.0000000 | 0.5910459 | -6.9092134 | 0.0000000 | 0.6075038 |
| C | -5.8238936 | 0.0000000 | -0.2137989 | -5.8120573 | 0.0000000 | -0.2008660 |
| C | -6.2094602 | 0.0000000 | -1.5247062 | -6.2120602 | 0.0000000 | -1.5263489 |
| C | -7.6235879 | 0.0000000 | -1.5242547 | -7.6095401 | 0.0000000 | -1.5223979 |
| C | -4.5502231 | 0.0000000 | 0.4266864 | -4.5508809 | 0.0000000 | 0.4111636 |
| O | -3.4580075 | 0.0000000 | -0.3777731 | -3.4544516 | 0.0000000 | -0.3990348 |
| C | -2.3658105 | 0.0000000 | 0.4268924 | -2.3562031 | 0.0000000 | 0.4105903 |
| C | -2.7511840 | 0.0000000 | 1.7380137 | -2.7588142 | 0.0000000 | 1.7405110 |
| C | -4.1650922 | 0.0000000 | 1.7379090 | -4.1504547 | 0.0000000 | 1.7385583 |
| C | -1.0922095 | 0.0000000 | -0.2135100 | -1.0978571 | 0.0000000 | -0.1959349 |
| O | 0.0000000 | 0.0000000 | 0.5910430 | 0.0000000 | 0.0000000 | 0.6147979 |
| C | 1.0922095 | 0.0000000 | -0.2135100 | 1.0978571 | 0.0000000 | -0.1959349 |
| C | 0.7069360 | 0.0000000 | -1.5247119 | 0.6947563 | 0.0000000 | -1.5263998 |
| C | -0.7069360 | 0.0000000 | -1.5247119 | -0.6947563 | 0.0000000 | -1.5263998 |
| C | 2.3658105 | 0.0000000 | 0.4268924 | 2.3562031 | 0.0000000 | 0.4105903 |
| O | 3.4580075 | 0.0000000 | -0.3777731 | 3.4544516 | 0.0000000 | -0.3990348 |
| C | 4.5502231 | 0.0000000 | 0.4266864 | 4.5508809 | 0.0000000 | 0.4111636 |
| C | 4.1650922 | 0.0000000 | 1.7379090 | 4.1504547 | 0.0000000 | 1.7385583 |
| C | 2.7511840 | 0.0000000 | 1.7380137 | 2.7588142 | 0.0000000 | 1.7405110 |
| C | 5.8238936 | 0.0000000 | -0.2137989 | 5.8120573 | 0.0000000 | -0.2008660 |
| C | 6.2094602 | 0.0000000 | -1.5247062 | 6.2120602 | 0.0000000 | -1.5263489 |
| C | 7.6235879 | 0.0000000 | -1.5242547 | 7.6095401 | 0.0000000 | -1.5223979 |
| C | 8.0082710 | 0.0000000 | -0.2131139 | 8.0039688 | 0.0000000 | -0.2000775 |
| O | 6.9160305 | 0.0000000 | 0.5910459 | 6.9092134 | 0.0000000 | 0.6075038 |
| C | 9.2821949 | 0.0000000 | 0.4280045 | 9.2699050 | 0.0000000 | 0.4219714 |
| O | 10.3742153 | 0.0000000 | -0.3770918 | 10.3647310 | 0.0000000 | -0.3860067 |
| C | 11.4659972 | 0.0000000 | 0.4266312 | 11.4577885 | 0.0000000 | 0.4180933 |
| C | 11.0830027 | 0.0000000 | 1.7368787 | 11.0719045 | 0.0000000 | 1.7344621 |
| C | 9.6679106 | 0.0000000 | 1.7383080 | 9.6660698 | 0.0000000 | 1.7405585 |
| H | -4.8249477 | 0.0000000 | 2.5891515 | -4.8123769 | 0.0000000 | 2.5885810 |
| H | -1.3666971 | 0.0000000 | -2.3760328 | -1.3561725 | 0.0000000 | -2.3767673 |
| H | 1.3666971 | 0.0000000 | -2.3760328 | 1.3561725 | 0.0000000 | -2.3767673 |
| H | -5.5499861 | 0.0000000 | -2.3762612 | -5.5529303 | 0.0000000 | -2.3783281 |
| H | -8.2837075 | 0.0000000 | -2.3752849 | -8.2721576 | 0.0000000 | -2.3718510 |
| H | 4.8249477 | 0.0000000 | 2.5891515 | 4.8123769 | 0.0000000 | 2.5885810 |
| H | 2.0915121 | 0.0000000 | 2.5894102 | 2.0982380 | 0.0000000 | 2.5914537 |
| H | -2.0915121 | 0.0000000 | 2.5894102 | -2.0982380 | 0.0000000 | 2.5914537 |
| H | 8.2837075 | 0.0000000 | -2.3752849 | 8.2721576 | 0.0000000 | -2.3718510 |
| H | 5.5499861 | 0.0000000 | -2.3762612 | 5.5529303 | 0.0000000 | -2.3783281 |
| H | 11.7442953 | 0.0000000 | 2.5870471 | 11.7361440 | 0.0000000 | 2.5825951 |
| C | 12.7428928 | 0.0000000 | -0.2157564 | 12.7311101 | 0.0000000 | -0.2162461 |
| H | 9.0089621 | 0.0000000 | 2.5902659 | 9.0088085 | 0.0000000 | 2.5938888 |
| H | -9.0089621 | 0.0000000 | 2.5902659 | -9.0088085 | 0.0000000 | 2.5938888 |
| H | -11.7442953 | 0.0000000 | 2.5870471 | -11.736144 | 0.0000000 | 2.5825951 |
| H | -12.4732790 | 0.0000000 | -2.3779592 | -12.468566 | 0.0000000 | -2.3825420 |
| H | -15.2117968 | 0.0000000 | -2.3653699 | -15.205055 | 0.0000000 | -2.3630418 |
| H | -15.8737127 | 0.0000000 | 0.2885114 | -15.863008 | 0.0000000 | 0.2915286 |
| O | 13.8321544 | 0.0000000 | 0.5907582 | 13.8212290 | 0.0000000 | 0.5923546 |
| C | 14.9202976 | 0.0000000 | -0.2112673 | 14.9096989 | 0.0000000 | -0.2086599 |
| C | 14.5510474 | 0.0000000 | -1.5140995 | 14.5419517 | 0.0000000 | -1.5134874 |
| C | 13.1291733 | 0.0000000 | -1.5237444 | 13.1226300 | 0.0000000 | -1.5269235 |
| H | 12.4732790 | 0.0000000 | -2.3779592 | 12.4685662 | 0.0000000 | -2.3825420 |
| H | 15.2117968 | 0.0000000 | -2.3653699 | 15.2050558 | 0.0000000 | -2.3630418 |
| H | 15.8737127 | 0.0000000 | 0.2885114 | 15.8630086 | 0.0000000 | 0.2915286 |

Part 5.

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| **2O/**  **MN15** | **Ground state** | | | **Excited state** | | |
| C | -0.675128 | 2.759693 | 0.0000000 | -0.688555 | 2.742964 | 0.000000 |
| C | 0.675128 | 2.861322 | 0.0000000 | 0.688555 | 2.840332 | 0.000000 |
| C | 1.175267 | 1.523793 | 0.0000000 | 1.199642 | 1.543930 | 0.000000 |
| C | 0.080960 | 0.714963 | 0.0000000 | 0.066450 | 0.685413 | 0.000000 |
| C | -0.080960 | -0.714963 | 0.0000000 | -0.066450 | -0.685413 | -0.000000 |
| C | -1.175267 | -1.523793 | 0.0000000 | -1.199642 | -1.543930 | -0.000000 |
| C | -0.675128 | -2.861322 | 0.0000000 | -0.688555 | -2.840332 | -0.000000 |
| C | 0.675128 | -2.759693 | 0.0000000 | 0.688555 | -2.742964 | -0.000000 |
| O | -1.050765 | 1.458875 | 0.0000000 | -1.089818 | 1.444383 | 0.000000 |
| O | 1.050765 | -1.458875 | 0.0000000 | 1.089818 | -1.444383 | -0.000000 |
| H | -1.470199 | 3.483640 | 0.0000000 | -1.469158 | 3.484068 | 0.000000 |
| H | 1.246152 | 3.773834 | 0.0000000 | 1.243871 | 3.763434 | 0.000000 |
| H | 2.200642 | 1.196954 | 0.0000000 | 2.224872 | 1.216497 | 0.000000 |
| H | -2.200642 | -1.196954 | 0.0000000 | -2.224872 | -1.216497 | -0.000000 |
| H | -1.246152 | -3.773834 | 0.0000000 | -1.243871 | -3.763434 | -0.000000 |
| H | 1.470199 | -3.483640 | 0.0000000 | 1.469158 | -3.484068 | -0.000000 |
|  |  |  |  |  |  |  |
| **3O/**  **MN15** | **Ground state** | | | **Excited state** | | |
| O | 0.000000 | 3.464974 | -0.713390 | -0.000000 | 3.463632 | -0.728483 |
| C | -0.000000 | 4.555854 | 0.088428 | -0.000000 | 4.538924 | 0.096144 |
| C | -0.000000 | 4.185007 | 1.390938 | -0.000000 | 4.146660 | 1.405127 |
| C | -0.000000 | 2.757546 | 1.398861 | -0.000000 | 2.737856 | 1.409939 |
| C | -0.000000 | 2.375683 | 0.091887 | -0.000000 | 2.351178 | 0.068551 |
| C | 0.000000 | 1.092100 | -0.553514 | -0.000000 | 1.100181 | -0.540676 |
| O | -0.000000 | 0.000000 | 0.250788 | 0.000000 | -0.000000 | 0.283644 |
| C | -0.000000 | -1.092100 | -0.553514 | -0.000000 | -1.100181 | -0.540676 |
| C | 0.000000 | -0.711449 | -1.861649 | 0.000000 | -0.689888 | -1.889845 |
| C | 0.000000 | 0.711449 | -1.861649 | 0.000000 | 0.689888 | -1.889845 |
| C | -0.000000 | -2.375683 | 0.091887 | -0.000000 | -2.351178 | 0.068551 |
| O | -0.000000 | -3.464974 | -0.713390 | -0.000000 | -3.463632 | -0.728483 |
| C | -0.000000 | -4.555854 | 0.088428 | -0.000000 | -4.538924 | 0.096144 |
| C | -0.000000 | -4.185007 | 1.390938 | -0.000000 | -4.146660 | 1.405127 |
| C | -0.000000 | -2.757546 | 1.398861 | -0.000000 | -2.737856 | 1.409939 |
| H | 0.000000 | 5.509876 | -0.407618 | -0.000000 | 5.504192 | -0.379141 |
| H | -0.000000 | 4.844355 | 2.241811 | -0.000000 | 4.804460 | 2.257951 |
| H | -0.000000 | 2.097488 | 2.248842 | -0.000000 | 2.067477 | 2.252281 |
| H | -0.000000 | -2.097488 | 2.248842 | -0.000000 | -2.067477 | 2.252281 |
| H | -0.000000 | -5.509876 | -0.407618 | -0.000000 | -5.504192 | -0.379141 |
| H | -0.000000 | -4.844355 | 2.241811 | -0.000000 | -4.804460 | 2.257951 |
| H | 0.000000 | 1.375323 | -2.708778 | -0.000000 | 1.359037 | -2.733244 |
| H | -0.000000 | -1.375323 | -2.708778 | -0.000000 | -1.359037 | -2.733244 |
|  |  |  |  |  |  |  |
| **4O/**  **MN15** | **Ground state** | | | **Excited state** | | |
| O | -0.307939 | 1.772253 | -0.000000 | -0.354471 | 1.769954 | -0.000000 |
| C | 0.600655 | 2.779161 | 0.000000 | 0.561627 | 2.784111 | -0.000000 |
| C | 1.864962 | 2.270620 | 0.000000 | 1.853469 | 2.259760 | -0.000000 |
| C | 1.724454 | 0.855376 | 0.000000 | 1.732139 | 0.877955 | -0.000000 |
| C | 0.384201 | 0.605386 | 0.000000 | 0.354471 | 0.595243 | -0.000000 |
| C | -0.384201 | -0.605386 | 0.000000 | -0.354471 | -0.595243 | -0.000000 |
| O | 0.307939 | -1.772253 | -0.000000 | 0.354471 | -1.769954 | -0.000000 |
| C | -0.600655 | -2.779161 | 0.000000 | -0.561627 | -2.784111 | -0.000000 |
| C | -1.864962 | -2.270620 | 0.000000 | -1.853469 | -2.259760 | -0.000000 |
| C | -1.724454 | -0.855376 | 0.000000 | -1.732139 | -0.877955 | -0.000000 |
| C | -0.086586 | -4.120444 | -0.000000 | -0.069359 | -4.100668 | 0.000000 |
| O | -0.996741 | -5.123848 | -0.000000 | -0.974717 | -5.119681 | 0.000000 |
| C | -0.307939 | -6.289287 | -0.000000 | -0.272255 | -6.276794 | 0.000000 |
| C | 1.025157 | -6.050521 | 0.000000 | 1.065835 | -6.025607 | 0.000000 |
| C | 1.175764 | -4.631090 | 0.000000 | 1.212844 | -4.617441 | 0.000000 |
| H | 2.773571 | 2.847466 | 0.000000 | 2.754948 | 2.848577 | -0.000000 |
| H | 2.502287 | 0.111583 | 0.000000 | 2.513262 | 0.137138 | -0.000000 |
| H | 2.087545 | -4.059443 | 0.000000 | 2.121109 | -4.039804 | 0.000000 |
| H | -0.896782 | -7.189000 | -0.000000 | -0.849502 | -7.184501 | 0.000000 |
| H | 1.805878 | -6.791566 | 0.000000 | 1.848147 | -6.765571 | 0.000000 |
| H | -2.502287 | -0.111583 | 0.000000 | -2.513262 | -0.137138 | -0.000000 |
| H | -2.773571 | -2.847466 | 0.000000 | -2.754948 | -2.848577 | -0.000000 |
| C | 0.086586 | 4.120444 | -0.000000 | 0.069359 | 4.100668 | 0.000000 |
| O | 0.996741 | 5.123848 | -0.000000 | 0.974717 | 5.119681 | 0.000000 |
| C | 0.307939 | 6.289287 | -0.000000 | 0.272255 | 6.276794 | 0.000000 |
| C | -1.025157 | 6.050521 | 0.000000 | -1.065835 | 6.025607 | 0.000000 |
| C | -1.175764 | 4.631090 | 0.000000 | -1.212844 | 4.617441 | 0.000000 |
| H | -2.087545 | 4.059443 | 0.000000 | -2.121109 | 4.039804 | 0.000000 |
| H | 0.896782 | 7.189000 | -0.000000 | 0.849502 | 7.184501 | 0.000000 |
| H | -1.805878 | 6.791566 | 0.000000 | -1.848147 | 6.765571 | 0.000000 |
|  |  |  |  |  |  |  |
| **5O/**  **MN15** | **Ground state** | | | **Excited state** | | |
| O | 3.4656174 | 0.0000000 | 0.2634834 | 0.000000 | 3.465535 | -0.342374 |
| C | 4.5579164 | 0.0000000 | -0.5403334 | 0.000000 | 4.557904 | 0.461324 |
| C | 4.1778183 | 0.0000000 | -1.8490906 | 0.000000 | 4.177932 | 1.770130 |
| C | 2.7557729 | 0.0000000 | -1.8503003 | 0.000000 | 2.755886 | 1.771469 |
| C | 2.3734238 | 0.0000000 | -0.5415039 | 0.000000 | 2.373424 | 0.462694 |
| C | 1.0924518 | 0.0000000 | 0.1023650 | 0.000000 | 1.092439 | -0.181143 |
| O | 0.0000000 | 0.0000000 | -0.7020291 | 0.000000 | -0.000000 | 0.623242 |
| C | -1.0924518 | 0.0000000 | 0.1023650 | -0.000000 | -1.092439 | -0.181143 |
| C | -0.7107322 | 0.0000000 | 1.4116147 | 0.000000 | -0.710728 | -1.490408 |
| C | 0.7107322 | 0.0000000 | 1.4116147 | 0.000000 | 0.710728 | -1.490408 |
| C | -2.3734238 | 0.0000000 | -0.5415039 | -0.000000 | -2.373424 | 0.462694 |
| O | -3.4656174 | 0.0000000 | 0.2634834 | -0.000000 | -3.465535 | -0.342374 |
| C | -4.5579164 | 0.0000000 | -0.5403334 | -0.000000 | -4.557904 | 0.461324 |
| C | -4.1778183 | 0.0000000 | -1.8490906 | -0.000000 | -4.177932 | 1.770130 |
| C | -2.7557729 | 0.0000000 | -1.8503003 | -0.000000 | -2.755886 | 1.771469 |
| C | 5.8413408 | 0.0000000 | 0.1046223 | 0.000000 | 5.841187 | -0.183904 |
| O | 6.9303757 | 0.0000000 | -0.7010950 | 0.000000 | 6.930464 | 0.621463 |
| C | 8.0213915 | 0.0000000 | 0.1003632 | 0.000000 | 8.021212 | -0.180356 |
| C | 7.6510317 | 0.0000000 | 1.4030803 | 0.000000 | 7.650424 | -1.482965 |
| C | 6.2237083 | 0.0000000 | 1.4115620 | 0.000000 | 6.223116 | -1.490980 |
| C | -5.8413408 | 0.0000000 | 0.1046223 | -0.000000 | -5.841187 | -0.183904 |
| O | -6.9303757 | 0.0000000 | -0.7010950 | -0.000000 | -6.930464 | 0.621463 |
| H | -4.8422747 | 0.0000000 | -2.6957347 | 0.000000 | -4.842507 | 2.616694 |
| H | -2.0932659 | 0.0000000 | -2.6984425 | 0.000000 | -2.093419 | 2.619656 |
| H | -1.3739771 | 0.0000000 | 2.2591697 | 0.000000 | -1.374017 | -2.337942 |
| H | 1.3739771 | 0.0000000 | 2.2591697 | 0.000000 | 1.374017 | -2.337942 |
| H | 2.0932659 | 0.0000000 | -2.6984425 | 0.000000 | 2.093419 | 2.619656 |
| H | 4.8422747 | 0.0000000 | -2.6957347 | 0.000000 | 4.842507 | 2.616694 |
| H | 5.5641254 | 0.0000000 | 2.2619012 | 0.000000 | 5.563209 | -2.341080 |
| H | 8.3106149 | 0.0000000 | 2.2537370 | 0.000000 | 8.309791 | -2.333803 |
| C | -8.0213915 | 0.0000000 | 0.1003632 | -0.000000 | -8.021212 | -0.180356 |
| C | -7.6510317 | 0.0000000 | 1.4030803 | -0.000000 | -7.650424 | -1.482965 |
| C | -6.2237083 | 0.0000000 | 1.4115620 | -0.000000 | -6.223116 | -1.490980 |
| H | -5.5641254 | 0.0000000 | 2.2619012 | -0.000000 | -5.563209 | -2.341080 |
| H | -8.9752988 | 0.0000000 | -0.3959153 | 0.000000 | -8.975263 | 0.315637 |
| H | -8.3106149 | 0.0000000 | 2.2537370 | -0.000000 | -8.309791 | -2.333803 |
| H | 8.9752988 | 0.0000000 | -0.3959153 | 0.000000 | 8.975263 | 0.315637 |
|  |  |  |  |  |  |  |
| **6O/**  **MN15** | **Ground state** | | | **Excited state** | | |
| O | -0.512586 | 1.724185 | 0.000000 | -0.549644 | 1.718290 | 0.000000 |
| C | 0.310692 | 0.645806 | 0.000000 | 0.285364 | 0.634380 | 0.000000 |
| C | 1.613237 | 1.050276 | 0.000000 | 1.615183 | 1.069399 | 0.000000 |
| C | 1.588535 | 2.471364 | 0.000000 | 1.582616 | 2.457632 | 0.000000 |
| C | 0.272740 | 2.830335 | 0.000000 | 0.240160 | 2.832758 | 0.000000 |
| C | -0.393063 | 4.099983 | 0.000000 | -0.392564 | 4.081703 | 0.000000 |
| O | 0.393063 | 5.205820 | 0.000000 | 0.392564 | 5.198363 | 0.000000 |
| C | -0.429338 | 6.284128 | 0.000000 | -0.438228 | 6.274345 | 0.000000 |
| C | -1.731432 | 5.881655 | 0.000000 | -1.751392 | 5.856627 | 0.000000 |
| C | -1.708256 | 4.459838 | 0.000000 | -1.729821 | 4.454928 | 0.000000 |
| H | -2.589345 | 6.531509 | 0.000000 | -2.609031 | 6.507481 | 0.000000 |
| H | 2.424408 | 3.149277 | 0.000000 | 2.413542 | 3.142225 | 0.000000 |
| H | 2.472259 | 0.401927 | 0.000000 | 2.475782 | 0.422626 | 0.000000 |
| C | 0.193591 | 7.578362 | 0.000000 | 0.160953 | 7.563111 | 0.000000 |
| O | -0.630496 | 8.653543 | 0.000000 | -0.671493 | 8.636668 | 0.000000 |
| C | 0.152353 | 9.757968 | 0.000000 | 0.104788 | 9.745086 | 0.000000 |
| C | 1.461191 | 9.409749 | 0.000000 | 1.419057 | 9.405302 | 0.000000 |
| C | 1.493868 | 7.982810 | 0.000000 | 1.465463 | 7.984026 | 0.000000 |
| H | 2.355288 | 7.337747 | 0.000000 | 2.332310 | 7.346165 | 0.000000 |
| H | -0.360046 | 10.703307 | 0.000000 | -0.412385 | 10.688058 | 0.000000 |
| H | 2.300503 | 10.083721 | 0.000000 | 2.251942 | 10.087509 | 0.000000 |
| C | -0.310692 | -0.645806 | 0.000000 | -0.285364 | -0.634380 | 0.000000 |
| O | 0.512586 | -1.724185 | 0.000000 | 0.549644 | -1.718290 | 0.000000 |
| C | -0.272740 | -2.830335 | 0.000000 | -0.240160 | -2.832758 | 0.000000 |
| C | -1.588535 | -2.471364 | 0.000000 | -1.582616 | -2.457632 | 0.000000 |
| C | -1.613237 | -1.050276 | 0.000000 | -1.615183 | -1.069399 | 0.000000 |
| H | -2.424408 | -3.149277 | 0.000000 | -2.413542 | -3.142225 | 0.000000 |
| H | -2.472259 | -0.401927 | 0.000000 | -2.475782 | -0.422626 | 0.000000 |
| H | -2.544898 | 3.782849 | 0.000000 | -2.564820 | 3.775589 | 0.000000 |
| C | 0.393063 | -4.099983 | 0.000000 | 0.392564 | -4.081703 | 0.000000 |
| C | 1.708256 | -4.459838 | 0.000000 | 1.729821 | -4.454928 | 0.000000 |
| C | 1.731432 | -5.881655 | 0.000000 | 1.751392 | -5.856627 | 0.000000 |
| C | 0.429338 | -6.284128 | 0.000000 | 0.438228 | -6.274345 | 0.000000 |
| O | -0.393063 | -5.205820 | 0.000000 | -0.392564 | -5.198363 | 0.000000 |
| H | 2.589345 | -6.531509 | 0.000000 | 2.609031 | -6.507481 | 0.000000 |
| H | 2.544898 | -3.782849 | 0.000000 | 2.564820 | -3.775589 | 0.000000 |
| C | -0.193591 | -7.578362 | 0.000000 | -0.160953 | -7.563111 | 0.000000 |
| C | -1.493868 | -7.982810 | 0.000000 | -1.465463 | -7.984026 | 0.000000 |
| C | -1.461191 | -9.409749 | 0.000000 | -1.419057 | -9.405302 | 0.000000 |
| C | -0.152353 | -9.757968 | 0.000000 | -0.104788 | -9.745086 | 0.000000 |
| O | 0.630496 | -8.653543 | 0.000000 | 0.671493 | -8.636668 | 0.000000 |
| H | -2.300503 | -10.083721 | 0.000000 | -2.251942 | -10.087509 | 0.000000 |
| H | 0.360046 | -10.703307 | 0.000000 | 0.412385 | -10.688058 | 0.000000 |
| H | -2.355288 | -7.337747 | 0.000000 | -2.332310 | -7.346165 | 0.000000 |
|  |  |  |  |  |  |  |
| **7O/**  **MN15** | **Ground state** | | | **Excited state** | | |
| C | 0.000000 | 9.688272 | 1.531453 | -0.000000 | 9.679534 | 1.536985 |
| C | 0.000000 | 9.306517 | 0.224320 | -0.000000 | 9.290517 | 0.225498 |
| O | 0.000000 | 10.395877 | -0.580921 | -0.000000 | 10.381538 | -0.582012 |
| C | 0.000000 | 11.486492 | 0.221020 | -0.000000 | 11.472377 | 0.218839 |
| C | 0.000000 | 11.115554 | 1.523608 | -0.000000 | 11.103059 | 1.524139 |
| C | 0.000000 | 8.023350 | -0.421113 | -0.000000 | 8.013266 | -0.407631 |
| O | 0.000000 | 6.930835 | 0.382295 | -0.000000 | 6.919027 | 0.396553 |
| C | 0.000000 | 5.838933 | -0.423085 | -0.000000 | 5.822294 | -0.412584 |
| C | 0.000000 | 6.221742 | -1.731773 | -0.000000 | 6.221773 | -1.735532 |
| C | 0.000000 | 7.643728 | -1.730069 | -0.000000 | 7.628629 | -1.726440 |
| C | 0.000000 | 4.557871 | 0.220441 | -0.000000 | 4.555243 | 0.199869 |
| O | 0.000000 | 3.465558 | -0.583957 | -0.000000 | 3.459554 | -0.611026 |
| C | 0.000000 | 2.373046 | 0.220502 | -0.000000 | 2.358537 | 0.198031 |
| C | 0.000000 | 2.754870 | 1.529882 | -0.000000 | 2.762227 | 1.532395 |
| C | 0.000000 | 4.176128 | 1.529845 | -0.000000 | 4.156011 | 1.528444 |
| C | 0.000000 | 1.092424 | -0.423113 | -0.000000 | 1.099578 | -0.402968 |
| O | -0.000000 | -0.000000 | 0.381349 | -0.000000 | 0.000000 | 0.408953 |
| C | -0.000000 | -1.092424 | -0.423113 | -0.000000 | -1.099578 | -0.402968 |
| C | -0.000000 | -0.710577 | -1.732582 | 0.000000 | -0.694108 | -1.739222 |
| C | 0.000000 | 0.710577 | -1.732582 | 0.000000 | 0.694108 | -1.739222 |
| C | -0.000000 | -2.373046 | 0.220502 | -0.000000 | -2.358537 | 0.198031 |
| O | -0.000000 | -3.465558 | -0.583957 | -0.000000 | -3.459554 | -0.611026 |
| C | -0.000000 | -4.557871 | 0.220441 | -0.000000 | -4.555243 | 0.199869 |
| C | -0.000000 | -4.176128 | 1.529845 | -0.000000 | -4.156011 | 1.528444 |
| C | -0.000000 | -2.754870 | 1.529882 | -0.000000 | -2.762227 | 1.532395 |
| C | -0.000000 | -5.838933 | -0.423085 | -0.000000 | -5.822294 | -0.412584 |
| O | -0.000000 | -6.930835 | 0.382295 | -0.000000 | -6.919027 | 0.396553 |
| C | -0.000000 | -8.023350 | -0.421113 | -0.000000 | -8.013266 | -0.407631 |
| C | -0.000000 | -7.643728 | -1.730069 | -0.000000 | -7.628629 | -1.726440 |
| C | -0.000000 | -6.221742 | -1.731773 | -0.000000 | -6.221773 | -1.735532 |
| C | -0.000000 | -9.306517 | 0.224320 | -0.000000 | -9.290517 | 0.225498 |
| C | -0.000000 | -9.688272 | 1.531453 | -0.000000 | -9.679534 | 1.536985 |
| C | -0.000000 | -11.115554 | 1.523608 | -0.000000 | -11.103059 | 1.524139 |
| C | -0.000000 | -11.486492 | 0.221020 | -0.000000 | -11.472377 | 0.218839 |
