

Supporting Information

Computational Studies on Mn(III)-Catalyzed Cyclopropanols: A Case of Mn(III)-Based Metalloradical Catalysis Involving α -Mn(II)-Bound-Alkyl Radical Key Intermediate

Pan Hong,^b Xiu-Yuan Zou,^a Peng-Cheng Zhang,^d Xin Lu,^b Long-Wu Ye,^b Yi-Dong Luo^c and Qing Sun^{*,a,c}

^aKey Laboratory of Jiangxi Province for Persistent Pollutants Prevention Control and Resource Reuse, Nanchang Hangkong University, Nanchang 330063, China

^bState Key Laboratory of Physical Chemistry of Solid Surface, Fujian Provincial Key Laboratory for Theoretical and Computational Chemistry, Department of Chemistry, College of Chemistry and Chemical Engineering, Xiamen University, Xiamen 361005, China

^cFoshan (Southern China) Institute for New Materials, Foshan 528200, China

^dCollege of Chemistry and Chemical Engineering, Zhoukou Normal University, Zhoukou 466001, China

***Correspondence:** sunqing@nchu.edu.cn

Relative Gibbs free energies of $\text{Mn}^{\text{II}}(\text{acac})_2$, **B**, **B1** and **B2** with different functionals

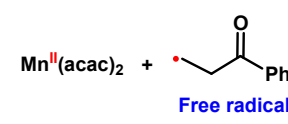
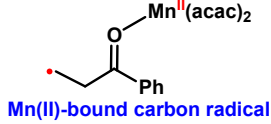
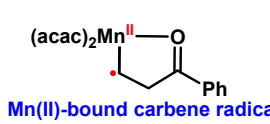
	 Free radical B	 Mn(II)-bound carbon radical B1	 Mn(II)-bound carbene radical B2
SMD-M06-D3/def2-TZVP// SMD-M06/6-31G(d,p)/SDD	0.0	3.5	-3.9
SMD-PWPB95-D3/def2-TZVP// SMD-M06/6-31G(d,p)/SDD	0.0	5.5	-6.6

Figure S1. Relative Gibbs free energies (in kcal/mol) of the lowest-lying electronic structures of $\text{Mn}^{\text{II}}(\text{acac})_2$, **B**, **B1** and **B2** at SMD-M06-D3/def2-TZVP//SMD-M06/6-31G(d,p)/SDD and SMD-PWPB95-D3/def2-TZVP//SMD-M06/6-31G(d,p)/SDD level with MeOH solvent.

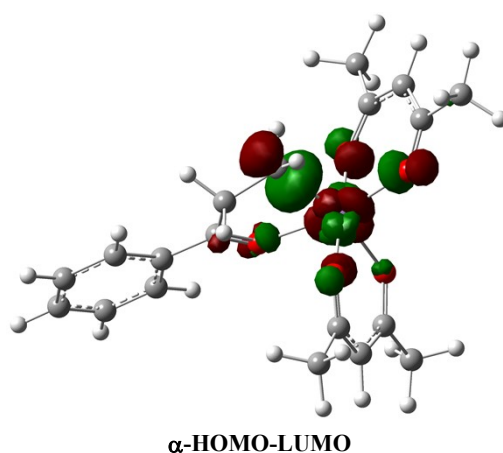


Figure S2. Molecular orbital analysis of intermediate **B2**. From the molecular orbital analysis of intermediate **B2**, the bond between the Mn(II) center and alkyl radical's carbon is a dative bond. This bond primarily arises from the weak coordinating interaction between the d orbitals of Mn(II) and the p orbitals of the carbon radical.

