

Supporting information

On the mechanism of water oxidation by a bimetallic manganese catalyst: a density functional study

W. M. C. Sameera,^a Christine J. McKenzie^b and John E. McGrady^{a*}

e-mail: john.mcgrady@chem.ox.ac.uk

^aInorganic Chemistry Laboratory, Department of Chemistry, University of Oxford, South Parks Road, Oxford OX1 3QR, United Kingdom.

^bDepartment of Physics and Chemistry, University of Southern Denmark, Odense, Campusvej 55, 5230 Odense M, Denmark.

Cartesian coordinates of the optimised structures

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|----|--------------|--------------|--------------|
| Mn | -2.020272000 | -0.220300000 | -0.325168000 |
| O | -2.371174000 | -0.137427000 | -2.484234000 |
| H | -1.516267000 | 0.083765000 | -3.042483000 |
| H | -3.125438000 | -0.426511000 | -3.024619000 |
| O | 0.323871000 | 0.179802000 | -1.269739000 |
| O | -0.166454000 | 0.357994000 | -3.497827000 |
| N | -4.340806000 | -1.210859000 | -0.344050000 |
| N | -2.947121000 | 0.162725000 | 1.913144000 |
| N | -2.746923000 | 1.961679000 | -0.250907000 |
| N | -1.839577000 | -2.488535000 | -0.328376000 |
| C | -4.674861000 | -1.463207000 | 1.093866000 |
| H | -4.080632000 | -2.315901000 | 1.439623000 |
| H | -5.735953000 | -1.745125000 | 1.206024000 |
| C | -4.388141000 | -0.238422000 | 1.970344000 |
| H | -4.990422000 | 0.610942000 | 1.632920000 |
| H | -4.696163000 | -0.453065000 | 3.006514000 |
| C | -2.094948000 | -0.645846000 | 2.826510000 |
| H | -2.342352000 | -1.707295000 | 2.710670000 |
| H | -2.236580000 | -0.386731000 | 3.885705000 |
| C | -2.774621000 | 1.623268000 | 2.180303000 |
| H | -1.723689000 | 1.802400000 | 2.437896000 |
| H | -3.375627000 | 1.948127000 | 3.043490000 |
| C | -3.113369000 | 2.465082000 | 0.963733000 |
| C | -3.729987000 | 3.723570000 | 1.083238000 |

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| H | -4.023601000 | 4.093039000 | 2.061299000 |
| C | -3.963422000 | 4.489335000 | -0.073953000 |
| H | -4.443705000 | 5.460882000 | -0.002626000 |
| C | -3.576193000 | 3.970348000 | -1.324144000 |
| H | -3.745335000 | 4.523920000 | -2.241904000 |
| C | -2.977158000 | 2.701531000 | -1.371053000 |
| H | -2.681867000 | 2.244677000 | -2.308027000 |
| C | -0.669416000 | -3.117292000 | -0.030868000 |
| H | 0.143082000 | -2.476662000 | 0.288198000 |
| C | -0.519533000 | -4.508667000 | -0.119666000 |
| H | 0.429855000 | -4.969874000 | 0.131321000 |
| C | -1.623188000 | -5.283101000 | -0.524461000 |
| H | -1.546172000 | -6.363915000 | -0.597431000 |
| C | -2.834072000 | -4.635027000 | -0.822199000 |
| H | -3.707050000 | -5.204673000 | -1.126659000 |
| C | -2.912077000 | -3.233776000 | -0.719358000 |
| C | -4.190290000 | -2.497860000 | -1.082156000 |
| H | -4.173468000 | -2.275560000 | -2.157182000 |
| H | -5.055093000 | -3.162311000 | -0.916212000 |
| C | -5.383091000 | -0.362092000 | -0.994899000 |
| H | -5.097627000 | -0.138022000 | -2.026927000 |
| H | -5.482546000 | 0.589186000 | -0.467950000 |
| H | -6.366991000 | -0.859741000 | -1.006037000 |
| C | 0.666181000 | 0.284110000 | -2.531159000 |
| Mn | 1.996998000 | 0.290841000 | 0.307290000 |
| O | 2.295036000 | 0.509992000 | 2.480300000 |
| H | 1.521051000 | 0.064670000 | 3.008253000 |
| H | 2.755441000 | 1.199776000 | 2.988256000 |
| O | -0.311970000 | -0.204676000 | 1.226258000 |
| C | -0.616665000 | -0.459152000 | 2.475608000 |
| O | 0.241809000 | -0.547854000 | 3.419439000 |
| N | 4.328970000 | 1.215278000 | 0.258023000 |
| C | 4.717043000 | 1.270582000 | -1.186687000 |
| H | 4.165098000 | 2.091964000 | -1.657550000 |
| H | 5.790910000 | 1.500212000 | -1.297114000 |
| C | 4.410180000 | -0.046154000 | -1.908295000 |
| N | 2.954668000 | -0.390318000 | -1.837476000 |
| N | 2.686531000 | -1.896709000 | 0.539436000 |
| C | 3.055153000 | -2.553829000 | -0.600011000 |
| C | 2.738431000 | -1.867388000 | -1.916417000 |
| C | 2.157201000 | 0.318663000 | -2.873161000 |
| H | 2.467412000 | 1.369145000 | -2.916969000 |
| H | 2.291979000 | -0.103318000 | -3.879770000 |
| H | 1.682944000 | -2.045257000 | -2.156687000 |
| H | 3.331756000 | -2.316785000 | -2.727682000 |
| C | 3.656709000 | -3.823917000 | -0.555834000 |
| H | 3.954920000 | -4.314758000 | -1.477554000 |
| C | 3.871841000 | -4.442259000 | 0.690466000 |
| H | 4.340865000 | -5.420349000 | 0.745837000 |
| C | 3.480829000 | -3.766922000 | 1.861535000 |
| H | 3.631429000 | -4.203994000 | 2.842985000 |
| C | 2.897986000 | -2.494477000 | 1.744879000 |

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| H | 2.601399000 | -1.930506000 | 2.620305000 |
| N | 1.866211000 | 2.557436000 | 0.085814000 |
| C | 0.707766000 | 3.177603000 | -0.269863000 |
| H | -0.126426000 | 2.525991000 | -0.498452000 |
| C | 0.594695000 | 4.573217000 | -0.345459000 |
| H | -0.347416000 | 5.026758000 | -0.634756000 |
| C | 1.724639000 | 5.359842000 | -0.051783000 |
| H | 1.676679000 | 6.443299000 | -0.108668000 |
| C | 2.923021000 | 4.719411000 | 0.307799000 |
| H | 3.814836000 | 5.297529000 | 0.531044000 |
| C | 2.962765000 | 3.314359000 | 0.375511000 |
| C | 4.223660000 | 2.591073000 | 0.820157000 |
| C | 5.301342000 | 0.408514000 | 1.056813000 |
| H | 4.923936000 | 0.282512000 | 2.074941000 |
| H | 5.416440000 | -0.586742000 | 0.621985000 |
| H | 6.294074000 | 0.886800000 | 1.094372000 |
| H | 4.223781000 | 2.512969000 | 1.915773000 |
| H | 5.105730000 | 3.200877000 | 0.561296000 |
| H | 4.975524000 | -0.862703000 | -1.448964000 |
| H | 4.747618000 | 0.023561000 | -2.954948000 |

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| Mn | -2.028903000 | -0.214552000 | -0.320713000 |
| O | -2.370642000 | -0.119368000 | -2.479302000 |
| H | -1.510189000 | 0.083400000 | -3.038057000 |
| H | -3.136033000 | -0.374701000 | -3.021077000 |
| O | 0.333589000 | 0.172518000 | -1.272304000 |
| O | -0.161197000 | 0.336172000 | -3.499855000 |
| N | -4.342708000 | -1.208626000 | -0.345408000 |
| N | -2.954895000 | 0.157839000 | 1.919748000 |
| N | -2.753454000 | 1.967281000 | -0.236703000 |
| N | -1.839576000 | -2.480926000 | -0.335682000 |
| C | -4.675932000 | -1.470718000 | 1.091123000 |
| H | -4.078427000 | -2.323078000 | 1.431992000 |
| H | -5.735921000 | -1.757394000 | 1.201363000 |
| C | -4.394149000 | -0.249901000 | 1.974942000 |
| H | -5.000151000 | 0.598982000 | 1.642880000 |
| H | -4.701039000 | -0.472158000 | 3.009820000 |
| C | -2.098413000 | -0.650887000 | 2.829233000 |
| H | -2.341528000 | -1.712845000 | 2.709077000 |
| H | -2.240009000 | -0.396453000 | 3.889529000 |
| C | -2.788334000 | 1.617886000 | 2.193244000 |
| H | -1.739049000 | 1.799552000 | 2.455841000 |
| H | -3.393600000 | 1.937267000 | 3.055468000 |
| C | -3.124578000 | 2.464316000 | 0.979121000 |
| C | -3.742710000 | 3.721731000 | 1.102520000 |
| H | -4.040166000 | 4.086146000 | 2.081314000 |
| C | -3.972198000 | 4.493188000 | -0.051623000 |
| H | -4.453344000 | 5.464073000 | 0.022785000 |
| C | -3.579502000 | 3.981009000 | -1.302932000 |
| H | -3.745282000 | 4.539302000 | -2.218452000 |
| C | -2.979555000 | 2.712851000 | -1.353906000 |

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| H | -2.679295000 | 2.260812000 | -2.291689000 |
| C | -0.668174000 | -3.108227000 | -0.040495000 |
| H | 0.142473000 | -2.466880000 | 0.281841000 |
| C | -0.515149000 | -4.498828000 | -0.136177000 |
| H | 0.434989000 | -4.959271000 | 0.113401000 |
| C | -1.616740000 | -5.273646000 | -0.545940000 |
| H | -1.537224000 | -6.353906000 | -0.624286000 |
| C | -2.828839000 | -4.626856000 | -0.841697000 |
| H | -3.700158000 | -5.196868000 | -1.150174000 |
| C | -2.909988000 | -3.226376000 | -0.731600000 |
| C | -4.188623000 | -2.490416000 | -1.092278000 |
| H | -4.168469000 | -2.259846000 | -2.165426000 |
| H | -5.052902000 | -3.157139000 | -0.933134000 |
| C | -5.387714000 | -0.358850000 | -0.990554000 |
| H | -5.105460000 | -0.131147000 | -2.022740000 |
| H | -5.487241000 | 0.590416000 | -0.459993000 |
| H | -6.370888000 | -0.857873000 | -1.001351000 |
| C | 0.673687000 | 0.267848000 | -2.534417000 |
| Mn | 2.002829000 | 0.289986000 | 0.302187000 |
| O | 2.290766000 | 0.517513000 | 2.475207000 |
| H | 1.515304000 | 0.073583000 | 3.003201000 |
| H | 2.747067000 | 1.211837000 | 2.980731000 |
| O | -0.319866000 | -0.200678000 | 1.227174000 |
| C | -0.621430000 | -0.456373000 | 2.476492000 |
| O | 0.239283000 | -0.540386000 | 3.419063000 |
| N | 4.331633000 | 1.214855000 | 0.251454000 |
| C | 4.720185000 | 1.265588000 | -1.193381000 |
| H | 4.165712000 | 2.083443000 | -1.667434000 |
| H | 5.793393000 | 1.498153000 | -1.304066000 |
| C | 4.417552000 | -0.054723000 | -1.910363000 |
| N | 2.962910000 | -0.402081000 | -1.839711000 |
| N | 2.689256000 | -1.895957000 | 0.545686000 |
| C | 3.061691000 | -2.558851000 | -0.589197000 |
| C | 2.749708000 | -1.879885000 | -1.910661000 |
| C | 2.164119000 | 0.299472000 | -2.879493000 |
| H | 2.474363000 | 1.349582000 | -2.931237000 |
| H | 2.297467000 | -0.129761000 | -3.883178000 |
| H | 1.695684000 | -2.061271000 | -2.154906000 |
| H | 3.347354000 | -2.333075000 | -2.716630000 |
| C | 3.662371000 | -3.829075000 | -0.536422000 |
| H | 3.963638000 | -4.324677000 | -1.454610000 |
| C | 3.872579000 | -4.441486000 | 0.713641000 |
| H | 4.340808000 | -5.419568000 | 0.775510000 |
| C | 3.477505000 | -3.760198000 | 1.879890000 |
| H | 3.623976000 | -4.192554000 | 2.864045000 |
| C | 2.895904000 | -2.488020000 | 1.754808000 |
| H | 2.596499000 | -1.919701000 | 2.626420000 |
| N | 1.868916000 | 2.555971000 | 0.075926000 |
| C | 0.709705000 | 3.174281000 | -0.280270000 |
| H | -0.124393000 | 2.521455000 | -0.505787000 |
| C | 0.595733000 | 4.569621000 | -0.359684000 |
| H | -0.347045000 | 5.021781000 | -0.648972000 |

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| C | 1.725583000 | 5.357760000 | -0.069615000 |
| H | 1.676932000 | 6.441018000 | -0.129646000 |
| C | 2.924728000 | 4.719105000 | 0.290684000 |
| H | 3.816394000 | 5.298404000 | 0.511465000 |
| C | 2.965210000 | 3.314293000 | 0.362566000 |
| C | 4.226290000 | 2.592570000 | 0.809105000 |
| C | 5.304019000 | 0.410967000 | 1.053300000 |
| H | 4.926835000 | 0.289346000 | 2.072055000 |
| H | 5.418793000 | -0.586095000 | 0.622531000 |
| H | 6.296877000 | 0.889143000 | 1.088676000 |
| H | 4.226546000 | 2.517790000 | 1.904979000 |
| H | 5.108274000 | 3.201574000 | 0.548159000 |
| H | 4.984388000 | -0.868144000 | -1.447346000 |
| H | 4.756110000 | 0.012007000 | -2.956825000 |

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| Mn | 1.817262000 | 0.246799000 | -0.175462000 |
| O | -0.142481000 | -0.006756000 | 0.892034000 |
| N | 2.823607000 | 0.517893000 | -2.354902000 |
| N | 4.013977000 | 0.759962000 | 0.403565000 |
| N | 1.741473000 | 2.435752000 | 0.199456000 |
| N | 1.635651000 | -1.721233000 | -1.200620000 |
| C | 4.260865000 | 0.203398000 | -2.037821000 |
| H | 4.326987000 | -0.866753000 | -1.811205000 |
| H | 4.898286000 | 0.391988000 | -2.918816000 |
| C | 4.798499000 | 1.016474000 | -0.845684000 |
| H | 4.748774000 | 2.087203000 | -1.070416000 |
| H | 5.862247000 | 0.772432000 | -0.701510000 |
| C | 4.483977000 | -0.429751000 | 1.184759000 |
| H | 4.773125000 | -1.224274000 | 0.485773000 |
| H | 5.361618000 | -0.200886000 | 1.805152000 |
| C | 3.912198000 | 1.963940000 | 1.281246000 |
| H | 3.646022000 | 1.619778000 | 2.288703000 |
| H | 4.879332000 | 2.482584000 | 1.367917000 |
| C | 2.837778000 | 2.944944000 | 0.832813000 |
| C | 2.926973000 | 4.315025000 | 1.141559000 |
| H | 3.810446000 | 4.699928000 | 1.642256000 |
| C | 1.860618000 | 5.168913000 | 0.810535000 |
| H | 1.911420000 | 6.227692000 | 1.046860000 |
| C | 0.724899000 | 4.631879000 | 0.173635000 |
| H | -0.122854000 | 5.255254000 | -0.090006000 |
| C | 0.707368000 | 3.260702000 | -0.116623000 |
| H | -0.149657000 | 2.802498000 | -0.600168000 |
| C | 1.316095000 | -2.841664000 | -0.494479000 |
| H | 1.131593000 | -2.700915000 | 0.564510000 |
| C | 1.258374000 | -4.105951000 | -1.098223000 |
| H | 0.999899000 | -4.976446000 | -0.504922000 |
| C | 1.554631000 | -4.215134000 | -2.470405000 |
| H | 1.526158000 | -5.181503000 | -2.965277000 |
| C | 1.901887000 | -3.058004000 | -3.191454000 |
| H | 2.148401000 | -3.114003000 | -4.247653000 |
| C | 1.928449000 | -1.820373000 | -2.526166000 |

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| C | 2.235256000 | -0.523403000 | -3.255857000 |
| H | 1.298690000 | -0.118489000 | -3.662632000 |
| H | 2.893184000 | -0.725592000 | -4.117011000 |
| C | 2.686182000 | 1.864641000 | -2.989908000 |
| H | 1.628726000 | 2.078314000 | -3.175273000 |
| H | 3.073719000 | 2.640725000 | -2.327757000 |
| H | 3.228210000 | 1.917222000 | -3.948293000 |
| C | 3.354850000 | -0.996651000 | 2.096420000 |
| O | 3.651940000 | -1.685260000 | 3.091896000 |
| O | 2.125574000 | -0.699619000 | 1.668410000 |
| H | 0.311110000 | -0.394736000 | 1.686194000 |
| H | -1.113578000 | -0.050478000 | 0.911145000 |

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| Mn | 1.942616000 | 0.316297000 | -0.244900000 |
| O | 0.373862000 | 0.410315000 | -0.773289000 |
| N | 2.735178000 | 0.537154000 | -2.270656000 |
| N | 4.071368000 | 0.711720000 | 0.268250000 |
| N | 1.863955000 | 2.281512000 | 0.333167000 |
| N | 1.954609000 | -1.658788000 | -0.916817000 |
| C | 4.211606000 | 0.230201000 | -2.180116000 |
| H | 4.322618000 | -0.852181000 | -2.063038000 |
| H | 4.720415000 | 0.516146000 | -3.112735000 |
| C | 4.852208000 | 0.955440000 | -0.992243000 |
| H | 4.861137000 | 2.034983000 | -1.174353000 |
| H | 5.898598000 | 0.637843000 | -0.878664000 |
| C | 4.421960000 | -0.526930000 | 1.029456000 |
| H | 4.567917000 | -1.362110000 | 0.335495000 |
| H | 5.333577000 | -0.418492000 | 1.630329000 |
| C | 4.116638000 | 1.902745000 | 1.185226000 |
| H | 4.037029000 | 1.551299000 | 2.220958000 |
| H | 5.077491000 | 2.427237000 | 1.101582000 |
| C | 2.957076000 | 2.837808000 | 0.925764000 |
| C | 2.950475000 | 4.173945000 | 1.353429000 |
| H | 3.834161000 | 4.599528000 | 1.819222000 |
| C | 1.780277000 | 4.937770000 | 1.192102000 |
| H | 1.751045000 | 5.971377000 | 1.523998000 |
| C | 0.646610000 | 4.341743000 | 0.607500000 |
| H | -0.279819000 | 4.891602000 | 0.483066000 |
| C | 0.721834000 | 3.008651000 | 0.184750000 |
| H | -0.110941000 | 2.477231000 | -0.262361000 |
| C | 1.722494000 | -2.737719000 | -0.119960000 |
| H | 1.661026000 | -2.558045000 | 0.945246000 |
| C | 1.524475000 | -4.017018000 | -0.658048000 |
| H | 1.339965000 | -4.851683000 | 0.009186000 |
| C | 1.559057000 | -4.185388000 | -2.053658000 |
| H | 1.412258000 | -5.166197000 | -2.495789000 |
| C | 1.767928000 | -3.059685000 | -2.871943000 |
| H | 1.774770000 | -3.150010000 | -3.953781000 |
| C | 1.944743000 | -1.805028000 | -2.274304000 |
| C | 2.026448000 | -0.521113000 | -3.066232000 |
| H | 1.004963000 | -0.163622000 | -3.240695000 |

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| H | 2.513970000 | -0.677749000 | -4.039119000 |
| C | 2.469806000 | 1.883034000 | -2.874191000 |
| H | 1.399061000 | 2.090904000 | -2.810296000 |
| H | 3.008845000 | 2.659513000 | -2.326999000 |
| H | 2.784691000 | 1.908039000 | -3.927511000 |
| C | 3.222980000 | -0.855519000 | 1.953756000 |
| O | 3.341909000 | -1.545429000 | 2.974213000 |
| O | 2.036877000 | -0.339004000 | 1.518034000 |

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| Mn | 1.997937000 | 0.303869000 | -0.256376000 |
| O | 0.381693000 | 0.404157000 | -0.780745000 |
| N | 2.708337000 | 0.547308000 | -2.223813000 |
| N | 4.060131000 | 0.687870000 | 0.267871000 |
| N | 1.872938000 | 2.265972000 | 0.297338000 |
| N | 1.971026000 | -1.653611000 | -0.912606000 |
| C | 4.202627000 | 0.233883000 | -2.171692000 |
| H | 4.315813000 | -0.850062000 | -2.085289000 |
| H | 4.666985000 | 0.546061000 | -3.115976000 |
| C | 4.858719000 | 0.944920000 | -0.992570000 |
| H | 4.884505000 | 2.025703000 | -1.157293000 |
| H | 5.895660000 | 0.608360000 | -0.870294000 |
| C | 4.455641000 | -0.538166000 | 1.044918000 |
| H | 4.636658000 | -1.379369000 | 0.367004000 |
| H | 5.359463000 | -0.380715000 | 1.644113000 |
| C | 4.107321000 | 1.888756000 | 1.193684000 |
| H | 4.017500000 | 1.540399000 | 2.229473000 |
| H | 5.077651000 | 2.391867000 | 1.110059000 |
| C | 2.960829000 | 2.824996000 | 0.910460000 |
| C | 2.944801000 | 4.157625000 | 1.340683000 |
| H | 3.819571000 | 4.583411000 | 1.822790000 |
| C | 1.775721000 | 4.922638000 | 1.164944000 |
| H | 1.740280000 | 5.954444000 | 1.501270000 |
| C | 0.650636000 | 4.327090000 | 0.562120000 |
| H | -0.275270000 | 4.875553000 | 0.427702000 |
| C | 0.729236000 | 2.996356000 | 0.136740000 |
| H | -0.116369000 | 2.489804000 | -0.312932000 |
| C | 1.748879000 | -2.735624000 | -0.108563000 |
| H | 1.700707000 | -2.570349000 | 0.959144000 |
| C | 1.539888000 | -4.010669000 | -0.649629000 |
| H | 1.366426000 | -4.847025000 | 0.018682000 |
| C | 1.543941000 | -4.174972000 | -2.047094000 |
| H | 1.384176000 | -5.154223000 | -2.488009000 |
| C | 1.736591000 | -3.047051000 | -2.869689000 |
| H | 1.718473000 | -3.138937000 | -3.951243000 |
| C | 1.929268000 | -1.795599000 | -2.276554000 |
| C | 2.005885000 | -0.509345000 | -3.057630000 |
| H | 0.992171000 | -0.150908000 | -3.269248000 |
| H | 2.530660000 | -0.637549000 | -4.012501000 |
| C | 2.452218000 | 1.912014000 | -2.825873000 |
| H | 1.381295000 | 2.123788000 | -2.807973000 |
| H | 2.979305000 | 2.683592000 | -2.263708000 |

| | | | |
|---|-------------|--------------|--------------|
| H | 2.803159000 | 1.924281000 | -3.865235000 |
| C | 3.260035000 | -0.873038000 | 1.956076000 |
| O | 3.293160000 | -1.538733000 | 2.979310000 |
| O | 2.063495000 | -0.336448000 | 1.451187000 |

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|----|--------------|--------------|--------------|
| Mn | 2.162739000 | 0.276530000 | -0.238822000 |
| O | 0.391678000 | 0.257005000 | -0.686792000 |
| N | 2.811544000 | 0.538388000 | -2.232918000 |
| N | 4.161335000 | 0.723347000 | 0.254376000 |
| N | 1.877268000 | 2.185525000 | 0.288194000 |
| N | 1.871369000 | -1.599646000 | -0.913862000 |
| C | 4.304147000 | 0.231229000 | -2.184223000 |
| H | 4.423128000 | -0.851539000 | -2.071093000 |
| H | 4.774838000 | 0.520815000 | -3.132681000 |
| C | 4.952379000 | 0.977403000 | -1.017914000 |
| H | 4.957328000 | 2.055026000 | -1.201869000 |
| H | 5.994826000 | 0.663042000 | -0.887825000 |
| C | 4.619201000 | -0.479493000 | 1.043425000 |
| H | 4.859549000 | -1.306576000 | 0.365594000 |
| H | 5.509945000 | -0.263746000 | 1.643942000 |
| C | 4.148082000 | 1.943593000 | 1.162782000 |
| H | 4.105392000 | 1.602750000 | 2.203981000 |
| H | 5.081236000 | 2.506533000 | 1.047370000 |
| C | 2.935969000 | 2.805433000 | 0.897799000 |
| C | 2.835066000 | 4.131259000 | 1.336541000 |
| H | 3.683429000 | 4.612405000 | 1.813800000 |
| C | 1.616295000 | 4.818245000 | 1.174697000 |
| H | 1.516567000 | 5.843049000 | 1.519535000 |
| C | 0.526257000 | 4.158317000 | 0.572884000 |
| H | -0.432492000 | 4.649633000 | 0.448335000 |
| C | 0.687145000 | 2.840682000 | 0.133865000 |
| H | -0.129330000 | 2.292808000 | -0.325575000 |
| C | 1.519947000 | -2.642756000 | -0.094796000 |
| H | 1.444214000 | -2.433037000 | 0.964721000 |
| C | 1.247139000 | -3.906901000 | -0.624654000 |
| H | 0.975244000 | -4.715520000 | 0.044892000 |
| C | 1.323140000 | -4.101075000 | -2.019185000 |
| H | 1.116561000 | -5.076457000 | -2.449775000 |
| C | 1.648004000 | -3.011415000 | -2.854896000 |
| H | 1.685691000 | -3.131431000 | -3.933112000 |
| C | 1.895016000 | -1.762722000 | -2.280255000 |
| C | 2.094624000 | -0.496656000 | -3.074392000 |
| H | 1.112168000 | -0.089617000 | -3.338850000 |
| H | 2.646254000 | -0.679626000 | -4.004972000 |
| C | 2.547501000 | 1.908255000 | -2.815682000 |
| H | 1.478153000 | 2.122014000 | -2.762535000 |
| H | 3.090823000 | 2.675072000 | -2.261919000 |
| H | 2.867152000 | 1.934868000 | -3.865074000 |
| C | 3.442194000 | -0.893047000 | 1.948345000 |
| O | 3.522812000 | -1.606310000 | 2.938685000 |
| O | 2.228243000 | -0.383330000 | 1.482941000 |

