

Supporting information for

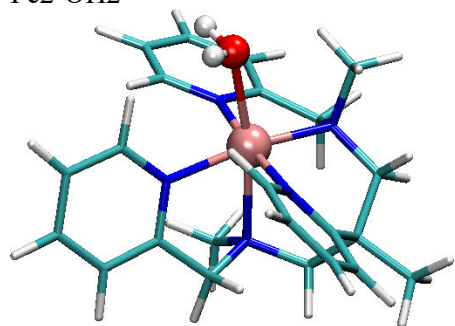
**Non-Heme Oxoiron complexes as active intermediates in water oxidation process with hydrogen/oxygen atom transfer reactions**

**Koteswara Rao Gorantla and Bhabani S. Mallik\***

Department of Chemistry, Indian Institute of Technology Hyderabad, Sangareddy 502285, Telangana, India

**Cartesian coordinates**

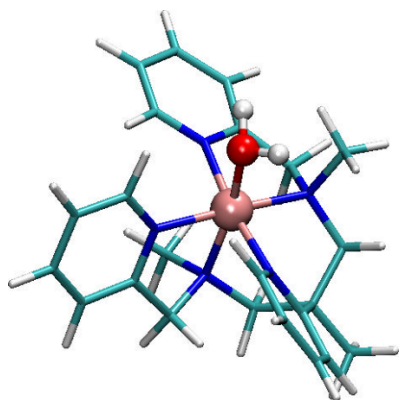
Fe2-OH2



|    |           |           |           |
|----|-----------|-----------|-----------|
| Fe | -0.259000 | -0.042000 | -0.523000 |
| O  | -0.825000 | 0.504000  | -2.855000 |
| N  | -0.395000 | -2.108000 | -0.609000 |
| C  | -0.651000 | -2.524000 | -2.006000 |
| H  | -0.713000 | -3.617000 | -2.071000 |
| H  | 0.157000  | -2.170000 | -2.647000 |
| H  | -1.594000 | -2.094000 | -2.350000 |
| C  | -0.847000 | -0.017000 | 2.660000  |
| H  | -0.524000 | 0.040000  | 3.710000  |
| H  | -1.514000 | -0.874000 | 2.550000  |
| H  | -1.415000 | 0.889000  | 2.425000  |
| N  | 0.298000  | -0.126000 | 1.748000  |
| C  | 1.096000  | -1.337000 | 2.021000  |
| H  | 0.437000  | -2.093000 | 2.461000  |
| H  | 1.862000  | -1.119000 | 2.779000  |
| C  | 1.788000  | -1.979000 | 0.792000  |
| C  | 0.830000  | -2.792000 | -0.107000 |
| H  | 1.403000  | -3.126000 | -0.977000 |
| H  | 0.523000  | -3.694000 | 0.436000  |
| C  | 2.767000  | -3.007000 | 1.359000  |
| H  | 3.516000  | -2.536000 | 2.000000  |
| H  | 3.283000  | -3.553000 | 0.564000  |
| H  | 2.222000  | -3.733000 | 1.969000  |

|   |           |           |           |
|---|-----------|-----------|-----------|
| N | 1.730000  | -0.094000 | -0.782000 |
| C | 2.311000  | 0.828000  | -1.574000 |
| H | 1.634000  | 1.489000  | -2.107000 |
| C | 3.683000  | 0.947000  | -1.705000 |
| H | 4.099000  | 1.703000  | -2.360000 |
| C | 4.490000  | 0.080000  | -0.977000 |
| H | 5.571000  | 0.142000  | -1.043000 |
| C | 3.895000  | -0.873000 | -0.159000 |
| H | 4.514000  | -1.553000 | 0.413000  |
| C | 2.506000  | -0.951000 | -0.069000 |
| N | -2.235000 | -0.220000 | -0.234000 |
| C | -3.151000 | 0.764000  | -0.316000 |
| H | -2.775000 | 1.752000  | -0.567000 |
| C | -4.501000 | 0.548000  | -0.092000 |
| H | -5.195000 | 1.377000  | -0.169000 |
| C | -4.932000 | -0.737000 | 0.224000  |
| H | -5.983000 | -0.940000 | 0.402000  |
| C | -3.994000 | -1.759000 | 0.303000  |
| H | -4.284000 | -2.777000 | 0.541000  |
| C | -2.655000 | -1.470000 | 0.075000  |
| C | -1.571000 | -2.483000 | 0.216000  |
| H | -1.260000 | -2.536000 | 1.265000  |
| H | -1.921000 | -3.489000 | -0.050000 |
| N | -0.089000 | 1.964000  | -0.037000 |
| C | -0.558000 | 2.987000  | -0.779000 |
| H | -1.046000 | 2.716000  | -1.710000 |
| C | -0.440000 | 4.312000  | -0.394000 |
| H | -0.837000 | 5.093000  | -1.033000 |
| C | 0.180000  | 4.603000  | 0.817000  |
| H | 0.278000  | 5.628000  | 1.159000  |
| C | 0.668000  | 3.554000  | 1.585000  |
| H | 1.156000  | 3.732000  | 2.539000  |
| C | 0.531000  | 2.247000  | 1.131000  |
| C | 1.113000  | 1.094000  | 1.890000  |
| H | 2.123000  | 0.903000  | 1.508000  |
| H | 1.236000  | 1.365000  | 2.949000  |
| H | -0.355000 | 1.255000  | -3.236000 |
| H | -1.752000 | 0.774000  | -2.885000 |

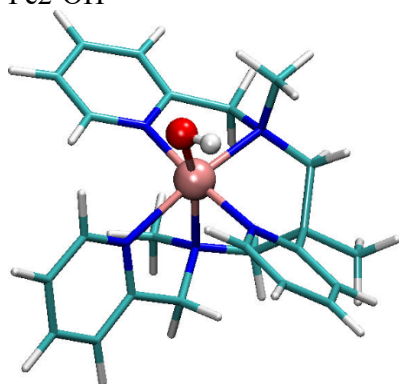
Fe3-OH2



|    |           |           |           |
|----|-----------|-----------|-----------|
| Fe | -0.245000 | -0.014000 | -0.396000 |
| O  | -0.624000 | 0.503000  | -2.345000 |
| N  | -0.381000 | -2.075000 | -0.591000 |
| C  | -0.556000 | -2.437000 | -2.024000 |
| H  | -0.621000 | -3.526000 | -2.107000 |
| H  | 0.304000  | -2.086000 | -2.597000 |
| H  | -1.476000 | -1.998000 | -2.412000 |
| C  | -0.975000 | 0.035000  | 2.481000  |
| H  | -0.652000 | 0.045000  | 3.526000  |
| H  | -1.653000 | -0.804000 | 2.332000  |
| H  | -1.498000 | 0.968000  | 2.259000  |
| N  | 0.224000  | -0.098000 | 1.608000  |
| C  | 0.985000  | -1.326000 | 1.982000  |
| H  | 0.283000  | -2.055000 | 2.398000  |
| H  | 1.677000  | -1.055000 | 2.786000  |
| C  | 1.754000  | -1.992000 | 0.830000  |
| C  | 0.814000  | -2.809000 | -0.067000 |
| H  | 1.386000  | -3.176000 | -0.922000 |
| H  | 0.461000  | -3.681000 | 0.491000  |
| C  | 2.711000  | -2.993000 | 1.473000  |
| H  | 3.460000  | -2.486000 | 2.087000  |
| H  | 3.225000  | -3.594000 | 0.719000  |
| H  | 2.149000  | -3.670000 | 2.121000  |
| N  | 1.722000  | -0.077000 | -0.697000 |
| C  | 2.296000  | 0.837000  | -1.504000 |
| H  | 1.631000  | 1.546000  | -1.987000 |
| C  | 3.662000  | 0.882000  | -1.709000 |
| H  | 4.081000  | 1.630000  | -2.372000 |
| C  | 4.459000  | -0.042000 | -1.045000 |
| H  | 5.536000  | -0.038000 | -1.176000 |
| C  | 3.866000  | -0.978000 | -0.207000 |
| H  | 4.476000  | -1.703000 | 0.317000  |
| C  | 2.485000  | -0.985000 | -0.037000 |
| N  | -2.235000 | -0.201000 | -0.207000 |
| C  | -3.126000 | 0.806000  | -0.282000 |
| H  | -2.729000 | 1.802000  | -0.441000 |
| C  | -4.487000 | 0.590000  | -0.150000 |
| H  | -5.166000 | 1.432000  | -0.210000 |

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -4.946000 | -0.708000 | 0.054000  |
| H | -6.008000 | -0.907000 | 0.156000  |
| C | -4.028000 | -1.748000 | 0.121000  |
| H | -4.342000 | -2.775000 | 0.273000  |
| C | -2.676000 | -1.463000 | -0.007000 |
| C | -1.613000 | -2.494000 | 0.137000  |
| H | -1.379000 | -2.639000 | 1.198000  |
| H | -1.945000 | -3.470000 | -0.234000 |
| N | -0.115000 | 1.971000  | -0.037000 |
| C | -0.577000 | 2.965000  | -0.821000 |
| H | -1.095000 | 2.665000  | -1.725000 |
| C | -0.388000 | 4.296000  | -0.497000 |
| H | -0.775000 | 5.063000  | -1.158000 |
| C | 0.293000  | 4.615000  | 0.675000  |
| H | 0.450000  | 5.652000  | 0.955000  |
| C | 0.767000  | 3.592000  | 1.483000  |
| H | 1.299000  | 3.795000  | 2.406000  |
| C | 0.554000  | 2.275000  | 1.097000  |
| C | 1.079000  | 1.109000  | 1.854000  |
| H | 2.107000  | 0.901000  | 1.541000  |
| H | 1.115000  | 1.308000  | 2.930000  |
| H | -0.026000 | 0.104000  | -2.996000 |
| H | -1.515000 | 0.279000  | -2.652000 |

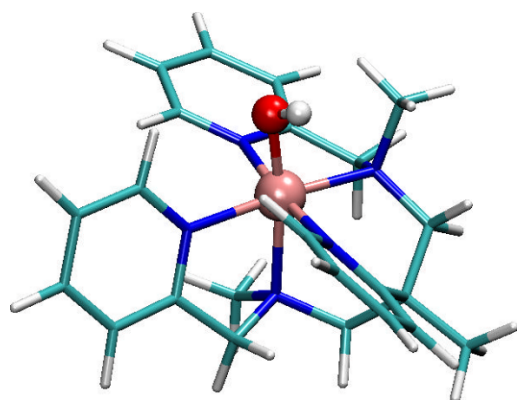
Fe2-OH



|    |           |           |           |
|----|-----------|-----------|-----------|
| Fe | -0.292000 | -0.036000 | -0.584000 |
| O  | -0.634000 | 0.369000  | -2.457000 |
| N  | -0.619000 | -2.226000 | -0.468000 |
| C  | -0.910000 | -2.721000 | -1.822000 |
| H  | -1.101000 | -3.803000 | -1.812000 |
| H  | -0.065000 | -2.511000 | -2.481000 |
| H  | -1.794000 | -2.213000 | -2.217000 |
| C  | -0.907000 | 0.263000  | 2.505000  |
| H  | -0.596000 | 0.326000  | 3.557000  |
| H  | -1.660000 | -0.521000 | 2.413000  |
| H  | -1.363000 | 1.215000  | 2.218000  |
| N  | 0.245000  | -0.011000 | 1.630000  |
| C  | 0.906000  | -1.278000 | 2.020000  |
| H  | 0.165000  | -1.922000 | 2.505000  |
| H  | 1.667000  | -1.066000 | 2.785000  |

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 1.561000  | -2.091000 | 0.878000  |
| C | 0.532000  | -2.947000 | 0.106000  |
| H | 1.063000  | -3.449000 | -0.710000 |
| H | 0.172000  | -3.740000 | 0.776000  |
| C | 2.474000  | -3.102000 | 1.574000  |
| H | 3.273000  | -2.607000 | 2.133000  |
| H | 2.928000  | -3.795000 | 0.860000  |
| H | 1.889000  | -3.691000 | 2.285000  |
| N | 1.645000  | -0.283000 | -0.814000 |
| C | 2.326000  | 0.542000  | -1.642000 |
| H | 1.723000  | 1.280000  | -2.165000 |
| C | 3.695000  | 0.481000  | -1.819000 |
| H | 4.180000  | 1.172000  | -2.498000 |
| C | 4.412000  | -0.473000 | -1.105000 |
| H | 5.488000  | -0.560000 | -1.212000 |
| C | 3.723000  | -1.313000 | -0.236000 |
| H | 4.270000  | -2.052000 | 0.336000  |
| C | 2.341000  | -1.207000 | -0.087000 |
| N | -2.243000 | -0.055000 | -0.284000 |
| C | -3.064000 | 0.995000  | -0.492000 |
| H | -2.583000 | 1.916000  | -0.805000 |
| C | -4.435000 | 0.922000  | -0.315000 |
| H | -5.044000 | 1.801000  | -0.492000 |
| C | -5.000000 | -0.289000 | 0.077000  |
| H | -6.072000 | -0.384000 | 0.218000  |
| C | -4.162000 | -1.381000 | 0.276000  |
| H | -4.556000 | -2.349000 | 0.570000  |
| C | -2.792000 | -1.237000 | 0.095000  |
| C | -1.833000 | -2.356000 | 0.360000  |
| H | -1.540000 | -2.337000 | 1.415000  |
| H | -2.322000 | -3.328000 | 0.200000  |
| N | 0.032000  | 2.138000  | -0.040000 |
| C | -0.304000 | 3.205000  | -0.783000 |
| H | -0.888000 | 2.997000  | -1.677000 |
| C | 0.067000  | 4.502000  | -0.458000 |
| H | -0.234000 | 5.328000  | -1.092000 |
| C | 0.821000  | 4.706000  | 0.694000  |
| H | 1.125000  | 5.707000  | 0.987000  |
| C | 1.179000  | 3.607000  | 1.465000  |
| H | 1.768000  | 3.720000  | 2.371000  |
| C | 0.775000  | 2.338000  | 1.061000  |
| C | 1.202000  | 1.105000  | 1.797000  |
| H | 2.182000  | 0.792000  | 1.421000  |
| H | 1.343000  | 1.322000  | 2.866000  |
| H | 0.172000  | 0.195000  | -2.958000 |

