Supporting Information

for

Multi-decker tricarbonyl-bridged sandwich complexes of transition metals: structure, stability and electron-counting rules

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Table of Contents: Total Energies, Harmonic Zero-Point Corrections, Frequencies, and Atomic Coordinates of optimized structures 5–7, 15–23 calculated by B3LYP/6-311+G(df,p) method:

5

E_{total} = -3177.186943 a.u.
ZPE = 0.156518 a.u.
λ=0
ω_1 = 10.6 cm^{-1}

C	-1.000992000	2.830982000	-0.020491000
C	0.005131000	2.818579000	1.021194000
C	1.046176000	2.810569000	0.017908000
C	0.044827000	2.823699000	-1.024352000
H	-2.076853000	2.907374000	-0.040425000
H	-0.016052000	2.874754000	2.098310000
H	2.123960000	2.850410000	0.038676000
H	0.064799000	2.883086000	-2.101327000
Fe	0.000142000	1.071752000	-0.006430000
Fe	0.003010000	-1.070932000	0.001751000
C	-0.647926000	-2.813961000	-0.808240000
C	0.784854000	-2.834017000	-0.618686000
C	0.594417000	-2.826412000	0.818736000
C	-0.839923000	-2.806816000	0.624378000
H	-1.302466000	-2.859622000	-1.664483000
H	1.640333000	-2.908751000	-1.271694000
H	1.247550000	-2.898669000	1.674247000
H	-1.695741000	-2.848546000	1.279849000
C	-0.849284000	0.053352000	-1.394934000
C	1.634029000	-0.070377000	-0.031286000
C	-0.781754000	0.016004000	1.425468000
O	-1.459276000	0.044872000	-2.379130000
O	2.791629000	-0.063884000	-0.045101000
O	-1.338140000	0.018467000	2.441143000

6

E_{total} = -3029.340349 a.u.
ZPE = 0.196689 a.u.
λ=0
ω_1 = 25.9 cm^{-1}

C	-2.865586000	-1.191983000	0.176484000
C	-2.863425000	-0.194268000	1.188897000
C	-2.857888000	1.073370000	0.556022000
C	-2.857786000	0.862892000	-0.850370000
C	-2.865777000	-0.536066000	-1.082213000
H	-2.847344000	-2.259125000	0.337753000
H	-2.839016000	-0.374244000	2.252753000
H	-2.829624000	2.032105000	1.050960000
H	-2.831287000	1.633486000	-1.605706000
H	-2.842726000	-1.018873000	-2.047052000
Mn	-1.082487000	-0.003374000	-0.002848000
Mn	1.082580000	-0.000299000	-0.000244000
C	2.853701000	1.082100000	0.561391000
C	2.861128000	-0.184612000	1.196095000
C	2.868477000	-1.183768000	0.185120000
C	2.869922000	-0.529657000	-1.074497000
C	2.857566000	0.869622000	-0.844684000
H	2.821619000	2.041458000	1.054887000
H	2.834647000	-0.363134000	2.260146000
H	2.852724000	-2.250720000	0.347892000
H	2.850555000	-1.013899000	-2.038697000
H	2.830812000	1.639053000	-1.601196000
C	0.002889000	-0.836798000	-1.397014000
C	-0.002139000	1.619919000	-0.029408000
C	-0.000574000	-0.806878000	1.409027000
O	-0.000870000	-1.394645000	2.416414000
O	0.004963000	-1.438848000	-2.396054000
O	-0.003821000	2.785990000	-0.057153000