³4.H₂O

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|----|--------------|--------------|--------------|
| Mn | 2.022732000 | 0.332356000 | -0.219463000 |
| O | 0.278860000 | 0.429961000 | -0.673659000 |
| N | 2.685017000 | 0.592670000 | -2.195518000 |
| N | 4.062198000 | 0.675636000 | 0.295449000 |
| N | 1.920208000 | 2.301470000 | 0.280239000 |
| N | 2.017735000 | -1.617923000 | -0.892665000 |
| C | 4.169662000 | 0.232805000 | -2.168927000 |
| H | 4.253316000 | -0.855297000 | -2.115349000 |
| H | 4.640375000 | 0.557907000 | -3.105764000 |
| C | 4.864752000 | 0.888804000 | -0.975568000 |
| H | 4.952656000 | 1.967723000 | -1.131071000 |
| H | 5.880952000 | 0.492168000 | -0.860244000 |
| C | 4.422263000 | -0.537326000 | 1.113626000 |
| H | 4.570839000 | -1.404399000 | 0.461720000 |
| H | 5.336616000 | -0.388435000 | 1.698855000 |
| C | 4.140893000 | 1.899619000 | 1.189991000 |
| H | 4.039378000 | 1.581335000 | 2.234158000 |
| H | 5.124671000 | 2.373865000 | 1.096658000 |
| C | 3.020264000 | 2.856189000 | 0.875545000 |
| C | 3.039170000 | 4.204593000 | 1.254284000 |
| H | 3.922881000 | 4.624799000 | 1.724773000 |
| C | 1.893814000 | 4.994269000 | 1.038729000 |
| H | 1.885852000 | 6.039693000 | 1.332041000 |
| C | 0.757095000 | 4.406940000 | 0.449292000 |
| H | -0.149546000 | 4.977850000 | 0.281013000 |
| C | 0.800331000 | 3.058154000 | 0.079378000 |
| H | -0.051165000 | 2.555321000 | -0.363601000 |
| C | 1.896366000 | -2.729397000 | -0.110855000 |
| H | 1.933854000 | -2.604659000 | 0.961141000 |
| C | 1.687366000 | -3.997442000 | -0.666249000 |
| H | 1.598979000 | -4.855736000 | -0.009453000 |
| C | 1.578747000 | -4.127046000 | -2.062316000 |
| H | 1.410683000 | -5.098941000 | -2.516066000 |
| C | 1.680794000 | -2.973883000 | -2.864416000 |
| H | 1.589291000 | -3.037272000 | -3.944181000 |
| C | 1.889575000 | -1.734269000 | -2.252777000 |
| C | 1.923488000 | -0.433134000 | -3.010217000 |
| H | 0.901344000 | -0.060644000 | -3.142739000 |
| H | 2.382109000 | -0.545719000 | -4.000644000 |
| C | 2.462080000 | 1.961006000 | -2.793608000 |
| H | 1.402892000 | 2.218817000 | -2.728616000 |
| H | 3.047468000 | 2.712599000 | -2.262023000 |
| H | 2.762790000 | 1.957754000 | -3.848826000 |
| C | 3.226208000 | -0.805623000 | 2.052970000 |
| O | 3.273974000 | -1.428048000 | 3.105852000 |
| O | 2.038898000 | -0.275990000 | 1.541851000 |
| O | -0.386738000 | -1.035892000 | 0.825695000 |
| H | -1.313778000 | -0.712449000 | 0.818404000 |
| H | 0.141881000 | -0.715937000 | 1.600029000 |

⁵4.H²O

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|----|--------------|--------------|--------------|
| Mn | 2.027078000 | 0.331938000 | -0.218572000 |
| O | 0.346745000 | 0.383153000 | -0.560239000 |
| N | 2.691295000 | 0.596151000 | -2.195080000 |
| N | 4.086604000 | 0.686684000 | 0.290937000 |
| N | 1.938481000 | 2.307601000 | 0.286848000 |
| N | 2.026447000 | -1.617444000 | -0.896352000 |
| C | 4.177270000 | 0.238013000 | -2.169544000 |
| H | 4.261394000 | -0.849812000 | -2.111006000 |
| H | 4.642448000 | 0.558893000 | -3.110627000 |
| C | 4.879814000 | 0.898768000 | -0.982773000 |
| H | 4.965711000 | 1.977311000 | -1.142539000 |
| H | 5.897859000 | 0.503833000 | -0.877131000 |
| C | 4.444407000 | -0.528167000 | 1.104230000 |
| H | 4.596939000 | -1.392339000 | 0.448990000 |
| H | 5.355354000 | -0.383690000 | 1.695911000 |
| C | 4.165375000 | 1.908689000 | 1.184560000 |
| H | 4.069055000 | 1.589893000 | 2.229261000 |
| H | 5.146410000 | 2.388426000 | 1.089069000 |
| C | 3.039849000 | 2.862799000 | 0.876771000 |
| C | 3.056922000 | 4.211731000 | 1.255558000 |
| H | 3.942041000 | 4.634188000 | 1.721343000 |
| C | 1.908660000 | 4.998378000 | 1.045728000 |
| H | 1.899580000 | 6.043800000 | 1.339009000 |
| C | 0.769835000 | 4.408522000 | 0.462157000 |
| H | -0.138999000 | 4.977359000 | 0.298860000 |
| C | 0.815844000 | 3.059996000 | 0.092381000 |
| H | -0.037270000 | 2.553789000 | -0.343907000 |
| C | 1.887623000 | -2.723268000 | -0.110611000 |
| H | 1.918046000 | -2.592456000 | 0.960859000 |
| C | 1.669478000 | -3.990803000 | -0.664496000 |
| H | 1.568901000 | -4.846464000 | -0.006044000 |
| C | 1.567065000 | -4.122472000 | -2.060669000 |
| H | 1.392994000 | -5.094012000 | -2.512963000 |
| C | 1.680283000 | -2.971989000 | -2.865702000 |
| H | 1.590179000 | -3.037528000 | -3.945470000 |
| C | 1.897461000 | -1.732809000 | -2.256331000 |
| C | 1.937003000 | -0.431726000 | -3.014926000 |
| H | 0.916484000 | -0.059597000 | -3.159815000 |
| H | 2.404976000 | -0.545330000 | -4.000891000 |
| C | 2.470859000 | 1.965235000 | -2.793310000 |
| H | 1.411015000 | 2.222107000 | -2.738455000 |
| H | 3.049176000 | 2.716600000 | -2.254044000 |
| H | 2.783325000 | 1.964058000 | -3.845132000 |
| C | 3.244777000 | -0.804570000 | 2.036489000 |
| O | 3.292033000 | -1.429459000 | 3.088706000 |
| O | 2.051079000 | -0.284244000 | 1.529103000 |
| O | -0.522894000 | -1.077559000 | 0.814468000 |
| H | -1.459357000 | -0.794569000 | 0.739165000 |
| H | -0.095563000 | -0.758769000 | 1.643101000 |

³TS4.H₂O-5

| | | | |
|----|--------------|--------------|--------------|
| Mn | -0.023707000 | -0.026538000 | 0.254404000 |
| O | 0.241965000 | -0.475881000 | 1.995913000 |
| N | 0.317479000 | -1.860711000 | -0.685869000 |
| N | -0.621722000 | 0.676823000 | -1.604985000 |
| N | -2.011502000 | -0.237934000 | 0.495502000 |
| N | 2.059362000 | -0.034965000 | 0.108714000 |
| C | 0.574148000 | -1.475088000 | -2.145205000 |
| H | 1.594447000 | -1.092689000 | -2.218119000 |
| H | 0.509375000 | -2.370226000 | -2.777555000 |
| C | -0.425998000 | -0.419955000 | -2.637772000 |
| H | -1.402342000 | -0.880264000 | -2.814341000 |
| H | -0.088130000 | 0.000646000 | -3.592769000 |
| C | 0.213654000 | 1.928248000 | -1.765698000 |
| H | 1.243344000 | 1.658886000 | -2.022528000 |
| H | -0.171927000 | 2.583394000 | -2.554907000 |
| C | -2.084194000 | 1.091291000 | -1.534596000 |
| H | -2.137836000 | 2.152162000 | -1.262255000 |
| H | -2.553914000 | 0.996120000 | -2.520051000 |
| C | -2.808482000 | 0.293805000 | -0.480675000 |
| C | -4.202877000 | 0.175995000 | -0.425547000 |
| H | -4.817815000 | 0.603387000 | -1.211676000 |
| C | -4.790740000 | -0.483188000 | 0.671019000 |
| H | -5.870222000 | -0.579976000 | 0.736976000 |
| C | -3.962342000 | -1.004426000 | 1.684624000 |
| H | -4.380205000 | -1.503809000 | 2.551872000 |
| C | -2.574717000 | -0.868512000 | 1.568553000 |
| H | -1.894364000 | -1.237756000 | 2.325325000 |
| C | 2.891225000 | 1.030538000 | 0.303005000 |
| H | 2.446852000 | 2.013335000 | 0.380154000 |
| C | 4.276988000 | 0.874276000 | 0.427864000 |
| H | 4.901142000 | 1.748740000 | 0.576647000 |
| C | 4.829946000 | -0.418842000 | 0.364119000 |
| H | 5.901052000 | -0.567690000 | 0.460376000 |
| C | 3.970637000 | -1.517555000 | 0.176310000 |
| H | 4.363567000 | -2.528275000 | 0.126617000 |
| C | 2.593050000 | -1.296405000 | 0.058980000 |
| C | 1.589673000 | -2.414897000 | -0.084954000 |
| H | 1.344212000 | -2.827960000 | 0.901056000 |
| H | 1.984693000 | -3.232445000 | -0.702381000 |
| C | -0.770125000 | -2.902056000 | -0.588235000 |
| H | -0.982324000 | -3.113992000 | 0.462089000 |
| H | -1.682764000 | -2.545852000 | -1.069046000 |
| H | -0.449752000 | -3.828926000 | -1.080840000 |
| C | 0.213802000 | 2.694035000 | -0.415194000 |
| O | 0.401839000 | 3.897865000 | -0.296239000 |
| O | 0.028911000 | 1.831929000 | 0.662946000 |
| O | -0.108496000 | 0.896189000 | 2.864894000 |
| H | 0.518994000 | 0.885600000 | 3.623439000 |
| H | -0.005328000 | 1.642934000 | 2.112127000 |

⁵TS4.H₂O-5

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|----|--------------|--------------|-------------|
| Mn | -0.029065313 | -0.065322250 | 0.293501019 |
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|---|--------------|--------------|--------------|
| O | 0.225199743 | -0.495372173 | 1.960236255 |
| N | 0.312416398 | -1.901084956 | -0.647586930 |
| N | -0.661367656 | 0.678366132 | -1.672496524 |
| N | -2.084221634 | -0.261778403 | 0.545590737 |
| N | 2.089505530 | -0.082333723 | 0.163151372 |
| C | 0.568789687 | -1.513872250 | -2.106107981 |
| H | 1.589088687 | -1.131473250 | -2.179021981 |
| H | 0.504016687 | -2.409010250 | -2.738457981 |
| C | -0.431356313 | -0.458739250 | -2.598674981 |
| H | -1.407700313 | -0.919048250 | -2.775243981 |
| H | -0.093488313 | -0.038138250 | -3.553671981 |
| C | 0.208295687 | 1.889463750 | -1.726600981 |
| H | 1.237985687 | 1.620101750 | -1.983430981 |
| H | -0.177285313 | 2.544609750 | -2.515809981 |
| C | -2.089552313 | 1.052506750 | -1.495498981 |
| H | -2.143194313 | 2.113377750 | -1.223157981 |
| H | -2.559272313 | 0.957335750 | -2.480953981 |
| C | -2.850696556 | 0.278249191 | -0.450266387 |
| C | -4.248024846 | 0.189169995 | -0.422083833 |
| H | -4.838424401 | 0.622692204 | -1.223519001 |
| C | -4.870818602 | -0.449244628 | 0.667465080 |
| H | -5.953146273 | -0.523604522 | 0.712598781 |
| C | -4.073464750 | -0.979113783 | 1.701289488 |
| H | -4.518524393 | -1.463030797 | 2.563761631 |
| C | -2.681327670 | -0.872280913 | 1.611906481 |
| H | -2.023770848 | -1.249227722 | 2.384858825 |
| C | 2.936834471 | 0.969240682 | 0.366293256 |
| H | 2.507208557 | 1.958228827 | 0.447738314 |
| C | 4.319643482 | 0.791178354 | 0.494666627 |
| H | 4.956532579 | 1.655164333 | 0.650526789 |
| C | 4.853077853 | -0.509820377 | 0.425166909 |
| H | 5.921474578 | -0.675513464 | 0.523977025 |
| C | 3.977779897 | -1.594219848 | 0.228226032 |
| H | 4.355454266 | -2.610502337 | 0.173909628 |
| C | 2.604108012 | -1.351446044 | 0.107785072 |
| C | 1.584314687 | -2.453681250 | -0.045856981 |
| H | 1.338853687 | -2.866744250 | 0.940153019 |
| H | 1.979334687 | -3.271229250 | -0.663283981 |
| C | -0.775187602 | -2.942429956 | -0.549952930 |
| H | -0.987386602 | -3.154365956 | 0.500371070 |
| H | -1.687826602 | -2.586225956 | -1.030763930 |
| H | -0.454814602 | -3.869299956 | -1.042557930 |
| C | 0.208443687 | 2.655250750 | -0.376096981 |
| O | 0.396480687 | 3.859080750 | -0.257141981 |
| O | 0.027600299 | 1.936106339 | 0.733469896 |
| O | -0.104448388 | 1.039150589 | 2.896320877 |
| H | 0.523041612 | 1.028561589 | 3.654865877 |
| H | -0.006638701 | 1.747111339 | 2.182650896 |

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|----|-------------|-------------|--------------|
| Mn | 1.854436000 | 0.400260000 | -0.295002000 |
| O | 0.080110000 | 0.509990000 | -0.832817000 |

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|---|--------------|--------------|--------------|
| N | 2.746530000 | 0.559179000 | -2.367843000 |
| N | 3.919618000 | 0.684179000 | 0.314173000 |
| N | 1.777142000 | 2.365720000 | 0.328588000 |
| N | 1.848449000 | -1.629397000 | -0.960339000 |
| C | 4.210205000 | 0.258270000 | -2.166190000 |
| H | 4.331077000 | -0.824548000 | -2.057925000 |
| H | 4.794931000 | 0.562095000 | -3.046425000 |
| C | 4.744885000 | 0.988716000 | -0.930379000 |
| H | 4.701548000 | 2.070358000 | -1.086586000 |
| H | 5.796608000 | 0.726122000 | -0.755862000 |
| C | 4.392856000 | -0.553556000 | 1.024935000 |
| H | 4.491190000 | -1.377976000 | 0.310292000 |
| H | 5.373789000 | -0.404918000 | 1.495169000 |
| C | 3.979598000 | 1.869521000 | 1.266658000 |
| H | 3.842131000 | 1.508074000 | 2.291955000 |
| H | 4.972012000 | 2.334614000 | 1.224589000 |
| C | 2.886307000 | 2.866251000 | 0.958639000 |
| C | 2.947826000 | 4.206068000 | 1.361488000 |
| H | 3.836419000 | 4.588601000 | 1.854427000 |
| C | 1.837721000 | 5.043100000 | 1.131673000 |
| H | 1.863987000 | 6.083191000 | 1.442438000 |
| C | 0.696214000 | 4.514621000 | 0.499286000 |
| H | -0.179788000 | 5.126388000 | 0.313791000 |
| C | 0.698445000 | 3.171113000 | 0.103504000 |
| H | -0.149517000 | 2.709510000 | -0.388358000 |
| C | 1.599577000 | -2.723798000 | -0.179900000 |
| H | 1.521957000 | -2.565956000 | 0.886962000 |
| C | 1.430622000 | -4.003889000 | -0.719267000 |
| H | 1.236088000 | -4.843492000 | -0.060747000 |
| C | 1.517645000 | -4.170584000 | -2.115126000 |
| H | 1.395021000 | -5.151643000 | -2.563760000 |
| C | 1.761744000 | -3.043581000 | -2.919575000 |
| H | 1.826066000 | -3.137418000 | -3.999330000 |
| C | 1.911563000 | -1.783383000 | -2.320220000 |
| C | 2.075937000 | -0.527761000 | -3.153050000 |
| H | 1.082465000 | -0.165462000 | -3.445841000 |
| H | 2.628790000 | -0.749869000 | -4.076883000 |
| C | 2.530293000 | 1.888519000 | -3.036402000 |
| H | 1.459824000 | 2.110284000 | -3.070615000 |
| H | 3.030703000 | 2.683533000 | -2.478217000 |
| H | 2.923615000 | 1.881433000 | -4.062333000 |
| C | 3.408737000 | -0.975785000 | 2.112829000 |
| O | 3.632768000 | -1.688368000 | 3.075563000 |
| O | 2.121217000 | -0.432485000 | 1.842431000 |
| H | 1.449547000 | -0.614886000 | 2.541443000 |
| O | -0.618207000 | -0.033978000 | 0.372603000 |
| H | -1.344187000 | -0.575832000 | -0.026416000 |

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|----|-------------|-------------|--------------|
| Mn | 1.995869000 | 0.352208000 | -0.312287000 |
| O | 0.201838000 | 0.334505000 | -0.703727000 |
| N | 2.695288000 | 0.588519000 | -2.230769000 |

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|---------------|--------------|--------------|--------------|
| N | 3.988235000 | 0.659753000 | 0.327880000 |
| N | 1.856148000 | 2.297788000 | 0.240994000 |
| N | 1.995948000 | -1.628677000 | -0.963641000 |
| C | 4.176231000 | 0.226807000 | -2.144964000 |
| H | 4.256425000 | -0.862070000 | -2.097208000 |
| H | 4.689528000 | 0.557206000 | -3.057441000 |
| C | 4.831927000 | 0.870538000 | -0.918795000 |
| H | 4.925216000 | 1.950112000 | -1.064682000 |
| H | 5.845246000 | 0.473520000 | -0.778235000 |
| C | 4.351203000 | -0.546634000 | 1.147467000 |
| H | 4.499523000 | -1.414238000 | 0.494905000 |
| H | 5.272060000 | -0.402485000 | 1.725803000 |
| C | 4.046615000 | 1.890284000 | 1.218660000 |
| H | 3.921570000 | 1.578741000 | 2.262895000 |
| H | 5.033649000 | 2.362823000 | 1.150593000 |
| C | 2.935393000 | 2.851231000 | 0.872343000 |
| C | 2.949173000 | 4.198946000 | 1.252987000 |
| H | 3.819194000 | 4.617941000 | 1.749548000 |
| C | 1.813929000 | 4.993395000 | 0.999499000 |
| H | 1.801085000 | 6.039316000 | 1.290636000 |
| C | 0.696229000 | 4.410040000 | 0.372986000 |
| H | -0.201550000 | 4.984991000 | 0.173835000 |
| C | 0.749183000 | 3.060303000 | 0.003043000 |
| H | -0.081819000 | 2.557322000 | -0.475885000 |
| C | 1.841658000 | -2.754033000 | -0.206831000 |
| H | 1.885562000 | -2.653980000 | 0.868170000 |
| C | 1.606480000 | -4.011408000 | -0.775658000 |
| H | 1.490512000 | -4.876696000 | -0.132195000 |
| C | 1.516261000 | -4.122447000 | -2.175611000 |
| H | 1.333516000 | -5.084632000 | -2.644005000 |
| C | 1.660808000 | -2.962470000 | -2.958375000 |
| H | 1.587411000 | -3.009837000 | -4.040407000 |
| C | 1.889910000 | -1.734307000 | -2.326173000 |
| C | 1.970796000 | -0.431100000 | -3.080501000 |
| H | 0.958495000 | -0.051622000 | -3.262031000 |
| H | 2.469662000 | -0.552111000 | -4.050849000 |
| C | 2.506257000 | 1.959082000 | -2.834157000 |
| H | 1.446303000 | 2.222214000 | -2.814718000 |
| H | 3.067072000 | 2.705597000 | -2.269734000 |
| H | 2.855075000 | 1.962336000 | -3.874545000 |
| C | 3.213261000 | -0.868548000 | 2.122040000 |
| O | 3.261586000 | -1.497518000 | 3.160420000 |
| O | 1.982868000 | -0.342180000 | 1.603720000 |
| H | 1.146677000 | -0.550118000 | 2.086703000 |
| O | -0.465149000 | -0.291023000 | 0.492175000 |
| H | -1.411843000 | -0.326241000 | 0.214149000 |
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| Mn | 1.917911000 | 0.340252000 | -0.116521000 |
| O | 0.095433000 | 0.467935000 | -0.489146000 |
| N | 2.728193000 | 0.558557000 | -2.291766000 |
| N | 3.995571000 | 0.728902000 | 0.328588000 |

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|---|--------------|--------------|--------------|
| N | 1.844406000 | 2.422840000 | 0.321114000 |
| N | 1.932430000 | -1.702189000 | -0.951073000 |
| C | 4.196464000 | 0.278832000 | -2.136938000 |
| H | 4.325084000 | -0.799273000 | -1.998841000 |
| H | 4.750307000 | 0.562884000 | -3.045847000 |
| C | 4.771075000 | 1.034302000 | -0.931493000 |
| H | 4.716801000 | 2.113978000 | -1.104192000 |
| H | 5.830843000 | 0.778046000 | -0.796267000 |
| C | 4.467564000 | -0.504402000 | 1.055470000 |
| H | 4.663545000 | -1.301435000 | 0.330299000 |
| H | 5.392347000 | -0.316697000 | 1.615213000 |
| C | 4.022293000 | 1.903870000 | 1.279362000 |
| H | 3.814311000 | 1.525279000 | 2.286427000 |
| H | 5.021070000 | 2.359444000 | 1.296898000 |
| C | 2.957626000 | 2.921330000 | 0.932019000 |
| C | 3.043488000 | 4.276229000 | 1.287117000 |
| H | 3.936960000 | 4.658066000 | 1.771448000 |
| C | 1.949560000 | 5.121476000 | 1.022179000 |
| H | 1.992495000 | 6.171945000 | 1.294239000 |
| C | 0.798518000 | 4.590203000 | 0.408734000 |
| H | -0.066866000 | 5.210059000 | 0.200980000 |
| C | 0.781207000 | 3.230499000 | 0.068159000 |
| H | -0.078373000 | 2.754582000 | -0.392240000 |
| C | 1.726085000 | -2.811541000 | -0.188633000 |
| H | 1.684640000 | -2.661041000 | 0.882906000 |
| C | 1.551030000 | -4.078155000 | -0.762691000 |
| H | 1.392096000 | -4.939386000 | -0.122996000 |
| C | 1.581537000 | -4.199545000 | -2.164259000 |
| H | 1.450286000 | -5.168318000 | -2.637264000 |
| C | 1.776554000 | -3.047266000 | -2.947084000 |
| H | 1.791588000 | -3.105844000 | -4.031350000 |
| C | 1.938795000 | -1.808384000 | -2.307483000 |
| C | 2.046556000 | -0.511491000 | -3.085737000 |
| H | 1.032200000 | -0.157590000 | -3.308700000 |
| H | 2.557495000 | -0.681852000 | -4.046319000 |
| C | 2.470742000 | 1.891824000 | -2.918220000 |
| H | 1.395034000 | 2.089790000 | -2.916797000 |
| H | 2.965000000 | 2.684556000 | -2.351876000 |
| H | 2.836039000 | 1.923952000 | -3.956460000 |
| C | 3.344707000 | -0.984617000 | 2.022263000 |
| O | 3.608971000 | -1.776897000 | 2.943810000 |
| O | 2.138166000 | -0.493251000 | 1.706353000 |
| O | -0.683658000 | -0.732575000 | -0.156853000 |
| H | -1.086184000 | -0.502652000 | 0.719164000 |

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|----|-------------|--------------|--------------|
| Mn | 2.027131000 | 0.355615000 | -0.206905000 |
| O | 0.231156000 | 0.522844000 | -0.630180000 |
| N | 2.691098000 | 0.584650000 | -2.208690000 |
| N | 4.078884000 | 0.702029000 | 0.280645000 |
| N | 1.920140000 | 2.325331000 | 0.315863000 |
| N | 1.994624000 | -1.604208000 | -0.848177000 |