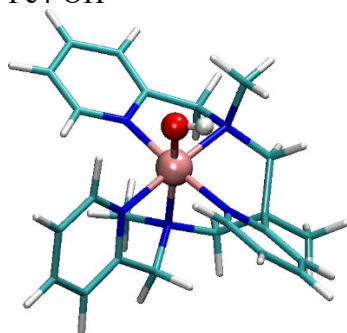
Fe3-OH



|    |           |           |           |
|----|-----------|-----------|-----------|
| Fe | -0.253000 | -0.017000 | -0.424000 |
| O  | -0.675000 | 0.300000  | -2.146000 |
| N  | -0.364000 | -2.073000 | -0.557000 |
| C  | -0.617000 | -2.498000 | -1.962000 |
| H  | -0.716000 | -3.588000 | -2.001000 |
| H  | 0.222000  | -2.192000 | -2.588000 |
| H  | -1.524000 | -2.022000 | -2.333000 |
| C  | -0.902000 | 0.053000  | 2.564000  |
| H  | -0.564000 | 0.088000  | 3.606000  |
| H  | -1.577000 | -0.793000 | 2.444000  |
| H  | -1.452000 | 0.968000  | 2.336000  |
| N  | 0.260000  | -0.063000 | 1.646000  |
| C  | 1.076000  | -1.262000 | 1.994000  |
| H  | 0.417000  | -2.003000 | 2.458000  |
| H  | 1.804000  | -0.982000 | 2.767000  |
| C  | 1.812000  | -1.940000 | 0.817000  |
| C  | 0.851000  | -2.778000 | -0.048000 |
| H  | 1.410000  | -3.153000 | -0.910000 |
| H  | 0.531000  | -3.658000 | 0.524000  |
| C  | 2.796000  | -2.931000 | 1.443000  |
| H  | 3.555000  | -2.422000 | 2.042000  |
| H  | 3.306000  | -3.532000 | 0.685000  |
| H  | 2.269000  | -3.621000 | 2.106000  |
| N  | 1.717000  | -0.065000 | -0.759000 |
| C  | 2.277000  | 0.843000  | -1.584000 |
| H  | 1.588000  | 1.530000  | -2.067000 |
| C  | 3.643000  | 0.920000  | -1.800000 |
| H  | 4.043000  | 1.664000  | -2.479000 |
| C  | 4.468000  | 0.028000  | -1.125000 |
| H  | 5.544000  | 0.054000  | -1.263000 |
| C  | 3.895000  | -0.902000 | -0.262000 |
| H  | 4.526000  | -1.602000 | 0.272000  |
| C  | 2.514000  | -0.935000 | -0.086000 |
| N  | -2.248000 | -0.195000 | -0.143000 |
| C  | -3.173000 | 0.761000  | -0.325000 |
| H  | -2.799000 | 1.764000  | -0.500000 |
| C  | -4.534000 | 0.495000  | -0.297000 |
| H  | -5.242000 | 1.302000  | -0.446000 |
| C  | -4.960000 | -0.813000 | -0.093000 |

|   |           |           |           |
|---|-----------|-----------|-----------|
| H | -6.017000 | -1.056000 | -0.079000 |
| C | -4.005000 | -1.812000 | 0.077000  |
| H | -4.296000 | -2.847000 | 0.223000  |
| C | -2.661000 | -1.468000 | 0.049000  |
| C | -1.558000 | -2.454000 | 0.255000  |
| H | -1.259000 | -2.476000 | 1.309000  |
| H | -1.872000 | -3.475000 | 0.002000  |
| N | -0.147000 | 1.957000  | -0.049000 |
| C | -0.626000 | 2.918000  | -0.864000 |
| H | -1.095000 | 2.558000  | -1.776000 |
| C | -0.504000 | 4.265000  | -0.559000 |
| H | -0.902000 | 5.006000  | -1.242000 |
| C | 0.129000  | 4.634000  | 0.625000  |
| H | 0.230000  | 5.681000  | 0.895000  |
| C | 0.636000  | 3.642000  | 1.458000  |
| H | 1.144000  | 3.892000  | 2.384000  |
| C | 0.493000  | 2.311000  | 1.086000  |
| C | 1.084000  | 1.169000  | 1.843000  |
| H | 2.099000  | 0.978000  | 1.476000  |
| H | 1.172000  | 1.390000  | 2.915000  |
| H | 0.077000  | 0.188000  | -2.746000 |

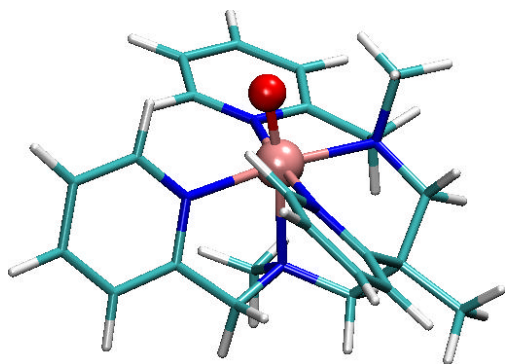
Fe4-OH



|    |           |           |           |
|----|-----------|-----------|-----------|
| Fe | -0.257000 | -0.021000 | -0.433000 |
| O  | -0.581000 | 0.267000  | -2.138000 |
| N  | -0.342000 | -2.100000 | -0.570000 |
| C  | -0.572000 | -2.523000 | -1.986000 |
| H  | -0.657000 | -3.614000 | -2.020000 |
| H  | 0.277000  | -2.224000 | -2.601000 |
| H  | -1.487000 | -2.072000 | -2.371000 |
| C  | -0.948000 | 0.043000  | 2.523000  |
| H  | -0.614000 | 0.058000  | 3.565000  |
| H  | -1.613000 | -0.807000 | 2.384000  |
| H  | -1.493000 | 0.964000  | 2.309000  |
| N  | 0.245000  | -0.058000 | 1.626000  |
| C  | 1.063000  | -1.260000 | 1.989000  |
| H  | 0.402000  | -1.996000 | 2.456000  |
| H  | 1.777000  | -0.957000 | 2.764000  |
| C  | 1.822000  | -1.937000 | 0.829000  |
| C  | 0.883000  | -2.787000 | -0.046000 |

|   |           |           |           |
|---|-----------|-----------|-----------|
| H | 1.451000  | -3.160000 | -0.903000 |
| H | 0.559000  | -3.665000 | 0.526000  |
| C | 2.813000  | -2.914000 | 1.471000  |
| H | 3.563000  | -2.393000 | 2.070000  |
| H | 3.330000  | -3.520000 | 0.723000  |
| H | 2.289000  | -3.601000 | 2.139000  |
| N | 1.728000  | -0.030000 | -0.724000 |
| C | 2.279000  | 0.902000  | -1.537000 |
| H | 1.591000  | 1.597000  | -2.009000 |
| C | 3.643000  | 0.974000  | -1.755000 |
| H | 4.041000  | 1.727000  | -2.426000 |
| C | 4.468000  | 0.062000  | -1.101000 |
| H | 5.543000  | 0.084000  | -1.248000 |
| C | 3.898000  | -0.882000 | -0.250000 |
| H | 4.529000  | -1.594000 | 0.268000  |
| C | 2.517000  | -0.921000 | -0.064000 |
| N | -2.237000 | -0.220000 | -0.145000 |
| C | -3.157000 | 0.752000  | -0.303000 |
| H | -2.786000 | 1.759000  | -0.454000 |
| C | -4.516000 | 0.484000  | -0.273000 |
| H | -5.224000 | 1.296000  | -0.400000 |
| C | -4.942000 | -0.830000 | -0.091000 |
| H | -6.001000 | -1.071000 | -0.076000 |
| C | -3.990000 | -1.837000 | 0.061000  |
| H | -4.287000 | -2.873000 | 0.193000  |
| C | -2.644000 | -1.504000 | 0.029000  |
| C | -1.546000 | -2.492000 | 0.230000  |
| H | -1.259000 | -2.540000 | 1.286000  |
| H | -1.853000 | -3.506000 | -0.050000 |
| N | -0.180000 | 1.966000  | -0.051000 |
| C | -0.667000 | 2.914000  | -0.880000 |
| H | -1.135000 | 2.561000  | -1.794000 |
| C | -0.552000 | 4.263000  | -0.580000 |
| H | -0.952000 | 4.997000  | -1.271000 |
| C | 0.080000  | 4.642000  | 0.604000  |
| H | 0.174000  | 5.692000  | 0.866000  |
| C | 0.595000  | 3.660000  | 1.445000  |
| H | 1.100000  | 3.921000  | 2.370000  |
| C | 0.462000  | 2.325000  | 1.085000  |
| C | 1.055000  | 1.191000  | 1.847000  |
| H | 2.083000  | 1.012000  | 1.513000  |
| H | 1.104000  | 1.396000  | 2.923000  |
| H | 0.113000  | 0.071000  | -2.788000 |

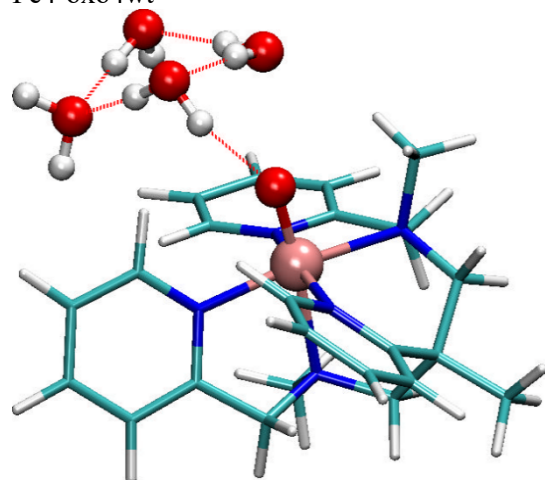
Fe4-oxo



|    |           |           |           |
|----|-----------|-----------|-----------|
| Fe | -0.261000 | -0.007000 | -0.495000 |
| O  | -0.519000 | 0.277000  | -2.081000 |
| N  | -0.354000 | -2.063000 | -0.617000 |
| C  | -0.566000 | -2.469000 | -2.036000 |
| H  | -0.611000 | -3.562000 | -2.100000 |
| H  | 0.254000  | -2.090000 | -2.645000 |
| H  | -1.495000 | -2.035000 | -2.405000 |
| C  | -0.961000 | 0.040000  | 2.543000  |
| H  | -0.647000 | 0.081000  | 3.593000  |
| H  | -1.628000 | -0.812000 | 2.413000  |
| H  | -1.516000 | 0.951000  | 2.305000  |
| N  | 0.218000  | -0.070000 | 1.650000  |
| C  | 1.024000  | -1.269000 | 2.010000  |
| H  | 0.354000  | -2.014000 | 2.453000  |
| H  | 1.736000  | -0.999000 | 2.802000  |
| C  | 1.786000  | -1.931000 | 0.843000  |
| C  | 0.861000  | -2.753000 | -0.081000 |
| H  | 1.454000  | -3.090000 | -0.936000 |
| H  | 0.537000  | -3.656000 | 0.450000  |
| C  | 2.753000  | -2.936000 | 1.473000  |
| H  | 3.489000  | -2.441000 | 2.112000  |
| H  | 3.292000  | -3.511000 | 0.716000  |
| H  | 2.208000  | -3.646000 | 2.099000  |
| N  | 1.732000  | -0.071000 | -0.745000 |
| C  | 2.290000  | 0.792000  | -1.615000 |
| H  | 1.592000  | 1.402000  | -2.180000 |
| C  | 3.661000  | 0.878000  | -1.790000 |
| H  | 4.070000  | 1.582000  | -2.506000 |
| C  | 4.479000  | 0.044000  | -1.037000 |
| H  | 5.559000  | 0.084000  | -1.142000 |
| C  | 3.897000  | -0.862000 | -0.156000 |
| H  | 4.522000  | -1.535000 | 0.419000  |
| C  | 2.512000  | -0.914000 | -0.024000 |
| N  | -2.248000 | -0.198000 | -0.172000 |
| C  | -3.168000 | 0.771000  | -0.308000 |
| H  | -2.789000 | 1.776000  | -0.465000 |
| C  | -4.528000 | 0.510000  | -0.257000 |
| H  | -5.236000 | 1.323000  | -0.369000 |
| C  | -4.955000 | -0.803000 | -0.078000 |
| H  | -6.013000 | -1.041000 | -0.048000 |

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -4.003000 | -1.810000 | 0.049000  |
| H | -4.298000 | -2.847000 | 0.176000  |
| C | -2.657000 | -1.475000 | -0.002000 |
| C | -1.555000 | -2.466000 | 0.172000  |
| H | -1.267000 | -2.522000 | 1.228000  |
| H | -1.868000 | -3.478000 | -0.115000 |
| N | -0.140000 | 1.959000  | -0.086000 |
| C | -0.582000 | 2.921000  | -0.920000 |
| H | -1.016000 | 2.568000  | -1.851000 |
| C | -0.465000 | 4.267000  | -0.609000 |
| H | -0.832000 | 5.011000  | -1.307000 |
| C | 0.124000  | 4.631000  | 0.599000  |
| H | 0.220000  | 5.677000  | 0.873000  |
| C | 0.595000  | 3.636000  | 1.449000  |
| H | 1.070000  | 3.882000  | 2.393000  |
| C | 0.461000  | 2.305000  | 1.073000  |
| C | 1.029000  | 1.166000  | 1.855000  |
| H | 2.054000  | 0.977000  | 1.517000  |
| H | 1.091000  | 1.403000  | 2.925000  |

Fe4-oxo4wt

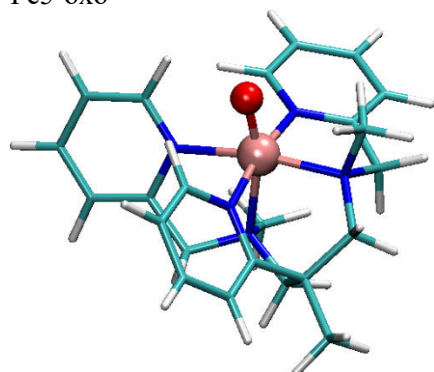


|    |           |           |           |
|----|-----------|-----------|-----------|
| Fe | 0.281000  | -0.112000 | -0.238000 |
| O  | -0.411000 | 0.188000  | -1.705000 |
| N  | 0.634000  | -2.118000 | -0.681000 |
| C  | 0.143000  | -2.487000 | -2.031000 |
| H  | 0.364000  | -3.545000 | -2.214000 |
| H  | 0.635000  | -1.872000 | -2.782000 |
| H  | -0.935000 | -2.328000 | -2.087000 |
| C  | 0.487000  | -0.548000 | 2.867000  |
| H  | 1.101000  | -0.506000 | 3.774000  |
| H  | 0.054000  | -1.545000 | 2.793000  |
| H  | -0.314000 | 0.189000  | 2.952000  |
| N  | 1.333000  | -0.245000 | 1.685000  |
| C  | 2.458000  | -1.220000 | 1.642000  |

|   |           |           |           |
|---|-----------|-----------|-----------|
| H | 2.123000  | -2.147000 | 2.116000  |
| H | 3.282000  | -0.835000 | 2.256000  |
| C | 2.994000  | -1.557000 | 0.239000  |
| C | 2.077000  | -2.488000 | -0.582000 |
| H | 2.478000  | -2.530000 | -1.597000 |
| H | 2.143000  | -3.502000 | -0.169000 |
| C | 4.294000  | -2.330000 | 0.447000  |
| H | 5.039000  | -1.724000 | 0.968000  |
| H | 4.718000  | -2.659000 | -0.505000 |
| H | 4.097000  | -3.217000 | 1.055000  |
| N | 2.103000  | 0.404000  | -0.888000 |
| C | 2.198000  | 1.530000  | -1.626000 |
| H | 1.266000  | 2.033000  | -1.857000 |
| C | 3.415000  | 2.010000  | -2.071000 |
| H | 3.444000  | 2.912000  | -2.670000 |
| C | 4.568000  | 1.309000  | -1.739000 |
| H | 5.542000  | 1.658000  | -2.067000 |
| C | 4.462000  | 0.147000  | -0.987000 |
| H | 5.347000  | -0.418000 | -0.723000 |
| C | 3.211000  | -0.298000 | -0.566000 |
| N | -1.320000 | -0.829000 | 0.654000  |
| C | -2.359000 | -0.084000 | 1.073000  |
| H | -2.254000 | 0.990000  | 0.992000  |
| C | -3.499000 | -0.662000 | 1.601000  |
| H | -4.313000 | -0.025000 | 1.929000  |
| C | -3.576000 | -2.050000 | 1.679000  |
| H | -4.462000 | -2.530000 | 2.081000  |
| C | -2.509000 | -2.814000 | 1.228000  |
| H | -2.528000 | -3.898000 | 1.265000  |
| C | -1.384000 | -2.175000 | 0.720000  |
| C | -0.149000 | -2.898000 | 0.318000  |
| H | 0.467000  | -3.063000 | 1.208000  |
| H | -0.378000 | -3.894000 | -0.077000 |
| N | 0.041000  | 1.779000  | 0.417000  |
| C | -0.833000 | 2.663000  | -0.096000 |
| H | -1.418000 | 2.315000  | -0.940000 |
| C | -0.971000 | 3.942000  | 0.416000  |
| H | -1.693000 | 4.619000  | -0.026000 |
| C | -0.175000 | 4.323000  | 1.493000  |
| H | -0.266000 | 5.315000  | 1.923000  |
| C | 0.738000  | 3.415000  | 2.011000  |
| H | 1.381000  | 3.671000  | 2.847000  |
| C | 0.832000  | 2.148000  | 1.447000  |
| C | 1.843000  | 1.143000  | 1.890000  |
| H | 2.766000  | 1.285000  | 1.321000  |
| H | 2.107000  | 1.290000  | 2.944000  |
| O | -3.387000 | -1.380000 | -1.969000 |
| H | -3.147000 | -0.530000 | -2.381000 |
| H | -4.224000 | -1.165000 | -1.511000 |
| O | -2.710000 | 1.269000  | -2.805000 |
| H | -1.831000 | 1.083000  | -2.428000 |

|   |           |           |           |
|---|-----------|-----------|-----------|
| H | -3.244000 | 1.545000  | -2.033000 |
| O | -4.399000 | 1.957000  | -0.675000 |
| H | -3.999000 | 2.296000  | 0.134000  |
| H | -4.959000 | 2.682000  | -0.979000 |
| O | -5.791000 | -0.483000 | -0.770000 |
| H | -5.378000 | 0.385000  | -0.600000 |
| H | -5.874000 | -0.875000 | 0.106000  |