| O | -0.000000 | -10.395877 | -0.580921 | -0.000000 | -10.381538 | -0.582012 |
| H | 0.000000 | 1.373755 | -2.580198 | -0.000000 | 1.359622 | -2.585444 |
| H | -0.000000 | -2.091708 | 2.377517 | 0.000000 | -2.098367 | 2.379809 |
| H | -0.000000 | -4.839415 | 2.377365 | 0.000000 | -4.822463 | 2.373967 |
| H | 0.000000 | 2.091708 | 2.377517 | 0.000000 | 2.098367 | 2.379809 |
| H | 0.000000 | 4.839415 | 2.377365 | 0.000000 | 4.822463 | 2.373967 |
| H | -0.000000 | -8.308520 | -2.576451 | 0.000000 | -8.297982 | -2.569609 |
| H | -0.000000 | -5.559548 | -2.580172 | 0.000000 | -5.561987 | -2.585988 |
| H | -0.000000 | -1.373755 | -2.580198 | -0.000000 | -1.359622 | -2.585444 |
| H | -0.000000 | -11.774806 | 2.374526 | 0.000000 | -11.765375 | 2.372850 |
| H | -0.000000 | -9.028294 | 2.381497 | 0.000000 | -9.021846 | 2.388848 |
| H | 0.000000 | 5.559548 | -2.580172 | 0.000000 | 5.561987 | -2.585988 |
| H | 0.000000 | 8.308520 | -2.576451 | 0.000000 | 8.297982 | -2.569609 |
| H | 0.000000 | 9.028294 | 2.381497 | 0.000000 | 9.021846 | 2.388848 |
| H | 0.000000 | 11.774806 | 2.374526 | 0.000000 | 11.765375 | 2.372850 |
| H | 0.000000 | 12.440611 | -0.274840 | -0.000000 | 12.426514 | -0.277309 |
| H | -0.000000 | -12.440611 | -0.274840 | -0.000000 | -12.426514 | -0.277309 |
|  |  |  |  |  |  |  |
| **8O/**  **MN15** | **Ground state** | | | **Excited state** | | |
| O | 5.016504 | 11.052781 | 0.000000 | 4.879182 | 11.097890 | 0.000000 |
| C | 5.247311 | 9.717917 | 0.000000 | 5.126710 | 9.764085 | 0.000000 |
| C | 6.586758 | 9.472566 | 0.000000 | 6.474006 | 9.537970 | 0.000000 |
| C | 7.220191 | 10.751622 | 0.000000 | 7.087846 | 10.823586 | 0.000000 |
| C | 6.222543 | 11.667590 | 0.000000 | 6.077135 | 11.727443 | 0.000000 |
| C | 4.094666 | 8.860888 | 0.000000 | 3.993997 | 8.893588 | 0.000000 |
| C | 2.754570 | 9.109175 | 0.000000 | 2.643143 | 9.126555 | 0.000000 |
| C | 2.114805 | 7.839244 | 0.000000 | 2.017818 | 7.862057 | 0.000000 |
| C | 3.112434 | 6.909757 | 0.000000 | 3.029825 | 6.928003 | 0.000000 |
| O | 4.322219 | 7.524016 | 0.000000 | 4.236493 | 7.558272 | 0.000000 |
| C | 3.112434 | 5.476154 | 0.000000 | 3.029825 | 5.514686 | 0.000000 |
| O | 1.903286 | 4.861234 | 0.000000 | 1.823414 | 4.884636 | 0.000000 |
| C | 2.131622 | 3.523848 | 0.000000 | 2.067834 | 3.542253 | 0.000000 |
| C | 3.473050 | 3.277190 | 0.000000 | 3.438506 | 3.320121 | 0.000000 |
| C | 4.111086 | 4.547175 | 0.000000 | 4.047310 | 4.579595 | 0.000000 |
| C | 0.981496 | 2.668626 | 0.000000 | 0.969534 | 2.673292 | 0.000000 |
| O | 1.209555 | 1.331306 | 0.000000 | 1.216780 | 1.330960 | 0.000000 |
| C | 0.000123 | 0.716596 | 0.000000 | 0.006225 | 0.697522 | 0.000000 |
| C | -0.998306 | 1.645954 | 0.000000 | -1.016038 | 1.646742 | 0.000000 |
| C | -0.359995 | 2.915646 | 0.000000 | -0.404447 | 2.895786 | 0.000000 |
| C | -0.000123 | -0.716596 | 0.000000 | -0.006225 | -0.697522 | 0.000000 |
| O | -1.209555 | -1.331306 | 0.000000 | -1.216780 | -1.330960 | 0.000000 |
| C | -0.981496 | -2.668626 | 0.000000 | -0.969534 | -2.673292 | 0.000000 |
| C | 0.359995 | -2.915646 | 0.000000 | 0.404447 | -2.895786 | 0.000000 |
| C | 0.998306 | -1.645954 | 0.000000 | 1.016038 | -1.646742 | 0.000000 |
| C | -2.131622 | -3.523848 | 0.000000 | -2.067834 | -3.542253 | 0.000000 |
| O | -1.903286 | -4.861234 | 0.000000 | -1.823414 | -4.884636 | 0.000000 |
| C | -3.112434 | -5.476154 | 0.000000 | -3.029825 | -5.514686 | 0.000000 |
| C | -4.111086 | -4.547175 | 0.000000 | -4.047310 | -4.579595 | 0.000000 |
| C | -3.473050 | -3.277190 | 0.000000 | -3.438506 | -3.320121 | 0.000000 |
| H | 0.819479 | -3.888849 | 0.000000 | 0.872849 | -3.865121 | 0.000000 |
| H | -2.053495 | 1.434234 | 0.000000 | -2.068605 | 1.420965 | 0.000000 |
| H | -0.819479 | 3.888849 | 0.000000 | -0.872849 | 3.865121 | 0.000000 |
| H | -3.932841 | -2.304118 | 0.000000 | -3.910581 | -2.352733 | 0.000000 |
| C | -3.112434 | -6.909757 | 0.000000 | -3.029825 | -6.928003 | 0.000000 |
| H | -5.166181 | -4.759306 | 0.000000 | -5.099311 | -4.808169 | 0.000000 |
| H | 5.166181 | 4.759306 | 0.000000 | 5.099311 | 4.808169 | 0.000000 |
| H | 3.932841 | 2.304118 | 0.000000 | 3.910581 | 2.352733 | 0.000000 |
| H | 2.053495 | -1.434234 | 0.000000 | 2.068605 | -1.420965 | 0.000000 |
| H | 2.296553 | 10.083102 | 0.000000 | 2.177738 | 10.097228 | 0.000000 |
| H | 1.059439 | 7.628348 | 0.000000 | 0.964292 | 7.641684 | 0.000000 |
| H | 8.276448 | 10.958939 | 0.000000 | 8.141114 | 11.046055 | 0.000000 |
| H | 6.207529 | 12.742765 | 0.000000 | 6.049170 | 12.802466 | 0.000000 |
| H | 7.050366 | 8.501372 | 0.000000 | 6.951022 | 8.573270 | 0.000000 |
| O | -4.322219 | -7.524016 | 0.000000 | -4.236493 | -7.558272 | 0.000000 |
| C | -4.094666 | -8.860888 | 0.000000 | -3.993997 | -8.893588 | 0.000000 |
| C | -2.754570 | -9.109175 | 0.000000 | -2.643143 | -9.126555 | 0.000000 |
| C | -2.114805 | -7.839244 | 0.000000 | -2.017818 | -7.862057 | 0.000000 |
| H | -1.059439 | -7.628348 | 0.000000 | -0.964292 | -7.641684 | 0.000000 |
| H | -2.296553 | -10.083102 | 0.000000 | -2.177738 | -10.097228 | 0.000000 |
| C | -5.247311 | -9.717917 | 0.000000 | -5.126710 | -9.764085 | 0.000000 |
| O | -5.016504 | -11.052781 | 0.000000 | -4.879182 | -11.097890 | 0.000000 |
| C | -6.222543 | -11.667590 | 0.000000 | -6.077135 | -11.727443 | 0.000000 |
| C | -7.220191 | -10.751622 | 0.000000 | -7.087846 | -10.823586 | 0.000000 |
| C | -6.586758 | -9.472566 | 0.000000 | -6.474006 | -9.537970 | 0.000000 |
| H | -7.050366 | -8.501372 | 0.000000 | -6.951022 | -8.573270 | 0.000000 |
| H | -8.276448 | -10.958939 | 0.000000 | -8.141114 | -11.046055 | 0.000000 |
| H | -6.207529 | -12.742765 | 0.000000 | -6.049170 | -12.802466 | 0.000000 |
|  |  |  |  |  |  |  |
| **9O/**  **MN15** | **Ground state** | | | **Excited state** | | |
| C | -0.000000 | 13.153255 | -1.554934 | 0.000000 | 13.141273 | -1.557887 |
| C | -0.000000 | 12.771770 | -0.247733 | 0.000000 | 12.755707 | -0.248596 |
| O | -0.000000 | 13.861277 | 0.557302 | 0.000000 | 13.845895 | 0.557843 |
| C | -0.000000 | 14.951719 | -0.244864 | 0.000000 | 14.936595 | -0.243419 |
| C | -0.000000 | 14.580534 | -1.547378 | 0.000000 | 14.566589 | -1.547438 |
| C | -0.000000 | 11.488738 | 0.397970 | 0.000000 | 11.475800 | 0.390685 |
| O | -0.000000 | 10.396059 | -0.405180 | 0.000000 | 10.382010 | -0.411963 |
| C | -0.000000 | 9.304345 | 0.400450 | 0.000000 | 9.287756 | 0.395973 |
| C | -0.000000 | 9.687445 | 1.709048 | 0.000000 | 9.681063 | 1.712107 |
| C | -0.000000 | 11.109420 | 1.707029 | 0.000000 | 11.094551 | 1.705216 |
| C | -0.000000 | 8.023154 | -0.242813 | 0.000000 | 8.014793 | -0.228924 |
| O | -0.000000 | 6.931009 | 0.561760 | 0.000000 | 6.920321 | 0.577636 |
| C | -0.000000 | 5.838369 | -0.242532 | 0.000000 | 5.822281 | -0.229639 |
| C | -0.000000 | 6.219966 | -1.551975 | 0.000000 | 6.220329 | -1.554658 |
| C | -0.000000 | 7.641201 | -1.552180 | 0.000000 | 7.623745 | -1.549961 |
| C | -0.000000 | 4.557886 | 0.401330 | 0.000000 | 4.556587 | 0.382784 |
| O | -0.000000 | 3.465302 | -0.402813 | 0.000000 | 3.459518 | -0.426065 |
| C | -0.000000 | 2.373088 | 0.401962 | 0.000000 | 2.360150 | 0.383227 |
| C | -0.000000 | 2.755300 | 1.711337 | 0.000000 | 2.763650 | 1.715076 |
| C | -0.000000 | 4.176403 | 1.710959 | 0.000000 | 4.158155 | 1.711436 |
| C | -0.000000 | 1.092388 | -0.241343 | 0.000000 | 1.099025 | -0.219728 |
| O | -0.000000 | 0.000000 | 0.563125 | -0.000000 | -0.000000 | 0.590448 |
| C | -0.000000 | -1.092388 | -0.241343 | -0.000000 | -1.099025 | -0.219728 |
| C | 0.000000 | -0.710532 | -1.550864 | -0.000000 | -0.695401 | -1.553107 |
| C | 0.000000 | 0.710532 | -1.550864 | 0.000000 | 0.695401 | -1.553107 |
| C | -0.000000 | -2.373088 | 0.401962 | -0.000000 | -2.360150 | 0.383227 |
| O | -0.000000 | -3.465302 | -0.402813 | -0.000000 | -3.459518 | -0.426065 |
| C | -0.000000 | -4.557886 | 0.401330 | -0.000000 | -4.556587 | 0.382784 |
| C | -0.000000 | -4.176403 | 1.710959 | -0.000000 | -4.158155 | 1.711436 |
| C | -0.000000 | -2.755300 | 1.711337 | -0.000000 | -2.763650 | 1.715076 |
| C | -0.000000 | -5.838369 | -0.242532 | -0.000000 | -5.822281 | -0.229639 |
| C | -0.000000 | -6.219966 | -1.551975 | -0.000000 | -6.220329 | -1.554658 |
| C | -0.000000 | -7.641201 | -1.552180 | -0.000000 | -7.623745 | -1.549961 |
| C | -0.000000 | -8.023154 | -0.242813 | -0.000000 | -8.014793 | -0.228924 |
| O | -0.000000 | -6.931009 | 0.561760 | -0.000000 | -6.920321 | 0.577636 |
| C | -0.000000 | -9.304345 | 0.400450 | -0.000000 | -9.287756 | 0.395973 |
| O | -0.000000 | -10.396059 | -0.405180 | -0.000000 | -10.382010 | -0.411963 |
| C | -0.000000 | -11.488738 | 0.397970 | -0.000000 | -11.475800 | 0.390685 |
| C | -0.000000 | -11.109420 | 1.707029 | -0.000000 | -11.094551 | 1.705216 |
| C | -0.000000 | -9.687445 | 1.709048 | -0.000000 | -9.681063 | 1.712107 |
| H | -0.000000 | 4.839809 | 2.558389 | 0.000000 | 4.824384 | 2.557082 |
| H | -0.000000 | 1.373700 | -2.398485 | 0.000000 | 1.360408 | -2.399688 |
| H | -0.000000 | -1.373700 | -2.398485 | -0.000000 | -1.360408 | -2.399688 |
| H | -0.000000 | 5.556685 | -2.399523 | 0.000000 | 5.558245 | -2.403330 |
| H | -0.000000 | 8.304342 | -2.399811 | 0.000000 | 8.290036 | -2.395477 |
| H | -0.000000 | -4.839809 | 2.558389 | -0.000000 | -4.824384 | 2.557082 |
| H | 0.000000 | -2.092400 | 2.559175 | -0.000000 | -2.100456 | 2.562990 |
| H | 0.000000 | 2.092400 | 2.559175 | 0.000000 | 2.100456 | 2.562990 |
| H | -0.000000 | -8.304342 | -2.399811 | -0.000000 | -8.290036 | -2.395477 |
| H | -0.000000 | -5.556685 | -2.399523 | -0.000000 | -5.558245 | -2.403330 |
| H | 0.000000 | -11.774403 | 2.553261 | -0.000000 | -11.762496 | 2.549333 |
| C | -0.000000 | -12.771770 | -0.247733 | -0.000000 | -12.755707 | -0.248596 |
| H | 0.000000 | -9.025455 | 2.557611 | -0.000000 | -9.021101 | 2.562331 |
| H | 0.000000 | 9.025455 | 2.557611 | 0.000000 | 9.021101 | 2.562331 |
| H | 0.000000 | 11.774403 | 2.553261 | 0.000000 | 11.762496 | 2.549333 |
| H | -0.000000 | 12.493112 | -2.404854 | 0.000000 | 12.482594 | -2.408956 |
| H | -0.000000 | 15.239620 | -2.398426 | 0.000000 | 15.227436 | -2.397204 |
| H | -0.000000 | 15.905939 | 0.250805 | 0.000000 | 15.890705 | 0.252635 |
| O | -0.000000 | -13.861277 | 0.557302 | -0.000000 | -13.845895 | 0.557843 |
| C | -0.000000 | -14.951719 | -0.244864 | -0.000000 | -14.936595 | -0.243419 |
| C | -0.000000 | -14.580534 | -1.547378 | -0.000000 | -14.566589 | -1.547438 |
| C | -0.000000 | -13.153255 | -1.554934 | -0.000000 | -13.141273 | -1.557887 |
| H | -0.000000 | -12.493112 | -2.404854 | -0.000000 | -12.482594 | -2.408956 |
| H | -0.000000 | -15.239620 | -2.398426 | -0.000000 | -15.227436 | -2.397204 |
| H | -0.000000 | -15.905939 | 0.250805 | -0.000000 | -15.890705 | 0.252635 |

Part 6.

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| **2O/**  **BHLYP** | **Ground state** | | | **Excited state** | | |
| C | -2.7942947 | 0.4306224 | 0.0000000 | -2.7798253 | 0.4424734 | 0.0000000 |
| C | -2.7795830 | -0.9121528 | 0.0000000 | -2.7559747 | -0.9274615 | 0.0000000 |
| C | -1.4078103 | -1.2929655 | 0.0000000 | -1.4268481 | -1.3206805 | 0.0000000 |
| C | -0.7020587 | -0.1414932 | 0.0000000 | -0.6719927 | -0.1245134 | 0.0000000 |
| C | 0.7020587 | 0.1414932 | 0.0000000 | 0.6719927 | 0.1245134 | 0.0000000 |
| C | 1.4078103 | 1.2929655 | 0.0000000 | 1.4268481 | 1.3206805 | 0.0000000 |
| C | 2.7795830 | 0.9121528 | 0.0000000 | 2.7559747 | 0.9274615 | 0.0000000 |
| C | 2.7942947 | -0.4306224 | 0.0000000 | 2.7798253 | -0.4424734 | 0.0000000 |
| O | -1.5380239 | 0.9152181 | 0.0000000 | -1.5290121 | 0.9530923 | 0.0000000 |
| O | 1.5380239 | -0.9152181 | 0.0000000 | 1.5290121 | -0.9530923 | 0.0000000 |
| H | -3.5788801 | 1.1541557 | 0.0000000 | -3.5811571 | 1.1487363 | 0.0000000 |
| H | -3.6326128 | -1.5559461 | 0.0000000 | -3.6197818 | -1.5579935 | 0.0000000 |
| H | -1.0003897 | -2.2802706 | 0.0000000 | -1.0187783 | -2.3075548 | 0.0000000 |
| H | 1.0003897 | 2.2802706 | 0.0000000 | 1.0187783 | 2.3075548 | 0.0000000 |
| H | 3.6326128 | 1.5559461 | 0.0000000 | 3.6197818 | 1.5579935 | 0.0000000 |
| H | 3.5788801 | -1.1541557 | 0.0000000 | 3.5811571 | -1.1487363 | 0.0000000 |
|  |  |  |  |  |  |  |
| **3O/**  **BHLYP** | **Ground state** | | | **Excited state** | | |
| O | 3.4496439 | 0.0000000 | 0.8248372 | 3.4466952 | 0.0000000 | 0.8428822 |
| C | 4.5343170 | 0.0000000 | 0.0271949 | 4.5182538 | 0.0000000 | 0.0266231 |
| C | 4.1674217 | 0.0000000 | -1.2647366 | 4.1343364 | 0.0000000 | -1.2733929 |
| C | 2.7442493 | 0.0000000 | -1.2722085 | 2.7314694 | 0.0000000 | -1.2833439 |
| C | 2.3650614 | 0.0000000 | 0.0248654 | 2.3405394 | 0.0000000 | 0.0477173 |
| C | 1.0872544 | 0.0000000 | 0.6669273 | 1.0964573 | 0.0000000 | 0.6493462 |
| O | 0.0000000 | 0.0000000 | -0.1318675 | 0.0000000 | 0.0000000 | -0.1684272 |
| C | -1.0872544 | 0.0000000 | 0.6669273 | -1.0964573 | 0.0000000 | 0.6493462 |
| C | -0.7091209 | 0.0000000 | 1.9646642 | -0.6852127 | 0.0000000 | 1.9906614 |
| C | 0.7091209 | 0.0000000 | 1.9646642 | 0.6852127 | 0.0000000 | 1.9906614 |
| C | -2.3650614 | 0.0000000 | 0.0248654 | -2.3405394 | 0.0000000 | 0.0477173 |
| O | -3.4496439 | 0.0000000 | 0.8248372 | -3.4466952 | 0.0000000 | 0.8428822 |
| C | -4.5343170 | 0.0000000 | 0.0271949 | -4.5182538 | 0.0000000 | 0.0266231 |
| C | -4.1674217 | 0.0000000 | -1.2647366 | -4.1343364 | 0.0000000 | -1.2733929 |
| C | -2.7442493 | 0.0000000 | -1.2722085 | -2.7314694 | 0.0000000 | -1.2833439 |
| H | 5.4814566 | 0.0000000 | 0.5191168 | 5.4750057 | 0.0000000 | 0.5008627 |
| H | 4.8214939 | 0.0000000 | -2.1098931 | 4.7898656 | 0.0000000 | -2.1181448 |
| H | 2.0926407 | 0.0000000 | -2.1184091 | 2.0735142 | 0.0000000 | -2.1248925 |
| H | -2.0926407 | 0.0000000 | -2.1184091 | -2.0735142 | 0.0000000 | -2.1248925 |
| H | -5.4814566 | 0.0000000 | 0.5191168 | -5.4750057 | 0.0000000 | 0.5008627 |
| H | -4.8214939 | 0.0000000 | -2.1098931 | -4.7898656 | 0.0000000 | -2.1181448 |
| H | 1.3638375 | 0.0000000 | 2.8085774 | 1.3451022 | 0.0000000 | 2.8308972 |
| H | -1.3638375 | 0.0000000 | 2.8085774 | -1.3451022 | 0.0000000 | 2.8308972 |
|  |  |  |  |  |  |  |
| **4O/**  **BHLYP** | **Ground state** | | | **Excited state** | | |
| O | -1.7576760 | 0.3395703 | 0.0000000 | -1.7566989 | 0.3764238 | 0.0000000 |
| C | -2.7780834 | -0.5429051 | 0.0000000 | -2.7793659 | -0.5191027 | 0.0000000 |
| C | -2.2981301 | -1.8068782 | 0.0000000 | -2.2742783 | -1.8094487 | 0.0000000 |
| C | -0.8849960 | -1.6949061 | 0.0000000 | -0.8993276 | -1.7087752 | 0.0000000 |
| C | -0.6100551 | -0.3704653 | 0.0000000 | -0.5958818 | -0.3429749 | 0.0000000 |
| C | 0.6100551 | 0.3704653 | 0.0000000 | 0.5958818 | 0.3429749 | 0.0000000 |
| O | 1.7576760 | -0.3395703 | 0.0000000 | 1.7566989 | -0.3764238 | 0.0000000 |
| C | 2.7780834 | 0.5429051 | 0.0000000 | 2.7793659 | 0.5191027 | 0.0000000 |
| C | 2.2981301 | 1.8068782 | 0.0000000 | 2.2742783 | 1.8094487 | 0.0000000 |
| C | 0.8849960 | 1.6949061 | 0.0000000 | 0.8993276 | 1.7087752 | 0.0000000 |
| C | 4.1026874 | 0.0047273 | 0.0000000 | 4.0819560 | 0.0133846 | 0.0000000 |
| O | 5.1201657 | 0.8885591 | 0.0000000 | 5.1085106 | 0.9001436 | 0.0000000 |
| C | 6.2647911 | 0.1797559 | 0.0000000 | 6.2499347 | 0.1871450 | 0.0000000 |
| C | 6.0019251 | -1.1373411 | 0.0000000 | 5.9850849 | -1.1369034 | 0.0000000 |
| C | 4.5839790 | -1.2581222 | 0.0000000 | 4.5802993 | -1.2657862 | 0.0000000 |
| H | -2.8840511 | -2.6999234 | 0.0000000 | -2.8669619 | -2.6985877 | 0.0000000 |
| H | -0.1662712 | -2.4849512 | 0.0000000 | -0.1795157 | -2.4981548 | 0.0000000 |
| H | 4.0018980 | -2.1535753 | 0.0000000 | 4.0000067 | -2.1625682 | 0.0000000 |
| H | 7.1698065 | 0.7454536 | 0.0000000 | 7.1582973 | 0.7481844 | 0.0000000 |
| H | 6.7211945 | -1.9277422 | 0.0000000 | 6.7095328 | -1.9230991 | 0.0000000 |
| H | 0.1662712 | 2.4849512 | 0.0000000 | 0.1795157 | 2.4981548 | 0.0000000 |
| H | 2.8840511 | 2.6999234 | 0.0000000 | 2.8669619 | 2.6985877 | 0.0000000 |
| C | -4.1026874 | -0.0047273 | 0.0000000 | -4.0819560 | -0.0133846 | 0.0000000 |
| O | -5.1201657 | -0.8885591 | 0.0000000 | -5.1085106 | -0.9001436 | 0.0000000 |
| C | -6.2647911 | -0.1797559 | 0.0000000 | -6.2499347 | -0.1871450 | 0.0000000 |
| C | -6.0019251 | 1.1373411 | 0.0000000 | -5.9850849 | 1.1369034 | 0.0000000 |
| C | -4.5839790 | 1.2581222 | 0.0000000 | -4.5802993 | 1.2657862 | 0.0000000 |
| H | -4.0018980 | 2.1535753 | 0.0000000 | -4.0000067 | 2.1625682 | 0.0000000 |
| H | -7.1698065 | -0.7454536 | 0.0000000 | -7.1582973 | -0.7481844 | 0.0000000 |
| H | -6.7211945 | 1.9277422 | 0.0000000 | -6.7095328 | 1.9230991 | 0.0000000 |
|  |  |  |  |  |  |  |
| **5O/**  **BHLYP** | **Ground state** | | | **Excited state** | | |
| O | 3.4501103 | 0.0000000 | 0.2606311 | 3.4427058 | 0.0000000 | 0.2893216 |
| C | 4.5374179 | 0.0000000 | -0.5378611 | 4.5311625 | 0.0000000 | -0.5168685 |
| C | 4.1595622 | 0.0000000 | -1.8361109 | 4.1372962 | 0.0000000 | -1.8340483 |
| C | 2.7421496 | 0.0000000 | -1.8370042 | 2.7493163 | 0.0000000 | -1.8429180 |
| C | 2.3625819 | 0.0000000 | -0.5385522 | 2.3441799 | 0.0000000 | -0.5149889 |
| C | 1.0876422 | 0.0000000 | 0.1027018 | 1.0961136 | 0.0000000 | 0.0790337 |
| O | 0.0000000 | 0.0000000 | -0.6960879 | 0.0000000 | 0.0000000 | -0.7306215 |
| C | -1.0876422 | 0.0000000 | 0.1027018 | -1.0961136 | 0.0000000 | 0.0790337 |
| C | -0.7084249 | 0.0000000 | 1.4015022 | -0.6879354 | 0.0000000 | 1.4118006 |
| C | 0.7084249 | 0.0000000 | 1.4015022 | 0.6879354 | 0.0000000 | 1.4118006 |
| C | -2.3625819 | 0.0000000 | -0.5385522 | -2.3441799 | 0.0000000 | -0.5149889 |
| O | -3.4501103 | 0.0000000 | 0.2606311 | -3.4427058 | 0.0000000 | 0.2893216 |
| C | -4.5374179 | 0.0000000 | -0.5378611 | -4.5311625 | 0.0000000 | -0.5168685 |
| C | -4.1595622 | 0.0000000 | -1.8361109 | -4.1372962 | 0.0000000 | -1.8340483 |
| C | -2.7421496 | 0.0000000 | -1.8370042 | -2.7493163 | 0.0000000 | -1.8429180 |
| C | 5.8150457 | 0.0000000 | 0.1038158 | 5.7971648 | 0.0000000 | 0.0983190 |
| O | 6.8994832 | 0.0000000 | -0.6964355 | 6.8851250 | 0.0000000 | -0.7067923 |
| C | 7.9841694 | 0.0000000 | 0.1010046 | 7.9702093 | 0.0000000 | 0.0888980 |
| C | 7.6175708 | 0.0000000 | 1.3930971 | 7.6066599 | 0.0000000 | 1.3865960 |
| C | 6.1945447 | 0.0000000 | 1.4009087 | 6.1918263 | 0.0000000 | 1.4051020 |
| C | -5.8150457 | 0.0000000 | 0.1038158 | -5.7971648 | 0.0000000 | 0.0983190 |
| O | -6.8994832 | 0.0000000 | -0.6964355 | -6.8851250 | 0.0000000 | -0.7067923 |
| H | -4.8146938 | 0.0000000 | -2.6796890 | -4.7976454 | 0.0000000 | -2.6741242 |
| H | -2.0886708 | 0.0000000 | -2.6818186 | -2.0961302 | 0.0000000 | -2.6882155 |
| H | -1.3624154 | 0.0000000 | 2.2459096 | -1.3451916 | 0.0000000 | 2.2540954 |
| H | 1.3624154 | 0.0000000 | 2.2459096 | 1.3451916 | 0.0000000 | 2.2540954 |