7

E_{total} = -2893.737955 a.u.
ZPE = 0.231015 a.u.
λ=0
ω_1 = 10.2 cm^{-1}

C	1.409085000	-0.002795000	2.834915000
C	0.701894000	1.221816000	2.833100000
C	-0.701894000	1.221816000	2.833100000
C	-1.409085000	-0.002795000	2.834915000
C	-0.707071000	-1.218257000	2.836636000
C	0.707071000	-1.218257000	2.836636000
H	2.489575000	0.002105000	2.777897000
H	1.246435000	2.154925000	2.774305000
H	-1.246435000	2.154925000	2.774305000
H	-2.489575000	0.002105000	2.777897000
H	-1.242695000	-2.156813000	2.781880000
H	1.242695000	-2.156813000	2.781880000
Cr	0.000000000	-0.000946000	1.119112000
Cr	0.000000000	-0.000946000	-1.119112000
C	-0.701894000	1.221816000	-2.833100000
C	-1.409085000	-0.002795000	-2.834915000
C	-0.707071000	-1.218257000	-2.836636000
C	0.707071000	-1.218257000	-2.836636000
C	1.409085000	-0.002795000	-2.834915000
C	0.701894000	1.221816000	-2.833100000
H	-1.246435000	2.154925000	-2.774305000
H	-2.489575000	0.002105000	-2.777897000
H	-1.242695000	-2.156813000	-2.781880000
H	1.242695000	-2.156813000	-2.781880000
H	2.489575000	0.002105000	-2.777897000
H	1.246435000	2.154925000	-2.774305000
C	1.447273000	0.835602000	0.000000000
C	-1.447273000	0.835602000	0.000000000
C	0.000000000	-1.673206000	0.000000000
O	2.462944000	1.423267000	0.000000000
O	0.000000000	-2.846562000	0.000000000
O	-2.462944000	1.423267000	0.000000000

15

E_{total} = -5974.126806 a.u.
ZPE = 0.249174 a.u.
λ=0
ω_1 = 6.5 cm^{-1}

C	-5.723208000	-0.997276000	-0.237640000
C	-5.726202000	-0.231182000	0.990766000
C	-5.720058000	0.997401000	0.226876000
C	-5.718441000	0.232195000	-1.001383000
H	-5.780001000	-2.046617000	-0.481823000
H	-5.784121000	-0.478025000	2.039455000
H	-5.775616000	2.046761000	0.470657000
H	-5.772799000	0.472929000	-2.051690000
Fe	-3.973268000	-0.000664000	0.000401000
Mn	-1.815312000	0.020342000	0.005839000
C	-2.902998000	-0.447047000	-1.550483000
C	-2.820764000	1.596655000	0.379458000
C	-2.917455000	-1.103382000	1.179920000
O	-2.918616000	-0.783837000	-2.662323000
O	-2.874702000	2.725041000	0.646956000
O	-2.930950000	-1.909110000	2.016773000
Fe	3.973326000	0.002704000	-0.001779000
Mn	1.815338000	-0.022868000	-0.002139000
C	0.016904000	0.596562000	0.863966000
C	-0.019713000	-0.861361000	0.601621000
C	-0.016726000	-0.597526000	-0.858656000
C	0.019799000	0.860126000	-0.595741000
H	0.026699000	1.208602000	1.751025000
H	-0.034742000	-1.746993000	1.215590000
H	-0.026844000	-1.213135000	-1.743242000
H	0.034993000	1.745090000	-1.210715000
C	2.897723000	0.391952000	1.567642000
C	2.822371000	-1.583218000	-0.432212000
C	2.920846000	1.143234000	-1.139237000
O	2.917315000	0.690345000	2.690235000
O	2.878646000	-2.701335000	-0.739478000
O	2.927896000	1.977500000	-1.947744000
C	5.719311000	-0.995877000	-0.232511000
C	5.721190000	-0.228402000	0.994805000
C	5.724073000	0.999413000	0.228779000
C	5.723423000	0.230956000	-0.998420000
H	5.774000000	-2.045660000	-0.474596000
H	5.779282000	-0.466990000	2.045366000
H	5.781854000	2.049316000	0.470259000
H	5.778014000	0.476630000	-2.047577000