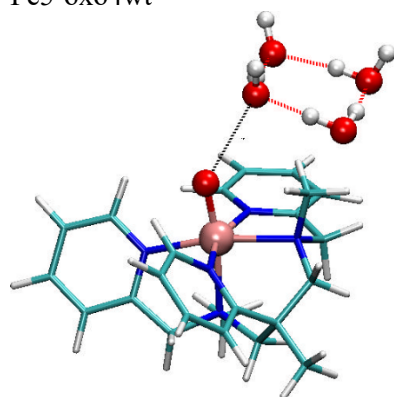
Fe5-oxo



|    |           |           |           |
|----|-----------|-----------|-----------|
| Fe | -0.257000 | -0.026000 | -0.587000 |
| O  | -0.368000 | 0.415000  | -2.104000 |
| N  | -0.351000 | -2.065000 | -0.672000 |
| C  | -0.508000 | -2.385000 | -2.135000 |
| H  | -0.566000 | -3.472000 | -2.231000 |
| H  | 0.356000  | -2.005000 | -2.678000 |
| H  | -1.425000 | -1.927000 | -2.507000 |
| C  | -1.091000 | -0.006000 | 2.407000  |
| H  | -0.798000 | 0.004000  | 3.461000  |
| H  | -1.746000 | -0.859000 | 2.241000  |
| H  | -1.624000 | 0.919000  | 2.180000  |
| N  | 0.139000  | -0.108000 | 1.574000  |
| C  | 0.902000  | -1.332000 | 1.950000  |
| H  | 0.201000  | -2.077000 | 2.335000  |
| H  | 1.568000  | -1.065000 | 2.778000  |
| C  | 1.735000  | -1.973000 | 0.826000  |
| C  | 0.847000  | -2.776000 | -0.143000 |
| H  | 1.454000  | -3.090000 | -0.994000 |
| H  | 0.491000  | -3.672000 | 0.375000  |
| C  | 2.666000  | -2.983000 | 1.491000  |
| H  | 3.370000  | -2.486000 | 2.162000  |
| H  | 3.229000  | -3.551000 | 0.747000  |
| H  | 2.076000  | -3.685000 | 2.084000  |
| N  | 1.754000  | -0.067000 | -0.703000 |
| C  | 2.350000  | 0.867000  | -1.467000 |
| H  | 1.701000  | 1.542000  | -2.015000 |
| C  | 3.728000  | 0.961000  | -1.559000 |
| H  | 4.166000  | 1.719000  | -2.197000 |
| C  | 4.506000  | 0.073000  | -0.828000 |
| H  | 5.589000  | 0.119000  | -0.872000 |
| C  | 3.882000  | -0.886000 | -0.042000 |

|   |           |           |           |
|---|-----------|-----------|-----------|
| H | 4.470000  | -1.591000 | 0.533000  |
| C | 2.490000  | -0.945000 | 0.016000  |
| N | -2.220000 | -0.207000 | -0.287000 |
| C | -3.101000 | 0.807000  | -0.320000 |
| H | -2.712000 | 1.801000  | -0.501000 |
| C | -4.454000 | 0.592000  | -0.126000 |
| H | -5.132000 | 1.436000  | -0.156000 |
| C | -4.910000 | -0.706000 | 0.091000  |
| H | -5.966000 | -0.901000 | 0.244000  |
| C | -3.998000 | -1.751000 | 0.108000  |
| H | -4.305000 | -2.777000 | 0.273000  |
| C | -2.650000 | -1.472000 | -0.079000 |
| C | -1.591000 | -2.503000 | 0.032000  |
| H | -1.370000 | -2.703000 | 1.086000  |
| H | -1.912000 | -3.460000 | -0.392000 |
| N | -0.157000 | 1.937000  | -0.082000 |
| C | -0.591000 | 2.913000  | -0.908000 |
| H | -1.060000 | 2.598000  | -1.834000 |
| C | -0.443000 | 4.247000  | -0.578000 |
| H | -0.808000 | 4.999000  | -1.268000 |
| C | 0.171000  | 4.584000  | 0.624000  |
| H | 0.295000  | 5.624000  | 0.907000  |
| C | 0.624000  | 3.574000  | 1.459000  |
| H | 1.104000  | 3.785000  | 2.408000  |
| C | 0.457000  | 2.248000  | 1.076000  |
| C | 0.961000  | 1.100000  | 1.865000  |
| H | 2.011000  | 0.912000  | 1.620000  |
| H | 0.931000  | 1.308000  | 2.940000  |

Fe5-oxo4wt

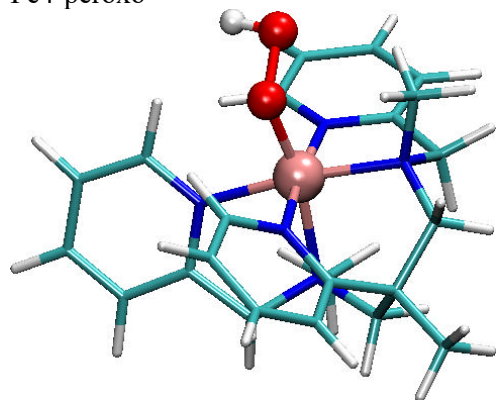


|    |           |           |           |
|----|-----------|-----------|-----------|
| Fe | -0.503000 | 0.196000  | 0.316000  |
| O  | 0.067000  | 0.524000  | 1.819000  |
| N  | 0.147000  | -1.959000 | 0.212000  |
| C  | 0.711000  | -2.293000 | 1.541000  |
| H  | 1.050000  | -3.335000 | 1.552000  |
| H  | -0.053000 | -2.149000 | 2.306000  |
| H  | 1.558000  | -1.639000 | 1.756000  |
| C  | -0.565000 | 0.492000  | -2.717000 |
| H  | -1.125000 | 0.496000  | -3.658000 |

|   |           |           |           |
|---|-----------|-----------|-----------|
| H | 0.292000  | -0.171000 | -2.826000 |
| H | -0.216000 | 1.506000  | -2.507000 |
| N | -1.450000 | 0.024000  | -1.618000 |
| C | -1.927000 | -1.355000 | -1.929000 |
| H | -1.167000 | -1.842000 | -2.547000 |
| H | -2.825000 | -1.265000 | -2.552000 |
| C | -2.240000 | -2.276000 | -0.733000 |
| C | -0.968000 | -2.896000 | -0.112000 |
| H | -1.255000 | -3.407000 | 0.811000  |
| H | -0.588000 | -3.663000 | -0.796000 |
| C | -3.034000 | -3.450000 | -1.305000 |
| H | -3.990000 | -3.122000 | -1.719000 |
| H | -3.228000 | -4.207000 | -0.540000 |
| H | -2.463000 | -3.921000 | -2.109000 |
| N | -2.350000 | -0.573000 | 1.009000  |
| C | -2.938000 | 0.088000  | 2.022000  |
| H | -2.345000 | 0.869000  | 2.490000  |
| C | -4.226000 | -0.202000 | 2.438000  |
| H | -4.667000 | 0.356000  | 3.255000  |
| C | -4.918000 | -1.214000 | 1.783000  |
| H | -5.929000 | -1.472000 | 2.081000  |
| C | -4.304000 | -1.901000 | 0.743000  |
| H | -4.828000 | -2.698000 | 0.231000  |
| C | -3.008000 | -1.562000 | 0.361000  |
| N | 1.493000  | 0.292000  | -0.516000 |
| C | 2.186000  | 1.440000  | -0.629000 |
| H | 1.671000  | 2.347000  | -0.321000 |
| C | 3.492000  | 1.487000  | -1.130000 |
| H | 3.988000  | 2.446000  | -1.227000 |
| C | 4.116000  | 0.309000  | -1.479000 |
| H | 5.130000  | 0.298000  | -1.862000 |
| C | 3.415000  | -0.904000 | -1.319000 |
| H | 3.802000  | -1.836000 | -1.714000 |
| C | 2.067000  | -0.860000 | -0.858000 |
| C | 1.228000  | -2.083000 | -0.789000 |
| H | 0.798000  | -2.235000 | -1.789000 |
| H | 1.846000  | -2.968000 | -0.590000 |
| N | -1.266000 | 2.116000  | 0.038000  |
| C | -0.893000 | 3.186000  | 0.764000  |
| H | -0.113000 | 3.013000  | 1.500000  |
| C | -1.475000 | 4.426000  | 0.575000  |
| H | -1.151000 | 5.270000  | 1.172000  |
| C | -2.474000 | 4.557000  | -0.388000 |
| H | -2.946000 | 5.519000  | -0.560000 |
| C | -2.861000 | 3.448000  | -1.130000 |
| H | -3.635000 | 3.513000  | -1.887000 |
| C | -2.238000 | 2.230000  | -0.890000 |
| C | -2.615000 | 0.962000  | -1.573000 |
| H | -3.442000 | 0.490000  | -1.035000 |
| H | -2.971000 | 1.146000  | -2.593000 |
| O | 4.075000  | -1.665000 | 0.668000  |

|   |          |           |          |
|---|----------|-----------|----------|
| H | 3.856000 | -0.842000 | 1.213000 |
| H | 5.060000 | -1.552000 | 0.445000 |
| O | 3.592000 | 0.590000  | 1.956000 |
| H | 3.668000 | 0.456000  | 2.909000 |
| H | 4.438000 | 1.023000  | 1.705000 |
| O | 6.074000 | 1.402000  | 1.020000 |
| H | 6.699000 | 1.796000  | 1.641000 |
| H | 6.034000 | 2.033000  | 0.291000 |
| O | 6.595000 | -1.174000 | 0.123000 |
| H | 6.561000 | -0.238000 | 0.418000 |
| H | 7.129000 | -1.612000 | 0.796000 |

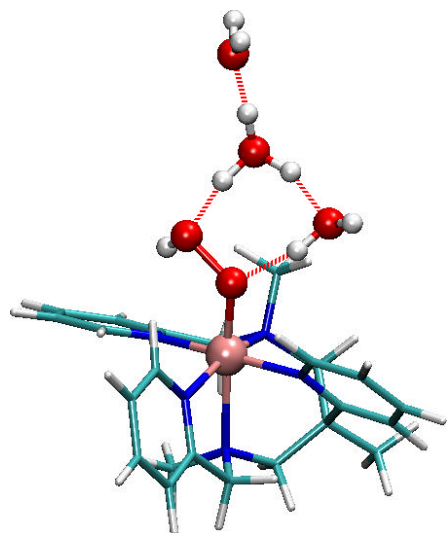
Fe4-peroxo



|    |           |           |           |
|----|-----------|-----------|-----------|
| Fe | -0.219000 | -0.033000 | -0.388000 |
| O  | -0.411000 | 0.340000  | -2.145000 |
| N  | -0.343000 | -2.074000 | -0.547000 |
| C  | -0.619000 | -2.471000 | -1.952000 |
| H  | -0.665000 | -3.564000 | -2.008000 |
| H  | 0.175000  | -2.101000 | -2.599000 |
| H  | -1.573000 | -2.054000 | -2.272000 |
| C  | -0.830000 | -0.024000 | 2.618000  |
| H  | -0.466000 | -0.010000 | 3.651000  |
| H  | -1.509000 | -0.868000 | 2.500000  |
| H  | -1.379000 | 0.900000  | 2.423000  |
| N  | 0.316000  | -0.131000 | 1.683000  |
| C  | 1.118000  | -1.346000 | 2.002000  |
| H  | 0.454000  | -2.097000 | 2.440000  |

|   |           |           |           |
|---|-----------|-----------|-----------|
| H | 1.848000  | -1.086000 | 2.778000  |
| C | 1.847000  | -1.983000 | 0.805000  |
| C | 0.889000  | -2.786000 | -0.092000 |
| H | 1.440000  | -3.100000 | -0.982000 |
| H | 0.581000  | -3.694000 | 0.438000  |
| C | 2.828000  | -2.996000 | 1.389000  |
| H | 3.582000  | -2.507000 | 2.010000  |
| H | 3.336000  | -3.559000 | 0.602000  |
| H | 2.288000  | -3.708000 | 2.019000  |
| N | 1.759000  | -0.066000 | -0.713000 |
| C | 2.312000  | 0.867000  | -1.509000 |
| H | 1.622000  | 1.548000  | -1.996000 |
| C | 3.679000  | 0.962000  | -1.704000 |
| H | 4.077000  | 1.729000  | -2.358000 |
| C | 4.504000  | 0.062000  | -1.042000 |
| H | 5.581000  | 0.105000  | -1.164000 |
| C | 3.934000  | -0.899000 | -0.216000 |
| H | 4.564000  | -1.608000 | 0.307000  |
| C | 2.551000  | -0.950000 | -0.057000 |
| N | -2.177000 | -0.200000 | -0.030000 |
| C | -3.081000 | 0.792000  | -0.058000 |
| H | -2.702000 | 1.790000  | -0.251000 |
| C | -4.432000 | 0.567000  | 0.151000  |
| H | -5.122000 | 1.402000  | 0.126000  |
| C | -4.869000 | -0.734000 | 0.380000  |
| H | -5.922000 | -0.944000 | 0.539000  |
| C | -3.938000 | -1.764000 | 0.397000  |
| H | -4.232000 | -2.794000 | 0.565000  |
| C | -2.596000 | -1.463000 | 0.195000  |
| C | -1.516000 | -2.485000 | 0.278000  |
| H | -1.197000 | -2.600000 | 1.319000  |
| H | -1.867000 | -3.473000 | -0.041000 |
| N | -0.078000 | 1.940000  | 0.048000  |
| C | -0.550000 | 2.938000  | -0.723000 |
| H | -1.070000 | 2.643000  | -1.627000 |
| C | -0.381000 | 4.270000  | -0.389000 |
| H | -0.780000 | 5.037000  | -1.043000 |
| C | 0.296000  | 4.589000  | 0.785000  |
| H | 0.437000  | 5.624000  | 1.077000  |
| C | 0.790000  | 3.561000  | 1.576000  |
| H | 1.327000  | 3.761000  | 2.498000  |
| C | 0.596000  | 2.245000  | 1.175000  |
| C | 1.161000  | 1.080000  | 1.906000  |
| H | 2.177000  | 0.889000  | 1.542000  |
| H | 1.248000  | 1.280000  | 2.980000  |
| O | -1.718000 | 0.201000  | -2.754000 |
| H | -2.032000 | 1.119000  | -2.771000 |

