

Alkene Epoxidations Mediated by Mn-Salen Macrocyclic Catalysts

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Supporting Information

B3LYP/6-31G(d) (for C, H, O, N atoms) and def2svp level (for Mn atom) Energies and Cartesian Coordinates

MnM20

$E_{\text{SCF}} = -3802.599465$

Gibbs free energy = -3801.73153

Mn -1.73369600 0.00000900 0.00012600
N -3.11202000 -1.18985000 -0.43953000
N -3.11214800 1.18982600 0.43958700
C -2.93719600 2.48492000 0.35057000
H -3.78528500 3.13843500 0.56669700
C -2.93694800 -2.48494200 -0.35065600
H -3.78494700 -3.13850800 -0.56698600
C -1.70947800 -3.09354100 0.06172300
C -1.70971300 3.09357200 -0.06171000
C -0.72296600 -2.35854700 0.79598900
C -0.72309700 2.35859100 -0.79582800
O -0.89699000 -1.08107300 1.14504900
O -0.89704000 1.08107200 -1.14483100
C -4.45836300 -0.58141600 -0.53849500
H -5.20374400 -1.31847300 -0.22093300
C -4.45844200 0.58126900 0.53845300
H -5.20387900 1.31826600 0.22087900
C -4.81079200 -0.09942800 -1.93902500
C -6.16723200 0.09770000 -2.23978200
C -3.85249500 0.16964200 -2.92302000
C -6.55824900 0.56581700 -3.49305300
H -6.92570400 -0.12634900 -1.49198600
C -4.24585400 0.63499000 -4.18053300
H -2.79869300 0.00990000 -2.72302500
C -5.59545100 0.83730800 -4.46845000
H -7.61280700 0.70713700 -3.71113400
H -3.49183900 0.83428000 -4.93662700
H -5.89759400 1.19551800 -5.44813200
C -4.81087200 0.09919300 1.93895700

C -6.16727300 -0.09849900 2.23953400
C -3.85260500 -0.16939900 2.92310900
C -6.55826900 -0.56669300 3.49278100
H -6.92573300 0.12516900 1.49161300
C -4.24594500 -0.63483300 4.18059900
H -2.79884300 -0.00922400 2.72325500
C -5.59549400 -0.83770300 4.46833700
H -7.61279700 -0.70844900 3.71072000
H -3.49195000 -0.83375400 4.93681000
H -5.89762700 -1.19597600 5.44800000
C -1.51763100 -4.48371500 -0.15538100
C 0.43011400 -3.03329600 1.26441000
C 0.42999500 3.03334800 -1.26419800
C -1.51794800 4.48377000 0.15532500
C -0.38187800 5.14802600 -0.27301300
C 0.57936700 -4.38033300 0.98449500
C 0.57917000 4.38040600 -0.98434900
H -2.29343900 5.01690000 0.69455900
H 1.48108900 4.86911100 -1.34178200
C -0.38158000 -5.14795600 0.27303200
H 1.48127700 -4.86901500 1.34198600
H -2.29305000 -5.01684200 -0.69472300
C 1.45021300 -2.25663200 2.05760900
H 0.92738800 -1.63764700 2.79513400
H 2.12425300 -2.93929500 2.59237000
C 1.45010600 2.25668800 -2.05739000
H 0.92727000 1.63797000 -2.79512800
H 2.12434100 2.93935100 -2.59190300
O 2.18503700 -1.44257800 1.14941300
O 2.18465500 1.44231900 -1.14925700
C 3.00410300 -0.45517500 1.64807800
C 3.79470400 0.21106300 0.71762400
C 3.05355400 -0.11786100 3.02475200
C 4.64099200 1.27686900 1.15813000
C 3.86597700 0.90643200 3.45453200
H 2.46377900 -0.66369000 3.75151800
C 4.67056600 1.63602800 2.54700500
H 3.90089500 1.15917400 4.51140900
C 3.00381700 0.45504100 -1.64800700
C 3.79465700 -0.21104000 -0.71763600
C 3.05313800 0.11767000 -3.02466600
C 4.64108400 -1.27670400 -1.15821200
C 3.86569200 -0.90649400 -3.45451600
H 2.46314400 0.66331800 -3.75139000
C 4.67054900 -1.63589900 -2.54708100
H 3.90049600 -1.15926900 -4.51138900
C 5.51306000 2.69628600 2.97992500
C 5.47809800 2.00324500 0.26304000
C 6.30322600 3.38033500 2.08618700
C 6.28360900 3.02414100 0.71482800
H 5.52379300 2.95307800 4.03669600