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|---|--------------|--------------|--------------|
| C | 4.171599000 | 0.260817000 | -2.175304000 |
| H | 4.275285000 | -0.824476000 | -2.092160000 |
| H | 4.647856000 | 0.570522000 | -3.116713000 |
| C | 4.852675000 | 0.946257000 | -0.988605000 |
| H | 4.888703000 | 2.028196000 | -1.151948000 |
| H | 5.889693000 | 0.596822000 | -0.891783000 |
| C | 4.444651000 | -0.523223000 | 1.061817000 |
| H | 4.574788000 | -1.372490000 | 0.383110000 |
| H | 5.366306000 | -0.399756000 | 1.644075000 |
| C | 4.150466000 | 1.904426000 | 1.191948000 |
| H | 4.049471000 | 1.561428000 | 2.228005000 |
| H | 5.128617000 | 2.395798000 | 1.111480000 |
| C | 3.021468000 | 2.866473000 | 0.909607000 |
| C | 3.049757000 | 4.209049000 | 1.315535000 |
| H | 3.940187000 | 4.616871000 | 1.784360000 |
| C | 1.904773000 | 5.003602000 | 1.126726000 |
| H | 1.901225000 | 6.043398000 | 1.440008000 |
| C | 0.762886000 | 4.429207000 | 0.536867000 |
| H | -0.144903000 | 5.003927000 | 0.388827000 |
| C | 0.804490000 | 3.086557000 | 0.140018000 |
| H | -0.040644000 | 2.576315000 | -0.307810000 |
| C | 1.811401000 | -2.690438000 | -0.048551000 |
| H | 1.790422000 | -2.520072000 | 1.019037000 |
| C | 1.612850000 | -3.972729000 | -0.578104000 |
| H | 1.471359000 | -4.809651000 | 0.097032000 |
| C | 1.593215000 | -4.143794000 | -1.973485000 |
| H | 1.445554000 | -5.127362000 | -2.409192000 |
| C | 1.750615000 | -3.014742000 | -2.796783000 |
| H | 1.713129000 | -3.102069000 | -3.878251000 |
| C | 1.930132000 | -1.759555000 | -2.203426000 |
| C | 1.954773000 | -0.474015000 | -2.991511000 |
| H | 0.921584000 | -0.132011000 | -3.118715000 |
| H | 2.407237000 | -0.609624000 | -3.983695000 |
| C | 2.425588000 | 1.927888000 | -2.823077000 |
| H | 1.359656000 | 2.149971000 | -2.736616000 |
| H | 2.990174000 | 2.703707000 | -2.301770000 |
| H | 2.713069000 | 1.930610000 | -3.883949000 |
| C | 3.251027000 | -0.815478000 | 2.010476000 |
| O | 3.376132000 | -1.504751000 | 3.032495000 |
| O | 2.081538000 | -0.268432000 | 1.582418000 |
| O | -0.558978000 | -0.646915000 | -1.142384000 |
| H | -1.304914000 | -0.671286000 | -0.496863000 |

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|----|-------------|--------------|--------------|
| Mn | 2.017921000 | 0.293981000 | -0.243570000 |
| O | 0.214608000 | 0.276877000 | -0.732455000 |
| N | 2.708685000 | 0.577687000 | -2.228295000 |
| N | 4.071989000 | 0.668831000 | 0.290928000 |
| N | 1.897401000 | 2.267758000 | 0.249916000 |
| N | 2.006904000 | -1.651204000 | -0.944640000 |
| C | 4.202353000 | 0.261919000 | -2.172983000 |
| H | 4.316999000 | -0.823725000 | -2.112110000 |

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|---|--------------|--------------|--------------|
| H | 4.678866000 | 0.595923000 | -3.103804000 |
| C | 4.861811000 | 0.942121000 | -0.971734000 |
| H | 4.893477000 | 2.026085000 | -1.113741000 |
| H | 5.897446000 | 0.596977000 | -0.861892000 |
| C | 4.458251000 | -0.562259000 | 1.062994000 |
| H | 4.648882000 | -1.397305000 | 0.380202000 |
| H | 5.355416000 | -0.408733000 | 1.673550000 |
| C | 4.096167000 | 1.861068000 | 1.227275000 |
| H | 3.967447000 | 1.504778000 | 2.255954000 |
| H | 5.072651000 | 2.357537000 | 1.180413000 |
| C | 2.970997000 | 2.810616000 | 0.904246000 |
| C | 2.971346000 | 4.149345000 | 1.313376000 |
| H | 3.834372000 | 4.558720000 | 1.829572000 |
| C | 1.836490000 | 4.944542000 | 1.064613000 |
| H | 1.812767000 | 5.981779000 | 1.384830000 |
| C | 0.734753000 | 4.374880000 | 0.398803000 |
| H | -0.160981000 | 4.950797000 | 0.193835000 |
| C | 0.793835000 | 3.035188000 | -0.000569000 |
| H | -0.036219000 | 2.562688000 | -0.505554000 |
| C | 1.829644000 | -2.758803000 | -0.163532000 |
| H | 1.812747000 | -2.622928000 | 0.909223000 |
| C | 1.636446000 | -4.025613000 | -0.727962000 |
| H | 1.503124000 | -4.881985000 | -0.075891000 |
| C | 1.610095000 | -4.158061000 | -2.129198000 |
| H | 1.463599000 | -5.130633000 | -2.589137000 |
| C | 1.761663000 | -3.008001000 | -2.928082000 |
| H | 1.725854000 | -3.075042000 | -4.010989000 |
| C | 1.943982000 | -1.766163000 | -2.310140000 |
| C | 1.997909000 | -0.463552000 | -3.067370000 |
| H | 0.977898000 | -0.105357000 | -3.251398000 |
| H | 2.496964000 | -0.574662000 | -4.038276000 |
| C | 2.458659000 | 1.942377000 | -2.826180000 |
| H | 1.392682000 | 2.172787000 | -2.773328000 |
| H | 3.017060000 | 2.706311000 | -2.283837000 |
| H | 2.774195000 | 1.950486000 | -3.877170000 |
| C | 3.252919000 | -0.909465000 | 1.963201000 |
| O | 3.292950000 | -1.603543000 | 2.969999000 |
| O | 2.062249000 | -0.363346000 | 1.472531000 |
| O | -0.690653000 | 0.553358000 | 0.375014000 |
| H | -1.126677000 | -0.319807000 | 0.559063000 |

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|----|--------------|--------------|--------------|
| Mn | 0.019079000 | -0.049829000 | -0.228537000 |
| O | -0.259543000 | -0.340845000 | -2.154578000 |
| N | -0.292332000 | -1.791716000 | 0.820984000 |
| N | 0.668244000 | 0.828351000 | 1.535738000 |
| N | 1.986672000 | -0.280554000 | -0.529904000 |
| N | -2.056367000 | -0.077770000 | -0.143587000 |
| C | -0.544322000 | -1.274210000 | 2.241912000 |
| H | -1.557685000 | -0.868519000 | 2.279248000 |
| H | -0.494362000 | -2.114170000 | 2.946815000 |
| C | 0.484383000 | -0.205320000 | 2.638774000 |

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|---|--------------|--------------|--------------|
| H | 1.459535000 | -0.666465000 | 2.816220000 |
| H | 0.179704000 | 0.278402000 | 3.574720000 |
| C | -0.153379000 | 2.085979000 | 1.673930000 |
| H | -1.170739000 | 1.832173000 | 1.991859000 |
| H | 0.265931000 | 2.782946000 | 2.409146000 |
| C | 2.137103000 | 1.206167000 | 1.390905000 |
| H | 2.197291000 | 2.241188000 | 1.032704000 |
| H | 2.635195000 | 1.180953000 | 2.366822000 |
| C | 2.818587000 | 0.313203000 | 0.380248000 |
| C | 4.209697000 | 0.178382000 | 0.292704000 |
| H | 4.853655000 | 0.655514000 | 1.025321000 |
| C | 4.758629000 | -0.564252000 | -0.771441000 |
| H | 5.834839000 | -0.676172000 | -0.862288000 |
| C | 3.896636000 | -1.145760000 | -1.722196000 |
| H | 4.284298000 | -1.706161000 | -2.565931000 |
| C | 2.513789000 | -0.986645000 | -1.574142000 |
| H | 1.813982000 | -1.399720000 | -2.291664000 |
| C | -2.900800000 | 0.949822000 | -0.456437000 |
| H | -2.475294000 | 1.933182000 | -0.603926000 |
| C | -4.278216000 | 0.758566000 | -0.611469000 |
| H | -4.909906000 | 1.603838000 | -0.862050000 |
| C | -4.813636000 | -0.533908000 | -0.450786000 |
| H | -5.877944000 | -0.710293000 | -0.571629000 |
| C | -3.944962000 | -1.595040000 | -0.136650000 |
| H | -4.323645000 | -2.604810000 | -0.012201000 |
| C | -2.575839000 | -1.337535000 | 0.003514000 |
| C | -1.559016000 | -2.421096000 | 0.270697000 |
| H | -1.299040000 | -2.932531000 | -0.664363000 |
| H | -1.943486000 | -3.177030000 | 0.967308000 |
| C | 0.809524000 | -2.826282000 | 0.813583000 |
| H | 1.021136000 | -3.132158000 | -0.213207000 |
| H | 1.719164000 | -2.419443000 | 1.257067000 |
| H | 0.495833000 | -3.706544000 | 1.388314000 |
| C | -0.238273000 | 2.786157000 | 0.304627000 |
| O | -0.500091000 | 3.946430000 | 0.066731000 |
| O | -0.002347000 | 1.812385000 | -0.713020000 |
| O | -0.349200000 | 0.824075000 | -2.877228000 |
| H | -0.158922000 | 1.837656000 | -1.779347000 |

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|----|--------------|--------------|--------------|
| Mn | 1.903161000 | 0.321478000 | -0.254099000 |
| O | -0.330109000 | 0.330937000 | -0.096710000 |
| N | 2.793577000 | 0.543840000 | -2.339371000 |
| N | 4.032482000 | 0.742277000 | 0.363635000 |
| N | 1.740348000 | 2.374686000 | 0.323147000 |
| N | 1.671143000 | -1.668828000 | -1.069378000 |
| C | 4.255353000 | 0.239810000 | -2.103558000 |
| H | 4.356460000 | -0.838989000 | -1.937054000 |
| H | 4.846130000 | 0.484782000 | -2.998859000 |
| C | 4.811972000 | 1.022952000 | -0.904811000 |
| H | 4.755423000 | 2.098139000 | -1.096900000 |
| H | 5.874325000 | 0.779673000 | -0.765771000 |

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|---|--------------|--------------|--------------|
| C | 4.565448000 | -0.445713000 | 1.101048000 |
| H | 4.751159000 | -1.265442000 | 0.396037000 |
| H | 5.518737000 | -0.234817000 | 1.605447000 |
| C | 3.988520000 | 1.954332000 | 1.262858000 |
| H | 3.822944000 | 1.617169000 | 2.293767000 |
| H | 4.954293000 | 2.476333000 | 1.255104000 |
| C | 2.864476000 | 2.910080000 | 0.895660000 |
| C | 2.936908000 | 4.274991000 | 1.213707000 |
| H | 3.837327000 | 4.682037000 | 1.664042000 |
| C | 1.828745000 | 5.104666000 | 0.957336000 |
| H | 1.867004000 | 6.161672000 | 1.202770000 |
| C | 0.671399000 | 4.545110000 | 0.382287000 |
| H | -0.205159000 | 5.149419000 | 0.175697000 |
| C | 0.666047000 | 3.178766000 | 0.074526000 |
| H | -0.208820000 | 2.712054000 | -0.366270000 |
| C | 1.329075000 | -2.778137000 | -0.346791000 |
| H | 1.165650000 | -2.642497000 | 0.715915000 |
| C | 1.185577000 | -4.039890000 | -0.934044000 |
| H | 0.908731000 | -4.892496000 | -0.323567000 |
| C | 1.409909000 | -4.171020000 | -2.318932000 |
| H | 1.311013000 | -5.136890000 | -2.804934000 |
| C | 1.763724000 | -3.031898000 | -3.064171000 |
| H | 1.938710000 | -3.103771000 | -4.133354000 |
| C | 1.879794000 | -1.790816000 | -2.417795000 |
| C | 2.164622000 | -0.519004000 | -3.196733000 |
| H | 1.217390000 | -0.120959000 | -3.583801000 |
| H | 2.792744000 | -0.742445000 | -4.071030000 |
| C | 2.616221000 | 1.887952000 | -2.993635000 |
| H | 1.550190000 | 2.106571000 | -3.105972000 |
| H | 3.063731000 | 2.674056000 | -2.382099000 |
| H | 3.084932000 | 1.907351000 | -3.987520000 |
| C | 3.593912000 | -0.951649000 | 2.160979000 |
| O | 3.859777000 | -1.602963000 | 3.155145000 |
| O | 2.241988000 | -0.580980000 | 1.852518000 |
| O | -1.089646000 | -0.660213000 | 0.178724000 |
| H | 1.630803000 | -0.828024000 | 2.587297000 |

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|----|-------------|--------------|--------------|
| Mn | 1.893213000 | 0.374317000 | -0.138660000 |
| O | 0.135161000 | 0.427645000 | -0.567538000 |
| N | 2.683694000 | 0.528289000 | -2.269256000 |
| N | 3.940594000 | 0.730896000 | 0.332424000 |
| N | 1.847714000 | 2.465067000 | 0.322154000 |
| N | 1.941986000 | -1.763222000 | -0.935775000 |
| C | 4.157890000 | 0.265692000 | -2.127938000 |
| H | 4.299592000 | -0.810774000 | -1.991614000 |
| H | 4.700092000 | 0.557951000 | -3.040648000 |
| C | 4.726852000 | 1.029378000 | -0.925421000 |
| H | 4.671025000 | 2.108024000 | -1.102887000 |
| H | 5.785289000 | 0.774565000 | -0.779496000 |
| C | 4.387925000 | -0.515489000 | 1.054960000 |
| H | 4.580928000 | -1.309426000 | 0.326198000 |

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|---|--------------|--------------|--------------|
| H | 5.306745000 | -0.343840000 | 1.628581000 |
| C | 3.998047000 | 1.901236000 | 1.293263000 |
| H | 3.784897000 | 1.518988000 | 2.297854000 |
| H | 5.008938000 | 2.328780000 | 1.308869000 |
| C | 2.954337000 | 2.943378000 | 0.955877000 |
| C | 3.045703000 | 4.289079000 | 1.341890000 |
| H | 3.934789000 | 4.657394000 | 1.844565000 |
| C | 1.956339000 | 5.143288000 | 1.083167000 |
| H | 2.000237000 | 6.187462000 | 1.378485000 |
| C | 0.808287000 | 4.630415000 | 0.448267000 |
| H | -0.052772000 | 5.258975000 | 0.248577000 |
| C | 0.788436000 | 3.278077000 | 0.076672000 |
| H | -0.062018000 | 2.804803000 | -0.402514000 |
| C | 1.765347000 | -2.885814000 | -0.184353000 |
| H | 1.748477000 | -2.753422000 | 0.890655000 |
| C | 1.591044000 | -4.148575000 | -0.770864000 |
| H | 1.452760000 | -5.019324000 | -0.139110000 |
| C | 1.601529000 | -4.253253000 | -2.174398000 |
| H | 1.475272000 | -5.218004000 | -2.656828000 |
| C | 1.772171000 | -3.089290000 | -2.946215000 |
| H | 1.774901000 | -3.135910000 | -4.031251000 |
| C | 1.927556000 | -1.855475000 | -2.293434000 |
| C | 2.003519000 | -0.548015000 | -3.057953000 |
| H | 0.980423000 | -0.203960000 | -3.252993000 |
| H | 2.499727000 | -0.698158000 | -4.029368000 |
| C | 2.401121000 | 1.857784000 | -2.896935000 |
| H | 1.325248000 | 2.048338000 | -2.858440000 |
| H | 2.910827000 | 2.655941000 | -2.352692000 |
| H | 2.733378000 | 1.880609000 | -3.946000000 |
| C | 3.242356000 | -0.984767000 | 1.998463000 |
| O | 3.474290000 | -1.785533000 | 2.920582000 |
| O | 2.045799000 | -0.477068000 | 1.661920000 |
| H | -0.512702000 | -0.144727000 | -0.106683000 |

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|----|-------------|--------------|--------------|
| Mn | 1.995254000 | 0.349381000 | -0.270345000 |
| O | 0.244467000 | 0.430705000 | -0.795092000 |
| N | 2.701564000 | 0.582499000 | -2.245625000 |
| N | 4.025158000 | 0.685169000 | 0.278674000 |
| N | 1.881795000 | 2.306282000 | 0.282491000 |
| N | 1.954249000 | -1.623148000 | -0.902148000 |
| C | 4.180114000 | 0.260279000 | -2.176448000 |
| H | 4.285135000 | -0.825245000 | -2.090527000 |
| H | 4.681477000 | 0.570985000 | -3.104328000 |
| C | 4.826946000 | 0.947523000 | -0.970718000 |
| H | 4.852490000 | 2.030627000 | -1.126708000 |
| H | 5.864793000 | 0.608998000 | -0.849866000 |
| C | 4.387058000 | -0.550074000 | 1.055022000 |
| H | 4.538133000 | -1.390458000 | 0.369071000 |
| H | 5.299248000 | -0.420768000 | 1.649833000 |
| C | 4.079911000 | 1.873603000 | 1.213350000 |
| H | 3.955340000 | 1.511863000 | 2.239629000 |

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|---|--------------|--------------|--------------|
| H | 5.062738000 | 2.358991000 | 1.159025000 |
| C | 2.961019000 | 2.842054000 | 0.918000000 |
| C | 2.974112000 | 4.179096000 | 1.341422000 |
| H | 3.848253000 | 4.581794000 | 1.844200000 |
| C | 1.834462000 | 4.974739000 | 1.124918000 |
| H | 1.817899000 | 6.010099000 | 1.451828000 |
| C | 0.716465000 | 4.406163000 | 0.486394000 |
| H | -0.186005000 | 4.981896000 | 0.311450000 |
| C | 0.773947000 | 3.068268000 | 0.073325000 |
| H | -0.046261000 | 2.559358000 | -0.419494000 |
| C | 1.767804000 | -2.719609000 | -0.114064000 |
| H | 1.752393000 | -2.558297000 | 0.955549000 |
| C | 1.568404000 | -3.995288000 | -0.660746000 |
| H | 1.423227000 | -4.841231000 | 0.002139000 |
| C | 1.556997000 | -4.147200000 | -2.059047000 |
| H | 1.410103000 | -5.125004000 | -2.507888000 |
| C | 1.727270000 | -3.009689000 | -2.869591000 |
| H | 1.705654000 | -3.088361000 | -3.952187000 |
| C | 1.910132000 | -1.759953000 | -2.262166000 |
| C | 1.980614000 | -0.470351000 | -3.045642000 |
| H | 0.959608000 | -0.105709000 | -3.202877000 |
| H | 2.458811000 | -0.619012000 | -4.024215000 |
| C | 2.450468000 | 1.928392000 | -2.857524000 |
| H | 1.383467000 | 2.151976000 | -2.789048000 |
| H | 3.003792000 | 2.699618000 | -2.317864000 |
| H | 2.758572000 | 1.941081000 | -3.912945000 |
| C | 3.179410000 | -0.863339000 | 1.986194000 |
| O | 3.312552000 | -1.582336000 | 2.991763000 |
| O | 2.027202000 | -0.313610000 | 1.556865000 |
| H | -0.409274000 | -0.130430000 | -0.329880000 |

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|----|--------------|-------------|--------------|
| Mn | 1.344137000 | 1.523514000 | -0.532525000 |
| O | 2.619110000 | 0.348192000 | -1.077656000 |
| N | 2.440061000 | 2.537199000 | 0.959896000 |
| N | 2.120662000 | 3.084923000 | -1.800148000 |
| N | 3.142145000 | 4.638107000 | -4.118358000 |
| N | -0.184068000 | 2.468809000 | 0.573464000 |
| C | 2.485285000 | 3.987537000 | 0.493878000 |
| H | 1.491425000 | 4.423831000 | 0.620073000 |
| H | 3.181952000 | 4.550295000 | 1.129784000 |
| C | 2.923231000 | 4.059232000 | -0.964666000 |
| H | 3.978506000 | 3.794553000 | -1.065516000 |
| H | 2.809953000 | 5.076073000 | -1.355406000 |
| C | 0.863682000 | 3.677103000 | -2.398357000 |
| H | 0.371232000 | 4.322704000 | -1.661266000 |
| H | 1.114778000 | 4.274387000 | -3.279655000 |
| C | 2.987264000 | 2.488279000 | -2.904378000 |
| H | 3.659844000 | 1.768131000 | -2.433538000 |
| H | 2.319103000 | 1.920013000 | -3.560637000 |
| C | 3.779613000 | 3.501707000 | -3.726926000 |
| C | 5.105260000 | 3.220081000 | -4.110127000 |

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|----|--------------|--------------|--------------|
| H | 5.595130000 | 2.309343000 | -3.775945000 |
| C | 5.783319000 | 4.134057000 | -4.941496000 |
| H | 6.803774000 | 3.938155000 | -5.257548000 |
| C | 5.120985000 | 5.304783000 | -5.351205000 |
| H | 5.606497000 | 6.033585000 | -5.991835000 |
| C | 3.801372000 | 5.520106000 | -4.908373000 |
| H | 3.253661000 | 6.412940000 | -5.195255000 |
| C | -1.481656000 | 2.605821000 | 0.184865000 |
| H | -1.721094000 | 2.363022000 | -0.842096000 |
| C | -2.476273000 | 3.018938000 | 1.082014000 |
| H | -3.497647000 | 3.129108000 | 0.734390000 |
| C | -2.123770000 | 3.283450000 | 2.418743000 |
| H | -2.873601000 | 3.611892000 | 3.132149000 |
| C | -0.784874000 | 3.116010000 | 2.820738000 |
| H | -0.483235000 | 3.307248000 | 3.845923000 |
| C | 0.162051000 | 2.699399000 | 1.876794000 |
| C | 1.611412000 | 2.430078000 | 2.214400000 |
| H | 1.722832000 | 1.408756000 | 2.594129000 |
| H | 1.981916000 | 3.124670000 | 2.980347000 |
| C | 3.835722000 | 2.020665000 | 1.211941000 |
| H | 3.792109000 | 0.980017000 | 1.532915000 |
| H | 4.416745000 | 2.066748000 | 0.290038000 |
| H | 4.320647000 | 2.636478000 | 1.981817000 |
| C | -0.074532000 | 2.517893000 | -2.747303000 |
| O | -0.987678000 | 2.569087000 | -3.573768000 |
| O | 0.175626000 | 1.383454000 | -1.999193000 |
| O | 0.829577000 | 0.005403000 | 0.407147000 |
| Mn | 2.104538000 | -1.169924000 | -0.138004000 |
| N | 1.008566000 | -2.183602000 | -1.630397000 |
| N | 1.328044000 | -2.731332000 | 1.129639000 |
| N | 0.306548000 | -4.284513000 | 3.447867000 |
| N | 3.632706000 | -2.115223000 | -1.244038000 |
| C | 0.963347000 | -3.633940000 | -1.164377000 |
| H | 1.957201000 | -4.070240000 | -1.290602000 |
| H | 0.266658000 | -4.196694000 | -1.800262000 |
| C | 0.525445000 | -3.705634000 | 0.294180000 |
| H | -0.529825000 | -3.440948000 | 0.395063000 |
| H | 0.638728000 | -4.722478000 | 0.684914000 |
| C | 2.585035000 | -3.323524000 | 1.727814000 |
| H | 3.077455000 | -3.969137000 | 0.990713000 |
| H | 2.333958000 | -3.920792000 | 2.609128000 |
| C | 0.461471000 | -2.134690000 | 2.233895000 |
| H | -0.211082000 | -1.414500000 | 1.763081000 |
| H | 1.129658000 | -1.566479000 | 2.890174000 |
| C | -0.330914000 | -3.148121000 | 3.056401000 |
| C | -1.656601000 | -2.866534000 | 3.439490000 |
| H | -2.146470000 | -1.955810000 | 3.105268000 |
| C | -2.334701000 | -3.780528000 | 4.270807000 |
| H | -3.355185000 | -3.584653000 | 4.586781000 |
| C | -1.672369000 | -4.951239000 | 4.680562000 |
| H | -2.157910000 | -5.680053000 | 5.321158000 |
| C | -0.352721000 | -5.166536000 | 4.237819000 |

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|---|--------------|--------------|--------------|
| H | 0.194993000 | -6.059352000 | 4.524749000 |
| C | 4.930306000 | -2.252237000 | -0.855477000 |
| H | 5.169774000 | -2.009440000 | 0.171476000 |
| C | 5.924896000 | -2.665352000 | -1.752656000 |
| H | 6.946280000 | -2.775525000 | -1.405061000 |
| C | 5.572355000 | -2.929861000 | -3.089376000 |
| H | 6.322165000 | -3.258303000 | -3.802804000 |
| C | 4.233447000 | -2.762419000 | -3.491331000 |
| H | 3.931778000 | -2.953653000 | -4.516509000 |
| C | 3.286550000 | -2.345809000 | -2.547360000 |
| C | 1.837180000 | -2.076484000 | -2.884924000 |
| H | 1.725750000 | -1.055163000 | -3.264651000 |
| H | 1.466652000 | -2.771076000 | -3.650860000 |
| C | -0.387100000 | -1.667059000 | -1.882403000 |
| H | -0.343485000 | -0.626419000 | -2.203402000 |
| H | -0.968090000 | -1.713117000 | -0.960479000 |
| H | -0.872057000 | -2.282882000 | -2.652251000 |
| C | 3.523272000 | -2.164322000 | 2.076724000 |
| O | 4.436453000 | -2.215527000 | 2.903149000 |
| O | 3.273089000 | -1.029876000 | 1.328633000 |

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|----|--------------|--------------|--------------|
| Mn | -0.627121000 | 1.657421000 | 0.087250000 |
| O | -0.234645000 | -0.050789000 | -0.192497000 |
| N | 1.300251000 | 2.423792000 | -0.138436000 |
| N | -1.113079000 | 3.568239000 | 0.819262000 |
| N | -1.074780000 | 5.628070000 | 3.266098000 |
| N | -0.509508000 | 1.974418000 | -2.023610000 |
| C | 1.109422000 | 3.927858000 | -0.289344000 |
| H | 0.754046000 | 4.123616000 | -1.303883000 |
| H | 2.077745000 | 4.433114000 | -0.172268000 |
| C | 0.117525000 | 4.458496000 | 0.746283000 |
| H | 0.549631000 | 4.501483000 | 1.746420000 |
| H | -0.170494000 | 5.486478000 | 0.500952000 |
| C | -2.253078000 | 3.989071000 | -0.070401000 |
| H | -1.867752000 | 4.296964000 | -1.048659000 |
| H | -2.812618000 | 4.827215000 | 0.354702000 |
| C | -1.623496000 | 3.463131000 | 2.270733000 |
| H | -0.800956000 | 3.051725000 | 2.860075000 |
| H | -2.436604000 | 2.734721000 | 2.269161000 |
| C | -2.071263000 | 4.780594000 | 2.879737000 |
| C | -3.432505000 | 5.076689000 | 3.089852000 |
| H | -4.205561000 | 4.376492000 | 2.784238000 |
| C | -3.775694000 | 6.288525000 | 3.723331000 |
| H | -4.816884000 | 6.538451000 | 3.904280000 |
| C | -2.749040000 | 7.161888000 | 4.121933000 |
| H | -2.969423000 | 8.100842000 | 4.619418000 |
| C | -1.411526000 | 6.792176000 | 3.870168000 |
| H | -0.589312000 | 7.436939000 | 4.166878000 |
| C | -1.540012000 | 1.984175000 | -2.914422000 |
| H | -2.544797000 | 1.998805000 | -2.513885000 |
| C | -1.321271000 | 1.958373000 | -4.297885000 |

