# Supplementary information

## Generation of Molecular Conformations using Generative Adversarial Neural Networks

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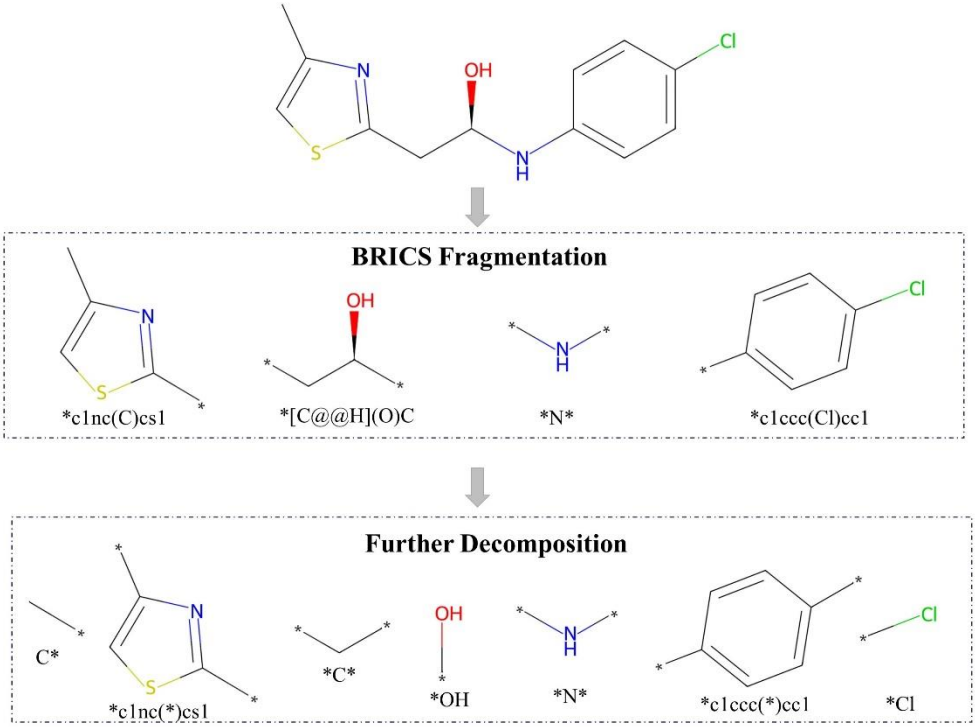


**Fig. S1.**
Schematic illustration of molecular motif generation.

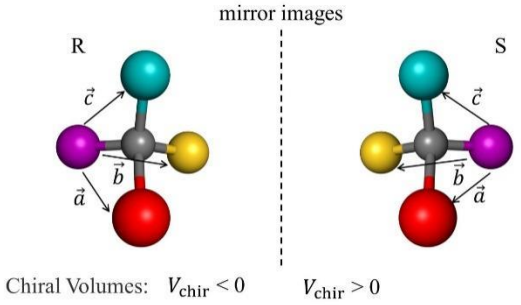


**Fig. S2.**
Schematic illustration of chirality volume violation. The volume is represented as $V_{chir} = \vec{a} + \vec{b} + \vec{c}$, where the molecule is R, then $V_{chir} < 0$,, and if the molecule is S, then $V_{chir} > 0$.

**Table S1.**

Performance comparison of different methods in molecular docking, including average affinity energy and average RMSD values.

| Method | Average Affinity Energy (kcal/mol) | Average RMSD (Å) |
|---|---|---|
| RDKit | -8.98 | 1.75 |
| CGCF | **-9.41** | 1.76 |
| ConfGF | -9.08 | 1.68 |
| ConfVAE | -9.38 | 1.94 |
| GeoDiff | -8.14 | 1.69 |
| GeoMol | -9.39 | 1.80 |
| **ConfGAN** | **-9.41** | **1.64** |

**Data 1. The molecular 3D coordinates in Figure 3 (ConfGAN)**

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Energy = -74.46961835 a.u.

| | | | |
|---|---|---|---|
| O | -5.46449668 | 6.74570153 | 2.82188698 |
| C | -4.76591202 | 5.77913134 | 2.69860124 |
| O | -3.56701337 | 5.84109226 | 2.12645526 |
| C | -5.16643122 | 4.38916670 | 3.18279090 |
| C | -4.20420115 | 3.88214054 | 4.27193938 |
| C | -3.75520351 | 2.44043487 | 4.03400261 |
| C | -2.86566643 | 2.31745327 | 2.80722547 |
| O | -2.56255277 | 3.26347069 | 2.10444291 |
| N | -2.44865944 | 1.04395875 | 2.58806920 |
| C | -1.61575865 | 0.54766722 | 1.57920097 |
| C | -1.11311607 | 1.33849198 | 0.55030787 |
| C | -0.29333418 | 0.78617652 | -0.41502303 |
| C | 0.03767794 | -0.56319457 | -0.36814502 |
| N | 0.87137631 | -1.15794130 | -1.32420866 |
| C | 1.47189486 | -0.59094262 | -2.39815996 |
| C | 2.19151286 | -1.57509805 | -3.02996697 |
| C | 1.95970692 | -2.72113240 | -2.25027350 |
| C | 2.49240646 | -4.09506512 | -2.46049774 |
| F | 3.23671797 | -4.52800764 | -1.42920068 |
| F | 1.52300397 | -5.00862395 | -2.63486844 |
| F | 3.27621445 | -4.16025018 | -3.54838947 |
| N | 1.16410142 | -2.44855259 | -1.23072678 |
| C | -0.46727653 | -1.35829764 | 0.65870900 |

| | | | |
|---|---|---|---|
| C | -1.28510330 | -0.80723551 | 1.61965257 |
| H | -3.13158733 | 4.95940991 | 2.07590342 |
| H | -6.18965188 | 4.43529799 | 3.55305966 |
| H | -5.14456469 | 3.72426244 | 2.31644697 |
| H | -3.31477297 | 4.51574809 | 4.31128592 |
| H | -4.68964889 | 3.94723210 | 5.24550324 |
| H | -3.19218195 | 2.08337154 | 4.90037055 |
| H | -4.62489358 | 1.79065890 | 3.90700531 |
| H | -2.75444689 | 0.34490346 | 3.25237662 |
| H | -1.36047604 | 2.38520935 | 0.50697248 |
| H | 0.08092923 | 1.42354595 | -1.19911437 |
| H | 1.36221808 | 0.44242166 | -2.64985355 |
| H | 2.79304959 | -1.50112718 | -3.91097036 |
| H | -0.20395236 | -2.40285376 | 0.68282153 |
| H | -1.67157714 | -1.43147157 | 2.41238250 |

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Energy = -56.81221120 a.u.

| | | | |
|---|---|---|---|
| C | 4.04292691 | 2.99415861 | -3.67370688 |
| C | 4.20794669 | 1.57416104 | -3.12775113 |
| C | 5.54474189 | 1.42656829 | -2.39819574 |
| C | 3.05502361 | 1.21211219 | -2.22361979 |
| C | 2.20060527 | 0.16736529 | -2.55234248 |
| C | 1.13972909 | -0.17112037 | -1.73642264 |
| C | 0.90296008 | 0.53256803 | -0.55714728 |
| N | -0.19721662 | 0.15103653 | 0.20948783 |
| C | -0.52637115 | 0.56736488 | 1.46675604 |
| O | 0.09196703 | 1.36176161 | 2.14642704 |
| N | -1.67373048 | -0.00556728 | 1.96608151 |
| C | -2.66022324 | -0.78113899 | 1.24281514 |
| C | -2.19254774 | -2.20478167 | 1.03493135 |
| C | -2.49006909 | -3.21968782 | 1.93596083 |
| C | -1.98652185 | -4.48863955 | 1.69905814 |
| C | -1.20214710 | -4.70090258 | 0.57612523 |
| C | -0.95695027 | -3.62461462 | -0.26121181 |
| N | -1.44093125 | -2.41531292 | -0.04065992 |
| C | 1.75134130 | 1.58241611 | -0.21954123 |
| C | 2.80886419 | 1.90823734 | -1.04639729 |
| H | 4.06447489 | 3.72157344 | -2.86625084 |
| H | 4.84640214 | 3.22808706 | -4.36921558 |

| | | | |
|---|---|---|---|
| H | 3.09317271 | 3.09031086 | -4.19551545 |
| H | 4.20545907 | 0.88068630 | -3.97684296 |
| H | 5.65569632 | 0.41525550 | -2.01283363 |
| H | 6.37021303 | 1.63190314 | -3.07688689 |
| H | 5.60699869 | 2.11932265 | -1.56293060 |
| H | 2.36733081 | -0.39190996 | -3.46286919 |
| H | 0.48322175 | -0.98624719 | -2.00761233 |
| H | -0.69701175 | -0.65796376 | -0.15566018 |
| H | -1.89786432 | 0.29742597 | 2.89983509 |
| H | -3.58645398 | -0.77757572 | 1.81967213 |
| H | -2.85394603 | -0.32300280 | 0.26537922 |
| H | -3.10178156 | -3.01832680 | 2.80175893 |
| H | -2.20141865 | -5.29857025 | 2.38061374 |
| H | -0.78968467 | -5.67296852 | 0.35769220 |
| H | -0.34670857 | -3.72772027 | -1.14875128 |
| H | 1.57948306 | 2.12906842 | 0.69232434 |
| H | 3.45307475 | 2.72662180 | -0.76119566 |

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Energy = -81.64711690 a.u.

| | | | |
|---|---|---|---|
| O | 2.66501218 | 1.04622856 | -2.37540886 |
| C | 2.06100147 | 1.03136548 | -1.32113568 |
| N | 1.87364490 | 2.09706137 | -0.53418659 |
| C | 2.19860768 | 3.43959404 | -0.95554825 |
| C | 0.95092161 | 4.32479207 | -0.98441120 |
| C | -0.19055509 | 3.79697567 | -1.81676472 |
| C | -1.49059937 | 4.14710241 | -1.46786962 |
| C | -2.56867155 | 3.73582111 | -2.23000866 |
| C | -2.36710128 | 2.94393029 | -3.34759859 |
| C | -1.07966476 | 2.57401088 | -3.69215595 |
| C | 0.00141985 | 3.00457922 | -2.94135851 |
| C | 1.43900625 | -0.28249880 | -0.79196458 |
| C | 1.79250735 | -0.60307188 | 0.63945067 |
| C | 0.97365062 | -1.40577750 | 1.42556071 |
| C | 1.37453578 | -1.70559340 | 2.71703240 |
| N | 2.50787936 | -1.28194816 | 3.24735156 |
| C | 3.29519325 | -0.53348601 | 2.49524951 |
| C | 2.99126041 | -0.16724205 | 1.19382945 |
| N | -0.00456260 | -0.27360537 | -1.03787825 |
| C | -0.79132627 | 0.54352875 | -0.30917625 |

| | | | |
|---|---|---|---|
| O | -0.37339801 | 1.18481989 | 0.65178904 |
| C | -2.21654570 | 0.67869739 | -0.68157605 |
| C | -3.12802035 | 1.30341647 | 0.14956018 |
| S | -4.62768080 | 1.35045800 | -0.63494458 |
| N | -3.99052908 | 0.58099276 | -1.96744014 |
| N | -2.77645797 | 0.30966510 | -1.85028355 |
| C | -0.48828755 | -1.06989176 | -2.12477596 |
| C | -0.08385085 | -2.51289068 | -2.20467113 |
| C | -1.49393126 | -2.15328452 | -1.86023919 |
| H | 1.25482613 | 1.99467582 | 0.26549899 |
| H | 2.92486690 | 3.87080134 | -0.25702489 |
| H | 2.66692640 | 3.37003543 | -1.93941604 |
| H | 0.59610403 | 4.46247556 | 0.04044274 |
| H | 1.23960213 | 5.30907242 | -1.36623243 |
| H | -1.65772835 | 4.75971009 | -0.59259806 |
| H | -3.56987146 | 4.03504386 | -1.95157421 |
| H | -3.20675508 | 2.61175658 | -3.93931306 |
| H | -0.91226746 | 1.95352237 | -4.56022685 |
| H | 0.99455418 | 2.71416193 | -3.24598668 |
| H | 1.85710138 | -1.07021277 | -1.42976812 |
| H | 0.03709951 | -1.78561954 | 1.04677613 |
| H | 0.75905758 | -2.32204986 | 3.35935087 |
| H | 4.21753397 | -0.21148161 | 2.96048499 |
| H | 3.67510243 | 0.43958550 | 0.62127962 |
| H | -2.95524923 | 1.70161348 | 1.12704700 |
| H | -0.57951298 | -0.51929094 | -3.05468702 |
| H | 0.12800175 | -2.92197676 | -3.17987726 |
| H | 0.53279459 | -2.92191257 | -1.41793968 |
| H | -2.27527770 | -2.30481393 | -2.58675058 |
| H | -1.81439696 | -2.30299876 | -0.84013566 |

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Energy = -82.11958469 a.u.

| | | | |
|---|---|---|---|
| C | -2.23333542 | -0.48227296 | -7.92008545 |
| O | -1.79329668 | -1.78674837 | -7.62179642 |
| C | -1.56919585 | -2.11357861 | -6.32141137 |
| C | -1.14086820 | -3.42088447 | -6.08412744 |
| C | -0.89224811 | -3.84016497 | -4.79345194 |
| C | -1.06123266 | -2.97672931 | -3.72559620 |
| C | -1.48686685 | -1.67341662 | -3.95978158 |

| | | | |
|---|---|---|---|
| N | -1.64422162 | -0.83809880 | -2.84772210 |
| C | -2.01819309 | 0.45388996 | -2.82577723 |
| O | -2.29619706 | 1.17541084 | -3.75600366 |
| N | -2.08369991 | 1.00650421 | -1.52531865 |
| C | -1.85564037 | 0.41650072 | -0.32985217 |
| N | -1.48206739 | -0.81050608 | -0.14849264 |
| N | -1.33203808 | -1.14155967 | 1.13126201 |
| C | -1.58298072 | -0.20503066 | 1.96174125 |
| C | -1.41703295 | -0.29353921 | 3.43274909 |
| C | -0.13454597 | 0.41781927 | 3.79554527 |
| C | -0.14126239 | 1.72245806 | 4.24360587 |
| C | 1.05360012 | 2.37804781 | 4.51315702 |
| C | 2.26642476 | 1.73839599 | 4.33077143 |
| O | 3.48918153 | 2.28949050 | 4.55984279 |
| C | 3.54805673 | 3.62373750 | 4.99694226 |
| C | 2.27893498 | 0.40158601 | 3.86697425 |
| O | 3.51025984 | -0.15415656 | 3.71454435 |
| C | 3.59086154 | -1.48350612 | 3.26350092 |
| C | 1.08098569 | -0.23542487 | 3.60255369 |
| S | -2.06069525 | 1.30713440 | 1.17654588 |
| C | -1.74289110 | -1.23918954 | -5.25563641 |
| H | -3.20024274 | -0.26873725 | -7.45417985 |
| H | -1.50537629 | 0.26993254 | -7.60152285 |
| H | -2.33817279 | -0.44852510 | -9.00347985 |
| H | -1.01102650 | -4.08227005 | -6.92529295 |
| H | -0.55757907 | -4.85086652 | -4.61529351 |
| H | -0.86568956 | -3.30386098 | -2.71558985 |
| H | -1.45114221 | -1.26193096 | -1.93852951 |
| H | -2.36805579 | 1.97682901 | -1.52066095 |
| H | -2.26530669 | 0.17636557 | 3.93229093 |
| H | -1.36680922 | -1.34768479 | 3.70754839 |
| H | -1.07513990 | 2.24477966 | 4.38853471 |
| H | 1.01918365 | 3.39619318 | 4.86561393 |
| H | 3.05404156 | 3.75406255 | 5.96575808 |
| H | 4.60770078 | 3.85119519 | 5.10097417 |
| H | 3.10189811 | 4.30770220 | 4.26698888 |
| H | 3.09936904 | -2.17432968 | 3.95670133 |
| H | 3.15421826 | -1.59922708 | 2.26602188 |
| H | 4.65412423 | -1.71365436 | 3.21977212 |
| H | 1.06525236 | -1.24871785 | 3.23391984 |
| H | -2.07250172 | -0.22646775 | -5.40546076 |