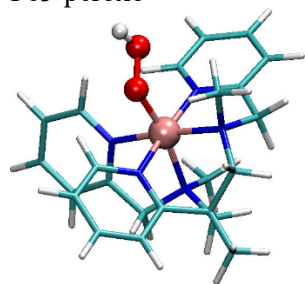
Fe4-peroxo4wt



|    |           |           |           |
|----|-----------|-----------|-----------|
| Fe | -0.024000 | 0.194000  | -0.032000 |
| O  | 1.489000  | -0.637000 | 0.850000  |
| N  | 0.364000  | -0.240000 | -2.119000 |
| C  | 1.683000  | -0.900000 | -2.204000 |
| H  | 1.957000  | -1.096000 | -3.249000 |
| H  | 1.663000  | -1.839000 | -1.649000 |
| H  | 2.443000  | -0.250000 | -1.761000 |
| C  | -2.169000 | 2.438000  | -0.863000 |
| H  | -3.192000 | 2.785000  | -1.065000 |
| H  | -1.541000 | 2.694000  | -1.717000 |
| H  | -1.787000 | 2.972000  | 0.011000  |
| N  | -2.131000 | 0.989000  | -0.599000 |
| C  | -2.671000 | 0.223000  | -1.744000 |
| H  | -2.539000 | 0.822000  | -2.653000 |
| H  | -3.759000 | 0.102000  | -1.630000 |
| C  | -2.043000 | -1.172000 | -2.002000 |
| C  | -0.682000 | -1.091000 | -2.736000 |
| H  | -0.287000 | -2.108000 | -2.814000 |
| H  | -0.862000 | -0.754000 | -3.766000 |
| C  | -2.985000 | -1.870000 | -2.989000 |
| H  | -3.982000 | -2.014000 | -2.566000 |
| H  | -2.601000 | -2.844000 | -3.302000 |
| H  | -3.103000 | -1.260000 | -3.889000 |
| N  | -1.002000 | -1.511000 | 0.211000  |
| C  | -0.861000 | -2.179000 | 1.377000  |
| H  | -0.154000 | -1.738000 | 2.075000  |
| C  | -1.560000 | -3.336000 | 1.674000  |
| H  | -1.413000 | -3.826000 | 2.630000  |
| C  | -2.450000 | -3.832000 | 0.729000  |
| H  | -3.020000 | -4.736000 | 0.918000  |
| C  | -2.608000 | -3.143000 | -0.469000 |
| H  | -3.302000 | -3.516000 | -1.211000 |
| C  | -1.885000 | -1.975000 | -0.716000 |
| N  | 0.890000  | 1.887000  | -0.533000 |

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 1.334000  | 2.831000  | 0.329000  |
| H | 1.174000  | 2.617000  | 1.382000  |
| C | 1.951000  | 3.999000  | -0.088000 |
| H | 2.284000  | 4.722000  | 0.648000  |
| C | 2.132000  | 4.215000  | -1.452000 |
| H | 2.615000  | 5.117000  | -1.813000 |
| C | 1.679000  | 3.251000  | -2.347000 |
| H | 1.801000  | 3.381000  | -3.417000 |
| C | 1.057000  | 2.106000  | -1.864000 |
| C | 0.447000  | 1.082000  | -2.773000 |
| H | -0.570000 | 1.400000  | -3.032000 |
| H | 0.997000  | 1.021000  | -3.724000 |
| N | -0.866000 | 0.908000  | 1.835000  |
| C | -0.155000 | 1.101000  | 2.960000  |
| H | 0.912000  | 0.901000  | 2.877000  |
| C | -0.737000 | 1.507000  | 4.152000  |
| H | -0.124000 | 1.650000  | 5.035000  |
| C | -2.112000 | 1.726000  | 4.182000  |
| H | -2.600000 | 2.055000  | 5.093000  |
| C | -2.852000 | 1.513000  | 3.024000  |
| H | -3.927000 | 1.667000  | 3.012000  |
| C | -2.198000 | 1.091000  | 1.871000  |
| C | -2.940000 | 0.739000  | 0.614000  |
| H | -3.205000 | -0.324000 | 0.647000  |
| H | -3.892000 | 1.289000  | 0.560000  |
| O | 2.228000  | -3.143000 | 0.289000  |
| H | 1.803000  | -2.320000 | 0.643000  |
| H | 2.032000  | -3.863000 | 0.896000  |
| O | 2.832000  | 0.068000  | 1.059000  |
| H | 2.762000  | 0.788000  | 0.413000  |
| H | 3.880000  | -0.984000 | 0.553000  |
| O | 4.357000  | -1.796000 | 0.159000  |
| H | 3.657000  | -2.539000 | 0.197000  |
| H | 5.219000  | -2.021000 | 0.641000  |
| O | 6.602000  | -2.253000 | 1.317000  |
| H | 7.402000  | -2.331000 | 0.789000  |
| H | 6.769000  | -2.736000 | 2.131000  |

Fe5-peroxo

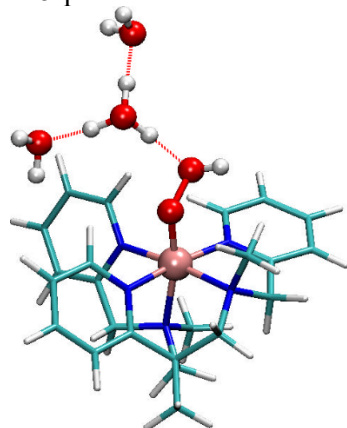


|    |          |           |          |
|----|----------|-----------|----------|
| Fe | 0.210000 | -0.030000 | 0.339000 |
| O  | 0.392000 | 0.327000  | 2.127000 |
| N  | 0.269000 | -2.088000 | 0.578000 |
| C  | 0.490000 | -2.421000 | 2.012000 |

|   |           |           |           |
|---|-----------|-----------|-----------|
| H | 0.518000  | -3.510000 | 2.112000  |
| H | -0.329000 | -2.018000 | 2.606000  |
| H | 1.437000  | -2.003000 | 2.353000  |
| C | 0.880000  | -0.098000 | -2.590000 |
| H | 0.524000  | -0.107000 | -3.624000 |
| H | 1.528000  | -0.958000 | -2.435000 |
| H | 1.441000  | 0.822000  | -2.412000 |
| N | -0.302000 | -0.156000 | -1.680000 |
| C | -1.125000 | -1.363000 | -1.991000 |
| H | -0.469000 | -2.133000 | -2.405000 |
| H | -1.831000 | -1.086000 | -2.781000 |
| C | -1.891000 | -1.960000 | -0.799000 |
| C | -0.970000 | -2.784000 | 0.112000  |
| H | -1.536000 | -3.088000 | 0.995000  |
| H | -0.665000 | -3.692000 | -0.418000 |
| C | -2.907000 | -2.938000 | -1.382000 |
| H | -3.639000 | -2.422000 | -2.006000 |
| H | -3.434000 | -3.478000 | -0.592000 |
| H | -2.389000 | -3.670000 | -2.007000 |
| N | -1.739000 | -0.028000 | 0.703000  |
| C | -2.249000 | 0.930000  | 1.503000  |
| H | -1.538000 | 1.597000  | 1.979000  |
| C | -3.608000 | 1.059000  | 1.709000  |
| H | -3.977000 | 1.841000  | 2.362000  |
| C | -4.463000 | 0.177000  | 1.059000  |
| H | -5.537000 | 0.250000  | 1.193000  |
| C | -3.932000 | -0.805000 | 0.230000  |
| H | -4.586000 | -1.499000 | -0.282000 |
| C | -2.556000 | -0.898000 | 0.055000  |
| N | 2.162000  | -0.276000 | 0.062000  |
| C | 3.082000  | 0.708000  | 0.067000  |
| H | 2.726000  | 1.718000  | 0.229000  |
| C | 4.423000  | 0.446000  | -0.137000 |
| H | 5.129000  | 1.268000  | -0.138000 |
| C | 4.833000  | -0.871000 | -0.327000 |
| H | 5.882000  | -1.105000 | -0.477000 |
| C | 3.885000  | -1.885000 | -0.315000 |
| H | 4.160000  | -2.925000 | -0.452000 |
| C | 2.551000  | -1.558000 | -0.128000 |
| C | 1.456000  | -2.559000 | -0.196000 |
| H | 1.172000  | -2.728000 | -1.240000 |
| H | 1.776000  | -3.533000 | 0.191000  |
| N | 0.134000  | 1.925000  | -0.088000 |
| C | 0.631000  | 2.905000  | 0.692000  |
| H | 1.144000  | 2.597000  | 1.597000  |
| C | 0.499000  | 4.236000  | 0.345000  |
| H | 0.916000  | 4.996000  | 0.995000  |
| C | -0.161000 | 4.565000  | -0.837000 |
| H | -0.267000 | 5.603000  | -1.136000 |
| C | -0.681000 | 3.553000  | -1.630000 |
| H | -1.204000 | 3.763000  | -2.556000 |

|   |           |          |           |
|---|-----------|----------|-----------|
| C | -0.528000 | 2.234000 | -1.225000 |
| C | -1.112000 | 1.078000 | -1.947000 |
| H | -2.143000 | 0.919000 | -1.615000 |
| H | -1.156000 | 1.251000 | -3.027000 |
| O | 1.665000  | 0.571000 | 2.613000  |
| H | 1.477000  | 0.768000 | 3.552000  |

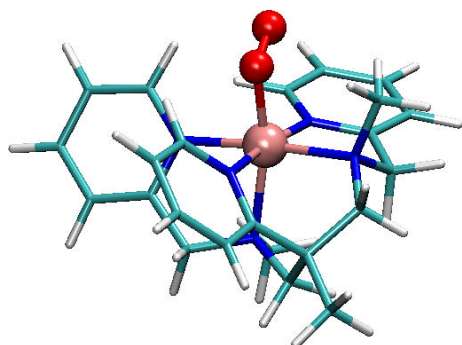
Fe5-peroxo4wt



|    |           |           |           |
|----|-----------|-----------|-----------|
| Fe | -0.324000 | 0.288000  | -0.141000 |
| O  | 1.015000  | 0.118000  | -1.336000 |
| N  | -1.687000 | 1.020000  | -1.499000 |
| C  | -1.054000 | 1.230000  | -2.827000 |
| H  | -1.811000 | 1.599000  | -3.526000 |
| H  | -0.641000 | 0.291000  | -3.191000 |
| H  | -0.262000 | 1.975000  | -2.744000 |
| C  | -1.901000 | 1.247000  | 2.297000  |
| H  | -2.628000 | 1.034000  | 3.088000  |
| H  | -2.224000 | 2.136000  | 1.756000  |
| H  | -0.928000 | 1.442000  | 2.753000  |
| N  | -1.800000 | 0.079000  | 1.386000  |
| C  | -3.144000 | -0.251000 | 0.833000  |
| H  | -3.737000 | 0.666000  | 0.791000  |
| H  | -3.653000 | -0.918000 | 1.538000  |
| C  | -3.135000 | -0.895000 | -0.565000 |
| C  | -2.878000 | 0.134000  | -1.679000 |
| H  | -2.752000 | -0.407000 | -2.620000 |
| H  | -3.761000 | 0.772000  | -1.787000 |
| C  | -4.547000 | -1.429000 | -0.800000 |
| H  | -4.808000 | -2.196000 | -0.067000 |
| H  | -4.652000 | -1.854000 | -1.802000 |
| H  | -5.268000 | -0.613000 | -0.702000 |
| N  | -0.797000 | -1.600000 | -0.622000 |
| C  | 0.185000  | -2.514000 | -0.748000 |
| H  | 1.199000  | -2.128000 | -0.706000 |
| C  | -0.073000 | -3.861000 | -0.930000 |
| H  | 0.752000  | -4.557000 | -1.025000 |
| C  | -1.397000 | -4.279000 | -0.981000 |

|   |           |           |           |
|---|-----------|-----------|-----------|
| H | -1.643000 | -5.327000 | -1.116000 |
| C | -2.410000 | -3.335000 | -0.863000 |
| H | -3.448000 | -3.642000 | -0.907000 |
| C | -2.092000 | -1.992000 | -0.680000 |
| N | -0.037000 | 2.233000  | 0.231000  |
| C | 0.970000  | 2.779000  | 0.935000  |
| H | 1.697000  | 2.094000  | 1.357000  |
| C | 1.085000  | 4.145000  | 1.123000  |
| H | 1.911000  | 4.536000  | 1.706000  |
| C | 0.137000  | 4.987000  | 0.547000  |
| H | 0.206000  | 6.063000  | 0.669000  |
| C | -0.900000 | 4.428000  | -0.187000 |
| H | -1.663000 | 5.041000  | -0.654000 |
| C | -0.966000 | 3.045000  | -0.317000 |
| C | -2.105000 | 2.356000  | -0.986000 |
| H | -2.922000 | 2.224000  | -0.270000 |
| H | -2.516000 | 2.956000  | -1.805000 |
| N | 0.818000  | -0.391000 | 1.379000  |
| C | 2.164000  | -0.352000 | 1.407000  |
| H | 2.653000  | 0.132000  | 0.570000  |
| C | 2.891000  | -0.901000 | 2.450000  |
| H | 3.974000  | -0.849000 | 2.427000  |
| C | 2.211000  | -1.509000 | 3.500000  |
| H | 2.754000  | -1.943000 | 4.333000  |
| C | 0.824000  | -1.555000 | 3.467000  |
| H | 0.251000  | -2.020000 | 4.262000  |
| C | 0.155000  | -0.996000 | 2.386000  |
| C | -1.321000 | -1.065000 | 2.217000  |
| H | -1.584000 | -2.009000 | 1.729000  |
| H | -1.840000 | -1.061000 | 3.182000  |
| O | 4.091000  | -2.560000 | -0.281000 |
| H | 3.250000  | -2.765000 | 0.146000  |
| H | 4.269000  | -3.338000 | -0.825000 |
| O | 2.053000  | 1.145000  | -1.335000 |
| H | 1.813000  | 1.681000  | -2.111000 |
| H | 3.292000  | 0.087000  | -1.726000 |
| O | 3.960000  | -0.611000 | -1.976000 |
| H | 3.954000  | -1.352000 | -1.277000 |
| H | 4.888000  | -0.174000 | -1.980000 |
| O | 6.272000  | 0.500000  | -2.017000 |
| H | 6.766000  | 0.083000  | -2.734000 |
| H | 6.747000  | 0.226000  | -1.223000 |