H 6.94655700 4.18658500 2.42690500
H 6.91688100 3.56067100 0.01325800
H 5.47944500 1.73516500 -0.78810100
C 5.47845100 -2.00289300 -0.26321200
C 5.51320000 -2.69600100 -2.98008600
C 6.30361600 -3.37986800 -2.08643400
C 6.28410400 -3.02364000 -0.71508100
H 5.47988400 -1.73479500 0.78792300
H 6.91757100 -3.56002800 -0.01357900
H 6.94706800 -4.18599800 -2.42720900
H 5.52384100 -2.95281300 -4.03685400
C -0.12724600 -6.64200100 0.01852300
C -0.12760700 6.64208800 -0.01853500
C -1.28385500 -7.30313100 -0.75426400
H -2.23011100 -7.24898300 -0.20307100
H -1.42942400 -6.84989500 -1.74178300
H -1.05946100 -8.36287300 -0.91238200
C 0.03315500 -7.37239100 1.37416000
H 0.22134100 -8.43836200 1.20447600
H 0.87242600 -6.98029200 1.95846900
H -0.87369900 -7.28128000 1.98269000
C 1.16978800 -6.80171000 -0.81177000
H 1.08130300 -6.30248500 -1.78309500
H 2.04293000 -6.38471400 -0.29885900
H 1.36934700 -7.86385100 -0.99276700
C -1.28430300 7.30321700 0.75412200
H -2.23050300 7.24904500 0.20283400
H -1.42996500 6.85000000 1.74163500
H -1.05994200 8.36296600 0.91224000
C 1.16934600 6.80185300 0.81187000
H 2.04254400 6.38485900 0.29905100
H 1.36886700 7.86400400 0.99285200
H 1.08078500 6.30265700 1.78320300
C 0.03290200 7.37244000 -1.37418100
H 0.87223600 6.98034600 -1.95840100
H -0.87389500 7.28128800 -1.98279200
H 0.22104500 8.43842000 -1.20451100

MnM20 activated

$E_{\text{SCF}} = -3877.812102$

Gibbs free energy = -3876.941245

$E_{\text{solv}} = -3877.870666$

Mn -1.30435600 -0.03804900 0.14615900
N -2.86779700 1.00678700 -0.27374600
N -2.58468500 -1.49813200 0.04516100
C -2.28816900 -2.76194000 -0.10332400

H -3.09346000 -3.48368800 0.03331500
C -2.86125000 2.29391100 -0.53901600
H -3.83615400 2.76177800 -0.67937400
C -1.73419300 3.14039200 -0.64592000
C -1.01236700 -3.26941400 -0.46303100
C -0.41534600 2.59080800 -0.62252600
C 0.02841000 -2.37293100 -0.82584800
O -0.21045800 1.29894300 -0.54761300
O -0.10697400 -1.05976200 -0.78354800
C -4.17805500 0.28142100 -0.29772500
H -4.38988600 0.06134600 -1.35077900
C -3.95334000 -1.05982000 0.42880200
H -3.90749300 -0.85559100 1.50600400
C -5.33648900 1.07133000 0.28320900
C -6.47745300 1.30968100 -0.49171800
C -5.29326800 1.55197300 1.60189500
C -7.56372600 2.00775800 0.04137600
H -6.52287600 0.94005300 -1.51320000
C -6.37577600 2.25197100 2.13218700
H -4.40871400 1.39014900 2.21361900
C -7.51444000 2.47931700 1.35330600
H -8.44451200 2.18191600 -0.56957200
H -6.33189000 2.61938800 3.15335200
H -8.35764600 3.02319800 1.76882000
C -5.06358300 -2.06042500 0.17070900
C -5.80012600 -2.56715900 1.24824600
C -5.38347800 -2.48304900 -1.12992900
C -6.84429300 -3.46949400 1.03440800
H -5.56301800 -2.24758800 2.25997500
C -6.42284800 -3.38774400 -1.34359000
H -4.81527300 -2.11585600 -1.98159800
C -7.15770700 -3.88040000 -0.26148000
H -7.41001300 -3.84893500 1.88014200
H -6.66022900 -3.70678200 -2.35431500
H -7.96916100 -4.58230900 -0.42970700
C -1.94464800 4.53525800 -0.80698300
C 0.68541200 3.48769500 -0.70766400
C 1.25088100 -2.90293900 -1.30398800
C -0.80729200 -4.67039200 -0.53782800
C 0.39955700 -5.20591800 -0.95470400
C 0.41296100 4.84341300 -0.83707300
C 1.40469400 -4.28100400 -1.34087900
H -1.62996600 -5.31645000 -0.25034500
H 2.36117300 -4.66235600 -1.68798600
C -0.88439900 5.41503200 -0.90228400
H 1.26898000 5.51300200 -0.89479900
H -2.96861400 4.89188200 -0.83754700
C 2.16634600 3.09719400 -0.67741000
H 2.66944200 3.71839800 0.07717400
H 2.60212000 3.35488600 -1.64947100
C 2.36923600 -1.98400900 -1.72570400

