## Supporting Information for:

# Study of Iron Dimers Reveals Angular Dependence of Valence-to-Core X-ray Emission Spectra

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*KEYWORDS x-ray emission spectroscopy, valence-to-core, dimers, bond angle*

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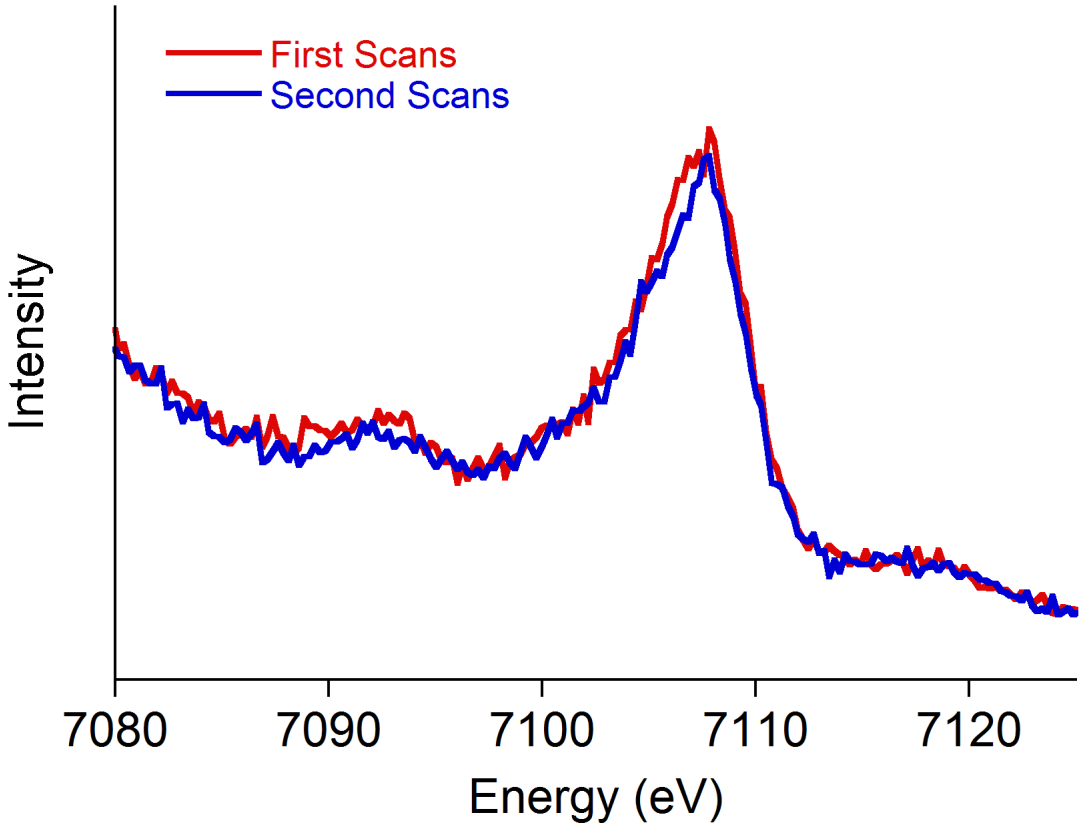


**Figure S1:** An overlay of the first and second scans for **8** shows evidence of slight damage.

**Broadening Modulation Using Matlab**

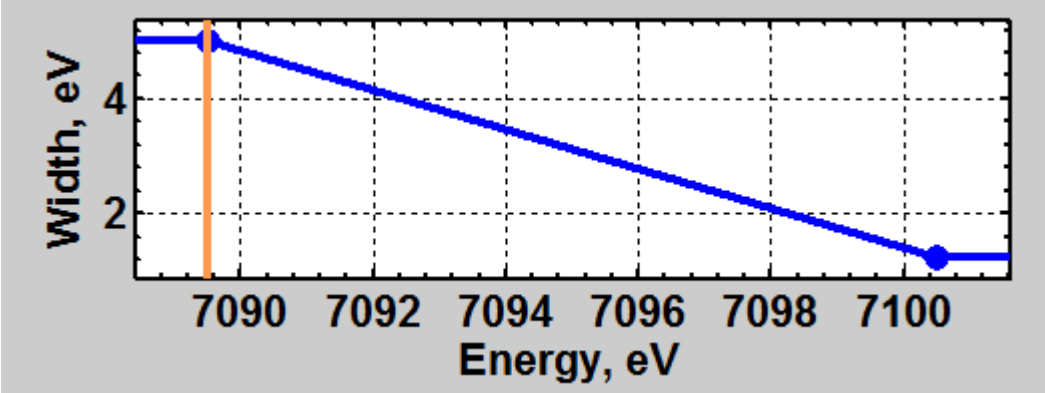


**Figure S2:** The broadening applied to these calculated spectra was modulated to account for the greater HWHM values observed for the Kβ" peaks relative to the $K\beta_{2,5}$. Namely, an initial HWHM broadening of 5 eV was applied below 7089.5 eV. Then, between 7089.5 and 7100.5 eV, this broadening linearly decreased to 1.25 eV, which was kept constant above 7100.5 eV. A 50:50 mixing of Gaussian / Lorentzian was used for the entire VtC spectrum.

**Contributions to Kβ”**

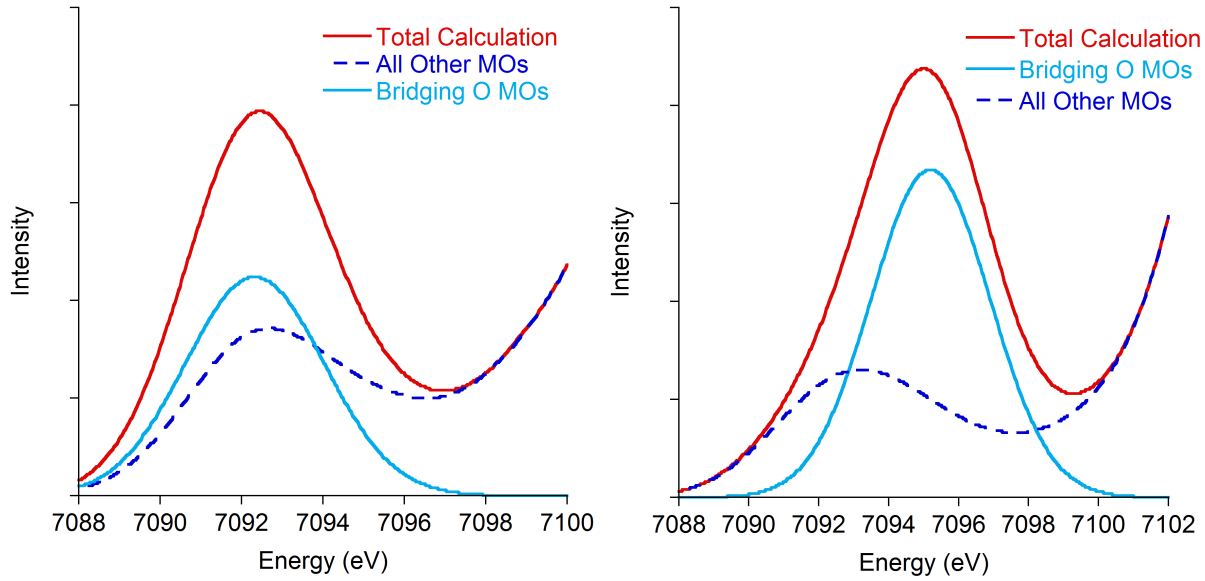


**Figure S3:** Plots showing the contributions of the bridging oxo and supporting ligands to the Kβ” feature for compounds **1** and **6**. As can clearly be seen, the 2s orbital from the bridging oxo constitutes the dominant contribution to the Kβ” intensity, even in cases where the Fe-$O_{bridging}$ bond length is relatively long (**1**). This can be attributed to the fact that the MOs from the supporting ligands are delocalized away from the metal centers and thus have less Fe *n*p mixing.

## Sample ORCA Geometry Optimization Input File

```
! UKS BP86 def2-TZVP def2-TZV/J TightSCF SlowConv SCFConv7 COSMO
! Grid4 NoFinalGrid Normalprint
! OPT
! PAL8

%geom Constraints
      {C 0 C}
      {C 1 C}
      {C 2 C}
      end
end

%scf
      MaxIter 500
      end

%maxcore 1024

%basis  newgto Fe "CP(PPP)" end
          end

%method SpecialGridAtoms 26
         SpecialGridIntAcc 7
         end

* xyzfile 4 11 FeTACN_bent.xyz
```

## Sample ORCA Broken Symmetry Calculation Input File

```
! UKS BP86 def2-TZVP def2-TZV/J TightSCF SlowConv SCFConv7 COSMO
! Grid4 NoFinalGrid Normalprint
! PAL4
! MOREAD

%moinp"HEDTA_opt.gbw"

%scf BrokenSym 5,5
      MaxIter 500
      end

%maxcore 1024

%basis  newgto Fe "CP(PPP)" end
          end

%method SpecialGridAtoms 26
         SpecialGridIntAcc 7
         end

%xes CoreOrb 0,1
           OrbOp 0,1
           end

* xyzfile -2 11 HEDTA_opt.xyz
```

## Sample ORCA XES Calculation Input File

```
! UKS BP86 def2-TZVP def2-TZV/J TightSCF SlowConv SCFConv7 COSMO
! Grid4 NoFinalGrid Normalprint
! PAL8
! MOREAD NOITER

%moinp"FeTACN_bentOpt.gbw"

%maxcore 1024

%basis  newgto Fe "CP(PPP)" end
          end

%method SpecialGridAtoms 26
         SpecialGridIntAcc 7
         end

%xes CoreOrb 0,0
          OrbOp 0,1
          end

* xyzfile 4 11 FeTACN_bentOpt.xyz
```