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|----|--------------|--------------|--------------|
| H | -2.168735000 | 1.981822000 | -4.974351000 |
| C | 0.000150000 | 1.903274000 | -4.780574000 |
| H | 0.198109000 | 1.881525000 | -5.847957000 |
| C | 1.061861000 | 1.876432000 | -3.859267000 |
| H | 2.092248000 | 1.822851000 | -4.195834000 |
| C | 0.774366000 | 1.912296000 | -2.488439000 |
| C | 1.838972000 | 1.835674000 | -1.421397000 |
| H | 2.082546000 | 0.782304000 | -1.242568000 |
| H | 2.753888000 | 2.361003000 | -1.726231000 |
| C | 2.228157000 | 2.105486000 | 1.000581000 |
| H | 2.245184000 | 1.026800000 | 1.152910000 |
| H | 1.869899000 | 2.574058000 | 1.917410000 |
| H | 3.238810000 | 2.470626000 | 0.771601000 |
| C | -3.174255000 | 2.767029000 | -0.257577000 |
| O | -4.365923000 | 2.844987000 | -0.580455000 |
| O | -2.520704000 | 1.579231000 | -0.079694000 |
| Mn | -0.006824000 | -1.824984000 | -0.469365000 |
| N | -0.748592000 | -2.668633000 | 1.394171000 |
| N | 0.082955000 | -3.809061000 | -1.122053000 |
| N | -1.938496000 | -2.039019000 | -1.583946000 |
| N | 1.852185000 | -1.855799000 | 1.073179000 |
| C | -0.313038000 | -4.122884000 | 1.342164000 |
| H | 0.742323000 | -4.170892000 | 1.620397000 |
| H | -0.877972000 | -4.711937000 | 2.078372000 |
| C | -0.521692000 | -4.708004000 | -0.057432000 |
| H | -1.589305000 | -4.799825000 | -0.277719000 |
| H | -0.083634000 | -5.712506000 | -0.120611000 |
| C | 1.547087000 | -4.043300000 | -1.404199000 |
| H | 2.081094000 | -4.218889000 | -0.465494000 |
| H | 1.700461000 | -4.910978000 | -2.055966000 |
| C | -0.687198000 | -3.940163000 | -2.424275000 |
| H | -0.054019000 | -3.549606000 | -3.228573000 |
| H | -0.874398000 | -5.001029000 | -2.633703000 |
| C | -1.971955000 | -3.144023000 | -2.380875000 |
| C | -3.098051000 | -3.467950000 | -3.151666000 |
| H | -3.102579000 | -4.358047000 | -3.773684000 |
| C | -4.217540000 | -2.614273000 | -3.105818000 |
| H | -5.103772000 | -2.843053000 | -3.690295000 |
| C | -4.173655000 | -1.467078000 | -2.290664000 |
| H | -5.016699000 | -0.787218000 | -2.226107000 |
| C | -3.016600000 | -1.208135000 | -1.537757000 |
| H | -2.943836000 | -0.336694000 | -0.894546000 |
| C | 3.184074000 | -1.695795000 | 0.829857000 |
| H | 3.501846000 | -1.707813000 | -0.206807000 |
| C | 4.117851000 | -1.523974000 | 1.862876000 |
| H | 5.171079000 | -1.414296000 | 1.626885000 |
| C | 3.660245000 | -1.512742000 | 3.195689000 |
| H | 4.358615000 | -1.390746000 | 4.018300000 |
| C | 2.285701000 | -1.671693000 | 3.446795000 |
| H | 1.902060000 | -1.669997000 | 4.462638000 |
| C | 1.409173000 | -1.839028000 | 2.360237000 |
| C | -0.086956000 | -1.961761000 | 2.552933000 |

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|---|--------------|--------------|--------------|
| H | -0.519906000 | -0.955373000 | 2.613751000 |
| H | -0.314384000 | -2.492222000 | 3.488977000 |
| C | -2.240399000 | -2.545824000 | 1.561172000 |
| H | -2.524200000 | -1.493448000 | 1.485655000 |
| H | -2.759961000 | -3.107543000 | 0.783841000 |
| H | -2.546625000 | -2.932447000 | 2.543110000 |
| C | 2.114356000 | -2.760988000 | -2.066431000 |
| O | 3.191005000 | -2.749829000 | -2.676495000 |
| O | 1.331687000 | -1.667549000 | -1.860955000 |
| O | -0.430597000 | 1.117855000 | 1.772591000 |

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|----|--------------|--------------|--------------|
| Mn | -0.542446000 | 1.605785000 | 0.416753000 |
| O | -0.229238000 | -0.094476000 | 0.085376000 |
| N | 1.401632000 | 2.323919000 | 0.194207000 |
| N | -1.033286000 | 3.644279000 | 0.955724000 |
| N | -1.614212000 | 6.178315000 | 2.473637000 |
| N | -0.349744000 | 1.854477000 | -1.740851000 |
| C | 1.263781000 | 3.828669000 | -0.036838000 |
| H | 0.967351000 | 3.980692000 | -1.076744000 |
| H | 2.245325000 | 4.301910000 | 0.101845000 |
| C | 0.248118000 | 4.455018000 | 0.913921000 |
| H | 0.634275000 | 4.489923000 | 1.934132000 |
| H | 0.038505000 | 5.493076000 | 0.642129000 |
| C | -2.079027000 | 3.983993000 | -0.068665000 |
| H | -1.614068000 | 4.155859000 | -1.044438000 |
| H | -2.647896000 | 4.877798000 | 0.199446000 |
| C | -1.675918000 | 3.718215000 | 2.346414000 |
| H | -0.887893000 | 3.506543000 | 3.070565000 |
| H | -2.401638000 | 2.903966000 | 2.417777000 |
| C | -2.348177000 | 5.046437000 | 2.668989000 |
| C | -3.647291000 | 5.077784000 | 3.210362000 |
| H | -4.213725000 | 4.160334000 | 3.343261000 |
| C | -4.199026000 | 6.319777000 | 3.584820000 |
| H | -5.196858000 | 6.371647000 | 4.010195000 |
| C | -3.439985000 | 7.487083000 | 3.393061000 |
| H | -3.825867000 | 8.463169000 | 3.668307000 |
| C | -2.155454000 | 7.369121000 | 2.825587000 |
| H | -1.541134000 | 8.248086000 | 2.652172000 |
| C | -1.342640000 | 1.843398000 | -2.673466000 |
| H | -2.364240000 | 1.896233000 | -2.322439000 |
| C | -1.070308000 | 1.753761000 | -4.044608000 |
| H | -1.890930000 | 1.763630000 | -4.753815000 |
| C | 0.267193000 | 1.656049000 | -4.472370000 |
| H | 0.506901000 | 1.585218000 | -5.528927000 |
| C | 1.289258000 | 1.647324000 | -3.508603000 |
| H | 2.330145000 | 1.550916000 | -3.799231000 |
| C | 0.947034000 | 1.744955000 | -2.154206000 |
| C | 1.965974000 | 1.671853000 | -1.046815000 |
| H | 2.164541000 | 0.618827000 | -0.826319000 |
| H | 2.908547000 | 2.160332000 | -1.327501000 |
| C | 2.291047000 | 2.029022000 | 1.373770000 |

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|----|--------------|--------------|--------------|
| H | 2.293602000 | 0.954125000 | 1.558003000 |
| H | 1.913152000 | 2.535749000 | 2.263784000 |
| H | 3.312804000 | 2.373624000 | 1.166389000 |
| C | -3.019532000 | 2.767341000 | -0.164581000 |
| O | -4.186051000 | 2.813105000 | -0.567766000 |
| O | -2.412858000 | 1.583505000 | 0.193539000 |
| Mn | -0.072928000 | -1.780451000 | -0.506348000 |
| N | -0.631750000 | -2.788316000 | 1.342743000 |
| N | -0.027755000 | -3.709170000 | -1.319374000 |
| N | -2.067051000 | -1.905201000 | -1.489983000 |
| N | 1.972606000 | -1.995384000 | 0.885286000 |
| C | -0.208342000 | -4.230235000 | 1.137174000 |
| H | 0.866716000 | -4.298808000 | 1.316193000 |
| H | -0.709608000 | -4.882578000 | 1.866379000 |
| C | -0.539521000 | -4.695707000 | -0.284822000 |
| H | -1.622505000 | -4.773388000 | -0.418833000 |
| H | -0.112512000 | -5.690234000 | -0.468897000 |
| C | 1.409812000 | -3.907664000 | -1.733708000 |
| H | 2.013352000 | -4.157647000 | -0.856499000 |
| H | 1.513496000 | -4.716753000 | -2.465926000 |
| C | -0.897936000 | -3.744064000 | -2.561116000 |
| H | -0.326295000 | -3.297684000 | -3.382562000 |
| H | -1.110530000 | -4.785539000 | -2.834418000 |
| C | -2.169075000 | -2.948803000 | -2.361438000 |
| C | -3.352205000 | -3.209840000 | -3.068040000 |
| H | -3.410879000 | -4.052072000 | -3.750992000 |
| C | -4.457097000 | -2.356662000 | -2.878494000 |
| H | -5.385306000 | -2.537540000 | -3.412459000 |
| C | -4.342440000 | -1.271693000 | -1.988552000 |
| H | -5.168704000 | -0.589706000 | -1.817645000 |
| C | -3.131401000 | -1.075336000 | -1.305074000 |
| H | -2.999447000 | -0.248504000 | -0.613906000 |
| C | 3.290686000 | -1.851895000 | 0.570585000 |
| H | 3.544518000 | -1.813726000 | -0.483553000 |
| C | 4.291900000 | -1.763835000 | 1.550637000 |
| H | 5.331395000 | -1.666916000 | 1.255535000 |
| C | 3.917587000 | -1.822467000 | 2.907861000 |
| H | 4.667954000 | -1.768595000 | 3.691036000 |
| C | 2.556856000 | -1.965355000 | 3.234378000 |
| H | 2.237095000 | -2.020654000 | 4.270764000 |
| C | 1.611071000 | -2.047139000 | 2.196062000 |
| C | 0.127537000 | -2.156295000 | 2.482317000 |
| H | -0.279075000 | -1.147152000 | 2.622869000 |
| H | -0.042329000 | -2.728433000 | 3.406278000 |
| C | -2.102931000 | -2.687646000 | 1.644517000 |
| H | -2.393395000 | -1.634780000 | 1.673031000 |
| H | -2.687424000 | -3.189122000 | 0.871737000 |
| H | -2.328625000 | -3.150388000 | 2.615489000 |
| C | 1.930558000 | -2.571949000 | -2.326058000 |
| O | 2.959264000 | -2.511430000 | -3.014307000 |
| O | 1.187111000 | -1.499188000 | -1.955673000 |
| O | -0.329508000 | 1.370753000 | 2.163610000 |

³11.H₂O

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|----|--------------|--------------|--------------|
| Mn | 0.180707000 | 1.374612000 | -0.801497000 |
| O | 0.363635000 | -0.288113000 | -0.234489000 |
| N | 1.804326000 | 1.476282000 | -2.123447000 |
| N | -0.174693000 | 3.441625000 | -1.426984000 |
| N | -1.595006000 | 6.134360000 | -1.895101000 |
| N | 1.892266000 | 1.769793000 | 0.510417000 |
| C | 2.136080000 | 2.957144000 | -2.289148000 |
| H | 2.704879000 | 3.272034000 | -1.412340000 |
| H | 2.783715000 | 3.082852000 | -3.167485000 |
| C | 0.880855000 | 3.810820000 | -2.442628000 |
| H | 0.439592000 | 3.660564000 | -3.431855000 |
| H | 1.139951000 | 4.873862000 | -2.367435000 |
| C | -0.125792000 | 4.162079000 | -0.100258000 |
| H | 0.908090000 | 4.252604000 | 0.245714000 |
| H | -0.565133000 | 5.161297000 | -0.194712000 |
| C | -1.560418000 | 3.674621000 | -2.040657000 |
| H | -1.734991000 | 2.877656000 | -2.762345000 |
| H | -2.287580000 | 3.560517000 | -1.230891000 |
| C | -1.748190000 | 5.040011000 | -2.691984000 |
| C | -2.124515000 | 5.150489000 | -4.044434000 |
| H | -2.246194000 | 4.262341000 | -4.658915000 |
| C | -2.367275000 | 6.430647000 | -4.583568000 |
| H | -2.671047000 | 6.542281000 | -5.620288000 |
| C | -2.213174000 | 7.557755000 | -3.758175000 |
| H | -2.394643000 | 8.560215000 | -4.131793000 |
| C | -1.817543000 | 7.362574000 | -2.419229000 |
| H | -1.684677000 | 8.204897000 | -1.746637000 |
| C | 1.877626000 | 2.199791000 | 1.801893000 |
| H | 0.930222000 | 2.521639000 | 2.214216000 |
| C | 3.036988000 | 2.223132000 | 2.588246000 |
| H | 2.985349000 | 2.599780000 | 3.603936000 |
| C | 4.246408000 | 1.758928000 | 2.037688000 |
| H | 5.161953000 | 1.770543000 | 2.621478000 |
| C | 4.252218000 | 1.277461000 | 0.717369000 |
| H | 5.160873000 | 0.893198000 | 0.265438000 |
| C | 3.060246000 | 1.301270000 | -0.020683000 |
| C | 2.968108000 | 0.796506000 | -1.438578000 |
| H | 2.802193000 | -0.285367000 | -1.415796000 |
| H | 3.894399000 | 0.995543000 | -1.994816000 |
| C | 1.529319000 | 0.818357000 | -3.447653000 |
| H | 1.258406000 | -0.224565000 | -3.276710000 |
| H | 0.695514000 | 1.315515000 | -3.947147000 |
| H | 2.421865000 | 0.867773000 | -4.085725000 |
| C | -0.931641000 | 3.316881000 | 0.903230000 |
| O | -1.430883000 | 3.752136000 | 1.942502000 |
| O | -1.025178000 | 1.978639000 | 0.546617000 |
| Mn | 0.674523000 | -2.019843000 | 0.147155000 |
| N | -1.099438000 | -2.459672000 | 1.316638000 |
| N | 1.044354000 | -4.086643000 | 0.317836000 |
| N | -0.124642000 | -2.818862000 | -1.793762000 |

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|---|--------------|--------------|--------------|
| N | 1.176566000 | -1.463379000 | 2.488135000 |
| C | -0.805895000 | -3.786146000 | 1.993427000 |
| H | -0.160689000 | -3.602052000 | 2.854553000 |
| H | -1.738571000 | -4.232698000 | 2.366264000 |
| C | -0.126616000 | -4.750803000 | 1.017010000 |
| H | -0.831312000 | -5.064303000 | 0.241085000 |
| H | 0.209507000 | -5.654138000 | 1.542671000 |
| C | 2.359270000 | -4.156430000 | 1.054798000 |
| H | 2.194541000 | -3.996069000 | 2.123706000 |
| H | 2.846579000 | -5.130071000 | 0.925389000 |
| C | 1.240404000 | -4.683862000 | -1.062691000 |
| H | 2.259054000 | -4.448615000 | -1.389599000 |
| H | 1.154452000 | -5.776640000 | -1.006716000 |
| C | 0.263466000 | -4.097715000 | -2.055814000 |
| C | -0.165282000 | -4.782715000 | -3.202711000 |
| H | 0.153125000 | -5.804574000 | -3.385906000 |
| C | -1.009897000 | -4.115965000 | -4.111028000 |
| H | -1.357747000 | -4.622064000 | -5.006700000 |
| C | -1.398485000 | -2.789840000 | -3.840684000 |
| H | -2.048669000 | -2.248041000 | -4.519513000 |
| C | -0.940912000 | -2.167870000 | -2.667141000 |
| H | -1.209802000 | -1.149026000 | -2.405168000 |
| C | 2.355374000 | -1.284174000 | 3.144536000 |
| H | 3.262190000 | -1.551181000 | 2.612916000 |
| C | 2.416710000 | -0.781711000 | 4.453799000 |
| H | 3.376689000 | -0.680863000 | 4.949251000 |
| C | 1.217690000 | -0.431222000 | 5.102879000 |
| H | 1.229236000 | -0.045251000 | 6.117959000 |
| C | -0.001002000 | -0.604614000 | 4.422081000 |
| H | -0.944266000 | -0.351756000 | 4.896861000 |
| C | 0.015579000 | -1.131023000 | 3.118968000 |
| C | -1.260237000 | -1.357452000 | 2.334657000 |
| H | -1.522095000 | -0.444404000 | 1.788470000 |
| H | -2.089538000 | -1.596596000 | 3.016018000 |
| C | -2.363698000 | -2.542357000 | 0.499619000 |
| H | -2.504633000 | -1.609962000 | -0.052175000 |
| H | -2.301439000 | -3.371441000 | -0.207595000 |
| H | -3.226414000 | -2.708482000 | 1.161011000 |
| C | 3.273620000 | -3.024245000 | 0.513930000 |
| O | 4.491518000 | -2.996158000 | 0.741576000 |
| O | 2.593841000 | -2.075482000 | -0.178301000 |
| O | -1.034111000 | 0.945597000 | -2.011599000 |
| O | -2.703373000 | 0.410121000 | -0.821754000 |
| H | -3.387534000 | 0.798124000 | -1.402849000 |
| H | -2.388462000 | 1.058904000 | -0.135610000 |

³TS11.H₂O-12

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|----|--------------|--------------|--------------|
| Mn | 0.254824000 | 1.382273000 | -0.760476000 |
| O | 0.377984000 | -0.309833000 | -0.198143000 |
| N | 1.765314000 | 1.421412000 | -2.173167000 |
| N | -0.123453000 | 3.454368000 | -1.440509000 |
| N | -1.094084000 | 6.132107000 | -2.161072000 |

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|----|--------------|--------------|--------------|
| N | 1.929145000 | 1.744493000 | 0.439728000 |
| C | 2.157748000 | 2.884437000 | -2.353799000 |
| H | 2.780861000 | 3.171391000 | -1.504950000 |
| H | 2.772948000 | 2.983903000 | -3.258918000 |
| C | 0.947927000 | 3.809393000 | -2.451851000 |
| H | 0.488928000 | 3.723121000 | -3.440556000 |
| H | 1.255206000 | 4.854507000 | -2.340209000 |
| C | -0.080451000 | 4.213737000 | -0.135983000 |
| H | 0.932067000 | 4.190307000 | 0.277021000 |
| H | -0.379305000 | 5.255742000 | -0.286760000 |
| C | -1.481335000 | 3.672462000 | -2.089765000 |
| H | -1.598812000 | 2.902371000 | -2.852937000 |
| H | -2.253609000 | 3.473093000 | -1.336533000 |
| C | -1.729872000 | 5.057128000 | -2.696725000 |
| C | -2.649234000 | 5.186959000 | -3.757285000 |
| H | -3.136683000 | 4.310841000 | -4.177368000 |
| C | -2.930028000 | 6.469867000 | -4.263424000 |
| H | -3.638719000 | 6.597333000 | -5.076450000 |
| C | -2.275406000 | 7.583166000 | -3.704351000 |
| H | -2.463486000 | 8.588853000 | -4.065456000 |
| C | -1.359337000 | 7.366607000 | -2.659524000 |
| H | -0.827239000 | 8.194865000 | -2.200969000 |
| C | 1.954176000 | 2.192228000 | 1.724449000 |
| H | 1.020901000 | 2.546729000 | 2.144743000 |
| C | 3.124276000 | 2.179945000 | 2.492914000 |
| H | 3.106551000 | 2.568488000 | 3.505360000 |
| C | 4.304117000 | 1.657155000 | 1.927978000 |
| H | 5.227755000 | 1.633430000 | 2.498460000 |
| C | 4.269247000 | 1.159745000 | 0.614453000 |
| H | 5.152665000 | 0.727009000 | 0.156859000 |
| C | 3.068600000 | 1.223970000 | -0.107015000 |
| C | 2.930372000 | 0.712174000 | -1.521221000 |
| H | 2.735921000 | -0.363260000 | -1.483501000 |
| H | 3.851563000 | 0.880223000 | -2.096495000 |
| C | 1.417106000 | 0.782737000 | -3.483854000 |
| H | 1.144631000 | -0.259082000 | -3.309816000 |
| H | 0.560805000 | 1.295539000 | -3.928562000 |
| H | 2.268184000 | 0.826277000 | -4.177873000 |
| C | -1.057411000 | 3.532280000 | 0.824048000 |
| O | -1.768858000 | 4.050375000 | 1.667863000 |
| O | -1.060505000 | 2.110038000 | 0.612746000 |
| Mn | 0.678977000 | -2.016519000 | 0.181183000 |
| N | -1.147510000 | -2.511773000 | 1.303313000 |
| N | 1.078856000 | -4.085078000 | 0.359388000 |
| N | -0.014579000 | -2.807540000 | -1.781505000 |
| N | 1.075803000 | -1.468780000 | 2.547651000 |
| C | -0.855293000 | -3.848554000 | 1.953121000 |
| H | -0.249364000 | -3.671028000 | 2.844370000 |
| H | -1.790731000 | -4.326837000 | 2.278399000 |
| C | -0.113294000 | -4.777328000 | 0.986801000 |
| H | -0.777249000 | -5.084221000 | 0.172581000 |
| H | 0.206769000 | -5.688835000 | 1.509349000 |

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|---|--------------|--------------|--------------|
| C | 2.352123000 | -4.145981000 | 1.162442000 |
| H | 2.128425000 | -4.000786000 | 2.222935000 |
| H | 2.860112000 | -5.111603000 | 1.050396000 |
| C | 1.350257000 | -4.660325000 | -1.015323000 |
| H | 2.379185000 | -4.405258000 | -1.291895000 |
| H | 1.280111000 | -5.755410000 | -0.982035000 |
| C | 0.411545000 | -4.074524000 | -2.044843000 |
| C | 0.051249000 | -4.747630000 | -3.222602000 |
| H | 0.398913000 | -5.759900000 | -3.405741000 |
| C | -0.762671000 | -4.083144000 | -4.159490000 |
| H | -1.057558000 | -4.580685000 | -5.078640000 |
| C | -1.188996000 | -2.768621000 | -3.887405000 |
| H | -1.814935000 | -2.227096000 | -4.589074000 |
| C | -0.798795000 | -2.157335000 | -2.684649000 |
| H | -1.092851000 | -1.143952000 | -2.422359000 |
| C | 2.232498000 | -1.241120000 | 3.227173000 |
| H | 3.158832000 | -1.466871000 | 2.711018000 |
| C | 2.247010000 | -0.742169000 | 4.539477000 |
| H | 3.192652000 | -0.599211000 | 5.051927000 |
| C | 1.022189000 | -0.453800000 | 5.170069000 |
| H | 0.998354000 | -0.076178000 | 6.188050000 |
| C | -0.174576000 | -0.678770000 | 4.465463000 |
| H | -1.137251000 | -0.477212000 | 4.926123000 |
| C | -0.109332000 | -1.189661000 | 3.157445000 |
| C | -1.361612000 | -1.447641000 | 2.343441000 |
| H | -1.647846000 | -0.533857000 | 1.810830000 |
| H | -2.194449000 | -1.726295000 | 3.006701000 |
| C | -2.367737000 | -2.577514000 | 0.428096000 |
| H | -2.477384000 | -1.626578000 | -0.100290000 |
| H | -2.266255000 | -3.379269000 | -0.305622000 |
| H | -3.266321000 | -2.766890000 | 1.033806000 |
| C | 3.280793000 | -2.996541000 | 0.687166000 |
| O | 4.484319000 | -2.964548000 | 0.994026000 |
| O | 2.637676000 | -2.050166000 | -0.031324000 |
| O | -1.173683580 | 0.920476543 | -1.807357939 |
| O | -2.529122492 | 0.687888739 | -0.846037310 |
| H | -3.300242492 | 0.834696739 | -1.439797310 |
| H | -2.132294467 | 1.324347732 | -0.041396105 |

³TS11.H₂O-12

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|----|--------------|--------------|--------------|
| Mn | 0.264018966 | 1.351447547 | -0.745734703 |
| O | 0.388739903 | -0.362104305 | -0.176274661 |
| N | 1.710909968 | 1.423369188 | -2.116041887 |
| N | -0.120514011 | 3.457811029 | -1.437014146 |
| N | -1.091145011 | 6.135550029 | -2.157577146 |
| N | 1.896580022 | 1.735214431 | 0.513692591 |
| C | 2.160686989 | 2.887880029 | -2.350304146 |
| H | 2.783799989 | 3.174834029 | -1.501455146 |
| H | 2.775886989 | 2.987346029 | -3.255423146 |
| C | 0.950865989 | 3.812836029 | -2.448356146 |
| H | 0.491866989 | 3.726564029 | -3.437061146 |
| H | 1.258144989 | 4.857950029 | -2.336714146 |