| H | 2.0886708 | 0.0000000 | -2.6818186 | 2.0961302 | 0.0000000 | -2.6882155 |
| H | 4.8146938 | 0.0000000 | -2.6796890 | 4.7976454 | 0.0000000 | -2.6741242 |
| H | 5.5432289 | 0.0000000 | 2.2473390 | 5.5449689 | 0.0000000 | 2.2550366 |
| H | 8.2718142 | 0.0000000 | 2.2381058 | 8.2673139 | 0.0000000 | 2.2269494 |
| C | -7.9841694 | 0.0000000 | 0.1010046 | -7.9702093 | 0.0000000 | 0.0888980 |
| C | -7.6175708 | 0.0000000 | 1.3930971 | -7.6066599 | 0.0000000 | 1.3865960 |
| C | -6.1945447 | 0.0000000 | 1.4009087 | -6.1918263 | 0.0000000 | 1.4051020 |
| H | -5.5432289 | 0.0000000 | 2.2473390 | -5.5449689 | 0.0000000 | 2.2550366 |
| H | -8.9312543 | 0.0000000 | -0.3910318 | -8.9174474 | 0.0000000 | -0.4034177 |
| H | -8.2718142 | 0.0000000 | 2.2381058 | -8.2673139 | 0.0000000 | 2.2269494 |
| H | 8.9312543 | 0.0000000 | -0.3910318 | 8.9174474 | 0.0000000 | -0.4034177 |
|  |  |  |  |  |  |  |
| **6O/**  **BHLYP** | **Ground state** | | | **Excited state** | | |
| O | 1.7900256 | -0.0195119 | 0.0000000 | 1.7953315 | 0.0123704 | 0.0000000 |
| C | 0.5232597 | -0.4848937 | 0.0000000 | 0.5172030 | -0.4575373 | 0.0000000 |
| C | 0.5269619 | -1.8380375 | 0.0000000 | 0.5391745 | -1.8489687 | 0.0000000 |
| C | 1.8879507 | -2.2314050 | 0.0000000 | 1.8661582 | -2.2284688 | 0.0000000 |
| C | 2.6129772 | -1.0889134 | 0.0000000 | 2.6213318 | -1.0667356 | 0.0000000 |
| C | 4.0158311 | -0.8271436 | 0.0000000 | 3.9935453 | -0.8372754 | 0.0000000 |
| O | 4.8384693 | -1.8970513 | 0.0000000 | 4.8224826 | -1.9132897 | 0.0000000 |
| C | 6.1047921 | -1.4321414 | 0.0000000 | 6.0909795 | -1.4457572 | 0.0000000 |
| C | 6.1025813 | -0.0799912 | 0.0000000 | 6.0835008 | -0.0779093 | 0.0000000 |
| C | 4.7412710 | 0.3147094 | 0.0000000 | 4.7455141 | 0.3187181 | 0.0000000 |
| H | 6.9663192 | 0.5483171 | 0.0000000 | 6.9511728 | 0.5455991 | 0.0000000 |
| H | 2.2817270 | -3.2242070 | 0.0000000 | 2.2643764 | -3.2199133 | 0.0000000 |
| H | -0.3357291 | -2.4677211 | 0.0000000 | -0.3245087 | -2.4777359 | 0.0000000 |
| C | 7.1538291 | -2.4035233 | 0.0000000 | 7.1372938 | -2.3973830 | 0.0000000 |
| O | 8.4178989 | -1.9360515 | 0.0000000 | 8.4043970 | -1.9269428 | 0.0000000 |
| C | 9.2383077 | -3.0034483 | 0.0000000 | 9.2259340 | -2.9926254 | 0.0000000 |
| C | 8.5271670 | -4.1428336 | 0.0000000 | 8.5163718 | -4.1365799 | 0.0000000 |
| C | 7.1580095 | -3.7549836 | 0.0000000 | 7.1503631 | -3.7578159 | 0.0000000 |
| H | 6.2971866 | -4.3871569 | 0.0000000 | 6.2922375 | -4.3937046 | 0.0000000 |
| H | 10.2848117 | -2.7939229 | 0.0000000 | 10.2724763 | -2.7823445 | 0.0000000 |
| H | 8.9208791 | -5.1363423 | 0.0000000 | 8.9155528 | -5.1281066 | 0.0000000 |
| C | -0.5232597 | 0.4848937 | 0.0000000 | -0.5172030 | 0.4575373 | 0.0000000 |
| O | -1.7900256 | 0.0195119 | 0.0000000 | -1.7953315 | -0.0123704 | 0.0000000 |
| C | -2.6129772 | 1.0889134 | 0.0000000 | -2.6213318 | 1.0667356 | 0.0000000 |
| C | -1.8879507 | 2.2314050 | 0.0000000 | -1.8661582 | 2.2284688 | 0.0000000 |
| C | -0.5269619 | 1.8380375 | 0.0000000 | -0.5391745 | 1.8489687 | 0.0000000 |
| H | -2.2817270 | 3.2242070 | 0.0000000 | -2.2643764 | 3.2199133 | 0.0000000 |
| H | 0.3357291 | 2.4677211 | 0.0000000 | 0.3245087 | 2.4777359 | 0.0000000 |
| H | 4.3483104 | 1.3078518 | 0.0000000 | 4.3549890 | 1.3129801 | 0.0000000 |
| C | -4.0158311 | 0.8271436 | 0.0000000 | -3.9935453 | 0.8372754 | 0.0000000 |
| C | -4.7412710 | -0.3147094 | 0.0000000 | -4.7455141 | -0.3187181 | 0.0000000 |
| C | -6.1025813 | 0.0799912 | 0.0000000 | -6.0835008 | 0.0779093 | 0.0000000 |
| C | -6.1047921 | 1.4321414 | 0.0000000 | -6.0909795 | 1.4457572 | 0.0000000 |
| O | -4.8384693 | 1.8970513 | 0.0000000 | -4.8224826 | 1.9132897 | 0.0000000 |
| H | -6.9663192 | -0.5483171 | 0.0000000 | -6.9511728 | -0.5455991 | 0.0000000 |
| H | -4.3483104 | -1.3078518 | 0.0000000 | -4.3549890 | -1.3129801 | 0.0000000 |
| C | -7.1538291 | 2.4035233 | 0.0000000 | -7.1372938 | 2.3973830 | 0.0000000 |
| C | -7.1580095 | 3.7549836 | 0.0000000 | -7.1503631 | 3.7578159 | 0.0000000 |
| C | -8.5271670 | 4.1428336 | 0.0000000 | -8.5163718 | 4.1365799 | 0.0000000 |
| C | -9.2383077 | 3.0034483 | 0.0000000 | -9.2259340 | 2.9926254 | 0.0000000 |
| O | -8.4178989 | 1.9360515 | 0.0000000 | -8.4043970 | 1.9269428 | 0.0000000 |
| H | -8.9208791 | 5.1363423 | 0.0000000 | -8.9155528 | 5.1281066 | 0.0000000 |
| H | -10.2848117 | 2.7939229 | 0.0000000 | -10.272476 | 2.7823445 | 0.0000000 |
| H | -6.2971866 | 4.3871569 | 0.0000000 | -6.2922375 | 4.3937046 | 0.0000000 |
|  |  |  |  |  |  |  |
| **7O/**  **BHLYP** | **Ground state** | | | **Excited state** | | |
| C | -9.6444763 | 0.0000000 | -1.4758579 | -9.6337910 | 0.0000000 | -1.4815556 |
| C | -9.2648830 | 0.0000000 | -0.1787996 | -9.2470235 | 0.0000000 | -0.1801939 |
| O | -10.3492333 | 0.0000000 | 0.6215585 | -10.333173 | 0.0000000 | 0.6222448 |
| C | -11.4339593 | 0.0000000 | -0.1757913 | -11.417961 | 0.0000000 | -0.1740543 |
| C | -11.0674825 | 0.0000000 | -1.4679284 | -11.052955 | 0.0000000 | -1.4687856 |
| C | -7.9872270 | 0.0000000 | 0.4628095 | -7.9754897 | 0.0000000 | 0.4495124 |
| O | -6.8999633 | 0.0000000 | -0.3356419 | -6.8865123 | 0.0000000 | -0.3492650 |
| C | -5.8124521 | 0.0000000 | 0.4635903 | -5.7939833 | 0.0000000 | 0.4538717 |
| C | -6.1920607 | 0.0000000 | 1.7620398 | -6.1915445 | 0.0000000 | 1.7669557 |
| C | -7.6094233 | 0.0000000 | 1.7611187 | -7.5927634 | 0.0000000 | 1.7579341 |
| C | -4.5375689 | 0.0000000 | -0.1776396 | -4.5342606 | 0.0000000 | -0.1556193 |
| O | -3.4499053 | 0.0000000 | 0.6209486 | -3.4427714 | 0.0000000 | 0.6487566 |
| C | -2.3623387 | 0.0000000 | -0.1781162 | -2.3462835 | 0.0000000 | -0.1553741 |
| C | -2.7419178 | 0.0000000 | -1.4769488 | -2.7508570 | 0.0000000 | -1.4808126 |
| C | -4.1585815 | 0.0000000 | -1.4766409 | -4.1371033 | 0.0000000 | -1.4752708 |
| C | -1.0876171 | 0.0000000 | 0.4626838 | -1.0954260 | 0.0000000 | 0.4401645 |
| O | 0.0000000 | 0.0000000 | -0.3361932 | 0.0000000 | 0.0000000 | -0.3661628 |
| C | 1.0876171 | 0.0000000 | 0.4626838 | 1.0954260 | 0.0000000 | 0.4401645 |
| C | 0.7082730 | 0.0000000 | 1.7616710 | 0.6897897 | 0.0000000 | 1.7682997 |
| C | -0.7082730 | 0.0000000 | 1.7616710 | -0.6897897 | 0.0000000 | 1.7682997 |
| C | 2.3623387 | 0.0000000 | -0.1781162 | 2.3462835 | 0.0000000 | -0.1553741 |
| O | 3.4499053 | 0.0000000 | 0.6209486 | 3.4427714 | 0.0000000 | 0.6487566 |
| C | 4.5375689 | 0.0000000 | -0.1776396 | 4.5342606 | 0.0000000 | -0.1556193 |
| C | 4.1585815 | 0.0000000 | -1.4766409 | 4.1371033 | 0.0000000 | -1.4752708 |
| C | 2.7419178 | 0.0000000 | -1.4769488 | 2.7508570 | 0.0000000 | -1.4808126 |
| C | 5.8124521 | 0.0000000 | 0.4635903 | 5.7939833 | 0.0000000 | 0.4538717 |
| O | 6.8999633 | 0.0000000 | -0.3356419 | 6.8865123 | 0.0000000 | -0.3492650 |
| C | 7.9872270 | 0.0000000 | 0.4628095 | 7.9754897 | 0.0000000 | 0.4495124 |
| C | 7.6094233 | 0.0000000 | 1.7611187 | 7.5927634 | 0.0000000 | 1.7579341 |
| C | 6.1920607 | 0.0000000 | 1.7620398 | 6.1915445 | 0.0000000 | 1.7669557 |
| C | 9.2648830 | 0.0000000 | -0.1787996 | 9.2470235 | 0.0000000 | -0.1801939 |
| C | 9.6444763 | 0.0000000 | -1.4758579 | 9.6337910 | 0.0000000 | -1.4815556 |
| C | 11.0674825 | 0.0000000 | -1.4679284 | 11.0529558 | 0.0000000 | -1.4687856 |
| C | 11.4339593 | 0.0000000 | -0.1757913 | 11.4179613 | 0.0000000 | -0.1740543 |
| O | 10.3492333 | 0.0000000 | 0.6215585 | 10.3331737 | 0.0000000 | 0.6222448 |
| H | -1.3621725 | 0.0000000 | 2.6061479 | -1.3460228 | 0.0000000 | 2.6113664 |
| H | 2.0882071 | 0.0000000 | -2.3215811 | 2.0972763 | 0.0000000 | -2.3258038 |
| H | 4.8127278 | 0.0000000 | -2.3209162 | 4.7951075 | 0.0000000 | -2.3170190 |
| H | -2.0882071 | 0.0000000 | -2.3215811 | -2.0972763 | 0.0000000 | -2.3258038 |
| H | -4.8127278 | 0.0000000 | -2.3209162 | -4.7951075 | 0.0000000 | -2.3170190 |
| H | 8.2645781 | 0.0000000 | 2.6046722 | 8.2527830 | 0.0000000 | 2.5980583 |
| H | 5.5386438 | 0.0000000 | 2.6069065 | 5.5410794 | 0.0000000 | 2.6142222 |
| H | 1.3621725 | 0.0000000 | 2.6061479 | 1.3460228 | 0.0000000 | 2.6113664 |
| H | 11.7217900 | 0.0000000 | -2.3128831 | 11.7101642 | 0.0000000 | -2.3116507 |
| H | 8.9932499 | 0.0000000 | -2.3223595 | 8.9848444 | 0.0000000 | -2.3298268 |
| H | -5.5386438 | 0.0000000 | 2.6069065 | -5.5410794 | 0.0000000 | 2.6142222 |
| H | -8.2645781 | 0.0000000 | 2.6046722 | -8.2527830 | 0.0000000 | 2.5980583 |
| H | -8.9932499 | 0.0000000 | -2.3223595 | -8.9848444 | 0.0000000 | -2.3298268 |
| H | -11.7217900 | 0.0000000 | -2.3128831 | -11.710164 | 0.0000000 | -2.3116507 |
| H | -12.3809925 | 0.0000000 | 0.3163476 | -12.365074 | 0.0000000 | 0.3182195 |
| H | 12.3809925 | 0.0000000 | 0.3163476 | 12.3650747 | 0.0000000 | 0.3182195 |
|  |  |  |  |  |  |  |
| **8O/**  **BHLYP** | **Ground state** | | | **Excited state** | | |
| O | -11.8119587 | 2.5478886 | 0.0000000 | -11.795926 | 2.5422622 | 0.0000000 |
| C | -10.5622291 | 3.0524403 | 0.0000000 | -10.5447425 | 3.0482398 | 0.0000000 |
| C | -10.6062567 | 4.4031861 | 0.0000000 | -10.593298 | 4.4031087 | 0.0000000 |
| C | -11.9862438 | 4.7504918 | 0.0000000 | -11.971599 | 4.7460874 | 0.0000000 |
| C | -12.6634705 | 3.5906196 | 0.0000000 | -12.647938 | 3.5839956 | 0.0000000 |
| C | -9.4850399 | 2.1123756 | 0.0000000 | -9.4695414 | 2.1175459 | 0.0000000 |
| C | -9.4430919 | 0.7608536 | 0.0000000 | -9.4263249 | 0.7581481 | 0.0000000 |
| C | -8.0707866 | 0.4063595 | 0.0000000 | -8.0670796 | 0.4005502 | 0.0000000 |
| C | -7.3792362 | 1.5690425 | 0.0000000 | -7.3597323 | 1.5700050 | 0.0000000 |
| O | -8.2329669 | 2.6143180 | 0.0000000 | -8.2163519 | 2.6189411 | 0.0000000 |
| C | -5.9847029 | 1.8719672 | 0.0000000 | -5.9823351 | 1.8526139 | 0.0000000 |
| O | -5.1306309 | 0.8273278 | 0.0000000 | -5.1259831 | 0.8042719 | 0.0000000 |
| C | -3.8781204 | 1.3298751 | 0.0000000 | -3.8656005 | 1.3090775 | 0.0000000 |
| C | -3.9217342 | 2.6823313 | 0.0000000 | -3.9251304 | 2.6872576 | 0.0000000 |
| C | -5.2936760 | 3.0353943 | 0.0000000 | -5.2749573 | 3.0282921 | 0.0000000 |
| C | -2.8035432 | 0.3913733 | 0.0000000 | -2.8003503 | 0.4136538 | 0.0000000 |
| O | -1.5510566 | 0.8936584 | 0.0000000 | -1.5404953 | 0.9205265 | 0.0000000 |
| C | -0.6971036 | -0.1512922 | 0.0000000 | -0.6799039 | -0.1321804 | 0.0000000 |
| C | -1.3885345 | -1.3145801 | 0.0000000 | -1.4031443 | -1.3158739 | 0.0000000 |
| C | -2.7602573 | -0.9612143 | 0.0000000 | -2.7413536 | -0.9686294 | 0.0000000 |
| C | 0.6971036 | 0.1512922 | 0.0000000 | 0.6799039 | 0.1321804 | 0.0000000 |
| O | 1.5510566 | -0.8936584 | 0.0000000 | 1.5404953 | -0.9205265 | 0.0000000 |
| C | 2.8035432 | -0.3913733 | 0.0000000 | 2.8003503 | -0.4136538 | 0.0000000 |
| C | 2.7602573 | 0.9612143 | 0.0000000 | 2.7413536 | 0.9686294 | 0.0000000 |
| C | 1.3885345 | 1.3145801 | 0.0000000 | 1.4031443 | 1.3158739 | 0.0000000 |
| C | 3.8781204 | -1.3298751 | 0.0000000 | 3.8656005 | -1.3090775 | 0.0000000 |
| O | 5.1306309 | -0.8273278 | 0.0000000 | 5.1259831 | -0.8042719 | 0.0000000 |
| C | 5.9847029 | -1.8719672 | 0.0000000 | 5.9823351 | -1.8526139 | 0.0000000 |
| C | 5.2936760 | -3.0353943 | 0.0000000 | 5.2749573 | -3.0282921 | 0.0000000 |
| C | 3.9217342 | -2.6823313 | 0.0000000 | 3.9251304 | -2.6872576 | 0.0000000 |
| H | 3.6041478 | 1.6158650 | 0.0000000 | 3.5875695 | 1.6208298 | 0.0000000 |
| H | -0.9660192 | -2.2955036 | 0.0000000 | -0.9794888 | -2.2965851 | 0.0000000 |
| H | -3.6041478 | -1.6158650 | 0.0000000 | -3.5875695 | -1.6208298 | 0.0000000 |
| H | 3.0780213 | -3.3372315 | 0.0000000 | 3.0824361 | -3.3437185 | 0.0000000 |
| C | 7.3792362 | -1.5690425 | 0.0000000 | 7.3597323 | -1.5700050 | 0.0000000 |
| H | 5.7165457 | -4.0161518 | 0.0000000 | 5.7023657 | -4.0074400 | 0.0000000 |
| H | -5.7165457 | 4.0161518 | 0.0000000 | -5.7023657 | 4.0074400 | 0.0000000 |
| H | -3.0780213 | 3.3372315 | 0.0000000 | -3.0824361 | 3.3437185 | 0.0000000 |
| H | 0.9660192 | 2.2955036 | 0.0000000 | 0.9794888 | 2.2965851 | 0.0000000 |
| H | -10.2879749 | 0.1074160 | 0.0000000 | -10.274172 | 0.1081995 | 0.0000000 |
| H | -7.6488331 | -0.5748187 | 0.0000000 | -7.6480579 | -0.5819542 | 0.0000000 |
| H | -12.4090913 | 5.7319524 | 0.0000000 | -12.397037 | 5.7265268 | 0.0000000 |
| H | -13.7033421 | 3.3503271 | 0.0000000 | -13.687817 | 3.3433029 | 0.0000000 |
| H | -9.7644655 | 5.0604908 | 0.0000000 | -9.7529596 | 5.0622823 | 0.0000000 |
| O | 8.2329669 | -2.6143180 | 0.0000000 | 8.2163519 | -2.6189411 | 0.0000000 |
| C | 9.4850399 | -2.1123756 | 0.0000000 | 9.4695414 | -2.1175459 | 0.0000000 |
| C | 9.4430919 | -0.7608536 | 0.0000000 | 9.4263249 | -0.7581481 | 0.0000000 |
| C | 8.0707866 | -0.4063595 | 0.0000000 | 8.0670796 | -0.4005502 | 0.0000000 |
| H | 7.6488331 | 0.5748187 | 0.0000000 | 7.6480579 | 0.5819542 | 0.0000000 |
| H | 10.2879749 | -0.1074160 | 0.0000000 | 10.2741720 | -0.1081995 | 0.0000000 |
| C | 10.5622291 | -3.0524403 | 0.0000000 | 10.5447425 | -3.0482398 | 0.0000000 |
| O | 11.8119587 | -2.5478886 | 0.0000000 | 11.7959262 | -2.5422622 | 0.0000000 |
| C | 12.6634705 | -3.5906196 | 0.0000000 | 12.6479387 | -3.5839956 | 0.0000000 |
| C | 11.9862438 | -4.7504918 | 0.0000000 | 11.9715997 | -4.7460874 | 0.0000000 |
| C | 10.6062567 | -4.4031861 | 0.0000000 | 10.5932983 | -4.4031087 | 0.0000000 |
| H | 9.7644655 | -5.0604908 | 0.0000000 | 9.7529596 | -5.0622823 | 0.0000000 |
| H | 12.4090913 | -5.7319524 | 0.0000000 | 12.3970373 | -5.7265268 | 0.0000000 |
| H | 13.7033421 | -3.3503271 | 0.0000000 | 13.6878170 | -3.3433029 | 0.0000000 |
|  |  |  |  |  |  |  |
| **9O/**  **BHLYP** | **Ground state** | | | **Excited state** | | |
| C | -13.0943270 | 0.0000000 | -1.5120234 | -13.079962 | 0.0000000 | -1.5147050 |
| C | -12.7146676 | 0.0000000 | -0.2149875 | -12.696394 | 0.0000000 | -0.2156734 |
| O | -13.7989667 | 0.0000000 | 0.5854345 | -13.781423 | 0.0000000 | 0.5860203 |
| C | -14.8837259 | 0.0000000 | -0.2118542 | -14.866350 | 0.0000000 | -0.2104197 |
| C | -14.5173256 | 0.0000000 | -1.5040172 | -14.501017 | 0.0000000 | -1.5039789 |
| C | -11.4369840 | 0.0000000 | 0.4265662 | -11.421806 | 0.0000000 | 0.4198310 |
| O | -10.3497571 | 0.0000000 | -0.3719035 | -10.333608 | 0.0000000 | -0.3780421 |
| C | -9.2622314 | 0.0000000 | 0.4273120 | -9.2434510 | 0.0000000 | 0.4233852 |
| C | -9.6418075 | 0.0000000 | 1.7257649 | -9.6334183 | 0.0000000 | 1.7293469 |
| C | -11.0591589 | 0.0000000 | 1.7248811 | -11.042034 | 0.0000000 | 1.7235201 |
| C | -7.9873756 | 0.0000000 | -0.2139676 | -7.9772151 | 0.0000000 | -0.1998790 |
| O | -6.8996863 | 0.0000000 | 0.5845326 | -6.8871129 | 0.0000000 | 0.6000936 |
| C | -5.8121793 | 0.0000000 | -0.2146307 | -5.7940656 | 0.0000000 | -0.2023140 |
| C | -6.1918510 | 0.0000000 | -1.5134271 | -6.1917792 | 0.0000000 | -1.5172291 |
| C | -7.6084938 | 0.0000000 | -1.5130222 | -7.5892622 | 0.0000000 | -1.5110811 |
| C | -4.5374399 | 0.0000000 | 0.4261079 | -4.5353496 | 0.0000000 | 0.4059817 |
| O | -3.4498616 | 0.0000000 | -0.3727233 | -3.4430006 | 0.0000000 | -0.3972380 |
| C | -2.3622525 | 0.0000000 | 0.4262047 | -2.3477381 | 0.0000000 | 0.4064628 |
| C | -2.7416478 | 0.0000000 | 1.7251859 | -2.7510072 | 0.0000000 | 1.7296376 |
| C | -4.1581423 | 0.0000000 | 1.7251577 | -4.1379792 | 0.0000000 | 1.7255070 |
| C | -1.0875944 | 0.0000000 | -0.2145768 | -1.0947896 | 0.0000000 | -0.1916383 |
| O | 0.0000000 | 0.0000000 | 0.5842866 | 0.0000000 | 0.0000000 | 0.6130074 |
| C | 1.0875944 | 0.0000000 | -0.2145768 | 1.0947896 | 0.0000000 | -0.1916383 |
| C | 0.7082383 | 0.0000000 | -1.5136096 | 0.6912419 | 0.0000000 | -1.5167108 |
| C | -0.7082383 | 0.0000000 | -1.5136096 | -0.6912419 | 0.0000000 | -1.5167108 |
| C | 2.3622525 | 0.0000000 | 0.4262047 | 2.3477381 | 0.0000000 | 0.4064628 |
| O | 3.4498616 | 0.0000000 | -0.3727233 | 3.4430006 | 0.0000000 | -0.3972380 |
| C | 4.5374399 | 0.0000000 | 0.4261079 | 4.5353496 | 0.0000000 | 0.4059817 |
| C | 4.1581423 | 0.0000000 | 1.7251577 | 4.1379792 | 0.0000000 | 1.7255070 |
| C | 2.7416478 | 0.0000000 | 1.7251859 | 2.7510072 | 0.0000000 | 1.7296376 |
| C | 5.8121793 | 0.0000000 | -0.2146307 | 5.7940656 | 0.0000000 | -0.2023140 |
| C | 6.1918510 | 0.0000000 | -1.5134271 | 6.1917792 | 0.0000000 | -1.5172291 |
| C | 7.6084938 | 0.0000000 | -1.5130222 | 7.5892622 | 0.0000000 | -1.5110811 |
| C | 7.9873756 | 0.0000000 | -0.2139676 | 7.9772151 | 0.0000000 | -0.1998790 |
| O | 6.8996863 | 0.0000000 | 0.5845326 | 6.8871129 | 0.0000000 | 0.6000936 |
| C | 9.2622314 | 0.0000000 | 0.4273120 | 9.2434510 | 0.0000000 | 0.4233852 |
| O | 10.3497571 | 0.0000000 | -0.3719035 | 10.3336087 | 0.0000000 | -0.3780421 |
| C | 11.4369840 | 0.0000000 | 0.4265662 | 11.4218063 | 0.0000000 | 0.4198310 |
| C | 11.0591589 | 0.0000000 | 1.7248811 | 11.0420349 | 0.0000000 | 1.7235201 |
| C | 9.6418075 | 0.0000000 | 1.7257649 | 9.6334183 | 0.0000000 | 1.7293469 |
| H | -4.8120656 | 0.0000000 | 2.5696092 | -4.7951502 | 0.0000000 | 2.5678536 |
| H | -1.3621108 | 0.0000000 | -2.3581055 | -1.3469584 | 0.0000000 | -2.3601470 |
| H | 1.3621108 | 0.0000000 | -2.3581055 | 1.3469584 | 0.0000000 | -2.3601470 |
| H | -5.5382248 | 0.0000000 | -2.3581284 | -5.5399283 | 0.0000000 | -2.3634438 |
| H | -8.2626976 | 0.0000000 | -2.3572489 | -8.2470331 | 0.0000000 | -2.3528777 |
| H | 4.8120656 | 0.0000000 | 2.5696092 | 4.7951502 | 0.0000000 | 2.5678536 |
| H | 2.0878110 | 0.0000000 | 2.5697162 | 2.0973620 | 0.0000000 | 2.5745750 |
| H | -2.0878110 | 0.0000000 | 2.5697162 | -2.0973620 | 0.0000000 | 2.5745750 |
| H | 8.2626976 | 0.0000000 | -2.3572489 | 8.2470331 | 0.0000000 | -2.3528777 |
| H | 5.5382248 | 0.0000000 | -2.3581284 | 5.5399283 | 0.0000000 | -2.3634438 |
| H | 11.7142953 | 0.0000000 | 2.5684466 | 11.7000934 | 0.0000000 | 2.5650149 |
| C | 12.7146676 | 0.0000000 | -0.2149875 | 12.6963945 | 0.0000000 | -0.2156734 |
| H | 8.9883829 | 0.0000000 | 2.5706275 | 8.9821469 | 0.0000000 | 2.5759244 |
| H | -8.9883829 | 0.0000000 | 2.5706275 | -8.9821469 | 0.0000000 | 2.5759244 |
| H | -11.7142953 | 0.0000000 | 2.5684466 | -11.700093 | 0.0000000 | 2.5650149 |
| H | -12.4431544 | 0.0000000 | -2.3585673 | -12.430190 | 0.0000000 | -2.3623304 |
| H | -15.1716786 | 0.0000000 | -2.3489351 | -15.157000 | 0.0000000 | -2.3477126 |
| H | -15.8307322 | 0.0000000 | 0.2803374 | -15.813286 | 0.0000000 | 0.2820624 |
| O | 13.7989667 | 0.0000000 | 0.5854345 | 13.7814235 | 0.0000000 | 0.5860203 |
| C | 14.8837259 | 0.0000000 | -0.2118542 | 14.8663505 | 0.0000000 | -0.2104197 |
| C | 14.5173256 | 0.0000000 | -1.5040172 | 14.5010179 | 0.0000000 | -1.5039789 |
| C | 13.0943270 | 0.0000000 | -1.5120234 | 13.0799625 | 0.0000000 | -1.5147050 |
| H | 12.4431544 | 0.0000000 | -2.3585673 | 12.4301908 | 0.0000000 | -2.3623304 |
| H | 15.1716786 | 0.0000000 | -2.3489351 | 15.1570007 | 0.0000000 | -2.3477126 |
| H | 15.8307322 | 0.0000000 | 0.2803374 | 15.8132862 | 0.0000000 | 0.2820624 |

Part 7.