H 1.99558700 -0.96984700 -1.89197900
H 2.81484200 -2.35186900 -2.65984600
O 2.50964600 1.73862400 -0.48632700
O 3.35475200 -1.97129600 -0.68051400
C 2.66185700 1.24904600 0.78995800
C 3.65692100 0.29791500 0.98231300
C 1.82291400 1.66053500 1.85469000
C 3.79249900 -0.31565400 2.27045600
C 1.95162300 1.08264200 3.09770900
H 1.07583300 2.42827200 1.69158600
C 2.92218200 0.07793500 3.34055600
H 1.30496500 1.39891400 3.91233900
C 4.42809000 -1.13253500 -0.92692600
C 4.61302200 -0.02148300 -0.12332600
C 5.33466000 -1.45686200 -1.96777100
C 5.75928900 0.81388500 -0.34987700
C 6.42375600 -0.65705900 -2.20832500
H 5.16421100 -2.35480800 -2.55426600
C 6.66582000 0.49621200 -1.41537600
H 7.12258800 -0.90566000 -3.00308300
C 3.06252200 -0.52988900 4.61623100
C 4.78138300 -1.30087300 2.54017800
C 4.02709700 -1.48723000 4.84073200
C 4.89333900 -1.87127400 3.79071000
H 2.39487700 -0.22042900 5.41699800
H 4.12840100 -1.94411000 5.82097100
H 5.65667300 -2.62273800 3.97257900
H 5.45293800 -1.60315600 1.74404600
C 6.03689900 1.95966100 0.44616900
C 7.79135600 1.33148600 -1.64567000
C 8.02573000 2.43724100 -0.86023500
C 7.13856900 2.74929300 0.19694300
H 5.37068000 2.20255200 1.26740100
H 7.33281800 3.61665100 0.82218500
H 8.89153600 3.06686600 -1.04429000
H 8.46971900 1.07695000 -2.45648700
C -1.04734600 6.93478500 -1.06364000
C 0.68131900 -6.71510100 -1.02153400
C -2.52913100 7.35390000 -1.09258200
H -3.04758600 7.08928700 -0.16353300
H -3.06776200 6.89982700 -1.93263500
H -2.60091500 8.44018900 -1.20876700
C -0.36106900 7.65527000 0.12218900
H -0.46953400 8.74035100 0.01523900
H 0.71112500 7.43709300 0.17454400
H -0.81172000 7.36226000 1.07715900
C -0.38736700 7.38080500 -2.39075900
H -0.85982100 6.89240000 -3.25042500
H 0.68259900 7.14765700 -2.41742500
H -0.49120900 8.46445400 -2.51681800
C -0.52875300 -7.54987100 -0.56187700