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|----|--------------|--------------|--------------|
| C | -0.077512011 | 4.217180029 | -0.132488146 |
| H | 0.935005989 | 4.193750029 | 0.280515854 |
| H | -0.376366011 | 5.259185029 | -0.283265146 |
| C | -1.478396011 | 3.675905029 | -2.086270146 |
| H | -1.595873011 | 2.905814029 | -2.849442146 |
| H | -2.250670011 | 3.476536029 | -1.333038146 |
| C | -1.726933011 | 5.060571029 | -2.693230146 |
| C | -2.646295011 | 5.190402029 | -3.753790146 |
| H | -3.133744011 | 4.314284029 | -4.173873146 |
| C | -2.927089011 | 6.473310029 | -4.259929146 |
| H | -3.635780011 | 6.600776029 | -5.072955146 |
| C | -2.272467011 | 7.586609029 | -3.700856146 |
| H | -2.460547011 | 8.592296029 | -4.061961146 |
| C | -1.356398011 | 7.370050029 | -2.656029146 |
| H | -0.824300011 | 8.198308029 | -2.197474146 |
| C | 1.934961057 | 2.172889133 | 1.801547001 |
| H | 1.006940809 | 2.527834601 | 2.232954424 |
| C | 3.111857198 | 2.150005954 | 2.559316867 |
| H | 3.104799162 | 2.530768332 | 3.574844778 |
| C | 4.284451395 | 1.626916973 | 1.979758742 |
| H | 5.213072853 | 1.595104637 | 2.541692818 |
| C | 4.235772135 | 1.139831220 | 0.662808344 |
| H | 5.113286239 | 0.707140665 | 0.193950200 |
| C | 3.028962766 | 1.214412136 | -0.047292337 |
| C | 2.875967968 | 0.714131188 | -1.464095887 |
| H | 2.681516968 | -0.361302812 | -1.426375887 |
| H | 3.797158968 | 0.882180188 | -2.039369887 |
| C | 1.362701968 | 0.784694188 | -3.426728887 |
| H | 1.090226968 | -0.257124812 | -3.252690887 |
| H | 0.506400968 | 1.297496188 | -3.871436887 |
| H | 2.213779968 | 0.828234188 | -4.120747887 |
| C | -1.054472011 | 3.535723029 | 0.827542854 |
| O | -1.765919011 | 4.053818029 | 1.671357854 |
| O | -1.066582569 | 2.118469846 | 0.625654267 |
| Mn | 0.692438630 | -2.084132273 | 0.206461227 |
| N | -0.983940943 | -2.488771060 | 1.537777464 |
| N | 1.055707713 | -4.146076648 | 0.381452568 |
| N | -0.245269598 | -2.872027814 | -1.621084640 |
| N | 1.399344293 | -1.484392070 | 2.481443976 |
| C | -0.664976320 | -3.824064762 | 2.190434502 |
| H | 0.048557596 | -3.646154577 | 2.998028169 |
| H | -1.566139097 | -4.269405086 | 2.636732946 |
| C | -0.069143685 | -4.792113640 | 1.163388815 |
| H | -0.834249850 | -5.096172079 | 0.442185109 |
| H | 0.288369344 | -5.701810148 | 1.664366304 |
| C | 2.417040188 | -4.240060233 | 1.027813326 |
| H | 2.326930660 | -4.067837042 | 2.103911477 |
| H | 2.882962439 | -5.221583019 | 0.877605291 |
| C | 1.144207232 | -4.755611000 | -1.002394843 |
| H | 2.138336049 | -4.535024558 | -1.406490859 |
| H | 1.050684283 | -5.847428690 | -0.935856896 |
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| C | -0.413851558 | -4.849737784 | -3.034811505 |
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| C | -1.317818496 | -4.181185543 | -3.881952705 |
| H | -1.734228667 | -4.688206591 | -4.747327962 |
| C | -1.674458832 | -2.850116747 | -3.590718260 |
| H | -2.366592749 | -2.305112539 | -4.224208115 |
| C | -1.126286174 | -2.226523735 | -2.457939428 |
| H | -1.360536845 | -1.200325285 | -2.185444578 |
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| C | 1.688980024 | -0.416991606 | 5.067348541 |
| H | 1.797994460 | -0.018926294 | 6.071894039 |
| C | 0.410482215 | -0.622057751 | 4.517149658 |
| H | -0.484002896 | -0.384532259 | 5.085528445 |
| C | 0.304105886 | -1.160173834 | 3.222818696 |
| C | -1.043545749 | -1.398820266 | 2.571478277 |
| H | -1.368646975 | -0.487995868 | 2.056392179 |
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| H | -2.450687079 | -1.594316042 | 0.284444940 |
| H | -2.310705291 | -3.355940296 | 0.095374816 |
| H | -3.125606472 | -2.689523764 | 1.531004462 |
| C | 3.310480308 | -3.126713465 | 0.418099225 |
| O | 4.542692617 | -3.122513580 | 0.577148376 |
| O | 2.609595318 | -2.176945054 | -0.239284371 |
| O | -1.211115346 | 0.874577974 | -1.826787048 |
| O | -2.656770538 | 0.726799691 | -0.619748749 |
| H | -3.427890538 | 0.873607691 | -1.213508749 |
| H | -2.048069500 | 1.398977116 | 0.026626243 |

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| Mn | 0.254824000 | 1.382273000 | -0.760476000 |
| O | 0.377984000 | -0.309833000 | -0.198143000 |
| N | 1.765314000 | 1.421412000 | -2.173167000 |
| N | -0.123453000 | 3.454368000 | -1.440509000 |
| N | -1.094084000 | 6.132107000 | -2.161072000 |
| N | 1.929145000 | 1.744493000 | 0.439728000 |
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| H | 2.780861000 | 3.171391000 | -1.504950000 |
| H | 2.772948000 | 2.983903000 | -3.258918000 |
| C | 0.947927000 | 3.809393000 | -2.451851000 |
| H | 0.488928000 | 3.723121000 | -3.440556000 |
| H | 1.255206000 | 4.854507000 | -2.340209000 |
| C | -0.080451000 | 4.213737000 | -0.135983000 |
| H | 0.932067000 | 4.190307000 | 0.277021000 |
| H | -0.379305000 | 5.255742000 | -0.286760000 |
| C | -1.481335000 | 3.672462000 | -2.089765000 |
| H | -1.598812000 | 2.902371000 | -2.852937000 |
| H | -2.253609000 | 3.473093000 | -1.336533000 |
| C | -1.729872000 | 5.057128000 | -2.696725000 |

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| H | -3.136683000 | 4.310841000 | -4.177368000 |
| C | -2.930028000 | 6.469867000 | -4.263424000 |
| H | -3.638719000 | 6.597333000 | -5.076450000 |
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| H | -2.463486000 | 8.588853000 | -4.065456000 |
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| C | 1.954176000 | 2.192228000 | 1.724449000 |
| H | 1.020901000 | 2.546729000 | 2.144743000 |
| C | 3.124276000 | 2.179945000 | 2.492914000 |
| H | 3.106551000 | 2.568488000 | 3.505360000 |
| C | 4.304117000 | 1.657155000 | 1.927978000 |
| H | 5.227755000 | 1.633430000 | 2.498460000 |
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| C | 3.068600000 | 1.223970000 | -0.107015000 |
| C | 2.930372000 | 0.712174000 | -1.521221000 |
| H | 2.735921000 | -0.363260000 | -1.483501000 |
| H | 3.851563000 | 0.880223000 | -2.096495000 |
| C | 1.417106000 | 0.782737000 | -3.483854000 |
| H | 1.144631000 | -0.259082000 | -3.309816000 |
| H | 0.560805000 | 1.295539000 | -3.928562000 |
| H | 2.268184000 | 0.826277000 | -4.177873000 |
| C | -1.057411000 | 3.532280000 | 0.824048000 |
| O | -1.768858000 | 4.050375000 | 1.667863000 |
| O | -1.060505000 | 2.110038000 | 0.612746000 |
| Mn | 0.678977000 | -2.016519000 | 0.181183000 |
| N | -1.147510000 | -2.511773000 | 1.303313000 |
| N | 1.078856000 | -4.085078000 | 0.359388000 |
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| C | -0.855293000 | -3.848554000 | 1.953121000 |
| H | -0.249364000 | -3.671028000 | 2.844370000 |
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| H | 0.206769000 | -5.688835000 | 1.509349000 |
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| H | 2.128425000 | -4.000786000 | 2.222935000 |
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| C | 1.022189000 | -0.453800000 | 5.170069000 |
| H | 0.998354000 | -0.076178000 | 6.188050000 |
| C | -0.174576000 | -0.678770000 | 4.465463000 |
| H | -1.137251000 | -0.477212000 | 4.926123000 |
| C | -0.109332000 | -1.189661000 | 3.157445000 |
| C | -1.361612000 | -1.447641000 | 2.343441000 |
| H | -1.647846000 | -0.533857000 | 1.810830000 |
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| C | -2.367737000 | -2.577514000 | 0.428096000 |
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| O | 4.484319000 | -2.964548000 | 0.994026000 |
| O | 2.637676000 | -2.050166000 | -0.031324000 |
| O | -1.251731000 | 0.895246000 | -1.864555000 |
| O | -2.448344000 | 0.701750000 | -0.903328000 |
| H | -3.219464000 | 0.848558000 | -1.497088000 |
| H | -1.931800000 | 1.645914000 | 0.365143000 |
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| Mn | 0.123700164 | 1.551146385 | -0.558931127 |
| O | 0.123504633 | -0.183260357 | 0.077231051 |
| N | 1.958817226 | 1.524989787 | -1.928288166 |
| N | -0.099158583 | 3.572824614 | -1.572793574 |
| N | -0.995961984 | 6.126962225 | -2.800241792 |
| N | 1.818728724 | 2.009256578 | 0.735238550 |
| C | 2.256600015 | 2.966150634 | -2.251650339 |
| H | 2.730859653 | 3.417859664 | -1.375426156 |
| H | 2.978697284 | 3.034322512 | -3.080055611 |
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| H | 0.583877827 | 3.360903566 | -3.562760789 |
| H | 1.215370074 | 4.794929949 | -2.766822449 |
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| H | 1.038852220 | 4.519095373 | -0.015232853 |
| H | -0.157975504 | 5.584314785 | -0.819274454 |
| C | -1.460739322 | 3.749002741 | -2.240271636 |
| H | -1.669603841 | 2.841116193 | -2.809849504 |
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| C | -2.054646794 | 7.249351362 | -4.670868619 |
| H | -2.198705519 | 8.164115617 | -5.236248541 |
| C | -1.202667282 | 7.237073722 | -3.550542974 |
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| C | 1.721728148 | 2.532763228 | 1.989724065 |
| H | 0.735464986 | 2.842575029 | 2.309904744 |
| C | 2.834394501 | 2.664101528 | 2.830188867 |
| H | 2.716672274 | 3.111406518 | 3.811370628 |
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| C | 4.181734118 | 1.650206132 | 1.090074138 |
| H | 5.129817915 | 1.284742806 | 0.708578288 |
| C | 3.030888674 | 1.568573409 | 0.287676987 |
| C | 3.062946958 | 0.957512571 | -1.091794584 |
| H | 2.930347588 | -0.127415449 | -0.984278006 |
| H | 4.041554061 | 1.137083146 | -1.562380896 |
| C | 1.764797283 | 0.697736054 | -3.160433928 |
| H | 1.515671128 | -0.326354786 | -2.869321236 |
| H | 0.945786846 | 1.099066560 | -3.764262714 |
| H | 2.676281570 | 0.679557752 | -3.777031566 |
| C | -0.991559480 | 4.252482414 | 0.643346248 |
| O | -1.691475828 | 5.040272974 | 1.261201223 |
| O | -1.034838248 | 2.852786449 | 0.862658739 |
| Mn | 0.584356144 | -1.878029455 | 0.309938167 |
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| N | 1.233105207 | -3.934580616 | 0.205316314 |
| N | -0.228748991 | -2.484897533 | -1.574415506 |
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| H | -1.272208776 | -5.007608869 | 2.354048408 |
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| H | -0.480340957 | -5.168196165 | 0.005778119 |
| H | 0.735524528 | -5.829337236 | 1.100656120 |
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| H | 1.511361685 | -5.318088605 | -1.425720441 |
| C | 0.291539174 | -3.645262546 | -2.074646718 |
| C | -0.163780260 | -4.192852076 | -3.283451071 |
| H | 0.264081047 | -5.117258275 | -3.659090733 |
| C | -1.176235902 | -3.523666511 | -3.996612994 |
| H | -1.549449229 | -3.932313447 | -4.930965487 |
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| H | -1.544993100 | -0.887874726 | -1.841937347 |
| C | 2.144752953 | -0.979121531 | 2.920594081 |
| H | 2.925328571 | -0.862581383 | 2.180476528 |
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| H | 3.321430636 | -0.250343565 | 4.572645056 |
| C | 1.297277204 | -0.778665515 | 5.178218052 |
| H | 1.429681507 | -0.523303066 | 6.225342401 |
| C | 0.066825563 | -1.279692015 | 4.716980160 |

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| H | -0.768120576 | -1.414635500 | 5.397946412 |
| C | -0.071449007 | -1.623798445 | 3.362039065 |
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| H | -2.012826054 | -1.291351378 | 2.511466019 |
| H | -1.938575965 | -2.688316428 | 3.590503996 |
| C | -2.443549673 | -3.185561523 | 0.873721089 |
| H | -2.832693301 | -2.218237623 | 0.539407473 |
| H | -2.290531039 | -3.811895518 | -0.007919231 |
| H | -3.200029658 | -3.661740643 | 1.516996256 |
| C | 3.373390497 | -2.701389844 | 0.488621332 |
| O | 4.598669613 | -2.617135551 | 0.685317479 |
| O | 2.591349659 | -1.732337751 | -0.018857521 |
| O | -1.666598000 | 1.191143000 | -1.259073000 |
| O | -2.573208000 | 1.028263000 | -0.079985000 |
| H | -2.575130355 | 0.055388302 | 0.074938619 |
| H | -1.916086501 | 2.386782181 | 0.944370637 |

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| Mn | 0.278463000 | 1.355226000 | -0.777521000 |
| O | 0.325642000 | -0.333496000 | -0.220015000 |
| N | 1.963058000 | 1.528849000 | -2.228442000 |
| N | -0.052725000 | 3.479773000 | -1.444309000 |
| N | -1.176784000 | 6.143439000 | -2.225836000 |
| N | 2.053095000 | 1.811575000 | 0.450623000 |
| C | 2.235343000 | 3.000468000 | -2.401639000 |
| H | 2.803735000 | 3.347519000 | -1.535315000 |
| H | 2.862785000 | 3.170050000 | -3.289756000 |
| C | 0.947461000 | 3.797307000 | -2.540856000 |
| H | 0.461213000 | 3.561121000 | -3.492636000 |
| H | 1.165454000 | 4.871002000 | -2.556565000 |
| C | 0.148976000 | 4.355092000 | -0.225044000 |
| H | 1.197461000 | 4.297502000 | 0.082553000 |
| H | -0.108352000 | 5.391959000 | -0.468372000 |
| C | -1.461291000 | 3.686034000 | -2.000927000 |
| H | -1.677290000 | 2.847949000 | -2.666076000 |
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| C | -1.723519000 | 5.004322000 | -2.729815000 |
| C | -2.572025000 | 5.020717000 | -3.854761000 |
| H | -2.991212000 | 4.096774000 | -4.244465000 |
| C | -2.879207000 | 6.254836000 | -4.460452000 |
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| C | 2.066978000 | 2.270987000 | 1.732549000 |
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| H | 3.220034000 | 2.762584000 | 3.485119000 |
| C | 4.456642000 | 1.927538000 | 1.894528000 |
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| C | 4.434881000 | 1.421770000 | 0.583435000 |

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| H | 5.342113000 | 1.064788000 | 0.107046000 |
| C | 3.218906000 | 1.386760000 | -0.117500000 |
| C | 3.120310000 | 0.868998000 | -1.534663000 |
| H | 2.958814000 | -0.214495000 | -1.495439000 |
| H | 4.058381000 | 1.056419000 | -2.078154000 |
| C | 1.666959000 | 0.855003000 | -3.531772000 |
| H | 1.427160000 | -0.195921000 | -3.349109000 |
| H | 0.810636000 | 1.329867000 | -4.019597000 |
| H | 2.530055000 | 0.908827000 | -4.211722000 |
| C | -0.730491000 | 3.885601000 | 0.912543000 |
| O | -1.317761000 | 4.576419000 | 1.733811000 |
| O | -0.796581000 | 2.474214000 | 0.914033000 |
| Mn | 0.578108000 | -2.031600000 | 0.243409000 |
| N | -1.377691000 | -2.794198000 | 1.316998000 |
| N | 1.035942000 | -4.111265000 | 0.371386000 |
| N | -0.094550000 | -2.710880000 | -1.647729000 |
| N | 0.768014000 | -1.492991000 | 2.398195000 |
| C | -0.962723000 | -4.106545000 | 1.920743000 |
| H | -0.383239000 | -3.909006000 | 2.826932000 |
| H | -1.842166000 | -4.697539000 | 2.220942000 |
| C | -0.120989000 | -4.919832000 | 0.931402000 |
| H | -0.742680000 | -5.235040000 | 0.087440000 |
| H | 0.260171000 | -5.829289000 | 1.414079000 |
| C | 2.304327000 | -4.208471000 | 1.180947000 |
| H | 2.068862000 | -4.107110000 | 2.245054000 |
| H | 2.802792000 | -5.174525000 | 1.033687000 |
| C | 1.338173000 | -4.567202000 | -1.045793000 |
| H | 2.351014000 | -4.236706000 | -1.298303000 |
| H | 1.319335000 | -5.662853000 | -1.100913000 |
| C | 0.367002000 | -3.941513000 | -2.016084000 |
| C | -0.004683000 | -4.527394000 | -3.235292000 |
| H | 0.371767000 | -5.508116000 | -3.509183000 |
| C | -0.866605000 | -3.819076000 | -4.093604000 |
| H | -1.168284000 | -4.251363000 | -5.043097000 |
| C | -1.333633000 | -2.547934000 | -3.705297000 |
| H | -2.000855000 | -1.978163000 | -4.343238000 |
| C | -0.929667000 | -2.018123000 | -2.470766000 |
| H | -1.255346000 | -1.042582000 | -2.119772000 |
| C | 1.941941000 | -1.162361000 | 3.004619000 |
| H | 2.838013000 | -1.222606000 | 2.401085000 |
| C | 1.998202000 | -0.755917000 | 4.345688000 |
| H | 2.958066000 | -0.529002000 | 4.797065000 |
| C | 0.802766000 | -0.664010000 | 5.081712000 |
| H | 0.815289000 | -0.359362000 | 6.123972000 |
| C | -0.411148000 | -0.985154000 | 4.447447000 |
| H | -1.352162000 | -0.932081000 | 4.986425000 |
| C | -0.396006000 | -1.399411000 | 3.105713000 |
| C | -1.664875000 | -1.765944000 | 2.364144000 |
| H | -2.061289000 | -0.882829000 | 1.847274000 |
| H | -2.432650000 | -2.111892000 | 3.073646000 |
| C | -2.563890000 | -2.940807000 | 0.418038000 |
| H | -2.764482000 | -1.984095000 | -0.071306000 |

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|---|--------------|--------------|--------------|
| H | -2.372987000 | -3.691255000 | -0.352225000 |
| H | -3.457733000 | -3.245921000 | 0.984470000 |
| C | 3.251840000 | -3.048307000 | 0.764350000 |
| O | 4.451136000 | -3.055762000 | 1.098437000 |
| O | 2.627080000 | -2.073580000 | 0.084819000 |
| O | -1.526306000 | 0.905966000 | -1.438389000 |
| O | -1.690576000 | 0.668520000 | 0.006285000 |
| H | -0.911324000 | -0.066366000 | 0.077571000 |
| H | -1.695250000 | 2.048433000 | 0.977721000 |

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| Mn | -0.212356000 | 0.951151000 | 0.179782000 |
| O | 0.857035000 | 0.806354000 | 2.042943000 |
| O | 1.558652000 | 1.082855000 | 4.544075000 |
| N | 0.351748000 | 1.051401000 | -2.140920000 |
| N | -2.249346000 | 1.591471000 | -0.739789000 |
| N | -0.202823000 | 3.210021000 | 0.308112000 |
| N | 0.164221000 | -1.189911000 | -0.519277000 |
| C | -0.986671000 | 0.798184000 | -2.786276000 |
| H | -1.252449000 | -0.250000000 | -2.616467000 |
| H | -0.920717000 | 0.944720000 | -3.877042000 |
| C | -2.094344000 | 1.709700000 | -2.231589000 |
| H | -1.866424000 | 2.754615000 | -2.464270000 |
| H | -3.039920000 | 1.472181000 | -2.741364000 |
| C | -3.197196000 | 0.517923000 | -0.312370000 |
| H | -3.029115000 | -0.373704000 | -0.928932000 |
| H | -4.250015000 | 0.807989000 | -0.435462000 |
| C | -2.604749000 | 2.906852000 | -0.121173000 |
| H | -3.013347000 | 2.713843000 | 0.878598000 |
| H | -3.393536000 | 3.417911000 | -0.692806000 |
| C | -1.392743000 | 3.815172000 | 0.026043000 |
| C | -1.496758000 | 5.215189000 | -0.065795000 |
| H | -2.450750000 | 5.675471000 | -0.305978000 |
| C | -0.353387000 | 6.006554000 | 0.151613000 |
| H | -0.411823000 | 7.088364000 | 0.075490000 |
| C | 0.868343000 | 5.375977000 | 0.460022000 |
| H | 1.772655000 | 5.950877000 | 0.630412000 |
| C | 0.900442000 | 3.974420000 | 0.526637000 |
| H | 1.818746000 | 3.442417000 | 0.755672000 |
| C | -0.256896000 | -2.295581000 | 0.156865000 |
| H | -0.810008000 | -2.120914000 | 1.070161000 |
| C | 0.012741000 | -3.596860000 | -0.289941000 |
| H | -0.339034000 | -4.448138000 | 0.282662000 |
| C | 0.742642000 | -3.766794000 | -1.480620000 |
| H | 0.970590000 | -4.760817000 | -1.853559000 |
| C | 1.161789000 | -2.626698000 | -2.190302000 |
| H | 1.711178000 | -2.723863000 | -3.121881000 |
| C | 0.855346000 | -1.352722000 | -1.684889000 |
| C | 1.289487000 | -0.088867000 | -2.402332000 |
| H | 2.285270000 | 0.211884000 | -2.048946000 |
| H | 1.381955000 | -0.287377000 | -3.482150000 |
| C | 0.968851000 | 2.317006000 | -2.650483000 |

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|----|--------------|--------------|--------------|
| H | 1.912720000 | 2.503289000 | -2.128739000 |
| H | 0.307902000 | 3.166593000 | -2.470429000 |
| H | 1.173063000 | 2.256365000 | -3.731163000 |
| C | 2.333116000 | 0.909995000 | 5.718593000 |
| Mn | -0.393619000 | 0.258176000 | 3.487056000 |
| C | -2.976149000 | 0.118933000 | 1.165087000 |
| O | -3.932265000 | -0.330518000 | 1.841031000 |
| N | -1.927585000 | -0.428649000 | 4.859956000 |
| C | -1.507648000 | -0.417169000 | 6.325886000 |
| H | -1.212273000 | 0.609637000 | 6.572702000 |
| H | -2.404588000 | -0.651169000 | 6.920488000 |
| C | -0.404890000 | -1.401006000 | 6.728170000 |
| N | 0.902021000 | -1.076704000 | 6.117639000 |
| N | 1.902333000 | -2.650310000 | 8.264931000 |
| C | 2.427722000 | -2.911072000 | 7.038600000 |
| C | 1.775358000 | -2.234964000 | 5.825206000 |
| C | 1.618486000 | 0.048197000 | 6.743671000 |
| H | 0.914430000 | 0.696616000 | 7.281527000 |
| H | 2.361982000 | -0.277622000 | 7.480409000 |
| H | 1.177635000 | -2.974130000 | 5.279147000 |
| H | 2.560149000 | -1.916277000 | 5.123911000 |
| C | 3.510153000 | -3.796598000 | 6.859804000 |
| H | 3.914922000 | -3.976999000 | 5.867121000 |
| C | 4.056992000 | -4.440531000 | 7.983978000 |
| H | 4.890725000 | -5.127986000 | 7.873478000 |
| C | 3.511381000 | -4.175624000 | 9.255050000 |
| H | 3.905190000 | -4.649058000 | 10.148538000 |
| C | 2.439137000 | -3.271578000 | 9.347699000 |
| H | 1.992173000 | -3.032706000 | 10.308663000 |
| N | -1.240895000 | 2.083139000 | 4.042313000 |
| C | -0.656235000 | 3.301187000 | 3.890046000 |
| H | 0.323241000 | 3.316288000 | 3.429345000 |
| C | -1.288529000 | 4.477084000 | 4.310624000 |
| H | -0.790649000 | 5.432811000 | 4.188510000 |
| C | -2.563404000 | 4.386762000 | 4.905196000 |
| H | -3.073056000 | 5.280595000 | 5.252600000 |
| C | -3.163809000 | 3.124112000 | 5.057553000 |
| H | -4.140594000 | 3.024030000 | 5.519935000 |
| C | -2.478091000 | 1.981057000 | 4.615442000 |
| C | -3.045623000 | 0.585674000 | 4.695225000 |
| C | -2.431977000 | -1.795366000 | 4.461141000 |
| H | -2.918108000 | -1.725187000 | 3.486247000 |
| H | -1.597631000 | -2.495329000 | 4.404383000 |
| H | -3.161291000 | -2.155110000 | 5.199888000 |
| H | -3.580932000 | 0.343478000 | 3.768347000 |
| H | -3.758242000 | 0.497880000 | 5.525667000 |
| H | -0.674285000 | -2.420695000 | 6.438728000 |
| H | -0.340201000 | -1.411939000 | 7.826037000 |
| O | 3.433199000 | 1.445199000 | 5.818965000 |
| O | -1.728633000 | 0.280262000 | 1.623951000 |
| H | 1.569905000 | 0.119789000 | 2.032414000 |
| H | 2.053471000 | 1.568365000 | 3.843768000 |