16

E_{total} = -5758.530186 a.u.
ZPE = 0.308478 a.u.
λ=0
ω_1 = 10.1 cm^{-1}

C	5.795690000	1.093644000	0.555472000
C	5.807811000	-0.173697000	1.195771000
C	5.810935000	-1.174058000	0.190193000
C	5.802886000	-0.524613000	-1.074490000
C	5.794385000	0.874855000	-0.848409000
H	5.765578000	2.054004000	1.047506000
H	5.782999000	-0.344280000	2.261116000
H	5.791537000	-2.241017000	0.352584000
H	5.774465000	-1.014843000	-2.035663000
H	5.757919000	1.641792000	-1.606815000
Mn	4.022149000	0.006700000	0.007378000
Cr	1.835547000	-0.015810000	-0.001357000
C	-0.040493000	-0.896529000	0.854439000
C	-0.030733000	0.523930000	1.094316000
C	-0.021957000	1.192454000	-0.184429000
C	-0.040007000	0.183204000	-1.213609000
C	-0.013958000	-1.108042000	-0.572030000
H	-0.061510000	-1.665718000	1.609241000
H	-0.050206000	1.002056000	2.060313000
H	-0.035620000	2.258649000	-0.343887000
H	-0.057515000	0.362856000	-2.276225000
H	-0.024869000	-2.063579000	-1.071547000
C	2.911644000	1.432919000	-0.761173000
C	2.939003000	-1.388151000	-0.858086000
C	2.916360000	-0.058504000	1.631217000
O	2.939226000	-0.095858000	2.806717000
O	2.937713000	2.472070000	-1.312062000
O	3.004040000	-2.384980000	-1.478932000
C	-5.780154000	-1.182894000	0.176943000
C	-5.769306000	-0.536468000	-1.082880000
C	-5.757230000	0.868115000	-0.856500000
C	-5.764246000	1.083913000	0.544399000
C	-5.771845000	-0.181990000	1.186525000
H	-5.768872000	-2.249067000	0.344235000
H	-5.749677000	-1.021332000	-2.046982000
H	-5.728899000	1.632299000	-1.618256000
H	-5.738742000	2.043307000	1.037940000
H	-5.758381000	-0.355200000	2.251866000
Mn	-3.986404000	-0.003295000	-0.001329000
Mn	-1.810605000	-0.018307000	-0.007672000
C	-2.948116000	-1.453679000	0.741300000
C	-2.920099000	1.352765000	0.875433000
C	-2.942453000	0.067949000	-1.625766000
O	-2.925360000	0.125421000	-2.786689000
O	-2.922158000	-2.485239000	1.276404000
O	-2.868856000	2.328729000	1.504947000

17

E_{total} = -5555.130480 a.u.
ZPE = 0.359929 a.u.
λ=0
ω_1 = 7.7 cm^{-1}

Cr	-0.000778000	0.003623000	1.765496000
Cr	0.001082000	0.013211000	4.001996000
C	-0.675453000	-1.212010000	5.729742000
C	-1.405078000	-0.012804000	5.724223000
C	-0.726197000	1.227075000	5.715546000
C	0.677300000	1.259292000	5.713691000
C	1.411789000	0.051534000	5.719467000
C	0.737781000	-1.179833000	5.727786000
H	-1.189910000	-2.162622000	5.680645000
H	-2.485533000	-0.033196000	5.669601000
H	-1.291649000	2.147454000	5.653764000
H	1.199771000	2.204638000	5.650324000
H	2.491827000	0.080420000	5.661227000
H	1.295156000	-2.105868000	5.677032000
C	0.002627000	-1.655825000	2.888726000
C	-1.441283000	0.839522000	2.882334000
C	1.438607000	0.844671000	2.877161000
O	0.004030000	-2.830020000	2.879671000
O	2.452263000	1.437042000	2.859609000
O	-2.457239000	1.428012000	2.865090000
C	0.656155000	-1.262863000	0.004141000
C	1.418809000	-0.067800000	-0.000219000
C	0.759582000	1.198697000	-0.002239000
C	-0.656511000	1.261893000	-0.001702000
C	-1.424339000	0.057437000	0.003061000
C	-0.770425000	-1.199854000	0.004459000
H	1.146507000	-2.225488000	0.006970000
H	2.498457000	-0.106892000	-0.002104000
H	1.348059000	2.104696000	-0.004580000
H	-1.162610000	2.216283000	-0.004374000
H	-2.503201000	0.113924000	0.004890000
H	-1.343582000	-2.115695000	0.007025000
Cr	-0.004636000	-0.004924000	-1.763380000
Cr	-0.004250000	-0.005504000	-3.999547000
C	0.651165000	-1.247534000	-5.723749000
C	1.401140000	-0.060923000	-5.721264000
C	0.743510000	1.190391000	-5.716586000
C	-0.659275000	1.246447000	-5.714471000
C	-1.414384000	0.051398000	-5.716653000
C	-0.761324000	-1.191197000	-5.721305000
H	1.149423000	-2.206595000	-5.671628000
H	2.481078000	-0.099422000	-5.666566000
H	1.324492000	2.101282000	-5.658058000
H	-1.165553000	2.200736000	-5.654055000
H	-2.493769000	0.098883000	-5.658523000
H	-1.334108000	-2.107585000	-5.667213000
C	-0.059416000	-1.668790000	-2.880683000
C	1.462826000	0.778519000	-2.881434000
C	-1.416336000	0.874439000	-2.877984000
O	-0.098575000	-2.842220000	-2.865282000
O	-2.412718000	1.495825000	-2.864918000
O	2.498599000	1.331801000	-2.865955000