**ORCA Input Keywords**

| | |
|---|---|
| UKS | Defines that the calculation will use the unrestricted Kohn-Sham method, allowing unpaired electrons. The spin-restricted analog is invoked with "RKS". |
| BP86 | Selects the BP86 functional |
| def2-TZVP | Selects the def2-TZVP basis set |
| def2-TZV/J | Selects the def2-TZV/J auxiliary basis set |
| TightSCF | Defines the criteria for SCF convergence |
| SlowConv | Specifies the strategy to be used to achieve SCF convergence. This keyword is often used for calculations on transition metal complexes. |
| SCFConv7 | Further specifies SCF convergence criteria |
| COSMO | Models the presence of solvent using the conductor-like screening model. A specific solvent may be chosen (e.g. COSMO(THF) for tetrahydrofuran) or, in the absence of this specification, an infinite dielectric is used. |
| Grid4, NoFinalGrid | Selects the integration grid to be used |
| OPT | Specifies a geometry optimization |
| PAL8 | Specifies that eight processors should be used for the calculation |
| MOREAD | Dictates that previously generated orbitals should be used as a starting point for the calculation. If used with "NOITER", no additional SCF iterations will be performed and the orbitals will be used exactly as they are read. |
| * xyzfile A B file.xyz | Dictates that the atomic coordinates for the calculation are found in "file.xyz". "A" is equal to the charge on the molecule and "B" is the multiplicity. |
| * xyz A B | Same as above, except the atomic coordinates are contained within the input file rather than a separate xyz file |
| %scf | This block contains the controls for parameters governing the SCF iterations |
| MaxIter | Specifies the maximum number of SCF iterations that can be carried out |
| %maxcore | Defines how much scratch memory is available for the calculation |
| %method | This block contains controls for a variety of parameters governing the computational model |
| SpecialGridAtoms | Defines that atoms with atomic number 26 (Fe) should have a special integration grid distinct from the general calculation |

| | |
|---|---|
| SpecialGridIntAcc | Dictates that an integration accuracy of 7 should be used for the atoms defined in SpecialGridAtoms. This is often necessary when calculating core properties and x-ray spectra. |
| %moinp | Used with MOREAD, this command specifies the orbitals that should be read as the starting point |
| %basis | This block contains variables that control the basis set |
| newgto | Dictates that additional basis functions should be added to the indicated element. In this cases, the large core properties CP(PPP) basis is being used for Fe. |
| %xes | This block controls the calculation of XES spectra |
| CoreOrb | Dictates the orbitals that will be the electron acceptors. For transition metal XES spectra, the metal 1s orbital is *usually* orbital 0. |
| OrbOp | Defines the operators of the electrons ($\alpha = 0$, $\beta = 1$) that will be calculated |
| BrokenSym 5,5 | Defines the desired spin coupling scheme with the number of unpaired electrons on each center specified (5,5). In this calculation, an antiferromagnetically coupled iron dimer is investigated, with five unpaired electrons on each iron, so the "5,5"formalism is used. Importantly, the two iron centers must be the first two atoms in the xyz file. The "spinflip" command could also be used to give identical results. |

**Optimized xyz Coordinates for 1:**

| | | | |
|---|---|---|---|
| Fe | 0.041135 | 0.101120 | -1.728409 |
| Fe | -0.192089 | 0.177126 | 1.902223 |
| C | -0.020163 | -2.778053 | -2.502542 |
| C | 2.128441 | 2.186562 | -2.422443 |
| C | -2.250018 | 2.194664 | 2.818065 |
| C | 0.226577 | -2.641145 | 2.810552 |
| C | 0.674963 | -4.016727 | -2.480265 |
| C | 3.511520 | 2.466445 | -2.579892 |
| C | -3.599966 | 2.415281 | 3.199172 |
| C | -0.366820 | -3.916361 | 3.008233 |
| C | 0.002515 | -5.222738 | -2.616706 |
| C | 3.956421 | 3.739726 | -2.912158 |
| C | -4.083641 | 3.696261 | 3.432521 |
| C | 0.407640 | -5.064264 | 3.101106 |
| C | -1.395216 | -5.259792 | -2.796840 |
| C | 3.047556 | 4.797748 | -3.106262 |
| C | -3.247116 | 4.821778 | 3.302449 |
| C | 1.813161 | -5.001665 | 3.016565 |
| C | -2.096853 | -4.065452 | -2.842707 |
| C | 1.690380 | 4.550987 | -2.959446 |
| C | -1.922725 | 4.633813 | 2.934812 |
| C | 2.419868 | -3.767565 | 2.844170 |
| C | -1.446008 | -2.815876 | -2.695352 |
| C | 1.201634 | 3.267317 | -2.619605 |
| C | -1.397125 | 3.344072 | 2.684048 |
| C | 1.661727 | -2.576299 | 2.734243 |
| C | -2.239826 | -1.623118 | -2.825370 |
| C | -0.224340 | 3.098595 | -2.497385 |
| C | -0.007588 | 3.241964 | 2.315407 |
| C | 2.374273 | -1.331851 | 2.624690 |
| C | -2.706959 | 0.713570 | -2.960580 |
| C | -2.275603 | 1.921170 | -2.123833 |
| C | 2.027037 | 2.140258 | 1.689358 |
| C | 2.690488 | 1.030438 | 2.508722 |
| H | 1.757104 | -3.991444 | -2.340597 |
| H | 3.405070 | 5.794013 | -3.367721 |
| H | 0.966320 | 5.356465 | -3.106652 |
| H | -0.836780 | 3.993709 | -2.696475 |
| H | -2.566561 | 1.762543 | -1.073004 |
| H | -2.753234 | 2.844902 | -2.487503 |
| H | -4.249751 | 1.544265 | 3.302922 |
| H | -5.128444 | 3.828107 | 3.722168 |
| H | -3.634155 | 5.823849 | 3.488900 |
| H | -1.254723 | 5.492585 | 2.830146 |
| H | 0.556611 | 4.188898 | 2.288205 |
| H | 0.568309 | -6.156503 | -2.584505 |
| H | 2.121137 | 1.909169 | 0.615411 |
| H | 2.501480 | 3.114863 | 1.885456 |
| H | -1.455159 | -3.967844 | 3.076033 |
| H | -0.083120 | -6.029637 | 3.243755 |
| H | 2.412763 | -5.909047 | 3.093987 |
| H | 3.509143 | -3.692993 | 2.791657 |
| H | 3.470906 | -1.399476 | 2.715975 |
| H | 2.766691 | 1.355958 | 3.559603 |

| | | | |
|---|---|---|---|
| H | 3.707302 | 0.817640 | 2.142418 |
| H | -1.913731 | -6.212658 | -2.906932 |
| H | -3.178931 | -4.068924 | -2.997709 |
| H | -3.292014 | -1.777403 | -3.116656 |
| H | -2.597458 | 0.960479 | -4.029839 |
| H | -3.761817 | 0.456258 | -2.774743 |
| H | 4.217930 | 1.647735 | -2.430967 |
| H | 5.028017 | 3.918415 | -3.024618 |
| N | -1.813060 | -0.408686 | -2.657655 |
| N | -0.819782 | 1.993675 | -2.182813 |
| N | 0.607527 | 2.140873 | 2.025841 |
| N | 1.836750 | -0.161352 | 2.460668 |
| O | 0.650986 | -1.656484 | -2.383494 |
| O | 1.752896 | 0.965448 | -2.110796 |
| O | -0.309959 | -0.071020 | 0.076066 |
| O | -1.834098 | 0.963444 | 2.618257 |
| O | -0.536845 | -1.575908 | 2.736865 |

**Optimized xyz Coordinates for 2:**

| | | | |
|---|---|---|---|
| Fe | -0.100824 | 0.125839 | -1.838186 |
| Fe | 0.012189 | 0.061595 | 1.802489 |
| C | 4.493395 | -0.149236 | -1.512652 |
| C | 0.257175 | -2.125781 | -3.710225 |
| C | -4.174129 | 1.964759 | 1.371780 |
| C | -2.931797 | 1.062701 | 1.312593 |
| C | -1.252905 | 2.832993 | 1.632296 |
| C | 0.261704 | 2.994929 | 1.816589 |
| C | -2.062562 | 1.539341 | 3.570958 |
| C | -0.804800 | 1.464191 | 4.432725 |
| C | 1.412697 | 0.350603 | 4.470165 |
| C | 2.272060 | -0.528179 | 3.542444 |
| C | -0.632538 | -0.983192 | 4.645261 |
| C | 2.974994 | -0.364014 | -1.423128 |
| C | -1.402925 | -1.800570 | 3.599179 |
| C | 2.306625 | 1.992549 | -1.661489 |
| C | 1.032977 | 2.840862 | -1.777875 |
| C | 2.384045 | 0.526264 | -3.645491 |
| C | 1.217921 | 1.067637 | -4.468597 |
| C | -1.263979 | 1.106980 | -4.452378 |
| C | -2.413254 | 0.690309 | -3.515247 |
| C | -0.072598 | -1.014560 | -4.716240 |
| N | 2.146020 | 0.614971 | -2.178433 |
| N | -0.035627 | 0.351348 | -4.154298 |
| N | -1.765830 | 1.530187 | 2.111938 |
| N | -0.015328 | 0.253797 | 4.123501 |
| O | 5.187343 | -1.155068 | -0.758765 |
| O | -5.238881 | 1.405881 | 0.587533 |
| O | 0.945953 | 1.897972 | 1.855423 |
| O | 0.747324 | 4.137456 | 1.874410 |
| O | 3.407408 | -0.871052 | 3.912556 |
| O | 1.746847 | -0.834627 | 2.396860 |
| O | -1.258447 | -1.453072 | 2.361520 |
| O | -2.091364 | -2.761914 | 3.986035 |
| O | -0.081074 | 2.185376 | -1.824579 |
| O | -0.099164 | -0.240332 | -0.022030 |
| O | 1.129027 | 4.079808 | -1.778964 |
| O | -3.586087 | 0.915089 | -3.856093 |
| O | -2.063388 | 0.144164 | -2.391481 |
| O | 0.316210 | -1.788417 | -2.462717 |
| O | 0.416537 | -3.283656 | -4.136680 |
| H | -1.076947 | 2.174073 | -4.265517 |
| H | -1.584113 | 0.998137 | -5.501527 |
| H | -1.085920 | -1.227817 | -5.088295 |
| H | 0.601519 | -1.107046 | -5.583316 |
| H | 1.472663 | 0.979638 | -5.540329 |
| H | 1.062352 | 2.134141 | -4.261652 |
| H | 3.297781 | 1.074561 | -3.931602 |
| H | 2.552240 | -0.532774 | -3.887362 |
| H | 5.060207 | -2.007119 | -1.214430 |
| H | 4.782223 | 0.811573 | -1.063919 |
| H | 4.833816 | -0.150071 | -2.562018 |
| H | 2.658108 | -0.325145 | -0.371092 |
| H | 2.725231 | -1.364558 | -1.805699 |

| | | | |
|---|---|---|---|
| H | -5.537256 | 0.591222 | 1.031485 |
| H | -3.966375 | 2.950288 | 0.931964 |
| H | -4.502633 | 2.120602 | 2.413483 |
| H | -2.600933 | 0.958347 | 0.269388 |
| H | -3.193597 | 0.058401 | 1.676851 |
| H | -1.424055 | 2.890168 | 0.545970 |
| H | -1.772951 | 3.681165 | 2.105698 |
| H | -2.625582 | 2.445034 | 3.854189 |
| H | -2.710729 | 0.676378 | 3.779606 |
| H | -1.105040 | 1.487007 | 5.495973 |
| H | -0.166793 | 2.340381 | 4.260500 |
| H | 1.744907 | 1.387361 | 4.317364 |
| H | 1.612040 | 0.083735 | 5.520923 |
| H | 0.154296 | -1.646297 | 5.034976 |
| H | -1.303047 | -0.767042 | 5.492902 |
| H | 2.521965 | 1.931981 | -0.583443 |
| H | 3.143389 | 2.520305 | -2.146529 |