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| O | 0.246590000 | -1.608744000 | 3.248515000 |
| O | 1.488529000 | -1.780130000 | 2.734713000 |

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|----|--------------|--------------|--------------|
| Mn | -0.140523000 | 0.971758000 | 0.056124000 |
| O | 1.004063000 | 0.671673000 | 1.830806000 |
| O | 1.359090000 | 1.081865000 | 4.292008000 |
| N | 0.369844000 | 1.084467000 | -2.262979000 |
| N | -2.183939000 | 1.731746000 | -0.810134000 |
| N | -0.058275000 | 3.208006000 | 0.307048000 |
| N | 0.156742000 | -1.178046000 | -0.667436000 |
| C | -0.991282000 | 0.919892000 | -2.888461000 |
| H | -1.311624000 | -0.115470000 | -2.731415000 |
| H | -0.934661000 | 1.081994000 | -3.977603000 |
| C | -2.036008000 | 1.882267000 | -2.298739000 |
| H | -1.745765000 | 2.917376000 | -2.505166000 |
| H | -2.998389000 | 1.717765000 | -2.806284000 |
| C | -3.183618000 | 0.696629000 | -0.405464000 |
| H | -3.070775000 | -0.182021000 | -1.052586000 |
| H | -4.220666000 | 1.046804000 | -0.504054000 |
| C | -2.468884000 | 3.044495000 | -0.149251000 |
| H | -2.891442000 | 2.840973000 | 0.842923000 |
| H | -3.226890000 | 3.615949000 | -0.705274000 |
| C | -1.212832000 | 3.883181000 | 0.037166000 |
| C | -1.245081000 | 5.288927000 | 0.003938000 |
| H | -2.171337000 | 5.806976000 | -0.226928000 |
| C | -0.066624000 | 6.010846000 | 0.272255000 |
| H | -0.069864000 | 7.096520000 | 0.243886000 |
| C | 1.116382000 | 5.306998000 | 0.572435000 |
| H | 2.043940000 | 5.827646000 | 0.786196000 |
| C | 1.078944000 | 3.903848000 | 0.577114000 |
| H | 1.962680000 | 3.314498000 | 0.800799000 |
| C | -0.254955000 | -2.275276000 | 0.027043000 |
| H | -0.771842000 | -2.087290000 | 0.960099000 |
| C | -0.036388000 | -3.580866000 | -0.434298000 |
| H | -0.380331000 | -4.427721000 | 0.149760000 |
| C | 0.628984000 | -3.761690000 | -1.661752000 |
| H | 0.813318000 | -4.759250000 | -2.049106000 |
| C | 1.041566000 | -2.629390000 | -2.387011000 |
| H | 1.544796000 | -2.736181000 | -3.343282000 |
| C | 0.791437000 | -1.349861000 | -1.862321000 |
| C | 1.241538000 | -0.092362000 | -2.583184000 |
| H | 2.265112000 | 0.157037000 | -2.272164000 |
| H | 1.275607000 | -0.276940000 | -3.668866000 |
| C | 1.041068000 | 2.336505000 | -2.738394000 |
| H | 2.004676000 | 2.452196000 | -2.232666000 |
| H | 0.429864000 | 3.210599000 | -2.506725000 |
| H | 1.216691000 | 2.310156000 | -3.825372000 |
| C | 2.314171000 | 0.495031000 | 5.129356000 |
| Mn | -0.594836000 | 0.291710000 | 3.301779000 |
| C | -2.962223000 | 0.235703000 | 1.051460000 |
| O | -3.912675000 | -0.181276000 | 1.748581000 |

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| N | -2.018464000 | -0.519053000 | 4.889093000 |
| C | -1.473425000 | -0.466687000 | 6.305708000 |
| H | -1.122348000 | 0.556132000 | 6.483435000 |
| H | -2.316611000 | -0.637515000 | 6.996408000 |
| C | -0.391214000 | -1.482842000 | 6.701333000 |
| N | 0.936852000 | -1.306206000 | 6.070391000 |
| N | 1.950027000 | -2.497107000 | 8.437070000 |
| C | 2.502198000 | -2.908471000 | 7.266210000 |
| C | 1.780748000 | -2.512134000 | 5.970207000 |
| C | 1.678621000 | -0.066113000 | 6.397142000 |
| H | 0.999995000 | 0.679450000 | 6.818671000 |
| H | 2.471233000 | -0.261883000 | 7.126620000 |
| H | 1.139842000 | -3.340690000 | 5.644722000 |
| H | 2.523537000 | -2.360998000 | 5.173838000 |
| C | 3.663995000 | -3.703508000 | 7.219002000 |
| H | 4.090676000 | -4.001345000 | 6.265023000 |
| C | 4.262257000 | -4.101703000 | 8.428758000 |
| H | 5.157027000 | -4.717376000 | 8.422997000 |
| C | 3.689004000 | -3.683098000 | 9.644621000 |
| H | 4.121427000 | -3.965330000 | 10.599003000 |
| C | 2.537484000 | -2.876951000 | 9.601056000 |
| H | 2.067634000 | -2.523519000 | 10.514428000 |
| N | -1.522713000 | 2.122615000 | 4.083611000 |
| C | -1.027414000 | 3.386552000 | 4.000695000 |
| H | -0.084637000 | 3.506803000 | 3.478622000 |
| C | -1.684789000 | 4.482071000 | 4.577152000 |
| H | -1.256781000 | 5.475766000 | 4.499571000 |
| C | -2.892731000 | 4.258169000 | 5.267166000 |
| H | -3.423486000 | 5.083990000 | 5.731653000 |
| C | -3.394447000 | 2.947890000 | 5.364505000 |
| H | -4.313727000 | 2.744052000 | 5.904598000 |
| C | -2.685669000 | 1.893753000 | 4.762738000 |
| C | -3.171317000 | 0.458809000 | 4.796533000 |
| C | -2.529350000 | -1.891986000 | 4.545406000 |
| H | -3.042918000 | -1.847696000 | 3.581031000 |
| H | -1.697896000 | -2.595466000 | 4.475963000 |
| H | -3.238428000 | -2.249534000 | 5.307259000 |
| H | -3.715038000 | 0.236090000 | 3.869623000 |
| H | -3.865016000 | 0.313138000 | 5.637364000 |
| H | -0.723344000 | -2.501774000 | 6.483137000 |
| H | -0.271523000 | -1.430635000 | 7.795334000 |
| O | 3.500727000 | 0.426429000 | 4.809654000 |
| O | -1.689151000 | 0.305768000 | 1.471386000 |
| H | 1.636960000 | -0.071185000 | 1.713700000 |
| H | 1.661727000 | 1.232276000 | 3.333133000 |
| O | 0.339938000 | -1.692783000 | 3.498007000 |
| O | 1.440360000 | -2.093968000 | 2.914600000 |

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|----|-------------|--------------|-------------|
| Mn | 1.001604000 | -0.239747000 | 0.047058000 |
| O | 2.219108000 | -1.202715000 | 1.398282000 |
| O | 1.051656000 | 1.016808000 | 3.602300000 |

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|----|--------------|--------------|--------------|
| N | 1.534253000 | -0.279950000 | -2.252076000 |
| N | -0.563538000 | 1.302762000 | -0.825880000 |
| N | 1.883913000 | 1.857190000 | 0.509469000 |
| N | 0.202863000 | -2.233692000 | -0.795260000 |
| C | 0.278267000 | 0.200043000 | -2.931600000 |
| H | -0.462477000 | -0.603947000 | -2.877550000 |
| H | 0.470934000 | 0.392888000 | -3.999780000 |
| C | -0.292598000 | 1.475365000 | -2.290770000 |
| H | 0.420031000 | 2.299124000 | -2.404599000 |
| H | -1.204826000 | 1.769268000 | -2.832930000 |
| C | -1.875571000 | 0.661534000 | -0.516264000 |
| H | -2.082894000 | -0.118726000 | -1.257060000 |
| H | -2.714972000 | 1.371946000 | -0.558337000 |
| C | -0.391679000 | 2.584493000 | -0.076944000 |
| H | -0.898215000 | 2.475404000 | 0.888714000 |
| H | -0.871951000 | 3.424068000 | -0.602300000 |
| C | 1.071336000 | 2.909371000 | 0.185959000 |
| C | 1.561305000 | 4.226865000 | 0.157558000 |
| H | 0.901610000 | 5.046697000 | -0.111107000 |
| C | 2.909640000 | 4.470239000 | 0.483554000 |
| H | 3.303130000 | 5.482235000 | 0.470549000 |
| C | 3.739668000 | 3.385438000 | 0.824524000 |
| H | 4.781547000 | 3.533211000 | 1.087704000 |
| C | 3.189450000 | 2.094478000 | 0.821255000 |
| H | 3.786445000 | 1.224125000 | 1.074886000 |
| C | -0.671448000 | -3.059743000 | -0.157277000 |
| H | -1.111562000 | -2.677336000 | 0.756125000 |
| C | -0.994124000 | -4.333023000 | -0.648615000 |
| H | -1.703985000 | -4.958119000 | -0.117090000 |
| C | -0.388692000 | -4.771122000 | -1.842419000 |
| H | -0.619567000 | -5.749531000 | -2.253063000 |
| C | 0.513452000 | -3.917831000 | -2.501843000 |
| H | 0.990992000 | -4.224142000 | -3.427846000 |
| C | 0.790369000 | -2.654175000 | -1.950276000 |
| C | 1.796211000 | -1.714722000 | -2.595061000 |
| H | 2.802819000 | -1.965754000 | -2.233994000 |
| H | 1.802843000 | -1.866575000 | -3.686492000 |
| C | 2.716036000 | 0.554250000 | -2.638814000 |
| H | 3.604992000 | 0.205687000 | -2.103176000 |
| H | 2.546052000 | 1.599748000 | -2.372149000 |
| H | 2.914862000 | 0.496902000 | -3.720561000 |
| C | 1.375589000 | 1.674918000 | 4.812047000 |
| Mn | -0.503740000 | -0.606450000 | 3.625963000 |
| C | -1.876986000 | -0.012104000 | 0.874525000 |
| O | -2.944219000 | -0.443166000 | 1.372870000 |
| N | -2.120868000 | -1.497644000 | 4.977614000 |
| C | -1.778760000 | -1.029008000 | 6.370673000 |
| H | -2.060583000 | 0.025459000 | 6.448001000 |
| H | -2.381525000 | -1.578460000 | 7.111912000 |
| C | -0.293789000 | -1.199658000 | 6.722665000 |
| N | 0.626802000 | -0.516297000 | 5.750144000 |
| N | 2.619177000 | -0.460827000 | 7.959195000 |

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| C | 2.665213000 | -1.455529000 | 7.029944000 |
| C | 1.965632000 | -1.212589000 | 5.692943000 |
| C | 0.789729000 | 0.949955000 | 6.014716000 |
| H | -0.191471000 | 1.397153000 | 6.218252000 |
| H | 1.440732000 | 1.126639000 | 6.879013000 |
| H | 1.815563000 | -2.162172000 | 5.173362000 |
| H | 2.618635000 | -0.613718000 | 5.045253000 |
| C | 3.369978000 | -2.654060000 | 7.259644000 |
| H | 3.384793000 | -3.436043000 | 6.504904000 |
| C | 4.059112000 | -2.821928000 | 8.476574000 |
| H | 4.613825000 | -3.734740000 | 8.673988000 |
| C | 4.013212000 | -1.792074000 | 9.433456000 |
| H | 4.529117000 | -1.880394000 | 10.384011000 |
| C | 3.274524000 | -0.631785000 | 9.133939000 |
| H | 3.207198000 | 0.186212000 | 9.845569000 |
| N | -2.082221000 | 1.084834000 | 3.994259000 |
| C | -1.942597000 | 2.420716000 | 3.774250000 |
| H | -0.946416000 | 2.770347000 | 3.523038000 |
| C | -3.012933000 | 3.320184000 | 3.874881000 |
| H | -2.853194000 | 4.379750000 | 3.704210000 |
| C | -4.284356000 | 2.817472000 | 4.216541000 |
| H | -5.136316000 | 3.484582000 | 4.307941000 |
| C | -4.430556000 | 1.440023000 | 4.449400000 |
| H | -5.395239000 | 1.022245000 | 4.720717000 |
| C | -3.310300000 | 0.597861000 | 4.329237000 |
| C | -3.422412000 | -0.901271000 | 4.525967000 |
| C | -2.193831000 | -2.991110000 | 4.905817000 |
| H | -2.419171000 | -3.297318000 | 3.879122000 |
| H | -1.237004000 | -3.430857000 | 5.200634000 |
| H | -2.978391000 | -3.387783000 | 5.568778000 |
| H | -3.683746000 | -1.347687000 | 3.558628000 |
| H | -4.228366000 | -1.131003000 | 5.240166000 |
| H | -0.028805000 | -2.262211000 | 6.721945000 |
| H | -0.128009000 | -0.838773000 | 7.747073000 |
| O | 2.026042000 | 2.716097000 | 4.810983000 |
| O | -0.681467000 | -0.121520000 | 1.467280000 |
| H | 3.151768000 | -1.479004000 | 1.375534000 |
| O | 0.695131000 | -2.199818000 | 2.976645000 |
| H | 1.497666000 | -1.802637000 | 2.227488000 |
| H | 0.567005000 | -3.163981000 | 2.972489000 |
| H | 1.482733000 | 1.384486000 | 2.795312000 |

Isomers:

¹⁵

| | | | |
|----|--------------|-------------|--------------|
| Mn | -0.317788000 | 1.856063000 | 0.429657000 |
| O | 0.102614000 | 0.158779000 | 0.075402000 |
| N | 1.387113000 | 2.816279000 | -0.520343000 |
| N | -0.855869000 | 3.803798000 | 0.996873000 |
| N | 0.499357000 | 2.007867000 | 2.540442000 |
| N | -0.857799000 | 2.077624000 | -1.947406000 |

| | | | |
|----|--------------|--------------|--------------|
| C | 0.987798000 | 4.272976000 | -0.653690000 |
| H | 0.341135000 | 4.371288000 | -1.528889000 |
| H | 1.876485000 | 4.897046000 | -0.825676000 |
| C | 0.254541000 | 4.758185000 | 0.602949000 |
| H | 0.948306000 | 4.812929000 | 1.447100000 |
| H | -0.149877000 | 5.766167000 | 0.441182000 |
| C | -2.180192000 | 4.028359000 | 0.311222000 |
| H | -2.016924000 | 4.251811000 | -0.746638000 |
| H | -2.734015000 | 4.862221000 | 0.758439000 |
| C | -1.086423000 | 3.849067000 | 2.493856000 |
| H | -2.071847000 | 3.415488000 | 2.694834000 |
| H | -1.109596000 | 4.893053000 | 2.832719000 |
| C | -0.037961000 | 3.051876000 | 3.233797000 |
| C | 0.325699000 | 3.331454000 | 4.559612000 |
| H | -0.114602000 | 4.174551000 | 5.083650000 |
| C | 1.269517000 | 2.501071000 | 5.193040000 |
| H | 1.571363000 | 2.696757000 | 6.217723000 |
| C | 1.824327000 | 1.426047000 | 4.474146000 |
| H | 2.568350000 | 0.775138000 | 4.921101000 |
| C | 1.420757000 | 1.207427000 | 3.146669000 |
| H | 1.848075000 | 0.407687000 | 2.549491000 |
| C | -2.043901000 | 1.941749000 | -2.601684000 |
| H | -2.941523000 | 1.907347000 | -1.993760000 |
| C | -2.121134000 | 1.853491000 | -4.001383000 |
| H | -3.088512000 | 1.763739000 | -4.484383000 |
| C | -0.929204000 | 1.909582000 | -4.749758000 |
| H | -0.956552000 | 1.869182000 | -5.834847000 |
| C | 0.297634000 | 2.035749000 | -4.072029000 |
| H | 1.232864000 | 2.093629000 | -4.621613000 |
| C | 0.297346000 | 2.109456000 | -2.666921000 |
| C | 1.586006000 | 2.184064000 | -1.871594000 |
| H | 1.959051000 | 1.167502000 | -1.689684000 |
| H | 2.351349000 | 2.737588000 | -2.436423000 |
| C | 2.664601000 | 2.655557000 | 0.262794000 |
| H | 2.848604000 | 1.592382000 | 0.439942000 |
| H | 2.586501000 | 3.163822000 | 1.224767000 |
| H | 3.509752000 | 3.083600000 | -0.295031000 |
| C | -3.003617000 | 2.715379000 | 0.425205000 |
| O | -4.225380000 | 2.692670000 | 0.215059000 |
| O | -2.243550000 | 1.635591000 | 0.728784000 |
| Mn | 0.671187000 | -1.495184000 | 0.366767000 |
| N | -0.445103000 | -2.608066000 | -1.206065000 |
| N | 1.265273000 | -3.421464000 | 0.964202000 |
| N | -0.721296000 | -1.881173000 | 2.030402000 |
| N | 2.110356000 | -1.751049000 | -2.743689000 |
| C | 0.194540000 | -3.975555000 | -1.245854000 |
| H | 1.118079000 | -3.914193000 | -1.825490000 |
| H | -0.460077000 | -4.703348000 | -1.748565000 |
| C | 0.508697000 | -4.467179000 | 0.172047000 |
| H | -0.416880000 | -4.683822000 | 0.713992000 |
| H | 1.086462000 | -5.400114000 | 0.126410000 |
| C | 2.761834000 | -3.422664000 | 0.752845000 |

| | | | |
|---|--------------|--------------|--------------|
| H | 2.982124000 | -3.565303000 | -0.307786000 |
| H | 3.249212000 | -4.220818000 | 1.325348000 |
| C | 0.973986000 | -3.574740000 | 2.444427000 |
| H | 1.775750000 | -3.072515000 | 2.996446000 |
| H | 0.997667000 | -4.636541000 | 2.721927000 |
| C | -0.347768000 | -2.933984000 | 2.812678000 |
| C | -1.111098000 | -3.336434000 | 3.918760000 |
| H | -0.799599000 | -4.182302000 | 4.524289000 |
| C | -2.282907000 | -2.619667000 | 4.229938000 |
| H | -2.893148000 | -2.912634000 | 5.079186000 |
| C | -2.653869000 | -1.524470000 | 3.426733000 |
| H | -3.550424000 | -0.950603000 | 3.635553000 |
| C | -1.849994000 | -1.179425000 | 2.328361000 |
| H | -2.102003000 | -0.344916000 | 1.680607000 |
| C | 3.294359000 | -1.835040000 | -3.431992000 |
| H | 4.176311000 | -1.582003000 | -2.856557000 |
| C | 3.307087000 | -2.227135000 | -4.770487000 |
| H | 4.256438000 | -2.286823000 | -5.291461000 |
| C | 2.093672000 | -2.546560000 | -5.412307000 |
| H | 2.082866000 | -2.861762000 | -6.450186000 |
| C | 0.896587000 | -2.458014000 | -4.679284000 |
| H | -0.052946000 | -2.702167000 | -5.144832000 |
| C | 0.902456000 | -2.054437000 | -3.335052000 |
| C | -0.359034000 | -1.861295000 | -2.528629000 |
| H | -0.485838000 | -0.801189000 | -2.279152000 |
| H | -1.199880000 | -2.167775000 | -3.164854000 |
| C | -1.905064000 | -2.692801000 | -0.844981000 |
| H | -2.311140000 | -1.681699000 | -0.756479000 |
| H | -2.032722000 | -3.197703000 | 0.112825000 |
| H | -2.464673000 | -3.244217000 | -1.614691000 |
| C | 3.318637000 | -2.037038000 | 1.180773000 |
| O | 4.524289000 | -1.856086000 | 1.393872000 |
| O | 2.352820000 | -1.092603000 | 1.291337000 |
| O | 2.154383000 | -1.365855000 | -1.432427000 |

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| | | | |
|----|--------------|--------------|--------------|
| Mn | -0.512794000 | 1.615863000 | 0.486086000 |
| O | -0.188960000 | -0.114347000 | 0.265094000 |
| N | 1.422444000 | 2.410642000 | -0.038610000 |
| N | -0.955155000 | 3.619017000 | 1.007203000 |
| N | 0.040957000 | 2.276460000 | 3.645610000 |
| N | -0.497393000 | 1.897851000 | -1.930474000 |
| C | 1.198642000 | 3.896587000 | -0.248458000 |
| H | 0.750348000 | 4.031337000 | -1.234647000 |
| H | 2.160481000 | 4.429225000 | -0.244085000 |
| C | 0.281114000 | 4.477164000 | 0.835805000 |
| H | 0.803731000 | 4.507704000 | 1.796125000 |
| H | 0.004612000 | 5.509462000 | 0.582180000 |
| C | -2.078399000 | 3.955544000 | 0.048601000 |
| H | -1.662288000 | 4.146634000 | -0.944049000 |
| H | -2.632807000 | 4.846157000 | 0.368323000 |
| C | -1.546550000 | 3.715077000 | 2.408709000 |

| | | | |
|----|--------------|--------------|--------------|
| H | -2.349072000 | 2.970062000 | 2.454640000 |
| H | -1.992375000 | 4.710620000 | 2.527468000 |
| C | -0.601320000 | 3.492214000 | 3.559602000 |
| C | -0.436484000 | 4.416904000 | 4.602165000 |
| H | -0.950854000 | 5.370434000 | 4.538292000 |
| C | 0.361746000 | 4.110482000 | 5.718301000 |
| H | 0.478053000 | 4.825046000 | 6.525976000 |
| C | 1.003264000 | 2.857273000 | 5.767650000 |
| H | 1.627989000 | 2.575192000 | 6.608036000 |
| C | 0.833808000 | 1.956417000 | 4.716242000 |
| H | 1.287549000 | 0.975161000 | 4.671206000 |
| C | -1.516536000 | 1.865081000 | -2.833988000 |
| H | -2.524592000 | 1.957492000 | -2.445590000 |
| C | -1.292605000 | 1.723421000 | -4.210949000 |
| H | -2.132823000 | 1.716596000 | -4.897307000 |
| C | 0.032804000 | 1.603958000 | -4.673958000 |
| H | 0.240503000 | 1.496960000 | -5.734524000 |
| C | 1.084543000 | 1.631304000 | -3.742999000 |
| H | 2.116687000 | 1.530982000 | -4.064060000 |
| C | 0.781433000 | 1.779172000 | -2.378945000 |
| C | 1.865768000 | 1.753591000 | -1.323973000 |
| H | 2.097475000 | 0.704121000 | -1.110409000 |
| H | 2.779069000 | 2.241824000 | -1.694937000 |
| C | 2.460870000 | 2.152628000 | 1.015532000 |
| H | 2.486844000 | 1.083234000 | 1.232715000 |
| H | 2.212780000 | 2.687636000 | 1.934404000 |
| H | 3.450456000 | 2.483805000 | 0.669450000 |
| C | -3.029965000 | 2.735712000 | -0.047853000 |
| O | -4.171901000 | 2.830865000 | -0.523784000 |
| O | -2.463146000 | 1.587281000 | 0.385399000 |
| Mn | -0.013771000 | -1.758977000 | -0.380985000 |
| N | -0.725620000 | -2.881322000 | 1.372911000 |
| N | 0.059791000 | -3.648561000 | -1.297084000 |
| N | -1.942864000 | -1.813011000 | -1.479675000 |
| N | 1.904340000 | -2.077403000 | 1.125498000 |
| C | -0.301433000 | -4.309886000 | 1.105545000 |
| H | 0.759408000 | -4.401955000 | 1.35012700 |
| H | -0.854012000 | -5.003472000 | 1.756095000 |
| C | -0.539534000 | -4.681998000 | -0.362718000 |
| H | -1.612240000 | -4.728439000 | -0.572810000 |
| H | -0.119196000 | -5.673721000 | -0.575984000 |
| C | 1.516857000 | -3.860322000 | -1.624438000 |
| H | 2.053494000 | -4.180792000 | -0.726609000 |
| H | 1.652261000 | -4.626779000 | -2.396674000 |
| C | -0.722674000 | -3.590163000 | -2.594339000 |
| H | -0.093237000 | -3.092922000 | -3.340751000 |
| H | -0.923598000 | -4.607547000 | -2.954143000 |
| C | -1.998662000 | -2.797274000 | -2.421994000 |
| C | -3.140697000 | -3.003769000 | -3.209431000 |
| H | -3.162316000 | -3.799433000 | -3.948151000 |
| C | -4.252714000 | -2.158456000 | -3.025338000 |
| H | -5.150264000 | -2.298334000 | -3.620656000 |

| | | | |
|---|--------------|--------------|--------------|
| C | -4.185636000 | -1.136383000 | -2.059906000 |
| H | -5.018123000 | -0.462097000 | -1.888291000 |
| C | -3.013563000 | -0.991471000 | -1.299127000 |
| H | -2.920561000 | -0.211921000 | -0.549077000 |
| C | 3.237387000 | -1.914659000 | 0.901542000 |
| H | 3.553104000 | -1.799993000 | -0.129587000 |
| C | 4.177656000 | -1.903579000 | 1.944584000 |
| H | 5.232810000 | -1.787700000 | 1.720220000 |
| C | 3.723088000 | -2.070528000 | 3.267305000 |
| H | 4.427093000 | -2.091050000 | 4.094210000 |
| C | 2.344677000 | -2.229539000 | 3.499207000 |
| H | 1.963216000 | -2.378822000 | 4.505497000 |
| C | 1.462263000 | -2.219624000 | 2.403422000 |
| C | -0.037842000 | -2.321690000 | 2.588137000 |
| H | -0.438817000 | -1.312337000 | 2.746367000 |
| H | -0.274132000 | -2.932841000 | 3.472482000 |
| C | -2.210760000 | -2.774936000 | 1.578283000 |
| H | -2.489778000 | -1.720314000 | 1.641271000 |
| H | -2.746141000 | -3.225116000 | 0.740962000 |
| H | -2.510599000 | -3.285811000 | 2.504743000 |
| C | 2.114084000 | -2.508227000 | -2.097343000 |
| O | 3.200824000 | -2.452153000 | -2.696157000 |
| O | 1.366188000 | -1.440156000 | -1.745455000 |
| O | -0.109495000 | 1.341769000 | 2.653058000 |