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| **2O/**  **CAM-B3LYP** | **Ground state** | | | **Excited state** | | |
| C | -2.8069982 | 0.4321278 | 0.0000000 | -2.7915557 | 0.4438111 | 0.0000000 |
| C | -2.7890134 | -0.9162819 | 0.0000000 | -2.7650333 | -0.9310852 | 0.0000000 |
| C | -1.4151178 | -1.2975944 | 0.0000000 | -1.4329128 | -1.3258813 | 0.0000000 |
| C | -0.7042793 | -0.1431766 | 0.0000000 | -0.6737216 | -0.1267289 | 0.0000000 |
| C | 0.7042793 | 0.1431766 | 0.0000000 | 0.6737216 | 0.1267289 | 0.0000000 |
| C | 1.4151178 | 1.2975944 | 0.0000000 | 1.4329128 | 1.3258813 | 0.0000000 |
| C | 2.7890134 | 0.9162819 | 0.0000000 | 2.7650333 | 0.9310852 | 0.0000000 |
| C | 2.8069982 | -0.4321278 | 0.0000000 | 2.7915557 | -0.4438111 | 0.0000000 |
| O | -1.5434843 | 0.9216052 | 0.0000000 | -1.5341415 | 0.9604119 | 0.0000000 |
| O | 1.5434843 | -0.9216052 | 0.0000000 | 1.5341415 | -0.9604119 | 0.0000000 |
| H | -3.5953909 | 1.1620968 | 0.0000000 | -3.5969815 | 1.1564078 | 0.0000000 |
| H | -3.6467412 | -1.5654675 | 0.0000000 | -3.6340400 | -1.5664761 | 0.0000000 |
| H | -1.0056051 | -2.2916376 | 0.0000000 | -1.0227187 | -2.3194262 | 0.0000000 |
| H | 1.0056051 | 2.2916376 | 0.0000000 | 1.0227187 | 2.3194262 | 0.0000000 |
| H | 3.6467412 | 1.5654675 | 0.0000000 | 3.6340400 | 1.5664761 | 0.0000000 |
| H | 3.5953909 | -1.1620968 | 0.0000000 | 3.5969815 | -1.1564078 | 0.0000000 |
|  |  |  |  |  |  |  |
| **3O/**  **CAM-B3LYP** | **Ground state** | | | **Excited state** | | |
| O | 3.4636806 | 0.0000000 | 0.8307793 | 3.4601217 | 0.0000000 | 0.8491542 |
| C | 4.5539626 | 0.0000000 | 0.0263544 | 4.5369712 | 0.0000000 | 0.0258074 |
| C | 4.1822288 | 0.0000000 | -1.2700525 | 4.1486534 | 0.0000000 | -1.2782988 |
| C | 2.7567961 | 0.0000000 | -1.2771940 | 2.7427451 | 0.0000000 | -1.2881158 |
| C | 2.3737816 | 0.0000000 | 0.0240387 | 2.3484524 | 0.0000000 | 0.0467134 |
| C | 1.0925440 | 0.0000000 | 0.6709158 | 1.1015879 | 0.0000000 | 0.6530121 |
| O | 0.0000000 | 0.0000000 | -0.1347980 | 0.0000000 | 0.0000000 | -0.1728940 |
| C | -1.0925440 | 0.0000000 | 0.6709158 | -1.1015879 | 0.0000000 | 0.6530121 |
| C | -0.7105149 | 0.0000000 | 1.9726903 | -0.6868370 | 0.0000000 | 1.9984862 |
| C | 0.7105149 | 0.0000000 | 1.9726903 | 0.6868370 | 0.0000000 | 1.9984862 |
| C | -2.3737816 | 0.0000000 | 0.0240387 | -2.3484524 | 0.0000000 | 0.0467134 |
| O | -3.4636806 | 0.0000000 | 0.8307793 | -3.4601217 | 0.0000000 | 0.8491542 |
| C | -4.5539626 | 0.0000000 | 0.0263544 | -4.5369712 | 0.0000000 | 0.0258074 |
| C | -4.1822288 | 0.0000000 | -1.2700525 | -4.1486534 | 0.0000000 | -1.2782988 |
| C | -2.7567961 | 0.0000000 | -1.2771940 | -2.7427451 | 0.0000000 | -1.2881158 |
| H | 5.5065255 | 0.0000000 | 0.5233731 | 5.4991990 | 0.0000000 | 0.5052139 |
| H | 4.8392695 | 0.0000000 | -2.1217600 | 4.8072930 | 0.0000000 | -2.1295297 |
| H | 2.1012901 | 0.0000000 | -2.1292648 | 2.0807481 | 0.0000000 | -2.1354002 |
| H | -2.1012901 | 0.0000000 | -2.1292648 | -2.0807481 | 0.0000000 | -2.1354002 |
| H | -5.5065255 | 0.0000000 | 0.5233731 | -5.4991990 | 0.0000000 | 0.5052139 |
| H | -4.8392695 | 0.0000000 | -2.1217600 | -4.8072930 | 0.0000000 | -2.1295297 |
| H | 1.3690805 | 0.0000000 | 2.8225211 | 1.3508887 | 0.0000000 | 2.8444066 |
| H | -1.3690805 | 0.0000000 | 2.8225211 | -1.3508887 | 0.0000000 | 2.8444066 |
|  |  |  |  |  |  |  |
| **4O/**  **CAM-B3LYP** | **Ground state** | | | **Excited state** | | |
| O | -1.7650332 | 0.3432868 | 0.0000000 | -1.7638355 | 0.3812312 | 0.0000000 |
| C | -2.7901351 | -0.5465590 | 0.0000000 | -2.7907832 | -0.5223304 | 0.0000000 |
| C | -2.3059544 | -1.8141624 | 0.0000000 | -2.2819645 | -1.8162115 | 0.0000000 |
| C | -0.8899219 | -1.7018469 | 0.0000000 | -0.9036273 | -1.7156113 | 0.0000000 |
| C | -0.6116205 | -0.3731702 | 0.0000000 | -0.5969494 | -0.3454042 | 0.0000000 |
| C | 0.6116205 | 0.3731702 | 0.0000000 | 0.5969494 | 0.3454042 | 0.0000000 |
| O | 1.7650332 | -0.3432868 | 0.0000000 | 1.7638355 | -0.3812312 | 0.0000000 |
| C | 2.7901351 | 0.5465590 | 0.0000000 | 2.7907832 | 0.5223304 | 0.0000000 |
| C | 2.3059544 | 1.8141624 | 0.0000000 | 2.2819645 | 1.8162115 | 0.0000000 |
| C | 0.8899219 | 1.7018469 | 0.0000000 | 0.9036273 | 1.7156113 | 0.0000000 |
| C | 4.1185892 | 0.0038401 | 0.0000000 | 4.0970805 | 0.0121268 | 0.0000000 |
| O | 5.1407925 | 0.8948621 | 0.0000000 | 5.1282309 | 0.9064490 | 0.0000000 |
| C | 6.2915781 | 0.1797744 | 0.0000000 | 6.2757841 | 0.1871856 | 0.0000000 |
| C | 6.0242719 | -1.1421629 | 0.0000000 | 6.0069279 | -1.1413911 | 0.0000000 |
| C | 4.6040315 | -1.2628246 | 0.0000000 | 4.5991837 | -1.2703024 | 0.0000000 |
| H | -2.8951840 | -2.7134503 | 0.0000000 | -2.8783753 | -2.7113500 | 0.0000000 |
| H | -0.1668670 | -2.4974641 | 0.0000000 | -0.1794073 | -2.5104720 | 0.0000000 |
| H | 4.0185538 | -2.1644540 | 0.0000000 | 4.0154749 | -2.1732348 | 0.0000000 |
| H | 7.2015723 | 0.7510189 | 0.0000000 | 7.1890221 | 0.7539968 | 0.0000000 |
| H | 6.7470394 | -1.9388427 | 0.0000000 | 6.7349733 | -1.9338031 | 0.0000000 |
| H | 0.1668670 | 2.4974641 | 0.0000000 | 0.1794073 | 2.5104720 | 0.0000000 |
| H | 2.8951840 | 2.7134503 | 0.0000000 | 2.8783753 | 2.7113500 | 0.0000000 |
| C | -4.1185892 | -0.0038401 | 0.0000000 | -4.0970805 | -0.0121268 | 0.0000000 |
| O | -5.1407925 | -0.8948621 | 0.0000000 | -5.1282309 | -0.9064490 | 0.0000000 |
| C | -6.2915781 | -0.1797744 | 0.0000000 | -6.2757841 | -0.1871856 | 0.0000000 |
| C | -6.0242719 | 1.1421629 | 0.0000000 | -6.0069279 | 1.1413911 | 0.0000000 |
| C | -4.6040315 | 1.2628246 | 0.0000000 | -4.5991837 | 1.2703024 | 0.0000000 |
| H | -4.0185538 | 2.1644540 | 0.0000000 | -4.0154749 | 2.1732348 | 0.0000000 |
| H | -7.2015723 | -0.7510189 | 0.0000000 | -7.1890221 | -0.7539968 | 0.0000000 |
| H | -6.7470394 | 1.9388427 | 0.0000000 | -6.7349733 | 1.9338031 | 0.0000000 |
|  |  |  |  |  |  |  |
| **5O/**  **CAM-B3LYP** | **Ground state** | | | **Excited state** | | |
| O | 3.4641773 | 0.0000000 | 0.2640775 | 3.4561443 | 0.0000000 | 0.2931210 |
| C | 4.5567745 | 0.0000000 | -0.5413693 | 4.5495609 | 0.0000000 | -0.5203194 |
| C | 4.1750216 | 0.0000000 | -1.8435630 | 4.1524758 | 0.0000000 | -1.8410925 |
| C | 2.7546642 | 0.0000000 | -1.8443638 | 2.7608548 | 0.0000000 | -1.8502766 |
| C | 2.3714198 | 0.0000000 | -0.5419852 | 2.3522305 | 0.0000000 | -0.5186129 |
| C | 1.0928780 | 0.0000000 | 0.1044464 | 1.1013192 | 0.0000000 | 0.0801626 |
| O | 0.0000000 | 0.0000000 | -0.7012612 | 0.0000000 | 0.0000000 | -0.7372372 |
| C | -1.0928780 | 0.0000000 | 0.1044464 | -1.1013192 | 0.0000000 | 0.0801626 |
| C | -0.7099537 | 0.0000000 | 1.4071130 | -0.6895763 | 0.0000000 | 1.4170177 |
| C | 0.7099537 | 0.0000000 | 1.4071130 | 0.6895763 | 0.0000000 | 1.4170177 |
| C | -2.3714198 | 0.0000000 | -0.5419852 | -2.3522305 | 0.0000000 | -0.5186129 |
| O | -3.4641773 | 0.0000000 | 0.2640775 | -3.4561443 | 0.0000000 | 0.2931210 |
| C | -4.5567745 | 0.0000000 | -0.5413693 | -4.5495609 | 0.0000000 | -0.5203194 |
| C | -4.1750216 | 0.0000000 | -1.8435630 | -4.1524758 | 0.0000000 | -1.8410925 |
| C | -2.7546642 | 0.0000000 | -1.8443638 | -2.7608548 | 0.0000000 | -1.8502766 |
| C | 5.8378721 | 0.0000000 | 0.1051798 | 5.8191376 | 0.0000000 | 0.1001060 |
| O | 6.9276026 | 0.0000000 | -0.7018432 | 6.9122719 | 0.0000000 | -0.7119114 |
| C | 8.0179204 | 0.0000000 | 0.1023732 | 8.0029537 | 0.0000000 | 0.0905896 |
| C | 7.6464839 | 0.0000000 | 1.3989265 | 7.6347769 | 0.0000000 | 1.3924724 |
| C | 6.2211751 | 0.0000000 | 1.4064098 | 6.2170651 | 0.0000000 | 1.4104633 |
| C | -5.8378721 | 0.0000000 | 0.1051798 | -5.8191376 | 0.0000000 | 0.1001060 |
| O | -6.9276026 | 0.0000000 | -0.7018432 | -6.9122719 | 0.0000000 | -0.7119114 |
| H | -4.8339608 | 0.0000000 | -2.6930916 | -4.8169508 | 0.0000000 | -2.6868960 |
| H | -2.0973275 | 0.0000000 | -2.6950888 | -2.1038051 | 0.0000000 | -2.7014604 |
| H | -1.3677630 | 0.0000000 | 2.2574608 | -1.3509017 | 0.0000000 | 2.2650669 |
| H | 1.3677630 | 0.0000000 | 2.2574608 | 1.3509017 | 0.0000000 | 2.2650669 |
| H | 2.0973275 | 0.0000000 | -2.6950888 | 2.1038051 | 0.0000000 | -2.7014604 |
| H | 4.8339608 | 0.0000000 | -2.6930916 | 4.8169508 | 0.0000000 | -2.6868960 |
| H | 5.5659676 | 0.0000000 | 2.2587152 | 5.5662079 | 0.0000000 | 2.2661820 |
| H | 8.3037000 | 0.0000000 | 2.2504846 | 8.2983409 | 0.0000000 | 2.2394441 |
| C | -8.0179204 | 0.0000000 | 0.1023732 | -8.0029537 | 0.0000000 | 0.0905896 |
| C | -7.6464839 | 0.0000000 | 1.3989265 | -7.6347769 | 0.0000000 | 1.3924724 |
| C | -6.2211751 | 0.0000000 | 1.4064098 | -6.2170651 | 0.0000000 | 1.4104633 |
| H | -5.5659676 | 0.0000000 | 2.2587152 | -5.5662079 | 0.0000000 | 2.2661820 |
| H | -8.9704161 | 0.0000000 | -0.3947829 | -8.9555497 | 0.0000000 | -0.4069694 |
| H | -8.3037000 | 0.0000000 | 2.2504846 | -8.2983409 | 0.0000000 | 2.2394441 |
| H | 8.9704161 | 0.0000000 | -0.3947829 | 8.9555497 | 0.0000000 | -0.4069694 |
|  |  |  |  |  |  |  |
| **6O/**  **CAM-B3LYP** | **Ground state** | | | **Excited state** | | |
| O | 1.7979777 | -0.0173306 | 0.0000000 | 1.8032517 | 0.0156501 | 0.0000000 |
| C | 0.5242841 | -0.4879137 | 0.0000000 | 0.5179053 | -0.4601501 | 0.0000000 |
| C | 0.5304537 | -1.8457693 | 0.0000000 | 0.5423088 | -1.8563907 | 0.0000000 |
| C | 1.8944106 | -2.2399922 | 0.0000000 | 1.8727512 | -2.2365162 | 0.0000000 |
| C | 2.6240532 | -1.0948279 | 0.0000000 | 2.6320549 | -1.0720108 | 0.0000000 |
| C | 4.0318150 | -0.8290555 | 0.0000000 | 4.0088497 | -0.8384016 | 0.0000000 |
| O | 4.8575682 | -1.9070148 | 0.0000000 | 4.8408517 | -1.9227881 | 0.0000000 |
| C | 6.1309057 | -1.4368871 | 0.0000000 | 6.1161267 | -1.4498317 | 0.0000000 |
| C | 6.1260359 | -0.0798711 | 0.0000000 | 6.1065113 | -0.0777634 | 0.0000000 |
| C | 4.7618610 | 0.3155524 | 0.0000000 | 4.7648570 | 0.3199930 | 0.0000000 |
| H | 6.9950818 | 0.5531005 | 0.0000000 | 6.9796156 | 0.5502536 | 0.0000000 |
| H | 2.2902090 | -3.2395609 | 0.0000000 | 2.2734158 | -3.2345720 | 0.0000000 |
| H | -0.3375522 | -2.4801040 | 0.0000000 | -0.3267325 | -2.4897385 | 0.0000000 |
| C | 7.1819227 | -2.4139175 | 0.0000000 | 7.1644699 | -2.4077410 | 0.0000000 |
| O | 8.4529585 | -1.9414157 | 0.0000000 | 8.4384361 | -1.9322460 | 0.0000000 |
| C | 9.2768944 | -3.0168896 | 0.0000000 | 9.2634278 | -3.0060773 | 0.0000000 |
| C | 8.5598629 | -4.1592115 | 0.0000000 | 8.5480998 | -4.1527293 | 0.0000000 |
| C | 7.1886030 | -3.7704087 | 0.0000000 | 7.1795884 | -3.7725717 | 0.0000000 |
| H | 6.3224078 | -4.4071426 | 0.0000000 | 6.3159725 | -4.4128556 | 0.0000000 |
| H | 10.3300185 | -2.8039489 | 0.0000000 | 10.3165871 | -2.7923444 | 0.0000000 |
| H | 8.9546092 | -5.1598387 | 0.0000000 | 8.9481316 | -5.1514575 | 0.0000000 |
| C | -0.5242841 | 0.4879137 | 0.0000000 | -0.5179053 | 0.4601501 | 0.0000000 |
| O | -1.7979777 | 0.0173306 | 0.0000000 | -1.8032517 | -0.0156501 | 0.0000000 |
| C | -2.6240532 | 1.0948279 | 0.0000000 | -2.6320549 | 1.0720108 | 0.0000000 |
| C | -1.8944106 | 2.2399922 | 0.0000000 | -1.8727512 | 2.2365162 | 0.0000000 |
| C | -0.5304537 | 1.8457693 | 0.0000000 | -0.5423088 | 1.8563907 | 0.0000000 |
| H | -2.2902090 | 3.2395609 | 0.0000000 | -2.2734158 | 3.2345720 | 0.0000000 |
| H | 0.3375522 | 2.4801040 | 0.0000000 | 0.3267325 | 2.4897385 | 0.0000000 |
| H | 4.3668306 | 1.3154419 | 0.0000000 | 4.3722186 | 1.3209704 | 0.0000000 |
| C | -4.0318150 | 0.8290555 | 0.0000000 | -4.0088497 | 0.8384016 | 0.0000000 |
| C | -4.7618610 | -0.3155524 | 0.0000000 | -4.7648570 | -0.3199930 | 0.0000000 |
| C | -6.1260359 | 0.0798711 | 0.0000000 | -6.1065113 | 0.0777634 | 0.0000000 |
| C | -6.1309057 | 1.4368871 | 0.0000000 | -6.1161267 | 1.4498317 | 0.0000000 |
| O | -4.8575682 | 1.9070148 | 0.0000000 | -4.8408517 | 1.9227881 | 0.0000000 |
| H | -6.9950818 | -0.5531005 | 0.0000000 | -6.9796156 | -0.5502536 | 0.0000000 |
| H | -4.3668306 | -1.3154419 | 0.0000000 | -4.3722186 | -1.3209704 | 0.0000000 |
| C | -7.1819227 | 2.4139175 | 0.0000000 | -7.1644699 | 2.4077410 | 0.0000000 |
| C | -7.1886030 | 3.7704087 | 0.0000000 | -7.1795884 | 3.7725717 | 0.0000000 |
| C | -8.5598629 | 4.1592115 | 0.0000000 | -8.5480998 | 4.1527293 | 0.0000000 |
| C | -9.2768944 | 3.0168896 | 0.0000000 | -9.2634278 | 3.0060773 | 0.0000000 |
| O | -8.4529585 | 1.9414157 | 0.0000000 | -8.4384361 | 1.9322460 | 0.0000000 |
| H | -8.9546092 | 5.1598387 | 0.0000000 | -8.9481316 | 5.1514575 | 0.0000000 |
| H | -10.3300185 | 2.8039489 | 0.0000000 | -10.316587 | 2.7923444 | 0.0000000 |
| H | -6.3224078 | 4.4071426 | 0.0000000 | -6.3159725 | 4.4128556 | 0.0000000 |
|  |  |  |  |  |  |  |
| **7O/**  **CAM-B3LYP** | **Ground state** | | | **Excited state** | | |
| C | -9.6852529 | 0.0000000 | -1.4814586 | -9.6729270 | 0.0000000 | -1.4872265 |
| C | -9.3018122 | 0.0000000 | -0.1802721 | -9.2830157 | 0.0000000 | -0.1820960 |
| O | -10.3914209 | 0.0000000 | 0.6268900 | -10.374420 | 0.0000000 | 0.6269815 |
| C | -11.4818060 | 0.0000000 | -0.1771908 | -11.464743 | 0.0000000 | -0.1762729 |
| C | -11.1105391 | 0.0000000 | -1.4738039 | -11.094790 | 0.0000000 | -1.4752039 |
| C | -8.0206541 | 0.0000000 | 0.4661430 | -8.0077906 | 0.0000000 | 0.4532163 |
| O | -6.9281386 | 0.0000000 | -0.3393139 | -6.9137053 | 0.0000000 | -0.3525366 |
| C | -5.8353670 | 0.0000000 | 0.4667299 | -5.8160509 | 0.0000000 | 0.4577119 |
| C | -6.2185739 | 0.0000000 | 1.7691291 | -6.2167113 | 0.0000000 | 1.7740583 |
| C | -7.6388819 | 0.0000000 | 1.7683726 | -7.6218256 | 0.0000000 | 1.7650866 |
| C | -4.5568992 | 0.0000000 | -0.1797400 | -4.5527113 | 0.0000000 | -0.1574205 |
| O | -3.4639718 | 0.0000000 | 0.6257387 | -3.4562745 | 0.0000000 | 0.6542167 |
| C | -2.3712117 | 0.0000000 | -0.1802538 | -2.3544734 | 0.0000000 | -0.1573365 |
| C | -2.7544797 | 0.0000000 | -1.4829220 | -2.7624681 | 0.0000000 | -1.4864153 |
| C | -4.1742339 | 0.0000000 | -1.4825928 | -4.1525217 | 0.0000000 | -1.4805790 |
| C | -1.0928382 | 0.0000000 | 0.4657889 | -1.1006111 | 0.0000000 | 0.4431881 |
| O | 0.0000000 | 0.0000000 | -0.3399953 | 0.0000000 | 0.0000000 | -0.3707147 |
| C | 1.0928382 | 0.0000000 | 0.4657889 | 1.1006111 | 0.0000000 | 0.4431881 |
| C | 0.7098288 | 0.0000000 | 1.7686056 | 0.6915378 | 0.0000000 | 1.7752220 |
| C | -0.7098288 | 0.0000000 | 1.7686056 | -0.6915378 | 0.0000000 | 1.7752220 |
| C | 2.3712117 | 0.0000000 | -0.1802538 | 2.3544734 | 0.0000000 | -0.1573365 |
| O | 3.4639718 | 0.0000000 | 0.6257387 | 3.4562745 | 0.0000000 | 0.6542167 |
| C | 4.5568992 | 0.0000000 | -0.1797400 | 4.5527113 | 0.0000000 | -0.1574205 |
| C | 4.1742339 | 0.0000000 | -1.4825928 | 4.1525217 | 0.0000000 | -1.4805790 |
| C | 2.7544797 | 0.0000000 | -1.4829220 | 2.7624681 | 0.0000000 | -1.4864153 |
| C | 5.8353670 | 0.0000000 | 0.4667299 | 5.8160509 | 0.0000000 | 0.4577119 |
| O | 6.9281386 | 0.0000000 | -0.3393139 | 6.9137053 | 0.0000000 | -0.3525366 |
| C | 8.0206541 | 0.0000000 | 0.4661430 | 8.0077906 | 0.0000000 | 0.4532163 |
| C | 7.6388819 | 0.0000000 | 1.7683726 | 7.6218256 | 0.0000000 | 1.7650866 |
| C | 6.2185739 | 0.0000000 | 1.7691291 | 6.2167113 | 0.0000000 | 1.7740583 |
| C | 9.3018122 | 0.0000000 | -0.1802721 | 9.2830157 | 0.0000000 | -0.1820960 |
| C | 9.6852529 | 0.0000000 | -1.4814586 | 9.6729270 | 0.0000000 | -1.4872265 |
| C | 11.1105391 | 0.0000000 | -1.4738039 | 11.0947904 | 0.0000000 | -1.4752039 |
| C | 11.4818060 | 0.0000000 | -0.1771908 | 11.4647431 | 0.0000000 | -0.1762729 |
| O | 10.3914209 | 0.0000000 | 0.6268900 | 10.3744203 | 0.0000000 | 0.6269815 |
| H | -1.3675678 | 0.0000000 | 2.6190056 | -1.3517972 | 0.0000000 | 2.6240712 |
| H | 2.0969570 | 0.0000000 | -2.3334979 | 2.1050317 | 0.0000000 | -2.3373046 |
| H | 4.8322253 | 0.0000000 | -2.3327880 | 4.8146208 | 0.0000000 | -2.3280664 |
| H | -2.0969570 | 0.0000000 | -2.3334979 | -2.1050317 | 0.0000000 | -2.3373046 |
| H | -4.8322253 | 0.0000000 | -2.3327880 | -4.8146208 | 0.0000000 | -2.3280664 |
| H | 8.2978273 | 0.0000000 | 2.6178892 | 8.2857369 | 0.0000000 | 2.6111003 |
| H | 5.5612311 | 0.0000000 | 2.6198515 | 5.5623584 | 0.0000000 | 2.6271987 |
| H | 1.3675678 | 0.0000000 | 2.6190056 | 1.3517972 | 0.0000000 | 2.6240712 |
| H | 11.7678786 | 0.0000000 | -2.3252614 | 11.7547438 | 0.0000000 | -2.3248015 |
| H | 9.0301373 | 0.0000000 | -2.3338351 | 9.0198638 | 0.0000000 | -2.3411989 |
| H | -5.5612311 | 0.0000000 | 2.6198515 | -5.5623584 | 0.0000000 | 2.6271987 |
| H | -8.2978273 | 0.0000000 | 2.6178892 | -8.2857369 | 0.0000000 | 2.6111003 |
| H | -9.0301373 | 0.0000000 | -2.3338351 | -9.0198638 | 0.0000000 | -2.3411989 |
| H | -11.7678786 | 0.0000000 | -2.3252614 | -11.754743 | 0.0000000 | -2.3248015 |
| H | -12.4342439 | 0.0000000 | 0.3200770 | -12.417302 | 0.0000000 | 0.3210573 |
| H | 12.4342439 | 0.0000000 | 0.3200770 | 12.4173027 | 0.0000000 | 0.3210573 |
|  |  |  |  |  |  |  |
| **8O/**  **CAM-B3LYP** | **Ground state** | | | **Excited state** | | |
| O | -11.8615544 | 2.5559043 | 0.0000000 | -11.843833 | 2.5500893 | 0.0000000 |
| C | -10.6050749 | 3.0657362 | 0.0000000 | -10.585905 | 3.0611773 | 0.0000000 |
| C | -10.6518207 | 4.4213912 | 0.0000000 | -10.636637 | 4.4205769 | 0.0000000 |
| C | -12.0339530 | 4.7695426 | 0.0000000 | -12.017302 | 4.7648877 | 0.0000000 |
| C | -12.7168961 | 3.6065475 | 0.0000000 | -12.699498 | 3.5999249 | 0.0000000 |
| C | -9.5255691 | 2.1202237 | 0.0000000 | -9.5084990 | 2.1242050 | 0.0000000 |
| C | -9.4807359 | 0.7639580 | 0.0000000 | -9.4628487 | 0.7606103 | 0.0000000 |
| C | -8.1055154 | 0.4088764 | 0.0000000 | -8.0998145 | 0.4022591 | 0.0000000 |
| C | -7.4094584 | 1.5743944 | 0.0000000 | -7.3887646 | 1.5741252 | 0.0000000 |
| O | -8.2666161 | 2.6275998 | 0.0000000 | -8.2485890 | 2.6310953 | 0.0000000 |
| C | -6.0099660 | 1.8811938 | 0.0000000 | -6.0061946 | 1.8615609 | 0.0000000 |
| O | -5.1525371 | 0.8285396 | 0.0000000 | -5.1467860 | 0.8051373 | 0.0000000 |
| C | -3.8932182 | 1.3364353 | 0.0000000 | -3.8795476 | 1.3157179 | 0.0000000 |
| C | -3.9394100 | 2.6934744 | 0.0000000 | -3.9413825 | 2.6979330 | 0.0000000 |
| C | -5.3144039 | 3.0473554 | 0.0000000 | -5.2951872 | 3.0397603 | 0.0000000 |
| C | -2.8162262 | 0.3920022 | 0.0000000 | -2.8123892 | 0.4142294 | 0.0000000 |
| O | -1.5569174 | 0.8996541 | 0.0000000 | -1.5458050 | 0.9270385 | 0.0000000 |
| C | -0.6996087 | -0.1532797 | 0.0000000 | -0.6819813 | -0.1342387 | 0.0000000 |
| C | -1.3955054 | -1.3193071 | 0.0000000 | -1.4094730 | -1.3207325 | 0.0000000 |
| C | -2.7703325 | -0.9651495 | 0.0000000 | -2.7512189 | -0.9723980 | 0.0000000 |
| C | 0.6996087 | 0.1532797 | 0.0000000 | 0.6819813 | 0.1342387 | 0.0000000 |
| O | 1.5569174 | -0.8996541 | 0.0000000 | 1.5458050 | -0.9270385 | 0.0000000 |
| C | 2.8162262 | -0.3920022 | 0.0000000 | 2.8123892 | -0.4142294 | 0.0000000 |
| C | 2.7703325 | 0.9651495 | 0.0000000 | 2.7512189 | 0.9723980 | 0.0000000 |
| C | 1.3955054 | 1.3193071 | 0.0000000 | 1.4094730 | 1.3207325 | 0.0000000 |
| C | 3.8932182 | -1.3364353 | 0.0000000 | 3.8795476 | -1.3157179 | 0.0000000 |
| O | 5.1525371 | -0.8285396 | 0.0000000 | 5.1467860 | -0.8051373 | 0.0000000 |
| C | 6.0099660 | -1.8811938 | 0.0000000 | 6.0061946 | -1.8615609 | 0.0000000 |
| C | 5.3144039 | -3.0473554 | 0.0000000 | 5.2951872 | -3.0397603 | 0.0000000 |
| C | 3.9394100 | -2.6934744 | 0.0000000 | 3.9413825 | -2.6979330 | 0.0000000 |
| H | 3.6196924 | 1.6242259 | 0.0000000 | 3.6028293 | 1.6291275 | 0.0000000 |
| H | -0.9703449 | -2.3067591 | 0.0000000 | -0.9834330 | -2.3080704 | 0.0000000 |
| H | -3.6196924 | -1.6242259 | 0.0000000 | -3.6028293 | -1.6291275 | 0.0000000 |
| H | 3.0902347 | -3.3527987 | 0.0000000 | 3.0934990 | -3.3591614 | 0.0000000 |
| C | 7.4094584 | -1.5743944 | 0.0000000 | 7.3887646 | -1.5741252 | 0.0000000 |
| H | 5.7398382 | -4.0346733 | 0.0000000 | 5.7250895 | -4.0254981 | 0.0000000 |
| H | -5.7398382 | 4.0346733 | 0.0000000 | -5.7250895 | 4.0254981 | 0.0000000 |
| H | -3.0902347 | 3.3527987 | 0.0000000 | -3.0934990 | 3.3591614 | 0.0000000 |
| H | 0.9703449 | 2.3067591 | 0.0000000 | 0.9834330 | 2.3080704 | 0.0000000 |
| H | -10.3308522 | 0.1058191 | 0.0000000 | -10.315853 | 0.1058343 | 0.0000000 |
| H | -7.6809165 | -0.5788126 | 0.0000000 | -7.6784066 | -0.5868685 | 0.0000000 |
| H | -12.4581065 | 5.7580374 | 0.0000000 | -12.443740 | 5.7525178 | 0.0000000 |
| H | -13.7632914 | 3.3626675 | 0.0000000 | -13.745914 | 3.3557111 | 0.0000000 |
| H | -9.8046135 | 5.0831539 | 0.0000000 | -9.7909047 | 5.0842611 | 0.0000000 |
| O | 8.2666161 | -2.6275998 | 0.0000000 | 8.2485890 | -2.6310953 | 0.0000000 |
| C | 9.5255691 | -2.1202237 | 0.0000000 | 9.5084990 | -2.1242050 | 0.0000000 |
| C | 9.4807359 | -0.7639580 | 0.0000000 | 9.4628487 | -0.7606103 | 0.0000000 |
| C | 8.1055154 | -0.4088764 | 0.0000000 | 8.0998145 | -0.4022591 | 0.0000000 |
| H | 7.6809165 | 0.5788126 | 0.0000000 | 7.6784066 | 0.5868685 | 0.0000000 |
| H | 10.3308522 | -0.1058191 | 0.0000000 | 10.3158538 | -0.1058343 | 0.0000000 |
| C | 10.6050749 | -3.0657362 | 0.0000000 | 10.5859054 | -3.0611773 | 0.0000000 |
| O | 11.8615544 | -2.5559043 | 0.0000000 | 11.8438331 | -2.5500893 | 0.0000000 |
| C | 12.7168961 | -3.6065475 | 0.0000000 | 12.6994989 | -3.5999249 | 0.0000000 |
| C | 12.0339530 | -4.7695426 | 0.0000000 | 12.0173021 | -4.7648877 | 0.0000000 |
| C | 10.6518207 | -4.4213912 | 0.0000000 | 10.6366378 | -4.4205769 | 0.0000000 |
| H | 9.8046135 | -5.0831539 | 0.0000000 | 9.7909047 | -5.0842611 | 0.0000000 |
| H | 12.4581065 | -5.7580374 | 0.0000000 | 12.4437409 | -5.7525178 | 0.0000000 |
| H | 13.7632914 | -3.3626675 | 0.0000000 | 13.7459140 | -3.3557111 | 0.0000000 |
|  |  |  |  |  |  |  |
| **9O/**  **CAM-B3LYP** | **Ground state** | | | **Excited state** | | |
| C | -13.1492556 | 0.0000000 | -1.5175576 | -13.133486 | 0.0000000 | -1.5202581 |
| C | -12.7657053 | 0.0000000 | -0.2164060 | -12.746509 | 0.0000000 | -0.2173303 |
| O | -13.8552356 | 0.0000000 | 0.5908563 | -13.836756 | 0.0000000 | 0.5910701 |
| C | -14.9456823 | 0.0000000 | -0.2131271 | -14.927304 | 0.0000000 | -0.2122248 |
| C | -14.5745348 | 0.0000000 | -1.5097775 | -14.557088 | 0.0000000 | -1.5100870 |
| C | -11.4844984 | 0.0000000 | 0.4299121 | -11.468217 | 0.0000000 | 0.4235372 |
| O | -10.3920442 | 0.0000000 | -0.3756005 | -10.374882 | 0.0000000 | -0.3813969 |
| C | -9.2992320 | 0.0000000 | 0.4303891 | -9.2795987 | 0.0000000 | 0.4269043 |
| C | -9.6823613 | 0.0000000 | 1.7328057 | -9.6724961 | 0.0000000 | 1.7362118 |
| C | -11.1026601 | 0.0000000 | 1.7321321 | -11.084859 | 0.0000000 | 1.7307218 |
| C | -8.0208137 | 0.0000000 | -0.2161754 | -8.0094919 | 0.0000000 | -0.2024628 |
| O | -6.9278293 | 0.0000000 | 0.5891806 | -6.9143832 | 0.0000000 | 0.6045058 |
| C | -5.8351584 | 0.0000000 | -0.2169458 | -5.8162190 | 0.0000000 | -0.2050822 |
| C | -6.2185588 | 0.0000000 | -1.5195654 | -6.2169886 | 0.0000000 | -1.5231738 |
| C | -7.6382955 | 0.0000000 | -1.5190897 | -7.6186185 | 0.0000000 | -1.5169455 |
| C | -4.5567447 | 0.0000000 | 0.4290005 | -4.5538705 | 0.0000000 | 0.4090236 |
| O | -3.4639654 | 0.0000000 | -0.3767769 | -3.4565556 | 0.0000000 | -0.4014430 |
| C | -2.3711163 | 0.0000000 | 0.4290191 | -2.3560557 | 0.0000000 | 0.4096558 |
| C | -2.7541201 | 0.0000000 | 1.7318394 | -2.7626324 | 0.0000000 | 1.7363589 |
| C | -4.1737372 | 0.0000000 | 1.7318571 | -4.1535383 | 0.0000000 | 1.7319971 |
| C | -1.0928172 | 0.0000000 | -0.2170675 | -1.0999335 | 0.0000000 | -0.1937035 |
| O | 0.0000000 | 0.0000000 | 0.5887045 | 0.0000000 | 0.0000000 | 0.6184191 |
| C | 1.0928172 | 0.0000000 | -0.2170675 | 1.0999335 | 0.0000000 | -0.1937035 |
| C | 0.7098041 | 0.0000000 | -1.5199160 | 0.6930949 | 0.0000000 | -1.5224958 |
| C | -0.7098041 | 0.0000000 | -1.5199160 | -0.6930949 | 0.0000000 | -1.5224958 |
| C | 2.3711163 | 0.0000000 | 0.4290191 | 2.3560557 | 0.0000000 | 0.4096558 |
| O | 3.4639654 | 0.0000000 | -0.3767769 | 3.4565556 | 0.0000000 | -0.4014430 |
| C | 4.5567447 | 0.0000000 | 0.4290005 | 4.5538705 | 0.0000000 | 0.4090236 |
| C | 4.1737372 | 0.0000000 | 1.7318571 | 4.1535383 | 0.0000000 | 1.7319971 |
| C | 2.7541201 | 0.0000000 | 1.7318394 | 2.7626324 | 0.0000000 | 1.7363589 |
| C | 5.8351584 | 0.0000000 | -0.2169458 | 5.8162190 | 0.0000000 | -0.2050822 |
| C | 6.2185588 | 0.0000000 | -1.5195654 | 6.2169886 | 0.0000000 | -1.5231738 |
| C | 7.6382955 | 0.0000000 | -1.5190897 | 7.6186185 | 0.0000000 | -1.5169455 |
| C | 8.0208137 | 0.0000000 | -0.2161754 | 8.0094919 | 0.0000000 | -0.2024628 |
| O | 6.9278293 | 0.0000000 | 0.5891806 | 6.9143832 | 0.0000000 | 0.6045058 |
| C | 9.2992320 | 0.0000000 | 0.4303891 | 9.2795987 | 0.0000000 | 0.4269043 |
| O | 10.3920442 | 0.0000000 | -0.3756005 | 10.3748820 | 0.0000000 | -0.3813969 |
| C | 11.4844984 | 0.0000000 | 0.4299121 | 11.4682173 | 0.0000000 | 0.4235372 |
| C | 11.1026601 | 0.0000000 | 1.7321321 | 11.0848594 | 0.0000000 | 1.7307218 |
| C | 9.6823613 | 0.0000000 | 1.7328057 | 9.6724961 | 0.0000000 | 1.7362118 |
| H | -4.8314718 | 0.0000000 | 2.5822542 | -4.8147802 | 0.0000000 | 2.5800935 |
| H | -1.3674977 | 0.0000000 | -2.3703496 | -1.3528207 | 0.0000000 | -2.3717238 |
| H | 1.3674977 | 0.0000000 | -2.3703496 | 1.3528207 | 0.0000000 | -2.3717238 |
| H | -5.5611531 | 0.0000000 | -2.3702349 | -5.5612998 | 0.0000000 | -2.3753010 |
| H | -8.2963727 | 0.0000000 | -2.3692147 | -8.2803224 | 0.0000000 | -2.3645943 |
| H | 4.8314718 | 0.0000000 | 2.5822542 | 4.8147802 | 0.0000000 | 2.5800935 |
| H | 2.0964193 | 0.0000000 | 2.5822731 | 2.1051206 | 0.0000000 | 2.5871880 |
| H | -2.0964193 | 0.0000000 | 2.5822731 | -2.1051206 | 0.0000000 | 2.5871880 |
| H | 8.2963727 | 0.0000000 | -2.3692147 | 8.2803224 | 0.0000000 | -2.3645943 |
| H | 5.5611531 | 0.0000000 | -2.3702349 | 5.5612998 | 0.0000000 | -2.3753010 |
| H | 11.7615581 | 0.0000000 | 2.5816834 | 11.7466087 | 0.0000000 | 2.5782547 |
| C | 12.7657053 | 0.0000000 | -0.2164060 | 12.7465096 | 0.0000000 | -0.2173303 |
| H | 9.0249849 | 0.0000000 | 2.5835037 | 9.0172245 | 0.0000000 | 2.5885834 |
| H | -9.0249849 | 0.0000000 | 2.5835037 | -9.0172245 | 0.0000000 | 2.5885834 |
| H | -11.7615581 | 0.0000000 | 2.5816834 | -11.746608 | 0.0000000 | 2.5782547 |
| H | -12.4942248 | 0.0000000 | -2.3700000 | -12.479716 | 0.0000000 | -2.3736763 |
| H | -15.2319488 | 0.0000000 | -2.3611760 | -15.215916 | 0.0000000 | -2.3604733 |
| H | -15.8980783 | 0.0000000 | 0.2842218 | -15.879661 | 0.0000000 | 0.2853564 |
| O | 13.8552356 | 0.0000000 | 0.5908563 | 13.8367566 | 0.0000000 | 0.5910701 |
| C | 14.9456823 | 0.0000000 | -0.2131271 | 14.9273046 | 0.0000000 | -0.2122248 |
| C | 14.5745348 | 0.0000000 | -1.5097775 | 14.5570881 | 0.0000000 | -1.5100870 |
| C | 13.1492556 | 0.0000000 | -1.5175576 | 13.1334868 | 0.0000000 | -1.5202581 |
| H | 12.4942248 | 0.0000000 | -2.3700000 | 12.4797166 | 0.0000000 | -2.3736763 |
| H | 15.2319488 | 0.0000000 | -2.3611760 | 15.2159160 | 0.0000000 | -2.3604733 |
| H | 15.8980783 | 0.0000000 | 0.2842218 | 15.8796611 | 0.0000000 | 0.2853564 |

Part 8.