**Optimized xyz Coordinates for 3:**

| | | | |
|---|---|---|---|
| Fe | -0.003770 | 0.180389 | -1.528702 |
| Fe | 0.003686 | -0.180697 | 1.532005 |
| O | -0.338280 | -1.368738 | -0.157777 |
| O | -0.073786 | 1.725744 | -2.713977 |
| O | 0.056981 | -1.047945 | -3.039379 |
| N | -2.121811 | 0.563616 | -1.140137 |
| N | 2.114499 | -0.290249 | -1.243220 |
| C | -2.700177 | -1.622006 | -0.180475 |
| C | -1.407869 | -2.183283 | -0.248997 |
| C | -1.261602 | -3.571908 | -0.408334 |
| C | -2.396905 | -4.381194 | -0.497743 |
| C | -3.681813 | -3.824960 | -0.430524 |
| C | -3.827834 | -2.442163 | -0.271695 |
| C | -2.787102 | -0.128722 | -0.008665 |
| C | 2.824279 | -1.007290 | -2.063179 |
| C | -2.840700 | 1.433703 | -1.785544 |
| C | 2.384667 | -1.618024 | -3.290190 |
| C | 1.010893 | -1.633977 | -3.714967 |
| C | 0.695358 | -2.329689 | -4.913052 |
| C | 1.681395 | -2.961113 | -5.658868 |
| C | 3.028548 | -2.940858 | -5.246617 |
| C | 3.361271 | -2.280818 | -4.073333 |
| C | -2.410511 | 2.294903 | -2.855652 |
| C | -1.036943 | 2.419200 | -3.263519 |
| C | -0.732976 | 3.347572 | -4.295288 |
| C | -1.729256 | 4.101621 | -4.900633 |
| C | -3.075402 | 3.979117 | -4.502820 |
| C | -3.397269 | 3.089740 | -3.488745 |
| H | -0.258072 | -3.996155 | -0.459548 |
| H | -2.277938 | -5.459606 | -0.621126 |
| H | -4.563065 | -4.463891 | -0.501129 |
| H | -4.824240 | -1.996447 | -0.217718 |
| H | -0.348246 | -2.349593 | -5.231751 |
| H | 1.404514 | -3.482327 | -6.577769 |
| H | 3.795680 | -3.441581 | -5.837542 |
| H | 4.398441 | -2.262643 | -3.729432 |
| H | 0.309891 | 3.447177 | -4.601201 |
| H | -1.461237 | 4.801188 | -5.695273 |
| H | -3.850529 | 4.577771 | -4.981573 |
| H | -4.433926 | 2.986184 | -3.158614 |
| H | 3.879981 | -1.197593 | -1.808382 |
| H | -3.897222 | 1.554484 | -1.494527 |
| H | -3.847976 | 0.179958 | 0.029521 |
| O | 0.338009 | 1.367698 | 0.160983 |
| C | 2.786891 | 0.128646 | 0.011359 |
| N | -2.114592 | 0.291242 | 1.245540 |
| C | 1.407430 | 2.182660 | 0.252654 |
| O | 0.073963 | -1.725934 | 2.717582 |
| O | -0.057347 | 1.047310 | 3.042579 |
| N | 2.121662 | -0.564744 | 1.142080 |
| C | 2.699804 | 1.621708 | 0.184162 |
| H | 3.847806 | -0.179882 | -0.027008 |
| C | -2.823529 | 1.011601 | 2.063373 |
| C | 1.260844 | 3.571152 | 0.412316 |

| | | | |
|---|---|---|---|
| C | 1.036811 | -2.422683 | 3.263553 |
| C | -1.010479 | 1.637127 | 3.715924 |
| C | 2.840125 | -1.436737 | 1.785266 |
| C | 3.827335 | 2.442005 | 0.275857 |
| C | -2.383797 | 1.623906 | 3.289558 |
| H | -3.878629 | 1.203555 | 1.807358 |
| C | 2.395965 | 4.380609 | 0.502305 |
| H | 0.257220 | 3.995069 | 0.463630 |
| C | 2.409901 | -2.299847 | 2.853792 |
| C | 0.732844 | -3.352992 | 4.293583 |
| C | -0.694549 | 2.334061 | 4.913204 |
| H | 3.896337 | -1.557962 | 1.493394 |
| C | 3.680978 | 3.824685 | 0.435171 |
| H | 4.823849 | 1.996478 | 0.221835 |
| C | -3.359624 | 2.290638 | 4.070308 |
| H | 2.276831 | 5.458966 | 0.626036 |
| C | 3.396258 | -3.097862 | 3.483520 |
| C | 1.728705 | -4.110294 | 4.895536 |
| H | -0.309725 | -3.451502 | 4.600882 |
| C | -1.679855 | 2.969344 | 5.656694 |
| H | 0.348713 | 2.351780 | 5.233140 |
| H | 4.562089 | 4.463760 | 0.506206 |
| C | -3.026540 | 2.951940 | 5.242776 |
| H | -4.396462 | 2.274594 | 3.725276 |
| C | 3.074415 | -3.989219 | 4.495863 |
| H | 4.432606 | -2.995187 | 3.152132 |
| H | 1.460691 | -4.811321 | 5.688889 |
| H | -1.402762 | 3.491390 | 6.575059 |
| H | -3.793052 | 3.455797 | 5.831843 |
| H | 3.849231 | -4.590456 | 4.971879 |

**Optimized xyz Coordinates for 4:**

| | | | |
|---|---|---|---|
| Fe | -0.253107 | -0.014684 | 1.268758 |
| Fe | -0.253051 | 0.015776 | -1.269701 |
| O | 0.518196 | -1.426352 | -0.018335 |
| O | -1.805476 | -0.001332 | -0.000558 |
| O | 0.518976 | 1.425657 | 0.017022 |
| N | 1.434881 | 0.023680 | 2.785420 |
| N | -1.142058 | 1.365756 | 2.794713 |
| N | -1.017020 | -1.528618 | 2.737785 |
| C | 1.302188 | 1.390481 | 3.360920 |
| C | -0.118332 | 1.679359 | 3.839410 |
| C | -2.273541 | 0.560648 | 3.329754 |
| C | -1.828605 | -0.829379 | 3.781868 |
| C | 0.233591 | -2.119581 | 3.284829 |
| C | 1.194308 | -1.051681 | 3.799571 |
| C | 2.771677 | -0.140555 | 2.175593 |
| C | -1.645819 | 2.608098 | 2.167457 |
| C | -1.815559 | -2.572879 | 2.057555 |
| N | 1.434580 | -0.022407 | -2.786558 |
| C | 1.301740 | -1.389295 | -3.361733 |
| C | -0.118920 | -1.678639 | -3.839728 |
| N | -1.142578 | -1.364548 | -2.795290 |
| N | -1.017548 | 1.529834 | -2.738915 |
| C | -1.828452 | 0.830364 | -3.783394 |
| C | -2.273814 | -0.559160 | -3.330663 |
| C | -1.647001 | -2.606176 | -2.167046 |
| C | 0.233301 | 2.120593 | -3.285387 |
| C | 1.193870 | 1.052914 | -3.800574 |
| C | 2.771683 | 0.141927 | -2.177266 |
| C | -1.816195 | 2.574388 | -2.059501 |
| H | -1.233477 | 2.985024 | -1.226428 |
| H | -2.735423 | 2.129302 | -1.661185 |
| H | -2.083422 | 3.383481 | -2.761234 |
| H | -1.242187 | 0.763644 | -4.708167 |
| H | -2.720045 | 1.426208 | -4.029758 |
| H | 0.698987 | 2.685624 | -2.465115 |
| H | 0.010262 | 2.835188 | -4.098350 |
| H | 0.808385 | 0.598017 | -4.721172 |
| H | 2.145776 | 1.532111 | -4.074041 |
| H | -0.186531 | -2.738863 | -4.126163 |
| H | -0.344393 | -1.104211 | -4.746714 |
| H | -3.014143 | -0.474075 | -2.522429 |
| H | -2.764130 | -1.079029 | -4.173514 |
| H | -2.336578 | -2.347462 | -1.354957 |
| H | -0.804461 | -3.164617 | -1.743022 |
| H | -2.170873 | -3.236464 | -2.906341 |
| H | 1.583423 | -2.097947 | -2.569555 |
| H | 2.005659 | -1.533640 | -4.201280 |
| H | 2.913698 | -0.596546 | -1.378281 |
| H | 2.863519 | 1.150162 | -1.754462 |
| H | 3.569827 | 0.003937 | -2.927151 |
| H | -2.337007 | 2.350856 | 1.356310 |
| H | -0.803255 | 3.165616 | 1.742321 |
| H | -2.168037 | 3.238806 | 2.907565 |
| H | -1.231365 | -2.984911 | 1.226176 |

| | | | |
|---|---|---|---|
| H | -2.733119 | -2.126549 | 1.656397 |
| H | -2.085333 | -3.381114 | 2.759542 |
| H | 2.913663 | 0.598298 | 1.377305 |
| H | 2.863098 | -1.148478 | 1.752197 |
| H | 3.569844 | -0.003590 | 2.925301 |
| H | 0.699188 | -2.685185 | 2.464966 |
| H | 0.010250 | -2.833506 | 4.098247 |
| H | 0.808792 | -0.596590 | 4.720026 |
| H | 2.146299 | -1.530790 | 4.073000 |
| H | -0.343619 | 1.104105 | 4.745889 |
| H | -0.186218 | 2.739352 | 4.126615 |
| H | 1.583626 | 2.099364 | 2.568989 |
| H | 2.006238 | 1.534514 | 4.200306 |
| H | -3.014103 | 0.475923 | 2.521719 |
| H | -2.763670 | 1.080154 | 4.172910 |
| H | -1.243163 | -0.763439 | 4.707318 |
| H | -2.720518 | -1.425180 | 4.027272 |
| H | 1.463791 | -1.650103 | -0.018077 |
| H | -2.774733 | 0.018603 | -0.000636 |
| H | 1.463365 | 1.654508 | 0.017050 |