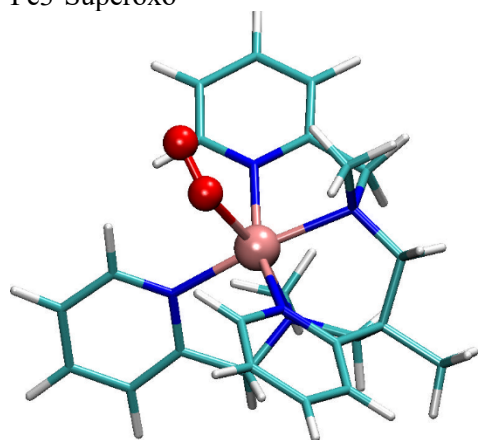
Fe2-superoxo



|    |           |           |           |
|----|-----------|-----------|-----------|
| Fe | -0.233000 | -0.015000 | -0.362000 |
| O  | -0.188000 | 0.288000  | -2.259000 |
| N  | -0.351000 | -2.069000 | -0.579000 |
| C  | -0.621000 | -2.457000 | -1.991000 |
| H  | -0.708000 | -3.546000 | -2.069000 |
| H  | 0.191000  | -2.107000 | -2.629000 |
| H  | -1.552000 | -1.997000 | -2.328000 |
| C  | -0.855000 | -0.012000 | 2.608000  |
| H  | -0.509000 | 0.002000  | 3.647000  |
| H  | -1.531000 | -0.856000 | 2.475000  |
| H  | -1.405000 | 0.909000  | 2.404000  |
| N  | 0.303000  | -0.113000 | 1.683000  |
| C  | 1.102000  | -1.331000 | 2.006000  |
| H  | 0.431000  | -2.068000 | 2.460000  |
| H  | 1.837000  | -1.077000 | 2.781000  |
| C  | 1.826000  | -1.993000 | 0.815000  |
| C  | 0.872000  | -2.785000 | -0.104000 |
| H  | 1.441000  | -3.098000 | -0.984000 |
| H  | 0.562000  | -3.705000 | 0.407000  |
| C  | 2.786000  | -3.023000 | 1.415000  |
| H  | 3.546000  | -2.551000 | 2.042000  |
| H  | 3.294000  | -3.603000 | 0.641000  |
| H  | 2.239000  | -3.729000 | 2.046000  |
| N  | 1.774000  | -0.049000 | -0.663000 |
| C  | 2.350000  | 0.886000  | -1.446000 |
| H  | 1.677000  | 1.591000  | -1.922000 |
| C  | 3.718000  | 0.950000  | -1.648000 |
| H  | 4.131000  | 1.717000  | -2.294000 |
| C  | 4.527000  | 0.018000  | -1.010000 |
| H  | 5.604000  | 0.034000  | -1.142000 |
| C  | 3.935000  | -0.943000 | -0.196000 |
| H  | 4.550000  | -1.679000 | 0.306000  |
| C  | 2.552000  | -0.963000 | -0.032000 |
| N  | -2.229000 | -0.218000 | -0.013000 |
| C  | -3.161000 | 0.752000  | -0.053000 |
| H  | -2.793000 | 1.765000  | -0.180000 |
| C  | -4.516000 | 0.486000  | 0.050000  |
| H  | -5.228000 | 1.302000  | 0.013000  |
| C  | -4.934000 | -0.836000 | 0.182000  |
| H  | -5.990000 | -1.079000 | 0.247000  |
| C  | -3.976000 | -1.843000 | 0.220000  |

|   |           |           |           |
|---|-----------|-----------|-----------|
| H | -4.262000 | -2.886000 | 0.316000  |
| C | -2.633000 | -1.500000 | 0.128000  |
| C | -1.525000 | -2.493000 | 0.237000  |
| H | -1.205000 | -2.574000 | 1.283000  |
| H | -1.850000 | -3.499000 | -0.061000 |
| N | -0.134000 | 1.956000  | 0.024000  |
| C | -0.622000 | 2.948000  | -0.748000 |
| H | -1.148000 | 2.641000  | -1.648000 |
| C | -0.462000 | 4.286000  | -0.421000 |
| H | -0.869000 | 5.049000  | -1.075000 |
| C | 0.217000  | 4.617000  | 0.748000  |
| H | 0.350000  | 5.655000  | 1.036000  |
| C | 0.722000  | 3.596000  | 1.545000  |
| H | 1.257000  | 3.815000  | 2.464000  |
| C | 0.542000  | 2.276000  | 1.151000  |
| C | 1.125000  | 1.118000  | 1.897000  |
| H | 2.144000  | 0.930000  | 1.544000  |
| H | 1.200000  | 1.332000  | 2.971000  |
| O | -1.399000 | 0.539000  | -2.568000 |

Fe3-Superoxo

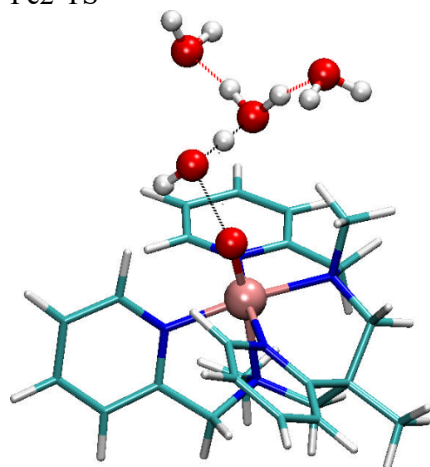


|    |           |           |          |
|----|-----------|-----------|----------|
| Fe | 0.261000  | 0.040000  | 0.232000 |
| O  | 0.693000  | 0.513000  | 2.436000 |
| N  | 0.346000  | -2.185000 | 0.320000 |
| C  | 0.557000  | -2.497000 | 1.762000 |
| H  | 0.608000  | -3.581000 | 1.910000 |
| H  | -0.272000 | -2.103000 | 2.354000 |

|   |           |           |           |
|---|-----------|-----------|-----------|
| H | 1.496000  | -2.062000 | 2.109000  |
| C | 0.634000  | 0.155000  | -2.726000 |
| H | 0.265000  | 0.179000  | -3.758000 |
| H | 1.313000  | -0.692000 | -2.619000 |
| H | 1.182000  | 1.079000  | -2.525000 |
| N | -0.506000 | 0.027000  | -1.776000 |
| C | -1.315000 | -1.197000 | -2.070000 |
| H | -0.674000 | -1.895000 | -2.618000 |
| H | -2.114000 | -0.909000 | -2.764000 |
| C | -1.933000 | -1.958000 | -0.869000 |
| C | -0.886000 | -2.865000 | -0.186000 |
| H | -1.365000 | -3.377000 | 0.654000  |
| H | -0.589000 | -3.646000 | -0.895000 |
| C | -2.968000 | -2.910000 | -1.480000 |
| H | -3.784000 | -2.370000 | -1.964000 |
| H | -3.395000 | -3.582000 | -0.732000 |
| H | -2.501000 | -3.537000 | -2.244000 |
| N | -1.717000 | -0.204000 | 0.859000  |
| C | -2.209000 | 0.603000  | 1.827000  |
| H | -1.502000 | 1.265000  | 2.321000  |
| C | -3.547000 | 0.611000  | 2.183000  |
| H | -3.894000 | 1.269000  | 2.971000  |
| C | -4.412000 | -0.240000 | 1.502000  |
| H | -5.468000 | -0.270000 | 1.751000  |
| C | -3.909000 | -1.061000 | 0.493000  |
| H | -4.577000 | -1.727000 | -0.040000 |
| C | -2.553000 | -1.041000 | 0.177000  |
| N | 2.303000  | -0.343000 | 0.057000  |
| C | 3.259000  | 0.605000  | 0.199000  |
| H | 2.917000  | 1.612000  | 0.423000  |
| C | 4.606000  | 0.322000  | 0.061000  |
| H | 5.340000  | 1.111000  | 0.182000  |
| C | 4.988000  | -0.990000 | -0.228000 |
| H | 6.038000  | -1.247000 | -0.329000 |
| C | 4.007000  | -1.968000 | -0.378000 |
| H | 4.275000  | -2.996000 | -0.601000 |
| C | 2.671000  | -1.618000 | -0.234000 |
| C | 1.549000  | -2.588000 | -0.449000 |
| H | 1.283000  | -2.614000 | -1.514000 |
| H | 1.852000  | -3.609000 | -0.185000 |
| N | 0.090000  | 2.124000  | -0.136000 |
| C | 0.640000  | 3.141000  | 0.570000  |
| H | 1.266000  | 2.870000  | 1.415000  |
| C | 0.423000  | 4.469000  | 0.249000  |
| H | 0.884000  | 5.250000  | 0.845000  |
| C | -0.387000 | 4.772000  | -0.846000 |
| H | -0.569000 | 5.804000  | -1.130000 |
| C | -0.959000 | 3.731000  | -1.574000 |
| H | -1.593000 | 3.935000  | -2.431000 |
| C | -0.711000 | 2.419000  | -1.192000 |
| C | -1.356000 | 1.251000  | -1.870000 |

|   |           |          |           |
|---|-----------|----------|-----------|
| H | -2.321000 | 1.034000 | -1.397000 |
| H | -1.565000 | 1.467000 | -2.925000 |
| O | 1.798000  | 0.675000 | 2.926000  |

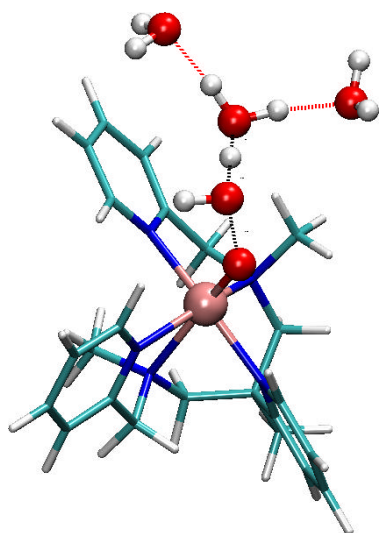
Fe2-TS



|    |           |           |           |
|----|-----------|-----------|-----------|
| Fe | -0.239000 | 0.043000  | 0.114000  |
| O  | 0.400000  | 0.052000  | 1.690000  |
| N  | 0.179000  | -1.978000 | -0.191000 |
| C  | 0.966000  | -2.565000 | 0.916000  |
| H  | 1.179000  | -3.619000 | 0.697000  |
| H  | 0.408000  | -2.487000 | 1.848000  |
| H  | 1.905000  | -2.022000 | 1.020000  |
| C  | -0.669000 | 0.613000  | -2.898000 |
| H  | -1.352000 | 0.739000  | -3.747000 |
| H  | 0.091000  | -0.117000 | -3.176000 |
| H  | -0.183000 | 1.570000  | -2.694000 |
| N  | -1.424000 | 0.167000  | -1.704000 |
| C  | -2.135000 | -1.101000 | -2.016000 |
| H  | -1.574000 | -1.634000 | -2.790000 |
| H  | -3.113000 | -0.864000 | -2.454000 |
| C  | -2.336000 | -2.055000 | -0.822000 |
| C  | -1.048000 | -2.799000 | -0.402000 |
| H  | -1.261000 | -3.323000 | 0.534000  |
| H  | -0.826000 | -3.568000 | -1.152000 |
| C  | -3.306000 | -3.135000 | -1.295000 |
| H  | -4.274000 | -2.710000 | -1.572000 |
| H  | -3.468000 | -3.894000 | -0.524000 |
| H  | -2.896000 | -3.634000 | -2.177000 |
| N  | -2.029000 | -0.411000 | 0.946000  |
| C  | -2.417000 | 0.280000  | 2.035000  |
| H  | -1.683000 | 0.969000  | 2.438000  |
| C  | -3.664000 | 0.116000  | 2.611000  |
| H  | -3.930000 | 0.694000  | 3.488000  |
| C  | -4.543000 | -0.796000 | 2.039000  |
| H  | -5.532000 | -0.952000 | 2.458000  |
| C  | -4.138000 | -1.515000 | 0.921000  |
| H  | -4.805000 | -2.236000 | 0.465000  |

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -2.869000 | -1.308000 | 0.383000  |
| N | 1.453000  | 0.287000  | -0.896000 |
| C | 2.177000  | 1.418000  | -0.968000 |
| H | 1.756000  | 2.295000  | -0.484000 |
| C | 3.389000  | 1.477000  | -1.633000 |
| H | 3.941000  | 2.410000  | -1.659000 |
| C | 3.873000  | 0.326000  | -2.249000 |
| H | 4.821000  | 0.340000  | -2.779000 |
| C | 3.128000  | -0.843000 | -2.174000 |
| H | 3.471000  | -1.765000 | -2.634000 |
| C | 1.921000  | -0.833000 | -1.486000 |
| C | 1.023000  | -2.018000 | -1.414000 |
| H | 0.373000  | -2.027000 | -2.295000 |
| H | 1.595000  | -2.954000 | -1.454000 |
| N | -0.762000 | 1.969000  | 0.199000  |
| C | -0.225000 | 2.874000  | 1.037000  |
| H | 0.548000  | 2.495000  | 1.697000  |
| C | -0.652000 | 4.191000  | 1.076000  |
| H | -0.190000 | 4.884000  | 1.769000  |
| C | -1.673000 | 4.590000  | 0.218000  |
| H | -2.024000 | 5.617000  | 0.217000  |
| C | -2.242000 | 3.653000  | -0.634000 |
| H | -3.050000 | 3.916000  | -1.309000 |
| C | -1.775000 | 2.343000  | -0.611000 |
| C | -2.406000 | 1.250000  | -1.408000 |
| H | -3.244000 | 0.836000  | -0.838000 |
| H | -2.834000 | 1.637000  | -2.342000 |
| O | 3.834000  | -2.599000 | 2.853000  |
| H | 3.526000  | -3.359000 | 2.343000  |
| H | 3.021000  | -2.261000 | 3.251000  |
| O | 2.360000  | 0.752000  | 2.125000  |
| H | 2.264000  | 1.533000  | 1.567000  |
| H | 3.208000  | 0.041000  | 1.533000  |
| O | 3.976000  | -0.621000 | 1.069000  |
| H | 4.093000  | -1.379000 | 1.703000  |
| H | 4.840000  | -0.127000 | 0.975000  |
| O | 6.159000  | 0.834000  | 0.694000  |
| H | 6.814000  | 0.266000  | 0.271000  |
| H | 6.547000  | 1.019000  | 1.557000  |