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|----|--------------|--------------|--------------|
| Mn | -0.350548000 | 1.643492000 | 0.552702000 |
| O | -0.360094000 | -0.166229000 | 0.669582000 |
| N | 2.177987000 | 2.709008000 | -0.681123000 |
| N | -0.565968000 | 3.780220000 | 0.714214000 |
| N | -0.006286000 | 1.974213000 | 2.749186000 |
| N | -0.269994000 | 1.701352000 | -1.977480000 |
| C | 1.440573000 | 4.057705000 | -0.855807000 |
| H | 0.750026000 | 3.954466000 | -1.691044000 |
| H | 2.195221000 | 4.801575000 | -1.128235000 |
| C | 0.717513000 | 4.515127000 | 0.415394000 |
| H | 1.371178000 | 4.395072000 | 1.283487000 |
| H | 0.498323000 | 5.587715000 | 0.303613000 |
| C | -1.707785000 | 4.133646000 | -0.204129000 |
| H | -1.356942000 | 4.194115000 | -1.238124000 |
| H | -2.161283000 | 5.096900000 | 0.058614000 |
| C | -1.004349000 | 4.093508000 | 2.136795000 |
| H | -2.078726000 | 3.888946000 | 2.202369000 |
| H | -0.860102000 | 5.162989000 | 2.339519000 |
| C | -0.291308000 | 3.237177000 | 3.158916000 |
| C | -0.010026000 | 3.672184000 | 4.463636000 |
| H | -0.247375000 | 4.686200000 | 4.771322000 |
| C | 0.574314000 | 2.763583000 | 5.366722000 |
| H | 0.798030000 | 3.071085000 | 6.383893000 |
| C | 0.867307000 | 1.456166000 | 4.934028000 |
| H | 1.321191000 | 0.734109000 | 5.604599000 |
| C | 0.566302000 | 1.099639000 | 3.609348000 |

| | | | |
|----|--------------|--------------|--------------|
| H | 0.780704000 | 0.115333000 | 3.210893000 |
| C | -1.434165000 | 1.491699000 | -2.655040000 |
| H | -2.340221000 | 1.468924000 | -2.063759000 |
| C | -1.485743000 | 1.308907000 | -4.045388000 |
| H | -2.443012000 | 1.160029000 | -4.533869000 |
| C | -0.285506000 | 1.345124000 | -4.777852000 |
| H | -0.286388000 | 1.219827000 | -5.856546000 |
| C | 0.918808000 | 1.561262000 | -4.086771000 |
| H | 1.864285000 | 1.590764000 | -4.619695000 |
| C | 0.891092000 | 1.731199000 | -2.690083000 |
| C | 2.207918000 | 1.863465000 | -1.959752000 |
| H | 2.517226000 | 0.862416000 | -1.638856000 |
| H | 2.966081000 | 2.294109000 | -2.621299000 |
| C | 3.611286000 | 2.956104000 | -0.235788000 |
| H | 4.083555000 | 1.984443000 | -0.090969000 |
| H | 3.585020000 | 3.491496000 | 0.714337000 |
| H | 4.141940000 | 3.535934000 | -0.996532000 |
| C | -2.764235000 | 3.005633000 | -0.122556000 |
| O | -3.928312000 | 3.165175000 | -0.519497000 |
| O | -2.268506000 | 1.844870000 | 0.364787000 |
| Mn | -0.000937000 | -1.710838000 | -0.114078000 |
| N | -0.679134000 | -3.427372000 | 1.415199000 |
| N | 0.216099000 | -3.465666000 | -1.360724000 |
| N | -1.862867000 | -1.734617000 | -1.105217000 |
| N | 1.680671000 | -2.021956000 | 1.329922000 |
| C | -0.047074000 | -4.662745000 | 0.840524000 |
| H | 1.023674000 | -4.641432000 | 1.065141000 |
| H | -0.460228000 | -5.571613000 | 1.306186000 |
| C | -0.262994000 | -4.726914000 | -0.673390000 |
| H | -1.328797000 | -4.841412000 | -0.893203000 |
| H | 0.251473000 | -5.601647000 | -1.093387000 |
| C | 1.667430000 | -3.519130000 | -1.764994000 |
| H | 2.256489000 | -3.948038000 | -0.947394000 |
| H | 1.816890000 | -4.145470000 | -2.653377000 |
| C | -0.630427000 | -3.200763000 | -2.589323000 |
| H | -0.078941000 | -2.508686000 | -3.235076000 |
| H | -0.786993000 | -4.129749000 | -3.152552000 |
| C | -1.939434000 | -2.560165000 | -2.191566000 |
| C | -3.138644000 | -2.724903000 | -2.897948000 |
| H | -3.183339000 | -3.392808000 | -3.752806000 |
| C | -4.278479000 | -2.007211000 | -2.481381000 |
| H | -5.219931000 | -2.122346000 | -3.010597000 |
| C | -4.181100000 | -1.139346000 | -1.377727000 |
| H | -5.029467000 | -0.554627000 | -1.038872000 |
| C | -2.953152000 | -1.025537000 | -0.706196000 |
| H | -2.814101000 | -0.342386000 | 0.123121000 |
| C | 2.931628000 | -1.526838000 | 1.124979000 |
| H | 3.106500000 | -1.057135000 | 0.166782000 |
| C | 3.936073000 | -1.613077000 | 2.100248000 |
| H | 4.926640000 | -1.223688000 | 1.890881000 |
| C | 3.636332000 | -2.222335000 | 3.332974000 |
| H | 4.396381000 | -2.317525000 | 4.102859000 |

| | | | |
|---|--------------|--------------|--------------|
| C | 2.336821000 | -2.716084000 | 3.549169000 |
| H | 2.072782000 | -3.197716000 | 4.486078000 |
| C | 1.377803000 | -2.595822000 | 2.528888000 |
| C | -0.052522000 | -3.059685000 | 2.718087000 |
| H | -0.645094000 | -2.241126000 | 3.147143000 |
| H | -0.086338000 | -3.897335000 | 3.433160000 |
| C | -2.156049000 | -3.584260000 | 1.592752000 |
| H | -2.589000000 | -2.629564000 | 1.904219000 |
| H | -2.625263000 | -3.880023000 | 0.652198000 |
| H | -2.389688000 | -4.346656000 | 2.352315000 |
| C | 2.176625000 | -2.081133000 | -2.035770000 |
| O | 3.230555000 | -1.877235000 | -2.673513000 |
| O | 1.411313000 | -1.131397000 | -1.486906000 |
| O | 1.604513000 | 1.914487000 | 0.399958000 |

Tetradentate ligand with COO replaced by -Me:

¹Dimer

| | | | |
|----|--------------|--------------|--------------|
| Mn | 1.273628000 | 0.521135000 | 0.516949000 |
| O | -0.432302000 | 0.031334000 | 1.081559000 |
| N | 2.124543000 | 0.902029000 | 2.463793000 |
| N | 3.203783000 | 1.108510000 | -0.249626000 |
| N | 1.023913000 | 2.547963000 | 0.186155000 |
| N | 2.009574000 | -1.334930000 | 1.050425000 |
| C | 3.631413000 | 1.011529000 | 2.224706000 |
| H | 4.058102000 | 0.006878000 | 2.182263000 |
| H | 4.097986000 | 1.529783000 | 3.071244000 |
| C | 3.912216000 | 1.776170000 | 0.930135000 |
| H | 3.570204000 | 2.810404000 | 1.009996000 |
| H | 4.991960000 | 1.801841000 | 0.739750000 |
| C | 4.110279000 | 0.068014000 | -0.866369000 |
| H | 4.455515000 | -0.640929000 | -0.114058000 |
| H | 4.987706000 | 0.562923000 | -1.301931000 |
| C | 2.859931000 | 2.113503000 | -1.333636000 |
| H | 2.453473000 | 1.556621000 | -2.185409000 |
| H | 3.764286000 | 2.636270000 | -1.668274000 |
| C | 1.844692000 | 3.071836000 | -0.781623000 |
| C | 1.764478000 | 4.418310000 | -1.159276000 |
| H | 2.435045000 | 4.809218000 | -1.918703000 |
| C | 0.836593000 | 5.261034000 | -0.516783000 |
| H | 0.774020000 | 6.312925000 | -0.780709000 |
| C | 0.021695000 | 4.723304000 | 0.498680000 |
| H | -0.676919000 | 5.347338000 | 1.046152000 |
| C | 0.137825000 | 3.365663000 | 0.820360000 |
| H | -0.457648000 | 2.926334000 | 1.604775000 |
| C | 2.383615000 | -2.329389000 | 0.197666000 |
| H | 2.338121000 | -2.111324000 | -0.857481000 |
| C | 2.838911000 | -3.569874000 | 0.660197000 |
| H | 3.152794000 | -4.326351000 | -0.051451000 |
| C | 2.905758000 | -3.803664000 | 2.047728000 |
| H | 3.263887000 | -4.753457000 | 2.434617000 |

| | | | |
|----|--------------|--------------|--------------|
| C | 2.536594000 | -2.768108000 | 2.928215000 |
| H | 2.613457000 | -2.900743000 | 4.003253000 |
| C | 2.103416000 | -1.543459000 | 2.404298000 |
| C | 1.776195000 | -0.347413000 | 3.250989000 |
| H | 0.705058000 | -0.308459000 | 3.479398000 |
| H | 2.327113000 | -0.364227000 | 4.199222000 |
| C | 1.647099000 | 2.091421000 | 3.264920000 |
| H | 0.561721000 | 2.051738000 | 3.378739000 |
| H | 1.940609000 | 3.025419000 | 2.785999000 |
| H | 2.098224000 | 2.060701000 | 4.264993000 |
| Mn | -1.246307000 | -0.355446000 | -0.546248000 |
| O | 0.455531000 | 0.133359000 | -1.111931000 |
| N | -2.297020000 | -0.301022000 | -2.454495000 |
| C | -3.744110000 | -0.673261000 | -2.126621000 |
| H | -4.266195000 | 0.215497000 | -1.765094000 |
| H | -4.252673000 | -0.999661000 | -3.042014000 |
| C | -3.793804000 | -1.789087000 | -1.083574000 |
| N | -3.016446000 | -1.394105000 | 0.173601000 |
| N | -0.758933000 | -2.333019000 | -0.829818000 |
| C | -1.436700000 | -3.239762000 | -0.056133000 |
| C | -2.450312000 | -2.622662000 | 0.866238000 |
| C | -3.938718000 | -0.703955000 | 1.152473000 |
| H | -4.454458000 | 0.129984000 | 0.675997000 |
| H | -4.694886000 | -1.416037000 | 1.507294000 |
| H | -1.991781000 | -2.294348000 | 1.806306000 |
| H | -3.254918000 | -3.326852000 | 1.109666000 |
| C | -1.237509000 | -4.619091000 | -0.205835000 |
| H | -1.791277000 | -5.318504000 | 0.413315000 |
| C | -0.352904000 | -5.082588000 | -1.200603000 |
| H | -0.212290000 | -6.148585000 | -1.356575000 |
| C | 0.319094000 | -4.142860000 | -2.008921000 |
| H | 0.986323000 | -4.461429000 | -2.803732000 |
| C | 0.107855000 | -2.776781000 | -1.785639000 |
| H | 0.613014000 | -2.018903000 | -2.369688000 |
| N | -2.225935000 | 1.451475000 | -0.476347000 |
| C | -2.617231000 | 2.064494000 | 0.678147000 |
| H | -2.320715000 | 1.588009000 | 1.603096000 |
| C | -3.378184000 | 3.239916000 | 0.664845000 |
| H | -3.705429000 | 3.679884000 | 1.601721000 |
| C | -3.717164000 | 3.824304000 | -0.572754000 |
| H | -4.312435000 | 4.732357000 | -0.612159000 |
| C | -3.300168000 | 3.194045000 | -1.762618000 |
| H | -3.570408000 | 3.603916000 | -2.731195000 |
| C | -2.573638000 | 1.997999000 | -1.684996000 |
| C | -2.192777000 | 1.156923000 | -2.870330000 |
| C | -1.797562000 | -1.140460000 | -3.607721000 |
| H | -0.743724000 | -0.925139000 | -3.795437000 |
| H | -1.930278000 | -2.202378000 | -3.400191000 |
| H | -2.367393000 | -0.894124000 | -4.512888000 |
| H | -1.156898000 | 1.341680000 | -3.177717000 |
| H | -2.843019000 | 1.354137000 | -3.731038000 |
| H | -3.371350000 | -2.711543000 | -1.487973000 |

| | | | |
|---|--------------|--------------|--------------|
| H | -4.836356000 | -1.999411000 | -0.815424000 |
| H | 3.584205000 | -0.458424000 | -1.665607000 |

⁴Monomer

| | | | |
|----|--------------|--------------|--------------|
| Mn | -1.559016000 | -0.480714000 | -0.865134000 |
| O | -0.046921000 | 0.110393000 | -0.779606000 |
| N | -2.704921000 | -0.300122000 | -2.597983000 |
| C | -4.109610000 | -0.769812000 | -2.241076000 |
| H | -4.645062000 | 0.071168000 | -1.792291000 |
| H | -4.642238000 | -1.053794000 | -3.157166000 |
| C | -4.042506000 | -1.950539000 | -1.273194000 |
| N | -3.229446000 | -1.579428000 | -0.040671000 |
| N | -0.810745000 | -2.377487000 | -0.881189000 |
| C | -1.482696000 | -3.332344000 | -0.164875000 |
| C | -2.685677000 | -2.835550000 | 0.603957000 |
| C | -4.085658000 | -0.841683000 | 0.961425000 |
| H | -4.554739000 | 0.027522000 | 0.497958000 |
| H | -4.871605000 | -1.502752000 | 1.349067000 |
| H | -2.385343000 | -2.589246000 | 1.630397000 |
| H | -3.467695000 | -3.603098000 | 0.672236000 |
| C | -1.010499000 | -4.649022000 | -0.095610000 |
| H | -1.554114000 | -5.393811000 | 0.477394000 |
| C | 0.184205000 | -4.984474000 | -0.762256000 |
| H | 0.568967000 | -5.998882000 | -0.717630000 |
| C | 0.883085000 | -3.987179000 | -1.472206000 |
| H | 1.817556000 | -4.205064000 | -1.977471000 |
| C | 0.363802000 | -2.688781000 | -1.506762000 |
| H | 0.885990000 | -1.876671000 | -1.999464000 |
| N | -2.315477000 | 1.394371000 | -0.539561000 |
| C | -2.211362000 | 2.090399000 | 0.627654000 |
| H | -1.784571000 | 1.574987000 | 1.481290000 |
| C | -2.610503000 | 3.429252000 | 0.714077000 |
| H | -2.511884000 | 3.960500000 | 1.654368000 |
| C | -3.123403000 | 4.063671000 | -0.435277000 |
| H | -3.438847000 | 5.101780000 | -0.394942000 |
| C | -3.209813000 | 3.342578000 | -1.642005000 |
| H | -3.584232000 | 3.815398000 | -2.544773000 |
| C | -2.785838000 | 2.007576000 | -1.668390000 |
| C | -2.714624000 | 1.181154000 | -2.936378000 |
| C | -2.138679000 | -1.091706000 | -3.757072000 |
| H | -1.095559000 | -0.809908000 | -3.924198000 |
| H | -2.191956000 | -2.161314000 | -3.543533000 |
| H | -2.713390000 | -0.883082000 | -4.668160000 |
| H | -1.784508000 | 1.410939000 | -3.470751000 |
| H | -3.548767000 | 1.403611000 | -3.613729000 |
| H | -3.567636000 | -2.813821000 | -1.749552000 |
| H | -5.054773000 | -2.252871000 | -0.974825000 |
| H | -3.468447000 | -0.504454000 | 1.798621000 |

Disproportionation:

bpy Mn-dimer model

¹Reactant

| | | | |
|----|--------------|--------------|--------------|
| Mn | 1.273628000 | 0.521135000 | 0.516949000 |
| O | -0.432302000 | 0.031334000 | 1.081559000 |
| N | 2.124543000 | 0.902029000 | 2.463793000 |
| N | 3.203783000 | 1.108510000 | -0.249626000 |
| N | 1.023913000 | 2.547963000 | 0.186155000 |
| N | 2.009574000 | -1.334930000 | 1.050425000 |
| C | 3.631413000 | 1.011529000 | 2.224706000 |
| H | 4.058102000 | 0.006878000 | 2.182263000 |
| H | 4.097986000 | 1.529783000 | 3.071244000 |
| C | 3.912216000 | 1.776170000 | 0.930135000 |
| H | 3.570204000 | 2.810404000 | 1.009996000 |
| H | 4.991960000 | 1.801841000 | 0.739750000 |
| C | 4.110279000 | 0.068014000 | -0.866369000 |
| H | 4.455515000 | -0.640929000 | -0.114058000 |
| H | 4.987706000 | 0.562923000 | -1.301931000 |
| C | 2.859931000 | 2.113503000 | -1.333636000 |
| H | 2.453473000 | 1.556621000 | -2.185409000 |
| H | 3.764286000 | 2.636270000 | -1.668274000 |
| C | 1.844692000 | 3.071836000 | -0.781623000 |
| C | 1.764478000 | 4.418310000 | -1.159276000 |
| H | 2.435045000 | 4.809218000 | -1.918703000 |
| C | 0.836593000 | 5.261034000 | -0.516783000 |
| H | 0.774020000 | 6.312925000 | -0.780709000 |
| C | 0.021695000 | 4.723304000 | 0.498680000 |
| H | -0.676919000 | 5.347338000 | 1.046152000 |
| C | 0.137825000 | 3.365663000 | 0.820360000 |
| H | -0.457648000 | 2.926334000 | 1.604775000 |
| C | 2.383615000 | -2.329389000 | 0.197666000 |
| H | 2.338121000 | -2.111324000 | -0.857481000 |
| C | 2.838911000 | -3.569874000 | 0.660197000 |
| H | 3.152794000 | -4.326351000 | -0.051451000 |
| C | 2.905758000 | -3.803664000 | 2.047728000 |
| H | 3.263887000 | -4.753457000 | 2.434617000 |
| C | 2.536594000 | -2.768108000 | 2.928215000 |
| H | 2.613457000 | -2.900743000 | 4.003253000 |
| C | 2.103416000 | -1.543459000 | 2.404298000 |
| C | 1.776195000 | -0.347413000 | 3.250989000 |
| H | 0.705058000 | -0.308459000 | 3.479398000 |
| H | 2.327113000 | -0.364227000 | 4.199222000 |
| C | 1.647099000 | 2.091421000 | 3.264920000 |
| H | 0.561721000 | 2.051738000 | 3.378739000 |
| H | 1.940609000 | 3.025419000 | 2.785999000 |
| H | 2.098224000 | 2.060701000 | 4.264993000 |
| Mn | -1.246307000 | -0.355446000 | -0.546248000 |
| O | 0.455531000 | 0.133359000 | -1.111931000 |
| N | -2.297020000 | -0.301022000 | -2.454495000 |
| C | -3.744110000 | -0.673261000 | -2.126621000 |
| H | -4.266195000 | 0.215497000 | -1.765094000 |
| H | -4.252673000 | -0.999661000 | -3.042014000 |

| | | | |
|---|--------------|--------------|--------------|
| C | -3.793804000 | -1.789087000 | -1.083574000 |
| N | -3.016446000 | -1.394105000 | 0.173601000 |
| N | -0.758933000 | -2.333019000 | -0.829818000 |
| C | -1.436700000 | -3.239762000 | -0.056133000 |
| C | -2.450312000 | -2.622662000 | 0.866238000 |
| C | -3.938718000 | -0.703955000 | 1.152473000 |
| H | -4.454458000 | 0.129984000 | 0.675997000 |
| H | -4.694886000 | -1.416037000 | 1.507294000 |
| H | -1.991781000 | -2.294348000 | 1.806306000 |
| H | -3.254918000 | -3.326852000 | 1.109666000 |
| C | -1.237509000 | -4.619091000 | -0.205835000 |
| H | -1.791277000 | -5.318504000 | 0.413315000 |
| C | -0.352904000 | -5.082588000 | -1.200603000 |
| H | -0.212290000 | -6.148585000 | -1.356575000 |
| C | 0.319094000 | -4.142860000 | -2.008921000 |
| H | 0.986323000 | -4.461429000 | -2.803732000 |
| C | 0.107855000 | -2.776781000 | -1.785639000 |
| H | 0.613014000 | -2.018903000 | -2.369688000 |
| N | -2.225935000 | 1.451475000 | -0.476347000 |
| C | -2.617231000 | 2.064494000 | 0.678147000 |
| H | -2.320715000 | 1.588009000 | 1.603096000 |
| C | -3.378184000 | 3.239916000 | 0.664845000 |
| H | -3.705429000 | 3.679884000 | 1.601721000 |
| C | -3.717164000 | 3.824304000 | -0.572754000 |
| H | -4.312435000 | 4.732357000 | -0.612159000 |
| C | -3.300168000 | 3.194045000 | -1.762618000 |
| H | -3.570408000 | 3.603916000 | -2.731195000 |
| C | -2.573638000 | 1.997999000 | -1.684996000 |
| C | -2.192777000 | 1.156923000 | -2.870330000 |
| C | -1.797562000 | -1.140460000 | -3.607721000 |
| H | -0.743724000 | -0.925139000 | -3.795437000 |
| H | -1.930278000 | -2.202378000 | -3.400191000 |
| H | -2.367393000 | -0.894124000 | -4.512888000 |
| H | -1.156898000 | 1.341680000 | -3.177717000 |
| H | -2.843019000 | 1.354137000 | -3.731038000 |
| H | -3.371350000 | -2.711543000 | -1.487973000 |
| H | -4.836356000 | -1.999411000 | -0.815424000 |
| H | 3.584205000 | -0.458424000 | -1.665607000 |
| H | -3.369069000 | -0.349276000 | 2.013726000 |

¹Transition_state

| | | | |
|----|--------------|--------------|--------------|
| Mn | 1.468548000 | 0.630460000 | 0.733483000 |
| O | -0.157962000 | 0.418220000 | 1.476438000 |
| N | 2.427714000 | 1.146916000 | 2.553187000 |
| N | 3.356445000 | 1.035807000 | -0.188149000 |
| N | 1.221660000 | 2.576028000 | 0.153610000 |
| N | 2.046714000 | -1.216767000 | 1.429334000 |
| C | 3.927621000 | 1.148265000 | 2.246583000 |
| H | 4.293273000 | 0.119459000 | 2.286229000 |
| H | 4.455611000 | 1.716429000 | 3.021992000 |
| C | 4.182729000 | 1.762371000 | 0.874058000 |
| H | 3.910895000 | 2.820921000 | 0.865781000 |

| | | | |
|----|--------------|--------------|--------------|
| H | 5.247923000 | 1.695547000 | 0.621387000 |
| C | 4.135350000 | -0.138891000 | -0.733848000 |
| H | 4.468537000 | -0.788024000 | 0.076584000 |
| H | 5.018139000 | 0.220428000 | -1.277373000 |
| C | 3.043814000 | 1.977597000 | -1.333695000 |
| H | 2.625758000 | 1.383791000 | -2.154959000 |
| H | 3.962784000 | 2.451805000 | -1.700232000 |
| C | 2.045521000 | 2.999594000 | -0.857140000 |
| C | 1.950521000 | 4.296708000 | -1.378959000 |
| H | 2.625513000 | 4.616978000 | -2.167059000 |
| C | 0.990504000 | 5.181901000 | -0.850905000 |
| H | 0.915137000 | 6.198059000 | -1.227287000 |
| C | 0.147453000 | 4.735075000 | 0.187148000 |
| H | -0.587832000 | 5.395900000 | 0.634041000 |
| C | 0.284746000 | 3.425361000 | 0.662142000 |
| H | -0.336129000 | 3.042430000 | 1.459557000 |
| C | 2.178957000 | -2.341964000 | 0.673363000 |
| H | 2.027820000 | -2.234426000 | -0.390416000 |
| C | 2.515413000 | -3.576046000 | 1.241991000 |
| H | 2.641432000 | -4.446816000 | 0.607325000 |
| C | 2.710922000 | -3.660225000 | 2.635746000 |
| H | 2.982600000 | -4.602879000 | 3.101971000 |
| C | 2.571697000 | -2.495107000 | 3.413981000 |
| H | 2.734317000 | -2.522308000 | 4.487288000 |
| C | 2.241644000 | -1.287409000 | 2.784553000 |
| C | 2.091231000 | 0.019723000 | 3.513168000 |
| H | 1.057437000 | 0.158357000 | 3.850292000 |
| H | 2.741963000 | 0.069267000 | 4.394930000 |
| C | 2.031557000 | 2.455083000 | 3.203700000 |
| H | 0.949403000 | 2.485792000 | 3.344939000 |
| H | 2.349090000 | 3.300279000 | 2.592662000 |
| H | 2.514342000 | 2.534618000 | 4.185682000 |
| Mn | -1.430555000 | -0.491800000 | -0.635091000 |
| O | 0.416922000 | 0.057100000 | -0.641862000 |
| N | -2.542600000 | -0.205392000 | -2.592202000 |
| C | -3.955703000 | -0.667239000 | -2.278775000 |
| H | -4.503191000 | 0.153389000 | -1.807444000 |
| H | -4.484492000 | -0.913311000 | -3.208648000 |
| C | -3.949770000 | -1.899446000 | -1.368385000 |
| N | -3.195948000 | -1.646299000 | -0.060807000 |
| N | -0.855147000 | -2.402362000 | -1.067732000 |
| C | -1.545689000 | -3.417317000 | -0.453254000 |
| C | -2.639375000 | -2.956342000 | 0.474553000 |
| C | -4.129872000 | -1.062725000 | 0.976504000 |
| H | -4.621747000 | -0.170269000 | 0.588344000 |
| H | -4.901833000 | -1.798682000 | 1.235342000 |
| H | -2.255306000 | -2.779784000 | 1.487262000 |
| H | -3.440312000 | -3.701932000 | 0.554528000 |
| C | -1.258629000 | -4.761055000 | -0.732030000 |
| H | -1.819834000 | -5.550818000 | -0.241551000 |
| C | -0.264637000 | -5.069453000 | -1.682227000 |
| H | -0.048423000 | -6.104347000 | -1.932876000 |

| | | | |
|---|--------------|--------------|--------------|
| C | 0.424559000 | -4.017532000 | -2.324252000 |
| H | 1.176693000 | -4.219897000 | -3.080160000 |
| C | 0.113543000 | -2.695523000 | -1.986146000 |
| H | 0.620874000 | -1.855872000 | -2.446544000 |
| N | -2.382864000 | 1.310831000 | -0.343587000 |
| C | -2.679433000 | 1.828616000 | 0.888207000 |
| H | -2.309990000 | 1.285265000 | 1.747962000 |
| C | -3.420509000 | 3.006940000 | 1.033690000 |
| H | -3.665057000 | 3.368544000 | 2.027381000 |
| C | -3.851670000 | 3.693705000 | -0.119919000 |
| H | -4.438924000 | 4.603938000 | -0.036102000 |
| C | -3.534085000 | 3.164760000 | -1.386037000 |
| H | -3.872723000 | 3.658204000 | -2.292141000 |
| C | -2.811074000 | 1.965876000 | -1.474448000 |
| C | -2.503728000 | 1.290554000 | -2.789869000 |
| C | -2.019286000 | -0.889315000 | -3.829717000 |
| H | -0.972289000 | -0.618069000 | -3.994161000 |
| H | -2.098614000 | -1.973568000 | -3.727574000 |
| H | -2.597494000 | -0.584788000 | -4.712210000 |
| H | -1.501449000 | 1.562059000 | -3.145172000 |
| H | -3.217705000 | 1.602264000 | -3.563419000 |
| H | -3.481651000 | -2.744149000 | -1.880160000 |
| H | -4.981960000 | -2.188233000 | -1.134312000 |
| H | 3.508962000 | -0.707747000 | -1.425029000 |
| H | -3.575187000 | -0.810002000 | 1.883905000 |