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| **2O/**  **tuned**  **CAM-**  **B3LYP** | **Ground state** | | | **Excited state** | | |
| C | -2.8154702 | 0.4351089 | 0.0000000 | -2.8019706 | 0.4462376 | 0.0000000 |
| C | -2.7949175 | -0.9216310 | 0.0000000 | -2.7737648 | -0.9352589 | 0.0000000 |
| C | -1.4203835 | -1.3041345 | 0.0000000 | -1.4359322 | -1.3314138 | 0.0000000 |
| C | -0.7024517 | -0.1437360 | 0.0000000 | -0.6765628 | -0.1298065 | 0.0000000 |
| C | 0.7024517 | 0.1437360 | 0.0000000 | 0.6765628 | 0.1298065 | 0.0000000 |
| C | 1.4203835 | 1.3041345 | 0.0000000 | 1.4359322 | 1.3314138 | 0.0000000 |
| C | 2.7949175 | 0.9216310 | 0.0000000 | 2.7737648 | 0.9352589 | 0.0000000 |
| C | 2.8154702 | -0.4351089 | 0.0000000 | 2.8019706 | -0.4462376 | 0.0000000 |
| O | -1.5451798 | 0.9288480 | 0.0000000 | -1.5366637 | 0.9685030 | 0.0000000 |
| O | 1.5451798 | -0.9288480 | 0.0000000 | 1.5366637 | -0.9685030 | 0.0000000 |
| H | -3.6046137 | 1.1700248 | 0.0000000 | -3.6080571 | 1.1641213 | 0.0000000 |
| H | -3.6556240 | -1.5737204 | 0.0000000 | -3.6456327 | -1.5737849 | 0.0000000 |
| H | -1.0086863 | -2.3019325 | 0.0000000 | -1.0224588 | -2.3282168 | 0.0000000 |
| H | 1.0086863 | 2.3019325 | 0.0000000 | 1.0224588 | 2.3282168 | 0.0000000 |
| H | 3.6556240 | 1.5737204 | 0.0000000 | 3.6456327 | 1.5737849 | 0.0000000 |
| H | 3.6046137 | -1.1700248 | 0.0000000 | 3.6080571 | -1.1641213 | 0.0000000 |
|  |  |  |  |  |  |  |
| **3O/**  **tuned**  **CAM-**  **B3LYP** | **Ground state** | | | **Excited state** | | |
| O | 3.4707821 | 0.0000000 | 0.8380634 | 3.4715436 | 0.0000000 | 0.8545795 |
| C | 4.5662467 | 0.0000000 | 0.0274333 | 4.5497382 | 0.0000000 | 0.0186253 |
| C | 4.1895810 | 0.0000000 | -1.2762584 | 4.1503801 | 0.0000000 | -1.2901229 |
| C | 2.7632162 | 0.0000000 | -1.2841166 | 2.7411388 | 0.0000000 | -1.2928738 |
| C | 2.3752233 | 0.0000000 | 0.0248869 | 2.3519124 | 0.0000000 | 0.0494479 |
| C | 1.0978822 | 0.0000000 | 0.6718883 | 1.1054495 | 0.0000000 | 0.6651984 |
| O | 0.0000000 | 0.0000000 | -0.1409397 | 0.0000000 | 0.0000000 | -0.1700297 |
| C | -1.0978822 | 0.0000000 | 0.6718883 | -1.1054495 | 0.0000000 | 0.6651984 |
| C | -0.7109240 | 0.0000000 | 1.9816205 | -0.6910643 | 0.0000000 | 2.0132531 |
| C | 0.7109240 | 0.0000000 | 1.9816205 | 0.6910643 | 0.0000000 | 2.0132531 |
| C | -2.3752233 | 0.0000000 | 0.0248869 | -2.3519124 | 0.0000000 | 0.0494479 |
| O | -3.4707821 | 0.0000000 | 0.8380634 | -3.4715436 | 0.0000000 | 0.8545795 |
| C | -4.5662467 | 0.0000000 | 0.0274333 | -4.5497382 | 0.0000000 | 0.0186253 |
| C | -4.1895810 | 0.0000000 | -1.2762584 | -4.1503801 | 0.0000000 | -1.2901229 |
| C | -2.7632162 | 0.0000000 | -1.2841166 | -2.7411388 | 0.0000000 | -1.2928738 |
| H | 5.5209718 | 0.0000000 | 0.5287736 | 5.5165809 | 0.0000000 | 0.4976519 |
| H | 4.8485878 | 0.0000000 | -2.1316616 | 4.8066139 | 0.0000000 | -2.1484555 |
| H | 2.1044003 | 0.0000000 | -2.1390823 | 2.0706056 | 0.0000000 | -2.1389224 |
| H | -2.1044003 | 0.0000000 | -2.1390823 | -2.0706056 | 0.0000000 | -2.1389224 |
| H | -5.5209718 | 0.0000000 | 0.5287736 | -5.5165809 | 0.0000000 | 0.4976519 |
| H | -4.8485878 | 0.0000000 | -2.1316616 | -4.8066139 | 0.0000000 | -2.1484555 |
| H | 1.3733693 | 0.0000000 | 2.8339253 | 1.3589157 | 0.0000000 | 2.8616355 |
| H | -1.3733693 | 0.0000000 | 2.8339253 | -1.3589157 | 0.0000000 | 2.8616355 |
|  |  |  |  |  |  |  |
| **4O/**  **tuned**  **CAM-**  **B3LYP** | **Ground state** | | | **Excited state** | | |
| O | -1.7690821 | 0.3501555 | 0.0000000 | -1.7690082 | 0.3843483 | 0.0000000 |
| C | -2.7988295 | -0.5473459 | 0.0000000 | -2.7991614 | -0.5294327 | 0.0000000 |
| C | -2.3090440 | -1.8224667 | 0.0000000 | -2.2867738 | -1.8271215 | 0.0000000 |
| C | -0.8921920 | -1.7100408 | 0.0000000 | -0.9019073 | -1.7234065 | 0.0000000 |
| C | -0.6097027 | -0.3729722 | 0.0000000 | -0.5974191 | -0.3497493 | 0.0000000 |
| C | 0.6097027 | 0.3729722 | 0.0000000 | 0.5974191 | 0.3497493 | 0.0000000 |
| O | 1.7690821 | -0.3501555 | 0.0000000 | 1.7690082 | -0.3843483 | 0.0000000 |
| C | 2.7988295 | 0.5473459 | 0.0000000 | 2.7991614 | 0.5294327 | 0.0000000 |
| C | 2.3090440 | 1.8224667 | 0.0000000 | 2.2867738 | 1.8271215 | 0.0000000 |
| C | 0.8921920 | 1.7100408 | 0.0000000 | 0.9019073 | 1.7234065 | 0.0000000 |
| C | 4.1234750 | 0.0043576 | 0.0000000 | 4.1045303 | 0.0146934 | 0.0000000 |
| O | 5.1506997 | 0.9023753 | 0.0000000 | 5.1416539 | 0.9148752 | 0.0000000 |
| C | 6.3072212 | 0.1816555 | 0.0000000 | 6.2935759 | 0.1868964 | 0.0000000 |
| C | 6.0357473 | -1.1479737 | 0.0000000 | 6.0179270 | -1.1485428 | 0.0000000 |
| C | 4.6146569 | -1.2696028 | 0.0000000 | 4.6078727 | -1.2752788 | 0.0000000 |
| H | -2.9019287 | -2.7245405 | 0.0000000 | -2.8854866 | -2.7259046 | 0.0000000 |
| H | -0.1649935 | -2.5077577 | 0.0000000 | -0.1720729 | -2.5189807 | 0.0000000 |
| H | 4.0262265 | -2.1744561 | 0.0000000 | 4.0186937 | -2.1797969 | 0.0000000 |
| H | 7.2189613 | 0.7574855 | 0.0000000 | 7.2098406 | 0.7563381 | 0.0000000 |
| H | 6.7608739 | -1.9480859 | 0.0000000 | 6.7467014 | -1.9459296 | 0.0000000 |
| H | 0.1649935 | 2.5077577 | 0.0000000 | 0.1720729 | 2.5189807 | 0.0000000 |
| H | 2.9019287 | 2.7245405 | 0.0000000 | 2.8854866 | 2.7259046 | 0.0000000 |
| C | -4.1234750 | -0.0043576 | 0.0000000 | -4.1045303 | -0.0146934 | 0.0000000 |
| O | -5.1506997 | -0.9023753 | 0.0000000 | -5.1416539 | -0.9148752 | 0.0000000 |
| C | -6.3072212 | -0.1816555 | 0.0000000 | -6.2935759 | -0.1868964 | 0.0000000 |
| C | -6.0357473 | 1.1479737 | 0.0000000 | -6.0179270 | 1.1485428 | 0.0000000 |
| C | -4.6146569 | 1.2696028 | 0.0000000 | -4.6078727 | 1.2752788 | 0.0000000 |
| H | -4.0262265 | 2.1744561 | 0.0000000 | -4.0186937 | 2.1797969 | 0.0000000 |
| H | -7.2189613 | -0.7574855 | 0.0000000 | -7.2098406 | -0.7563381 | 0.0000000 |
| H | -6.7608739 | 1.9480859 | 0.0000000 | -6.7467014 | 1.9459296 | 0.0000000 |
|  |  |  |  |  |  |  |
| **5O/**  **tuned**  **CAM-**  **B3LYP** | **Ground state** | | | **Excited state** | | |
| O | 3.4710422 | 0.0000000 | 0.2707202 | 3.4654277 | 0.0000000 | 0.2988331 |
| C | 4.5689731 | 0.0000000 | -0.5418495 | 4.5631949 | 0.0000000 | -0.5241846 |
| C | 4.1824026 | 0.0000000 | -1.8520395 | 4.1615705 | 0.0000000 | -1.8505340 |
| C | 2.7612279 | 0.0000000 | -1.8529812 | 2.7651473 | 0.0000000 | -1.8573093 |
| C | 2.3729664 | 0.0000000 | -0.5426147 | 2.3569592 | 0.0000000 | -0.5204547 |
| C | 1.0981990 | 0.0000000 | 0.1035594 | 1.1052136 | 0.0000000 | 0.0849574 |
| O | 0.0000000 | 0.0000000 | -0.7094230 | 0.0000000 | 0.0000000 | -0.7411551 |
| C | -1.0981990 | 0.0000000 | 0.1035594 | -1.1052136 | 0.0000000 | 0.0849574 |
| C | -0.7103693 | 0.0000000 | 1.4142401 | -0.6932107 | 0.0000000 | 1.4251692 |
| C | 0.7103693 | 0.0000000 | 1.4142401 | 0.6932107 | 0.0000000 | 1.4251692 |
| C | -2.3729664 | 0.0000000 | -0.5426147 | -2.3569592 | 0.0000000 | -0.5204547 |
| O | -3.4710422 | 0.0000000 | 0.2707202 | -3.4654277 | 0.0000000 | 0.2988331 |
| C | -4.5689731 | 0.0000000 | -0.5418495 | -4.5631949 | 0.0000000 | -0.5241846 |
| C | -4.1824026 | 0.0000000 | -1.8520395 | -4.1615705 | 0.0000000 | -1.8505340 |
| C | -2.7612279 | 0.0000000 | -1.8529812 | -2.7651473 | 0.0000000 | -1.8573093 |
| C | 5.8461784 | 0.0000000 | 0.1048052 | 5.8305848 | 0.0000000 | 0.0982548 |
| O | 6.9415563 | 0.0000000 | -0.7086790 | 6.9296368 | 0.0000000 | -0.7200675 |
| C | 8.0370516 | 0.0000000 | 0.1017226 | 8.0248446 | 0.0000000 | 0.0899814 |
| C | 7.6607149 | 0.0000000 | 1.4055750 | 7.6508120 | 0.0000000 | 1.3988074 |
| C | 6.2344849 | 0.0000000 | 1.4138063 | 6.2315819 | 0.0000000 | 1.4163449 |
| C | -5.8461784 | 0.0000000 | 0.1048052 | -5.8305848 | 0.0000000 | 0.0982548 |
| O | -6.9415563 | 0.0000000 | -0.7086790 | -6.9296368 | 0.0000000 | -0.7200675 |
| H | -4.8453235 | 0.0000000 | -2.7039640 | -4.8287759 | 0.0000000 | -2.6996967 |
| H | -2.1000405 | 0.0000000 | -2.7062161 | -2.1025502 | 0.0000000 | -2.7096643 |
| H | -1.3721298 | 0.0000000 | 2.2670215 | -1.3586127 | 0.0000000 | 2.2755084 |
| H | 1.3721298 | 0.0000000 | 2.2670215 | 1.3586127 | 0.0000000 | 2.2755084 |
| H | 2.1000405 | 0.0000000 | -2.7062161 | 2.1025502 | 0.0000000 | -2.7096643 |
| H | 4.8453235 | 0.0000000 | -2.7039640 | 4.8287759 | 0.0000000 | -2.6996967 |
| H | 5.5759900 | 0.0000000 | 2.2690235 | 5.5763947 | 0.0000000 | 2.2741849 |
| H | 8.3199230 | 0.0000000 | 2.2608089 | 8.3157867 | 0.0000000 | 2.2499539 |
| C | -8.0370516 | 0.0000000 | 0.1017226 | -8.0248446 | 0.0000000 | 0.0899814 |
| C | -7.6607149 | 0.0000000 | 1.4055750 | -7.6508120 | 0.0000000 | 1.3988074 |
| C | -6.2344849 | 0.0000000 | 1.4138063 | -6.2315819 | 0.0000000 | 1.4163449 |
| H | -5.5759900 | 0.0000000 | 2.2690235 | -5.5763947 | 0.0000000 | 2.2741849 |
| H | -8.9917087 | 0.0000000 | -0.3997589 | -8.9800930 | 0.0000000 | -0.4110383 |
| H | -8.3199230 | 0.0000000 | 2.2608089 | -8.3157867 | 0.0000000 | 2.2499539 |
| H | 8.9917087 | 0.0000000 | -0.3997589 | 8.9800930 | 0.0000000 | -0.4110383 |
|  |  |  |  |  |  |  |
| **6O/**  **tuned**  **CAM-**  **B3LYP** | **Ground state** | | | **Excited state** | | |
| O | 1.8033412 | -0.0110325 | 0.0000000 | 1.8090104 | 0.0188916 | 0.0000000 |
| C | 0.5225420 | -0.4872248 | 0.0000000 | 0.5175202 | -0.4636064 | 0.0000000 |
| C | 0.5313049 | -1.8541485 | 0.0000000 | 0.5405713 | -1.8635146 | 0.0000000 |
| C | 1.8960825 | -2.2484966 | 0.0000000 | 1.8767395 | -2.2466586 | 0.0000000 |
| C | 2.6325786 | -1.0969337 | 0.0000000 | 2.6393063 | -1.0785852 | 0.0000000 |
| C | 4.0366243 | -0.8302811 | 0.0000000 | 4.0169831 | -0.8406356 | 0.0000000 |
| O | 4.8655232 | -1.9166643 | 0.0000000 | 4.8515658 | -1.9336660 | 0.0000000 |
| C | 6.1459333 | -1.4411086 | 0.0000000 | 6.1338461 | -1.4533313 | 0.0000000 |
| C | 6.1385895 | -0.0750701 | 0.0000000 | 6.1213124 | -0.0735283 | 0.0000000 |
| C | 4.7736520 | 0.3206446 | 0.0000000 | 4.7760240 | 0.3235495 | 0.0000000 |
| H | 7.0120944 | 0.5591404 | 0.0000000 | 6.9982843 | 0.5565473 | 0.0000000 |
| H | 2.2950824 | -3.2514682 | 0.0000000 | 2.2799114 | -3.2483626 | 0.0000000 |
| H | -0.3411242 | -2.4897900 | 0.0000000 | -0.3335775 | -2.4971854 | 0.0000000 |
| C | 7.1932387 | -2.4170962 | 0.0000000 | 7.1792323 | -2.4112185 | 0.0000000 |
| O | 8.4714639 | -1.9398770 | 0.0000000 | 8.4605673 | -1.9309531 | 0.0000000 |
| C | 9.2987189 | -3.0226769 | 0.0000000 | 9.2883435 | -3.0127339 | 0.0000000 |
| C | 8.5750251 | -4.1706962 | 0.0000000 | 8.5659768 | -4.1648581 | 0.0000000 |
| C | 7.2026503 | -3.7824425 | 0.0000000 | 7.1962123 | -3.7847324 | 0.0000000 |
| H | 6.3325290 | -4.4211159 | 0.0000000 | 6.3282891 | -4.4264478 | 0.0000000 |
| H | 10.3551087 | -2.8061201 | 0.0000000 | 10.3449002 | -2.7958906 | 0.0000000 |
| H | 8.9707289 | -5.1753821 | 0.0000000 | 8.9667325 | -5.1677711 | 0.0000000 |
| C | -0.5225420 | 0.4872248 | 0.0000000 | -0.5175202 | 0.4636064 | 0.0000000 |
| O | -1.8033412 | 0.0110325 | 0.0000000 | -1.8090104 | -0.0188916 | 0.0000000 |
| C | -2.6325786 | 1.0969337 | 0.0000000 | -2.6393063 | 1.0785852 | 0.0000000 |
| C | -1.8960825 | 2.2484966 | 0.0000000 | -1.8767395 | 2.2466586 | 0.0000000 |
| C | -0.5313049 | 1.8541485 | 0.0000000 | -0.5405713 | 1.8635146 | 0.0000000 |
| H | -2.2950824 | 3.2514682 | 0.0000000 | -2.2799114 | 3.2483626 | 0.0000000 |
| H | 0.3411242 | 2.4897900 | 0.0000000 | 0.3335775 | 2.4971854 | 0.0000000 |
| H | 4.3755703 | 1.3239958 | 0.0000000 | 4.3788197 | 1.3273836 | 0.0000000 |
| C | -4.0366243 | 0.8302811 | 0.0000000 | -4.0169831 | 0.8406356 | 0.0000000 |
| C | -4.7736520 | -0.3206446 | 0.0000000 | -4.7760240 | -0.3235495 | 0.0000000 |
| C | -6.1385895 | 0.0750701 | 0.0000000 | -6.1213124 | 0.0735283 | 0.0000000 |
| C | -6.1459333 | 1.4411086 | 0.0000000 | -6.1338461 | 1.4533313 | 0.0000000 |
| O | -4.8655232 | 1.9166643 | 0.0000000 | -4.8515658 | 1.9336660 | 0.0000000 |
| H | -7.0120944 | -0.5591404 | 0.0000000 | -6.9982843 | -0.5565473 | 0.0000000 |
| H | -4.3755703 | -1.3239958 | 0.0000000 | -4.3788197 | -1.3273836 | 0.0000000 |
| C | -7.1932387 | 2.4170962 | 0.0000000 | -7.1792323 | 2.4112185 | 0.0000000 |
| C | -7.2026503 | 3.7824425 | 0.0000000 | -7.1962123 | 3.7847324 | 0.0000000 |
| C | -8.5750251 | 4.1706962 | 0.0000000 | -8.5659768 | 4.1648581 | 0.0000000 |
| C | -9.2987189 | 3.0226769 | 0.0000000 | -9.2883435 | 3.0127339 | 0.0000000 |
| O | -8.4714639 | 1.9398770 | 0.0000000 | -8.4605673 | 1.9309531 | 0.0000000 |
| H | -8.9707289 | 5.1753821 | 0.0000000 | -8.9667325 | 5.1677711 | 0.0000000 |
| H | -10.3551087 | 2.8061201 | 0.0000000 | -10.344900 | 2.7958906 | 0.0000000 |
| H | -6.3325290 | 4.4211159 | 0.0000000 | -6.3282891 | 4.4264478 | 0.0000000 |
|  |  |  |  |  |  |  |
| **7O/**  **tuned**  **CAM-**  **B3LYP** | **Ground state** | | | **Excited state** | | |
| C | -9.7053444 | 0.0000000 | -1.4892442 | -9.6966289 | 0.0000000 | -1.4940902 |
| C | -9.3169604 | 0.0000000 | -0.1802740 | -9.3018199 | 0.0000000 | -0.1811149 |
| O | -10.4122600 | 0.0000000 | 0.6333064 | -10.398847 | 0.0000000 | 0.6348066 |
| C | -11.5077836 | 0.0000000 | -0.1770166 | -11.494292 | 0.0000000 | -0.1748571 |
| C | -11.1315580 | 0.0000000 | -1.4809079 | -11.119503 | 0.0000000 | -1.4811643 |
| C | -8.0397441 | 0.0000000 | 0.4663467 | -8.0298247 | 0.0000000 | 0.4542509 |
| O | -6.9418382 | 0.0000000 | -0.3461614 | -6.9308930 | 0.0000000 | -0.3601331 |
| C | -5.8437997 | 0.0000000 | 0.4672511 | -5.8280598 | 0.0000000 | 0.4576474 |
| C | -6.2321223 | 0.0000000 | 1.7776012 | -6.2313168 | 0.0000000 | 1.7812491 |
| C | -7.6532560 | 0.0000000 | 1.7765989 | -7.6386748 | 0.0000000 | 1.7733839 |
| C | -4.5690830 | 0.0000000 | -0.1789133 | -4.5662175 | 0.0000000 | -0.1601390 |
| O | -3.4708546 | 0.0000000 | 0.6338640 | -3.4652480 | 0.0000000 | 0.6604551 |
| C | -2.3727520 | 0.0000000 | -0.1794098 | -2.3591619 | 0.0000000 | -0.1591133 |
| C | -2.7609170 | 0.0000000 | -1.4900958 | -2.7676267 | 0.0000000 | -1.4931173 |
| C | -4.1815041 | 0.0000000 | -1.4897809 | -4.1626734 | 0.0000000 | -1.4888007 |
| C | -1.0981638 | 0.0000000 | 0.4663893 | -1.1046577 | 0.0000000 | 0.4472090 |
| O | 0.0000000 | 0.0000000 | -0.3466884 | 0.0000000 | 0.0000000 | -0.3751125 |
| C | 1.0981638 | 0.0000000 | 0.4663893 | 1.1046577 | 0.0000000 | 0.4472090 |
| C | 0.7102448 | 0.0000000 | 1.7772236 | 0.6948308 | 0.0000000 | 1.7831200 |
| C | -0.7102448 | 0.0000000 | 1.7772236 | -0.6948308 | 0.0000000 | 1.7831200 |
| C | 2.3727520 | 0.0000000 | -0.1794098 | 2.3591619 | 0.0000000 | -0.1591133 |
| O | 3.4708546 | 0.0000000 | 0.6338640 | 3.4652480 | 0.0000000 | 0.6604551 |
| C | 4.5690830 | 0.0000000 | -0.1789133 | 4.5662175 | 0.0000000 | -0.1601390 |
| C | 4.1815041 | 0.0000000 | -1.4897809 | 4.1626734 | 0.0000000 | -1.4888007 |
| C | 2.7609170 | 0.0000000 | -1.4900958 | 2.7676267 | 0.0000000 | -1.4931173 |
| C | 5.8437997 | 0.0000000 | 0.4672511 | 5.8280598 | 0.0000000 | 0.4576474 |
| O | 6.9418382 | 0.0000000 | -0.3461614 | 6.9308930 | 0.0000000 | -0.3601331 |
| C | 8.0397441 | 0.0000000 | 0.4663467 | 8.0298247 | 0.0000000 | 0.4542509 |
| C | 7.6532560 | 0.0000000 | 1.7765989 | 7.6386748 | 0.0000000 | 1.7733839 |
| C | 6.2321223 | 0.0000000 | 1.7776012 | 6.2313168 | 0.0000000 | 1.7812491 |
| C | 9.3169604 | 0.0000000 | -0.1802740 | 9.3018199 | 0.0000000 | -0.1811149 |
| C | 9.7053444 | 0.0000000 | -1.4892442 | 9.6966289 | 0.0000000 | -1.4940902 |
| C | 11.1315580 | 0.0000000 | -1.4809079 | 11.1195034 | 0.0000000 | -1.4811643 |
| C | 11.5077836 | 0.0000000 | -0.1770166 | 11.4942927 | 0.0000000 | -0.1748571 |
| O | 10.4122600 | 0.0000000 | 0.6333064 | 10.3988475 | 0.0000000 | 0.6348066 |
| H | -1.3719010 | 0.0000000 | 2.6300851 | -1.3591886 | 0.0000000 | 2.6342531 |
| H | 2.0994619 | 0.0000000 | -2.3431214 | 2.1052072 | 0.0000000 | -2.3456211 |
| H | 4.8434188 | 0.0000000 | -2.3424322 | 4.8281046 | 0.0000000 | -2.3391773 |
| H | -2.0994619 | 0.0000000 | -2.3431214 | -2.1052072 | 0.0000000 | -2.3456211 |
| H | -4.8434188 | 0.0000000 | -2.3424322 | -4.8281046 | 0.0000000 | -2.3391773 |
| H | 8.3162086 | 0.0000000 | 2.6284924 | 8.3060176 | 0.0000000 | 2.6222333 |
| H | 5.5710343 | 0.0000000 | 2.6309171 | 5.5720971 | 0.0000000 | 2.6361191 |
| H | 1.3719010 | 0.0000000 | 2.6300851 | 1.3591886 | 0.0000000 | 2.6342531 |
| H | 11.7908100 | 0.0000000 | -2.3361035 | 11.7816005 | 0.0000000 | -2.3343518 |
| H | 9.0469457 | 0.0000000 | -2.3445377 | 9.0401981 | 0.0000000 | -2.3509169 |
| H | -5.5710343 | 0.0000000 | 2.6309171 | -5.5720971 | 0.0000000 | 2.6361191 |
| H | -8.3162086 | 0.0000000 | 2.6284924 | -8.3060176 | 0.0000000 | 2.6222333 |
| H | -9.0469457 | 0.0000000 | -2.3445377 | -9.0401981 | 0.0000000 | -2.3509169 |
| H | -11.7908100 | 0.0000000 | -2.3361035 | -11.781600 | 0.0000000 | -2.3343518 |
| H | -12.4623931 | 0.0000000 | 0.3245602 | -12.449084 | 0.0000000 | 0.3267186 |
| H | 12.4623931 | 0.0000000 | 0.3245602 | 12.4490842 | 0.0000000 | 0.3267186 |
|  |  |  |  |  |  |  |
| **8O/**  **tuned**  **CAM-**  **B3LYP** | **Ground state** | | | **Excited state** | | |
| O | -11.8862147 | 2.5556973 | 0.0000000 | -11.872693 | 2.5502642 | 0.0000000 |
| C | -10.6226283 | 3.0702730 | 0.0000000 | -10.607592 | 3.0665140 | 0.0000000 |
| C | -10.6721424 | 4.4346926 | 0.0000000 | -10.661286 | 4.4348334 | 0.0000000 |
| C | -12.0553345 | 4.7824708 | 0.0000000 | -12.043076 | 4.7784274 | 0.0000000 |
| C | -12.7449218 | 3.6136878 | 0.0000000 | -12.731770 | 3.6074896 | 0.0000000 |
| C | -9.5470433 | 2.1255189 | 0.0000000 | -9.5335873 | 2.1306002 | 0.0000000 |
| C | -9.4996092 | 0.7603174 | 0.0000000 | -9.4848876 | 0.7582708 | 0.0000000 |
| C | -8.1236239 | 0.4048686 | 0.0000000 | -8.1202331 | 0.4000554 | 0.0000000 |
| C | -7.4207065 | 1.5768495 | 0.0000000 | -7.4036988 | 1.5785094 | 0.0000000 |
| O | -8.2811603 | 2.6384285 | 0.0000000 | -8.2667538 | 2.6441569 | 0.0000000 |
| C | -6.0249654 | 1.8844156 | 0.0000000 | -6.0230805 | 1.8677197 | 0.0000000 |
| O | -5.1642559 | 0.8233795 | 0.0000000 | -5.1612507 | 0.8015427 | 0.0000000 |
| C | -3.8979799 | 1.3369657 | 0.0000000 | -3.8875584 | 1.3186255 | 0.0000000 |
| C | -3.9468446 | 2.7029782 | 0.0000000 | -3.9493401 | 2.7070328 | 0.0000000 |
| C | -5.3226529 | 3.0571144 | 0.0000000 | -5.3063710 | 3.0511181 | 0.0000000 |
| C | -2.8246366 | 0.3937289 | 0.0000000 | -2.8217687 | 0.4130135 | 0.0000000 |
| O | -1.5584817 | 0.9073099 | 0.0000000 | -1.5489009 | 0.9330677 | 0.0000000 |
| C | -0.6976814 | -0.1538294 | 0.0000000 | -0.6831294 | -0.1370822 | 0.0000000 |
| C | -1.4000867 | -1.3265340 | 0.0000000 | -1.4120704 | -1.3275136 | 0.0000000 |
| C | -2.7758010 | -0.9723993 | 0.0000000 | -2.7598382 | -0.9785274 | 0.0000000 |
| C | 0.6976814 | 0.1538294 | 0.0000000 | 0.6831294 | 0.1370822 | 0.0000000 |
| O | 1.5584817 | -0.9073099 | 0.0000000 | 1.5489009 | -0.9330677 | 0.0000000 |
| C | 2.8246366 | -0.3937289 | 0.0000000 | 2.8217687 | -0.4130135 | 0.0000000 |
| C | 2.7758010 | 0.9723993 | 0.0000000 | 2.7598382 | 0.9785274 | 0.0000000 |
| C | 1.4000867 | 1.3265340 | 0.0000000 | 1.4120704 | 1.3275136 | 0.0000000 |
| C | 3.8979799 | -1.3369657 | 0.0000000 | 3.8875584 | -1.3186255 | 0.0000000 |
| O | 5.1642559 | -0.8233795 | 0.0000000 | 5.1612507 | -0.8015427 | 0.0000000 |
| C | 6.0249654 | -1.8844156 | 0.0000000 | 6.0230805 | -1.8677197 | 0.0000000 |
| C | 5.3226529 | -3.0571144 | 0.0000000 | 5.3063710 | -3.0511181 | 0.0000000 |
| C | 3.9468446 | -2.7029782 | 0.0000000 | 3.9493401 | -2.7070328 | 0.0000000 |
| H | 3.6294559 | 1.6330046 | 0.0000000 | 3.6156494 | 1.6368833 | 0.0000000 |
| H | -0.9715678 | -2.3172518 | 0.0000000 | -0.9821046 | -2.3178656 | 0.0000000 |
| H | -3.6294559 | -1.6330046 | 0.0000000 | -3.6156494 | -1.6368833 | 0.0000000 |
| H | 3.0932151 | -3.3636283 | 0.0000000 | 3.0962487 | -3.3686232 | 0.0000000 |
| C | 7.4207065 | -1.5768495 | 0.0000000 | 7.4036988 | -1.5785094 | 0.0000000 |
| H | 5.7512577 | -4.0477817 | 0.0000000 | 5.7388515 | -4.0404628 | 0.0000000 |
| H | -5.7512577 | 4.0477817 | 0.0000000 | -5.7388515 | 4.0404628 | 0.0000000 |
| H | -3.0932151 | 3.3636283 | 0.0000000 | -3.0962487 | 3.3686232 | 0.0000000 |
| H | 0.9715678 | 2.3172518 | 0.0000000 | 0.9821046 | 2.3178656 | 0.0000000 |
| H | -10.3542000 | 0.1008914 | 0.0000000 | -10.342148 | 0.1018907 | 0.0000000 |