**Optimized xyz Coordinates for 5:**

| | | | |
|---|---|---|---|
| Fe | 0.027562 | 0.002271 | 1.608074 |
| Fe | -0.000158 | 0.003628 | -1.600324 |
| N | -0.020888 | -1.014277 | 3.697741 |
| N | 1.467669 | 1.293844 | 2.805249 |
| N | -1.417325 | 1.324279 | 2.747977 |
| N | -1.495990 | 1.234704 | -2.793188 |
| N | 1.385479 | 1.392878 | -2.732992 |
| N | 0.094307 | -1.000251 | -3.695093 |
| O | -0.007260 | 0.967561 | 0.004643 |
| O | -1.455750 | -1.362921 | 1.127122 |
| O | -1.512983 | -1.319751 | -1.128473 |
| O | 1.598398 | -1.251309 | 1.132597 |
| O | 1.540677 | -1.297087 | -1.122914 |
| C | 1.015615 | -0.396780 | 4.582916 |
| C | 2.075369 | 0.356976 | 3.788479 |
| C | 0.710335 | 2.405869 | 3.463375 |
| C | -0.662145 | 2.604634 | 2.833886 |
| C | -1.737862 | 0.751072 | 4.093213 |
| C | -1.400570 | -0.733542 | 4.175134 |
| C | 0.188653 | -2.476265 | 3.601103 |
| C | 2.514844 | 1.845246 | 1.916775 |
| C | -2.655624 | 1.521308 | 1.961740 |
| C | -0.787995 | 2.382765 | -3.444457 |
| C | 0.574036 | 2.638785 | -2.812735 |
| C | 1.731333 | 0.840904 | -4.080731 |
| C | 1.460773 | -0.656912 | -4.169273 |
| C | -0.967330 | -0.424870 | -4.578825 |
| C | -2.060326 | 0.277034 | -3.782062 |
| C | -2.567710 | 1.734198 | -1.903302 |
| C | 2.613774 | 1.640614 | -1.945583 |
| C | -0.051498 | -2.470394 | -3.604617 |
| C | -1.924480 | -1.740974 | 0.003535 |
| C | -3.031131 | -2.817310 | 0.001627 |
| C | -2.315522 | -4.172848 | -0.219790 |
| C | -4.023851 | -2.564881 | -1.147352 |
| C | -3.781925 | -2.845454 | 1.342165 |
| C | 2.023286 | -1.658185 | 0.000461 |
| C | 3.166094 | -2.696023 | 0.000584 |
| C | 2.493485 | -4.077516 | 0.195752 |
| C | 4.138325 | -2.427524 | 1.163110 |
| C | 3.930525 | -2.680569 | -1.332610 |
| H | 1.507389 | -1.175426 | 5.184799 |
| H | 0.523382 | 0.272528 | 5.299088 |
| H | 2.692627 | -0.346091 | 3.213619 |
| H | 2.740038 | 0.900349 | 4.483032 |
| H | 1.280613 | 3.342996 | 3.385912 |
| H | 0.619875 | 2.191179 | 4.534812 |
| H | -1.230004 | 3.354816 | 3.411829 |
| H | -0.557824 | 2.978463 | 1.805655 |
| H | -1.195785 | 1.315361 | 4.861374 |
| H | -2.807089 | 0.889432 | 4.311012 |
| H | -2.080653 | -1.312770 | 3.536761 |
| H | -1.535449 | -1.082206 | 5.214741 |
| H | 1.203584 | -2.673790 | 3.239254 |

| | | | |
|---|---|---|---|
| H | -0.529069 | -2.899730 | 2.889331 |
| H | 0.053226 | -2.955628 | 4.585836 |
| H | 2.051754 | 2.528978 | 1.196680 |
| H | 3.005118 | 1.027656 | 1.376031 |
| H | 3.271314 | 2.394300 | 2.502467 |
| H | -2.390887 | 1.868706 | 0.957619 |
| H | -3.309342 | 2.265401 | 2.446897 |
| H | -3.194163 | 0.569962 | 1.883262 |
| H | -1.399145 | 3.293350 | -3.362257 |
| H | -0.687502 | 2.178153 | -4.516954 |
| H | 0.452558 | 3.002028 | -1.782610 |
| H | 1.108291 | 3.416528 | -3.386291 |
| H | 1.164235 | 1.383689 | -4.846241 |
| H | 2.793214 | 1.028149 | -4.297870 |
| H | 2.165121 | -1.208031 | -3.532260 |
| H | 1.612487 | -0.994871 | -5.210084 |
| H | -0.504588 | 0.269232 | -5.291121 |
| H | -1.423360 | -1.221508 | -5.185295 |
| H | -2.646550 | -0.455762 | -3.211844 |
| H | -2.747708 | 0.793913 | -4.474733 |
| H | -2.136140 | 2.433446 | -1.178568 |
| H | -3.022145 | 0.892624 | -1.368076 |
| H | -3.346896 | 2.252795 | -2.486941 |
| H | 3.194140 | 0.713743 | -1.872813 |
| H | 2.334018 | 1.969974 | -0.939506 |
| H | 3.233690 | 2.415759 | -2.426461 |
| H | -1.057321 | -2.713388 | -3.244907 |
| H | 0.683195 | -2.864949 | -2.893515 |
| H | 0.105750 | -2.939500 | -4.591032 |
| H | -4.278277 | -1.885734 | 1.546584 |
| H | -3.108898 | -3.072034 | 2.178969 |
| H | -4.556602 | -3.625262 | 1.307684 |
| H | -3.523213 | -2.581122 | -2.123614 |
| H | -4.532589 | -1.596356 | -1.033076 |
| H | -4.792081 | -3.351732 | -1.143027 |
| H | -1.601484 | -4.385913 | 0.588592 |
| H | -1.777221 | -4.188724 | -1.177379 |
| H | -3.064640 | -4.978118 | -0.233363 |
| H | 1.794718 | -4.302294 | -0.622692 |
| H | 1.946772 | -4.125009 | 1.147556 |
| H | 3.268594 | -4.857849 | 0.205745 |
| H | 3.629035 | -2.474107 | 2.133900 |
| H | 4.615998 | -1.441277 | 1.068012 |
| H | 4.932025 | -3.188647 | 1.155802 |
| H | 4.395772 | -1.701858 | -1.519739 |
| H | 3.273805 | -2.918587 | -2.179074 |
| H | 4.731176 | -3.433758 | -1.300546 |

**Optimized xyz Coordinates for 6:**

| | | | |
|---|---|---|---|
| Fe | 0.125923 | -0.073705 | 1.553563 |
| Fe | 0.115624 | -0.157154 | -1.523974 |
| O | 1.176493 | -0.173189 | 0.013127 |
| O | -0.932614 | 1.629799 | 1.099030 |
| O | -1.137594 | -1.719387 | -1.061680 |
| O | 2.951509 | 4.781367 | -4.310487 |
| O | 2.865441 | -4.313054 | -5.387573 |
| O | 2.406614 | -5.188036 | 4.497255 |
| O | 3.445241 | 3.789341 | 5.305099 |
| N | -1.410485 | 1.260508 | -1.111654 |
| N | -0.885817 | -0.005217 | -3.586319 |
| N | 1.185718 | 1.492563 | -2.520706 |
| N | 1.162151 | -1.551830 | -2.836904 |
| N | -1.560060 | -1.295042 | 1.150241 |
| N | -0.888244 | -0.092079 | 3.623150 |
| N | 1.011161 | -1.802844 | 2.564452 |
| N | 1.330693 | 1.212355 | 2.862696 |
| C | -0.155363 | 0.928033 | -4.479932 |
| H | -0.876230 | 1.532877 | -5.054086 |
| H | 0.400449 | 0.337330 | -5.226157 |
| C | 0.834482 | 1.828901 | -3.772601 |
| C | 1.397087 | 2.933749 | -4.439388 |
| C | 1.040066 | 3.246571 | -5.867564 |
| H | 1.747862 | 3.964746 | -6.296494 |
| H | 0.027285 | 3.671845 | -5.949838 |
| H | 1.061225 | 2.338694 | -6.487034 |
| C | 2.333586 | 3.701760 | -3.724007 |
| C | 2.154130 | 5.990617 | -4.364941 |
| H | 2.771613 | 6.736047 | -4.877335 |
| H | 1.915425 | 6.337431 | -3.348327 |
| H | 1.222689 | 5.829686 | -4.926882 |
| C | 2.725425 | 3.342390 | -2.418087 |
| C | 3.760506 | 4.125226 | -1.661081 |
| H | 3.932499 | 3.682157 | -0.672236 |
| H | 3.450994 | 5.170937 | -1.519937 |
| H | 4.716732 | 4.143434 | -2.203819 |
| C | 2.110285 | 2.221641 | -1.867892 |
| H | 2.348748 | 1.876630 | -0.859681 |
| C | -0.867286 | -1.383734 | -4.125679 |
| H | -1.183240 | -1.399072 | -5.179701 |
| H | -1.594024 | -1.976697 | -3.551082 |
| C | 0.510693 | -1.987603 | -3.939923 |
| C | 1.079361 | -2.926579 | -4.806651 |
| C | 0.377186 | -3.457868 | -6.026738 |
| H | -0.528289 | -2.890557 | -6.265068 |
| H | 0.083241 | -4.508584 | -5.877821 |
| H | 1.046205 | -3.436755 | -6.897493 |
| C | 2.387094 | -3.394302 | -4.508947 |
| C | 4.263755 | -4.321843 | -5.767864 |
| H | 4.287060 | -4.787161 | -6.759533 |
| H | 4.865466 | -4.917372 | -5.071046 |
| H | 4.651745 | -3.297304 | -5.833976 |
| C | 3.063848 | -2.956221 | -3.347651 |
| C | 4.393641 | -3.478312 | -2.866633 |