H -1.40796900 -7.38255300 -1.19532300
H -0.80314000 -7.33509400 0.47755700
H -0.28286100 -8.61507700 -0.62129600
C 1.88146600 -7.04871600 -0.10213500
H 2.79002000 -6.51473800 -0.40007600
H 2.09960400 -8.12185700 -0.14511700
H 1.66510900 -6.78727600 0.93968800
C 1.02198500 -7.11053700 -2.47888400
H 1.90271200 -6.57894800 -2.85483800
H 0.18536900 -6.89584600 -3.15352900
H 1.23644700 -8.18360900 -2.53589700
O -1.04421000 0.01522100 1.64714600

cis- β -methyl-styrene

E_{SCF} = -348.963676

Gibbs free energy = -348.834433

Esolv = -348.966662

C -2.58426700 -0.46315600 -0.10007100
C -1.38773300 -1.01425500 -0.36724500
H -3.45933600 -1.07656800 -0.31516000
H -1.39263800 -2.04118200 -0.73361000
C -2.88384100 0.88167700 0.50053200
H -2.01559100 1.31627800 1.00311900
H -3.22569200 1.59878300 -0.25995100
H -3.69591900 0.79580100 1.23318200
C -0.03930000 -0.44172600 -0.19469700
C 0.25412300 0.92101000 -0.38548200
C 1.02405400 -1.30138500 0.13912800
C 1.55033800 1.40657600 -0.21391700
H -0.53084200 1.59874400 -0.70418400
C 2.31807600 -0.81719100 0.31476300
H 0.82293700 -2.36212000 0.27154000
C 2.58676900 0.54285500 0.14378800
H 1.75242400 2.46291700 -0.37219700
H 3.11905100 -1.50206000 0.58118500
H 3.59629100 0.92297500 0.27528200

(2S,3R)-TS (A)

E_{SCF} = -4226.763970

Imaginary frequency= -391.14

Gibbs free energy = -4225.741609

Esolv = -4226.820382

Mn 1.72827500 0.12647500 0.66732400
N 2.90460700 -1.19723300 -0.02924800

N 2.99383200 1.34116200 -0.22101200
C 2.71465300 2.44864200 -0.83368600
H 3.52791100 3.01931400 -1.28367700
C 2.62437500 -2.47888000 -0.18204900
H 3.40616900 -3.09380800 -0.63260300
C 1.42473600 -3.14352500 0.14860200
C 1.38552600 2.96630900 -0.99162000
C 0.33722600 -2.45779600 0.78786100
C 0.25506400 2.19968400 -0.60842100
O 0.40042800 -1.21262900 1.13984800
O 0.33982900 0.97204200 -0.09601000
C 4.22145600 -0.71309200 -0.55572500
H 4.16487900 -0.75866600 -1.64988800
C 4.36316400 0.77819400 -0.14781100
H 4.62657100 0.80420800 0.91621600
C 5.39885100 -1.55229500 -0.09165400
C 6.29564300 -2.08524700 -1.02479200
C 5.61739700 -1.78918400 1.27431800
C 7.39638500 -2.83564500 -0.60427800
H 6.13926700 -1.90584200 -2.08572900
C 6.71362400 -2.54048800 1.69449400
H 4.92081700 -1.39312200 2.00950200
C 7.60710500 -3.06451600 0.75549100
H 8.08515100 -3.24075100 -1.33990300
H 6.87196600 -2.71894100 2.75435300
H 8.46112700 -3.64951700 1.08421700
C 5.44622600 1.50343400 -0.92448500
C 6.47610000 2.14748900 -0.22729600
C 5.45462100 1.54556700 -2.32850500
C 7.49709400 2.81062200 -0.91051000
H 6.48459000 2.12215100 0.85967200
C 6.47088200 2.21220600 -3.01311600
H 4.66156600 1.06471100 -2.89643500
C 7.49652500 2.84414300 -2.30534900
H 8.29106400 3.29830400 -0.35247500
H 6.46304300 2.23583400 -4.09909500
H 8.28970100 3.35903400 -2.83956400
C 1.30382100 -4.52349800 -0.19294400
C -0.85651200 -3.20605000 1.03676200
C -1.03733600 2.73623400 -0.81028400
C 1.20575300 4.22887400 -1.60066000
C -0.05638900 4.76537500 -1.82345500
C -0.91690700 -4.53414500 0.66608900
C -1.15978000 3.98531200 -1.40768800
H 2.09596800 4.77747800 -1.89050000
H -2.16705200 4.36129700 -1.56463700
C 0.15497100 -5.24361300 0.05002300
H -1.84859100 -5.06235200 0.85199200
H 2.15728500 -4.99313000 -0.67124400
C -2.04445600 -2.52106400 1.65729400
H -1.72723800 -1.90362700 2.50741700