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Energy = -70.58580400 a.u.

| | | | |
|---|---|---|---|
| C | 4.07561677 | 3.42553648 | -2.83086201 |
| O | 2.94441436 | 2.59675739 | -2.69188381 |
| C | 2.92812832 | 1.66758512 | -1.70602346 |
| C | 3.97850407 | 1.41843655 | -0.82656996 |
| C | 3.87119794 | 0.43872109 | 0.14353646 |
| C | 2.71001241 | -0.31908797 | 0.25973363 |
| C | 2.51064386 | -1.39192063 | 1.25779495 |
| C | 3.63874692 | -1.64919451 | 2.22784328 |
| O | 1.48606360 | -2.04203642 | 1.29391420 |
| C | 1.65937279 | -0.05718831 | -0.62394733 |
| C | 1.74645172 | 0.91472170 | -1.59325612 |
| C | 0.60270290 | 1.19437516 | -2.53377170 |
| O | -0.57215463 | 0.51973235 | -2.11940242 |
| C | -1.51996013 | 1.24943603 | -1.49663492 |
| O | -1.49434272 | 2.45504024 | -1.43857354 |
| C | -2.56718964 | 0.39986242 | -0.89180576 |
| C | -3.77815345 | 0.98438352 | -0.52811863 |
| C | -4.73299442 | 0.20015521 | 0.08999718 |
| C | -4.48984748 | -1.13047084 | 0.37216580 |
| C | -3.27061637 | -1.73623399 | 0.02592523 |
| N | -3.01149601 | -3.05294483 | 0.29662923 |
| C | -1.66586472 | -3.56554567 | 0.16674146 |
| C | -3.98726024 | -3.85952403 | 0.98440751 |
| C | -2.32121300 | -0.94037131 | -0.62829019 |
| H | 4.25413228 | 4.01514107 | -1.92657616 |
| H | 4.97127008 | 2.84522342 | -3.07307480 |
| H | 3.84648857 | 4.09549233 | -3.65785048 |
| H | 4.89148192 | 1.98925103 | -0.89122071 |
| H | 4.70783965 | 0.27607698 | 0.80463097 |
| H | 4.53605094 | -1.94162626 | 1.68702488 |
| H | 3.85306585 | -0.74956322 | 2.79996459 |
| H | 3.35282407 | -2.44831557 | 2.90674727 |
| H | 0.75757347 | -0.64067840 | -0.52606572 |
| H | 0.41288983 | 2.27384967 | -2.57668327 |
| H | 0.84565953 | 0.83849536 | -3.54048901 |
| H | -3.94647353 | 2.02898256 | -0.73412334 |
| H | -5.68173480 | 0.63237801 | 0.37370495 |
| H | -5.25514891 | -1.69468206 | 0.87958995 |

| | | | |
|---|---|---|---|
| H | -0.93800950 | -2.94081954 | 0.69266047 |
| H | -1.61856613 | -4.56515040 | 0.59092790 |
| H | -1.37468329 | -3.63143730 | -0.88578388 |
| H | -4.13679027 | -3.53633847 | 2.02210805 |
| H | -4.94745191 | -3.82071488 | 0.46495362 |
| H | -3.65644913 | -4.89581081 | 0.99282313 |
| H | -1.37794257 | -1.35771629 | -0.93198146 |

**Data 2. Molecular SMILES and Molecular Conformation Counts Used in Benchmark Testing**

| **Smiles** | **count** |
|---|---|
| COc1c(N)ccn1C | 4 |
| OCC(O)C1=CCOC1 | 70 |
| c1n[nH]c2c1CCCO2 | 1 |
| [H]N=c1oc(N)ccc1C | 1 |
| CCC1CC2C(C#N)N12 | 3 |
| CCC1CC(C(N)=O)O1 | 3 |
| OCC12CC=CC1OC2 | 9 |
| O=C1C2C3C4C1N2C34 | 1 |
| O=CC12CCC3C1OC32 | 1 |
| CC12CC1C1(C#N)CC21 | 1 |
| CCC1(C(C)O)NC1C | 34 |
| C#CC(C)C1(O)COC1 | 9 |
| CC(C)Nc1nc[nH]n1 | 5 |
| C#CC1OCC2OCC12 | 2 |
| C1COC2CC2C1 | 4 |
| [H]N=COC(CO)C1CO1 | 51 |
| O=c1[nH]cno1 | 1 |
| OC12CCCC(O)(C1)C2 | 3 |
| C1CCC2C(C1)C1CC21 | 3 |
| CC1=CCC(=O)COC1 | 6 |
| N#CC(O)(C#N)CN | 12 |
| C1OC2CC3C1C3C2 | 1 |
| O=C1CC2(O)CC(C2)N1 | 1 |
| CCOC1(C)COC1 | 13 |
| C=C1CC(C(O)=C=O)N1 | 10 |
| CC(O)CC(C#N)C=O | 77 |
| OCC(CO)CN1CC1 | 117 |

| | |
|---|---|
| OC1COC2CC1CO2 | 3 |
| COCC1C2CC(C)N12 | 11 |
| O=C1NCC2=CCOC12 | 1 |
| CC1COC2(C#N)CC12 | 1 |
| [H]N=C1OC2(C3CC3)CC12 | 3 |
| [H]N=C1CNCC(CC)O1 | 22 |
| c1[nH]nnc1C1CCO1 | 1 |
| CCC12CC(C1)C2(C)O | 11 |
| OC1C2C(O)C3C1N23 | 2 |
| C1COC23CN(C2)C3C1 | 2 |
| CCCCCOC(C)C | 313 |
| CCC#CC1NC1CO | 99 |
| CC#CC(C)(C=O)OC | 7 |
| O=C1OC2CCC1OC2 | 1 |
| CC1CCOC(C)CO1 | 16 |
| C1=NC2CC2OCCO1 | 5 |
| [H]N=C1NCC1(N)C#N | 3 |
| CN=COC1COC1=O | 2 |
| COC1CNC1(C)C=O | 17 |
| C1C2C3OC3C1C21CN1 | 3 |
| O=C1CN2C3COC1C32 | 1 |
| N#CC1=CC2(CC1)CN2 | 1 |
| CCCC1=C(C)CCC1 | 10 |
| NC(=O)c1nccnn1 | 2 |
| CC1NC1(C)C#CC#N | 1 |
| Nc1cc(O)ccn1 | 2 |
| CCCc1n[nH]c(=O)o1 | 7 |
| C1CC2(CCC23CN3)O1 | 1 |
| O=CC(O)C1(O)CC1O | 33 |
| CCC(O)C1CC1CC | 50 |
| CC(C)C(N)(C#N)CN | 84 |
| OC1C2CC2C2CC12 | 2 |
| CC(C)N=C(N)C=O | 6 |
| CC#CC1C2C3CC2N13 | 1 |
| CC#CCC(N)C(=O)O | 13 |
| OCCOC1CCOC1 | 164 |
| CC12CC1C1(CC1)O2 | 1 |
| OCCCc1conn1 | 40 |
| CC1N2CCC3C2C31O | 3 |
| CC1(O)CC(C#N)C1 | 2 |
| [H]N=C(C)OCC#N | 6 |

| | |
|---|---|
| CCC12NC(C1=O)C2C | 3 |
| CNC(=O)N1CC(O)C1 | 11 |
| COCC12CC1CCO2 | 13 |
| Cn1nncc1N | 1 |
| CC(C#N)OCC1CN1 | 32 |
| CCCC1CC1OCC | 75 |
| c1cc(C2CCC2)n[nH]1 | 2 |
| OC12C3CC4CC1C2C43 | 2 |
| C1=NCC2C(O1)C1CN21 | 1 |
| [H]N=COC1CC1OC=N[H] | 8 |
| O=CC1OC=NC1CO | 15 |
| CC(C#N)N1CCC1C | 7 |
| FC(F)(F)C(F)(F)F | 1 |
| CC1(C)C2CC(O)C21 | 3 |
| Nc1cnc(C2CN2)o1 | 3 |
| O=C1NCC(CO)N1 | 14 |
| CC12CC1C1OC1C2O | 1 |
| CC1=CCOCOCC1 | 5 |
| C1=CC(=C2CCC2)CC1 | 1 |
| N#CCN=c1[nH]cc[nH]1 | 2 |
| CCNC(=NC)C(N)=O | 4 |
| CN(C=O)C1CC1C=O | 4 |
| CCC(O)C(C#N)CC | 84 |
| OC12C3CC1N1C3CC12 | 2 |
| c1cc2c[nH]ccc-2n1 | 1 |
| [H]N=C1OCC(=O)C2OC12 | 1 |
| CC12C3COC1C2OC3 | 1 |
| [H]N=CN1C=NCC1=O | 2 |
| CNC(=O)C1(O)COC1 | 4 |
| CC1C(=O)OC2CC21 | 1 |
| [H]N=C(N)C(=O)N(C)CC | 4 |
| C#Cc1coc(CC)n1 | 7 |

**Data 3. 3D Coordinates of Molecules Used in Quantum Computing Testing (ConfGAN)**

27

Energy = -42.21514935 a.u.

| | | | |
|---|---|---|---|
| N | -3.32907576 | 0.65830901 | 3.39438091 |
| C | -2.57028712 | 0.87780259 | 2.26618111 |
| C | -2.89476894 | 1.97540341 | 1.42343398 |

| | | | |
|---|---|---|---|
| C | -2.13217111 | 2.26951133 | 0.33869296 |
| C | -0.99402339 | 1.49151672 | 0.01647586 |
| C | -0.17674614 | 1.74603189 | -1.07917659 |
| C | 0.92099259 | 0.93018589 | -1.32925516 |
| C | 1.80476229 | 1.12300763 | -2.41840651 |
| C | 2.86184850 | 0.29323404 | -2.61528863 |
| C | 3.10959931 | -0.79306459 | -1.73278424 |
| N | 4.15072212 | -1.65102960 | -2.00978459 |
| C | 2.27137183 | -1.00373172 | -0.66523728 |
| C | 1.16401396 | -0.16268296 | -0.42954264 |
| N | 0.38804091 | -0.40943639 | 0.62362070 |
| C | -0.65894996 | 0.37812896 | 0.85968261 |
| C | -1.47374831 | 0.10263272 | 1.97743104 |
| H | -3.23101554 | -0.24218252 | 3.83329822 |
| H | -4.26096419 | 1.03885029 | 3.40011638 |
| H | -3.76292786 | 2.57249852 | 1.66629562 |
| H | -2.38423544 | 3.10493188 | -0.30023875 |
| H | -0.39495101 | 2.57879288 | -1.73704963 |
| H | 1.62147758 | 1.94905235 | -3.09201946 |
| H | 3.53412717 | 0.44370448 | -3.44871788 |
| H | 4.44674333 | -2.25451620 | -1.26056573 |
| H | 4.89064536 | -1.29876675 | -2.59436273 |
| H | 2.43942040 | -1.82023680 | 0.02008371 |
| H | -1.20777160 | -0.73726503 | 2.60065971 |

37

Energy = -51.66658912 a.u.

| | | | |
|---|---|---|---|
| C | 4.22705193 | -1.88845366 | -0.46867976 |
| C | 2.98669661 | -1.39461150 | -1.13903623 |
| C | 1.82736739 | -1.08040856 | -0.57875655 |
| C | 1.50558893 | -1.13936620 | 0.88542341 |
| C | 0.19653376 | -1.84059110 | 1.12113482 |
| C | -0.69515682 | -2.08726438 | 0.17302700 |
| C | -1.99554871 | -2.78034138 | 0.43798512 |
| C | -0.44404469 | -1.69848644 | -1.25447243 |
| C | 0.62146444 | -0.58714251 | -1.35945733 |
| N | 0.84797275 | -0.31091769 | -2.77287994 |
| C | 0.09557915 | 0.68342404 | -0.71815616 |
| C | -0.87275268 | 1.49270950 | -1.51764013 |
| C | -1.30364627 | 2.74559214 | -0.87618237 |
| C | -0.89045258 | 3.14722952 | 0.40942491 |

| | | | |
|---|---|---|---|
| O | -1.21589863 | 4.17398967 | 0.99791067 |
| N | -0.02338440 | 2.25004450 | 1.04861290 |
| C | 0.46086022 | 1.08425238 | 0.51334874 |
| C | 1.40743460 | 0.31138275 | 1.38410795 |
| H | 4.10746679 | -1.99591910 | 0.60462125 |
| H | 4.51163712 | -2.85474370 | -0.88495382 |
| H | 5.04707038 | -1.19541241 | -0.65777430 |
| H | 3.09655375 | -1.29673189 | -2.21360711 |
| H | 2.28677245 | -1.65609050 | 1.44896724 |
| H | -0.00028855 | -2.12543527 | 2.14568238 |
| H | -2.06194069 | -3.10659684 | 1.47230141 |
| H | -2.82801723 | -2.10809204 | 0.23106091 |
| H | -2.10040414 | -3.64817246 | -0.21236920 |
| H | -0.09322616 | -2.57450195 | -1.81096999 |
| H | -1.36810019 | -1.36327087 | -1.72805269 |
| H | 1.61428356 | 0.34551685 | -2.87891761 |
| H | 1.09289085 | -1.16366082 | -3.26280974 |
| H | -0.44159751 | 1.69799135 | -2.50824095 |
| H | -1.75799273 | 0.87884796 | -1.74735158 |
| H | -1.98124200 | 3.39366197 | -1.40752017 |
| H | 0.27621241 | 2.52611188 | 1.97367428 |
| H | 2.39694818 | 0.77918240 | 1.35479176 |
| H | 1.05509069 | 0.33096538 | 2.41888033 |

99

Energy = -149.96439232 a.u.