XYZ Coordinates

1a

C	-2.25573200	-0.76133000	0.80179500
C	-2.27435400	-0.83862300	-0.69463200
C	-1.42519900	0.19205300	-0.00251900
H	-3.12647200	-0.33351700	1.29360200
H	-1.73746900	-1.53751600	1.36105900
H	-3.15663000	-0.45449100	-1.20167500
H	-1.78153900	-1.67419800	-1.18759200
O	-1.92503200	1.50001700	-0.00440000
H	-1.77462000	1.87553600	-0.88303600
C	0.06188700	0.06959100	-0.00350700
C	0.69349800	-1.18019000	-0.04272500
C	0.86020100	1.21532700	0.04291400
C	2.07977700	-1.27661300	-0.03970600

H	0.10098900	-2.09369700	-0.07454300
C	2.24940800	1.11775700	0.04316400
H	0.38608500	2.19297500	0.08491400
C	2.86697400	-0.12742800	0.00095600
H	2.54870100	-2.25825100	-0.07133400
H	2.85031200	2.02459900	0.07845700
H	3.95213500	-0.20484500	0.00092000

2a

C	-1.45799600	1.69204400	0.33518700
H	-2.53055000	1.87271800	0.33752800
C	-0.93860200	0.48814100	0.06451900
C	0.50165700	0.17362500	0.01966200
C	1.44591000	1.18941300	-0.17720900
C	0.95225400	-1.14204900	0.17592700
C	2.80328500	0.89839800	-0.19344300
H	1.11501800	2.21312400	-0.34021900
C	2.31246900	-1.43115000	0.15723800
H	0.23069600	-1.94265200	0.32182400
C	3.24308400	-0.41302500	-0.02402700
H	3.52240500	1.69926600	-0.35128500
H	2.64482900	-2.45899100	0.28617100
H	4.30683800	-0.63981600	-0.04155400
N	-1.74413200	-0.66202000	-0.20803300
N	-2.96240300	-0.53242500	-0.12775800
N	-4.10007500	-0.52096300	-0.08395000
H	-0.81534000	2.53181900	0.57859500

3a

C	-1.16248700	0.85536000	0.00000000
C	-0.00002900	2.94950700	0.00000400
C	-1.19997700	2.25438200	0.00000500
H	-2.13907200	2.79906500	0.00001000
C	-2.39912400	0.03227200	0.00000100
C	-2.30941200	-1.36590500	-0.00000800
C	-3.67450300	0.61215200	0.00001000
C	-3.45190200	-2.15589300	-0.00000700
H	-1.32550300	-1.82800000	-0.00001500
C	-4.81793400	-0.17820800	0.00001100
H	-3.79179300	1.69298700	0.00001700
C	-4.71339900	-1.56609700	0.00000200
H	-3.35613700	-3.23982000	-0.00001400
H	-5.79711600	0.29601800	0.00001800
H	-5.60891200	-2.18381000	0.00000200

H	-0.00010000	4.03722800	0.00001300
C	1.19999800	2.25443600	-0.00001000
H	2.13909900	2.79912300	-0.00001000
C	1.16255900	0.85538800	-0.00002100
C	2.39913600	0.03228500	-0.00000900
C	3.67446500	0.61214300	-0.00000100
C	2.30940900	-1.36592500	-0.00000500
C	4.81793600	-0.17825000	0.00001000
H	3.79190800	1.69297300	-0.00000300
C	3.45184700	-2.15589100	0.00000600
H	1.32544100	-1.82790800	-0.00001100
C	4.71339900	-1.56610400	0.00001300
H	5.79707600	0.29606100	0.00001500
H	3.35610100	-3.23982100	0.00000800
H	5.60887100	-2.18387200	0.00002100
N	0.00003500	0.19083800	-0.00000800

Mn(acac)₃ (Quintet)