| | | | |
|---|---|---|---|
| H | 4.402720 | -4.576882 | -2.833886 |
| H | 4.589178 | -3.107190 | -1.852305 |
| H | 5.231311 | -3.156989 | -3.500238 |
| C | 2.384407 | -2.026672 | -2.559204 |
| H | 2.842453 | -1.648493 | -1.642044 |
| C | -2.252201 | 0.471632 | -3.262850 |
| H | -2.783653 | -0.363710 | -2.788377 |
| H | -2.800566 | 0.757736 | -4.177476 |
| C | -2.193473 | 1.644912 | -2.290931 |
| H | -1.745326 | 2.528259 | -2.782855 |
| H | -3.226925 | 1.920295 | -2.030168 |
| C | -1.566215 | 1.932746 | 0.017940 |
| C | -2.504543 | 3.118717 | 0.111649 |
| H | -2.320300 | 3.842579 | -0.694763 |
| H | -2.374022 | 3.610729 | 1.080907 |
| H | -3.551028 | 2.789003 | 0.021606 |
| C | -0.272924 | -1.102637 | 4.520369 |
| H | -1.063499 | -1.641717 | 5.067771 |
| H | 0.316558 | -0.579190 | 5.290494 |
| C | 0.639977 | -2.089827 | 3.824767 |
| C | 1.112528 | -3.221629 | 4.505633 |
| C | 0.696828 | -3.498291 | 5.925923 |
| H | 0.801387 | -2.601753 | 6.553933 |
| H | 1.304385 | -4.298720 | 6.359718 |
| H | -0.358853 | -3.809649 | 5.977651 |
| C | 2.002742 | -4.078167 | 3.818051 |
| C | 3.802053 | -5.580525 | 4.470989 |
| H | 3.983621 | -6.076604 | 5.431349 |
| H | 4.450599 | -4.698785 | 4.385717 |
| H | 4.003030 | -6.283322 | 3.653135 |
| C | 2.365871 | -3.804307 | 2.477190 |
| C | 3.195165 | -4.722824 | 1.618397 |
| H | 2.845779 | -5.761985 | 1.696677 |
| H | 4.260396 | -4.708395 | 1.888336 |
| H | 3.113692 | -4.419152 | 0.567041 |
| C | 1.839524 | -2.642044 | 1.918597 |
| H | 2.069020 | -2.364623 | 0.887519 |
| C | -0.704973 | 1.275775 | 4.155729 |
| H | -1.005826 | 1.337381 | 5.213522 |
| H | -1.361850 | 1.949540 | 3.585626 |
| C | 0.729143 | 1.719292 | 3.958039 |
| C | 1.386298 | 2.609654 | 4.825059 |
| C | 0.728376 | 3.144449 | 6.068981 |
| H | 1.478756 | 3.542912 | 6.761414 |
| H | 0.168280 | 2.357280 | 6.591851 |
| H | 0.014047 | 3.949317 | 5.836875 |
| C | 2.712692 | 2.957850 | 4.493061 |
| C | 3.135232 | 5.201093 | 5.189598 |
| H | 3.777440 | 5.710022 | 5.916162 |
| H | 2.079662 | 5.400304 | 5.423122 |
| H | 3.362038 | 5.558506 | 4.174088 |
| C | 3.359562 | 2.398740 | 3.373600 |
| C | 4.791111 | 2.715032 | 3.046120 |
| H | 5.107344 | 2.183623 | 2.139593 |
| H | 5.457031 | 2.419928 | 3.870173 |
| H | 4.938351 | 3.793022 | 2.886965 |
| C | 2.606602 | 1.528936 | 2.587730 |

| | | | |
|---|---|---|---|
| H | 3.033964 | 1.061885 | 1.697520 |
| C | -2.301120 | -0.405933 | 3.300462 |
| H | -2.731083 | 0.484341 | 2.823190 |
| H | -2.879646 | -0.623239 | 4.215436 |
| C | -2.379427 | -1.581662 | 2.333111 |
| H | -2.033649 | -2.508310 | 2.827861 |
| H | -3.438187 | -1.738060 | 2.075656 |
| C | -1.799944 | -1.943478 | 0.021792 |
| C | -2.875152 | -3.007012 | -0.068500 |
| H | -2.807499 | -3.512394 | -1.037287 |
| H | -3.873615 | -2.552370 | 0.022856 |
| H | -2.778059 | -3.746786 | 0.738645 |

**Optimized xyz Coordinates for 7:**

| | | | |
|---|---|---|---|
| Fe | 1.507808 | -0.031629 | -0.176865 |
| Fe | -1.388199 | 0.001828 | 0.082782 |
| O | 0.066260 | -1.207861 | -0.091336 |
| O | 0.003512 | 1.419937 | -0.046846 |
| O | 2.616703 | 0.749882 | -6.328459 |
| N | 3.215608 | 1.460621 | -0.365339 |
| C | 2.925078 | 2.253630 | -1.585294 |
| H | 3.787491 | 2.874942 | -1.868861 |
| H | 2.095824 | 2.940002 | -1.354624 |
| N | 1.784055 | 0.260406 | -2.312488 |
| C | 2.502389 | 1.333720 | -2.707556 |
| N | 2.175520 | 0.336676 | 1.867913 |
| C | 2.809361 | 1.572111 | -4.057383 |
| N | 3.186331 | -1.344967 | -0.246005 |
| C | 2.324113 | 0.633164 | -4.995135 |
| C | 1.609666 | -0.509998 | -4.583831 |
| C | 1.363651 | -0.638822 | -3.219145 |
| H | 0.806990 | -1.492783 | -2.828251 |
| C | 3.656271 | 2.738740 | -4.490260 |
| H | 4.493888 | 2.899901 | -3.798507 |
| H | 3.077318 | 3.674506 | -4.520016 |
| H | 4.074017 | 2.562476 | -5.488052 |
| C | 1.904979 | 1.785221 | -7.053226 |
| H | 2.341074 | 1.802153 | -8.057357 |
| H | 2.026662 | 2.768754 | -6.579226 |
| H | 0.836109 | 1.532848 | -7.116337 |
| C | 1.147708 | -1.548503 | -5.565111 |
| H | 0.569611 | -2.331180 | -5.058519 |
| H | 2.005736 | -2.021337 | -6.065463 |
| H | 0.523986 | -1.107104 | -6.355231 |
| C | 3.187354 | 2.287578 | 0.865126 |
| H | 2.360139 | 3.008715 | 0.773731 |
| H | 4.110843 | 2.878702 | 0.964757 |
| C | 2.960815 | 1.413495 | 2.077855 |
| C | 3.509402 | 1.704647 | 3.335904 |
| C | 2.438552 | -0.347805 | 4.162008 |
| C | 4.342751 | 2.936802 | 3.565663 |
| H | 3.781136 | 3.847486 | 3.311533 |
| H | 5.250298 | 2.927747 | 2.943016 |
| H | 4.647829 | 3.004703 | 4.614659 |
| C | 4.852436 | 0.261072 | 6.075919 |
| H | 5.065619 | 0.589522 | 7.098373 |
| H | 5.726373 | 0.441670 | 5.432940 |
| H | 4.605119 | -0.809107 | 6.073915 |
| C | 2.103819 | -1.328049 | 5.249975 |
| H | 1.183156 | -1.873274 | 5.006013 |
| H | 1.976861 | -0.819875 | 6.215228 |
| H | 2.900147 | -2.077650 | 5.375049 |
| C | 4.502476 | 0.712287 | -0.496784 |
| H | 5.228835 | 1.111592 | 0.228631 |
| H | 4.936901 | 0.925939 | -1.486578 |
| C | 4.407703 | -0.791525 | -0.338882 |
| C | 5.577020 | -1.569841 | -0.322757 |
| C | 5.423540 | -2.965277 | -0.187356 |

| | | | |
|---|---|---|---|
| C | 4.140512 | -3.552783 | -0.112004 |
| C | 3.055663 | -2.681854 | -0.145573 |
| H | 2.031250 | -3.057962 | -0.102992 |
| C | 6.933157 | -0.933603 | -0.451643 |
| H | 7.025277 | -0.389313 | -1.404247 |
| H | 7.722505 | -1.690736 | -0.413336 |
| H | 7.111632 | -0.205619 | 0.354657 |
| C | 6.934208 | -4.369814 | 1.027820 |
| H | 7.804541 | -4.991920 | 0.794616 |
| H | 6.128322 | -4.996464 | 1.432905 |
| H | 7.209134 | -3.598519 | 1.762412 |
| C | 3.922962 | -5.038689 | -0.049221 |
| H | 2.923541 | -5.294409 | -0.423867 |
| H | 3.993951 | -5.415668 | 0.982645 |
| H | 4.672851 | -5.571352 | -0.649421 |
| C | 3.248311 | 0.788336 | 4.378478 |
| C | 1.920818 | -0.511672 | 2.878525 |
| H | 1.272485 | -1.358737 | 2.645172 |
| O | 3.731787 | 1.067425 | 5.628990 |
| O | 6.548243 | -3.746033 | -0.223571 |
| O | -2.741687 | -1.023809 | 6.175563 |
| N | -3.047018 | -1.482364 | 0.184519 |
| C | -2.725227 | -2.330025 | 1.361238 |
| H | -3.543824 | -3.032930 | 1.573979 |
| H | -1.834159 | -2.925358 | 1.108728 |
| N | -1.731099 | -0.324288 | 2.230676 |
| C | -2.407663 | -1.449447 | 2.546338 |
| N | -2.106002 | -0.167565 | -1.970600 |
| C | -2.769025 | -1.761350 | 3.867557 |
| N | -3.139539 | 1.328587 | 0.290882 |
| C | -2.384678 | -0.838079 | 4.866095 |
| C | -1.714075 | 0.356950 | 4.537544 |
| C | -1.407631 | 0.555158 | 3.192837 |
| H | -0.883829 | 1.458171 | 2.873362 |
| C | -3.571081 | -2.988362 | 4.209054 |
| H | -4.355548 | -3.172045 | 3.462971 |
| H | -2.940517 | -3.890019 | 4.242397 |
| H | -4.055595 | -2.872695 | 5.185334 |
| C | -2.014083 | -2.048176 | 6.900256 |
| H | -2.502855 | -2.129049 | 7.876598 |
| H | -2.054708 | -3.016678 | 6.383416 |
| H | -0.965899 | -1.741969 | 7.033477 |
| C | -1.363141 | 1.379472 | 5.579534 |
| H | -0.797374 | 2.208162 | 5.135910 |
| H | -2.272157 | 1.790899 | 6.042830 |
| H | -0.765317 | 0.940232 | 6.390485 |
| C | -2.949906 | -2.241088 | -1.089924 |
| H | -2.042797 | -2.862962 | -1.038220 |
| H | -3.810582 | -2.915776 | -1.211652 |
| C | -2.825477 | -1.275141 | -2.244269 |
| C | -3.396326 | -1.502839 | -3.504962 |
| C | -2.475790 | 0.670058 | -4.195863 |
| C | -4.161954 | -2.762959 | -3.808294 |
| H | -3.531488 | -3.652857 | -3.666446 |
| H | -5.033104 | -2.870759 | -3.144568 |
| H | -4.517890 | -2.757842 | -4.843331 |
| C | -4.908762 | 0.074689 | -6.083283 |