H -2.75960000 -3.26748000 2.02684500
C -2.26381400 1.96788400 -0.35587200
H -2.75555500 2.51063200 0.46018800
H -1.97382700 0.98149400 0.00794900
O -2.66131500 -1.70275500 0.66149700
O -3.24190100 1.85615700 -1.39977900
C -3.81339400 -1.02696400 0.97583600
C -4.45694000 -0.37709700 -0.07756400
C -4.32518500 -0.96596100 2.29807800
C -5.65701300 0.35716600 0.18994300
C -5.47498700 -0.25413800 2.56011500
H -3.82627100 -1.48885500 3.10599300
C -6.17019400 0.42223600 1.52947400
H -5.86823600 -0.21792600 3.57332000
C -3.30658600 0.64145500 -2.05805100
C -3.90136400 -0.46462400 -1.46490500
C -2.80085300 0.59709500 -3.37990000
C -4.00266100 -1.67850600 -2.22577700
C -2.88376700 -0.56085200 -4.11311600
H -2.35947800 1.50076100 -3.78813100
C -3.47932700 -1.72553600 -3.56100800
H -2.49775400 -0.59759000 -5.12891800
C -7.36553800 1.14745400 1.79040800
C -6.38667800 1.02528800 -0.83491100
C -8.04008400 1.78396700 0.77577000
C -7.54202600 1.71625400 -0.54912400
H -7.74000700 1.18204500 2.81097400
H -8.95460700 2.33224800 0.98303000
H -8.08205500 2.21388300 -1.34999900
H -6.02186500 0.97894600 -1.85454100
C -4.62982500 -2.84803800 -1.71309400
C -3.58424500 -2.92892200 -4.30976900
C -4.18727700 -4.04516700 -3.77725800
C -4.71984200 -3.99773200 -2.46647600
H -5.05570600 -2.81979500 -0.71582700
H -5.21326100 -4.87474200 -2.05566300
H -4.26740600 -4.95725800 -4.36208500
H -3.18359000 -2.94725000 -5.32065900
C -0.02279500 -6.72413800 -0.32019300
C -0.28854100 6.13729900 -2.47831100
C 1.24392100 -7.31197600 -0.97006300
H 2.10923300 -7.26390300 -0.29843000
H 1.50085300 -6.79767900 -1.90349200
H 1.07640900 -8.36636600 -1.21351700
C -0.33706100 -7.54008800 0.95697900
H -0.47769500 -8.59737400 0.70473900
H -1.25253400 -7.19567900 1.45018100
H 0.48252600 -7.47068100 1.68137500
C -1.19393800 -6.86459500 -1.32286100
H -0.99590200 -6.30207300 -2.24194000
H -2.13921100 -6.49908500 -0.90765000

H -1.33578800 -7.91801800 -1.59088200
C 1.03279700 6.82805200 -2.86509500
H 1.60630400 6.23890400 -3.59033000
H 1.66827800 7.01620900 -1.99176800
H 0.81822800 7.79693400 -3.32815000
C -1.04471100 7.05559100 -1.48796800
H -2.01837800 6.64070900 -1.20601900
H -1.22266500 8.03679900 -1.94296500
H -0.46456900 7.20740800 -0.57046000
C -1.13549600 5.95600800 -3.76098300
H -2.11157900 5.50743900 -3.54865900
H -0.62065800 5.31425900 -4.48509300
H -1.31380600 6.92769800 -4.23596600
O 2.07979400 0.58609400 2.18985600
C 1.36502800 -0.03553400 3.69184100
C 0.07384400 0.55270000 3.65506500
C -0.45914400 1.74408000 4.22928300
C -1.81267900 2.05486400 3.90875300
C 0.23485100 2.62555100 5.10447400
C -2.43347400 3.18128100 4.42628200
H -2.36554700 1.38678500 3.25337500
C -0.39331700 3.75177300 5.61419800
H 1.25981400 2.42328800 5.38281500
C -1.72473600 4.03555700 5.27938400
H -3.46620900 3.39731800 4.17047200
H 0.14968700 4.41561500 6.28007800
H -2.20795000 4.91879800 5.68694200
H -0.60872800 0.02833500 2.99162500
C 2.46076100 0.30036300 4.67317700
H 2.11803500 0.15995900 5.70538300
H 3.31863100 -0.35796400 4.51125900
H 2.80540500 1.33099600 4.55531700
H 1.33105300 -1.08153300 3.39689400