Mn	0.22178500	-0.18352500	-0.04617000
O	1.57574200	-0.31940800	-1.41836900
O	-0.46358000	-2.18151100	-0.52419700
O	-1.01376300	0.57061800	-1.38057700
O	0.70590000	1.93267300	0.40917600
O	-1.15373500	-0.12777300	1.30103000
O	1.51749300	-0.75977600	1.32838200
C	2.84482300	-0.28449100	-1.22335400
C	2.78951800	-0.67020900	1.21187200
C	3.46740200	-0.38846500	0.02050800
H	4.55170900	-0.34713100	0.04979200
C	3.66485200	-0.14696600	-2.46226500
H	4.73562600	-0.11459300	-2.24936500
H	3.36863300	0.76611200	-2.99185700
H	3.45258200	-0.98925700	-3.13131000
C	3.56176300	-0.92214300	2.46444300
H	3.21587000	-0.23471700	3.24510900
H	4.63811200	-0.80215000	2.32215300
H	3.35410300	-1.93925900	2.81755500
C	-1.71681400	1.64307200	-1.22207000
C	-0.16538700	2.84311500	0.31038600
C	-1.37407100	2.72314900	-0.41895200
H	-2.05381300	3.57084300	-0.40966100
C	0.12345300	4.13933000	1.00519900
H	-0.67944300	4.87258700	0.89300500
H	1.05305400	4.56252400	0.60589600

H	0.29258500	3.94779700	2.07151400
C	-2.99011300	1.66383000	-2.00544400
H	-3.53433400	2.60580300	-1.90129800
H	-3.62693500	0.83782400	-1.66146300
H	-2.77622100	1.48173100	-3.06528800
C	-2.29275000	-0.74153600	1.25377300
C	-1.64223300	-2.57517800	-0.29516700
C	-2.57970100	-1.86960900	0.49915400
H	-3.57600400	-2.29152700	0.59739600
C	-2.04355300	-3.89224100	-0.88362800
H	-1.77737400	-3.91518800	-1.94624900
H	-3.10908800	-4.10489900	-0.76591500
H	-1.46941700	-4.68784100	-0.39218100
C	-3.34176400	-0.13414400	2.12690700
H	-4.27575600	-0.70098100	2.11331700
H	-3.53364600	0.89154000	1.78475600
H	-2.97189400	-0.06474700	3.15661100

Mn(acac)₃ (Triplet)

Mn	0.00000000	0.00000000	0.00925400
O	0.00000000	1.93271400	-0.07347900
O	1.34953500	0.10941400	1.39391900
O	1.42687400	0.02235000	-1.29727000
O	-1.42687400	-0.02235000	-1.29727000
O	0.00000000	-1.93271400	-0.07347900
O	-1.34953500	-0.10941400	1.39391900
C	-0.75267900	2.68629100	0.63692900
C	-1.92527600	0.90616400	1.92131300
C	-1.67608700	2.24253500	1.58970400
H	-2.24417400	3.00033800	2.12100200
C	-0.58402400	4.15109400	0.39480600
H	-1.26514500	4.75607400	0.99775100
H	-0.75063400	4.36539200	-0.66741500
H	0.44965200	4.43871600	0.62129800
C	-2.93992900	0.58094900	2.96869200
H	-3.73515000	-0.03040000	2.52571000
H	-3.38114300	1.47506000	3.41526000
H	-2.47061200	-0.02340100	3.75382600
C	1.24412800	0.02109200	-2.56466600
C	-1.24412800	-0.02109200	-2.56466600
C	0.00000000	0.00000000	-3.20429100
H	0.00000000	0.00000000	-4.29021100
C	-2.49544600	-0.04229900	-3.38098900
H	-2.29478800	-0.03162500	-4.45484700

H	-3.11288400	0.82530400	-3.11945400
H	-3.07768600	-0.93702800	-3.13090900
C	2.49544600	0.04229900	-3.38098900
H	2.29478800	0.03162500	-4.45484700
H	3.11288400	-0.82530400	-3.11945400
H	3.07768600	0.93702800	-3.13090900
C	0.75267900	-2.68629100	0.63692900
C	1.92527600	-0.90616400	1.92131300
C	1.67608700	-2.24253500	1.58970400
H	2.24417400	-3.00033800	2.12100200
C	2.93992900	-0.58094900	2.96869200
H	3.73515000	0.03040000	2.52571000
H	3.38114300	-1.47506000	3.41526000
H	2.47061200	0.02340100	3.75382600
C	0.58402400	-4.15109400	0.39480600
H	1.26514500	-4.75607400	0.99775100
H	0.75063400	-4.36539200	-0.66741500
H	-0.44965200	-4.43871600	0.62129800