| | | | |
|---|---|---|---|
| C | 3.33323774 | -2.09804147 | -8.07712930 |
| C | 3.59914928 | -1.26146736 | -6.82659592 |
| C | 4.04191281 | 0.14376710 | -7.22521806 |
| C | 2.33760493 | -1.22356802 | -5.95291304 |
| C | 2.62218705 | -0.75147195 | -4.51892707 |
| N | 1.44720462 | -0.21544861 | -3.87238384 |
| C | 1.51256771 | 0.90682693 | -3.11648328 |
| O | 2.55859831 | 1.49874363 | -2.93996664 |
| C | 0.16484484 | 1.34414504 | -2.55362036 |
| C | -0.36497908 | 0.31564156 | -1.53445742 |
| C | 0.63220371 | -0.03859182 | -0.49033447 |
| C | 0.35154716 | -0.43462349 | 0.80829722 |
| C | 1.42686643 | -0.75612664 | 1.68464212 |
| C | 1.20545693 | -1.20150236 | 2.95707243 |
| C | -0.09780375 | -1.37720859 | 3.45206187 |

| | | | |
|---|---|---|---|
| C | -0.32277882 | -1.91913474 | 4.78734766 |
| C | 0.55672117 | -1.63761379 | 5.83618265 |
| C | 0.36723229 | -2.17715051 | 7.09205438 |
| C | -0.71505193 | -3.01167466 | 7.30306018 |
| F | -0.90783288 | -3.54174867 | 8.53167113 |
| C | -1.60923712 | -3.31063845 | 6.29140138 |
| C | -1.40953543 | -2.75999662 | 5.04195618 |
| C | -1.16751784 | -1.04597550 | 2.60589875 |
| C | -0.96060756 | -0.57443703 | 1.33822113 |
| C | 0.20969514 | 2.76136367 | -1.96423267 |
| C | 1.13255788 | 2.92584231 | -0.75641681 |
| C | 0.84016232 | 4.19311133 | 0.05639428 |
| C | 0.01259477 | 3.92795417 | 1.31737237 |
| C | -1.37711854 | 3.36844403 | 1.01938638 |
| C | -2.35060377 | 3.44401375 | 2.19908330 |
| N | -2.15737676 | 2.45047968 | 3.22324462 |
| C | -1.14439849 | 2.55269225 | 4.24739235 |
| C | -1.59466212 | 1.55456778 | 5.26836989 |
| C | -1.07753499 | 1.24341493 | 6.50823385 |
| C | -1.74205449 | 0.29820269 | 7.27709383 |
| C | -2.88580047 | -0.33238606 | 6.80921620 |
| C | -3.39626789 | -0.03460450 | 5.55660636 |
| C | -2.74009329 | 0.91691293 | 4.79645729 |
| C | -3.10122086 | 1.50026552 | 3.48596999 |
| O | -4.04698580 | 1.23835110 | 2.77054234 |
| C | 4.71850042 | 0.38067741 | -1.97142217 |
| O | 4.07176446 | -0.25088258 | -1.26390313 |
| O | 5.41031491 | 0.99328195 | -2.63973088 |
| C | 3.36170704 | -1.82298324 | -3.71721280 |
| O | 4.56575901 | -1.94164440 | -3.83756245 |
| N | 2.71310824 | -2.61395026 | -2.82043414 |
| C | 1.37113883 | -2.83164852 | -2.48419458 |
| C | 0.36694849 | -2.96365500 | -3.43946999 |
| C | -0.93592941 | -3.22016866 | -3.04713957 |
| C | -1.25075673 | -3.36698961 | -1.70654199 |
| C | -0.24800481 | -3.27570227 | -0.75547255 |
| C | 1.05287431 | -3.01224083 | -1.13920503 |
| H | 3.06713119 | -3.11933807 | -7.81319036 |
| H | 2.51885328 | -1.66749937 | -8.65721201 |
| H | 4.21962018 | -2.13048599 | -8.70514875 |
| H | 4.40116428 | -1.73261847 | -6.25086967 |
| H | 4.27285803 | 0.74918419 | -6.35306594 |

| | | | |
|---|---|---|---|
| H | 4.93608450 | 0.09190087 | -7.84110832 |
| H | 3.26048644 | 0.64210618 | -7.79658706 |
| H | 1.60916899 | -0.54191721 | -6.40003522 |
| H | 1.89823151 | -2.22353750 | -5.93351060 |
| H | 3.33157993 | 0.08549647 | -4.56492951 |
| H | 0.56902694 | -0.69373011 | -3.99333421 |
| H | -0.53765110 | 1.36630539 | -3.39729232 |
| H | -1.27762342 | 0.71366160 | -1.08500768 |
| H | -0.65446249 | -0.59925821 | -2.06806896 |
| H | 1.66533407 | -0.05167088 | -0.80462473 |
| H | 1.02925455 | 2.05526157 | -0.10481268 |
| H | 2.43535866 | -0.64783101 | 1.31190451 |
| H | 2.04673244 | -1.46373999 | 3.58221279 |
| H | 1.38792559 | -0.96910559 | 5.67178853 |
| H | 1.04233585 | -1.95895607 | 7.90475299 |
| H | -2.44085965 | -3.96893276 | 6.48818162 |
| H | -2.09116268 | -3.00692004 | 4.24279729 |
| H | -2.17876024 | -1.14234258 | 2.97045298 |
| H | -1.81479303 | -0.32678417 | 0.72732371 |
| H | 0.53401129 | 3.44821416 | -2.74944585 |
| H | -0.81098078 | 3.03219614 | -1.68790358 |
| H | 2.16099483 | 2.93883827 | -1.11474275 |
| H | 1.78348437 | 4.64553019 | 0.36864631 |
| H | 0.32343786 | 4.92342897 | -0.57002723 |
| H | 0.56339393 | 3.23298793 | 1.95399869 |
| H | -0.09318035 | 4.86904900 | 1.86450127 |
| H | -1.81819969 | 3.95046778 | 0.20700980 |
| H | -1.30098103 | 2.33014047 | 0.69871045 |
| H | -2.30204664 | 4.44181946 | 2.65385149 |
| H | -3.36642170 | 3.27786613 | 1.82648648 |
| H | -0.15566575 | 2.29295746 | 3.85018027 |
| H | -1.09348373 | 3.57070582 | 4.65205896 |
| H | -0.19063842 | 1.73329353 | 6.88170346 |
| H | -1.36794887 | 0.05595112 | 8.26040669 |
| H | -3.38448831 | -1.05757053 | 7.43415485 |
| H | -4.28780450 | -0.51205353 | 5.18023802 |
| H | 3.37058009 | -3.09404289 | -2.21440809 |
| H | 0.60651842 | -2.90134698 | -4.48933880 |
| H | -1.70598593 | -3.31882624 | -3.79823457 |
| H | -2.26779261 | -3.56645506 | -1.40711594 |
| H | -0.47870840 | -3.40251202 | 0.29099683 |
| H | 1.83247512 | -2.94282897 | -0.39603910 |

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Energy = -101.75378003 a.u.

| | | | |
|---|---|---|---|
| C | -3.31938406 | 2.75938363 | -0.28514871 |
| N | -2.06084608 | 2.56339553 | 0.40444803 |
| C | -2.18087707 | 2.09997182 | 1.77315332 |
| C | -2.67109416 | 0.65523545 | 1.90297995 |
| C | -1.60520468 | -0.40414491 | 1.58471426 |
| O | -0.36400248 | -0.15284386 | 2.17463435 |
| C | 0.22903409 | 1.13890808 | 2.14516018 |
| C | 1.24256981 | 1.05283756 | 3.30061260 |
| C | -0.82625143 | 2.23439072 | 2.50482774 |
| O | -0.21629356 | 3.48363676 | 2.27194993 |
| C | -0.71954886 | 4.54705510 | 3.04423684 |
| N | 0.90003132 | 1.35764656 | 0.88716086 |
| C | 2.04326012 | 2.09088390 | 0.63378079 |
| C | 2.83066686 | 2.87399397 | 1.46468001 |
| C | 3.97492445 | 3.46668810 | 0.95091082 |
| C | 4.35157530 | 3.30664621 | -0.37576718 |
| C | 3.56185473 | 2.56683046 | -1.23369375 |
| C | 2.40586278 | 1.97254634 | -0.73821143 |
| C | 1.41643073 | 1.18547466 | -1.38880569 |
| C | 1.36600789 | 0.52850980 | -2.58966407 |
| C | 0.36296133 | -0.40862450 | -2.89495950 |
| C | -0.56441952 | -0.77900190 | -1.89257955 |
| C | -1.61314796 | -1.75311508 | -1.81976750 |
| C | -2.13837535 | -2.66636158 | -2.72783637 |
| C | -3.18312229 | -3.46829003 | -2.31707151 |
| C | -3.70618185 | -3.37451477 | -1.02736644 |
| C | -3.20204481 | -2.47321417 | -0.10885702 |
| C | -2.15167657 | -1.66320797 | -0.51383655 |
| N | -1.47503376 | -0.67474113 | 0.17397213 |
| C | -0.51271695 | -0.16656356 | -0.64225361 |
| C | 0.28660868 | 1.05151723 | -0.40183796 |
| C | 0.58500558 | -0.92855202 | -4.23937100 |
| O | -0.04124601 | -1.74604258 | -4.88560404 |
| N | 1.70866789 | -0.28252247 | -4.69936184 |
| C | 2.32099259 | 0.61822008 | -3.75772993 |
| O | 2.49120641 | 1.90599071 | -4.28534505 |
| H | -4.04113352 | 3.35393888 | 0.29451373 |
| H | -3.12361566 | 3.26581769 | -1.22758428 |

| | | | |
|---|---|---|---|
| H | -3.76745343 | 1.79172491 | -0.50890728 |
| H | -0.43643945 | 1.87899255 | -0.59928207 |
| H | -1.53776272 | 3.43615291 | 0.42741258 |
| H | -2.91585543 | 2.73092798 | 2.31896325 |
| H | -2.98547690 | 0.50556680 | 2.93815553 |
| H | -3.53253394 | 0.48649691 | 1.25787325 |
| H | -1.92194230 | -1.35177654 | 2.04889927 |
| H | 0.82229251 | 0.39397817 | 4.05640440 |
| H | 2.17451480 | 0.62401706 | 2.94760520 |
| H | 1.42460998 | 2.02571262 | 3.74182191 |
| H | -1.03471661 | 2.10996297 | 3.58105047 |
| H | -0.65228052 | 4.32463916 | 4.11565913 |
| H | -0.09497047 | 5.40739614 | 2.81183918 |
| H | -1.76126933 | 4.78221549 | 2.79969087 |
| H | 2.56660911 | 3.06634342 | 2.48798865 |
| H | 4.58114436 | 4.07662263 | 1.60507779 |
| H | 5.24993511 | 3.78154392 | -0.74028753 |
| H | 3.80808813 | 2.47153181 | -2.27881332 |
| H | -1.72502299 | -2.72886158 | -3.72193720 |
| H | -3.60939702 | -4.18410956 | -3.00339104 |
| H | -4.52559642 | -4.01713709 | -0.74027726 |
| H | -3.62022034 | -2.40550316 | 0.88517709 |
| H | 2.12831205 | -0.50222928 | -5.58646648 |
| H | 3.33715186 | 0.29279343 | -3.48789083 |
| H | 1.62350200 | 2.27146261 | -4.49650709 |

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Energy = -167.22686015 a.u.

| | | | |
|---|---|---|---|
| C | 4.04866474 | -1.15464161 | -0.98120431 |
| C | 3.33787905 | -2.33859396 | -0.40101146 |
| C | 2.96961000 | -2.33017362 | 0.89558324 |
| N | 2.00219138 | -3.13703124 | 1.40510280 |
| C | 1.24944134 | -2.64867055 | 2.56085081 |
| C | 0.17505411 | -1.66836567 | 2.03344343 |
| C | 0.73189043 | -0.37538038 | 1.40258241 |
| O | 1.10515514 | -0.63711687 | 0.08018046 |
| P | 1.89661268 | 0.47131389 | -0.81846776 |
| O | 2.27556113 | 1.67907716 | -0.11957232 |
| O | 3.03717339 | -0.34068991 | -1.57312356 |
| O | 0.92719499 | 0.67777186 | -2.05081473 |
| P | 0.41839244 | -0.36994342 | -3.19094759 |

| | | | |
|---|---|---|---|
| O | 1.69391670 | -0.96563003 | -3.85845341 |
| O | -0.50745162 | 0.26688745 | -4.10175352 |
| O | -0.17825510 | -1.56092873 | -2.28236692 |
| C | -1.48618692 | -2.02908717 | -2.55251590 |
| C | -2.60107338 | -1.24627806 | -1.84133432 |
| O | -3.18338803 | -0.29483518 | -2.72457052 |
| C | -3.38980980 | 0.96111089 | -2.11731671 |
| N | -2.52002610 | 1.94130318 | -2.72407930 |
| C | -2.60956448 | 2.24307150 | -4.06909215 |
| N | -1.68830566 | 3.03527267 | -4.49841998 |
| C | -0.89434467 | 3.27696371 | -3.40733973 |
| C | 0.26514428 | 4.04559534 | -3.20561229 |
| N | 0.85884863 | 4.73400957 | -4.19083559 |
| N | 0.76377656 | 4.13786888 | -1.96657135 |
| C | 0.17971476 | 3.49203422 | -0.98408396 |
| N | -0.88310721 | 2.69767099 | -1.05945684 |
| C | -1.39837671 | 2.59414380 | -2.29072413 |
| C | -3.17766343 | 0.71100379 | -0.60980813 |
| O | -2.83825228 | 1.74190560 | 0.21998199 |
| C | -2.17810257 | -0.46965506 | -0.59626642 |
| O | -2.41409702 | -1.15897505 | 0.59590845 |
| P | -3.91985625 | -0.80638497 | 1.16150666 |
| O | -3.67548405 | 0.14930863 | 2.38984779 |
| O | -4.76403098 | -1.94476252 | 1.43631399 |
| O | -4.35366580 | 0.13592127 | -0.09011677 |
| C | 1.87343257 | -1.41069036 | 4.58687367 |
| C | 3.13648586 | -0.58090728 | 4.92408063 |
| O | 2.97812147 | 0.65743124 | 4.25432590 |
| P | 1.55275537 | 0.76020841 | 3.54131027 |
| O | 1.85428741 | 0.09269389 | 2.10016418 |
| O | 0.87230147 | -0.47204715 | 4.37339789 |
| O | 0.81005837 | 1.99545151 | 3.52627078 |
| O | 2.22654525 | -2.12719753 | 3.43502004 |
| C | 1.38076362 | -4.10107493 | 0.61618996 |
| O | 0.51332873 | -4.82523427 | 1.03016135 |
| N | 1.84446236 | -4.15672357 | -0.67752733 |
| C | 2.63533961 | -3.21589833 | -1.31727792 |
| O | 2.68071596 | -3.16677746 | -2.53274998 |
| H | 4.59521207 | -0.59767696 | -0.21663734 |
| H | 4.70745680 | -1.42743222 | -1.80963992 |
| H | 2.16182599 | -1.69239655 | -3.40259842 |
| H | 3.38876855 | -1.62210094 | 1.59392849 |

| | | | |
|---|---|---|---|
| H | 0.73957990 | -3.51238196 | 3.01677068 |
| H | -0.40263020 | -2.19098883 | 1.26949757 |
| H | -0.51328214 | -1.40383634 | 2.83502782 |
| H | -0.04200001 | 0.40630574 | 1.42519082 |
| H | -1.68955296 | -1.97060630 | -3.62500425 |
| H | -1.49970935 | -3.06813476 | -2.21668781 |
| H | -3.38975631 | -1.95612179 | -1.54582880 |
| H | -4.43009883 | 1.26194568 | -2.31014799 |
| H | -3.39376385 | 1.83458109 | -4.67312641 |
| H | 1.73653090 | 5.18411137 | -3.99877144 |
| H | 0.55112409 | 4.58083596 | -5.13484680 |
| H | 0.60186905 | 3.62354129 | 0.00075518 |
| H | -1.98674461 | 2.20814532 | -0.12949769 |
| H | -3.31553952 | 1.00929291 | 2.13603194 |
| H | -1.14233026 | -0.13129403 | -0.64357553 |
| H | 1.54420112 | -2.08281370 | 5.39162054 |
| H | 3.21620848 | -0.39086733 | 5.99686553 |
| H | 4.02609975 | -1.09330678 | 4.55438523 |
| H | 1.35338953 | -4.81198239 | -1.27902325 |

45

Energy = -74.15372811 a.u.

| | | | |
|---|---|---|---|
| O | 0.08010872 | -0.98932337 | 1.19781254 |
| C | -0.49759482 | -1.66054567 | 0.38348672 |
| C | -1.51582077 | -2.71695186 | 0.75180554 |
| C | -2.09187594 | -2.50667114 | 2.15092874 |
| C | -3.12798317 | -1.38332183 | 2.18530347 |
| C | -3.60297946 | -1.09971057 | 3.61158444 |
| C | -2.61196127 | -0.23465899 | 4.40740247 |
| C | -2.86914618 | 1.22526013 | 4.19592353 |
| C | -2.12167669 | 2.09193558 | 3.53026140 |
| C | -0.84710620 | 1.81183725 | 2.79660706 |
| C | -0.82648047 | 2.57294364 | 1.46724097 |
| O | 0.18108963 | 2.04182908 | 0.61337078 |
| C | -0.21299858 | 1.23555101 | -0.36199436 |
| O | -1.36880295 | 1.00258258 | -0.63260967 |
| C | 0.94966068 | 0.64942420 | -1.09069579 |
| C | 2.06376019 | 1.44115364 | -1.39948287 |
| O | 2.03970611 | 2.75609042 | -1.10160886 |
| C | 3.15462237 | 0.87685347 | -2.04561886 |
| C | 3.16350486 | -0.46953135 | -2.38014881 |

| | | | |
|---|---|---|---|
| O | 4.24530464 | -0.98297768 | -2.99176596 |
| C | 2.04100877 | -1.24277544 | -2.07521562 |
| Cl | 2.10258471 | -2.93223752 | -2.51921610 |
| C | 0.92585947 | -0.70163595 | -1.45266544 |
| C | -0.26724949 | -1.54113036 | -1.11565441 |
| H | -2.30942309 | -2.73891337 | 0.00365090 |
| H | -0.99235124 | -3.67732028 | 0.70872895 |
| H | -2.55805191 | -3.43330156 | 2.49375698 |
| H | -1.26895973 | -2.27400738 | 2.82861892 |
| H | -2.70881136 | -0.47482364 | 1.75069699 |
| H | -3.98343238 | -1.67729795 | 1.57162664 |
| H | -4.56678672 | -0.58719104 | 3.57928234 |
| H | -3.75453864 | -2.05191034 | 4.12574660 |
| H | -2.73542889 | -0.44493456 | 5.47317892 |
| H | -1.59051789 | -0.49239964 | 4.13444158 |
| H | -3.78388442 | 1.58125754 | 4.65465637 |
| H | -2.44059914 | 3.12631493 | 3.48379495 |
| H | 0.01200281 | 2.11978223 | 3.39914410 |
| H | -0.73549156 | 0.74945529 | 2.58065687 |
| H | -1.79676480 | 2.48147219 | 0.96667055 |
| H | -0.58620278 | 3.62878908 | 1.61412409 |
| H | 2.87338347 | 3.16797890 | -1.36254385 |
| H | 4.02157549 | 1.47017911 | -2.29516812 |
| H | 4.09459506 | -1.92836822 | -3.15670448 |
| H | -1.16397049 | -1.06037133 | -1.51618180 |
| H | -0.19068997 | -2.53881723 | -1.54777340 |