| H | -7.6960294 | -0.5862412 | 0.0000000 | -7.6949696 | -0.5921461 | 0.0000000 |
| H | -12.4804415 | 5.7750477 | 0.0000000 | -12.470723 | 5.7700519 | 0.0000000 |
| H | -13.7944961 | 3.3661990 | 0.0000000 | -13.781383 | 3.3596466 | 0.0000000 |
| H | -9.8209998 | 5.0984068 | 0.0000000 | -9.8116472 | 5.1005254 | 0.0000000 |
| O | 8.2811603 | -2.6384285 | 0.0000000 | 8.2667538 | -2.6441569 | 0.0000000 |
| C | 9.5470433 | -2.1255189 | 0.0000000 | 9.5335873 | -2.1306002 | 0.0000000 |
| C | 9.4996092 | -0.7603174 | 0.0000000 | 9.4848876 | -0.7582708 | 0.0000000 |
| C | 8.1236239 | -0.4048686 | 0.0000000 | 8.1202331 | -0.4000554 | 0.0000000 |
| H | 7.6960294 | 0.5862412 | 0.0000000 | 7.6949696 | 0.5921461 | 0.0000000 |
| H | 10.3542000 | -0.1008914 | 0.0000000 | 10.3421484 | -0.1018907 | 0.0000000 |
| C | 10.6226283 | -3.0702730 | 0.0000000 | 10.6075928 | -3.0665140 | 0.0000000 |
| O | 11.8862147 | -2.5556973 | 0.0000000 | 11.8726933 | -2.5502642 | 0.0000000 |
| C | 12.7449218 | -3.6136878 | 0.0000000 | 12.7317700 | -3.6074896 | 0.0000000 |
| C | 12.0553345 | -4.7824708 | 0.0000000 | 12.0430768 | -4.7784274 | 0.0000000 |
| C | 10.6721424 | -4.4346926 | 0.0000000 | 10.6612864 | -4.4348334 | 0.0000000 |
| H | 9.8209998 | -5.0984068 | 0.0000000 | 9.8116472 | -5.1005254 | 0.0000000 |
| H | 12.4804415 | -5.7750477 | 0.0000000 | 12.4707239 | -5.7700519 | 0.0000000 |
| H | 13.7944961 | -3.3661990 | 0.0000000 | 13.7813835 | -3.3596466 | 0.0000000 |
|  |  |  |  |  |  |  |
| **9O/**  **tuned**  **CAM-**  **B3LYP** | **Ground state** | | | **Excited state** | | |
| C | -13.1761832 | 0.0000000 | -1.5255997 | -13.164501 | 0.0000000 | -1.5282725 |
| C | -12.7877059 | 0.0000000 | -0.2166575 | -12.772385 | 0.0000000 | -0.2174040 |
| O | -13.8829278 | 0.0000000 | 0.5970090 | -13.868346 | 0.0000000 | 0.5976870 |
| C | -14.9785043 | 0.0000000 | -0.2132261 | -14.964018 | 0.0000000 | -0.2118929 |
| C | -14.6023860 | 0.0000000 | -1.5171499 | -14.588957 | 0.0000000 | -1.5171610 |
| C | -11.5104444 | 0.0000000 | 0.4298666 | -11.497880 | 0.0000000 | 0.4232402 |
| O | -10.4125884 | 0.0000000 | -0.3826733 | -10.399320 | 0.0000000 | -0.3894667 |
| C | -9.3145279 | 0.0000000 | 0.4307095 | -9.2987277 | 0.0000000 | 0.4265390 |
| C | -9.7028019 | 0.0000000 | 1.7410705 | -9.6961147 | 0.0000000 | 1.7438624 |
| C | -11.1239174 | 0.0000000 | 1.7401208 | -11.109548 | 0.0000000 | 1.7384193 |
| C | -8.0398472 | 0.0000000 | -0.2155107 | -8.0315081 | 0.0000000 | -0.2029709 |
| O | -6.9415788 | 0.0000000 | 0.5971589 | -6.9314923 | 0.0000000 | 0.6127125 |
| C | -5.8435545 | 0.0000000 | -0.2162377 | -5.8283400 | 0.0000000 | -0.2046405 |
| C | -6.2318374 | 0.0000000 | -1.5268805 | -6.2315649 | 0.0000000 | -1.5296621 |
| C | -7.6523970 | 0.0000000 | -1.5264398 | -7.6357781 | 0.0000000 | -1.5245982 |
| C | -4.5689422 | 0.0000000 | 0.4294825 | -4.5673023 | 0.0000000 | 0.4123613 |
| O | -3.4708129 | 0.0000000 | -0.3835415 | -3.4653618 | 0.0000000 | -0.4066742 |
| C | -2.3726697 | 0.0000000 | 0.4296000 | -2.3606348 | 0.0000000 | 0.4124932 |
| C | -2.7606439 | 0.0000000 | 1.7404228 | -2.7681481 | 0.0000000 | 1.7440895 |
| C | -4.1810809 | 0.0000000 | 1.7403806 | -4.1640223 | 0.0000000 | 1.7408522 |
| C | -1.0981359 | 0.0000000 | -0.2161812 | -1.1040765 | 0.0000000 | -0.1962448 |
| O | 0.0000000 | 0.0000000 | 0.5968879 | 0.0000000 | 0.0000000 | 0.6240912 |
| C | 1.0981359 | 0.0000000 | -0.2161812 | 1.1040765 | 0.0000000 | -0.1962448 |
| C | 0.7102114 | 0.0000000 | -1.5270562 | 0.6962035 | 0.0000000 | -1.5292018 |
| C | -0.7102114 | 0.0000000 | -1.5270562 | -0.6962035 | 0.0000000 | -1.5292018 |
| C | 2.3726697 | 0.0000000 | 0.4296000 | 2.3606348 | 0.0000000 | 0.4124932 |
| O | 3.4708129 | 0.0000000 | -0.3835415 | 3.4653618 | 0.0000000 | -0.4066742 |
| C | 4.5689422 | 0.0000000 | 0.4294825 | 4.5673023 | 0.0000000 | 0.4123613 |
| C | 4.1810809 | 0.0000000 | 1.7403806 | 4.1640223 | 0.0000000 | 1.7408522 |
| C | 2.7606439 | 0.0000000 | 1.7404228 | 2.7681481 | 0.0000000 | 1.7440895 |
| C | 5.8435545 | 0.0000000 | -0.2162377 | 5.8283400 | 0.0000000 | -0.2046405 |
| C | 6.2318374 | 0.0000000 | -1.5268805 | 6.2315649 | 0.0000000 | -1.5296621 |
| C | 7.6523970 | 0.0000000 | -1.5264398 | 7.6357781 | 0.0000000 | -1.5245982 |
| C | 8.0398472 | 0.0000000 | -0.2155107 | 8.0315081 | 0.0000000 | -0.2029709 |
| O | 6.9415788 | 0.0000000 | 0.5971589 | 6.9314923 | 0.0000000 | 0.6127125 |
| C | 9.3145279 | 0.0000000 | 0.4307095 | 9.2987277 | 0.0000000 | 0.4265390 |
| O | 10.4125884 | 0.0000000 | -0.3826733 | 10.3993200 | 0.0000000 | -0.3894667 |
| C | 11.5104444 | 0.0000000 | 0.4298666 | 11.4978808 | 0.0000000 | 0.4232402 |
| C | 11.1239174 | 0.0000000 | 1.7401208 | 11.1095482 | 0.0000000 | 1.7384193 |
| C | 9.7028019 | 0.0000000 | 1.7410705 | 9.6961147 | 0.0000000 | 1.7438624 |
| H | -4.8427771 | 0.0000000 | 2.5932052 | -4.8288256 | 0.0000000 | 2.5916554 |
| H | -1.3718527 | 0.0000000 | -2.3799284 | -1.3600183 | 0.0000000 | -2.3807254 |
| H | 1.3718527 | 0.0000000 | -2.3799284 | 1.3600183 | 0.0000000 | -2.3807254 |
| H | -5.5704771 | 0.0000000 | -2.3799839 | -5.5710171 | 0.0000000 | -2.3835229 |
| H | -8.3143995 | 0.0000000 | -2.3790197 | -8.3009741 | 0.0000000 | -2.3750349 |
| H | 4.8427771 | 0.0000000 | 2.5932052 | 4.8288256 | 0.0000000 | 2.5916554 |
| H | 2.0990581 | 0.0000000 | 2.5933443 | 2.1059278 | 0.0000000 | 2.5967512 |
| H | -2.0990581 | 0.0000000 | 2.5933443 | -2.1059278 | 0.0000000 | 2.5967512 |
| H | 8.3143995 | 0.0000000 | -2.3790197 | 8.3009741 | 0.0000000 | -2.3750349 |
| H | 5.5704771 | 0.0000000 | -2.3799839 | 5.5710171 | 0.0000000 | -2.3835229 |
| H | 11.7868488 | 0.0000000 | 2.5920293 | 11.7752848 | 0.0000000 | 2.5883640 |
| C | 12.7877059 | 0.0000000 | -0.2166575 | 12.7723857 | 0.0000000 | -0.2174040 |
| H | 9.0416941 | 0.0000000 | 2.5943734 | 9.0366609 | 0.0000000 | 2.5984965 |
| H | -9.0416941 | 0.0000000 | 2.5943734 | -9.0366609 | 0.0000000 | 2.5984965 |
| H | -11.7868488 | 0.0000000 | 2.5920293 | -11.775284 | 0.0000000 | 2.5883640 |
| H | -12.5178633 | 0.0000000 | -2.3809546 | -12.507468 | 0.0000000 | -2.3846249 |
| H | -15.2617026 | 0.0000000 | -2.3722946 | -15.249918 | 0.0000000 | -2.3711366 |
| H | -15.9330788 | 0.0000000 | 0.2884173 | -15.918581 | 0.0000000 | 0.2899648 |
| O | 13.8829278 | 0.0000000 | 0.5970090 | 13.8683469 | 0.0000000 | 0.5976870 |
| C | 14.9785043 | 0.0000000 | -0.2132261 | 14.9640180 | 0.0000000 | -0.2118929 |
| C | 14.6023860 | 0.0000000 | -1.5171499 | 14.5889577 | 0.0000000 | -1.5171610 |
| C | 13.1761832 | 0.0000000 | -1.5255997 | 13.1645010 | 0.0000000 | -1.5282725 |
| H | 12.5178633 | 0.0000000 | -2.3809546 | 12.5074685 | 0.0000000 | -2.3846249 |
| H | 15.2617026 | 0.0000000 | -2.3722946 | 15.2499189 | 0.0000000 | -2.3711366 |
| H | 15.9330788 | 0.0000000 | 0.2884173 | 15.9185817 | 0.0000000 | 0.2899648 |

Part 9.

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| **2O/**  **ωB97X** | **Ground state** | | | **Excited state** | | |
| C | -2.8067887 | 0.4318525 | 0.0000000 | -2.7891546 | 0.4436938 | 0.0000000 |
| C | -2.7922279 | -0.9176872 | 0.0000000 | -2.7662993 | -0.9326693 | 0.0000000 |
| C | -1.4153695 | -1.3002742 | 0.0000000 | -1.4330497 | -1.3292765 | 0.0000000 |
| C | -0.7077119 | -0.1442062 | 0.0000000 | -0.6743198 | -0.1260607 | 0.0000000 |
| C | 0.7077119 | 0.1442062 | 0.0000000 | 0.6743198 | 0.1260607 | 0.0000000 |
| C | 1.4153695 | 1.3002742 | 0.0000000 | 1.4330497 | 1.3292765 | 0.0000000 |
| C | 2.7922279 | 0.9176872 | 0.0000000 | 2.7662993 | 0.9326693 | 0.0000000 |
| C | 2.8067887 | -0.4318525 | 0.0000000 | 2.7891546 | -0.4436938 | 0.0000000 |
| O | -1.5435821 | 0.9213667 | 0.0000000 | -1.5331691 | 0.9606076 | 0.0000000 |
| O | 1.5435821 | -0.9213667 | 0.0000000 | 1.5331691 | -0.9606076 | 0.0000000 |
| H | -3.5952348 | 1.1644547 | 0.0000000 | -3.5952566 | 1.1583279 | 0.0000000 |
| H | -3.6523890 | -1.5660668 | 0.0000000 | -3.6382771 | -1.5664786 | 0.0000000 |
| H | -1.0029248 | -2.2949731 | 0.0000000 | -1.0201807 | -2.3236109 | 0.0000000 |
| H | 1.0029248 | 2.2949731 | 0.0000000 | 1.0201807 | 2.3236109 | 0.0000000 |
| H | 3.6523890 | 1.5660668 | 0.0000000 | 3.6382771 | 1.5664786 | 0.0000000 |
| H | 3.5952348 | -1.1644547 | 0.0000000 | 3.5952566 | -1.1583279 | 0.0000000 |
|  |  |  |  |  |  |  |
| **3O/**  **ωB97X** | **Ground state** | | | **Excited state** | | |
| O | 3.4645687 | 0.0000000 | 0.8302645 | 3.4585995 | 0.0000000 | 0.8493106 |
| C | 4.5540662 | 0.0000000 | 0.0252049 | 4.5351334 | 0.0000000 | 0.0268878 |
| C | 4.1845202 | 0.0000000 | -1.2729024 | 4.1511706 | 0.0000000 | -1.2792162 |
| C | 2.7557625 | 0.0000000 | -1.2795006 | 2.7420465 | 0.0000000 | -1.2904539 |
| C | 2.3773291 | 0.0000000 | 0.0225505 | 2.3499357 | 0.0000000 | 0.0453520 |
| C | 1.0901608 | 0.0000000 | 0.6743712 | 1.0995348 | 0.0000000 | 0.6513529 |
| O | 0.0000000 | 0.0000000 | -0.1324390 | 0.0000000 | 0.0000000 | -0.1754311 |
| C | -1.0901608 | 0.0000000 | 0.6743712 | -1.0995348 | 0.0000000 | 0.6513529 |
| C | -0.7126512 | 0.0000000 | 1.9767866 | -0.6866359 | 0.0000000 | 2.0013878 |
| C | 0.7126512 | 0.0000000 | 1.9767866 | 0.6866359 | 0.0000000 | 2.0013878 |
| C | -2.3773291 | 0.0000000 | 0.0225505 | -2.3499357 | 0.0000000 | 0.0453520 |
| O | -3.4645687 | 0.0000000 | 0.8302645 | -3.4585995 | 0.0000000 | 0.8493106 |
| C | -4.5540662 | 0.0000000 | 0.0252049 | -4.5351334 | 0.0000000 | 0.0268878 |
| C | -4.1845202 | 0.0000000 | -1.2729024 | -4.1511706 | 0.0000000 | -1.2792162 |
| C | -2.7557625 | 0.0000000 | -1.2795006 | -2.7420465 | 0.0000000 | -1.2904539 |
| H | 5.5076838 | 0.0000000 | 0.5241371 | 5.4978850 | 0.0000000 | 0.5093632 |
| H | 4.8435894 | 0.0000000 | -2.1248789 | 4.8131297 | 0.0000000 | -2.1296731 |
| H | 2.0965433 | 0.0000000 | -2.1309087 | 2.0775186 | 0.0000000 | -2.1380215 |
| H | -2.0965433 | 0.0000000 | -2.1309087 | -2.0775186 | 0.0000000 | -2.1380215 |
| H | -5.5076838 | 0.0000000 | 0.5241371 | -5.4978850 | 0.0000000 | 0.5093632 |
| H | -4.8435894 | 0.0000000 | -2.1248789 | -4.8131297 | 0.0000000 | -2.1296731 |
| H | 1.3746510 | 0.0000000 | 2.8260975 | 1.3546637 | 0.0000000 | 2.8464282 |
| H | -1.3746510 | 0.0000000 | 2.8260975 | -1.3546637 | 0.0000000 | 2.8464282 |
|  |  |  |  |  |  |  |
| **4O/**  **ωB97X** | **Ground state** | | | **Excited state** | | |
| O | -1.7655283 | 0.3407221 | 0.0000000 | -1.7636007 | 0.3818177 | 0.0000000 |
| C | -2.7878208 | -0.5504095 | 0.0000000 | -2.7871738 | -0.5226352 | 0.0000000 |
| C | -2.3076012 | -1.8187453 | 0.0000000 | -2.2817265 | -1.8191500 | 0.0000000 |
| C | -0.8871599 | -1.7053706 | 0.0000000 | -0.9021106 | -1.7197088 | 0.0000000 |
| C | -0.6142746 | -0.3764964 | 0.0000000 | -0.5976860 | -0.3453885 | 0.0000000 |
| C | 0.6142746 | 0.3764964 | 0.0000000 | 0.5976860 | 0.3453885 | 0.0000000 |
| O | 1.7655283 | -0.3407221 | 0.0000000 | 1.7636007 | -0.3818177 | 0.0000000 |
| C | 2.7878208 | 0.5504095 | 0.0000000 | 2.7871738 | 0.5226352 | 0.0000000 |
| C | 2.3076012 | 1.8187453 | 0.0000000 | 2.2817265 | 1.8191500 | 0.0000000 |
| C | 0.8871599 | 1.7053706 | 0.0000000 | 0.9021106 | 1.7197088 | 0.0000000 |
| C | 4.1226649 | 0.0032169 | 0.0000000 | 4.0992338 | 0.0104816 | 0.0000000 |
| O | 5.1422492 | 0.8948110 | 0.0000000 | 5.1268963 | 0.9058097 | 0.0000000 |
| C | 6.2921887 | 0.1788240 | 0.0000000 | 6.2740870 | 0.1869940 | 0.0000000 |
| C | 6.0269736 | -1.1445868 | 0.0000000 | 6.0090558 | -1.1427988 | 0.0000000 |
| C | 4.6033408 | -1.2646981 | 0.0000000 | 4.5973789 | -1.2721826 | 0.0000000 |
| H | -2.8998118 | -2.7180985 | 0.0000000 | -2.8825013 | -2.7134875 | 0.0000000 |
| H | -0.1603227 | -2.4998628 | 0.0000000 | -0.1746014 | -2.5139391 | 0.0000000 |
| H | 4.0139566 | -2.1658614 | 0.0000000 | 4.0105335 | -2.1751930 | 0.0000000 |
| H | 7.2031517 | 0.7519484 | 0.0000000 | 7.1876168 | 0.7567824 | 0.0000000 |
| H | 6.7515926 | -1.9415484 | 0.0000000 | 6.7395592 | -1.9348673 | 0.0000000 |
| H | 0.1603227 | 2.4998628 | 0.0000000 | 0.1746014 | 2.5139391 | 0.0000000 |
| H | 2.8998118 | 2.7180985 | 0.0000000 | 2.8825013 | 2.7134875 | 0.0000000 |
| C | -4.1226649 | -0.0032169 | 0.0000000 | -4.0992338 | -0.0104816 | 0.0000000 |
| O | -5.1422492 | -0.8948110 | 0.0000000 | -5.1268963 | -0.9058097 | 0.0000000 |
| C | -6.2921887 | -0.1788240 | 0.0000000 | -6.2740870 | -0.1869940 | 0.0000000 |
| C | -6.0269736 | 1.1445868 | 0.0000000 | -6.0090558 | 1.1427988 | 0.0000000 |
| C | -4.6033408 | 1.2646981 | 0.0000000 | -4.5973789 | 1.2721826 | 0.0000000 |
| H | -4.0139566 | 2.1658614 | 0.0000000 | -4.0105335 | 2.1751930 | 0.0000000 |
| H | -7.2031517 | -0.7519484 | 0.0000000 | -7.1876168 | -0.7567824 | 0.0000000 |
| H | -6.7515926 | 1.9415484 | 0.0000000 | -6.7395592 | 1.9348673 | 0.0000000 |
|  |  |  |  |  |  |  |
| **5O/**  **ωB97X** | **Ground state** | | | **Excited state** | | |
| O | 3.4658470 | 0.0000000 | 0.2636695 | 3.4560776 | 0.0000000 | 0.2936333 |
| C | 4.5550359 | 0.0000000 | -0.5443049 | 4.5451848 | 0.0000000 | -0.5220322 |
| C | 4.1761684 | 0.0000000 | -1.8465506 | 4.1514517 | 0.0000000 | -1.8431194 |
| C | 2.7513377 | 0.0000000 | -1.8453776 | 2.7564717 | 0.0000000 | -1.8515429 |
| C | 2.3746685 | 0.0000000 | -0.5420941 | 2.3527727 | 0.0000000 | -0.5172266 |
| C | 1.0903659 | 0.0000000 | 0.1108704 | 1.0993070 | 0.0000000 | 0.0834495 |
| O | 0.0000000 | 0.0000000 | -0.6958360 | 0.0000000 | 0.0000000 | -0.7350137 |
| C | -1.0903659 | 0.0000000 | 0.1108704 | -1.0993070 | 0.0000000 | 0.0834495 |
| C | -0.7123166 | 0.0000000 | 1.4139017 | -0.6898214 | 0.0000000 | 1.4243273 |
| C | 0.7123166 | 0.0000000 | 1.4139017 | 0.6898214 | 0.0000000 | 1.4243273 |
| C | -2.3746685 | 0.0000000 | -0.5420941 | -2.3527727 | 0.0000000 | -0.5172266 |
| O | -3.4658470 | 0.0000000 | 0.2636695 | -3.4560776 | 0.0000000 | 0.2936333 |
| C | -4.5550359 | 0.0000000 | -0.5443049 | -4.5451848 | 0.0000000 | -0.5220322 |
| C | -4.1761684 | 0.0000000 | -1.8465506 | -4.1514517 | 0.0000000 | -1.8431194 |
| C | -2.7513377 | 0.0000000 | -1.8453776 | -2.7564717 | 0.0000000 | -1.8515429 |
| C | 5.8430050 | 0.0000000 | 0.1055483 | 5.8221780 | 0.0000000 | 0.1012906 |
| O | 6.9289103 | 0.0000000 | -0.7039695 | 6.9106569 | 0.0000000 | -0.7133968 |
| C | 8.0195852 | 0.0000000 | 0.0993548 | 8.0021216 | 0.0000000 | 0.0873974 |
| C | 7.6521520 | 0.0000000 | 1.3981058 | 7.6390120 | 0.0000000 | 1.3911518 |
| C | 6.2234952 | 0.0000000 | 1.4070280 | 6.2171359 | 0.0000000 | 1.4107276 |
| C | -5.8430050 | 0.0000000 | 0.1055483 | -5.8221780 | 0.0000000 | 0.1012906 |
| O | -6.9289103 | 0.0000000 | -0.7039695 | -6.9106569 | 0.0000000 | -0.7133968 |
| H | -4.8373569 | 0.0000000 | -2.6964706 | -4.8189240 | 0.0000000 | -2.6887470 |
| H | -2.0893330 | 0.0000000 | -2.6946488 | -2.0950906 | 0.0000000 | -2.7015732 |
| H | -1.3735495 | 0.0000000 | 2.2637617 | -1.3549941 | 0.0000000 | 2.2716173 |
| H | 1.3735495 | 0.0000000 | 2.2637617 | 1.3549941 | 0.0000000 | 2.2716173 |
| H | 2.0893330 | 0.0000000 | -2.6946488 | 2.0950906 | 0.0000000 | -2.7015732 |
| H | 4.8373569 | 0.0000000 | -2.6964706 | 4.8189240 | 0.0000000 | -2.6887470 |
| H | 5.5657747 | 0.0000000 | 2.2595991 | 5.5640381 | 0.0000000 | 2.2669536 |
| H | 8.3125650 | 0.0000000 | 2.2490241 | 8.3059062 | 0.0000000 | 2.2372984 |
| C | -8.0195852 | 0.0000000 | 0.0993548 | -8.0021216 | 0.0000000 | 0.0873974 |
| C | -7.6521520 | 0.0000000 | 1.3981058 | -7.6390120 | 0.0000000 | 1.3911518 |
| C | -6.2234952 | 0.0000000 | 1.4070280 | -6.2171359 | 0.0000000 | 1.4107276 |
| H | -5.5657747 | 0.0000000 | 2.2595991 | -5.5640381 | 0.0000000 | 2.2669536 |
| H | -8.9724281 | 0.0000000 | -0.4010608 | -8.9546256 | 0.0000000 | -0.4142332 |
| H | -8.3125650 | 0.0000000 | 2.2490241 | -8.3059062 | 0.0000000 | 2.2372984 |
| H | 8.9724281 | 0.0000000 | -0.4010608 | 8.9546256 | 0.0000000 | -0.4142332 |
|  |  |  |  |  |  |  |
| **6O/**  **ωB97X** | **Ground state** | | | **Excited state** | | |
| O | 1.7979234 | -0.0194548 | 0.0000000 | 1.8030182 | 0.0167403 | 0.0000000 |
| C | 0.5263967 | -0.4916734 | 0.0000000 | 0.5190486 | -0.4607229 | 0.0000000 |
| C | 0.5276558 | -1.8484881 | 0.0000000 | 0.5405730 | -1.8597414 | 0.0000000 |
| C | 1.8961094 | -2.2441167 | 0.0000000 | 1.8729790 | -2.2390283 | 0.0000000 |
| C | 2.6212258 | -1.0972898 | 0.0000000 | 2.6289617 | -1.0709577 | 0.0000000 |
| C | 4.0364771 | -0.8274488 | 0.0000000 | 4.0112251 | -0.8351040 | 0.0000000 |
| O | 4.8598072 | -1.9054214 | 0.0000000 | 4.8409846 | -1.9192984 | 0.0000000 |
| C | 6.1310179 | -1.4331832 | 0.0000000 | 6.1134478 | -1.4447160 | 0.0000000 |
| C | 6.1302155 | -0.0769019 | 0.0000000 | 6.1090366 | -0.0741916 | 0.0000000 |
| C | 4.7615456 | 0.3191776 | 0.0000000 | 4.7627533 | 0.3251106 | 0.0000000 |
| H | 7.0020525 | 0.5551021 | 0.0000000 | 6.9853008 | 0.5523041 | 0.0000000 |
| H | 2.2952047 | -3.2442148 | 0.0000000 | 2.2781617 | -3.2371598 | 0.0000000 |
| H | -0.3435045 | -2.4813975 | 0.0000000 | -0.3313863 | -2.4920481 | 0.0000000 |
| C | 7.1864796 | -2.4166652 | 0.0000000 | 7.1665716 | -2.4103758 | 0.0000000 |
| O | 8.4551642 | -1.9424448 | 0.0000000 | 8.4376811 | -1.9334386 | 0.0000000 |
| C | 9.2782378 | -3.0182674 | 0.0000000 | 9.2618261 | -3.0075648 | 0.0000000 |
| C | 8.5628756 | -4.1628585 | 0.0000000 | 8.5484115 | -4.1560251 | 0.0000000 |
| C | 7.1885413 | -3.7726394 | 0.0000000 | 7.1762553 | -3.7734957 | 0.0000000 |
| H | 6.3190556 | -4.4078320 | 0.0000000 | 6.3091299 | -4.4119823 | 0.0000000 |
| H | 10.3328800 | -2.8036403 | 0.0000000 | 10.3164473 | -2.7919477 | 0.0000000 |
| H | 8.9594198 | -5.1643363 | 0.0000000 | 8.9497511 | -5.1557545 | 0.0000000 |
| C | -0.5263967 | 0.4916734 | 0.0000000 | -0.5190486 | 0.4607229 | 0.0000000 |
| O | -1.7979234 | 0.0194548 | 0.0000000 | -1.8030182 | -0.0167403 | 0.0000000 |
| C | -2.6212258 | 1.0972898 | 0.0000000 | -2.6289617 | 1.0709577 | 0.0000000 |
| C | -1.8961094 | 2.2441167 | 0.0000000 | -1.8729790 | 2.2390283 | 0.0000000 |
| C | -0.5276558 | 1.8484881 | 0.0000000 | -0.5405730 | 1.8597414 | 0.0000000 |
| H | -2.2952047 | 3.2442148 | 0.0000000 | -2.2781617 | 3.2371598 | 0.0000000 |
| H | 0.3435045 | 2.4813975 | 0.0000000 | 0.3313863 | 2.4920481 | 0.0000000 |
| H | 4.3626997 | 1.3193998 | 0.0000000 | 4.3667904 | 1.3266450 | 0.0000000 |
| C | -4.0364771 | 0.8274488 | 0.0000000 | -4.0112251 | 0.8351040 | 0.0000000 |
| C | -4.7615456 | -0.3191776 | 0.0000000 | -4.7627533 | -0.3251106 | 0.0000000 |
| C | -6.1302155 | 0.0769019 | 0.0000000 | -6.1090366 | 0.0741916 | 0.0000000 |
| C | -6.1310179 | 1.4331832 | 0.0000000 | -6.1134478 | 1.4447160 | 0.0000000 |
| O | -4.8598072 | 1.9054214 | 0.0000000 | -4.8409846 | 1.9192984 | 0.0000000 |
| H | -7.0020525 | -0.5551021 | 0.0000000 | -6.9853008 | -0.5523041 | 0.0000000 |
| H | -4.3626997 | -1.3193998 | 0.0000000 | -4.3667904 | -1.3266450 | 0.0000000 |
| C | -7.1864796 | 2.4166652 | 0.0000000 | -7.1665716 | 2.4103758 | 0.0000000 |
| C | -7.1885413 | 3.7726394 | 0.0000000 | -7.1762553 | 3.7734957 | 0.0000000 |
| C | -8.5628756 | 4.1628585 | 0.0000000 | -8.5484115 | 4.1560251 | 0.0000000 |
| C | -9.2782378 | 3.0182674 | 0.0000000 | -9.2618261 | 3.0075648 | 0.0000000 |
| O | -8.4551642 | 1.9424448 | 0.0000000 | -8.4376811 | 1.9334386 | 0.0000000 |
| H | -8.9594198 | 5.1643363 | 0.0000000 | -8.9497511 | 5.1557545 | 0.0000000 |
| H | -10.3328800 | 2.8036403 | 0.0000000 | -10.316447 | 2.7919477 | 0.0000000 |
| H | -6.3190556 | 4.4078320 | 0.0000000 | -6.3091299 | 4.4119823 | 0.0000000 |
|  |  |  |  |  |  |  |
| **7O/**  **ωB97X** | **Ground state** | | | **Excited state** | | |
| C | -9.6917992 | 0.0000000 | -1.4751685 | -9.6752417 | 0.0000000 | -1.4814416 |
| C | -9.3086759 | 0.0000000 | -0.1744690 | -9.2873162 | 0.0000000 | -0.1774348 |
| O | -10.3929125 | 0.0000000 | 0.6372715 | -10.373339 | 0.0000000 | 0.6353719 |
| C | -11.4851965 | 0.0000000 | -0.1638295 | -11.465203 | 0.0000000 | -0.1654204 |
| C | -11.1204196 | 0.0000000 | -1.4633384 | -11.101135 | 0.0000000 | -1.4666333 |
| C | -8.0194159 | 0.0000000 | 0.4728265 | -8.0034835 | 0.0000000 | 0.4607196 |
| O | -6.9318057 | 0.0000000 | -0.3372028 | -6.9144815 | 0.0000000 | -0.3488367 |
| C | -5.8391216 | 0.0000000 | 0.4665168 | -5.8173585 | 0.0000000 | 0.4590376 |
| C | -6.2133093 | 0.0000000 | 1.7705090 | -6.2087441 | 0.0000000 | 1.7760391 |