Mn(acac)₃ (Singlet)

Mn	-0.12919000	-0.13668100	0.01618600
O	-1.46585900	-0.88357400	-1.25341100
O	-0.62343400	1.59231800	-0.65455000
O	1.18612400	-0.23552100	-1.34855000
O	0.34056100	-1.93275200	0.58988800
O	1.16465800	0.56193700	1.24265100
O	-1.44787300	-0.09899500	1.41676700
C	-2.72501100	-0.78432300	-1.12372600
C	-2.72487300	-0.09000500	1.24731000
C	-3.37576700	-0.34918500	0.04605400
H	-4.46159600	-0.32695700	0.04254600
C	-3.53752900	-1.19887800	-2.30817100
H	-4.61233500	-1.16083500	-2.11577300
H	-3.25600600	-2.21577400	-2.60535000
H	-3.30020100	-0.54175300	-3.15366200
C	-3.51873700	0.18321400	2.48245600
H	-3.33777600	-0.61678800	3.21101400
H	-4.59136900	0.24639300	2.28371000
H	-3.17553700	1.11746700	2.94183800
C	2.31412300	-0.84446000	-1.21017400
C	1.50873800	-2.43273300	0.48402900
C	2.53383000	-1.87332600	-0.29959700
H	3.49820100	-2.37280600	-0.31374600
C	1.73784300	-3.72473600	1.19532400

H	1.39090600	-3.64612700	2.23128800
H	2.78815300	-4.02576400	1.17912600
H	1.14066200	-4.50834900	0.71236100
C	3.39173600	-0.39738700	-2.13822200
H	4.31077000	-0.97694700	-2.02388900
H	3.60575200	0.66167600	-1.94182100
H	3.04196200	-0.46587300	-3.17483800
C	1.70991600	1.71528500	1.12098300
C	0.10308400	2.64030500	-0.52614500
C	1.26057300	2.72106200	0.25772100
H	1.79076900	3.66894400	0.27415200
C	-0.38160300	3.84665800	-1.26114300
H	-0.50770100	3.60483800	-2.32273500
H	0.29539200	4.69824100	-1.15975900
H	-1.36934300	4.12927500	-0.87688700
C	2.89506100	1.95032600	1.99782300
H	3.29128800	2.96453900	1.90852000
H	3.67966200	1.23134500	1.72754800
H	2.62637400	1.75409000	3.04221200

Mn(acac)₂

Mn	0.00000400	0.11579500	-0.00005500
O	1.40505400	-1.04393000	-0.98635400
O	-1.40499400	-1.04403700	0.98621600
O	-1.55104400	1.13519000	-0.94365400
O	1.55098200	1.13527900	0.94356300
C	2.67285800	-0.96336000	-0.86555300
C	2.79834800	0.91368000	0.79493600
C	3.36534800	-0.06026200	-0.04315100
H	4.45047000	-0.12195400	-0.05526200
C	3.46435800	-1.93446700	-1.68967400
H	4.54395500	-1.83782100	-1.54843600
H	3.22658100	-1.78661300	-2.75023700
H	3.15894700	-2.95686100	-1.43579000
C	3.71140800	1.78692200	1.60243700
H	3.52099500	2.83788800	1.35296800
H	4.76987700	1.56667300	1.44160700
H	3.47756200	1.66662200	2.66735400
C	-2.79840400	0.91366700	-0.79486800
C	-2.67281100	-0.96338400	0.86559600
C	-3.36535700	-0.06021000	0.04332600
H	-4.45048100	-0.12183600	0.05558000
C	-3.46425100	-1.93451300	1.68974800
H	-3.15916600	-2.95691200	1.43548200

H	-4.54387500	-1.83759100	1.54890100
H	-3.22606600	-1.78700000	2.75026500
C	-3.71151300	1.78686400	-1.60236300
H	-4.76999000	1.56711700	-1.44090100
H	-3.47825900	1.66587000	-2.66733500
H	-3.52053600	2.83788700	-1.35358000