(2R,3S)-TS (B)

$E_{\text{SCF}} = -4226.762172$

Imaginary frequency = -382.67

Gibbs free energy = -4225.740393

$E_{\text{solv}} = -4226.819766$

Mn 1.52297700 0.42372200 0.50540300
N 2.55683900 -0.42938400 -0.84238500
N 2.48186200 2.00963700 -0.14725900
C 2.00293900 3.20330800 -0.30907200
H 2.66039500 3.98514900 -0.69144300
C 2.29077100 -1.60017000 -1.39295500
C 1.21251500 -2.46217300 -1.10241800
C 0.63713600 3.56304700 -0.05419600

C 0.29070100 -2.17665800 -0.03814000
C -0.32933400 2.57540500 0.26624900
O 0.41993300 -1.15403100 0.74631300
O -0.04671200 1.27451300 0.36144600
C 3.71853200 0.34405700 -1.38588500
H 3.45196600 0.64871900 -2.40485500
C 3.86401200 1.62861300 -0.52367300
H 4.34755300 1.33870700 0.41655900
C 5.00273900 -0.46513000 -1.43443600
C 5.73636500 -0.55325600 -2.62297200
C 5.48087700 -1.11826100 -0.28772000
C 6.93226900 -1.27395800 -2.66738500
H 5.37766900 -0.04844300 -3.51662200
C 6.67261700 -1.83975300 -0.33284200
H 4.91333800 -1.07051600 0.63854900
C 7.40219500 -1.91816400 -1.52286400
H 7.49262200 -1.33173000 -3.59599900
H 7.03265800 -2.34243600 0.56047200
H 8.33092000 -2.48040500 -1.55649500
C 4.71442200 2.69665700 -1.18584300
C 5.81206000 3.22454800 -0.49419300
C 4.43756600 3.17724400 -2.47633300
C 6.62244000 4.20105000 -1.07597700
H 6.03976000 2.86222500 0.50535700
C 5.24323900 4.15643200 -3.05786100
H 3.58502300 2.79542200 -3.03304500
C 6.33957700 4.66891700 -2.35968500
H 7.47312300 4.59349700 -0.52649000
H 5.01579200 4.51749300 -4.05677200
H 6.96837300 5.42848200 -2.81495800
C 1.03858500 -3.62445400 -1.91189800
C -0.80136000 -3.08062200 0.14745700
C -1.67459600 2.96438400 0.45684000
C 0.24089700 4.91154500 -0.20248600
C -1.07847200 5.31276600 -0.03167100
C -0.92766300 -4.17388300 -0.68659700
C -2.01210700 4.30386100 0.29959300
H 1.00813400 5.63509500 -0.45786700
H -3.05830700 4.56589000 0.42898100
C -0.01613400 -4.49297700 -1.73421600
H -1.78981600 -4.81849500 -0.53582200
H 1.76483900 -3.79506600 -2.70013500
C -1.84766800 -2.77874100 1.18766100
H -1.38537400 -2.37769600 2.09813300
H -2.39175300 -3.69543800 1.45026400
C -2.72390400 1.93820600 0.84535200
H -3.03052300 2.10089900 1.88530500
H -2.31511400 0.93045800 0.76157100
O -2.74618100 -1.81662000 0.63312300
O -3.91384000 2.07257900 0.05512500
C -3.84964900 -1.43903400 1.35892400