18

E_{total} = -5838.581342 a.u.
ZPE = 0.285551 a.u.
λ=0
ω_1 = 2.2 cm^{-1}

C	5.698276000	-0.939746000	-0.393629000
C	5.690399000	0.393069000	-0.962602000
C	5.702501000	0.958746000	0.369983000
C	5.710035000	-0.371414000	0.936184000
H	5.754230000	-1.938126000	-0.798535000
H	5.740114000	0.793731000	-1.963050000
H	5.759822000	1.959189000	0.769342000
H	5.772587000	-0.774375000	1.934781000
Fe	3.948453000	0.007120000	-0.000512000
Cr	1.761433000	0.000480000	0.018661000
C	2.884607000	-0.806440000	1.444659000
C	2.904658000	1.646738000	-0.024693000
C	2.926865000	-0.830316000	-1.402195000
O	2.984678000	-1.388350000	2.449195000
O	2.983902000	2.808985000	-0.060609000
O	3.001423000	-1.410443000	-2.410432000
Fe	-3.948323000	-0.006393000	-0.007949000
Cr	-1.761236000	-0.007988000	-0.015212000
C	-0.002571000	-1.277484000	0.636416000
C	0.011558000	-1.189298000	-0.784586000
C	0.011019000	0.085227000	-1.418064000
C	0.003040000	1.271014000	-0.629545000
C	-0.011458000	1.183957000	0.791332000
C	-0.012318000	-0.090956000	1.423667000
H	-0.004739000	-2.244978000	1.117214000
H	0.020244000	-2.089570000	-1.381796000
H	0.021973000	0.153006000	-2.496277000
H	0.005679000	2.238506000	-1.110407000
H	-0.020307000	2.084098000	1.388692000
H	-0.022491000	-0.158816000	2.501925000
C	-2.884856000	0.931624000	-1.364685000
C	-2.898942000	-1.647586000	-0.125676000
C	-2.932345000	0.698398000	1.468346000
O	-2.973184000	1.601875000	-2.313854000
O	-2.985101000	-2.808105000	-0.188120000
O	-3.011180000	1.194130000	2.520213000
C	-5.703977000	-0.942723000	-0.410491000
C	-5.704708000	0.402440000	-0.940443000
C	-5.696574000	0.934369000	0.404806000
C	-5.695626000	-0.413686000	0.936678000
H	-5.762511000	-1.931363000	-0.838026000
H	-5.763255000	0.832684000	-1.927827000
H	-5.751024000	1.921656000	0.836301000
H	-5.749811000	-0.841800000	1.925453000

19

E_{total} = -5826.281070 a.u.
ZPE = 0.289495 a.u.
λ=0
ω_1 = 15.7 cm^{-1}

Mn	3.980299000	-0.014981000	0.001770000
Mn	1.813483000	-0.002116000	-0.008304000
C	2.918581000	-1.122311000	1.174050000
C	2.868690000	1.565535000	0.364541000
C	2.896417000	-0.461807000	-1.558433000
O	2.873401000	-1.925218000	2.018400000
O	2.865667000	2.702199000	0.625930000
O	2.869337000	-0.788090000	-2.677725000
Mn	-3.980861000	0.009518000	-0.011273000
Mn	-1.813899000	-0.004088000	-0.010752000
C	-0.008812000	0.816761000	-0.664569000
C	0.004755000	-0.655847000	-0.830774000
C	0.007979000	-0.823369000	0.642530000
C	-0.005264000	0.649604000	0.808952000
H	-0.010066000	1.659325000	-1.336738000
H	0.006007000	-1.326976000	-1.674151000
H	0.009757000	-1.666240000	1.314302000
H	-0.006235000	1.320729000	1.652341000
C	-2.924889000	1.105556000	-1.199180000
C	-2.864505000	-1.573228000	-0.382136000
C	-2.895278000	0.452958000	1.541958000
O	-2.883404000	1.893581000	-2.057543000
O	-2.851548000	-2.708164000	-0.650465000
O	-2.874314000	0.772916000	2.663289000
C	-5.745833000	-0.513402000	1.097756000
C	-5.756690000	0.883479000	0.830173000
C	-5.772122000	1.058905000	-0.575383000
C	-5.769360000	-0.227665000	-1.180784000
C	-5.757224000	-1.197361000	-0.144500000
H	-5.709802000	-0.969696000	2.075348000
H	-5.730201000	1.669174000	1.569683000
H	-5.759158000	2.002943000	-1.098283000
H	-5.756967000	-0.429660000	-2.241054000
H	-5.729354000	-2.267712000	-0.279600000
C	5.775552000	-1.189148000	-0.145562000
C	5.762112000	-0.505495000	1.100972000
C	5.743721000	0.886873000	0.839103000
C	5.747091000	1.068039000	-0.571084000
C	5.770051000	-0.214203000	-1.176999000
H	5.770731000	-2.259854000	-0.282095000
H	5.740611000	-0.968993000	2.075383000
H	5.705151000	1.673404000	1.577186000
H	5.712466000	2.015453000	-1.087261000
H	5.754418000	-0.414749000	-2.237311000