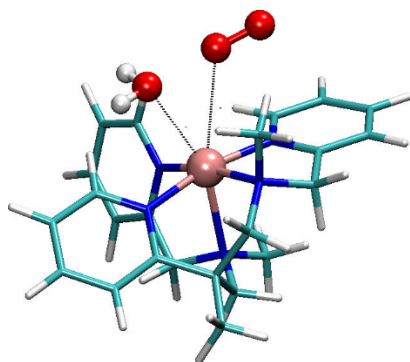
Fe3-TS



|    |           |           |           |
|----|-----------|-----------|-----------|
| Fe | -0.138000 | 0.101000  | 0.362000  |
| O  | 0.699000  | 0.288000  | 1.960000  |
| N  | 0.258000  | -1.980000 | -0.521000 |
| C  | 1.135000  | -2.641000 | 0.457000  |
| H  | 1.408000  | -3.658000 | 0.133000  |
| H  | 0.636000  | -2.700000 | 1.427000  |
| H  | 2.050000  | -2.056000 | 0.569000  |
| C  | -0.920000 | 0.934000  | -2.795000 |
| H  | -1.620000 | 1.130000  | -3.624000 |
| H  | -0.116000 | 0.297000  | -3.167000 |
| H  | -0.479000 | 1.887000  | -2.488000 |
| N  | -1.599000 | 0.316000  | -1.652000 |
| C  | -2.229000 | -0.955000 | -2.049000 |
| H  | -1.683000 | -1.361000 | -2.908000 |
| H  | -3.252000 | -0.764000 | -2.413000 |
| C  | -2.300000 | -2.068000 | -0.974000 |
| C  | -0.951000 | -2.797000 | -0.749000 |
| H  | -1.081000 | -3.450000 | 0.121000  |
| H  | -0.776000 | -3.464000 | -1.606000 |
| C  | -3.228000 | -3.135000 | -1.560000 |
| H  | -4.229000 | -2.741000 | -1.751000 |
| H  | -3.320000 | -4.000000 | -0.897000 |
| H  | -2.826000 | -3.487000 | -2.515000 |
| N  | -2.014000 | -0.719000 | 1.063000  |
| C  | -2.466000 | -0.226000 | 2.237000  |
| H  | -1.780000 | 0.441000  | 2.755000  |
| C  | -3.709000 | -0.522000 | 2.766000  |
| H  | -4.010000 | -0.092000 | 3.716000  |
| C  | -4.548000 | -1.369000 | 2.046000  |
| H  | -5.534000 | -1.629000 | 2.418000  |
| C  | -4.097000 | -1.878000 | 0.832000  |
| H  | -4.738000 | -2.537000 | 0.260000  |
| C  | -2.831000 | -1.544000 | 0.352000  |
| N  | 1.587000  | 0.404000  | -0.974000 |
| C  | 2.415000  | 1.460000  | -0.886000 |

|   |           |           |           |
|---|-----------|-----------|-----------|
| H | 2.042000  | 2.308000  | -0.311000 |
| C | 3.664000  | 1.496000  | -1.488000 |
| H | 4.294000  | 2.373000  | -1.385000 |
| C | 4.083000  | 0.383000  | -2.216000 |
| H | 5.058000  | 0.369000  | -2.695000 |
| C | 3.233000  | -0.715000 | -2.311000 |
| H | 3.523000  | -1.605000 | -2.861000 |
| C | 1.994000  | -0.671000 | -1.682000 |
| C | 1.013000  | -1.800000 | -1.775000 |
| H | 0.298000  | -1.592000 | -2.578000 |
| H | 1.528000  | -2.731000 | -2.060000 |
| N | -0.929000 | 2.150000  | 0.302000  |
| C | -0.381000 | 3.160000  | 1.009000  |
| H | 0.475000  | 2.892000  | 1.624000  |
| C | -0.858000 | 4.460000  | 0.975000  |
| H | -0.372000 | 5.229000  | 1.567000  |
| C | -1.955000 | 4.752000  | 0.165000  |
| H | -2.350000 | 5.761000  | 0.101000  |
| C | -2.529000 | 3.716000  | -0.568000 |
| H | -3.383000 | 3.891000  | -1.217000 |
| C | -2.003000 | 2.433000  | -0.469000 |
| C | -2.619000 | 1.268000  | -1.180000 |
| H | -3.298000 | 0.752000  | -0.494000 |
| H | -3.239000 | 1.622000  | -2.021000 |
| O | 3.984000  | -2.904000 | 2.590000  |
| H | 3.799000  | -2.628000 | 3.496000  |
| H | 4.896000  | -3.216000 | 2.632000  |
| O | 2.215000  | 0.805000  | 2.427000  |
| H | 2.267000  | 1.642000  | 1.945000  |
| H | 3.093000  | 0.046000  | 1.757000  |
| O | 3.867000  | -0.662000 | 1.153000  |
| H | 4.003000  | -1.481000 | 1.706000  |
| H | 4.736000  | -0.177000 | 1.075000  |
| O | 6.105000  | 0.747000  | 0.781000  |
| H | 5.765000  | 1.650000  | 0.817000  |
| H | 6.255000  | 0.608000  | -0.162000 |

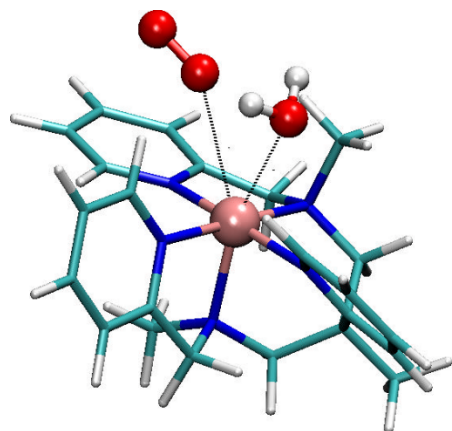
Fe2-oxy-re -ts



|    |           |           |           |
|----|-----------|-----------|-----------|
| Fe | 0.167000  | -0.044000 | 0.426000  |
| O  | 2.299000  | 0.805000  | 2.359000  |
| N  | 0.244000  | -2.075000 | 0.657000  |
| C  | 0.595000  | -2.367000 | 2.067000  |
| H  | 0.721000  | -3.447000 | 2.205000  |
| H  | -0.200000 | -2.005000 | 2.719000  |
| H  | 1.529000  | -1.863000 | 2.325000  |
| C  | 0.575000  | -0.299000 | -2.827000 |
| H  | 0.170000  | -0.332000 | -3.849000 |
| H  | 1.226000  | -1.164000 | -2.686000 |
| H  | 1.177000  | 0.608000  | -2.726000 |
| N  | -0.507000 | -0.288000 | -1.831000 |
| C  | -1.350000 | -1.494000 | -1.961000 |
| H  | -0.734000 | -2.296000 | -2.383000 |
| H  | -2.155000 | -1.312000 | -2.687000 |
| C  | -1.993000 | -2.033000 | -0.656000 |
| C  | -1.025000 | -2.768000 | 0.298000  |
| H  | -1.567000 | -2.966000 | 1.227000  |
| H  | -0.771000 | -3.742000 | -0.134000 |
| C  | -2.995000 | -3.100000 | -1.100000 |
| H  | -3.757000 | -2.686000 | -1.766000 |
| H  | -3.497000 | -3.561000 | -0.245000 |
| H  | -2.471000 | -3.887000 | -1.649000 |
| N  | -1.849000 | -0.015000 | 0.710000  |
| C  | -2.397000 | 1.050000  | 1.334000  |
| H  | -1.702000 | 1.764000  | 1.764000  |
| C  | -3.762000 | 1.251000  | 1.425000  |
| H  | -4.142000 | 2.123000  | 1.944000  |
| C  | -4.608000 | 0.319000  | 0.836000  |
| H  | -5.686000 | 0.437000  | 0.884000  |
| C  | -4.052000 | -0.764000 | 0.169000  |
| H  | -4.693000 | -1.492000 | -0.313000 |
| C  | -2.666000 | -0.912000 | 0.105000  |
| N  | 2.076000  | -0.275000 | -0.197000 |
| C  | 2.974000  | 0.689000  | -0.477000 |
| H  | 2.648000  | 1.712000  | -0.319000 |
| C  | 4.253000  | 0.407000  | -0.922000 |
| H  | 4.934000  | 1.221000  | -1.138000 |
| C  | 4.639000  | -0.924000 | -1.058000 |
| H  | 5.643000  | -1.179000 | -1.383000 |

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 3.719000  | -1.923000 | -0.771000 |
| H | 3.971000  | -2.973000 | -0.873000 |
| C | 2.438000  | -1.566000 | -0.364000 |
| C | 1.348000  | -2.569000 | -0.215000 |
| H | 0.936000  | -2.778000 | -1.208000 |
| H | 1.724000  | -3.527000 | 0.163000  |
| N | 0.061000  | 1.881000  | -0.209000 |
| C | 0.565000  | 2.912000  | 0.496000  |
| H | 1.102000  | 2.651000  | 1.404000  |
| C | 0.418000  | 4.228000  | 0.094000  |
| H | 0.843000  | 5.024000  | 0.695000  |
| C | -0.270000 | 4.490000  | -1.087000 |
| H | -0.393000 | 5.508000  | -1.442000 |
| C | -0.797000 | 3.427000  | -1.810000 |
| H | -1.341000 | 3.589000  | -2.735000 |
| C | -0.635000 | 2.128000  | -1.340000 |
| C | -1.274000 | 0.958000  | -2.029000 |
| H | -2.289000 | 0.836000  | -1.635000 |
| H | -1.394000 | 1.176000  | -3.099000 |
| O | 3.426000  | 0.301000  | 2.373000  |
| O | -0.159000 | 0.456000  | 3.264000  |
| H | -1.092000 | 0.384000  | 3.495000  |
| H | -0.005000 | 1.408000  | 3.241000  |

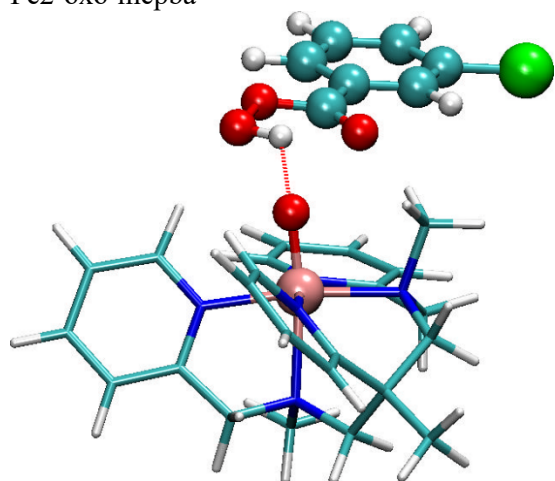
Fe3-oxo-re-ts



|    |           |           |           |
|----|-----------|-----------|-----------|
| Fe | 0.131000  | -0.078000 | 0.199000  |
| O  | 2.406000  | 0.314000  | 2.115000  |
| N  | 0.123000  | -2.074000 | 0.584000  |
| C  | 0.365000  | -2.225000 | 2.043000  |
| H  | 0.422000  | -3.291000 | 2.286000  |
| H  | -0.459000 | -1.772000 | 2.594000  |
| H  | 1.308000  | -1.750000 | 2.317000  |
| C  | 0.459000  | -0.213000 | -2.779000 |
| H  | -0.030000 | -0.240000 | -3.757000 |
| H  | 1.084000  | -1.098000 | -2.674000 |
| H  | 1.066000  | 0.691000  | -2.713000 |
| N  | -0.603000 | -0.190000 | -1.737000 |

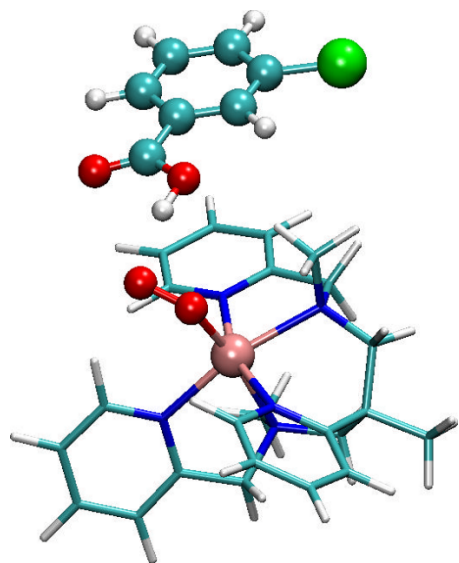
|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -1.472000 | -1.394000 | -1.915000 |
| H | -0.861000 | -2.176000 | -2.373000 |
| H | -2.254000 | -1.126000 | -2.633000 |
| C | -2.126000 | -1.969000 | -0.646000 |
| C | -1.144000 | -2.776000 | 0.218000  |
| H | -1.657000 | -3.059000 | 1.140000  |
| H | -0.882000 | -3.699000 | -0.308000 |
| C | -3.181000 | -2.962000 | -1.128000 |
| H | -3.949000 | -2.468000 | -1.727000 |
| H | -3.663000 | -3.466000 | -0.286000 |
| H | -2.707000 | -3.724000 | -1.752000 |
| N | -1.839000 | 0.041000  | 0.691000  |
| C | -2.296000 | 1.113000  | 1.369000  |
| H | -1.560000 | 1.832000  | 1.700000  |
| C | -3.643000 | 1.306000  | 1.619000  |
| H | -3.959000 | 2.186000  | 2.168000  |
| C | -4.551000 | 0.368000  | 1.147000  |
| H | -5.615000 | 0.487000  | 1.324000  |
| C | -4.082000 | -0.720000 | 0.423000  |
| H | -4.773000 | -1.451000 | 0.024000  |
| C | -2.717000 | -0.860000 | 0.190000  |
| N | 2.034000  | -0.402000 | -0.406000 |
| C | 2.959000  | 0.522000  | -0.724000 |
| H | 2.619000  | 1.548000  | -0.808000 |
| C | 4.286000  | 0.188000  | -0.920000 |
| H | 4.998000  | 0.965000  | -1.173000 |
| C | 4.678000  | -1.138000 | -0.759000 |
| H | 5.718000  | -1.424000 | -0.877000 |
| C | 3.720000  | -2.096000 | -0.453000 |
| H | 3.977000  | -3.143000 | -0.342000 |
| C | 2.398000  | -1.702000 | -0.301000 |
| C | 1.279000  | -2.671000 | -0.153000 |
| H | 0.947000  | -2.944000 | -1.163000 |
| H | 1.591000  | -3.596000 | 0.341000  |
| N | 0.147000  | 1.866000  | -0.251000 |
| C | 0.807000  | 2.811000  | 0.444000  |
| H | 1.439000  | 2.462000  | 1.255000  |
| C | 0.686000  | 4.153000  | 0.129000  |
| H | 1.229000  | 4.890000  | 0.709000  |
| C | -0.131000 | 4.521000  | -0.936000 |
| H | -0.238000 | 5.566000  | -1.210000 |
| C | -0.804000 | 3.541000  | -1.655000 |
| H | -1.442000 | 3.789000  | -2.496000 |
| C | -0.653000 | 2.213000  | -1.281000 |
| C | -1.372000 | 1.083000  | -1.935000 |
| H | -2.378000 | 0.979000  | -1.518000 |
| H | -1.495000 | 1.253000  | -3.009000 |
| O | 3.570000  | 0.635000  | 2.275000  |
| O | -0.053000 | 0.660000  | 2.998000  |
| H | 0.316000  | 1.549000  | 3.064000  |
| H | 0.599000  | 0.121000  | 3.462000  |