26

Energy = -42.46868271 a.u.

| | | | |
|---|---|---|---|
| C | 0.71456268 | -0.28823867 | 2.60638756 |
| O | 0.82300974 | 0.24893436 | 1.30288434 |
| C | 1.41713855 | -0.62036442 | 0.37403518 |
| O | 0.59542457 | -1.71367112 | 0.06520565 |
| C | -0.66542961 | -1.33355664 | -0.49562696 |
| C | -1.49786842 | -2.59579036 | -0.66427217 |
| C | -0.42330585 | -0.61344683 | -1.83219783 |
| O | 0.15518671 | -1.47927868 | -2.77390424 |
| C | 0.47477123 | 0.62754440 | -1.60106222 |
| O | -0.17246259 | 1.64378491 | -0.87952417 |
| C | 1.77305794 | 0.19817884 | -0.89208981 |
| O | 2.57671436 | 1.29635655 | -0.57893717 |

| | | | |
|---|---|---|---|
| H | 0.20379474 | 0.46410166 | 3.20330722 |
| H | 0.13800960 | -1.21720543 | 2.60081534 |
| H | 1.70768791 | -0.48335319 | 3.02227809 |
| H | 2.33092915 | -1.06285094 | 0.80036648 |
| H | -1.17679091 | -0.64678606 | 0.19390533 |
| H | -1.52690848 | -3.14339068 | 0.27335025 |
| H | -2.50820959 | -2.32864428 | -0.95939770 |
| H | -1.06254599 | -3.23258327 | -1.42932705 |
| H | -1.37665142 | -0.28126425 | -2.25569895 |
| H | 0.81699570 | -2.01348456 | -2.31552565 |
| H | 0.72116117 | 1.06467648 | -2.57514861 |
| H | -0.22688059 | 1.37244937 | 0.04944464 |
| H | 2.36354616 | -0.44473821 | -1.55321111 |
| H | 1.99583723 | 2.00053502 | -0.25505942 |

88

Energy = -152.07625084 a.u.

| | | | |
|---|---|---|---|
| C | -2.45111674 | -2.52123904 | 3.49150494 |
| C | -2.98929046 | -2.01144999 | 2.15990842 |
| O | -2.56488526 | -2.93324655 | 1.16964134 |
| C | -3.06856524 | -2.68304374 | -0.12622192 |
| O | -2.76990821 | -3.76543753 | -0.94060960 |
| C | -1.43695870 | -4.04242067 | -1.39250523 |
| C | -0.35337638 | -3.79504939 | -0.33075198 |
| O | -0.43866177 | -4.72206153 | 0.72278066 |
| C | 1.02884573 | -3.92586557 | -0.96793685 |
| O | 2.03963904 | -3.58037967 | -0.05528884 |
| C | 1.08253042 | -2.95340687 | -2.15421393 |
| O | 0.75834510 | -1.67358299 | -1.68533786 |
| C | 1.64757632 | -0.60673209 | -1.98702060 |
| C | 1.41829463 | -0.03301563 | -3.40307528 |
| O | 1.65148859 | -0.98279338 | -4.40229280 |
| C | 0.00637416 | 0.57476406 | -3.47523527 |
| O | -0.27805156 | 1.15279518 | -4.71216348 |
| C | -0.13989663 | 1.61535391 | -2.34496337 |
| O | 0.72738960 | 2.66082453 | -2.59087021 |
| O | 0.08253841 | 1.01241748 | -1.07782034 |
| C | 1.39208005 | 0.47473159 | -0.92867168 |
| C | 1.47228144 | -0.09088105 | 0.50405881 |
| O | 2.63488698 | -0.82035779 | 0.74827865 |
| O | 0.19134970 | -3.37032605 | -3.14782526 |
| C | -1.17545972 | -3.34297182 | -2.74925540 |

| | | | |
|---|---|---|---|
| C | -1.97074622 | -4.03565395 | -3.86795912 |
| O | -3.34538767 | -3.80796914 | -3.77716356 |
| C | -2.62192794 | -1.29182726 | -0.61587218 |
| O | -3.25578223 | -1.03611373 | -1.84043310 |
| C | -2.99831983 | -0.22209415 | 0.41962519 |
| O | -2.53725591 | 1.03084315 | -0.02068834 |
| C | -2.47473437 | -0.59297115 | 1.81486015 |
| N | -2.85374916 | 0.44556066 | 2.75631820 |
| C | 1.69520493 | 4.35040451 | 0.51944294 |
| C | 2.31702875 | 3.67338996 | 1.53470869 |
| C | 1.64000001 | 3.05112798 | 2.56873536 |
| C | 2.38119340 | 2.34242796 | 3.66344372 |
| O | 1.68437492 | 2.23515646 | 4.87350610 |
| C | 0.13746946 | 3.04731994 | 2.58919924 |
| O | -0.33490726 | 1.81032678 | 3.09822019 |
| C | -0.43337921 | 3.27417762 | 1.17892999 |
| O | -1.83376702 | 3.47629010 | 1.21991721 |
| C | 0.21486362 | 4.49221378 | 0.50523608 |
| O | -0.25484818 | 4.60066336 | -0.82862481 |
| H | -2.74376568 | -3.55904170 | 3.62254796 |
| H | -1.36604745 | -2.46046579 | 3.50325817 |
| H | -2.85430116 | -1.94210569 | 4.31730404 |
| H | -4.09341000 | -1.99413907 | 2.17939936 |
| H | -4.17333850 | -2.68301594 | -0.09822568 |
| H | -1.45671807 | -5.12843538 | -1.56428116 |
| H | -0.42814907 | -2.77656870 | 0.06742902 |
| H | -1.28272175 | -4.56503504 | 1.16937301 |
| H | 1.17264543 | -4.94984564 | -1.33942589 |
| H | 1.87559857 | -4.08812500 | 0.75138566 |
| H | 2.08032197 | -2.97379089 | -2.60825277 |
| H | 2.68524452 | -0.95519601 | -1.90816761 |
| H | 2.15284452 | 0.76308121 | -3.57276957 |
| H | 0.96026262 | -1.66020537 | -4.37535624 |
| H | -0.73771674 | -0.21703606 | -3.33322085 |
| H | 0.34297626 | 1.87975338 | -4.85152350 |
| H | -1.18520865 | 1.96205212 | -2.30306041 |
| H | 0.52003483 | 3.40813405 | -1.98899150 |
| H | 2.13252190 | 1.27376248 | -1.06042982 |
| H | 1.46218309 | 0.74442343 | 1.20907150 |
| H | 0.57560762 | -0.70071859 | 0.67104732 |
| H | 2.54645992 | -1.70862873 | 0.36336715 |
| H | -1.52126443 | -2.30514504 | -2.68896553 |

| | | | |
|---|---|---|---|
| H | -1.64459965 | -3.63354075 | -4.83053559 |
| H | -1.74207325 | -5.11253305 | -3.84878123 |
| H | -3.61202673 | -3.89801773 | -2.85240928 |
| H | -1.52695120 | -1.26330450 | -0.73878442 |
| H | -3.24727995 | -0.08154688 | -1.99576546 |
| H | -4.09238368 | -0.12999708 | 0.45946407 |
| H | -1.59182765 | 0.95219384 | -0.24538964 |
| H | -1.37737759 | -0.61920841 | 1.79359442 |
| H | -3.85660698 | 0.59909329 | 2.73909203 |
| H | -2.58885742 | 0.17766868 | 3.69741657 |
| H | 2.24191336 | 4.81127115 | -0.28415826 |
| H | 3.39659799 | 3.62528645 | 1.54048047 |
| H | 2.66692410 | 1.33498271 | 3.30366633 |
| H | 3.30851192 | 2.87863149 | 3.88796031 |
| H | 0.81305313 | 1.87057164 | 4.66009960 |
| H | -0.22558471 | 3.86747309 | 3.23754299 |
| H | -1.29071709 | 1.74742397 | 2.92996713 |
| H | -0.18327418 | 2.39538055 | 0.57657856 |
| H | -2.28912763 | 2.64940402 | 0.99510301 |
| H | -0.09142375 | 5.39611739 | 1.06186136 |
| H | -1.22014635 | 4.60035278 | -0.77902347 |

66

| | | | |
|---|---|---|---|
| C | -3.659300 | -2.776100 | 3.465300 |
| O | -3.577400 | -1.720400 | 2.515500 |
| C | -2.354500 | -1.754000 | 1.769100 |
| C | -1.269200 | -0.870000 | 2.455200 |
| O | -1.550800 | 0.008000 | 3.277500 |
| N | 0.048400 | -1.193300 | 2.183400 |
| C | 1.128700 | -0.832200 | 3.141100 |
| C | 2.279600 | -1.104300 | 2.288600 |
| N | 3.620000 | -1.169500 | 2.417400 |
| N | 4.215200 | -1.420100 | 1.223100 |
| C | 3.208300 | -1.444300 | 0.334000 |
| N | 3.474600 | -1.490300 | -1.013100 |
| C | 2.824900 | -0.790000 | -2.007300 |
| O | 2.981800 | -1.056200 | -3.195300 |
| C | 1.983200 | 0.379800 | -1.645400 |
| C | 2.450200 | 1.335200 | -0.739600 |
| C | 1.592200 | 2.336500 | -0.284300 |
| C | 0.265100 | 2.423800 | -0.733000 |

| | | | |
|---|---|---|---|
| N | -0.580500 | 3.372900 | -0.127100 |
| C | -1.732500 | 3.847000 | -0.915700 |
| C | -2.392800 | 5.053000 | -0.213900 |
| N | -2.783500 | 4.730800 | 1.228500 |
| C | -4.020700 | 3.894700 | 1.347700 |
| C | -1.596800 | 4.160200 | 2.004000 |
| C | -0.927500 | 2.981400 | 1.265600 |
| C | -0.138200 | 1.540100 | -1.744800 |
| C | 0.713900 | 0.524500 | -2.205100 |
| C | 1.979400 | -1.404700 | 0.997200 |
| C | 0.531300 | -1.516400 | 0.807700 |
| C | -2.709400 | -1.324900 | 0.357500 |
| C | -3.363900 | -0.108400 | 0.115400 |
| C | -3.756500 | 0.246600 | -1.177800 |
| C | -3.490100 | -0.610300 | -2.246000 |
| C | -2.847700 | -1.824500 | -2.020000 |
| C | -2.467200 | -2.185600 | -0.727400 |
| H | -3.626849 | -2.357809 | 4.482148 |
| H | -4.602647 | -3.323974 | 3.324126 |
| H | -2.811738 | -3.462911 | 3.324126 |
| H | -1.905227 | -2.757448 | 1.733795 |
| H | 1.077948 | 0.224413 | 3.442749 |
| H | 1.111199 | -1.367281 | 4.102028 |
| H | 4.126360 | -1.045421 | 3.305715 |
| H | 4.239170 | -2.112724 | -1.311296 |
| H | 3.491300 | 1.298099 | -0.386422 |
| H | 1.963883 | 3.073906 | 0.442393 |
| H | -1.389129 | 4.150704 | -1.915630 |
| H | -2.468123 | 3.034010 | -1.004617 |
| H | -1.683970 | 5.894160 | -0.210690 |
| H | -3.309376 | 5.308166 | -0.765967 |
| H | -3.039368 | 5.625111 | 1.670811 |
| H | -4.255156 | 3.736255 | 2.410680 |
| H | -4.860621 | 4.411089 | 0.859976 |
| H | -3.854828 | 2.922789 | 0.859976 |
| H | -0.851833 | 4.956732 | 2.147387 |
| H | -1.973056 | 3.784416 | 2.966922 |
| H | -0.010607 | 2.692314 | 1.800143 |
| H | -1.629140 | 2.134803 | 1.234385 |
| H | -1.140584 | 1.645026 | -2.185501 |
| H | 0.382060 | -0.154756 | -3.004158 |
| H | 0.161941 | -0.791438 | 0.067427 |

| | | | |
|---|---|---|---|
| H | 0.194302 | -2.489689 | 0.421513 |
| H | -3.570531 | 0.574018 | 0.953021 |
| H | -4.275054 | 1.200681 | -1.353391 |
| H | -3.787506 | -0.326672 | -3.266346 |
| H | -2.639714 | -2.500560 | -2.862428 |
| H | -1.972895 | -3.153101 | -0.555340 |

50

Energy = -85.37484735 a.u.

| | | | |
|---|---|---|---|
| C | -0.96335206 | 4.32865334 | 5.07046096 |
| C | -2.19072256 | 3.42666731 | 5.04077749 |
| C | -2.22729875 | 2.56795405 | 3.77668714 |
| C | -1.14282377 | 1.51125531 | 3.78578768 |
| O | -0.65530440 | 1.05463642 | 4.80749651 |
| N | -0.78516816 | 1.08082366 | 2.55864086 |
| C | 0.26482805 | 0.11708458 | 2.31773594 |
| C | 0.42631429 | -0.08679602 | 0.83840764 |
| N | -0.26142321 | 0.65061118 | 0.07123424 |
| O | -0.09757294 | 0.41272483 | -1.30145487 |
| C | -0.82161382 | 1.26219735 | -2.07184884 |
| O | -1.49861229 | 2.16510976 | -1.65542156 |
| N | -0.69563661 | 0.99058319 | -3.39933619 |
| C | -0.02893590 | -0.01074229 | -4.11807720 |
| C | -0.10371527 | 0.06277032 | -5.50926511 |
| C | 0.51329811 | -0.88797591 | -6.29838967 |
| C | 1.21310538 | -1.93063039 | -5.71375239 |
| C | 1.28841203 | -2.00773590 | -4.33438884 |
| C | 0.67631319 | -1.05835936 | -3.53434898 |
| O | 1.28886877 | -1.00661141 | 0.40905386 |
| C | 1.77101717 | -1.93327736 | 1.36762031 |
| C | 2.46088729 | -3.06512566 | 0.58828459 |
| O | 1.67657268 | -3.60055516 | -0.43264813 |
| C | 0.60146236 | -2.42167803 | 2.23696800 |
| O | -0.35402426 | -3.01892842 | 1.38918173 |
| C | 0.01425354 | -1.24123057 | 3.03809129 |
| O | 0.60640949 | -1.25811665 | 4.29802158 |
| H | -0.96666166 | 4.94358829 | 5.96698617 |
| H | -0.05671606 | 3.72887808 | 5.07110333 |
| H | -0.94626015 | 4.98480682 | 4.20229289 |
| H | -2.17584049 | 2.76772745 | 5.91029060 |
| H | -3.09592633 | 4.03487011 | 5.08539449 |
| H | -3.18484756 | 2.04332354 | 3.71578640 |

| | | | |
|---|---|---|---|
| H | -2.12673624 | 3.19004304 | 2.88631241 |
| H | -1.18002515 | 1.47833746 | 1.71596011 |
| H | 1.21985234 | 0.50138412 | 2.71609052 |
| H | -1.20983740 | 1.64863267 | -3.97201373 |
| H | -0.65127887 | 0.87286755 | -5.97099089 |
| H | 0.44504457 | -0.81386540 | -7.37368707 |
| H | 1.69352781 | -2.67534397 | -6.32987948 |
| H | 1.82564909 | -2.81580372 | -3.86157798 |
| H | 0.75437365 | -1.14547083 | -2.46531087 |
| H | 2.50608603 | -1.45554812 | 2.03117115 |
| H | 3.36152927 | -2.66969021 | 0.11072972 |
| H | 2.75641288 | -3.83957306 | 1.31454063 |
| H | 0.76189310 | -3.64509431 | -0.11850956 |
| H | 0.98710427 | -3.14587253 | 2.96852001 |
| H | -1.08444873 | -3.35707268 | 1.91847612 |
| H | -1.07977234 | -1.37767577 | 3.11089335 |
| H | 0.27247162 | -0.46622066 | 4.77912661 |