20

E_{total} = -5690.733133 a.u.
ZPE = 0.325735 a.u.
λ=0
ω_1 = 11.3 cm^{-1}

Mn	3.962107000	-0.001147000	-0.006936000
Cr	1.759948000	-0.008615000	-0.006138000
C	2.916266000	-1.096024000	1.216368000
C	2.909807000	1.599411000	0.319481000
C	2.916299000	-0.529525000	-1.560017000
O	2.953657000	-1.875893000	2.088114000
O	2.949798000	2.746640000	0.547299000
O	2.947520000	-0.911630000	-2.665683000
Mn	-3.962024000	-0.007112000	-0.000286000
Cr	-1.759833000	-0.012317000	-0.003420000
C	0.002397000	-1.297615000	0.605883000
C	-0.000491000	-1.184626000	-0.812877000
C	-0.000230000	0.100748000	-1.423658000
C	-0.003309000	1.273737000	-0.616976000
C	-0.001048000	1.159395000	0.801672000
C	0.000982000	-0.125800000	1.413646000
H	0.004707000	-2.273320000	1.069725000
H	-0.000746000	-2.074315000	-1.425966000
H	-0.000256000	0.186404000	-2.500661000
H	-0.006548000	2.249372000	-1.081072000
H	-0.001075000	2.048790000	1.415093000
H	0.000515000	-0.211534000	2.490682000
C	-2.915722000	0.837320000	-1.402609000
C	-2.916398000	-1.649514000	-0.029001000
C	-2.909203000	0.773325000	1.437753000
O	-2.958557000	1.444588000	-2.402077000
O	-2.950268000	-2.819097000	-0.045615000
O	-2.939799000	1.324568000	2.469646000
C	-5.752772000	-0.566722000	1.057182000
C	-5.742932000	0.841316000	0.866660000
C	-5.734222000	1.096784000	-0.526328000
C	-5.742661000	-0.154979000	-1.202468000
C	-5.757631000	-1.179540000	-0.223791000
H	-5.740551000	-1.079080000	2.007130000
H	-5.714290000	1.584033000	1.649035000
H	-5.699412000	2.068151000	-0.995458000
H	-5.716991000	-0.295834000	-2.272255000
H	-5.741252000	-2.241246000	-0.416296000
C	5.758757000	-1.175977000	-0.186628000
C	5.748756000	-0.526385000	1.077118000
C	5.732341000	0.872029000	0.853110000
C	5.735679000	1.091574000	-0.552442000
C	5.755495000	-0.172860000	-1.191685000
H	5.751674000	-2.242500000	-0.352517000
H	5.724996000	-1.016026000	2.038517000
H	5.696169000	1.638453000	1.612118000
H	5.703802000	2.052807000	-1.042302000
H	5.736608000	-0.345546000	-2.256772000