| C | -7.6380977 | 0.0000000 | 1.7743866 | -7.6195200 | 0.0000000 | 1.7711740 |
| C | -4.5560519 | 0.0000000 | -0.1888286 | -4.5493345 | 0.0000000 | -0.1645263 |
| O | -3.4642679 | 0.0000000 | 0.6158148 | -3.4547456 | 0.0000000 | 0.6459936 |
| C | -2.3754004 | 0.0000000 | -0.1930010 | -2.3560860 | 0.0000000 | -0.1681323 |
| C | -2.7559050 | 0.0000000 | -1.4953421 | -2.7630321 | 0.0000000 | -1.4985485 |
| C | -4.1804530 | 0.0000000 | -1.4926437 | -4.1565725 | 0.0000000 | -1.4892551 |
| C | -1.0902259 | 0.0000000 | 0.4578160 | -1.0983622 | 0.0000000 | 0.4332227 |
| O | 0.0000000 | 0.0000000 | -0.3491275 | 0.0000000 | 0.0000000 | -0.3819995 |
| C | 1.0902259 | 0.0000000 | 0.4578160 | 1.0983622 | 0.0000000 | 0.4332227 |
| C | 0.7121758 | 0.0000000 | 1.7609278 | 0.6921673 | 0.0000000 | 1.7685957 |
| C | -0.7121758 | 0.0000000 | 1.7609278 | -0.6921673 | 0.0000000 | 1.7685957 |
| C | 2.3754004 | 0.0000000 | -0.1930010 | 2.3560860 | 0.0000000 | -0.1681323 |
| O | 3.4642679 | 0.0000000 | 0.6158148 | 3.4547456 | 0.0000000 | 0.6459936 |
| C | 4.5560519 | 0.0000000 | -0.1888286 | 4.5493345 | 0.0000000 | -0.1645263 |
| C | 4.1804530 | 0.0000000 | -1.4926437 | 4.1565725 | 0.0000000 | -1.4892551 |
| C | 2.7559050 | 0.0000000 | -1.4953421 | 2.7630321 | 0.0000000 | -1.4985485 |
| C | 5.8391216 | 0.0000000 | 0.4665168 | 5.8173585 | 0.0000000 | 0.4590376 |
| O | 6.9318057 | 0.0000000 | -0.3372028 | 6.9144815 | 0.0000000 | -0.3488367 |
| C | 8.0194159 | 0.0000000 | 0.4728265 | 8.0034835 | 0.0000000 | 0.4607196 |
| C | 7.6380977 | 0.0000000 | 1.7743866 | 7.6195200 | 0.0000000 | 1.7711740 |
| C | 6.2133093 | 0.0000000 | 1.7705090 | 6.2087441 | 0.0000000 | 1.7760391 |
| C | 9.3086759 | 0.0000000 | -0.1744690 | 9.2873162 | 0.0000000 | -0.1774348 |
| C | 9.6917992 | 0.0000000 | -1.4751685 | 9.6752417 | 0.0000000 | -1.4814416 |
| C | 11.1204196 | 0.0000000 | -1.4633384 | 11.1011357 | 0.0000000 | -1.4666333 |
| C | 11.4851965 | 0.0000000 | -0.1638295 | 11.4652030 | 0.0000000 | -0.1654204 |
| O | 10.3929125 | 0.0000000 | 0.6372715 | 10.3733390 | 0.0000000 | 0.6353719 |
| H | -1.3733789 | 0.0000000 | 2.6107997 | -1.3563341 | 0.0000000 | 2.6166138 |
| H | 2.0963955 | 0.0000000 | -2.3465448 | 2.1039201 | 0.0000000 | -2.3503434 |
| H | 4.8432300 | 0.0000000 | -2.3412848 | 4.8242129 | 0.0000000 | -2.3345999 |
| H | -2.0963955 | 0.0000000 | -2.3465448 | -2.1039201 | 0.0000000 | -2.3503434 |
| H | -4.8432300 | 0.0000000 | -2.3412848 | -4.8242129 | 0.0000000 | -2.3345999 |
| H | 8.2976794 | 0.0000000 | 2.6255481 | 8.2844088 | 0.0000000 | 2.6185348 |
| H | 5.5497524 | 0.0000000 | 2.6185719 | 5.5485054 | 0.0000000 | 2.6268185 |
| H | 1.3733789 | 0.0000000 | 2.6107997 | 1.3563341 | 0.0000000 | 2.6166138 |
| H | 11.7825626 | 0.0000000 | -2.3129028 | 11.7651008 | 0.0000000 | -2.3149046 |
| H | 9.0358243 | 0.0000000 | -2.3290888 | 9.0206177 | 0.0000000 | -2.3364235 |
| H | -5.5497524 | 0.0000000 | 2.6185719 | -5.5485054 | 0.0000000 | 2.6268185 |
| H | -8.2976794 | 0.0000000 | 2.6255481 | -8.2844088 | 0.0000000 | 2.6185348 |
| H | -9.0358243 | 0.0000000 | -2.3290888 | -9.0206177 | 0.0000000 | -2.3364235 |
| H | -11.7825626 | 0.0000000 | -2.3129028 | -11.765100 | 0.0000000 | -2.3149046 |
| H | -12.4370265 | 0.0000000 | 0.3385129 | -12.417300 | 0.0000000 | 0.3366719 |
| H | 12.4370265 | 0.0000000 | 0.3385129 | 12.4173004 | 0.0000000 | 0.3366719 |
|  |  |  |  |  |  |  |
| **8O/**  **ωB97X** | **Ground state** | | | **Excited state** | | |
| O | -11.8641856 | 2.5573716 | 0.0000000 | -11.844186 | 2.5508014 | 0.0000000 |
| C | -10.6099093 | 3.0683089 | 0.0000000 | -10.588966 | 3.0631243 | 0.0000000 |
| C | -10.6513892 | 4.4235823 | 0.0000000 | -10.634079 | 4.4212927 | 0.0000000 |
| C | -12.0364516 | 4.7736841 | 0.0000000 | -12.018209 | 4.7679071 | 0.0000000 |
| C | -12.7181737 | 3.6087781 | 0.0000000 | -12.698827 | 3.6012117 | 0.0000000 |
| C | -9.5261669 | 2.1161388 | 0.0000000 | -9.5066372 | 2.1182401 | 0.0000000 |
| C | -9.4856623 | 0.7605004 | 0.0000000 | -9.4655140 | 0.7564205 | 0.0000000 |
| C | -8.1059756 | 0.4046892 | 0.0000000 | -8.0964141 | 0.3977701 | 0.0000000 |
| C | -7.4148163 | 1.5719908 | 0.0000000 | -7.3920688 | 1.5708011 | 0.0000000 |
| O | -8.2693530 | 2.6253629 | 0.0000000 | -8.2493832 | 2.6272191 | 0.0000000 |
| C | -6.0080510 | 1.8832403 | 0.0000000 | -6.0013275 | 1.8639943 | 0.0000000 |
| O | -5.1531965 | 0.8303838 | 0.0000000 | -5.1448943 | 0.8080925 | 0.0000000 |
| C | -3.8962705 | 1.3401519 | 0.0000000 | -3.8798781 | 1.3203186 | 0.0000000 |
| C | -3.9377506 | 2.6962617 | 0.0000000 | -3.9376230 | 2.7019561 | 0.0000000 |
| C | -5.3173596 | 3.0510846 | 0.0000000 | -5.2965196 | 3.0438551 | 0.0000000 |
| C | -2.8148259 | 0.3884644 | 0.0000000 | -2.8092461 | 0.4138160 | 0.0000000 |
| O | -1.5578300 | 0.8977986 | 0.0000000 | -1.5449437 | 0.9279526 | 0.0000000 |
| C | -0.7033144 | -0.1554557 | 0.0000000 | -0.6836822 | -0.1343275 | 0.0000000 |
| C | -1.3944340 | -1.3230446 | 0.0000000 | -1.4096767 | -1.3241513 | 0.0000000 |
| C | -2.7738421 | -0.9677397 | 0.0000000 | -2.7531411 | -0.9739596 | 0.0000000 |
| C | 0.7033144 | 0.1554557 | 0.0000000 | 0.6836822 | 0.1343275 | 0.0000000 |
| O | 1.5578300 | -0.8977986 | 0.0000000 | 1.5449437 | -0.9279526 | 0.0000000 |
| C | 2.8148259 | -0.3884644 | 0.0000000 | 2.8092461 | -0.4138160 | 0.0000000 |
| C | 2.7738421 | 0.9677397 | 0.0000000 | 2.7531411 | 0.9739596 | 0.0000000 |
| C | 1.3944340 | 1.3230446 | 0.0000000 | 1.4096767 | 1.3241513 | 0.0000000 |
| C | 3.8962705 | -1.3401519 | 0.0000000 | 3.8798781 | -1.3203186 | 0.0000000 |
| O | 5.1531965 | -0.8303838 | 0.0000000 | 5.1448943 | -0.8080925 | 0.0000000 |
| C | 6.0080510 | -1.8832403 | 0.0000000 | 6.0013275 | -1.8639943 | 0.0000000 |
| C | 5.3173596 | -3.0510846 | 0.0000000 | 5.2965196 | -3.0438551 | 0.0000000 |
| C | 3.9377506 | -2.6962617 | 0.0000000 | 3.9376230 | -2.7019561 | 0.0000000 |
| H | 3.6263283 | 1.6255317 | 0.0000000 | 3.6087248 | 1.6283783 | 0.0000000 |
| H | -0.9659017 | -2.3108772 | 0.0000000 | -0.9806598 | -2.3120940 | 0.0000000 |
| H | -3.6263283 | -1.6255317 | 0.0000000 | -3.6087248 | -1.6283783 | 0.0000000 |
| H | 3.0855202 | -3.3544100 | 0.0000000 | 3.0870188 | -3.3625000 | 0.0000000 |
| C | 7.4148163 | -1.5719908 | 0.0000000 | 7.3920688 | -1.5708011 | 0.0000000 |
| H | 5.7464207 | -4.0386744 | 0.0000000 | 5.7306545 | -4.0296017 | 0.0000000 |
| H | -5.7464207 | 4.0386744 | 0.0000000 | -5.7306545 | 4.0296017 | 0.0000000 |
| H | -3.0855202 | 3.3544100 | 0.0000000 | -3.0870188 | 3.3625000 | 0.0000000 |
| H | 0.9659017 | 2.3108772 | 0.0000000 | 0.9806598 | 2.3120940 | 0.0000000 |
| H | -10.3387590 | 0.1034813 | 0.0000000 | -10.321052 | 0.1022268 | 0.0000000 |
| H | -7.6776925 | -0.5832707 | 0.0000000 | -7.6709378 | -0.5914885 | 0.0000000 |
| H | -12.4620419 | 5.7631494 | 0.0000000 | -12.445903 | 5.7565514 | 0.0000000 |
| H | -13.7661278 | 3.3635891 | 0.0000000 | -13.746710 | 3.3553310 | 0.0000000 |
| H | -9.8004751 | 5.0834167 | 0.0000000 | -9.7846767 | 5.0831198 | 0.0000000 |
| O | 8.2693530 | -2.6253629 | 0.0000000 | 8.2493832 | -2.6272191 | 0.0000000 |
| C | 9.5261669 | -2.1161388 | 0.0000000 | 9.5066372 | -2.1182401 | 0.0000000 |
| C | 9.4856623 | -0.7605004 | 0.0000000 | 9.4655140 | -0.7564205 | 0.0000000 |
| C | 8.1059756 | -0.4046892 | 0.0000000 | 8.0964141 | -0.3977701 | 0.0000000 |
| H | 7.6776925 | 0.5832707 | 0.0000000 | 7.6709378 | 0.5914885 | 0.0000000 |
| H | 10.3387590 | -0.1034813 | 0.0000000 | 10.3210523 | -0.1022268 | 0.0000000 |
| C | 10.6099093 | -3.0683089 | 0.0000000 | 10.5889668 | -3.0631243 | 0.0000000 |
| O | 11.8641856 | -2.5573716 | 0.0000000 | 11.8441864 | -2.5508014 | 0.0000000 |
| C | 12.7181737 | -3.6087781 | 0.0000000 | 12.6988278 | -3.6012117 | 0.0000000 |
| C | 12.0364516 | -4.7736841 | 0.0000000 | 12.0182098 | -4.7679071 | 0.0000000 |
| C | 10.6513892 | -4.4235823 | 0.0000000 | 10.6340798 | -4.4212927 | 0.0000000 |
| H | 9.8004751 | -5.0834167 | 0.0000000 | 9.7846767 | -5.0831198 | 0.0000000 |
| H | 12.4620419 | -5.7631494 | 0.0000000 | 12.4459032 | -5.7565514 | 0.0000000 |
| H | 13.7661278 | -3.3635891 | 0.0000000 | 13.7467107 | -3.3553310 | 0.0000000 |
|  |  |  |  |  |  |  |
| **9O/**  **ωB97X** | **Ground state** | | | **Excited state** | | |
| C | -13.1605404 | 0.0000000 | -1.4978356 | -13.141343 | 0.0000000 | -1.4997772 |
| C | -12.7743733 | 0.0000000 | -0.1980396 | -12.752673 | 0.0000000 | -0.1986794 |
| O | -13.8566988 | 0.0000000 | 0.6162403 | -13.835554 | 0.0000000 | 0.6163715 |
| C | -14.9508534 | 0.0000000 | -0.1822932 | -14.929731 | 0.0000000 | -0.1816699 |
| C | -14.5891275 | 0.0000000 | -1.4826572 | -14.568701 | 0.0000000 | -1.4829010 |
| C | -11.4836024 | 0.0000000 | 0.4462536 | -11.464229 | 0.0000000 | 0.4414297 |
| O | -10.3978736 | 0.0000000 | -0.3662754 | -10.377904 | 0.0000000 | -0.3704761 |
| C | -9.3033425 | 0.0000000 | 0.4349292 | -9.2812602 | 0.0000000 | 0.4325902 |
| C | -9.6745209 | 0.0000000 | 1.7397775 | -9.6607141 | 0.0000000 | 1.7432184 |
| C | -11.0992884 | 0.0000000 | 1.7469408 | -11.078976 | 0.0000000 | 1.7461539 |
| C | -8.0217898 | 0.0000000 | -0.2233778 | -8.0071106 | 0.0000000 | -0.2105005 |
| O | -6.9281730 | 0.0000000 | 0.5787311 | -6.9118605 | 0.0000000 | 0.5926025 |
| C | -5.8411773 | 0.0000000 | -0.2326044 | -5.8196058 | 0.0000000 | -0.2220191 |
| C | -6.2246757 | 0.0000000 | -1.5340553 | -6.2202140 | 0.0000000 | -1.5380903 |
| C | -7.6492025 | 0.0000000 | -1.5280741 | -7.6277745 | 0.0000000 | -1.5259170 |
| C | -4.5545727 | 0.0000000 | 0.4153835 | -4.5494411 | 0.0000000 | 0.3939477 |
| O | -3.4660479 | 0.0000000 | -0.3937866 | -3.4569584 | 0.0000000 | -0.4197079 |
| C | -2.3741880 | 0.0000000 | 0.4109529 | -2.3568834 | 0.0000000 | 0.3902573 |
| C | -2.7495648 | 0.0000000 | 1.7148317 | -2.7573121 | 0.0000000 | 1.7196892 |
| C | -4.1738650 | 0.0000000 | 1.7177546 | -4.1517024 | 0.0000000 | 1.7170711 |
| C | -1.0902947 | 0.0000000 | -0.2423497 | -1.0977063 | 0.0000000 | -0.2167820 |
| O | 0.0000000 | 0.0000000 | 0.5643868 | 0.0000000 | 0.0000000 | 0.5965435 |
| C | 1.0902947 | 0.0000000 | -0.2423497 | 1.0977063 | 0.0000000 | -0.2167820 |
| C | 0.7122359 | 0.0000000 | -1.5454824 | 0.6940329 | 0.0000000 | -1.5484975 |
| C | -0.7122359 | 0.0000000 | -1.5454824 | -0.6940329 | 0.0000000 | -1.5484975 |
| C | 2.3741880 | 0.0000000 | 0.4109529 | 2.3568834 | 0.0000000 | 0.3902573 |
| O | 3.4660479 | 0.0000000 | -0.3937866 | 3.4569584 | 0.0000000 | -0.4197079 |
| C | 4.5545727 | 0.0000000 | 0.4153835 | 4.5494411 | 0.0000000 | 0.3939477 |
| C | 4.1738650 | 0.0000000 | 1.7177546 | 4.1517024 | 0.0000000 | 1.7170711 |
| C | 2.7495648 | 0.0000000 | 1.7148317 | 2.7573121 | 0.0000000 | 1.7196892 |
| C | 5.8411773 | 0.0000000 | -0.2326044 | 5.8196058 | 0.0000000 | -0.2220191 |
| C | 6.2246757 | 0.0000000 | -1.5340553 | 6.2202140 | 0.0000000 | -1.5380903 |
| C | 7.6492025 | 0.0000000 | -1.5280741 | 7.6277745 | 0.0000000 | -1.5259170 |
| C | 8.0217898 | 0.0000000 | -0.2233778 | 8.0071106 | 0.0000000 | -0.2105005 |
| O | 6.9281730 | 0.0000000 | 0.5787311 | 6.9118605 | 0.0000000 | 0.5926025 |
| C | 9.3033425 | 0.0000000 | 0.4349292 | 9.2812602 | 0.0000000 | 0.4325902 |
| O | 10.3978736 | 0.0000000 | -0.3662754 | 10.3779049 | 0.0000000 | -0.3704761 |
| C | 11.4836024 | 0.0000000 | 0.4462536 | 11.4642296 | 0.0000000 | 0.4414297 |
| C | 11.0992884 | 0.0000000 | 1.7469408 | 11.0789765 | 0.0000000 | 1.7461539 |
| C | 9.6745209 | 0.0000000 | 1.7397775 | 9.6607141 | 0.0000000 | 1.7432184 |
| H | -4.8333337 | 0.0000000 | 2.5689661 | -4.8154448 | 0.0000000 | 2.5654060 |
| H | -1.3732947 | 0.0000000 | -2.3954742 | -1.3575034 | 0.0000000 | -2.3970232 |
| H | 1.3732947 | 0.0000000 | -2.3954742 | 1.3575034 | 0.0000000 | -2.3970232 |
| H | -5.5671733 | 0.0000000 | -2.3868172 | -5.5647417 | 0.0000000 | -2.3925581 |
| H | -8.3139441 | 0.0000000 | -2.3751754 | -8.2964502 | 0.0000000 | -2.3702381 |
| H | 4.8333337 | 0.0000000 | 2.5689661 | 4.8154448 | 0.0000000 | 2.5654060 |
| H | 2.0866658 | 0.0000000 | 2.5633850 | 2.0948465 | 0.0000000 | 2.5688586 |
| H | -2.0866658 | 0.0000000 | 2.5633850 | -2.0948465 | 0.0000000 | 2.5688586 |
| H | 8.3139441 | 0.0000000 | -2.3751754 | 8.2964502 | 0.0000000 | -2.3702381 |
| H | 5.5671733 | 0.0000000 | -2.3868172 | 5.5647417 | 0.0000000 | -2.3925581 |
| H | 11.7568888 | 0.0000000 | 2.5996319 | 11.7391110 | 0.0000000 | 2.5970470 |
| C | 12.7743733 | 0.0000000 | -0.1980396 | 12.7526732 | 0.0000000 | -0.1986794 |
| H | 9.0090281 | 0.0000000 | 2.5863240 | 8.9970543 | 0.0000000 | 2.5912584 |
| H | -9.0090281 | 0.0000000 | 2.5863240 | -8.9970543 | 0.0000000 | 2.5912584 |
| H | -11.7568888 | 0.0000000 | 2.5996319 | -11.739111 | 0.0000000 | 2.5970470 |
| H | -12.5065998 | 0.0000000 | -2.3533117 | -12.488295 | 0.0000000 | -2.3559469 |
| H | -15.2532517 | 0.0000000 | -2.3306759 | -15.233856 | 0.0000000 | -2.3301694 |
| H | -15.9014975 | 0.0000000 | 0.3222897 | -15.880353 | 0.0000000 | 0.3230799 |
| O | 13.8566988 | 0.0000000 | 0.6162403 | 13.8355541 | 0.0000000 | 0.6163715 |
| C | 14.9508534 | 0.0000000 | -0.1822932 | 14.9297318 | 0.0000000 | -0.1816699 |
| C | 14.5891275 | 0.0000000 | -1.4826572 | 14.5687015 | 0.0000000 | -1.4829010 |
| C | 13.1605404 | 0.0000000 | -1.4978356 | 13.1413435 | 0.0000000 | -1.4997772 |
| H | 12.5065998 | 0.0000000 | -2.3533117 | 12.4882957 | 0.0000000 | -2.3559469 |
| H | 15.2532517 | 0.0000000 | -2.3306759 | 15.2338567 | 0.0000000 | -2.3301694 |
| H | 15.9014975 | 0.0000000 | 0.3222897 | 15.8803535 | 0.0000000 | 0.3230799 |

Part 10.

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| **2O/**  **CC2** | **Ground state** | | | **Excited state** | | |
| C | -2.8191046 | 0.4361825 | 0.0000000 | -2.8010893 | 0.4502933 | 0.0000000 |
| C | -2.7984455 | -0.9288921 | 0.0000000 | -2.7725994 | -0.9421680 | 0.0000000 |
| C | -1.4255912 | -1.3126309 | 0.0000000 | -1.4377773 | -1.3440648 | 0.0000000 |
| C | -0.7021728 | -0.1460385 | 0.0000000 | -0.6722342 | -0.1353455 | 0.0000000 |
| C | 0.7021728 | 0.1460385 | 0.0000000 | 0.6722342 | 0.1353455 | 0.0000000 |
| C | 1.4255912 | 1.3126309 | 0.0000000 | 1.4377773 | 1.3440648 | 0.0000000 |
| C | 2.7984455 | 0.9288921 | 0.0000000 | 2.7725994 | 0.9421680 | 0.0000000 |
| C | 2.8191046 | -0.4361825 | 0.0000000 | 2.8010893 | -0.4502933 | 0.0000000 |
| O | -1.5433475 | 0.9354033 | 0.0000000 | -1.5350652 | 0.9739632 | 0.0000000 |
| O | 1.5433475 | -0.9354033 | 0.0000000 | 1.5350652 | -0.9739632 | 0.0000000 |
| H | -3.6027594 | 1.1716188 | 0.0000000 | -3.6037101 | 1.1675264 | 0.0000000 |
| H | -3.6585261 | -1.5759251 | 0.0000000 | -3.6465226 | -1.5728789 | 0.0000000 |
| H | -1.0140409 | -2.3069428 | 0.0000000 | -1.0260996 | -2.3384746 | 0.0000000 |
| H | 1.0140409 | 2.3069428 | 0.0000000 | 1.0260996 | 2.3384746 | 0.0000000 |
| H | 3.6585261 | 1.5759251 | 0.0000000 | 3.6465226 | 1.5728789 | 0.0000000 |
| H | 3.6027594 | -1.1716188 | 0.0000000 | 3.6037101 | -1.1675264 | 0.0000000 |
|  |  |  |  |  |  |  |
| **3O/**  **CC2** | **Ground state** | | | **Excited state** | | |
| O | 3.4730317 | 0.0000000 | 0.8436679 | 3.4712753 | 0.0000000 | 0.8627926 |
| C | 4.5697412 | 0.0000000 | 0.0226257 | 4.5525950 | 0.0000000 | 0.0230776 |
| C | 4.1864400 | 0.0000000 | -1.2880010 | 4.1516194 | 0.0000000 | -1.2961930 |
| C | 2.7615591 | 0.0000000 | -1.2931529 | 2.7452928 | 0.0000000 | -1.3045899 |
| C | 2.3739077 | 0.0000000 | 0.0249759 | 2.3490542 | 0.0000000 | 0.0473573 |
| C | 1.1005680 | 0.0000000 | 0.6785335 | 1.1088564 | 0.0000000 | 0.6629274 |
| O | 0.0000000 | 0.0000000 | -0.1417334 | 0.0000000 | 0.0000000 | -0.1783493 |
| C | -1.1005680 | 0.0000000 | 0.6785335 | -1.1088564 | 0.0000000 | 0.6629274 |
| C | -0.7098425 | 0.0000000 | 1.9968941 | -0.6900978 | 0.0000000 | 2.0208156 |
| C | 0.7098425 | 0.0000000 | 1.9968941 | 0.6900978 | 0.0000000 | 2.0208156 |
| H | 1.3721057 | 0.0000000 | 2.8456549 | 1.3587985 | 0.0000000 | 2.8655155 |
| H | -1.3721057 | 0.0000000 | 2.8456549 | -1.3587985 | 0.0000000 | 2.8655155 |
| H | 2.1008227 | 0.0000000 | -2.1426668 | 2.0766375 | 0.0000000 | -2.1489570 |
| H | 5.5209837 | 0.0000000 | 0.5228422 | 5.5149118 | 0.0000000 | 0.5042737 |
| H | 4.8435015 | 0.0000000 | -2.1405067 | 4.8115506 | 0.0000000 | -2.1478452 |
| C | -2.3739077 | 0.0000000 | 0.0249759 | -2.3490542 | 0.0000000 | 0.0473573 |
| O | -3.4730317 | 0.0000000 | 0.8436679 | -3.4712753 | 0.0000000 | 0.8627926 |
| C | -4.5697412 | 0.0000000 | 0.0226257 | -4.5525950 | 0.0000000 | 0.0230776 |
| C | -4.1864400 | 0.0000000 | -1.2880010 | -4.1516194 | 0.0000000 | -1.2961930 |
| C | -2.7615591 | 0.0000000 | -1.2931529 | -2.7452928 | 0.0000000 | -1.3045899 |
| H | -2.1008227 | 0.0000000 | -2.1426668 | -2.0766375 | 0.0000000 | -2.1489570 |
| H | -5.5209837 | 0.0000000 | 0.5228422 | -5.5149118 | 0.0000000 | 0.5042737 |
| H | -4.8435015 | 0.0000000 | -2.1405067 | -4.8115506 | 0.0000000 | -2.1478452 |
|  |  |  |  |  |  |  |
| **4O/**  **CC2** | **Ground state** | | | **Excited state** | | |
| O | -1.5209479 | 0.9728153 | 0.0000000 | -1.5064155 | 1.0097914 | 0.0000000 |
| C | -2.8108006 | 0.5031317 | 0.0000000 | -2.8029584 | 0.5286744 | 0.0000000 |
| C | -2.8151192 | -0.8725185 | 0.0000000 | -2.7958125 | -0.8789099 | 0.0000000 |
| C | -1.4564907 | -1.2807896 | 0.0000000 | -1.4720583 | -1.2865191 | 0.0000000 |
| C | -0.7019455 | -0.1293685 | 0.0000000 | -0.6802417 | -0.1087082 | 0.0000000 |
| C | 0.7019455 | 0.1293685 | 0.0000000 | 0.6802417 | 0.1087082 | 0.0000000 |
| O | 1.5209479 | -0.9728153 | 0.0000000 | 1.5064155 | -1.0097914 | 0.0000000 |
| C | 2.8108006 | -0.5031317 | 0.0000000 | 2.8029584 | -0.5286744 | 0.0000000 |
| C | 2.8151192 | 0.8725185 | 0.0000000 | 2.7958125 | 0.8789099 | 0.0000000 |
| C | 1.4564907 | 1.2807896 | 0.0000000 | 1.4720583 | 1.2865191 | 0.0000000 |
| H | 1.0667387 | 2.2844450 | 0.0000000 | 1.0801736 | 2.2902566 | 0.0000000 |
| H | 3.6935727 | 1.4949653 | 0.0000000 | 3.6807197 | 1.4939827 | 0.0000000 |
| H | -1.0667387 | -2.2844450 | 0.0000000 | -1.0801736 | -2.2902566 | 0.0000000 |
| H | -3.6935727 | -1.4949653 | 0.0000000 | -3.6807197 | -1.4939827 | 0.0000000 |
| C | 3.8429327 | -1.4939487 | 0.0000000 | 3.8273570 | -1.4802636 | 0.0000000 |
| O | 5.1307465 | -1.0247803 | 0.0000000 | 5.1253709 | -1.0096041 | 0.0000000 |
| C | 5.9458468 | -2.1258748 | 0.0000000 | 5.9361968 | -2.1122349 | 0.0000000 |
| C | 5.2027479 | -3.2716142 | 0.0000000 | 5.1899305 | -3.2651334 | 0.0000000 |
| C | 3.8363687 | -2.8681131 | 0.0000000 | 3.8315792 | -2.8759505 | 0.0000000 |
| H | 2.9598227 | -3.4925820 | 0.0000000 | 2.9560717 | -3.5030307 | 0.0000000 |
| H | 7.0006123 | -1.9195298 | 0.0000000 | 6.9927780 | -1.9109937 | 0.0000000 |
| H | 5.5877685 | -4.2767365 | 0.0000000 | 5.5835521 | -4.2677273 | 0.0000000 |
| C | -3.8429327 | 1.4939487 | 0.0000000 | -3.8273570 | 1.4802636 | 0.0000000 |
| O | -5.1307465 | 1.0247803 | 0.0000000 | -5.1253709 | 1.0096041 | 0.0000000 |
| C | -5.9458468 | 2.1258748 | 0.0000000 | -5.9361968 | 2.1122349 | 0.0000000 |
| C | -5.2027479 | 3.2716142 | 0.0000000 | -5.1899305 | 3.2651334 | 0.0000000 |
| C | -3.8363687 | 2.8681131 | 0.0000000 | -3.8315792 | 2.8759505 | 0.0000000 |
| H | -7.0006123 | 1.9195298 | 0.0000000 | -6.9927780 | 1.9109937 | 0.0000000 |
| H | -5.5877685 | 4.2767365 | 0.0000000 | -5.5835521 | 4.2677273 | 0.0000000 |
| H | -2.9598227 | 3.4925820 | 0.0000000 | -2.9560717 | 3.5030307 | 0.0000000 |
|  |  |  |  |  |  |  |
| **5O/**  **CC2** | **Ground state** | | | **Excited state** | | |
| O | 0.0000000 | 0.0000000 | 0.7160720 | 0.0000000 | 0.0000000 | 0.7524122 |
| C | 1.1011363 | 0.0000000 | -0.1045293 | 1.1092399 | 0.0000000 | -0.0807231 |
| C | 0.7087424 | 0.0000000 | -1.4247847 | 0.6909588 | 0.0000000 | -1.4329479 |
| C | -0.7087424 | 0.0000000 | -1.4247847 | -0.6909588 | 0.0000000 | -1.4329479 |
| C | -1.1011363 | 0.0000000 | -0.1045293 | -1.1092399 | 0.0000000 | -0.0807231 |
| C | -2.3713930 | 0.0000000 | 0.5453666 | -2.3547339 | 0.0000000 | 0.5206767 |
| O | -3.4720856 | 0.0000000 | -0.2758613 | -3.4665006 | 0.0000000 | -0.3078825 |
| C | -4.5731184 | 0.0000000 | 0.5438845 | -4.5685374 | 0.0000000 | 0.5194769 |
| C | -4.1828029 | 0.0000000 | 1.8631978 | -4.1633571 | 0.0000000 | 1.8580365 |