Fe2-oxo-mcpba



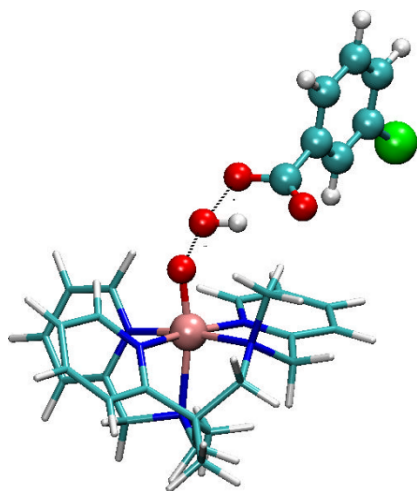
|    |           |           |           |
|----|-----------|-----------|-----------|
| Fe | 1.421000  | -0.003000 | -0.126000 |
| O  | 0.697000  | 0.434000  | -1.523000 |
| N  | 0.889000  | -1.994000 | -0.224000 |
| C  | 0.118000  | -2.246000 | -1.478000 |
| H  | -0.148000 | -3.307000 | -1.529000 |
| H  | 0.734000  | -1.973000 | -2.334000 |
| H  | -0.782000 | -1.631000 | -1.482000 |
| C  | 1.864000  | -0.071000 | 2.962000  |
| H  | 2.531000  | -0.173000 | 3.827000  |
| H  | 1.041000  | -0.777000 | 3.070000  |
| H  | 1.452000  | 0.941000  | 2.950000  |
| N  | 2.606000  | -0.317000 | 1.702000  |
| C  | 3.234000  | -1.665000 | 1.734000  |
| H  | 2.633000  | -2.308000 | 2.386000  |
| H  | 4.220000  | -1.592000 | 2.213000  |
| C  | 3.385000  | -2.365000 | 0.368000  |
| C  | 2.051000  | -2.932000 | -0.164000 |
| H  | 2.227000  | -3.308000 | -1.175000 |
| H  | 1.765000  | -3.799000 | 0.445000  |
| C  | 4.293000  | -3.576000 | 0.603000  |
| H  | 5.291000  | -3.276000 | 0.930000  |
| H  | 4.398000  | -4.185000 | -0.299000 |
| H  | 3.875000  | -4.216000 | 1.383000  |
| N  | 3.154000  | -0.403000 | -1.074000 |
| C  | 3.534000  | 0.409000  | -2.080000 |
| H  | 2.826000  | 1.189000  | -2.342000 |
| C  | 4.736000  | 0.242000  | -2.747000 |
| H  | 4.999000  | 0.913000  | -3.557000 |
| C  | 5.572000  | -0.798000 | -2.358000 |
| H  | 6.523000  | -0.959000 | -2.856000 |
| C  | 5.168000  | -1.645000 | -1.331000 |
| H  | 5.799000  | -2.473000 | -1.033000 |
| C  | 3.944000  | -1.438000 | -0.698000 |
| N  | -0.299000 | 0.144000  | 0.909000  |
| C  | -0.969000 | 1.280000  | 1.165000  |

|    |           |           |           |
|----|-----------|-----------|-----------|
| H  | -0.477000 | 2.206000  | 0.890000  |
| C  | -2.231000 | 1.276000  | 1.738000  |
| H  | -2.737000 | 2.217000  | 1.923000  |
| C  | -2.835000 | 0.056000  | 2.030000  |
| H  | -3.835000 | 0.021000  | 2.451000  |
| C  | -2.146000 | -1.120000 | 1.753000  |
| H  | -2.589000 | -2.091000 | 1.954000  |
| C  | -0.877000 | -1.043000 | 1.196000  |
| C  | -0.019000 | -2.234000 | 0.935000  |
| H  | 0.600000  | -2.442000 | 1.817000  |
| H  | -0.616000 | -3.137000 | 0.758000  |
| N  | 2.048000  | 1.872000  | 0.235000  |
| C  | 1.517000  | 2.961000  | -0.356000 |
| H  | 0.687000  | 2.774000  | -1.034000 |
| C  | 1.999000  | 4.236000  | -0.101000 |
| H  | 1.545000  | 5.086000  | -0.596000 |
| C  | 3.056000  | 4.392000  | 0.792000  |
| H  | 3.448000  | 5.379000  | 1.016000  |
| C  | 3.605000  | 3.265000  | 1.394000  |
| H  | 4.431000  | 3.349000  | 2.094000  |
| C  | 3.086000  | 2.013000  | 1.088000  |
| C  | 3.660000  | 0.734000  | 1.608000  |
| H  | 4.444000  | 0.385000  | 0.928000  |
| H  | 4.136000  | 0.877000  | 2.587000  |
| C  | -6.457000 | -0.796000 | -0.228000 |
| C  | -7.260000 | 0.308000  | 0.063000  |
| C  | -6.738000 | 1.592000  | -0.075000 |
| C  | -5.427000 | 1.783000  | -0.493000 |
| C  | -4.631000 | 0.667000  | -0.782000 |
| C  | -5.145000 | -0.629000 | -0.651000 |
| H  | -8.284000 | 0.157000  | 0.388000  |
| H  | -7.367000 | 2.448000  | 0.145000  |
| H  | -5.027000 | 2.785000  | -0.605000 |
| H  | -4.524000 | -1.485000 | -0.894000 |
| C  | -3.228000 | 0.782000  | -1.194000 |
| O  | -2.445000 | -0.139000 | -1.385000 |
| O  | -2.835000 | 2.077000  | -1.325000 |
| O  | -1.443000 | 2.156000  | -1.680000 |
| H  | -1.223000 | 1.207000  | -1.846000 |
| Cl | -7.099000 | -2.394000 | -0.057000 |



|    |           |           |           |
|----|-----------|-----------|-----------|
| Fe | 1.235000  | 0.181000  | -0.292000 |
| O  | 0.708000  | 0.728000  | -2.057000 |
| N  | 0.352000  | -1.916000 | -0.218000 |
| C  | -0.339000 | -2.078000 | -1.516000 |
| H  | -0.792000 | -3.076000 | -1.579000 |
| H  | 0.379000  | -1.957000 | -2.329000 |
| H  | -1.124000 | -1.326000 | -1.618000 |
| C  | 1.441000  | 0.122000  | 2.857000  |
| H  | 2.012000  | -0.013000 | 3.783000  |
| H  | 0.523000  | -0.461000 | 2.929000  |
| H  | 1.181000  | 1.179000  | 2.753000  |
| N  | 2.247000  | -0.318000 | 1.694000  |
| C  | 2.597000  | -1.757000 | 1.845000  |
| H  | 1.834000  | -2.229000 | 2.470000  |
| H  | 3.539000  | -1.826000 | 2.404000  |
| C  | 2.728000  | -2.589000 | 0.551000  |
| C  | 1.361000  | -2.993000 | -0.045000 |
| H  | 1.543000  | -3.443000 | -1.025000 |
| H  | 0.929000  | -3.777000 | 0.587000  |
| C  | 3.394000  | -3.900000 | 0.968000  |
| H  | 4.398000  | -3.735000 | 1.364000  |
| H  | 3.459000  | -4.598000 | 0.129000  |
| H  | 2.801000  | -4.375000 | 1.754000  |
| N  | 2.980000  | -0.762000 | -1.058000 |
| C  | 3.634000  | -0.079000 | -2.018000 |
| H  | 3.128000  | 0.801000  | -2.405000 |
| C  | 4.877000  | -0.465000 | -2.487000 |
| H  | 5.366000  | 0.114000  | -3.261000 |
| C  | 5.461000  | -1.599000 | -1.937000 |
| H  | 6.435000  | -1.938000 | -2.276000 |
| C  | 4.788000  | -2.303000 | -0.946000 |
| H  | 5.234000  | -3.191000 | -0.515000 |
| C  | 3.538000  | -1.868000 | -0.510000 |
| N  | -0.652000 | 0.458000  | 0.625000  |

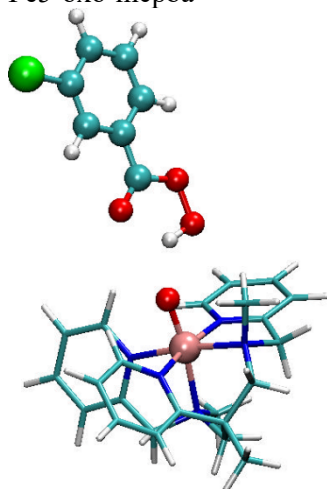
|    |           |           |           |
|----|-----------|-----------|-----------|
| C  | -1.156000 | 1.688000  | 0.837000  |
| H  | -0.597000 | 2.519000  | 0.413000  |
| C  | -2.323000 | 1.886000  | 1.554000  |
| H  | -2.702000 | 2.892000  | 1.701000  |
| C  | -2.995000 | 0.772000  | 2.053000  |
| H  | -3.921000 | 0.892000  | 2.607000  |
| C  | -2.486000 | -0.496000 | 1.811000  |
| H  | -2.995000 | -1.389000 | 2.163000  |
| C  | -1.304000 | -0.624000 | 1.090000  |
| C  | -0.653000 | -1.951000 | 0.868000  |
| H  | -0.165000 | -2.261000 | 1.799000  |
| H  | -1.411000 | -2.718000 | 0.657000  |
| N  | 2.244000  | 2.001000  | 0.272000  |
| C  | 1.968000  | 3.202000  | -0.265000 |
| H  | 1.180000  | 3.220000  | -1.014000 |
| C  | 2.647000  | 4.346000  | 0.118000  |
| H  | 2.395000  | 5.299000  | -0.332000 |
| C  | 3.644000  | 4.238000  | 1.084000  |
| H  | 4.189000  | 5.117000  | 1.412000  |
| C  | 3.932000  | 2.993000  | 1.632000  |
| H  | 4.699000  | 2.871000  | 2.389000  |
| C  | 3.216000  | 1.884000  | 1.199000  |
| C  | 3.488000  | 0.499000  | 1.685000  |
| H  | 4.229000  | 0.026000  | 1.030000  |
| H  | 3.928000  | 0.517000  | 2.690000  |
| C  | -5.606000 | -1.078000 | -0.081000 |
| C  | -6.605000 | -0.287000 | 0.480000  |
| C  | -6.541000 | 1.095000  | 0.313000  |
| C  | -5.491000 | 1.670000  | -0.391000 |
| C  | -4.497000 | 0.861000  | -0.949000 |
| C  | -4.554000 | -0.528000 | -0.800000 |
| H  | -7.414000 | -0.743000 | 1.040000  |
| H  | -7.314000 | 1.719000  | 0.749000  |
| H  | -5.420000 | 2.747000  | -0.504000 |
| H  | -3.776000 | -1.162000 | -1.212000 |
| C  | -3.337000 | 1.510000  | -1.599000 |
| O  | -2.458000 | 0.634000  | -2.099000 |
| O  | -3.173000 | 2.723000  | -1.648000 |
| O  | 0.015000  | 1.787000  | -2.321000 |
| H  | -1.646000 | 1.131000  | -2.368000 |
| Cl | -5.653000 | -2.811000 | 0.153000  |



|    |           |           |           |
|----|-----------|-----------|-----------|
| Fe | -1.488000 | -0.034000 | 0.094000  |
| O  | -0.704000 | 0.210000  | 1.556000  |
| N  | -1.410000 | -2.096000 | 0.155000  |
| C  | -0.624000 | -2.547000 | 1.340000  |
| H  | -0.624000 | -3.642000 | 1.377000  |
| H  | -1.070000 | -2.140000 | 2.247000  |
| H  | 0.405000  | -2.192000 | 1.256000  |
| C  | -2.058000 | 0.033000  | -2.964000 |
| H  | -2.770000 | 0.098000  | -3.795000 |
| H  | -1.423000 | -0.840000 | -3.116000 |
| H  | -1.425000 | 0.923000  | -2.969000 |
| N  | -2.778000 | -0.053000 | -1.670000 |
| C  | -3.699000 | -1.225000 | -1.676000 |
| H  | -3.290000 | -1.981000 | -2.356000 |
| H  | -4.660000 | -0.921000 | -2.114000 |
| C  | -3.952000 | -1.884000 | -0.305000 |
| C  | -2.758000 | -2.737000 | 0.182000  |
| H  | -2.961000 | -3.038000 | 1.213000  |
| H  | -2.712000 | -3.660000 | -0.410000 |
| C  | -5.115000 | -2.859000 | -0.503000 |
| H  | -6.030000 | -2.343000 | -0.802000 |
| H  | -5.326000 | -3.430000 | 0.405000  |
| H  | -4.876000 | -3.576000 | -1.293000 |
| N  | -3.231000 | -0.035000 | 1.119000  |
| C  | -3.388000 | 0.854000  | 2.119000  |
| H  | -2.512000 | 1.447000  | 2.359000  |
| C  | -4.582000 | 0.986000  | 2.809000  |
| H  | -4.663000 | 1.710000  | 3.611000  |
| C  | -5.648000 | 0.170000  | 2.452000  |
| H  | -6.601000 | 0.245000  | 2.966000  |
| C  | -5.477000 | -0.761000 | 1.431000  |
| H  | -6.293000 | -1.419000 | 1.156000  |
| C  | -4.253000 | -0.854000 | 0.773000  |
| N  | 0.178000  | -0.270000 | -0.994000 |
| C  | 1.084000  | 0.683000  | -1.270000 |

|    |           |           |           |
|----|-----------|-----------|-----------|
| H  | 0.867000  | 1.680000  | -0.905000 |
| C  | 2.248000  | 0.409000  | -1.970000 |
| H  | 2.942000  | 1.216000  | -2.182000 |
| C  | 2.505000  | -0.899000 | -2.367000 |
| H  | 3.416000  | -1.147000 | -2.905000 |
| C  | 1.583000  | -1.892000 | -2.058000 |
| H  | 1.757000  | -2.927000 | -2.332000 |
| C  | 0.426000  | -1.543000 | -1.375000 |
| C  | -0.667000 | -2.513000 | -1.069000 |
| H  | -1.374000 | -2.553000 | -1.905000 |
| H  | -0.281000 | -3.532000 | -0.942000 |
| N  | -1.684000 | 1.937000  | -0.234000 |
| C  | -0.908000 | 2.870000  | 0.354000  |
| H  | -0.125000 | 2.490000  | 1.005000  |
| C  | -1.110000 | 4.224000  | 0.134000  |
| H  | -0.466000 | 4.945000  | 0.625000  |
| C  | -2.136000 | 4.627000  | -0.716000 |
| H  | -2.310000 | 5.680000  | -0.912000 |
| C  | -2.940000 | 3.660000  | -1.311000 |
| H  | -3.754000 | 3.937000  | -1.973000 |
| C  | -2.698000 | 2.320000  | -1.039000 |
| C  | -3.565000 | 1.208000  | -1.535000 |
| H  | -4.380000 | 1.043000  | -0.823000 |
| H  | -4.035000 | 1.460000  | -2.496000 |
| C  | 6.916000  | 0.059000  | -0.043000 |
| C  | 7.653000  | -0.161000 | 1.130000  |
| C  | 6.982000  | -0.360000 | 2.334000  |
| C  | 5.595000  | -0.339000 | 2.378000  |
| C  | 4.869000  | -0.153000 | 1.188000  |
| C  | 5.529000  | 0.081000  | -0.019000 |
| H  | 8.737000  | -0.162000 | 1.089000  |
| H  | 7.552000  | -0.521000 | 3.244000  |
| H  | 5.069000  | -0.478000 | 3.317000  |
| H  | 4.975000  | 0.256000  | -0.935000 |
| C  | 3.374000  | -0.205000 | 1.221000  |
| O  | 2.701000  | -1.234000 | 1.115000  |
| O  | 2.921000  | 0.992000  | 1.394000  |
| O  | 0.990000  | 0.706000  | 1.560000  |
| H  | 1.285000  | -0.235000 | 1.550000  |
| Cl | 7.748000  | 0.306000  | -1.534000 |