¹Product

| | | | |
|----|--------------|--------------|--------------|
| Mn | 1.390024000 | 0.865731000 | 0.737464000 |
| O | -0.065831000 | 1.794582000 | 1.161134000 |
| N | 2.451796000 | 2.060210000 | 2.126495000 |
| N | 3.356015000 | 0.167175000 | 0.151522000 |
| N | 1.767088000 | 2.042219000 | -0.888844000 |
| N | 1.288308000 | -0.301494000 | 2.410375000 |
| C | 3.876311000 | 1.511501000 | 2.192217000 |
| H | 3.885194000 | 0.643109000 | 2.856015000 |
| H | 4.537101000 | 2.269388000 | 2.630372000 |
| C | 4.349029000 | 1.133285000 | 0.796258000 |
| H | 4.434322000 | 2.020255000 | 0.162625000 |
| H | 5.341021000 | 0.667049000 | 0.842168000 |
| C | 3.710163000 | -1.256974000 | 0.511989000 |
| H | 3.780432000 | -1.370174000 | 1.594672000 |
| H | 4.678306000 | -1.527887000 | 0.072170000 |
| C | 3.426946000 | 0.324397000 | -1.350521000 |
| H | 2.919091000 | -0.535863000 | -1.801512000 |
| H | 4.470697000 | 0.299943000 | -1.689257000 |
| C | 2.751645000 | 1.615756000 | -1.743487000 |
| C | 3.080633000 | 2.346466000 | -2.894099000 |
| H | 3.880964000 | 2.007094000 | -3.545154000 |
| C | 2.379133000 | 3.534831000 | -3.180823000 |
| H | 2.631804000 | 4.123875000 | -4.057881000 |
| C | 1.357479000 | 3.954918000 | -2.304328000 |
| H | 0.804586000 | 4.870795000 | -2.486321000 |

| | | | |
|----|--------------|--------------|--------------|
| C | 1.074004000 | 3.185662000 | -1.168668000 |
| H | 0.306692000 | 3.470128000 | -0.459268000 |
| C | 1.013717000 | -1.637604000 | 2.415319000 |
| H | 0.894793000 | -2.114212000 | 1.449892000 |
| C | 0.917820000 | -2.362759000 | 3.608929000 |
| H | 0.727846000 | -3.430871000 | 3.581498000 |
| C | 1.097741000 | -1.689450000 | 4.836679000 |
| H | 1.041181000 | -2.230378000 | 5.776992000 |
| C | 1.371807000 | -0.308573000 | 4.825475000 |
| H | 1.527528000 | 0.233037000 | 5.753728000 |
| C | 1.463052000 | 0.361224000 | 3.596393000 |
| C | 1.756943000 | 1.831679000 | 3.458491000 |
| H | 0.826179000 | 2.409999000 | 3.460988000 |
| H | 2.386831000 | 2.199365000 | 4.277687000 |
| C | 2.472599000 | 3.547691000 | 1.838962000 |
| H | 1.451119000 | 3.913714000 | 1.719539000 |
| H | 3.045034000 | 3.752968000 | 0.933715000 |
| H | 2.942929000 | 4.075712000 | 2.677593000 |
| Mn | -1.497957000 | -0.816352000 | -0.657408000 |
| O | 0.171366000 | -0.143211000 | -0.164030000 |
| N | -2.807498000 | 0.576177000 | -1.816612000 |
| C | -4.119293000 | -0.169876000 | -1.989590000 |
| H | -4.748131000 | 0.016323000 | -1.114368000 |
| H | -4.660942000 | 0.218004000 | -2.861448000 |
| C | -3.872321000 | -1.669404000 | -2.169916000 |
| N | -3.089899000 | -2.249487000 | -0.990242000 |
| N | -0.687777000 | -1.983619000 | -2.114405000 |
| C | -1.249988000 | -3.222334000 | -2.312503000 |
| C | -2.414611000 | -3.544094000 | -1.411933000 |
| C | -4.032629000 | -2.556443000 | 0.156033000 |
| H | -4.605520000 | -1.670765000 | 0.431164000 |
| H | -4.732943000 | -3.346130000 | -0.143627000 |
| H | -2.077239000 | -4.069821000 | -0.509238000 |
| H | -3.137922000 | -4.201000000 | -1.911543000 |
| C | -0.755786000 | -4.096830000 | -3.289521000 |
| H | -1.213732000 | -5.071269000 | -3.431159000 |
| C | 0.325385000 | -3.688778000 | -4.094666000 |
| H | 0.714826000 | -4.348386000 | -4.864988000 |
| C | 0.880534000 | -2.405036000 | -3.901146000 |
| H | 1.695655000 | -2.053673000 | -4.525129000 |
| C | 0.357304000 | -1.581050000 | -2.900134000 |
| H | 0.742929000 | -0.586257000 | -2.714014000 |
| N | -2.481375000 | 0.104062000 | 0.853795000 |
| C | -2.504347000 | -0.362254000 | 2.137834000 |
| H | -1.969841000 | -1.283396000 | 2.345019000 |
| C | -3.197475000 | 0.307694000 | 3.149728000 |
| H | -3.216791000 | -0.100121000 | 4.154935000 |
| C | -3.882786000 | 1.499913000 | 2.833081000 |
| H | -4.444421000 | 2.032493000 | 3.595331000 |
| C | -3.840578000 | 1.984229000 | 1.512184000 |
| H | -4.363205000 | 2.896964000 | 1.241938000 |
| C | -3.126349000 | 1.273187000 | 0.537113000 |

| | | | |
|---|--------------|--------------|--------------|
| C | -2.990046000 | 1.753073000 | -0.892096000 |
| C | -2.261740000 | 1.025397000 | -3.147152000 |
| H | -1.267807000 | 1.463013000 | -3.011433000 |
| H | -2.186843000 | 0.174393000 | -3.828815000 |
| H | -2.918416000 | 1.776514000 | -3.605576000 |
| H | -2.103025000 | 2.392773000 | -0.975020000 |
| H | -3.858238000 | 2.356025000 | -1.188706000 |
| H | -3.303203000 | -1.856798000 | -3.084911000 |
| H | -4.829629000 | -2.198285000 | -2.259642000 |
| H | 2.946095000 | -1.936658000 | 0.126414000 |
| H | -3.469129000 | -2.906311000 | 1.024867000 |

Mn-dimer system with Me in place of COO-

¹Reactant

| | | | |
|---|--------------|--------------|--------------|
| O | 2.440616000 | 0.490632000 | 0.005181000 |
| O | 0.167534000 | -0.077470000 | -0.001789000 |
| N | 1.366937000 | -1.467025000 | 2.014526000 |
| C | 0.231644000 | -1.087581000 | 2.670292000 |
| C | 0.025360000 | -1.405128000 | 4.018351000 |
| C | 1.017960000 | -2.129159000 | 4.710924000 |
| C | 2.184283000 | -2.518851000 | 4.029035000 |
| C | 2.340934000 | -2.183548000 | 2.672080000 |
| N | 3.392518000 | -2.207705000 | 0.514717000 |
| C | 4.415360000 | -2.512798000 | -0.329906000 |
| C | 5.567348000 | -3.188994000 | 0.100089000 |
| C | 5.673792000 | -3.567339000 | 1.450022000 |
| C | 4.621266000 | -3.248397000 | 2.328287000 |
| C | 3.493672000 | -2.568449000 | 1.841571000 |
| N | 0.600868000 | -2.924132000 | -0.393120000 |
| C | -0.167455000 | -3.638848000 | 0.473828000 |
| C | -0.859647000 | -4.795765000 | 0.084721000 |
| C | -0.758728000 | -5.237260000 | -1.246365000 |
| C | 0.029184000 | -4.497525000 | -2.147957000 |
| C | 0.697158000 | -3.346090000 | -1.702119000 |
| N | 2.055721000 | -1.381072000 | -1.942025000 |
| C | 2.887387000 | -0.540384000 | -2.623336000 |
| C | 3.234546000 | -0.779315000 | -3.958650000 |
| C | 2.706639000 | -1.912826000 | -4.611049000 |
| C | 1.852842000 | -2.776700000 | -3.902555000 |
| C | 1.541371000 | -2.498574000 | -2.559528000 |
| N | 1.210069000 | 1.961367000 | 1.944231000 |
| C | 2.333289000 | 1.607012000 | 2.633887000 |
| C | 2.518525000 | 1.980352000 | 3.970662000 |
| C | 1.517480000 | 2.736101000 | 4.615619000 |
| C | 0.363881000 | 3.100046000 | 3.898791000 |
| C | 0.227955000 | 2.707774000 | 2.554978000 |
| N | -0.790771000 | 2.639950000 | 0.382942000 |
| C | -1.800779000 | 2.907992000 | -0.489273000 |
| C | -2.957286000 | 3.604700000 | -0.106860000 |
| C | -3.082086000 | 4.043967000 | 1.222898000 |

| | | | |
|----|--------------|--------------|--------------|
| C | -2.043384000 | 3.762634000 | 2.129967000 |
| C | -0.910622000 | 3.059258000 | 1.690818000 |
| N | 2.015865000 | 3.319342000 | -0.506397000 |
| C | 2.770526000 | 4.068226000 | 0.343559000 |
| C | 3.469891000 | 5.208460000 | -0.080415000 |
| C | 3.391191000 | 5.595953000 | -1.429681000 |
| C | 2.617598000 | 4.820648000 | -2.313602000 |
| C | 1.941461000 | 3.688190000 | -1.832762000 |
| N | 0.585900000 | 1.715047000 | -2.015375000 |
| C | -0.234966000 | 0.847519000 | -2.675745000 |
| C | -0.559738000 | 1.031951000 | -4.025244000 |
| C | -0.019819000 | 2.137689000 | -4.714377000 |
| C | 0.822629000 | 3.029637000 | -4.027406000 |
| C | 1.111122000 | 2.806596000 | -2.669029000 |
| H | -0.504586000 | -0.555883000 | 2.080173000 |
| H | -0.896391000 | -1.107498000 | 4.507048000 |
| H | 0.880489000 | -2.397585000 | 5.754409000 |
| H | 2.945152000 | -3.090912000 | 4.547369000 |
| H | 4.321424000 | -2.215263000 | -1.363789000 |
| H | 6.356070000 | -3.411215000 | -0.610828000 |
| H | 6.551255000 | -4.094645000 | 1.812077000 |
| H | 4.691905000 | -3.529759000 | 3.372797000 |
| H | -0.237170000 | -3.287995000 | 1.492759000 |
| H | -1.459123000 | -5.332710000 | 0.812162000 |
| H | -1.279429000 | -6.131116000 | -1.576501000 |
| H | 0.111881000 | -4.823162000 | -3.178604000 |
| H | 3.281217000 | 0.297884000 | -2.062214000 |
| H | 3.914035000 | -0.104113000 | -4.467992000 |
| H | 2.966223000 | -2.127962000 | -5.643600000 |
| H | 1.456585000 | -3.660361000 | -4.389376000 |
| H | 3.077376000 | 1.049403000 | 2.078566000 |
| H | 3.430987000 | 1.700748000 | 4.486661000 |
| H | 1.638833000 | 3.047769000 | 5.649032000 |
| H | -0.403385000 | 3.695524000 | 4.379994000 |
| H | -1.692758000 | 2.563746000 | -1.507169000 |
| H | -3.735324000 | 3.795742000 | -0.838330000 |
| H | -3.963329000 | 4.588784000 | 1.547977000 |
| H | -2.128703000 | 4.090297000 | 3.159768000 |
| H | 2.823388000 | 3.758423000 | 1.376723000 |
| H | 4.057802000 | 5.774204000 | 0.634534000 |
| H | 3.918032000 | 6.475666000 | -1.786952000 |
| H | 2.552230000 | 5.104602000 | -3.357742000 |
| H | -0.638470000 | 0.032848000 | -2.087449000 |
| H | -1.231296000 | 0.336761000 | -4.517954000 |
| H | -0.261682000 | 2.310487000 | -5.759112000 |
| H | 1.227990000 | 3.892478000 | -4.543164000 |
| Mn | 0.960616000 | 1.586404000 | -0.029664000 |
| Mn | 1.647927000 | -1.173306000 | 0.030987000 |

¹Transition state

| | | | |
|---|--------------|-------------|--------------|
| O | 1.863158000 | 0.424641000 | -0.009567000 |
| O | -0.350917000 | 0.372405000 | 0.283555000 |

| | | | |
|---|--------------|--------------|--------------|
| N | 1.393334000 | -1.768843000 | 1.969059000 |
| C | 0.230889000 | -1.437979000 | 2.610177000 |
| C | 0.006370000 | -1.782678000 | 3.948217000 |
| C | 1.009733000 | -2.480569000 | 4.650441000 |
| C | 2.208949000 | -2.804515000 | 3.992101000 |
| C | 2.390978000 | -2.444472000 | 2.643952000 |
| N | 3.590134000 | -2.343509000 | 0.557174000 |
| C | 4.673599000 | -2.572177000 | -0.232320000 |
| C | 5.826020000 | -3.217121000 | 0.245024000 |
| C | 5.856119000 | -3.644671000 | 1.585039000 |
| C | 4.736438000 | -3.407389000 | 2.405431000 |
| C | 3.614045000 | -2.752505000 | 1.869723000 |
| N | 0.675072000 | -3.204606000 | -0.523580000 |
| C | -0.085233000 | -3.978127000 | 0.301755000 |
| C | -0.687087000 | -5.168866000 | -0.133120000 |
| C | -0.494632000 | -5.584857000 | -1.462665000 |
| C | 0.287981000 | -4.787249000 | -2.320232000 |
| C | 0.859567000 | -3.602116000 | -1.833928000 |
| N | 2.092827000 | -1.546231000 | -1.983548000 |
| C | 2.860347000 | -0.616340000 | -2.621606000 |
| C | 3.261352000 | -0.790693000 | -3.951879000 |
| C | 2.849514000 | -1.949609000 | -4.642734000 |
| C | 2.048138000 | -2.898961000 | -3.982524000 |
| C | 1.679958000 | -2.683594000 | -2.643410000 |
| N | 1.064624000 | 2.165254000 | 1.997403000 |
| C | 2.130917000 | 1.653389000 | 2.671730000 |
| C | 2.368656000 | 1.976251000 | 4.014288000 |
| C | 1.474602000 | 2.841423000 | 4.678082000 |
| C | 0.371812000 | 3.360311000 | 3.976745000 |
| C | 0.184637000 | 3.012905000 | 2.627133000 |
| N | -0.866408000 | 3.062272000 | 0.468872000 |
| C | -1.847920000 | 3.441400000 | -0.395279000 |
| C | -2.902088000 | 4.280067000 | -0.004674000 |
| C | -2.950824000 | 4.743879000 | 1.322260000 |
| C | -1.941735000 | 4.345835000 | 2.218970000 |
| C | -0.911517000 | 3.502517000 | 1.774899000 |
| N | 1.920642000 | 3.379749000 | -0.530162000 |
| C | 2.753016000 | 4.095983000 | 0.274290000 |
| C | 3.512766000 | 5.174887000 | -0.203184000 |
| C | 3.409269000 | 5.534849000 | -1.558775000 |
| C | 2.553685000 | 4.793640000 | -2.395313000 |
| C | 1.822344000 | 3.719989000 | -1.862416000 |
| N | 0.297118000 | 1.866281000 | -1.934575000 |
| C | -0.576124000 | 1.017760000 | -2.547427000 |
| C | -0.888527000 | 1.147393000 | -3.907421000 |
| C | -0.280563000 | 2.178709000 | -4.652492000 |
| C | 0.627030000 | 3.044528000 | -4.015585000 |
| C | 0.905345000 | 2.873173000 | -2.647630000 |
| H | -0.504788000 | -0.897888000 | 2.025704000 |
| H | -0.933919000 | -1.519704000 | 4.421069000 |
| H | 0.860414000 | -2.771501000 | 5.686221000 |
| H | 2.983048000 | -3.343098000 | 4.525764000 |

| | | | |
|----|--------------|--------------|--------------|
| H | 4.621240000 | -2.235333000 | -1.260655000 |
| H | 6.670344000 | -3.379961000 | -0.416355000 |
| H | 6.729422000 | -4.151288000 | 1.984712000 |
| H | 4.756261000 | -3.733883000 | 3.438708000 |
| H | -0.218075000 | -3.643773000 | 1.321282000 |
| H | -1.287296000 | -5.751175000 | 0.557876000 |
| H | -0.942509000 | -6.504950000 | -1.826074000 |
| H | 0.439033000 | -5.095642000 | -3.348553000 |
| H | 3.147890000 | 0.250432000 | -2.038489000 |
| H | 3.887793000 | -0.045743000 | -4.430778000 |
| H | 3.152093000 | -2.114735000 | -5.672760000 |
| H | 1.732454000 | -3.794243000 | -4.505701000 |
| H | 2.787315000 | 1.003335000 | 2.106967000 |
| H | 3.237271000 | 1.571269000 | 4.522494000 |
| H | 1.637097000 | 3.113651000 | 5.716797000 |
| H | -0.317117000 | 4.031655000 | 4.476260000 |
| H | -1.796899000 | 3.070205000 | -1.408365000 |
| H | -3.662545000 | 4.557448000 | -0.726836000 |
| H | -3.754322000 | 5.394788000 | 1.653477000 |
| H | -1.970045000 | 4.691122000 | 3.246114000 |
| H | 2.815818000 | 3.807216000 | 1.313903000 |
| H | 4.162595000 | 5.717168000 | 0.475381000 |
| H | 3.977838000 | 6.370153000 | -1.956321000 |
| H | 2.465305000 | 5.060617000 | -3.442222000 |
| H | -1.032661000 | 0.263099000 | -1.917998000 |
| H | -1.603917000 | 0.471203000 | -4.363492000 |
| H | -0.516188000 | 2.313365000 | -5.704160000 |
| H | 1.092911000 | 3.844912000 | -4.578859000 |
| Mn | 0.699708000 | 1.804177000 | 0.047260000 |
| Mn | 1.693841000 | -1.456325000 | -0.012646000 |

¹Product

| | | | |
|---|--------------|--------------|--------------|
| O | 1.423075000 | 0.313787000 | 0.066645000 |
| O | -0.799136000 | 0.723805000 | 0.685047000 |
| N | 1.217980000 | -1.932284000 | 1.906933000 |
| C | -0.009073000 | -1.637927000 | 2.431505000 |
| C | -0.372469000 | -2.052228000 | 3.719581000 |
| C | 0.555783000 | -2.781432000 | 4.489205000 |
| C | 1.825211000 | -3.063408000 | 3.951106000 |
| C | 2.147260000 | -2.631584000 | 2.652782000 |
| N | 3.570075000 | -2.345506000 | 0.730199000 |
| C | 4.743041000 | -2.489795000 | 0.054814000 |
| C | 5.848223000 | -3.155399000 | 0.608078000 |
| C | 5.734560000 | -3.697853000 | 1.901721000 |
| C | 4.523286000 | -3.548066000 | 2.604142000 |
| C | 3.454395000 | -2.864445000 | 2.000594000 |
| N | 0.887371000 | -3.306828000 | -0.707624000 |
| C | 0.101382000 | -4.177951000 | -0.014557000 |
| C | -0.349904000 | -5.384145000 | -0.572750000 |
| C | 0.027803000 | -5.709649000 | -1.888072000 |
| C | 0.837741000 | -4.810266000 | -2.609248000 |
| C | 1.252197000 | -3.614599000 | -2.003432000 |

| | | | |
|---|--------------|--------------|--------------|
| N | 2.341360000 | -1.471746000 | -1.906375000 |
| C | 3.080950000 | -0.444742000 | -2.413973000 |
| C | 3.618133000 | -0.501362000 | -3.705580000 |
| C | 3.370524000 | -1.643076000 | -4.496867000 |
| C | 2.589908000 | -2.690025000 | -3.974246000 |
| C | 2.081308000 | -2.590755000 | -2.667455000 |
| N | 1.104867000 | 2.291844000 | 2.022786000 |
| C | 2.142792000 | 1.670414000 | 2.645194000 |
| C | 2.532179000 | 2.019289000 | 3.945050000 |
| C | 1.821762000 | 3.030949000 | 4.622768000 |
| C | 0.746575000 | 3.664840000 | 3.976059000 |
| C | 0.402828000 | 3.281837000 | 2.667571000 |
| N | -0.831389000 | 3.354599000 | 0.608589000 |
| C | -1.833471000 | 3.812137000 | -0.192135000 |
| C | -2.724771000 | 4.809499000 | 0.228653000 |
| C | -2.584834000 | 5.351604000 | 1.519043000 |
| C | -1.555857000 | 4.872110000 | 2.350543000 |
| C | -0.692452000 | 3.870765000 | 1.879667000 |
| N | 1.800141000 | 3.206525000 | -0.697116000 |
| C | 2.778739000 | 3.896798000 | -0.049800000 |
| C | 3.559553000 | 4.869600000 | -0.692781000 |
| C | 3.319818000 | 5.146964000 | -2.051072000 |
| C | 2.313612000 | 4.430350000 | -2.725548000 |
| C | 1.568201000 | 3.462871000 | -2.031101000 |
| N | -0.136898000 | 1.791544000 | -1.767543000 |
| C | -1.150181000 | 0.991329000 | -2.201678000 |
| C | -1.589263000 | 1.026099000 | -3.532967000 |
| C | -0.965179000 | 1.912120000 | -4.434170000 |
| C | 0.086086000 | 2.730056000 | -3.979390000 |
| C | 0.490312000 | 2.655163000 | -2.634919000 |
| H | -0.683480000 | -1.053504000 | 1.814923000 |
| H | -1.357914000 | -1.810392000 | 4.103114000 |
| H | 0.298815000 | -3.123049000 | 5.487698000 |
| H | 2.545697000 | -3.617817000 | 4.541045000 |
| H | 4.799404000 | -2.067757000 | -0.941446000 |
| H | 6.766838000 | -3.247310000 | 0.038394000 |
| H | 6.568249000 | -4.225516000 | 2.355270000 |
| H | 4.430771000 | -3.962847000 | 3.601306000 |
| H | -0.173615000 | -3.908080000 | 0.996490000 |
| H | -0.977977000 | -6.046947000 | 0.012988000 |
| H | -0.300004000 | -6.638833000 | -2.344580000 |
| H | 1.130468000 | -5.049938000 | -3.625209000 |
| H | 3.233939000 | 0.408281000 | -1.762871000 |
| H | 4.219856000 | 0.319748000 | -4.080097000 |
| H | 3.779285000 | -1.717644000 | -5.500397000 |
| H | 2.394298000 | -3.568356000 | -4.578596000 |
| H | 2.653090000 | 0.903404000 | 2.077188000 |
| H | 3.373204000 | 1.517912000 | 4.411885000 |
| H | 2.101393000 | 3.323353000 | 5.630493000 |
| H | 0.195438000 | 4.445821000 | 4.486949000 |
| H | -1.931495000 | 3.375744000 | -1.175361000 |
| H | -3.508775000 | 5.145386000 | -0.441609000 |

| | | | |
|----|--------------|--------------|--------------|
| H | -3.261848000 | 6.123232000 | 1.872866000 |
| H | -1.441399000 | 5.275697000 | 3.349987000 |
| H | 2.938731000 | 3.673022000 | 0.996044000 |
| H | 4.326386000 | 5.398695000 | -0.136984000 |
| H | 3.897523000 | 5.904423000 | -2.572292000 |
| H | 2.115933000 | 4.638752000 | -3.770903000 |
| H | -1.613228000 | 0.355134000 | -1.456625000 |
| H | -2.410990000 | 0.390715000 | -3.846056000 |
| H | -1.296654000 | 1.973592000 | -5.466593000 |
| H | 0.565849000 | 3.419958000 | -4.664205000 |
| Mn | 0.478804000 | 1.844155000 | 0.155899000 |
| Mn | 1.725800000 | -1.517569000 | 0.003533000 |