21

E_{total} = -3035.465381 a.u.
ZPE = 0.194000 a.u.
λ=0
ω_1 = 11.7 cm^{-1}

Cr	-0.909852000	-0.038233000	0.000000000
Fe	1.272611000	0.083280000	0.000000000
C	0.091852000	1.675516000	0.000000000
C	0.288916000	-0.804782000	1.421074000
C	0.288916000	-0.804782000	-1.421074000
O	0.135543000	2.840151000	0.000000000
O	0.426337000	-1.395779000	2.416441000
O	0.426337000	-1.395779000	-2.416441000
C	3.075124000	-0.841367000	0.000000000
C	3.020188000	0.183031000	-1.023293000
C	2.964809000	1.203151000	0.000000000
C	3.020188000	0.183031000	1.023293000
H	3.191355000	-1.913919000	0.000000000
H	3.073354000	0.183598000	-2.100737000
H	2.953865000	2.281764000	0.000000000
H	3.073354000	0.183598000	2.100737000
C	-2.712166000	1.054697000	-0.707225000
C	-2.625712000	-0.157112000	-1.409621000
C	-2.540319000	-1.378185000	-0.701776000
C	-2.540319000	-1.378185000	0.701776000
C	-2.625712000	-0.157112000	1.409621000
C	-2.712166000	1.054697000	0.707225000
H	-2.726701000	1.994024000	-1.243990000
H	-2.574872000	-0.157369000	-2.490367000
H	-2.420526000	-2.306325000	-1.244768000
H	-2.420526000	-2.306326000	1.244768000
H	-2.574872000	-0.157369000	2.490367000
H	-2.726701000	1.994024000	1.243990000

22

E_{total} = -3103.264084 a.u.
ZPE = 0.176618 a.u.
λ=0
ω_1 = 12.3 cm^{-1}

Mn	0.938833000	0.183320000	0.008604000
Fe	-1.179997000	-0.213681000	-0.002123000
C	0.074554000	-0.986685000	1.295207000
C	-0.372100000	1.584928000	0.189337000
C	-0.024813000	-0.650797000	-1.487884000
O	0.152089000	-1.703727000	2.206098000
O	-0.635663000	2.709772000	0.311168000
O	0.013865000	-1.116532000	-2.552016000
C	-2.949882000	-0.234113000	-0.987669000
C	-2.721683000	-1.493205000	-0.309410000
C	-2.847657000	-0.826386000	0.968781000
C	-3.075621000	0.431834000	0.290742000
H	-3.054789000	0.065595000	-2.018784000
H	-2.587042000	-2.515358000	-0.627442000
H	-2.848251000	-1.150519000	1.997716000
H	-3.317334000	1.435093000	0.604886000
C	2.904808000	-0.690410000	0.001376000
C	2.762632000	0.135396000	1.150663000
C	2.520341000	1.459649000	0.713374000
C	2.513380000	1.458535000	-0.710261000
C	2.755037000	0.131674000	-1.145967000
H	3.078766000	-1.755623000	0.002878000
H	2.804237000	-0.196981000	2.176594000
H	2.346538000	2.316593000	1.345996000
H	2.336079000	2.314213000	-1.343684000
H	2.788121000	-0.202069000	-2.171732000

23

E_{total} = -2961.540302 a.u.
ZPE = 0.213929 a.u.
λ=0
ω_1 = 7.4 cm^{-1}

C	2.876019000	0.931290000	-0.706862000
C	2.754160000	-0.278704000	-1.409111000
C	2.630164000	-1.496484000	-0.702261000
C	2.630164000	-1.496484000	0.702261000
C	2.754160000	-0.278704000	1.409111000
C	2.876019000	0.931290000	0.706862000
H	2.915411000	1.870178000	-1.243154000
H	2.698516000	-0.277701000	-2.489663000
H	2.479924000	-2.419677000	-1.246149000
H	2.479924000	-2.419677000	1.246149000
H	2.698516000	-0.277701000	2.489663000
H	2.915411000	1.870178000	1.243154000
Cr	1.044713000	-0.107319000	0.000000000
Mn	-1.143671000	0.116804000	0.000000000
C	-2.881460000	0.662953000	1.148541000
C	-2.803894000	1.491502000	0.000000000
C	-2.881460000	0.662953000	-1.148541000
C	-3.015207000	-0.682594000	-0.707844000
C	-3.015207000	-0.682594000	0.707844000
H	-2.827842000	0.991099000	2.175406000
H	-2.671323000	2.562430000	0.000000000
H	-2.827842000	0.991099000	-2.175406000
H	-3.073982000	-1.552054000	-1.344446000
H	-3.073982000	-1.552054000	1.344446000
C	0.073172000	1.647781000	0.000000000
C	-0.181834000	-0.803058000	-1.427823000
C	-0.181834000	-0.803058000	1.427823000
O	0.143036000	2.815889000	0.000000000
O	-0.299792000	-1.369734000	2.444746000
O	-0.299792000	-1.369734000	-2.444746000