| | | | |
|---|---|---|---|
| H | -5.139411 | -0.188539 | -7.120726 |
| H | -5.751011 | -0.197443 | -5.430221 |
| H | -4.715283 | 1.153321 | -6.008280 |
| C | -2.229522 | 1.746844 | -5.214338 |
| H | -1.331356 | 2.322402 | -4.956929 |
| H | -2.107651 | 1.320269 | -6.218994 |
| H | -3.068370 | 2.458245 | -5.258880 |
| C | -4.368478 | -0.805587 | 0.331568 |
| H | -5.024933 | -1.119140 | -0.495708 |
| H | -4.861881 | -1.179161 | 1.243053 |
| C | -4.330274 | 0.709753 | 0.381484 |
| C | -5.535857 | 1.420316 | 0.516759 |
| C | -5.459309 | 2.827227 | 0.541719 |
| C | -4.213793 | 3.485940 | 0.457353 |
| C | -3.090201 | 2.672831 | 0.332510 |
| H | -2.098819 | 3.124873 | 0.270022 |
| C | -6.851865 | 0.701973 | 0.631226 |
| H | -6.870964 | 0.044354 | 1.514293 |
| H | -7.676144 | 1.415920 | 0.723825 |
| H | -7.039278 | 0.066665 | -0.247978 |
| C | -7.132661 | 4.233869 | -0.426442 |
| H | -8.014689 | 4.781943 | -0.079056 |
| H | -6.396739 | 4.938214 | -0.837994 |
| H | -7.422752 | 3.506973 | -1.199649 |
| C | -4.072117 | 4.979634 | 0.540547 |
| H | -3.057299 | 5.251890 | 0.857556 |
| H | -4.252216 | 5.457279 | -0.434850 |
| H | -4.792204 | 5.402991 | 1.253747 |
| C | -3.224914 | -0.493020 | -4.477989 |
| C | -1.931241 | 0.769335 | -2.916409 |
| H | -1.326049 | 1.633678 | -2.635393 |
| O | -3.735901 | -0.703426 | -5.731123 |
| O | -6.612762 | 3.542541 | 0.737747 |
| H | 0.023956 | 2.320591 | 0.318626 |

**Optimized xyz Coordinates for 8:**

| | | | |
|---|---|---|---|
| Fe | 1.301087 | 0.017662 | -0.117634 |
| Fe | -1.299665 | -0.018561 | 0.116518 |
| O | 0.070429 | -1.271049 | -0.019389 |
| O | -0.068819 | 1.270082 | 0.017688 |
| O | 2.429294 | 0.490564 | -6.108471 |
| N | 2.728564 | 1.476861 | -0.224621 |
| C | 2.371069 | 2.265834 | -1.441875 |
| H | 3.172973 | 2.969565 | -1.701145 |
| H | 1.470510 | 2.849525 | -1.202271 |
| N | 1.435085 | 0.167031 | -2.110720 |
| C | 2.064721 | 1.288711 | -2.546541 |
| N | 1.772289 | 0.131871 | 1.820459 |
| C | 2.408530 | 1.475413 | -3.892987 |
| N | 2.873393 | -1.208791 | -0.261272 |
| C | 2.072526 | 0.434100 | -4.789251 |
| C | 1.465580 | -0.752170 | -4.331017 |
| C | 1.164647 | -0.827607 | -2.973168 |
| H | 0.686632 | -1.710566 | -2.548244 |
| C | 3.160468 | 2.693277 | -4.358906 |
| H | 3.911988 | 3.005945 | -3.622509 |
| H | 2.489539 | 3.551093 | -4.518361 |
| H | 3.679137 | 2.485661 | -5.301954 |
| C | 1.693803 | 1.418819 | -6.946246 |
| H | 2.199556 | 1.410088 | -7.917073 |
| H | 1.703737 | 2.435982 | -6.532546 |
| H | 0.656190 | 1.074256 | -7.065156 |
| C | 1.174910 | -1.896720 | -5.258593 |
| H | 0.668793 | -2.711760 | -4.726909 |
| H | 2.105848 | -2.291762 | -5.690855 |
| H | 0.542840 | -1.581463 | -6.100595 |
| C | 2.570094 | 2.255842 | 1.041236 |
| H | 1.652807 | 2.854619 | 0.947422 |
| H | 3.415256 | 2.942605 | 1.187116 |
| C | 2.430375 | 1.265439 | 2.167505 |
| C | 2.948595 | 1.460421 | 3.453627 |
| C | 2.158168 | -0.799227 | 4.003539 |
| C | 3.637189 | 2.744430 | 3.831565 |
| H | 2.999291 | 3.614904 | 3.623161 |
| H | 4.569298 | 2.877397 | 3.261381 |
| H | 3.885370 | 2.747197 | 4.897721 |
| C | 4.518099 | -0.103371 | 5.974616 |
| H | 4.703642 | 0.111590 | 7.031931 |
| H | 5.336221 | 0.298907 | 5.359449 |
| H | 4.439250 | -1.188670 | 5.824069 |
| C | 1.983930 | -1.951654 | 4.951589 |
| H | 1.135596 | -2.578938 | 4.650604 |
| H | 1.823216 | -1.597451 | 5.978309 |
| H | 2.876295 | -2.595963 | 4.963901 |
| C | 4.104978 | 0.880503 | -0.337577 |
| H | 4.722632 | 1.239702 | 0.499300 |
| H | 4.590841 | 1.265643 | -1.246748 |
| C | 4.084437 | -0.625550 | -0.356824 |
| C | 5.266083 | -1.373010 | -0.462903 |
| C | 5.144202 | -2.777223 | -0.454771 |

| | | | |
|---|---|---|---|
| C | 3.876509 | -3.393540 | -0.368965 |
| C | 2.771179 | -2.551699 | -0.273703 |
| H | 1.757212 | -2.949497 | -0.213495 |
| C | 6.599235 | -0.688597 | -0.579796 |
| H | 6.633527 | -0.037955 | -1.467238 |
| H | 7.406548 | -1.422687 | -0.664653 |
| H | 6.797313 | -0.052137 | 0.296204 |
| C | 6.766007 | -4.207495 | 0.566099 |
| H | 7.635486 | -4.787872 | 0.240514 |
| H | 6.007061 | -4.880773 | 0.987489 |
| H | 7.068955 | -3.469228 | 1.323165 |
| C | 3.692582 | -4.884300 | -0.420022 |
| H | 2.675083 | -5.135327 | -0.745185 |
| H | 3.845645 | -5.342984 | 0.568799 |
| H | 4.410626 | -5.343631 | -1.112518 |
| C | 2.814025 | 0.394987 | 4.371072 |
| C | 1.646260 | -0.867914 | 2.709086 |
| H | 1.108387 | -1.750189 | 2.361178 |
| O | 3.272980 | 0.568398 | 5.648947 |
| O | 6.275831 | -3.531771 | -0.620584 |
| O | -2.430612 | -0.489758 | 6.106906 |
| N | -2.727300 | -1.477397 | 0.223622 |
| C | -2.369568 | -2.266521 | 1.440718 |
| H | -3.170978 | -2.970966 | 1.699543 |
| H | -1.468439 | -2.849346 | 1.201131 |
| N | -1.433823 | -0.167850 | 2.109704 |
| C | -2.064002 | -1.289263 | 2.545484 |
| N | -1.771309 | -0.132495 | -1.821515 |
| C | -2.408595 | -1.475555 | 3.891774 |
| N | -2.871532 | 1.208372 | 0.260474 |
| C | -2.073121 | -0.433920 | 4.787923 |
| C | -1.466089 | 0.752275 | 4.329588 |
| C | -1.164186 | 0.827203 | 2.971927 |
| H | -0.686439 | 1.710288 | 2.546971 |
| C | -3.160926 | -2.693169 | 4.357721 |
| H | -3.910362 | -3.007565 | 3.619961 |
| H | -2.489949 | -3.550333 | 4.520442 |
| H | -3.682108 | -2.484244 | 5.299113 |
| C | -1.697124 | -1.418902 | 6.945458 |
| H | -2.204809 | -1.410762 | 7.915278 |
| H | -1.706489 | -2.435748 | 6.531028 |
| H | -0.659670 | -1.074657 | 7.066659 |
| C | -1.176066 | 1.897166 | 5.256940 |
| H | -0.670185 | 2.712270 | 4.725134 |
| H | -2.107233 | 2.291927 | 5.688958 |
| H | -0.544079 | 1.582309 | 6.099166 |
| C | -2.569455 | -2.256349 | -1.042351 |
| H | -1.652373 | -2.855466 | -0.948774 |
| H | -3.414918 | -2.942765 | -1.188058 |
| C | -2.429912 | -1.265794 | -2.168509 |
| C | -2.949180 | -1.460144 | -3.454280 |
| C | -2.158810 | 0.799598 | -4.003890 |
| C | -3.638515 | -2.743784 | -3.832201 |
| H | -3.001828 | -3.614747 | -3.622222 |
| H | -4.571616 | -2.875338 | -3.263275 |
| H | -3.885179 | -2.747087 | -4.898717 |
| C | -4.520750 | 0.105842 | -5.972961 |