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Energy = -106.72030528 a.u.

| | | | |
|---|---|---|---|
| C | -5.13708129 | -0.72479337 | -2.15214885 |
| C | -3.89310804 | -0.29912205 | -1.41098110 |
| O | -3.90685343 | 0.09161024 | -0.25797209 |
| N | -2.77027531 | -0.36207636 | -2.15700883 |
| C | -1.44974079 | -0.15336455 | -1.61121261 |
| C | -0.53517795 | 0.46700189 | -2.68459856 |
| C | -0.06401659 | 1.87624478 | -2.35472553 |
| O | 0.14994529 | 1.99253259 | -1.04356494 |
| O | 0.18171277 | 2.72447202 | -3.16713604 |
| C | -0.97342243 | -1.49835802 | -1.03774384 |
| O | -1.54457694 | -2.53023314 | -1.31373755 |
| N | 0.06343654 | -1.51017044 | -0.15922216 |
| C | 1.00200932 | -0.50159844 | 0.21516001 |
| C | 2.23794222 | -1.18062074 | 0.84015197 |
| C | 1.84626146 | -2.11507182 | 1.95328571 |
| C | 1.54522987 | -1.61901914 | 3.21613077 |
| C | 1.14529267 | -2.47987126 | 4.22289821 |
| C | 1.04546825 | -3.84043894 | 3.98280498 |
| C | 1.34785289 | -4.34184053 | 2.72886021 |
| C | 1.74333000 | -3.48234627 | 1.71785180 |
| P | 1.02885799 | 1.83711628 | 1.57164439 |
| O | 0.42901132 | 0.40439235 | 1.15185608 |

| | | | |
|---|---|---|---|
| O | 1.10303175 | 1.95324853 | 3.01864661 |
| C | 2.47590990 | 2.29924801 | 0.50776422 |
| C | 1.94515697 | 3.46483555 | -0.32758481 |
| C | 2.27038954 | 4.80107585 | 0.32690798 |
| C | 0.41028153 | 3.26462474 | -0.34358237 |
| O | 0.01936588 | 2.95542149 | 0.95312110 |
| N | -0.28095604 | 4.38022217 | -0.84805549 |
| C | -1.68585723 | 4.52066753 | -0.45329260 |
| C | -2.31062654 | 5.64914768 | -1.26104585 |
| C | -2.44075075 | 3.20878276 | -0.70975705 |
| N | -2.97061699 | 2.62827108 | 0.37193255 |
| O | -2.52152089 | 2.73949309 | -1.83290656 |
| H | -6.00459382 | -0.57610976 | -1.51580779 |
| H | -5.24711908 | -0.13510381 | -3.05925135 |
| H | -5.06377894 | -1.77719262 | -2.41836701 |
| H | -2.81610017 | -0.85408944 | -3.03594600 |
| H | -1.55868174 | 0.52741710 | -0.76139279 |
| H | 0.35531687 | -0.14774113 | -2.84449986 |
| H | -1.06849937 | 0.53126012 | -3.63381412 |
| H | 0.14529857 | -2.38261830 | 0.35517036 |
| H | 1.29196578 | 0.05739385 | -0.68256401 |
| H | 2.76454103 | -1.72615103 | 0.05391900 |
| H | 2.88835861 | -0.39675197 | 1.23338883 |
| H | 1.61389379 | -0.55911069 | 3.40653979 |
| H | 0.91110892 | -2.08520506 | 5.19980938 |
| H | 0.73386922 | -4.50907392 | 4.77126535 |
| H | 1.27374812 | -5.40127677 | 2.53400250 |
| H | 1.98964040 | -3.88164876 | 0.74278628 |
| H | 3.28381256 | 2.61420140 | 1.16638930 |
| H | 2.83231163 | 1.48120261 | -0.11412306 |
| H | 2.31616553 | 3.44284753 | -1.35562618 |
| H | 3.34626616 | 4.95667693 | 0.34435276 |
| H | 1.80058000 | 5.61162124 | -0.22258209 |
| H | 1.89321846 | 4.80582008 | 1.34754110 |
| H | -0.18866237 | 4.40806575 | -1.86154573 |
| H | -1.68751387 | 4.75816095 | 0.61509098 |
| H | -2.37768080 | 5.35216100 | -2.30566016 |
| H | -3.31148164 | 5.85774348 | -0.89257162 |
| H | -1.70368116 | 6.54695806 | -1.18006114 |
| H | -3.39804902 | 1.70600092 | 0.27662730 |
| H | -2.76184361 | 2.96202972 | 1.29654614 |

87

Energy = -147.76919743 a.u.

| | | | |
|---|---|---|---|
| O | 3.78661514 | -3.82142814 | 2.14824375 |
| C | 3.29500684 | -3.59169040 | 1.07118165 |
| N | 2.65483421 | -2.44431857 | 0.74077914 |
| C | 2.37733269 | -1.42347384 | 1.71193204 |
| C | 1.25833196 | -1.80772009 | 2.69625022 |
| C | 0.02772220 | -2.35047488 | 2.02744336 |
| C | -1.12162509 | -1.58276258 | 1.90461639 |
| C | -2.24982425 | -2.08914067 | 1.28527782 |
| C | -2.25067788 | -3.38426061 | 0.79796239 |
| C | -1.12062000 | -4.17085203 | 0.93995876 |
| C | 0.00869808 | -3.65544126 | 1.54851897 |
| P | 2.18925915 | 0.09784076 | 0.67831451 |
| O | 3.27762784 | 0.27060589 | -0.28394953 |
| O | 0.74209506 | -0.17074018 | 0.00600368 |
| C | 1.92159501 | 1.54870050 | 1.79769131 |
| C | 0.93825293 | 2.56956765 | 1.21905232 |
| C | -0.53493431 | 2.19886049 | 1.45756868 |
| C | -1.41373037 | 3.04637670 | 0.60510585 |
| C | -1.58439607 | 4.39506041 | 0.50543595 |
| C | -2.52247830 | 4.54989111 | -0.55290409 |
| C | -3.07626970 | 5.78019546 | -1.09537310 |
| C | -4.25880523 | 5.74255009 | -1.83269776 |
| C | -4.78996785 | 6.90670222 | -2.35155021 |
| C | -4.14837245 | 8.11770803 | -2.14386362 |
| C | -2.96938817 | 8.16007872 | -1.41818616 |
| C | -2.43302823 | 6.99894239 | -0.89362282 |
| N | -2.86224963 | 3.37050954 | -1.02337593 |
| O | -2.18085429 | 2.43630110 | -0.31644658 |
| C | 1.22278597 | 2.83677201 | -0.25859377 |
| O | 1.66040231 | 3.91262757 | -0.61078242 |
| N | 0.99513185 | 1.87357652 | -1.18211688 |
| C | 0.38631776 | 0.56875702 | -1.14513273 |
| C | 0.80169627 | -0.18359236 | -2.41659300 |
| C | 0.33036523 | -1.60963777 | -2.37422056 |
| C | 1.23972261 | -2.65143316 | -2.23787894 |
| C | 0.81581370 | -3.96396759 | -2.16100766 |
| C | -0.54044690 | -4.25827488 | -2.23437324 |
| O | -0.92706285 | -5.56043405 | -2.16506150 |
| C | -1.45613638 | -3.22358485 | -2.38650926 |

| | | | |
|---|---|---|---|
| C | -1.02233825 | -1.91334063 | -2.44748593 |
| C | -1.63540333 | 3.55461434 | -3.54548153 |
| O | -2.30816815 | 4.42077790 | -3.86383725 |
| O | -0.93939117 | 2.68702606 | -3.26813061 |
| O | 3.31604578 | -4.42735712 | 0.01180571 |
| C | 3.72692576 | -5.77579554 | 0.27071482 |
| C | 2.51228541 | -6.59323307 | 0.62750336 |
| C | 2.07880733 | -6.65302190 | 1.94679077 |
| C | 0.90692360 | -7.31619129 | 2.26686347 |
| C | 0.15851581 | -7.92275776 | 1.27202135 |
| C | 0.58824833 | -7.87143143 | -0.04323883 |
| C | 1.75897676 | -7.20778397 | -0.36389800 |
| H | 2.12577725 | -2.43292068 | -0.12180950 |
| H | 3.29891922 | -1.25744051 | 2.28882635 |
| H | 1.67578728 | -2.57682650 | 3.35156572 |
| H | 1.00640706 | -0.93723654 | 3.30401672 |
| H | -1.14386930 | -0.58741137 | 2.32299092 |
| H | -3.13423182 | -1.47517784 | 1.19444399 |
| H | -3.13872469 | -3.78338482 | 0.32986823 |
| H | -1.11070638 | -5.19207530 | 0.58883318 |
| H | 0.87300506 | -4.28933590 | 1.67401868 |
| H | 1.58239082 | 1.22323478 | 2.78145348 |
| H | 2.90430296 | 2.01031180 | 1.90678607 |
| H | 1.12330837 | 3.53418820 | 1.70749584 |
| H | -0.72034300 | 1.15569403 | 1.20965202 |
| H | -0.77586776 | 2.35766937 | 2.51246759 |
| H | -1.12542170 | 5.15851046 | 1.09527637 |
| H | -4.74409079 | 4.79140278 | -1.98526935 |
| H | -5.70694060 | 6.87237639 | -2.92096152 |
| H | -4.56476556 | 9.02761500 | -2.55025613 |
| H | -2.46392707 | 9.10196099 | -1.26234609 |
| H | -1.50427310 | 7.03485782 | -0.34441779 |
| H | 1.27672298 | 2.17094241 | -2.10844272 |
| H | -0.71233404 | 0.65233046 | -1.10250188 |
| H | 0.37053844 | 0.33876141 | -3.27273647 |
| H | 1.89080896 | -0.15440202 | -2.47766901 |
| H | 2.29911498 | -2.43653256 | -2.21942357 |
| H | 1.52249305 | -4.76735471 | -2.03861000 |
| H | -1.88835077 | -5.61724407 | -2.22527606 |
| H | -2.51249889 | -3.44708854 | -2.45725490 |
| H | -1.74509920 | -1.11934525 | -2.56435988 |
| H | 4.19025241 | -6.12497532 | -0.65410616 |

| | | | |
|---|---|---|---|
| H | 4.45806018 | -5.77556494 | 1.08523151 |
| H | 2.66028117 | -6.16995653 | 2.71893561 |
| H | 0.57457416 | -7.35427969 | 3.29397103 |
| H | -0.75878708 | -8.43538011 | 1.52319447 |
| H | 0.00787284 | -8.33952013 | -0.82402445 |
| H | 2.08878978 | -7.16662045 | -1.39157763 |

41

Energy = -76.78652051 a.u.

| | | | |
|---|---|---|---|
| O | -1.07999904 | -1.59367488 | 0.08531480 |
| P | 0.38303988 | -1.03138013 | -0.03026821 |
| O | 0.26748111 | 0.55124700 | -0.40018703 |
| O | 1.34722298 | -1.27595876 | 1.01891039 |
| C | -0.16270699 | 0.86252298 | -1.68093315 |
| C | -1.54204705 | 1.49767533 | -1.77323312 |
| C | -2.69294237 | 0.75503364 | -1.08359682 |
| C | -2.84079850 | 1.04286263 | 0.42231884 |
| C | -1.92908172 | 0.28634667 | 1.33860287 |
| C | -1.92863816 | -1.20008646 | 1.24840577 |
| C | -1.40691989 | -1.86618997 | 2.46629066 |
| C | -0.62131014 | -1.20525466 | 3.34488326 |
| C | -0.37091469 | 0.17528541 | 3.18493519 |
| O | 0.46095277 | 0.76032441 | 4.07527585 |
| C | 1.17607897 | 1.87612158 | 3.72311205 |
| C | 1.67502819 | 2.06959076 | 2.43779068 |
| C | 2.43614816 | 3.19213061 | 2.16975474 |
| C | 2.70641447 | 4.11745921 | 3.16526893 |
| C | 2.22286770 | 3.91026498 | 4.44697380 |
| C | 1.45955081 | 2.79389077 | 4.73109825 |
| C | -1.09368994 | 0.90152084 | 2.21839776 |
| S | -0.06200970 | -0.71792197 | -2.63342164 |
| O | -1.33711514 | -1.30595165 | -2.85437113 |
| O | 0.74714982 | -1.56768072 | -1.50110195 |
| O | 0.78940593 | -0.55168618 | -3.76055326 |
| H | 0.58938054 | 1.49785266 | -2.16156072 |
| H | -1.47579734 | 2.51221952 | -1.36898131 |
| H | -1.76207550 | 1.56994759 | -2.84087573 |
| H | -3.61353243 | 1.09206701 | -1.56505668 |
| H | -2.60162993 | -0.31264458 | -1.27121366 |
| H | -2.71945471 | 2.11389674 | 0.59874796 |
| H | -3.86826554 | 0.77861670 | 0.69769469 |

| | | | |
|---|---|---|---|
| H | -2.90247163 | -1.59897935 | 0.94272135 |
| H | -1.58425327 | -2.92444199 | 2.56067568 |
| H | -0.16649943 | -1.70887801 | 4.18254094 |
| H | 1.48708349 | 1.32877951 | 1.67479088 |
| H | 2.82869290 | 3.33844924 | 1.17470341 |
| H | 3.30035456 | 4.99166655 | 2.94553590 |
| H | 2.43924948 | 4.62192922 | 5.22948145 |
| H | 1.07621995 | 2.61497967 | 5.72353787 |
| H | -1.02183764 | 1.98093207 | 2.22727248 |

52

Energy = -85.40067627 a.u.