| C | -2.7644449 | 0.0000000 | 1.8650206 | -2.7717627 | 0.0000000 | 1.8688426 |
| H | -4.8459926 | 0.0000000 | 2.7113278 | -4.8334201 | 0.0000000 | 2.7020166 |
| H | -1.3707417 | 0.0000000 | -2.2739758 | -1.3576151 | 0.0000000 | -2.2797262 |
| H | 1.3707417 | 0.0000000 | -2.2739758 | 1.3576151 | 0.0000000 | -2.2797262 |
| C | -5.8459885 | 0.0000000 | -0.1091603 | -5.8304628 | 0.0000000 | -0.1045304 |
| O | -6.9450703 | 0.0000000 | 0.7097591 | -6.9323413 | 0.0000000 | 0.7217628 |
| C | -8.0417720 | 0.0000000 | -0.1111947 | -8.0303089 | 0.0000000 | -0.0955119 |
| C | -7.6586246 | 0.0000000 | -1.4219935 | -7.6527221 | 0.0000000 | -1.4130449 |
| C | -6.2339782 | 0.0000000 | -1.4274939 | -6.2359891 | 0.0000000 | -1.4322591 |
| H | -5.5734942 | 0.0000000 | -2.2772381 | -5.5809030 | 0.0000000 | -2.2867651 |
| H | -8.9930026 | 0.0000000 | 0.3890795 | -8.9812980 | 0.0000000 | 0.4064354 |
| H | -8.3158353 | 0.0000000 | -2.2743931 | -8.3185942 | 0.0000000 | -2.2593609 |
| C | 2.3713930 | 0.0000000 | 0.5453666 | 2.3547339 | 0.0000000 | 0.5206767 |
| O | 3.4720856 | 0.0000000 | -0.2758613 | 3.4665006 | 0.0000000 | -0.3078825 |
| C | 4.5731184 | 0.0000000 | 0.5438845 | 4.5685374 | 0.0000000 | 0.5194769 |
| C | 4.1828029 | 0.0000000 | 1.8631978 | 4.1633571 | 0.0000000 | 1.8580365 |
| C | 2.7644449 | 0.0000000 | 1.8650206 | 2.7717627 | 0.0000000 | 1.8688426 |
| H | 4.8459926 | 0.0000000 | 2.7113278 | 4.8334201 | 0.0000000 | 2.7020166 |
| H | 2.1034620 | 0.0000000 | 2.7149530 | 2.1100893 | 0.0000000 | 2.7192985 |
| H | -2.1034620 | 0.0000000 | 2.7149530 | -2.1100893 | 0.0000000 | 2.7192985 |
| C | 5.8459885 | 0.0000000 | -0.1091603 | 5.8304628 | 0.0000000 | -0.1045304 |
| C | 6.2339782 | 0.0000000 | -1.4274939 | 6.2359891 | 0.0000000 | -1.4322591 |
| C | 7.6586246 | 0.0000000 | -1.4219935 | 7.6527221 | 0.0000000 | -1.4130449 |
| C | 8.0417720 | 0.0000000 | -0.1111947 | 8.0303089 | 0.0000000 | -0.0955119 |
| O | 6.9450703 | 0.0000000 | 0.7097591 | 6.9323413 | 0.0000000 | 0.7217628 |
| H | 8.3158353 | 0.0000000 | -2.2743931 | 8.3185942 | 0.0000000 | -2.2593609 |
| H | 8.9930026 | 0.0000000 | 0.3890795 | 8.9812980 | 0.0000000 | 0.4064354 |
| H | 5.5734942 | 0.0000000 | -2.2772381 | 5.5809030 | 0.0000000 | -2.2867651 |
|  |  |  |  |  |  |  |
| **6O/**  **CC2** | **Ground state** | | | **Excited state** | | |
| O | 1.8055341 | 0.0096084 | 0.0000000 | 1.8123930 | 0.0441333 | 0.0000000 |
| C | 0.5238156 | -0.4838230 | 0.0000000 | 0.5189731 | -0.4557841 | 0.0000000 |
| C | 0.5459667 | -1.8613206 | 0.0000000 | 0.5580386 | -1.8696675 | 0.0000000 |
| C | 1.9107136 | -2.2431969 | 0.0000000 | 1.8923847 | -2.2386179 | 0.0000000 |
| C | 2.6446576 | -1.0774563 | 0.0000000 | 2.6545088 | -1.0534497 | 0.0000000 |
| C | 4.0429809 | -0.7943722 | 0.0000000 | 4.0229230 | -0.8059216 | 0.0000000 |
| O | 4.8813573 | -1.8820852 | 0.0000000 | 4.8671899 | -1.9017008 | 0.0000000 |
| C | 6.1626737 | -1.3897371 | 0.0000000 | 6.1507858 | -1.4074628 | 0.0000000 |
| C | 6.1427176 | -0.0139815 | 0.0000000 | 6.1268329 | -0.0154501 | 0.0000000 |
| C | 4.7775223 | 0.3703853 | 0.0000000 | 4.7843202 | 0.3729793 | 0.0000000 |
| H | 7.0101363 | 0.6237756 | 0.0000000 | 6.9997709 | 0.6161577 | 0.0000000 |
| H | 2.3193579 | -3.2393910 | 0.0000000 | 2.3069920 | -3.2334454 | 0.0000000 |
| H | -0.3203840 | -2.5007430 | 0.0000000 | -0.3104969 | -2.5076948 | 0.0000000 |
| C | 7.2122619 | -2.3618148 | 0.0000000 | 7.1981726 | -2.3580771 | 0.0000000 |
| O | 8.4914468 | -1.8695856 | 0.0000000 | 8.4804013 | -1.8611371 | 0.0000000 |
| C | 9.3261288 | -2.9558584 | 0.0000000 | 9.3171410 | -2.9446081 | 0.0000000 |
| C | 8.6037150 | -4.1147987 | 0.0000000 | 8.5977856 | -4.1093240 | 0.0000000 |
| C | 7.2303769 | -3.7359498 | 0.0000000 | 7.2269957 | -3.7414855 | 0.0000000 |
| H | 6.3652243 | -4.3761218 | 0.0000000 | 6.3649628 | -4.3863939 | 0.0000000 |
| H | 10.3770291 | -2.7306320 | 0.0000000 | 10.3680670 | -2.7176220 | 0.0000000 |
| H | 9.0067347 | -5.1128387 | 0.0000000 | 9.0079773 | -5.1048285 | 0.0000000 |
| C | -0.5238156 | 0.4838230 | 0.0000000 | -0.5189731 | 0.4557841 | 0.0000000 |
| O | -1.8055341 | -0.0096084 | 0.0000000 | -1.8123930 | -0.0441333 | 0.0000000 |
| C | -2.6446576 | 1.0774563 | 0.0000000 | -2.6545088 | 1.0534497 | 0.0000000 |
| C | -1.9107136 | 2.2431969 | 0.0000000 | -1.8923847 | 2.2386179 | 0.0000000 |
| C | -0.5459667 | 1.8613206 | 0.0000000 | -0.5580386 | 1.8696675 | 0.0000000 |
| H | -2.3193579 | 3.2393910 | 0.0000000 | -2.3069920 | 3.2334454 | 0.0000000 |
| H | 0.3203840 | 2.5007430 | 0.0000000 | 0.3104969 | 2.5076948 | 0.0000000 |
| H | 4.3703412 | 1.3671306 | 0.0000000 | 4.3793720 | 1.3714078 | 0.0000000 |
| C | -4.0429809 | 0.7943722 | 0.0000000 | -4.0229230 | 0.8059216 | 0.0000000 |
| C | -4.7775223 | -0.3703853 | 0.0000000 | -4.7843202 | -0.3729793 | 0.0000000 |
| C | -6.1427176 | 0.0139815 | 0.0000000 | -6.1268329 | 0.0154501 | 0.0000000 |
| C | -6.1626737 | 1.3897371 | 0.0000000 | -6.1507858 | 1.4074628 | 0.0000000 |
| O | -4.8813573 | 1.8820852 | 0.0000000 | -4.8671899 | 1.9017008 | 0.0000000 |
| H | -7.0101363 | -0.6237756 | 0.0000000 | -6.9997709 | -0.6161577 | 0.0000000 |
| H | -4.3703412 | -1.3671306 | 0.0000000 | -4.3793720 | -1.3714078 | 0.0000000 |
| C | -7.2122619 | 2.3618148 | 0.0000000 | -7.1981726 | 2.3580771 | 0.0000000 |
| C | -7.2303769 | 3.7359498 | 0.0000000 | -7.2269957 | 3.7414855 | 0.0000000 |
| C | -8.6037150 | 4.1147987 | 0.0000000 | -8.5977856 | 4.1093240 | 0.0000000 |
| C | -9.3261288 | 2.9558584 | 0.0000000 | -9.3171410 | 2.9446081 | 0.0000000 |
| O | -8.4914468 | 1.8695856 | 0.0000000 | -8.4804013 | 1.8611371 | 0.0000000 |
| H | -9.0067347 | 5.1128387 | 0.0000000 | -9.0079773 | 5.1048285 | 0.0000000 |
| H | -10.3770291 | 2.7306320 | 0.0000000 | -10.368067 | 2.7176220 | 0.0000000 |
| H | -6.3652243 | 4.3761218 | 0.0000000 | -6.3649628 | 4.3863939 | 0.0000000 |
|  |  |  |  |  |  |  |
| **7O/**  **CC2** | **Ground state** | | | **Excited state** | | |
| C | -9.7061488 | 0.0000000 | -1.4878127 | -9.6999763 | 0.0000000 | -1.4954639 |
| C | -9.3179805 | 0.0000000 | -0.1695154 | -9.3036077 | 0.0000000 | -0.1728228 |
| O | -10.4169294 | 0.0000000 | 0.6495701 | -10.404285 | 0.0000000 | 0.6492531 |
| C | -11.5137222 | 0.0000000 | -0.1712364 | -11.501397 | 0.0000000 | -0.1698530 |
| C | -11.1307635 | 0.0000000 | -1.4821010 | -11.120812 | 0.0000000 | -1.4837948 |
| C | -8.0450888 | 0.0000000 | 0.4833999 | -8.0370066 | 0.0000000 | 0.4672243 |
| O | -6.9440530 | 0.0000000 | -0.3362831 | -6.9336165 | 0.0000000 | -0.3516669 |
| C | -5.8433864 | 0.0000000 | 0.4850264 | -5.8280116 | 0.0000000 | 0.4755163 |
| C | -6.2365758 | 0.0000000 | 1.8047424 | -6.2407820 | 0.0000000 | 1.8100419 |
| C | -7.6548165 | 0.0000000 | 1.8028074 | -7.6432485 | 0.0000000 | 1.7979034 |
| C | -4.5732772 | 0.0000000 | -0.1646991 | -4.5723788 | 0.0000000 | -0.1391252 |
| O | -3.4720077 | 0.0000000 | 0.6556634 | -3.4669720 | 0.0000000 | 0.6873898 |
| C | -2.3709121 | 0.0000000 | -0.1652745 | -2.3567718 | 0.0000000 | -0.1402749 |
| C | -2.7639438 | 0.0000000 | -1.4857846 | -2.7739933 | 0.0000000 | -1.4871851 |
| C | -4.1810244 | 0.0000000 | -1.4852770 | -4.1627617 | 0.0000000 | -1.4807829 |
| C | -1.1012247 | 0.0000000 | 0.4837805 | -1.1091389 | 0.0000000 | 0.4603572 |
| O | 0.0000000 | 0.0000000 | -0.3369205 | 0.0000000 | 0.0000000 | -0.3690875 |
| C | 1.1012247 | 0.0000000 | 0.4837805 | 1.1091389 | 0.0000000 | 0.4603572 |
| C | 0.7084227 | 0.0000000 | 1.8044901 | 0.6916654 | 0.0000000 | 1.8095622 |
| C | -0.7084227 | 0.0000000 | 1.8044901 | -0.6916654 | 0.0000000 | 1.8095622 |
| C | 2.3709121 | 0.0000000 | -0.1652745 | 2.3567718 | 0.0000000 | -0.1402749 |
| O | 3.4720077 | 0.0000000 | 0.6556634 | 3.4669720 | 0.0000000 | 0.6873898 |
| C | 4.5732772 | 0.0000000 | -0.1646991 | 4.5723788 | 0.0000000 | -0.1391252 |
| C | 4.1810244 | 0.0000000 | -1.4852770 | 4.1627617 | 0.0000000 | -1.4807829 |
| C | 2.7639438 | 0.0000000 | -1.4857846 | 2.7739933 | 0.0000000 | -1.4871851 |
| C | 5.8433864 | 0.0000000 | 0.4850264 | 5.8280116 | 0.0000000 | 0.4755163 |
| O | 6.9440530 | 0.0000000 | -0.3362831 | 6.9336165 | 0.0000000 | -0.3516669 |
| C | 8.0450888 | 0.0000000 | 0.4833999 | 8.0370066 | 0.0000000 | 0.4672243 |
| C | 7.6548165 | 0.0000000 | 1.8028074 | 7.6432485 | 0.0000000 | 1.7979034 |
| C | 6.2365758 | 0.0000000 | 1.8047424 | 6.2407820 | 0.0000000 | 1.8100419 |
| C | 9.3179805 | 0.0000000 | -0.1695154 | 9.3036077 | 0.0000000 | -0.1728228 |
| C | 9.7061488 | 0.0000000 | -1.4878127 | 9.6999763 | 0.0000000 | -1.4954639 |
| C | 11.1307635 | 0.0000000 | -1.4821010 | 11.1208127 | 0.0000000 | -1.4837948 |
| C | 11.5137222 | 0.0000000 | -0.1712364 | 11.5013979 | 0.0000000 | -0.1698530 |
| O | 10.4169294 | 0.0000000 | 0.6495701 | 10.4042850 | 0.0000000 | 0.6492531 |
| H | -1.3703591 | 0.0000000 | 2.6537771 | -1.3573146 | 0.0000000 | 2.6572048 |
| H | 2.1022872 | 0.0000000 | -2.3352843 | 2.1114009 | 0.0000000 | -2.3370326 |
| H | 4.8432763 | 0.0000000 | -2.3342879 | 4.8303461 | 0.0000000 | -2.3268235 |
| H | -2.1022872 | 0.0000000 | -2.3352843 | -2.1114009 | 0.0000000 | -2.3370326 |
| H | -4.8432763 | 0.0000000 | -2.3342879 | -4.8303461 | 0.0000000 | -2.3268235 |
| H | 8.3180632 | 0.0000000 | 2.6508952 | 8.3132787 | 0.0000000 | 2.6414796 |
| H | 5.5756960 | 0.0000000 | 2.6547677 | 5.5830166 | 0.0000000 | 2.6631975 |
| H | 1.3703591 | 0.0000000 | 2.6537771 | 1.3573146 | 0.0000000 | 2.6572048 |
| H | 11.7880856 | 0.0000000 | -2.3344128 | 11.7819125 | 0.0000000 | -2.3334930 |
| H | 9.0458130 | 0.0000000 | -2.3376759 | 9.0421551 | 0.0000000 | -2.3475581 |
| H | -5.5756960 | 0.0000000 | 2.6547677 | -5.5830166 | 0.0000000 | 2.6631975 |
| H | -8.3180632 | 0.0000000 | 2.6508952 | -8.3132787 | 0.0000000 | 2.6414796 |
| H | -9.0458130 | 0.0000000 | -2.3376759 | -9.0421551 | 0.0000000 | -2.3475581 |
| H | -11.7880856 | 0.0000000 | -2.3344128 | -11.781912 | 0.0000000 | -2.3334930 |
| H | -12.4648778 | 0.0000000 | 0.3291847 | -12.452487 | 0.0000000 | 0.3312904 |
| H | 12.4648778 | 0.0000000 | 0.3291847 | 12.4524873 | 0.0000000 | 0.3312904 |
|  |  |  |  |  |  |  |
| **8O/**  **CC2** | **Ground state** | | | **Excited state** | | |
| O | -11.8921393 | 2.5513182 | 0.0000000 | -11.879824 | 2.5471693 | 0.0000000 |
| C | -10.6238342 | 3.0709671 | 0.0000000 | -10.609996 | 3.0688549 | 0.0000000 |
| C | -10.6715058 | 4.4443927 | 0.0000000 | -10.662898 | 4.4466236 | 0.0000000 |
| C | -12.0526747 | 4.7936019 | 0.0000000 | -12.042597 | 4.7907486 | 0.0000000 |
| C | -12.7499677 | 3.6193575 | 0.0000000 | -12.738474 | 3.6138202 | 0.0000000 |
| C | -9.5536543 | 2.1216013 | 0.0000000 | -9.5417411 | 2.1296436 | 0.0000000 |
| C | -9.5042527 | 0.7465608 | 0.0000000 | -9.4923851 | 0.7460559 | 0.0000000 |
| C | -8.1311699 | 0.3915092 | 0.0000000 | -8.1327619 | 0.3861991 | 0.0000000 |
| C | -7.4217295 | 1.5717442 | 0.0000000 | -7.4058797 | 1.5731001 | 0.0000000 |
| O | -8.2831936 | 2.6412707 | 0.0000000 | -8.2699113 | 2.6477301 | 0.0000000 |
| C | -6.0298496 | 1.8847971 | 0.0000000 | -6.0316644 | 1.8629495 | 0.0000000 |
| O | -5.1675021 | 0.8161032 | 0.0000000 | -5.1664407 | 0.7905770 | 0.0000000 |
| C | -3.8966942 | 1.3370766 | 0.0000000 | -3.8870977 | 1.3153822 | 0.0000000 |
| C | -3.9485988 | 2.7138775 | 0.0000000 | -3.9553890 | 2.7183700 | 0.0000000 |
| C | -5.3211705 | 3.0661642 | 0.0000000 | -5.3070533 | 3.0577017 | 0.0000000 |
| C | -2.8286371 | 0.3923311 | 0.0000000 | -2.8263376 | 0.4171320 | 0.0000000 |
| O | -1.5577390 | 0.9129056 | 0.0000000 | -1.5475131 | 0.9431145 | 0.0000000 |
| C | -0.6955794 | -0.1562033 | 0.0000000 | -0.6787765 | -0.1351522 | 0.0000000 |
| C | -1.4050056 | -1.3375279 | 0.0000000 | -1.4189390 | -1.3369958 | 0.0000000 |
| C | -2.7771236 | -0.9846566 | 0.0000000 | -2.7598978 | -0.9894472 | 0.0000000 |
| C | 0.6955794 | 0.1562033 | 0.0000000 | 0.6787765 | 0.1351522 | 0.0000000 |
| O | 1.5577390 | -0.9129056 | 0.0000000 | 1.5475131 | -0.9431145 | 0.0000000 |
| C | 2.8286371 | -0.3923311 | 0.0000000 | 2.8263376 | -0.4171320 | 0.0000000 |
| C | 2.7771236 | 0.9846566 | 0.0000000 | 2.7598978 | 0.9894472 | 0.0000000 |
| C | 1.4050056 | 1.3375279 | 0.0000000 | 1.4189390 | 1.3369958 | 0.0000000 |
| C | 3.8966942 | -1.3370766 | 0.0000000 | 3.8870977 | -1.3153822 | 0.0000000 |
| O | 5.1675021 | -0.8161032 | 0.0000000 | 5.1664407 | -0.7905770 | 0.0000000 |
| C | 6.0298496 | -1.8847971 | 0.0000000 | 6.0316644 | -1.8629495 | 0.0000000 |
| C | 5.3211705 | -3.0661642 | 0.0000000 | 5.3070533 | -3.0577017 | 0.0000000 |
| C | 3.9485988 | -2.7138775 | 0.0000000 | 3.9553890 | -2.7183700 | 0.0000000 |
| H | 3.6297141 | 1.6423321 | 0.0000000 | 3.6161223 | 1.6440192 | 0.0000000 |
| H | -0.9755086 | -2.3249442 | 0.0000000 | -0.9869032 | -2.3243258 | 0.0000000 |
| H | -3.6297141 | -1.6423321 | 0.0000000 | -3.6161223 | -1.6440192 | 0.0000000 |
| H | 3.0963116 | -3.3719421 | 0.0000000 | 3.1034371 | -3.3780777 | 0.0000000 |
| C | 7.4217295 | -1.5717442 | 0.0000000 | 7.4058797 | -1.5731001 | 0.0000000 |
| H | 5.7511829 | -4.0533225 | 0.0000000 | 5.7434189 | -4.0429864 | 0.0000000 |
| H | -5.7511829 | 4.0533225 | 0.0000000 | -5.7434189 | 4.0429864 | 0.0000000 |
| H | -3.0963116 | 3.3719421 | 0.0000000 | -3.1034371 | 3.3780777 | 0.0000000 |
| H | 0.9755086 | 2.3249442 | 0.0000000 | 0.9869032 | 2.3243258 | 0.0000000 |
| H | -10.3577968 | 0.0903537 | 0.0000000 | -10.350181 | 0.0945868 | 0.0000000 |
| H | -7.7028123 | -0.5963242 | 0.0000000 | -7.7076800 | -0.6035272 | 0.0000000 |
| H | -12.4770499 | 5.7827457 | 0.0000000 | -12.470256 | 5.7786678 | 0.0000000 |
| H | -13.7958086 | 3.3716878 | 0.0000000 | -13.784307 | 3.3652736 | 0.0000000 |
| H | -9.8203473 | 5.1030582 | 0.0000000 | -9.8133001 | 5.1075565 | 0.0000000 |
| O | 8.2831936 | -2.6412707 | 0.0000000 | 8.2699113 | -2.6477301 | 0.0000000 |
| C | 9.5536543 | -2.1216013 | 0.0000000 | 9.5417411 | -2.1296436 | 0.0000000 |
| C | 9.5042527 | -0.7465608 | 0.0000000 | 9.4923851 | -0.7460559 | 0.0000000 |
| C | 8.1311699 | -0.3915092 | 0.0000000 | 8.1327619 | -0.3861991 | 0.0000000 |
| H | 7.7028123 | 0.5963242 | 0.0000000 | 7.7076800 | 0.6035272 | 0.0000000 |
| H | 10.3577968 | -0.0903537 | 0.0000000 | 10.3501817 | -0.0945868 | 0.0000000 |
| C | 10.6238342 | -3.0709671 | 0.0000000 | 10.6099962 | -3.0688549 | 0.0000000 |
| O | 11.8921393 | -2.5513182 | 0.0000000 | 11.8798246 | -2.5471693 | 0.0000000 |
| C | 12.7499677 | -3.6193575 | 0.0000000 | 12.7384742 | -3.6138202 | 0.0000000 |
| C | 12.0526747 | -4.7936019 | 0.0000000 | 12.0425978 | -4.7907486 | 0.0000000 |
| C | 10.6715058 | -4.4443927 | 0.0000000 | 10.6628989 | -4.4466236 | 0.0000000 |
| H | 9.8203473 | -5.1030582 | 0.0000000 | 9.8133001 | -5.1075565 | 0.0000000 |
| H | 12.4770499 | -5.7827457 | 0.0000000 | 12.4702568 | -5.7786678 | 0.0000000 |
| H | 13.7958086 | -3.3716878 | 0.0000000 | 13.7843074 | -3.3652736 | 0.0000000 |
|  |  |  |  |  |  |  |
| **9O/**  **CC2** | **Ground state** | | | **Excited state** | | |
| C | -13.1781107 | 0.0000000 | -1.5220002 | -13.168586 | 0.0000000 | -1.5258058 |
| C | -12.7898800 | 0.0000000 | -0.2037205 | -12.776021 | 0.0000000 | -0.2054874 |
| O | -13.8887769 | 0.0000000 | 0.6154249 | -13.875641 | 0.0000000 | 0.6152882 |
| C | -14.9855978 | 0.0000000 | -0.2053169 | -14.972719 | 0.0000000 | -0.2043459 |
| C | -14.6027175 | 0.0000000 | -1.5162126 | -14.591277 | 0.0000000 | -1.5168442 |
| C | -11.5169660 | 0.0000000 | 0.4491447 | -11.506363 | 0.0000000 | 0.4409500 |
| O | -10.4159569 | 0.0000000 | -0.3705378 | -10.403919 | 0.0000000 | -0.3772716 |
| C | -9.3152865 | 0.0000000 | 0.4507604 | -9.3006272 | 0.0000000 | 0.4474443 |
| C | -9.7084616 | 0.0000000 | 1.7704902 | -9.7056997 | 0.0000000 | 1.7749198 |
| C | -11.1266844 | 0.0000000 | 1.7685689 | -11.115137 | 0.0000000 | 1.7665525 |
| C | -8.0452157 | 0.0000000 | -0.1990018 | -8.0391436 | 0.0000000 | -0.1819203 |
| O | -6.9438987 | 0.0000000 | 0.6212554 | -6.9348572 | 0.0000000 | 0.6394323 |
| C | -5.8428748 | 0.0000000 | -0.1997862 | -5.8279711 | 0.0000000 | -0.1862918 |
| C | -6.2360311 | 0.0000000 | -1.5202890 | -6.2403017 | 0.0000000 | -1.5235110 |
| C | -7.6530672 | 0.0000000 | -1.5196502 | -7.6384889 | 0.0000000 | -1.5158106 |
| C | -4.5732128 | 0.0000000 | 0.4491844 | -4.5737834 | 0.0000000 | 0.4264953 |
| O | -3.4719523 | 0.0000000 | -0.3714094 | -3.4671792 | 0.0000000 | -0.3989258 |
| C | -2.3707695 | 0.0000000 | 0.4494008 | -2.3579993 | 0.0000000 | 0.4281089 |
| C | -2.7637638 | 0.0000000 | 1.7701713 | -2.7747475 | 0.0000000 | 1.7733724 |
| C | -4.1804824 | 0.0000000 | 1.7700140 | -4.1634374 | 0.0000000 | 1.7685276 |
| C | -1.1012335 | 0.0000000 | -0.1994534 | -1.1088190 | 0.0000000 | -0.1740930 |
| O | 0.0000000 | 0.0000000 | 0.6212389 | 0.0000000 | 0.0000000 | 0.6534950 |
| C | 1.1012335 | 0.0000000 | -0.1994534 | 1.1088190 | 0.0000000 | -0.1740930 |
| C | 0.7083306 | 0.0000000 | -1.5203010 | 0.6924721 | 0.0000000 | -1.5211085 |
| C | -0.7083306 | 0.0000000 | -1.5203010 | -0.6924721 | 0.0000000 | -1.5211085 |
| C | 2.3707695 | 0.0000000 | 0.4494008 | 2.3579993 | 0.0000000 | 0.4281089 |
| O | 3.4719523 | 0.0000000 | -0.3714094 | 3.4671792 | 0.0000000 | -0.3989258 |
| C | 4.5732128 | 0.0000000 | 0.4491844 | 4.5737834 | 0.0000000 | 0.4264953 |
| C | 4.1804824 | 0.0000000 | 1.7700140 | 4.1634374 | 0.0000000 | 1.7685276 |
| C | 2.7637638 | 0.0000000 | 1.7701713 | 2.7747475 | 0.0000000 | 1.7733724 |
| C | 5.8428748 | 0.0000000 | -0.1997862 | 5.8279711 | 0.0000000 | -0.1862918 |
| C | 6.2360311 | 0.0000000 | -1.5202890 | 6.2403017 | 0.0000000 | -1.5235110 |
| C | 7.6530672 | 0.0000000 | -1.5196502 | 7.6384889 | 0.0000000 | -1.5158106 |
| C | 8.0452157 | 0.0000000 | -0.1990018 | 8.0391436 | 0.0000000 | -0.1819203 |
| O | 6.9438987 | 0.0000000 | 0.6212554 | 6.9348572 | 0.0000000 | 0.6394323 |
| C | 9.3152865 | 0.0000000 | 0.4507604 | 9.3006272 | 0.0000000 | 0.4474443 |
| O | 10.4159569 | 0.0000000 | -0.3705378 | 10.4039193 | 0.0000000 | -0.3772716 |
| C | 11.5169660 | 0.0000000 | 0.4491447 | 11.5063636 | 0.0000000 | 0.4409500 |
| C | 11.1266844 | 0.0000000 | 1.7685689 | 11.1151378 | 0.0000000 | 1.7665525 |
| C | 9.7084616 | 0.0000000 | 1.7704902 | 9.7056997 | 0.0000000 | 1.7749198 |
| H | -4.8425121 | 0.0000000 | 2.6192293 | -4.8302325 | 0.0000000 | 2.6151851 |
| H | -1.3702548 | 0.0000000 | -2.3696074 | -1.3576402 | 0.0000000 | -2.3691039 |
| H | 1.3702548 | 0.0000000 | -2.3696074 | 1.3576402 | 0.0000000 | -2.3691039 |
| H | -5.5744697 | 0.0000000 | -2.3698675 | -5.5801552 | 0.0000000 | -2.3749649 |
| H | -8.3153984 | 0.0000000 | -2.3685974 | -8.3059455 | 0.0000000 | -2.3616183 |
| H | 4.8425121 | 0.0000000 | 2.6192293 | 4.8302325 | 0.0000000 | 2.6151851 |
| H | 2.1019517 | 0.0000000 | 2.6195672 | 2.1120471 | 0.0000000 | 2.6231498 |
| H | -2.1019517 | 0.0000000 | 2.6195672 | -2.1120471 | 0.0000000 | 2.6231498 |
| H | 8.3153984 | 0.0000000 | -2.3685974 | 8.3059455 | 0.0000000 | -2.3616183 |
| H | 5.5744697 | 0.0000000 | -2.3698675 | 5.5801552 | 0.0000000 | -2.3749649 |
| H | 11.7899280 | 0.0000000 | 2.6166583 | 11.7825974 | 0.0000000 | 2.6118022 |
| C | 12.7898800 | 0.0000000 | -0.2037205 | 12.7760212 | 0.0000000 | -0.2054874 |
| H | 9.0475868 | 0.0000000 | 2.6205213 | 9.0472507 | 0.0000000 | 2.6272501 |
| H | -9.0475868 | 0.0000000 | 2.6205213 | -9.0472507 | 0.0000000 | 2.6272501 |
| H | -11.7899280 | 0.0000000 | 2.6166583 | -11.782597 | 0.0000000 | 2.6118022 |
| H | -12.5178333 | 0.0000000 | -2.3719085 | -12.509786 | 0.0000000 | -2.3770018 |
| H | -15.2600863 | 0.0000000 | -2.3684861 | -15.250638 | 0.0000000 | -2.3677295 |
| H | -15.9367364 | 0.0000000 | 0.2951353 | -15.923754 | 0.0000000 | 0.2966084 |
| O | 13.8887769 | 0.0000000 | 0.6154249 | 13.8756417 | 0.0000000 | 0.6152882 |
| C | 14.9855978 | 0.0000000 | -0.2053169 | 14.9727196 | 0.0000000 | -0.2043459 |
| C | 14.6027175 | 0.0000000 | -1.5162126 | 14.5912778 | 0.0000000 | -1.5168442 |
| C | 13.1781107 | 0.0000000 | -1.5220002 | 13.1685863 | 0.0000000 | -1.5258058 |
| H | 12.5178333 | 0.0000000 | -2.3719085 | 12.5097869 | 0.0000000 | -2.3770018 |
| H | 15.2600863 | 0.0000000 | -2.3684861 | 15.2506389 | 0.0000000 | -2.3677295 |
| H | 15.9367364 | 0.0000000 | 0.2951353 | 15.9237544 | 0.0000000 | 0.2966084 |