| | | | |
|---|---|---|---|
| H | -4.708753 | -0.110698 | -7.029518 |
| H | -5.338117 | -0.294292 | -5.355409 |
| H | -4.440169 | 1.191304 | -5.824496 |
| C | -1.985423 | 1.952546 | -4.951465 |
| H | -1.136083 | 2.579026 | -4.651638 |
| H | -1.826912 | 1.598920 | -5.978722 |
| H | -2.877322 | 2.597544 | -4.961634 |
| C | -4.103553 | -0.880723 | 0.337106 |
| H | -4.721383 | -1.239295 | -0.499920 |
| H | -4.589492 | -1.266279 | 1.246074 |
| C | -4.082596 | 0.625322 | 0.357047 |
| C | -5.264036 | 1.372983 | 0.464480 |
| C | -5.141858 | 2.777139 | 0.456815 |
| C | -3.874179 | 3.393209 | 0.369834 |
| C | -2.769049 | 2.551248 | 0.273250 |
| H | -1.755043 | 2.948887 | 0.212680 |
| C | -6.597084 | 0.688628 | 0.582786 |
| H | -6.631193 | 0.039796 | 1.471569 |
| H | -7.404539 | 1.422734 | 0.666231 |
| H | -6.795066 | 0.050388 | -0.291932 |
| C | -6.766193 | 4.205386 | -0.562541 |
| H | -7.633114 | 4.788717 | -0.235417 |
| H | -6.007306 | 4.875603 | -0.988922 |
| H | -7.073750 | 3.465500 | -1.316177 |
| C | -3.690222 | 4.883961 | 0.420512 |
| H | -2.671503 | 5.135064 | 0.741731 |
| H | -3.847363 | 5.342978 | -0.567509 |
| H | -4.405684 | 5.342950 | 1.115920 |
| C | -2.815322 | -0.394280 | -4.371363 |
| C | -1.645765 | 0.867609 | -2.709849 |
| H | -1.107648 | 1.749732 | -2.361928 |
| O | -3.275831 | -0.566998 | -5.648742 |
| O | -6.272888 | 3.532243 | 0.624303 |

**Optimized xyz Coordinates for 90° Mono-μ-oxo Model:**

| | | | |
|---|---|---|---|
| Fe | 0.000000 | -0.000000 | 1.308100 |
| Fe | 0.000000 | 0.000000 | -1.308100 |
| O | -0.000000 | 1.308100 | -0.000000 |
| N | 0.881298 | -1.738775 | 2.002017 |
| N | -1.726371 | -0.608715 | 2.293155 |
| N | 0.537496 | 0.881645 | 3.124900 |
| N | -0.001769 | 0.837437 | -3.218402 |
| N | 1.420737 | -1.335264 | -2.002400 |
| N | -1.440168 | -1.316312 | -2.017962 |
| H | 1.568922 | -2.187811 | 1.390921 |
| C | -0.294408 | -2.663407 | 2.157568 |
| C | -1.455235 | -1.972256 | 2.868670 |
| H | -2.555350 | -0.641171 | 1.691943 |
| C | -1.911662 | 0.483799 | 3.307860 |
| C | -0.612681 | 0.734070 | 4.071656 |
| H | 0.753703 | 1.870286 | 2.961033 |
| C | 1.786260 | 0.124186 | 3.429720 |
| C | 1.563355 | -1.380632 | 3.307498 |
| H | 0.177662 | 1.844551 | -3.150409 |
| C | 1.081214 | 0.149568 | -3.991448 |
| C | 2.100144 | -0.497626 | -3.054864 |
| H | 2.135347 | -1.630546 | -1.330670 |
| C | 0.682710 | -2.541355 | -2.528863 |
| C | -0.731388 | -2.636157 | -1.957900 |
| H | -2.290904 | -1.365826 | -1.449875 |
| C | -1.805577 | -0.863179 | -3.413180 |
| C | -1.409289 | 0.591664 | -3.648543 |
| H | -0.590894 | -2.991817 | 1.151612 |
| H | 0.008253 | -3.561530 | 2.714364 |
| H | -1.249811 | -1.858444 | 3.938605 |
| H | -2.355930 | -2.589940 | 2.772926 |
| H | -2.224935 | 1.379336 | 2.756689 |
| H | -2.716587 | 0.211946 | 4.005726 |
| H | -0.385292 | -0.084503 | 4.763941 |
| H | -0.708452 | 1.652151 | 4.664185 |
| H | 2.137652 | 0.371239 | 4.443584 |
| H | 2.548143 | 0.468870 | 2.717853 |
| H | 2.528748 | -1.896277 | 3.354685 |
| H | 0.943133 | -1.762441 | 4.126457 |
| H | 0.615189 | -0.588668 | -4.653557 |
| H | 1.591486 | 0.886578 | -4.623757 |
| H | 2.685463 | 0.262774 | -2.523191 |
| H | 2.795829 | -1.124265 | -3.631096 |
| H | 1.241348 | -3.447318 | -2.269927 |
| H | 0.660745 | -2.475039 | -3.622121 |
| H | -0.717735 | -2.946221 | -0.903359 |
| H | -1.304762 | -3.399245 | -2.503682 |
| H | -2.886961 | -0.973917 | -3.550905 |
| H | -1.311303 | -1.533898 | -4.125492 |
| H | -1.524834 | 0.847052 | -4.713247 |
| H | -2.042980 | 1.273666 | -3.067317 |

**Optimized xyz Coordinates for 120° Mono-μ-oxo Model:**

| | | | |
|---|---|---|---|
| Fe | 0.92500001441428 | 1.60215006349232 | -0.00000000000000 |
| Fe | -1.84999994004900 | 0.00000001628546 | -0.00000000000000 |
| O | -0.00000007760534 | -0.00000007737634 | 0.00000000000000 |
| N | 2.64521214774086 | 1.86213077842761 | 1.12350351522232 |
| N | 0.43422719025687 | 3.55717214591408 | 0.45470330878733 |
| N | 2.00910178781675 | 2.35519533738272 | -1.59643943898847 |
| H | 2.92163296302792 | 1.00124706283526 | 1.60472684099086 |
| C | 2.17570859414279 | 2.86822149760360 | 2.12935030848044 |
| C | 1.46815687697764 | 4.03706022549891 | 1.44571795815104 |
| H | -0.49926716430683 | 3.69258575140719 | 0.85395506560011 |
| C | 0.48647052460003 | 4.21874693857416 | -0.89319715359458 |
| C | 1.76125922461858 | 3.83774490325860 | -1.64444511657211 |
| H | 1.73949841510357 | 1.92239299354798 | -2.48474731287541 |
| C | 3.41004120258512 | 1.94679512131075 | -1.25142203370294 |
| C | 3.73777386644858 | 2.31419439034347 | 0.19488846110802 |
| H | 1.49543740510252 | 2.34104736651601 | 2.81150308350737 |
| H | 3.02632517091227 | 3.24000135892675 | 2.71966582560615 |
| H | 2.17926721509360 | 4.67414774707385 | 0.90778500852911 |
| H | 0.97602024943769 | 4.65822870231272 | 2.20262449199486 |
| H | -0.40709813510086 | 3.89342200788638 | -1.44245144329136 |
| H | 0.42948632712690 | 5.31066800263578 | -0.77762109752116 |
| H | 2.63548050665796 | 4.34393414083400 | -1.21884454673260 |
| H | 1.67510627293293 | 4.15682782342012 | -2.68976873236093 |
| H | 4.12329767140913 | 2.42725548358751 | -1.93700844971052 |
| H | 3.47027868183906 | 0.86133414935738 | -1.40330417002858 |
| H | 4.68152873117141 | 1.84027930141205 | 0.48924183018604 |
| H | 3.86341092233773 | 3.39699882404751 | 0.31388062487146 |
| N | -2.90324054585431 | -1.49150334874196 | -0.97584049068269 |
| N | -3.30812925000676 | 1.32429297640312 | -0.62739039298799 |
| N | -3.06470804121382 | -0.38752579789421 | 1.63401135040270 |
| H | -2.28068448643306 | -2.20100657929132 | -1.37356725614363 |
| C | -3.54089265967315 | -0.70847062769160 | -2.08263217566575 |
| C | -4.22522745832581 | 0.54521706635682 | -1.53989418956762 |
| H | -2.96150633674252 | 2.14891474477946 | -1.12673592499831 |
| C | -3.92159497298081 | 1.76154857398414 | 0.67164159339544 |
| C | -4.23050680767507 | 0.56024757211978 | 1.56413786542236 |
| H | -2.56683779074863 | -0.26690956496639 | 2.52110846821909 |
| C | -3.39548131820141 | -1.83853249189086 | 1.44967747844390 |
| C | -3.84472052614898 | -2.11710352056402 | 0.01555613992262 |
| H | -2.74165750539722 | -0.44626984656476 | -2.78871586559359 |
| H | -4.27273504045344 | -1.33368261391038 | -2.61542253301608 |
| H | -5.12678601728549 | 0.29003585414749 | -0.97107022118270 |
| H | -4.53042241893328 | 1.18659608330627 | -2.37451364563600 |
| H | -3.20085217077896 | 2.43585595714557 | 1.15345832310629 |
| H | -4.83951833977623 | 2.33600104389730 | 0.48090856313748 |
| H | -5.09966277328671 | 0.00691504958457 | 1.19178597061041 |
| H | -4.47353048648845 | 0.91076995320534 | 2.57400471111247 |
| H | -4.18016066056827 | -2.14016644731908 | 2.15875597503320 |
| H | -2.48458062971692 | -2.40164454884270 | 1.69029504516941 |
| H | -3.88005705393942 | -3.19970606246369 | -0.15327784666505 |
| H | -4.84946604671025 | -1.72167011147195 | -0.17427946211793 |