| | | | |
|---|---|---|---|
| C | 4.17615402 | 2.64615832 | 4.58772739 |
| C | 4.85559448 | 1.76544318 | 5.63005640 |
| C | 5.56648539 | 0.54639680 | 5.03755504 |
| C | 4.63991152 | -0.64472549 | 4.74914617 |
| C | 3.67248072 | -0.39450794 | 3.63279433 |
| C | 4.12339327 | -0.26153188 | 2.32144091 |
| C | 3.24885467 | -0.00907594 | 1.28912360 |
| C | 1.86963837 | 0.12565605 | 1.52030275 |
| C | 0.95322976 | 0.42688069 | 0.44685493 |
| C | -0.37161121 | 1.04242459 | 0.77946911 |
| C | -1.08959151 | 1.60196198 | -0.38797649 |
| C | -0.80430202 | 1.22722628 | -1.66138997 |
| C | -1.75225111 | 1.55991527 | -2.77812288 |
| C | -2.09410579 | 0.37931615 | -3.70874620 |
| C | -2.17292718 | -1.02847439 | -3.09719166 |
| C | -2.96912430 | -1.16499845 | -1.78778204 |
| P | -2.49347633 | -0.64659251 | 0.77021672 |
| O | -1.23542591 | -0.00338863 | 1.41177185 |
| O | -3.08237181 | -1.76638492 | 1.49313935 |
| O | -3.57495472 | 0.53626728 | 0.56262413 |
| S | -4.85793067 | -0.05835953 | -0.33583727 |
| O | -5.69667681 | 1.05866010 | -0.60701055 |
| O | -2.04678028 | -0.99969237 | -0.73518624 |
| O | -4.00639153 | -0.25029097 | -1.75249016 |
| C | 0.38154036 | 0.49806038 | -1.91255676 |
| C | 1.23655155 | 0.15601061 | -0.87990358 |
| C | 1.42187356 | -0.01780086 | 2.84312738 |
| C | 2.30518213 | -0.28151466 | 3.86772997 |
| H | 3.73784445 | 3.52005910 | 5.06507654 |
| H | 4.89957215 | 2.98755892 | 3.85005091 |

| | | | |
|---|---|---|---|
| H | 3.38829816 | 2.10790252 | 4.06937942 |
| H | 5.59483313 | 2.37044342 | 6.16138868 |
| H | 4.11798120 | 1.43346580 | 6.36379123 |
| H | 6.08009817 | 0.84059720 | 4.12039729 |
| H | 6.32487598 | 0.20672259 | 5.74721573 |
| H | 5.26656315 | -1.50125929 | 4.48391021 |
| H | 4.09385431 | -0.89784393 | 5.66001653 |
| H | 5.18000402 | -0.35293903 | 2.11294697 |
| H | 3.64025016 | 0.11971573 | 0.29189495 |
| H | -0.27021987 | 1.77825235 | 1.58652972 |
| H | -1.96100785 | 2.19829129 | -0.16384024 |
| H | -2.67581281 | 1.93844365 | -2.33851334 |
| H | -1.33021367 | 2.35816060 | -3.39619222 |
| H | -3.05708200 | 0.60517574 | -4.16877682 |
| H | -1.35357063 | 0.32033518 | -4.50978739 |
| H | -2.62607532 | -1.68540265 | -3.84102542 |
| H | -1.17451836 | -1.40300456 | -2.86833295 |
| H | -3.38240690 | -2.18856226 | -1.70590669 |
| H | 0.63561519 | 0.23101641 | -2.92637444 |
| H | 2.15146315 | -0.36293377 | -1.12484863 |
| H | 0.36687542 | 0.04197324 | 3.05639290 |
| H | 1.92919316 | -0.39533936 | 4.87465286 |

30

Energy = -41.35152929 a.u.

| | | | |
|---|---|---|---|
| C | -0.85098988 | -0.01751399 | 2.75538087 |
| C | -0.28205425 | -1.29320723 | 2.14431818 |
| C | -1.29012885 | -2.43561186 | 2.24399942 |
| C | 0.20016345 | -1.09081983 | 0.67773385 |
| N | -0.89861793 | -0.88182276 | -0.26009944 |
| C | -0.37978528 | -0.60290613 | -1.58883765 |
| C | 0.23364763 | 0.81038867 | -1.64945825 |
| O | 1.11236393 | 0.91706168 | -2.74248834 |
| C | 0.91687296 | 1.20008316 | -0.30543515 |
| O | 0.17985666 | 2.20267294 | 0.37615864 |
| C | 1.17343684 | 0.01469490 | 0.55317067 |
| O | -2.53040563 | 1.27338193 | 0.30184611 |
| H | -1.07233528 | -0.18425104 | 3.80714857 |
| H | -0.13226808 | 0.79401421 | 2.67779726 |
| H | -1.76696458 | 0.28366419 | 2.25781966 |
| H | 0.61543654 | -1.57441614 | 2.70693503 |
| H | -1.46952087 | -2.67536362 | 3.28937417 |

| | | | |
|---|---|---|---|
| H | -2.24129223 | -2.15034071 | 1.80038569 |
| H | -0.92052827 | -3.33309843 | 1.74999232 |
| H | 0.73263709 | -2.03741731 | 0.41930506 |
| H | -1.48449667 | -1.71047987 | -0.27964360 |
| H | -2.05411851 | 0.45019726 | 0.06079552 |
| H | 0.40380475 | -1.32754970 | -1.87607112 |
| H | -1.18813085 | -0.68295795 | -2.31893091 |
| H | -0.54398033 | 1.55353033 | -1.85217888 |
| H | 1.86649252 | 0.33396279 | -2.59785410 |
| H | 1.86726532 | 1.69559007 | -0.54367564 |
| H | -0.72804279 | 1.89029051 | 0.54721092 |
| H | 2.02366361 | 0.01536041 | 1.21166677 |
| H | -2.91885000 | 1.63007149 | -0.49839558 |

49

Energy = -97.19790339 a.u.

| | | | |
|---|---|---|---|
| C | 0.40525936 | -5.56446401 | 1.61982957 |
| C | 0.61544060 | -4.07847379 | 1.73602315 |
| O | 0.30523344 | -3.42770670 | 2.71175856 |
| N | 1.17088176 | -3.52641904 | 0.61379708 |
| C | 1.58367400 | -2.20712202 | 0.42518995 |
| C | 1.88102120 | -1.36356782 | 1.49281472 |
| C | 2.32058424 | -0.07724223 | 1.25584723 |
| C | 2.47156636 | 0.39702660 | -0.04350077 |
| O | 2.94771200 | 1.68969639 | -0.19305300 |
| C | 2.27788875 | 2.53296216 | -1.10512332 |
| C | 0.93072086 | 2.98662781 | -0.49191136 |
| C | 0.33098370 | 4.15277801 | -1.27476972 |
| O | 1.13747779 | 3.36097467 | 0.85550737 |
| C | -0.01793935 | 1.77357180 | -0.58919052 |
| O | -0.30564018 | 1.28053726 | -1.65483694 |
| N | -0.44988823 | 1.34975895 | 0.63217527 |
| C | -1.06374929 | 0.16253605 | 0.96892802 |
| C | -1.29951178 | -0.11305678 | 2.31793334 |
| C | -1.84993020 | -1.31712888 | 2.68900550 |
| C | -2.16284895 | -2.27701043 | 1.73234619 |
| N | -2.64539225 | -3.54825404 | 2.21260550 |
| O | -3.21582787 | -3.55570094 | 3.27738921 |
| O | -2.43301931 | -4.52346560 | 1.52747227 |
| C | -1.95575135 | -2.00047665 | 0.37712583 |
| C | -2.31638882 | -2.97025797 | -0.72588818 |
| F | -1.41455020 | -3.95833207 | -0.86337054 |

| | | | |
|---|---|---|---|
| F | -3.51908357 | -3.53027432 | -0.56864116 |
| F | -2.35427553 | -2.36329432 | -1.92339467 |
| C | -1.42187290 | -0.78000195 | 0.00296921 |
| C | 2.19274342 | -0.44732667 | -1.11103226 |
| C | 1.75299415 | -1.73442099 | -0.87462343 |
| H | 0.25009840 | -5.98122968 | 2.61077588 |
| H | -0.49252209 | -5.74585704 | 1.03096128 |
| H | 1.25247328 | -6.04745887 | 1.14039651 |
| H | 1.20183271 | -4.11224993 | -0.20906825 |
| H | 1.76005063 | -1.71695953 | 2.50255328 |
| H | 2.56552314 | 0.57112175 | 2.08367477 |
| H | 2.93463581 | 3.39655460 | -1.23739089 |
| H | 2.09693036 | 2.06009781 | -2.07317305 |
| H | -0.56637830 | 4.50050171 | -0.76995484 |
| H | 1.04241532 | 4.97256829 | -1.32533611 |
| H | 0.07487467 | 3.82550871 | -2.27778255 |
| H | 2.00895333 | 3.02322071 | 1.11577904 |
| H | -0.15109902 | 1.95350721 | 1.39662157 |
| H | -1.03278074 | 0.61414685 | 3.06925774 |
| H | -2.01980711 | -1.55992994 | 3.72618164 |
| H | -1.26741921 | -0.54642403 | -1.03816485 |
| H | 2.31550757 | -0.10924749 | -2.12777109 |
| H | 1.53865037 | -2.38360561 | -1.71084620 |

57

Energy = -99.75649711 a.u.

| | | | |
|---|---|---|---|
| C | -2.82598179 | -4.53530017 | -0.58950530 |
| C | -3.37722890 | -3.49038032 | -1.56186807 |
| C | -3.14910566 | -3.96389826 | -3.00288802 |
| C | -4.87863782 | -3.30513846 | -1.32808255 |
| C | -2.67961773 | -2.12120111 | -1.33863463 |
| N | -1.32109087 | -2.11644092 | -1.90844208 |
| C | -2.64464244 | -1.77162304 | 0.15977018 |
| O | -3.65074885 | -1.33798881 | 0.70625983 |
| N | -1.49911391 | -1.99988133 | 0.78706614 |
| S | 0.48559006 | -2.09186588 | 0.35693485 |
| O | 0.38989951 | -3.33799293 | -0.43833328 |
| O | 0.50753012 | -0.91825540 | -0.54221267 |
| O | 2.12960824 | -2.19407247 | 0.91350516 |
| C | 2.59662830 | -0.97495335 | 1.37666494 |
| C | 1.85380615 | -0.56307046 | 2.65934309 |
| O | 0.44942163 | -0.52741032 | 2.43169962 |

| | | | |
|---|---|---|---|
| C | -0.03675463 | 0.79829933 | 2.40057541 |
| N | -0.25162401 | 1.27765020 | 1.06423016 |
| C | -1.41143821 | 1.14543956 | 0.34099368 |
| N | -1.31383474 | 1.52330520 | -0.89276780 |
| C | -0.00829181 | 1.92630991 | -1.03672049 |
| C | 0.73628881 | 2.44026492 | -2.10933755 |
| N | 0.22495267 | 2.60820733 | -3.34594066 |
| N | 2.01834590 | 2.75313422 | -1.90226787 |
| C | 2.53702357 | 2.56180813 | -0.70340961 |
| N | 1.95084465 | 2.08957503 | 0.38315842 |
| C | 0.67239931 | 1.76806571 | 0.18101344 |
| C | 0.96685696 | 1.66465928 | 3.17430703 |
| O | 0.46526255 | 1.87036827 | 4.46925279 |
| C | 2.27630230 | 0.82335556 | 3.18930778 |
| O | 2.85298124 | 0.77561471 | 4.46075269 |
| H | -3.20273461 | -5.52079006 | -0.85320551 |
| H | -1.73897148 | -4.56425858 | -0.60139309 |
| H | -3.14341922 | -4.30822864 | 0.42430543 |
| H | -3.80346917 | -4.80762157 | -3.20845007 |
| H | -3.38945611 | -3.17978597 | -3.71952761 |
| H | -2.12656089 | -4.30065285 | -3.15716406 |
| H | -5.38098010 | -4.26896239 | -1.32646220 |
| H | -5.05232168 | -2.81886524 | -0.37248969 |
| H | -5.31706251 | -2.68878159 | -2.11008913 |
| H | -3.27250224 | -1.33888295 | -1.82701425 |
| H | -0.71590467 | -2.88119061 | -1.44103857 |
| H | -1.33474153 | -2.19523316 | -2.92263815 |
| H | -0.75632224 | -1.28741733 | -1.57587735 |
| H | -1.53229493 | -1.76880092 | 1.76915367 |
| H | 3.66245735 | -1.08822421 | 1.59896834 |
| H | 2.45772195 | -0.20281760 | 0.61061314 |
| H | 2.01798199 | -1.34057031 | 3.41725889 |
| H | -1.00930807 | 0.79291121 | 2.91022447 |
| H | -2.31629175 | 0.78099826 | 0.78625132 |
| H | 0.78071927 | 3.10200947 | -4.02194501 |
| H | -0.76989119 | 2.53684103 | -3.46406726 |
| H | 3.57827992 | 2.83474917 | -0.59283717 |
| H | 1.12382828 | 2.62033589 | 2.66192630 |
| H | 1.13091045 | 2.35682895 | 4.97389681 |
| H | 3.01658790 | 1.27717411 | 2.52843910 |
| H | 2.20757971 | 0.39938675 | 5.07657303 |

55

Energy = -77.31225205 a.u.

| | | | |
|---|---|---|---|
| O | 4.38818704 | -1.34721224 | -1.30421624 |
| C | 4.52756411 | -1.67208490 | 0.00993504 |
| C | 5.67855594 | -2.36777429 | 0.39398963 |
| C | 6.63627552 | -2.75471321 | -0.58118635 |
| C | 7.77043914 | -3.43781309 | -0.23697058 |
| C | 8.05065711 | -3.79315475 | 1.08869605 |
| C | 9.32569226 | -4.55119259 | 1.41040727 |
| C | 10.53316099 | -3.69288022 | 1.00425475 |
| C | 9.34327712 | -5.87029971 | 0.62360849 |
| C | 9.45660624 | -4.88518458 | 2.89903611 |
| C | 7.12016691 | -3.40925184 | 2.05492235 |
| C | 5.97496141 | -2.72080353 | 1.73375729 |
| C | 3.45471358 | -1.24448886 | 0.97309791 |
| C | 2.06952103 | -1.12813517 | 0.32466589 |
| N | 2.04857862 | -0.09585762 | -0.70986842 |
| C | 2.47909166 | 1.25505018 | -0.34057795 |
| C | 1.81085740 | 2.19660134 | -1.35144556 |
| O | 0.96007090 | 3.09540412 | -0.68978511 |
| C | 0.99030665 | 1.25338610 | -2.27560313 |
| O | -0.16562927 | 1.89382760 | -2.74159374 |
| C | 0.76829275 | 0.02218671 | -1.38588407 |
| C | -0.40785129 | 0.21640572 | -0.40570899 |
| O | -1.60535632 | 0.17771803 | -1.17151966 |
| C | -0.39070720 | -0.88300060 | 0.65831007 |
| C | 0.96084516 | -0.92360782 | 1.36557474 |
| H | 6.44531103 | -2.49431676 | -1.60998512 |
| H | 8.46492785 | -3.70478035 | -1.02025696 |
| H | 10.52239861 | -2.75013584 | 1.54748998 |
| H | 11.46048991 | -4.21435422 | 1.23376343 |
| H | 10.51941489 | -3.47200534 | -0.05939279 |
| H | 10.24599681 | -6.43305683 | 0.85348900 |
| H | 8.48010965 | -6.47705794 | 0.88951659 |
| H | 9.31678990 | -5.69284936 | -0.44770323 |
| H | 9.48996525 | -3.98077821 | 3.50208881 |
| H | 8.62894106 | -5.50638732 | 3.23375404 |
| H | 10.38046452 | -5.43539622 | 3.06790874 |
| H | 7.28754157 | -3.64954313 | 3.09309491 |
| H | 5.29942568 | -2.43984312 | 2.52739621 |
| H | 3.38525096 | -1.98163991 | 1.77432704 |
| H | 3.72246839 | -0.28813778 | 1.43698583 |

| | | | |
|---|---|---|---|
| H | 1.86165614 | -2.07260213 | -0.20003739 |
| H | 3.55462563 | -0.85072534 | -1.42097691 |
| H | 2.16000238 | 1.55508829 | 0.66368557 |
| H | 3.56740653 | 1.31843100 | -0.39587821 |
| H | 2.55403809 | 2.75797501 | -1.93394439 |
| H | 0.27315218 | 3.32999975 | -1.33435905 |
| H | 1.60929092 | 0.96679193 | -3.13597773 |
| H | -0.93447201 | 1.39017154 | -2.43031148 |
| H | 0.57335576 | -0.87916023 | -1.97739113 |
| H | -0.31144115 | 1.19789189 | 0.08190610 |
| H | -2.35973706 | 0.20873938 | -0.57317709 |
| H | -1.19304097 | -0.70481891 | 1.38008894 |
| H | -0.58067734 | -1.84283492 | 0.16985674 |
| H | 0.97774063 | -1.74075343 | 2.08744725 |
| H | 1.12460072 | 0.00930076 | 1.90864749 |

37

Energy = -74.42337496 a.u.