Hacac

O	1.27530300	1.26476500	0.00000500
O	-1.29964800	1.23856600	-0.00000900
C	1.24740100	0.01389400	0.00001000
C	-1.19506600	-0.08411000	-0.00000700
C	0.01460300	-0.72260800	0.00000300
H	0.03854100	-1.80875100	-0.00002100
C	-2.50160200	-0.78307500	0.00000100
H	-2.37870600	-1.86843300	-0.00017700
H	-3.08188800	-0.48372600	-0.88125000
H	-3.08171300	-0.48402100	0.88147000
C	2.52523400	-0.76530900	-0.00000400
H	2.56812900	-1.41865100	-0.88005000
H	2.56844100	-1.41821800	0.88034600
H	3.38639600	-0.09231600	-0.00033000
H	-0.36785600	1.59472000	0.00002800

A

C	2.34889300	-0.75464600	-0.71920400
C	2.34886900	-0.75463700	0.71929600
C	1.42304400	0.35161500	-0.00005100
H	3.17235600	-0.28569500	-1.25007800
H	1.77796200	-1.50242500	-1.26531600
H	3.17228400	-0.28564900	1.25021300
H	1.77785300	-1.50235900	1.26539200
O	1.90066400	1.53791500	-0.00006100
C	-0.04908500	0.11676900	-0.00000800
C	-0.62710300	-1.15895500	-0.00002600
C	-0.89032200	1.23459800	0.00003000
C	-2.00930800	-1.30721000	-0.00002600
H	-0.00563000	-2.05301000	-0.00002800
C	-2.27160500	1.08464200	0.00003200
H	-0.44439300	2.22644400	0.00005500
C	-2.83772500	-0.18771300	-0.00000400
H	-2.44098000	-2.30589300	-0.00004800
H	-2.90975800	1.96599600	0.00006600
H	-3.91894300	-0.30750500	-0.00001500

TS_A

C	2.35669300	-0.77174000	-0.57933000
C	2.34889600	-0.75713000	0.86790500
C	1.41603800	0.37690500	-0.16645800
H	3.24538000	-0.38539700	-1.07447500
H	1.87331100	-1.60624100	-1.08550600
H	3.09949300	-0.19023300	1.41043800
H	1.69342000	-1.41117400	1.43647200
O	1.88218200	1.54847800	-0.12740500
C	-0.04984100	0.12489600	-0.07794600
C	-0.62053600	-1.15343800	-0.12806700
C	-0.89413700	1.23506100	0.03764500
C	-1.99960600	-1.31186200	-0.06138700
H	0.00634900	-2.03936700	-0.21348000
C	-2.27225600	1.07509200	0.10166900
H	-0.45086100	2.22742100	0.07386400
C	-2.83076400	-0.19991800	0.05252600
H	-2.42741200	-2.31132600	-0.10060400
H	-2.91416200	1.94906700	0.19036000
H	-3.90989800	-0.32777100	0.10283800

B

C	2.40831000	-0.39510800	-0.39712700
C	2.45618400	-1.34186800	0.74682700
C	1.34813500	0.66721900	-0.19181100
H	3.35933800	0.14408500	-0.53042700
H	2.20608600	-0.93149600	-1.33387800
H	2.46921700	-0.96499600	1.76697200
H	2.55956100	-2.41184000	0.59166500
O	1.66378500	1.84621800	-0.08367200
C	-0.07661200	0.25065000	-0.10135800
C	-0.48731300	-1.07504400	-0.28905000
C	-1.03845000	1.23289700	0.16374100
C	-1.83439100	-1.40761500	-0.21016000
H	0.24260900	-1.85422200	-0.49856900
C	-2.38248200	0.89933300	0.24557100
H	-0.71203300	2.26054600	0.30599500
C	-2.78189000	-0.42295700	0.05846800
H	-2.14606300	-2.43883200	-0.35894500
H	-3.12241300	1.66859600	0.45434900
H	-3.83553400	-0.68662200	0.12160800