**Optimized xyz Coordinates for 150° Mono-μ-oxo Model:**

| | | | |
|---|---|---|---|
| Fe | 1.60214995368452 | 0.92499995602940 | 0.00000000000000 |
| Fe | -1.85000006433787 | -0.00000001194443 | 0.00000000000000 |
| O | 0.00000011186642 | 0.00000005386333 | -0.00000000000000 |
| N | 2.91171317826354 | 1.01925096139329 | 1.60644917908247 |
| N | 2.09580427497598 | 2.89574193194068 | -0.37135930333668 |
| N | 3.25075694420037 | 0.40697532543340 | -1.14495208403127 |
| H | 2.59622190892498 | 0.44449579648285 | 2.39338968488952 |
| C | 2.82637587123065 | 2.46629206735756 | 1.98534720803810 |
| C | 2.97888817962876 | 3.36186677148263 | 0.75570386117207 |
| H | 1.27673952181175 | 3.50588544657671 | -0.44823465015773 |
| C | 2.75748752304113 | 2.79480649760386 | -1.71452822010182 |
| C | 3.80292963970639 | 1.67957251852535 | -1.72727332426210 |
| H | 3.00824122957982 | -0.24782068394266 | -1.89433477956629 |
| C | 4.12700655976721 | -0.28611563526021 | -0.14565780802354 |
| C | 4.25795271971760 | 0.54704445047132 | 1.12862519759745 |
| H | 1.84532851082167 | 2.61191884791591 | 2.45699873805308 |
| H | 3.59916090592065 | 2.71126102852337 | 2.72882204362323 |
| H | 4.01353668119437 | 3.36715243148454 | 0.39383524713231 |
| H | 2.71625533617128 | 4.39293566568433 | 1.01912208794385 |
| H | 1.96076817715819 | 2.59417948693452 | -2.44327444590413 |
| H | 3.22513922930106 | 3.75426442090311 | -1.97970918653736 |
| H | 4.69118777427828 | 1.96229567076427 | -1.15053663782913 |
| H | 4.12632954200119 | 1.49536173383566 | -2.75848596601685 |
| H | 5.12026181122065 | -0.47631166082539 | -0.57823183538389 |
| H | 3.65727709266018 | -1.25538253210978 | 0.06680445756719 |
| H | 4.73260377577636 | -0.05223693447671 | 1.91431129693082 |
| H | 4.88762358723784 | 1.42890125990494 | 0.96181565488991 |
| N | -3.04602046315678 | -0.82298656310725 | -1.47963782606514 |
| N | -3.24974406091821 | 1.51448850765011 | 0.13009463227712 |
| N | -3.01941689840935 | -1.04680075354486 | 1.35388659452258 |
| H | -2.49330302511263 | -1.29630346845586 | -2.20048866160298 |
| C | -3.68538737056258 | 0.39767110702707 | -2.06824411517703 |
| C | -4.25385580669643 | 1.29750246559176 | -0.97139705528400 |
| H | -2.83554695876632 | 2.44723085586398 | 0.04328333767196 |
| C | -3.76729270363388 | 1.33756753863216 | 1.52720876788279 |
| C | -4.12096614881374 | -0.12500812278342 | 1.80083921411145 |
| H | -2.47748576720584 | -1.36728919223521 | 2.16178662478119 |
| C | -3.45071227286300 | -2.23344493586261 | 0.54584025473441 |
| C | -3.98171649602115 | -1.79867014509395 | -0.81975554255816 |
| H | -2.90463541113646 | 0.91957433583266 | -2.63756198660550 |
| H | -4.48147792500301 | 0.10922822229815 | -2.77048041244500 |
| H | -5.15693349786847 | 0.86328049552948 | -0.52723623091966 |
| H | -4.53337892520046 | 2.26636141106839 | -1.40136105285379 |
| H | -2.97237324939247 | 1.68055314842587 | 2.20265507491018 |
| H | -4.64841196295057 | 1.97561308949878 | 1.68839757745762 |
| H | -5.04100260747142 | -0.41644471163345 | 1.28147279719667 |
| H | -4.29388077848257 | -0.26188260554090 | 2.87475076612547 |
| H | -4.22040819422760 | -2.80268310671485 | 1.08739643469510 |
| H | -2.56758299061563 | -2.87606517795385 | 0.43513065454276 |
| H | -4.09972551662503 | -2.67846481392486 | -1.46316367449955 |
| H | -4.96569198294477 | -1.32323834147254 | -0.73265202320772 |

**Optimized xyz Coordinates for 180° Mono-μ-oxo Model:**

| | | | |
|---|---|---|---|
| Fe | -0.000000 | -0.000000 | 1.850000 |
| Fe | -0.000000 | -0.000000 | -1.850000 |
| O | 0.000000 | 0.000000 | 0.000000 |
| N | -0.790352 | -1.421909 | 3.131232 |
| N | -0.872123 | 1.420160 | 3.082425 |
| N | 1.632104 | 0.071391 | 3.123000 |
| N | -0.171877 | 1.682630 | -3.050888 |
| N | 1.498163 | -0.615765 | -3.139289 |
| N | -1.333249 | -0.911897 | -3.144570 |
| H | -1.063374 | -2.276150 | 2.636111 |
| C | -2.019388 | -0.732796 | 3.642640 |
| C | -1.694053 | 0.687264 | 4.107445 |
| H | -1.462504 | 2.073016 | 2.558658 |
| C | 0.325817 | 2.150790 | 3.610408 |
| C | 1.380888 | 1.168944 | 4.121304 |
| H | 2.506737 | 0.245911 | 2.619176 |
| C | 1.650674 | -1.320802 | 3.679059 |
| C | 0.259815 | -1.733975 | 4.162488 |
| H | -0.101536 | 2.549893 | -2.510479 |
| C | 0.926111 | 1.621965 | -4.077574 |
| C | 2.051314 | 0.689515 | -3.627327 |
| H | 2.235355 | -1.134562 | -2.652626 |
| C | 0.859321 | -1.484768 | -4.188882 |
| C | -0.496762 | -2.014857 | -3.720693 |
| H | -2.134465 | -1.318190 | -2.652275 |
| C | -1.803271 | 0.131248 | -4.122270 |
| C | -1.566571 | 1.541581 | -3.581268 |
| H | -2.740624 | -0.717956 | 2.814821 |
| H | -2.461675 | -1.308342 | 4.468926 |
| H | -1.133999 | 0.677612 | 5.049742 |
| H | -2.625686 | 1.236896 | 4.285377 |
| H | 0.720328 | 2.751640 | 2.780347 |
| H | 0.027771 | 2.837816 | 4.415885 |
| H | 1.068683 | 0.706400 | 5.064783 |
| H | 2.317319 | 1.705342 | 4.313607 |
| H | 2.373221 | -1.390384 | 4.505344 |
| H | 1.995184 | -1.979011 | 2.870489 |
| H | 0.250912 | -2.809443 | 4.374508 |
| H | -0.008413 | -1.215009 | 5.090162 |
| H | 0.488213 | 1.286485 | -5.024940 |
| H | 1.327436 | 2.629129 | -4.240127 |
| H | 2.612056 | 1.127724 | -2.791230 |
| H | 2.754017 | 0.518024 | -4.455844 |
| H | 1.522798 | -2.327652 | -4.414754 |
| H | 0.757976 | -0.892287 | -5.105612 |
| H | -0.371372 | -2.763233 | -2.926996 |
| H | -1.024015 | -2.493588 | -4.558835 |
| H | -2.872516 | -0.010542 | -4.317855 |
| H | -1.273533 | -0.025242 | -5.069185 |
| H | -1.750168 | 2.284869 | -4.370970 |
| H | -2.245660 | 1.759205 | -2.746283 |

**Optimized xyz Coordinates for 90° Bis-μ-oxo Model:**

| | | | |
|---|---|---|---|
| Fe | -0.000000 | 0.000000 | 1.308100 |
| Fe | -0.000000 | 0.000000 | -1.308100 |
| O | 0.000000 | 1.308100 | 0.000000 |
| O | 0.000000 | -1.308100 | 0.000000 |
| N | -0.172546 | -1.587285 | 2.932755 |
| N | -1.338393 | 0.952704 | 2.730728 |
| N | 1.534260 | 0.617752 | 2.688744 |
| N | 1.270999 | 1.027199 | -2.751186 |
| N | 0.269004 | -1.576980 | -2.925713 |
| N | -1.575978 | 0.520514 | -2.674916 |
| H | -0.106502 | -2.479902 | 2.441261 |
| C | -1.539278 | -1.416957 | 3.472471 |
| C | -1.789436 | 0.049578 | 3.830911 |
| H | -2.151799 | 1.337806 | 2.246035 |
| C | -0.466644 | 2.086222 | 3.159070 |
| C | 0.908171 | 1.601260 | 3.633897 |
| H | 2.291570 | 1.076224 | 2.177243 |
| C | 2.071935 | -0.608002 | 3.342089 |
| C | 0.932554 | -1.457115 | 3.914513 |
| H | 2.060950 | 1.463674 | -2.271415 |
| C | 1.770445 | 0.151793 | -3.851430 |
| C | 1.615388 | -1.326563 | -3.484994 |
| H | 0.263663 | -2.469630 | -2.429566 |
| C | -0.854392 | -1.520737 | -3.894801 |
| C | -2.038951 | -0.744623 | -3.311982 |
| H | -2.358018 | 0.935173 | -2.163120 |
| C | -1.020042 | 1.532919 | -3.633653 |
| C | 0.327243 | 2.103086 | -3.174777 |
| H | -2.236644 | -1.734036 | 2.683950 |
| H | -1.722929 | -2.049821 | 4.357212 |
| H | -1.247872 | 0.319649 | 4.747230 |
| H | -2.856934 | 0.204682 | 4.034883 |
| H | -0.357339 | 2.744199 | 2.286789 |
| H | -0.939800 | 2.665644 | 3.968441 |
| H | 0.827565 | 1.125180 | 4.619195 |
| H | 1.566585 | 2.471366 | 3.755232 |
| H | 2.787018 | -0.352499 | 4.140549 |
| H | 2.615976 | -1.166732 | 2.567763 |
| H | 1.325888 | -2.442629 | 4.201967 |
| H | 0.536689 | -0.999065 | 4.830679 |
| H | 1.207513 | 0.383691 | -4.765446 |
| H | 2.825098 | 0.372034 | -4.062737 |
| H | 2.341625 | -1.597246 | -2.705086 |
| H | 1.824281 | -1.951654 | -4.369548 |
| H | -1.186718 | -2.530256 | -4.175212 |
| H | -0.499044 | -1.040718 | -4.816146 |
| H | -2.533200 | -1.332639 | -2.526284 |
| H | -2.780672 | -0.543333 | -4.101636 |
| H | -1.731213 | 2.360569 | -3.754102 |
| H | -0.920291 | 1.055633 | -4.616602 |
| H | 0.755366 | 2.707891 | -3.990651 |
| H | 0.186278 | 2.756259 | -2.303412 |