| | | | |
|---|---|---|---|
| C | -1.67505754 | 3.15279736 | 1.62816984 |
| C | -0.38751675 | 2.49313945 | 2.00565009 |
| C | -0.10371777 | 1.18594202 | 1.57253711 |
| N | -1.07916803 | 0.50608227 | 0.87929372 |
| C | -0.91050732 | -0.20808613 | -0.14187132 |
| O | -1.94477639 | -0.95517639 | -0.60873149 |
| C | -1.54459006 | -1.66496286 | -1.75553759 |
| C | -1.44622042 | -3.16020274 | -1.41074355 |
| F | -0.59805441 | -3.38351607 | -0.40311738 |
| F | -0.98987995 | -3.86058966 | -2.46219433 |
| F | -2.62166871 | -3.68280272 | -1.07340922 |
| C | -0.16715065 | -1.10372989 | -2.13081136 |
| C | -0.12208382 | -0.06324147 | -3.27534766 |
| O | -0.05766300 | -0.60558803 | -4.55208456 |
| C | 1.08457409 | 0.79042863 | -2.84604794 |
| C | 1.02781175 | 0.79848305 | -1.31147694 |
| N | 0.20171281 | -0.34986523 | -0.95066379 |
| C | 1.09319032 | 0.56360225 | 1.94506775 |
| C | 2.01517849 | 1.22705344 | 2.72044251 |
| C | 1.76710276 | 2.53735438 | 3.13401509 |
| C | 2.72555213 | 3.22281675 | 3.91015375 |
| N | 3.51894426 | 3.76502212 | 4.53565447 |
| C | 0.56358072 | 3.15124788 | 2.76951601 |

| | | | |
|---|---|---|---|
| Cl | 0.27400354 | 4.77512432 | 3.29168781 |
| H | -2.11776347 | 3.63809204 | 2.49523181 |
| H | -1.50413266 | 3.91852622 | 0.87124102 |
| H | -2.36221262 | 2.40857771 | 1.23615502 |
| H | -2.29716586 | -1.55317483 | -2.54522096 |
| H | 0.55326594 | -1.90791508 | -2.32920236 |
| H | -1.03983283 | 0.53494773 | -3.25764244 |
| H | 0.76417391 | -1.10000861 | -4.66243616 |
| H | 2.00017048 | 0.30700351 | -3.19276337 |
| H | 1.04582750 | 1.79311050 | -3.26347079 |
| H | 2.01893477 | 0.69442036 | -0.86303128 |
| H | 0.57241891 | 1.71393135 | -0.92640484 |
| H | 1.27152780 | -0.45341753 | 1.63062462 |
| H | 2.93788306 | 0.74867194 | 3.01242575 |

22

Energy = -38.22356284 a.u.

| | | | |
|---|---|---|---|
| O | 2.51271077 | -0.06045839 | -4.10154854 |
| C | 1.57992350 | -0.08302674 | -3.32466347 |
| C | 1.76404700 | -0.27602290 | -1.89469465 |
| C | 0.74527616 | -0.31805012 | -1.01460619 |
| N | 1.02118328 | -0.58563159 | 0.31450040 |
| C | 0.14785426 | -0.70866801 | 1.34054847 |
| N | -1.16523391 | -0.59045451 | 1.35524579 |
| N | -1.54719008 | -0.80599848 | 2.60885825 |
| N | -0.57589728 | -1.04822239 | 3.36782434 |
| N | 0.54416996 | -1.00207374 | 2.61793787 |
| C | -0.67166746 | -0.09077311 | -1.42002781 |
| C | -0.72823185 | 0.70208784 | -2.72248132 |
| C | 0.13979775 | 0.03813816 | -3.78231655 |
| H | 2.78587018 | -0.41739322 | -1.56820136 |
| H | 1.99716308 | -0.73574317 | 0.53522463 |
| H | 1.45830493 | -1.16353203 | 3.00732058 |
| H | -1.15872840 | -1.06254987 | -1.54907979 |
| H | -1.20950442 | 0.42308953 | -0.62307480 |
| H | -1.76072102 | 0.76783919 | -3.06732563 |
| H | -0.36632577 | 1.71720370 | -2.54461364 |
| H | -0.22219994 | -0.97570083 | -3.97954226 |
| H | 0.11463722 | 0.58765669 | -4.72400735 |

48

Energy = -78.77067849 a.u.

| | | | |
|---|---|---|---|
| O | -5.73159633 | -1.74757381 | 2.47179351 |
| C | -4.52479430 | -1.36081426 | 1.86654279 |
| C | -4.73295036 | -0.76105017 | 0.47185318 |
| C | -3.44500185 | -0.15608171 | -0.08062751 |
| O | -2.94505525 | 0.85876370 | 0.77551891 |
| C | -3.66541785 | 0.40121838 | -1.50827799 |
| O | -4.54434187 | 1.50148655 | -1.48189726 |
| C | -2.34654253 | 0.79944344 | -2.17013790 |
| S | -1.26437926 | -0.64166017 | -2.46737627 |
| C | 0.39171618 | 0.14015488 | -2.32174205 |
| C | 1.14469936 | -0.26628820 | -1.05511040 |
| O | 1.53448352 | -1.62211825 | -1.11521104 |
| C | 0.30855771 | -0.00180259 | 0.21979354 |
| O | -0.22267695 | 1.30718812 | 0.18316613 |
| C | 1.07181893 | -0.22869583 | 1.54524813 |
| O | 1.80773334 | -1.42772912 | 1.57040866 |
| C | 1.93885394 | 0.95563313 | 2.07022678 |
| O | 2.58786924 | 0.48370719 | 3.23356234 |
| C | 2.99284743 | 1.63031631 | 1.15817263 |
| O | 2.45633425 | 2.14764219 | -0.03793661 |
| C | 4.18722895 | 0.71989343 | 0.82612875 |
| O | 5.09704186 | 0.63937588 | 1.89098198 |
| H | -6.15865574 | -2.41725251 | 1.92532285 |
| H | -4.09005446 | -0.61627185 | 2.53794591 |
| H | -3.82886168 | -2.20968061 | 1.79986431 |
| H | -5.50084596 | 0.01581570 | 0.52227041 |
| H | -2.66623448 | -0.92332350 | -0.12385255 |
| H | -3.68737122 | 1.42585391 | 1.01991256 |
| H | -4.16483693 | -0.36384055 | -2.11009747 |
| H | -4.07611652 | 2.25879583 | -1.10825815 |
| H | -2.55336602 | 1.26748916 | -3.13403692 |
| H | -1.79875106 | 1.48990674 | -1.52871895 |
| H | -5.08245278 | -1.53479755 | -0.21427764 |
| H | 0.96575273 | -0.19296443 | -3.18583286 |
| H | 0.26283034 | 1.21716900 | -2.36404908 |
| H | 2.07101559 | 0.31558239 | -1.02540524 |
| H | 0.76500692 | -2.15455288 | -1.35905330 |
| H | -0.50720661 | -0.74004246 | 0.20230419 |
| H | -1.08390437 | 1.29486263 | 0.63250482 |
| H | 0.30445650 | -0.34507362 | 2.33026127 |
| H | 2.06796832 | -1.66227116 | 0.66412822 |
| H | 1.24121220 | 1.74690873 | 2.38314809 |

| | | | |
|---|---|---|---|
| H | 2.66255689 | -0.47952397 | 3.12692434 |
| H | 3.39902564 | 2.46509892 | 1.75797894 |
| H | 1.51673142 | 2.33730966 | 0.09269633 |
| H | 3.84434099 | -0.28267571 | 0.53412923 |
| H | 4.72375149 | 1.15987470 | -0.01875133 |
| H | 4.58488461 | 0.53229830 | 2.70622971 |

32

Energy = -49.46480868 a.u.

| | | | |
|---|---|---|---|
| O | 1.42881489 | -3.61043157 | 1.45342690 |
| C | 0.13719161 | -3.09200372 | 1.32217813 |
| C | -0.06112218 | -2.26906669 | 0.03633979 |
| N | 0.24423897 | -0.85043605 | 0.21930312 |
| C | 0.58964280 | -0.22866432 | -1.05820298 |
| C | 0.66717742 | 1.28661092 | -0.91977780 |
| O | 1.14916683 | 1.80364575 | -2.13332426 |
| C | -0.71777864 | 1.86978306 | -0.54815083 |
| O | -0.59505697 | 2.91926943 | 0.37400796 |
| C | -1.65150386 | 0.78931549 | 0.01903273 |
| O | -2.26567215 | 0.08061534 | -1.02078327 |
| C | -0.80038277 | -0.13644913 | 0.96087310 |
| C | -0.25790940 | 0.66767824 | 2.07148542 |
| O | 2.70762365 | -1.13656620 | 1.54290720 |
| H | 2.06872960 | -2.87136834 | 1.44661477 |
| H | -0.52592144 | -3.96136212 | 1.29646976 |
| H | -0.13004978 | -2.48350058 | 2.20065934 |
| H | 0.62764499 | -2.66424777 | -0.71273060 |
| H | -1.08407569 | -2.40779027 | -0.34276141 |
| H | 1.88615018 | -0.87917122 | 1.07859374 |
| H | 1.56887083 | -0.60062958 | -1.36829656 |
| H | -0.13694975 | -0.46047318 | -1.84677249 |
| H | 1.36776094 | 1.53693507 | -0.10464872 |
| H | 1.16827190 | 2.76546723 | -2.07199209 |
| H | -1.18134152 | 2.28898340 | -1.44740083 |
| H | -0.32088211 | 2.51754495 | 1.22414996 |
| H | -2.40559020 | 1.29900806 | 0.63739093 |
| H | -3.01091746 | -0.42316255 | -0.67616274 |
| H | -1.51910533 | -0.87157455 | 1.36046609 |
| H | 0.79811745 | 0.79831862 | 2.19590733 |
| H | -0.91519150 | 0.99715633 | 2.85413728 |
| H | 2.60636672 | -0.89397905 | 2.46476104 |

33

Energy = -52.03555730 a.u.

| | | | |
|---|---|---|---|
| C | 0.11679877 | -3.74564653 | -0.35873485 |
| C | -0.69426367 | -2.66570467 | 0.33618891 |
| C | -1.77123629 | -3.24586830 | 1.23562060 |
| S | 0.45370108 | -1.61203072 | 1.32045377 |
| C | -0.47055026 | -0.01227715 | 1.17411573 |
| O | -0.53051032 | 0.43003581 | -0.13486043 |
| C | 0.70805356 | 0.82137492 | -0.70597486 |
| C | 0.35198285 | 1.40138715 | -2.09094996 |
| O | 1.35199211 | 2.21305856 | -2.62979488 |
| C | 1.47462284 | 1.84481394 | 0.14734821 |
| O | 0.85138318 | 3.10470256 | 0.07760973 |
| C | 1.56129809 | 1.36797051 | 1.60300637 |
| O | 2.11909883 | 2.41213595 | 2.36629085 |
| C | 0.15970942 | 1.01440216 | 2.11752269 |
| O | 0.20016774 | 0.58742217 | 3.45161486 |
| H | 0.88884313 | -3.30415843 | -0.98431398 |
| H | 0.59431080 | -4.39109020 | 0.37523870 |
| H | -0.53629205 | -4.35043230 | -0.98448944 |
| H | -1.12524700 | -1.98200627 | -0.40040225 |
| H | -1.32479787 | -3.90011021 | 1.98146899 |
| H | -2.31959545 | -2.45928320 | 1.75018572 |
| H | -2.47678040 | -3.82284731 | 0.64090662 |
| H | -1.50174015 | -0.22411615 | 1.47341496 |
| H | 1.35562586 | -0.06320380 | -0.80487654 |
| H | 0.19459113 | 0.58393533 | -2.79707476 |
| H | -0.58957984 | 1.95067639 | -1.97099262 |
| H | 1.40166352 | 3.01014190 | -2.08593747 |
| H | 2.49998107 | 1.91597323 | -0.25124269 |
| H | 1.18944845 | 3.61567898 | 0.82688767 |
| H | 2.19689107 | 0.46884769 | 1.65937836 |
| H | 1.89838837 | 2.24157294 | 3.29166805 |
| H | -0.45964238 | 1.92034258 | 2.10519571 |
| H | 0.55966981 | -0.31128652 | 3.47541122 |

31

Energy = -39.20043442 a.u.

| | | | |
|---|---|---|---|
| C | -2.12181311 | 4.61382548 | 1.94958230 |
| C | -1.80536681 | 3.13996525 | 1.72775173 |

| | | | |
|---|---|---|---|
| C | -0.70008415 | 2.94527504 | 0.69268366 |
| C | -0.39155216 | 1.46948867 | 0.45304965 |
| C | 0.70679571 | 1.27494231 | -0.58947332 |
| C | 0.98172811 | -0.20323024 | -0.85371965 |
| C | 2.04913001 | -0.39702161 | -1.92934949 |
| C | 2.41584222 | -1.86360278 | -2.14619629 |
| C | 1.34195977 | -2.68893995 | -2.77785257 |
| C | 0.15419897 | -3.20358400 | -1.56218071 |
| O | -0.92011123 | -3.01540985 | -2.04616799 |
| O | 0.73417966 | -3.61927147 | -0.61135131 |
| H | -2.91003522 | 4.72959646 | 2.68977840 |
| H | -1.23995263 | 5.14505311 | 2.30129716 |
| H | -2.45169330 | 5.07667967 | 1.02192101 |
| H | -1.49729451 | 2.68811356 | 2.67331928 |
| H | -2.70672248 | 2.62189813 | 1.39273309 |
| H | -1.00495258 | 3.40741293 | -0.24943738 |
| H | 0.20536675 | 3.45456578 | 1.03171632 |
| H | -0.08354609 | 1.00596368 | 1.39301198 |
| H | -1.29851560 | 0.96132843 | 0.11777997 |
| H | 0.40687938 | 1.75818143 | -1.52260639 |
| H | 1.62313549 | 1.76114216 | -0.24583905 |
| H | 1.30599999 | -0.68430393 | 0.07158431 |
| H | 0.05412062 | -0.68422539 | -1.16811677 |
| H | 1.69907309 | 0.03414250 | -2.87022281 |
| H | 2.95000553 | 0.14513422 | -1.63256136 |
| H | 3.27738656 | -1.90974717 | -2.82673589 |
| H | 2.73219330 | -2.31853992 | -1.20418194 |
| H | 0.75042907 | -2.16940003 | -3.52402042 |
| H | 1.66647360 | -3.66966448 | -3.11189653 |

50

Energy = -94.83517227 a.u.

| | | | |
|---|---|---|---|
| O | -1.31903571 | -1.62060768 | -0.78486206 |
| C | -0.40962014 | -1.78099089 | 0.05550944 |
| N | -0.72712676 | -2.02621696 | 1.32305284 |
| C | 0.09496425 | -1.91494036 | 2.50916495 |
| C | -0.69485781 | -1.36617152 | 3.66358426 |
| C | -1.46988832 | -0.29177757 | 3.67402632 |
| C | -1.78542000 | 0.66692862 | 2.57226816 |
| O | -0.84766219 | 0.67999567 | 1.50455795 |
| C | -1.45090359 | 1.34649191 | 0.44683216 |
| S | -1.23056004 | 3.17680227 | 0.56793562 |

| | | | |
|---|---|---|---|
| C | 0.43215381 | 3.35920881 | -0.01148447 |
| C | 1.38299371 | 2.35127860 | 0.08701348 |
| C | 2.65225499 | 2.60891160 | -0.40969341 |
| N | 3.00896234 | 3.75544599 | -0.95811447 |
| C | 2.10244863 | 4.71562300 | -1.03001276 |
| C | 0.80224858 | 4.57580296 | -0.57649439 |
| C | -2.95811159 | 1.01522902 | 0.47907039 |
| O | -3.37093792 | 0.15288572 | -0.52969945 |
| C | -3.14742384 | 0.38802481 | 1.89459530 |
| O | -3.39095590 | -0.99072079 | 1.80011764 |
| C | 1.00582259 | -1.65852515 | -0.36903546 |
| C | 2.06321020 | -2.29429780 | 0.27308915 |
| C | 3.36201889 | -2.06953370 | -0.15096951 |
| N | 4.43791384 | -2.74038877 | 0.52708306 |
| O | 5.56345604 | -2.56451720 | 0.11627848 |
| O | 4.15035138 | -3.44103509 | 1.47701950 |
| C | 3.65139355 | -1.21221673 | -1.21004836 |
| C | 2.61215909 | -0.60924428 | -1.88979522 |
| O | 2.85588056 | 0.19306365 | -2.94028185 |
| C | 1.27803910 | -0.85857151 | -1.49252283 |
| O | 0.31587331 | -0.29179481 | -2.24063798 |
| H | -1.73149733 | -1.98972394 | 1.51478696 |
| H | 0.47713353 | -2.90260144 | 2.78903256 |
| H | 0.94566250 | -1.25684594 | 2.30227623 |
| H | -0.59676780 | -1.92341231 | 4.58379098 |
| H | -1.99077765 | -0.03888436 | 4.58666833 |
| H | -1.82989150 | 1.68426852 | 2.99550512 |
| H | -0.97586694 | 1.05111006 | -0.48963546 |
| H | 1.15775151 | 1.40369862 | 0.55000650 |
| H | 3.42421728 | 1.85235049 | -0.35831759 |
| H | 2.43464729 | 5.64139778 | -1.47981757 |
| H | 0.08779174 | 5.37891257 | -0.65670752 |
| H | -3.55618154 | 1.92473638 | 0.37497035 |
| H | -2.70815341 | -0.56309822 | -0.65776040 |
| H | -3.96353297 | 0.87129485 | 2.44535061 |
| H | -3.91367759 | -1.12380221 | 0.98955548 |
| H | 1.89911178 | -3.00082159 | 1.06876291 |
| H | 4.67140968 | -1.04122440 | -1.51447412 |
| H | 2.01165782 | 0.50692997 | -3.29766806 |
| H | -0.54257852 | -0.70633869 | -1.96058173 |