TS_B

O	0.50635500	-0.03686000	-1.93427100
C	-0.45946700	0.59786500	-1.52655400
C	-0.74660400	2.73640500	-0.17950200
C	-0.41388200	2.11002000	-1.48932000
H	-0.42991200	3.76460900	-0.01932100
H	-1.11265500	2.46750600	-2.27128600
H	0.58887400	2.40395400	-1.82373500
C	-1.68723900	-0.10792300	-1.07614400
C	-1.57911800	-1.45467600	-0.70808100
C	-2.93627800	0.52156400	-1.02073800
C	-2.69479700	-2.15371300	-0.26896600
H	-0.60432800	-1.93643300	-0.75837400
C	-4.05693100	-0.18642100	-0.60129800
H	-3.04169500	1.56180800	-1.32225400
C	-3.93535100	-1.51917500	-0.21628400
H	-2.60145500	-3.19512500	0.03046200
H	-5.02694000	0.30425900	-0.57128800
H	-4.81132800	-2.06745400	0.12380500
H	-1.63624000	2.42253900	0.36224900
C	0.78744900	1.87177700	1.57462000
H	-0.00243300	2.21594400	2.23711300
C	1.02207100	0.54727200	1.39663400
C	2.15829800	-0.03550800	0.67613600
C	3.09437000	0.78196300	0.02309700
C	2.31147800	-1.42621500	0.58113400
C	4.13997200	0.22594700	-0.69938800
H	2.99915400	1.86499500	0.06309900
C	3.36240000	-1.97918300	-0.14171700
H	1.59501700	-2.07932000	1.07370700
C	4.28069000	-1.15819900	-0.78836200
H	4.84914300	0.87961700	-1.20301900
H	3.45949800	-3.06124100	-0.20215300
H	5.09901600	-1.59128000	-1.35928400
N	0.11305600	-0.43997200	1.88448800
N	-1.00600400	-0.07166100	2.22453000
N	-2.07554100	0.15416800	2.55167500
H	1.52250100	2.61197800	1.27799900
C			
O	-0.64799200	0.05357600	-2.44107200
C	0.36379900	-0.35862200	-1.88026100
C	0.93512900	-2.51530500	-0.55550200
C	0.68674800	-1.83371500	-1.90147700
H	1.12075300	-3.57896000	-0.74922400

H	1.57982200	-1.96703100	-2.53068800
H	-0.14739400	-2.32008700	-2.42318900
C	1.27418400	0.59285800	-1.19096700
C	0.76161400	1.84301400	-0.82268500
C	2.60126500	0.27761400	-0.87772300
C	1.54540000	2.74321800	-0.11575500
H	-0.26893300	2.08265700	-1.07773000
C	3.39136200	1.18790600	-0.18435600
H	3.03025000	-0.67274500	-1.18930100
C	2.86070700	2.41362300	0.20941600
H	1.13351000	3.70404800	0.18491900
H	4.42309100	0.93800200	0.05242700
H	3.47564500	3.11772900	0.76594600
H	1.85643600	-2.13485700	-0.09928400
C	-0.22998000	-2.41897900	0.43873000
H	0.01497600	-3.04826300	1.30978700
C	-0.53584400	-1.04089800	0.93185700
C	-1.73331800	-0.29910800	0.67466500
C	-2.72825900	-0.78067000	-0.20872600
C	-1.95032700	0.96584700	1.27583100
C	-3.87176000	-0.04173400	-0.46550400
H	-2.59594600	-1.73463500	-0.71396000
C	-3.09681800	1.69532000	1.01110800
H	-1.20101700	1.36692400	1.95459900
C	-4.06953500	1.19951500	0.14049900
H	-4.61807000	-0.43711100	-1.15157300
H	-3.23684900	2.66271300	1.48948100
H	-4.96904500	1.77523300	-0.06534100
N	0.36822200	-0.41730800	1.78651300
N	1.41759400	-0.96598800	2.12003000
N	2.42647900	-1.34507700	2.50845800
H	-1.12556300	-2.86290600	-0.00820100