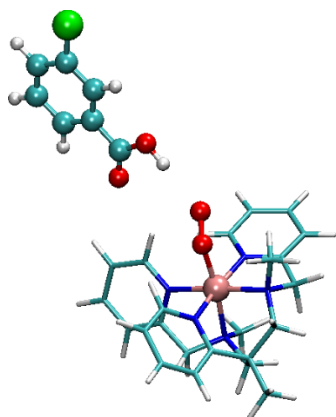
Fe5-oxo-mcpba



|    |           |           |           |
|----|-----------|-----------|-----------|
| Fe | -1.570000 | 0.104000  | -0.047000 |
| O  | -0.006000 | -0.232000 | -0.441000 |
| N  | -2.082000 | 0.873000  | -1.922000 |
| C  | -0.909000 | 0.723000  | -2.830000 |
| H  | -1.190000 | 1.120000  | -3.810000 |
| H  | -0.650000 | -0.331000 | -2.918000 |
| H  | -0.063000 | 1.287000  | -2.435000 |
| C  | -3.788000 | 1.618000  | 1.467000  |
| H  | -4.807000 | 1.614000  | 1.868000  |
| H  | -3.675000 | 2.477000  | 0.807000  |
| H  | -3.081000 | 1.694000  | 2.296000  |
| N  | -3.565000 | 0.346000  | 0.722000  |
| C  | -4.607000 | 0.207000  | -0.335000 |
| H  | -4.910000 | 1.209000  | -0.653000 |
| H  | -5.487000 | -0.264000 | 0.117000  |
| C  | -4.183000 | -0.595000 | -1.575000 |
| C  | -3.273000 | 0.204000  | -2.531000 |
| H  | -2.911000 | -0.473000 | -3.306000 |
| H  | -3.871000 | 0.984000  | -3.013000 |
| C  | -5.455000 | -0.905000 | -2.359000 |
| H  | -6.138000 | -1.523000 | -1.773000 |
| H  | -5.228000 | -1.419000 | -3.296000 |
| H  | -5.968000 | 0.030000  | -2.598000 |
| N  | -2.187000 | -1.678000 | -0.677000 |
| C  | -1.381000 | -2.728000 | -0.412000 |
| H  | -0.400000 | -2.504000 | -0.010000 |
| C  | -1.800000 | -4.023000 | -0.643000 |
| H  | -1.130000 | -4.844000 | -0.418000 |
| C  | -3.074000 | -4.230000 | -1.162000 |
| H  | -3.435000 | -5.236000 | -1.349000 |
| C  | -3.881000 | -3.139000 | -1.454000 |
| H  | -4.868000 | -3.280000 | -1.878000 |
| C  | -3.422000 | -1.849000 | -1.209000 |
| N  | -1.127000 | 2.036000  | 0.307000  |

|    |           |           |           |
|----|-----------|-----------|-----------|
| C  | -0.439000 | 2.463000  | 1.381000  |
| H  | -0.164000 | 1.727000  | 2.127000  |
| C  | -0.111000 | 3.799000  | 1.531000  |
| H  | 0.427000  | 4.111000  | 2.418000  |
| C  | -0.460000 | 4.698000  | 0.529000  |
| H  | -0.193000 | 5.746000  | 0.612000  |
| C  | -1.153000 | 4.242000  | -0.586000 |
| H  | -1.445000 | 4.907000  | -1.391000 |
| C  | -1.491000 | 2.899000  | -0.666000 |
| C  | -2.356000 | 2.331000  | -1.726000 |
| H  | -3.406000 | 2.465000  | -1.443000 |
| H  | -2.229000 | 2.842000  | -2.685000 |
| N  | -1.303000 | -0.572000 | 1.800000  |
| C  | -0.082000 | -0.746000 | 2.348000  |
| H  | 0.770000  | -0.463000 | 1.735000  |
| C  | 0.052000  | -1.252000 | 3.626000  |
| H  | 1.044000  | -1.377000 | 4.044000  |
| C  | -1.095000 | -1.587000 | 4.345000  |
| H  | -1.013000 | -1.981000 | 5.352000  |
| C  | -2.345000 | -1.416000 | 3.765000  |
| H  | -3.258000 | -1.669000 | 4.292000  |
| C  | -2.427000 | -0.909000 | 2.476000  |
| C  | -3.694000 | -0.763000 | 1.717000  |
| H  | -3.913000 | -1.704000 | 1.200000  |
| H  | -4.544000 | -0.567000 | 2.379000  |
| C  | 7.245000  | -1.051000 | -0.411000 |
| C  | 8.079000  | 0.064000  | -0.430000 |
| C  | 7.511000  | 1.332000  | -0.345000 |
| C  | 6.133000  | 1.487000  | -0.253000 |
| C  | 5.312000  | 0.353000  | -0.238000 |
| C  | 5.866000  | -0.929000 | -0.313000 |
| H  | 9.154000  | -0.058000 | -0.506000 |
| H  | 8.154000  | 2.205000  | -0.353000 |
| H  | 5.701000  | 2.479000  | -0.185000 |
| H  | 5.223000  | -1.802000 | -0.302000 |
| C  | 3.847000  | 0.440000  | -0.155000 |
| O  | 3.066000  | -0.484000 | 0.006000  |
| O  | 3.415000  | 1.723000  | -0.304000 |
| O  | 1.981000  | 1.808000  | -0.228000 |
| H  | 1.724000  | 0.861000  | -0.109000 |
| Cl | 7.947000  | -2.645000 | -0.517000 |

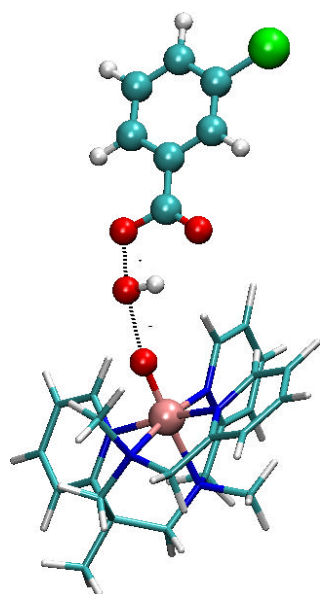
Fe3-peroxo-mcpba-b



|    |           |           |           |
|----|-----------|-----------|-----------|
| Fe | -1.873000 | 0.216000  | -0.098000 |
| O  | -0.243000 | 0.262000  | -1.016000 |
| N  | -2.925000 | 1.172000  | -1.606000 |
| C  | -2.057000 | 1.395000  | -2.797000 |
| H  | -2.636000 | 1.875000  | -3.593000 |
| H  | -1.675000 | 0.438000  | -3.154000 |
| H  | -1.218000 | 2.039000  | -2.530000 |
| C  | -3.715000 | 1.119000  | 2.133000  |
| H  | -4.576000 | 0.910000  | 2.778000  |
| H  | -3.880000 | 2.070000  | 1.629000  |
| H  | -2.817000 | 1.196000  | 2.750000  |
| N  | -3.543000 | 0.021000  | 1.144000  |
| C  | -4.807000 | -0.159000 | 0.365000  |
| H  | -5.329000 | 0.803000  | 0.332000  |
| H  | -5.464000 | -0.837000 | 0.926000  |
| C  | -4.643000 | -0.678000 | -1.077000 |
| C  | -4.153000 | 0.428000  | -2.033000 |
| H  | -3.952000 | -0.026000 | -3.007000 |
| H  | -4.961000 | 1.154000  | -2.188000 |
| C  | -6.043000 | -1.071000 | -1.557000 |
| H  | -6.455000 | -1.895000 | -0.970000 |
| H  | -6.043000 | -1.366000 | -2.609000 |
| H  | -6.730000 | -0.227000 | -1.455000 |
| N  | -2.367000 | -1.559000 | -0.868000 |
| C  | -1.424000 | -2.514000 | -1.009000 |
| H  | -0.411000 | -2.221000 | -0.749000 |
| C  | -1.720000 | -3.789000 | -1.458000 |
| H  | -0.929000 | -4.522000 | -1.564000 |
| C  | -3.043000 | -4.093000 | -1.759000 |
| H  | -3.318000 | -5.084000 | -2.107000 |
| C  | -4.016000 | -3.107000 | -1.619000 |
| H  | -5.048000 | -3.328000 | -1.865000 |
| C  | -3.662000 | -1.836000 | -1.177000 |
| N  | -1.479000 | 2.106000  | 0.452000  |
| C  | -0.496000 | 2.502000  | 1.284000  |
| H  | 0.071000  | 1.715000  | 1.770000  |
| C  | -0.225000 | 3.840000  | 1.523000  |
| H  | 0.565000  | 4.112000  | 2.214000  |
| C  | -0.975000 | 4.808000  | 0.862000  |

|    |           |           |           |
|----|-----------|-----------|-----------|
| H  | -0.781000 | 5.864000  | 1.022000  |
| C  | -1.976000 | 4.402000  | -0.016000 |
| H  | -2.573000 | 5.128000  | -0.559000 |
| C  | -2.208000 | 3.046000  | -0.196000 |
| C  | -3.304000 | 2.505000  | -1.051000 |
| H  | -4.215000 | 2.383000  | -0.452000 |
| H  | -3.564000 | 3.192000  | -1.865000 |
| N  | -0.976000 | -0.686000 | 1.469000  |
| C  | 0.351000  | -0.765000 | 1.709000  |
| H  | 1.023000  | -0.284000 | 1.004000  |
| C  | 0.859000  | -1.435000 | 2.811000  |
| H  | 1.933000  | -1.470000 | 2.952000  |
| C  | -0.021000 | -2.037000 | 3.706000  |
| H  | 0.348000  | -2.558000 | 4.584000  |
| C  | -1.388000 | -1.959000 | 3.459000  |
| H  | -2.106000 | -2.415000 | 4.133000  |
| C  | -1.833000 | -1.287000 | 2.328000  |
| C  | -3.268000 | -1.226000 | 1.928000  |
| H  | -3.515000 | -2.093000 | 1.306000  |
| H  | -3.935000 | -1.266000 | 2.798000  |
| C  | 8.018000  | -0.192000 | -0.711000 |
| C  | 8.484000  | -0.628000 | 0.555000  |
| C  | 7.567000  | -0.853000 | 1.559000  |
| C  | 6.196000  | -0.652000 | 1.319000  |
| C  | 5.731000  | -0.218000 | 0.056000  |
| C  | 6.635000  | 0.015000  | -0.963000 |
| H  | 9.548000  | -0.776000 | 0.710000  |
| H  | 7.903000  | -1.186000 | 2.535000  |
| H  | 5.466000  | -0.825000 | 2.103000  |
| H  | 6.310000  | 0.349000  | -1.943000 |
| C  | 4.265000  | -0.032000 | -0.127000 |
| O  | 3.963000  | 0.411000  | -1.350000 |
| O  | 3.444000  | -0.262000 | 0.744000  |
| O  | 0.798000  | 0.968000  | -0.909000 |
| H  | 3.000000  | 0.516000  | -1.406000 |
| Cl | 9.130000  | 0.085000  | -1.950000 |

Fe3-mcpba-TS



|    |          |           |           |
|----|----------|-----------|-----------|
| Fe | 1.689000 | -0.237000 | -0.138000 |
| O  | 0.355000 | -0.085000 | -1.106000 |
| N  | 2.973000 | -0.866000 | -1.683000 |
| C  | 2.207000 | -0.846000 | -2.960000 |
| H  | 2.886000 | -1.152000 | -3.762000 |
| H  | 1.844000 | 0.163000  | -3.150000 |
| H  | 1.372000 | -1.544000 | -2.904000 |
| C  | 3.384000 | -1.576000 | 2.036000  |
| H  | 4.146000 | -1.488000 | 2.816000  |
| H  | 3.669000 | -2.383000 | 1.364000  |
| H  | 2.422000 | -1.805000 | 2.499000  |
| N  | 3.300000 | -0.285000 | 1.301000  |
| C  | 4.628000 | 0.050000  | 0.712000  |
| H  | 5.180000 | -0.877000 | 0.544000  |
| H  | 5.193000 | 0.622000  | 1.456000  |
| C  | 4.578000 | 0.848000  | -0.600000 |
| C  | 4.194000 | -0.015000 | -1.818000 |
| H  | 4.045000 | 0.646000  | -2.674000 |
| H  | 5.027000 | -0.686000 | -2.049000 |
| C  | 5.993000 | 1.355000  | -0.862000 |
| H  | 6.326000 | 2.017000  | -0.060000 |
| H  | 6.053000 | 1.892000  | -1.812000 |
| H  | 6.680000 | 0.507000  | -0.902000 |
| N  | 2.266000 | 1.633000  | -0.481000 |
| C  | 1.286000 | 2.563000  | -0.500000 |
| H  | 0.264000 | 2.199000  | -0.475000 |
| C  | 1.586000 | 3.910000  | -0.545000 |
| H  | 0.778000 | 4.631000  | -0.555000 |
| C  | 2.922000 | 4.295000  | -0.579000 |
| H  | 3.191000 | 5.345000  | -0.612000 |
| C  | 3.917000 | 3.326000  | -0.585000 |
| H  | 4.961000 | 3.610000  | -0.628000 |

|    |           |           |           |
|----|-----------|-----------|-----------|
| C  | 3.575000  | 1.979000  | -0.534000 |
| N  | 1.374000  | -2.223000 | -0.042000 |
| C  | 0.315000  | -2.765000 | 0.586000  |
| H  | -0.366000 | -2.092000 | 1.093000  |
| C  | 0.108000  | -4.132000 | 0.580000  |
| H  | -0.746000 | -4.536000 | 1.109000  |
| C  | 0.998000  | -4.948000 | -0.111000 |
| H  | 0.850000  | -6.023000 | -0.139000 |
| C  | 2.067000  | -4.374000 | -0.786000 |
| H  | 2.771000  | -4.969000 | -1.357000 |
| C  | 2.234000  | -2.998000 | -0.736000 |
| C  | 3.362000  | -2.278000 | -1.371000 |
| H  | 4.234000  | -2.286000 | -0.712000 |
| H  | 3.682000  | -2.760000 | -2.300000 |
| N  | 0.701000  | 0.301000  | 1.524000  |
| C  | -0.644000 | 0.297000  | 1.629000  |
| H  | -1.202000 | -0.022000 | 0.757000  |
| C  | -1.272000 | 0.693000  | 2.793000  |
| H  | -2.354000 | 0.671000  | 2.840000  |
| C  | -0.495000 | 1.109000  | 3.873000  |
| H  | -0.965000 | 1.420000  | 4.800000  |
| C  | 0.888000  | 1.122000  | 3.753000  |
| H  | 1.530000  | 1.438000  | 4.568000  |
| C  | 1.468000  | 0.716000  | 2.560000  |
| C  | 2.925000  | 0.763000  | 2.298000  |
| H  | 3.190000  | 1.755000  | 1.914000  |
| H  | 3.507000  | 0.619000  | 3.213000  |
| C  | -7.480000 | -0.030000 | -0.088000 |
| C  | -7.979000 | 1.215000  | -0.461000 |
| C  | -7.106000 | 2.159000  | -0.994000 |
| C  | -5.757000 | 1.868000  | -1.151000 |
| C  | -5.276000 | 0.610000  | -0.770000 |
| C  | -6.139000 | -0.352000 | -0.235000 |
| H  | -9.033000 | 1.440000  | -0.336000 |
| H  | -7.489000 | 3.131000  | -1.287000 |
| H  | -5.084000 | 2.610000  | -1.565000 |
| H  | -5.756000 | -1.323000 | 0.057000  |
| C  | -3.853000 | 0.228000  | -0.901000 |
| O  | -3.386000 | -0.855000 | -0.566000 |
| O  | -3.118000 | 1.208000  | -1.447000 |
| O  | -1.525000 | 0.699000  | -1.441000 |
| H  | -1.754000 | -0.242000 | -1.250000 |
| Cl | -8.569000 | -1.222000 | 0.579000  |