35

Energy = -57.58684806 a.u.

| | | | |
|---|---|---|---|
| C | 1.35227049 | 3.40589287 | -1.75527612 |
| C | 0.49224899 | 2.25116988 | -1.32042615 |
| C | -0.86509470 | 2.08162457 | -1.62601076 |
| C | -1.55231815 | 3.04964531 | -2.43236572 |
| C | -2.85173560 | 2.89860453 | -2.73672464 |
| N | -3.53765695 | 1.81999076 | -2.27876047 |
| C | -3.01056563 | 0.81269509 | -1.49433473 |
| O | -3.78094652 | -0.08295681 | -1.17813878 |
| C | -1.59226072 | 0.94347920 | -1.14355857 |
| C | -0.95962650 | -0.03337987 | -0.35078786 |
| C | -1.64344161 | -1.23798517 | 0.21500765 |
| C | 0.39447307 | 0.13285147 | -0.06856795 |
| C | 1.09209253 | 1.26655602 | -0.55034856 |
| N | 2.39301303 | 1.20397103 | -0.13450491 |
| C | 2.58093834 | 0.05811084 | 0.59942766 |
| C | 3.73743429 | -0.41014263 | 1.20075901 |
| C | 3.67663802 | -1.60610877 | 1.88484926 |
| C | 2.47819564 | -2.32077121 | 1.96394296 |
| O | 2.49939156 | -3.49893210 | 2.65593907 |
| C | 1.31912967 | -1.85386658 | 1.36437534 |
| C | 1.35764900 | -0.64782794 | 0.67079316 |
| H | 1.73760681 | 3.92998694 | -0.87941579 |
| H | 2.20210153 | 3.03852740 | -2.33225311 |
| H | 0.82256339 | 4.12596969 | -2.36661189 |
| H | -1.03079774 | 3.91153736 | -2.80749653 |
| H | -3.40247712 | 3.60245864 | -3.34211940 |
| H | -4.51609805 | 1.70083072 | -2.50626968 |
| H | -1.51510915 | -1.24873834 | 1.29666837 |
| H | -2.70072861 | -1.24436675 | -0.01576642 |
| H | -1.18950977 | -2.13875378 | -0.19711777 |
| H | 3.10591333 | 1.88100384 | -0.33943081 |
| H | 4.66214126 | 0.14332605 | 1.13506312 |
| H | 4.54769587 | -2.01633137 | 2.36956224 |
| H | 1.62186368 | -3.89832758 | 2.63901981 |
| H | 0.41226431 | -2.43313532 | 1.44252397 |

67

Energy = -116.43467571 a.u.

| | | | |
|---|---|---|---|
| C | 1.45917984 | 3.32946021 | 3.48732454 |
| C | 2.14961297 | 2.01402452 | 3.75641154 |

| | | | |
|---|---|---|---|
| O | 2.38377638 | 1.57843672 | 4.86075101 |
| N | 2.48145972 | 1.33727050 | 2.62130792 |
| C | 3.21490266 | 0.09969044 | 2.64711635 |
| C | 4.50597127 | 0.18576762 | 1.78279947 |
| C | 4.03668476 | 0.14963532 | 0.36120954 |
| C | 3.50223654 | 1.28806912 | -0.23533898 |
| C | 2.57260255 | 1.17271755 | -1.25448516 |
| C | 2.19917942 | -0.09237996 | -1.67989055 |
| O | 0.98612998 | -0.26899876 | -2.34299100 |
| P | -0.21827741 | -0.41041975 | -1.28838343 |
| O | -1.48366650 | -0.63162503 | -1.99769210 |
| O | -0.16603270 | 0.88750303 | -0.37102433 |
| O | 0.25944707 | -1.57499776 | -0.33742194 |
| C | 2.91627996 | -1.20814664 | -1.27600556 |
| C | 3.83784974 | -1.08222673 | -0.25627666 |
| C | 2.39318601 | -1.12746695 | 2.18952686 |
| O | 2.85801869 | -2.23798461 | 2.30169305 |
| N | 1.16342775 | -0.83290855 | 1.69928318 |
| C | 0.16895150 | -1.69449709 | 1.09381047 |
| C | -1.88097947 | 3.09059241 | 0.55015029 |
| O | -1.32513675 | 2.92736701 | 1.55409624 |
| N | -2.62257905 | 3.36963403 | -0.33798777 |
| C | -2.75355000 | 3.24393096 | -1.74251209 |
| C | -3.38400870 | 1.88626326 | -2.10362919 |
| C | -3.45467533 | 1.68335204 | -3.61138667 |
| N | -3.18324829 | 0.43542448 | -4.00327438 |
| O | -3.74709807 | 2.58711715 | -4.37975539 |
| C | -1.38092339 | 3.36828178 | -2.41926144 |
| N | -1.41449085 | 3.86555575 | -3.65366304 |
| O | -0.34465275 | 3.05996990 | -1.84226919 |
| C | -1.20660964 | -1.25216967 | 1.59761619 |
| C | -2.32000495 | -2.12545683 | 1.02880975 |
| C | -2.07861915 | -3.58813234 | 1.38386753 |
| C | -0.72912433 | -4.03200477 | 0.83232860 |
| C | 0.40129574 | -3.17505614 | 1.39637163 |
| H | 1.28202994 | 3.84018127 | 4.42904652 |
| H | 2.07447531 | 3.95744386 | 2.84650366 |
| H | 0.50693251 | 3.15425769 | 2.99227457 |
| H | 2.32203074 | 1.76491240 | 1.72049250 |
| H | 3.48771569 | -0.07374170 | 3.69538008 |
| H | 5.03842426 | 1.10403749 | 2.03142834 |
| H | 5.13247207 | -0.67409888 | 2.01313645 |

| | | | |
|---|---|---|---|
| H | 3.75866222 | 2.26831538 | 0.14188819 |
| H | 2.06550150 | 2.04178354 | -1.64552568 |
| H | 2.66154283 | -2.17384053 | -1.68245656 |
| H | 4.32197206 | -1.96208073 | 0.13727443 |
| H | 0.91638744 | 0.14770838 | 1.66058269 |
| H | -0.22134508 | 1.72619716 | -0.88737482 |
| H | -3.40326736 | 4.05421755 | -2.08914160 |
| H | -2.81146254 | 1.07762866 | -1.65161991 |
| H | -4.40049838 | 1.85913993 | -1.70579670 |
| H | -3.18170613 | 0.22956425 | -4.98990709 |
| H | -2.72393336 | -0.21001199 | -3.37083894 |
| H | -0.55738238 | 3.89480670 | -4.18540706 |
| H | -2.29743698 | 3.90562454 | -4.15258486 |
| H | -1.19524215 | -1.32296793 | 2.68750786 |
| H | -1.36803913 | -0.20948131 | 1.32096924 |
| H | -3.27887915 | -1.78928503 | 1.42782851 |
| H | -2.34456825 | -2.01137139 | -0.05610302 |
| H | -2.08962358 | -3.70875479 | 2.46964286 |
| H | -2.87406976 | -4.20777672 | 0.96672273 |
| H | -0.54094832 | -5.07633374 | 1.08566756 |
| H | -0.73735872 | -3.93904948 | -0.25481353 |
| H | 0.46925849 | -3.29408895 | 2.47775153 |
| H | 1.35366297 | -3.47647283 | 0.96388875 |

27

Energy = -40.05461477 a.u.

| | | | |
|---|---|---|---|
| O | -2.55061744 | -0.50697979 | -1.31933323 |
| C | -1.65629186 | -0.90215005 | -0.36419091 |
| N | -1.95215764 | -0.75793870 | 0.97107112 |
| C | -0.81460684 | -0.84182940 | 1.72374874 |
| C | -0.65965049 | -0.85149334 | 3.10616635 |
| C | 0.62352896 | -0.93531072 | 3.61152711 |
| C | 1.73051122 | -1.01254496 | 2.77291037 |
| C | 1.57175010 | -1.01110539 | 1.38920863 |
| C | 0.30517436 | -0.93354959 | 0.86470623 |
| C | -0.16941211 | -0.90691429 | -0.55940891 |
| C | 0.30186138 | -2.07369315 | -1.46944831 |
| C | 0.34108703 | -1.47690781 | -2.88649379 |
| N | -0.14446468 | -0.10575078 | -2.72837222 |
| C | 0.27975402 | 0.31330515 | -1.40406973 |
| H | -2.89109253 | -0.70665529 | 1.32674191 |
| H | -1.51673547 | -0.78879534 | 3.75969387 |

| | | | |
|---|---|---|---|
| H | 0.77084362 | -0.94017383 | 4.68177813 |
| H | 2.72017176 | -1.07639699 | 3.19823829 |
| H | 2.43692641 | -1.07364944 | 0.74438545 |
| H | 1.29008644 | -2.40687540 | -1.15629342 |
| H | -0.38296532 | -2.91634920 | -1.39755826 |
| H | 1.36379140 | -1.51200371 | -3.28682975 |
| H | -0.31458688 | -2.00750056 | -3.58116477 |
| H | 0.18836092 | 0.50708643 | -3.46522760 |
| H | -2.01903018 | -0.31342527 | -2.11504139 |
| H | 1.36707457 | 0.45540510 | -1.30815762 |
| H | -0.22633372 | 1.23403029 | -1.10935626 |

18

Energy = -29.82565926 a.u.

| | | | |
|---|---|---|---|
| O | 1.21490233 | 0.67626440 | -1.58867741 |
| C | 0.15569552 | 0.02678170 | -1.06686534 |
| C | -1.07756323 | 0.04195134 | -1.67385650 |
| C | -2.15363451 | -0.64613903 | -1.09922941 |
| C | -2.01357071 | -1.34612599 | 0.06913863 |
| C | -0.76600652 | -1.38504876 | 0.72029310 |
| C | -0.51685657 | -2.07557114 | 1.92533660 |
| C | 0.73782626 | -2.04602830 | 2.47205666 |
| C | 1.74913198 | -1.32459053 | 1.81430161 |
| N | 1.56055556 | -0.67333449 | 0.69972377 |
| C | 0.33001200 | -0.69201772 | 0.14731849 |
| H | 1.96051159 | 0.51610652 | -0.98396898 |
| H | -1.20446802 | 0.58865233 | -2.59465084 |
| H | -3.11112522 | -0.61687551 | -1.59802374 |
| H | -2.84910956 | -1.87380575 | 0.50492360 |
| H | -1.32212733 | -2.61900691 | 2.40024106 |
| H | 0.96206618 | -2.56314364 | 3.39228942 |
| H | 2.75073924 | -1.28359050 | 2.22332331 |

59

Energy = -98.95391407 a.u.

| | | | |
|---|---|---|---|
| N | 5.23891092 | 0.46856791 | 2.55802388 |
| C | 3.78563452 | 0.49003897 | 2.38845028 |
| C | 3.10382528 | -0.05347465 | 3.65828917 |
| C | 1.62491707 | -0.37766356 | 3.44588739 |
| C | 0.89046053 | 0.80035871 | 2.82233950 |
| O | 1.15885139 | 1.95699217 | 3.07691250 |
| N | -0.07570066 | 0.44573124 | 1.95023807 |

| | | | |
|---|---|---|---|
| C | -1.00174265 | 1.40410294 | 1.40812122 |
| C | -2.37570842 | 1.33000562 | 2.09476623 |
| S | -2.89926744 | -0.35430880 | 2.53791769 |
| C | -3.39984696 | -1.05302943 | 0.92460950 |
| C | -2.26668709 | -1.62366502 | 0.12770892 |
| C | -2.25549165 | -1.49406781 | -1.25494981 |
| C | -1.21876002 | -2.02480025 | -2.00184563 |
| C | -0.17521522 | -2.68528342 | -1.37509167 |
| C | -0.18585748 | -2.83411412 | 0.00081672 |
| C | -1.23113881 | -2.31663335 | 0.74642866 |
| C | -1.15934279 | 1.31566156 | -0.10922470 |
| O | -2.16914864 | 1.73828392 | -0.65849575 |
| N | -0.09985621 | 0.81716786 | -0.80087631 |
| C | -0.10431111 | 0.79470479 | -2.16602259 |
| C | -4.06917616 | 1.54714786 | -2.32342026 |
| O | -3.40011812 | 1.76074851 | -3.22659853 |
| O | -4.80067125 | 1.31016698 | -1.47539306 |
| C | 0.87358110 | 0.24879754 | -3.00161421 |
| C | 2.03091570 | -0.42116875 | -2.54027775 |
| C | 2.93842153 | -0.94617413 | -3.43026542 |
| C | 2.74140227 | -0.83248144 | -4.80156111 |
| C | 1.60902170 | -0.17948691 | -5.27794007 |
| C | 0.69227385 | 0.35090491 | -4.40396728 |
| C | 3.45130658 | -0.42537349 | 1.20983675 |
| O | 4.41501358 | -1.27552186 | 0.90612487 |
| O | 2.39762420 | -0.39081892 | 0.62514786 |
| H | 5.49388439 | 0.69434083 | 3.51237280 |
| H | 5.17624997 | -1.06635016 | 1.50029324 |
| H | 5.68029102 | 1.15447847 | 1.95427520 |
| H | 3.37508265 | 1.48596746 | 2.17793559 |
| H | 3.63234637 | -0.95147027 | 3.98674820 |
| H | 3.19084109 | 0.70911447 | 4.43434667 |
| H | 1.50561930 | -1.26266435 | 2.82160546 |
| H | 1.16214731 | -0.57745218 | 4.41537408 |
| H | -0.30350355 | -0.52959053 | 1.81035986 |
| H | -0.57427253 | 2.39564733 | 1.62298390 |
| H | -2.35213007 | 1.85819120 | 3.04687516 |
| H | -3.13289782 | 1.76949535 | 1.44561170 |
| H | -4.11322015 | -1.83888176 | 1.18395318 |
| H | -3.92049707 | -0.27024827 | 0.37406628 |
| H | -3.06441799 | -0.97423654 | -1.74660920 |
| H | -1.22366502 | -1.92176165 | -3.07638795 |

| | | | |
|---|---|---|---|
| H | 0.64026068 | -3.08338567 | -1.95878441 |
| H | 0.61810073 | -3.36044082 | 0.49392147 |
| H | -1.26667942 | -2.46785482 | 1.81812871 |
| H | 0.69640542 | 0.44040892 | -0.29426972 |
| H | -0.97327676 | 1.26335615 | -2.60420516 |
| H | 2.19909188 | -0.53085252 | -1.48251685 |
| H | 3.81497336 | -1.45633481 | -3.05646846 |
| H | 3.45976708 | -1.24865410 | -5.49165094 |
| H | 1.45069486 | -0.09077946 | -6.34326490 |
| H | -0.18733524 | 0.85615715 | -4.77484299 |