C -4.74460100 -0.58425600 0.71732300
C -4.07288600 -1.87146000 2.69063200
C -5.91106900 -0.14497000 1.42157400
C -5.18951500 -1.44646200 3.37355500
H -3.36916900 -2.53573500 3.17870100
C -6.13345500 -0.58052400 2.77124600
H -5.35781800 -1.78075300 4.39441800
C -4.07868200 1.15074400 -0.96345000
C -4.48849200 -0.14784500 -0.69148900
C -3.87034200 1.60425900 -2.28872700
C -4.69444000 -1.04653900 -1.79223700
C -4.06015300 0.75217300 -3.34886200
H -3.56719300 2.63611500 -2.43542600
C -4.46874200 -0.59055900 -3.13383900
H -3.90241500 1.09816900 -4.36754400
C -7.29321700 -0.14364400 3.46822800
C -6.88423100 0.70928700 0.82836200
C -8.20843300 0.68618700 2.86503200
C -7.99809200 1.11114600 1.52987700
H -7.44390400 -0.48383900 4.49014900
H -9.09287000 1.01311900 3.40431700
H -8.72733400 1.76088900 1.05360900
H -6.73973000 1.03995100 -0.19398800
C -5.13698700 -2.38594300 -1.60699000
C -4.67427100 -1.48572400 -4.21850700
C -5.09226900 -2.77871500 -4.00152700
C -5.32996200 -3.22803400 -2.68007800
H -5.33610000 -2.73651800 -0.59986400
H -5.67909600 -4.24377100 -2.51318200
H -5.25264300 -3.45129700 -4.83959700
H -4.50105600 -1.12417800 -5.22952900
C -0.26610200 -5.73080100 -2.61017400
C -1.54571400 6.76949100 -0.18758000
C 0.83861100 -5.92381400 -3.66540900
H 1.82463900 -6.06023500 -3.20555800
H 0.89318300 -5.07675400 -4.35896200
H 0.62702500 -6.81862000 -4.26005600
C -0.31257900 -6.99599000 -1.72005400
H -0.50203300 -7.88307700 -2.33519200
H -1.10750700 -6.94324700 -0.96826900
H 0.63817600 -7.14508100 -1.19518500
C -1.61891500 -5.56689600 -3.34558100
H -1.60625300 -4.68919800 -4.00116100
H -2.45656300 -5.44605100 -2.65037300
H -1.82271800 -6.45055900 -3.96157600
C -0.38300900 7.71833100 -0.53412600
H 0.09333900 7.45286100 -1.48524800
H 0.38529700 7.72643700 0.24789600
H -0.76063600 8.74142900 -0.63254700
C -2.18452800 7.24900100 1.13826200
H -3.05053800 6.64128100 1.42119200

H -2.52737700 8.28523600 1.03803400
H -1.46188500 7.20925700 1.96137000
C -2.59526500 6.85047100 -1.32246400
H -3.46951400 6.22333400 -1.11882400
H -2.16662000 6.53003300 -2.27900000
H -2.94743900 7.88212200 -1.43747700
O 2.18975800 0.39515200 1.99781400
C 1.48573200 -0.38486700 3.38810600
C 2.05958000 -1.68556900 3.31105700
H 0.44908200 -0.39423200 3.06115100
H 1.51104700 -2.36126200 2.66077800
C 1.77495100 0.64457400 4.45639100
H 1.58931700 0.23160300 5.45497200
H 2.80626700 1.00215600 4.40899700
H 1.11926700 1.50813800 4.31805500
C 3.26446500 -2.22975200 3.84835800
C 4.15384000 -1.55599100 4.73112800
C 3.58361000 -3.56921500 3.48354500
C 5.28919000 -2.19207400 5.21128200
H 3.94672800 -0.54215500 5.04360500
C 4.71925700 -4.19851300 3.96921000
H 2.91497300 -4.10112500 2.81209200
C 5.57749400 -3.51118800 4.83616700
H 5.95520100 -1.66458700 5.88741300
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H 6.46597500 -4.00200100 5.22257500
H 2.97459100 -1.93040900 -2.17797100