TS_c

O	0.43600000	-0.65800000	-1.89300000
C	-0.46600000	0.11300000	-1.58300000
C	-0.44300000	2.43400000	-0.48200000
C	-0.29900000	1.60300000	-1.76000000
H	-0.49300000	3.49200000	-0.76500000
H	-1.05500000	1.94400000	-2.48200000
H	0.68400000	1.76500000	-2.22000000
C	-1.73300000	-0.41400000	-1.00900000
C	-1.70100000	-1.66700000	-0.38500000
C	-2.93700000	0.29600000	-1.06500000

C	-2.85000000	-2.19400000	0.18800000
H	-0.75700000	-2.20600000	-0.34100000
C	-4.09100000	-0.24200000	-0.50700000
H	-2.98300000	1.26400000	-1.56000000
C	-4.04700000	-1.48200000	0.12500000
H	-2.81500000	-3.16100000	0.68600000
H	-5.02700000	0.30800000	-0.56400000
H	-4.94900000	-1.89600000	0.57100000
H	-1.39600000	2.20500000	0.00900000
C	0.70500000	2.29000000	0.52600000
H	0.45800000	2.88800000	1.41200000
C	0.94400000	0.87900000	0.99100000
C	2.14700000	0.12300000	0.55900000
C	3.11200000	0.68300000	-0.28700000
C	2.31200000	-1.20900000	0.97400000
C	4.21200000	-0.06400000	-0.69800000
H	3.02100000	1.70500000	-0.64300000
C	3.40800000	-1.95000000	0.56300000
H	1.56500000	-1.65900000	1.62300000
C	4.36400000	-1.37900000	-0.27700000
H	4.95000000	0.39000000	-1.35500000
H	3.51700000	-2.98000000	0.89500000
H	5.22300000	-1.96200000	-0.60200000
N	0.12600000	0.22300000	1.74600000
N	-1.04100000	1.09000000	2.21000000
N	-2.06500000	0.61900000	2.49300000
H	1.61600000	2.71600000	0.10200000

D

O	0.76786400	0.51587900	1.98456900
C	1.50060900	0.91518000	1.08321200
C	0.47520200	2.42839000	-0.68789800
C	1.34972600	2.32297800	0.56940300
H	0.44520000	3.48736700	-0.96863200
H	2.32987100	2.77030800	0.36771800
H	0.87933600	2.89905000	1.37592700
C	2.52396700	0.01660500	0.48706200
C	2.59347300	-1.30556600	0.94301900
C	3.40081800	0.43914500	-0.51820600
C	3.52466700	-2.18546400	0.41264900
H	1.90243300	-1.62804600	1.71845800
C	4.33288900	-0.44422900	-1.05147700
H	3.36187500	1.45967900	-0.89239200
C	4.39714200	-1.75460700	-0.58638100

H	3.57269200	-3.21033100	0.77368200
H	5.01142100	-0.10803500	-1.83205000
H	5.12824400	-2.44378800	-1.00372000
H	0.94139600	1.89614900	-1.52767300
C	-0.95641000	1.94538700	-0.48503600
H	-1.62748100	2.44560800	-1.19758600
C	-1.17868000	0.45717300	-0.66416200
C	-2.51888300	-0.11558400	-0.35343300
C	-3.60603700	0.70120500	-0.03055600
C	-2.69644100	-1.50480700	-0.39477200
C	-4.84816500	0.13681600	0.24452100
H	-3.49483700	1.78223200	0.00562800
C	-3.93520700	-2.06398900	-0.11842800
H	-1.84891200	-2.14225700	-0.64109200
C	-5.01582300	-1.24326800	0.20212000
H	-5.68777300	0.78178500	0.49385300
H	-4.06020200	-3.14404500	-0.15045100
H	-5.98728200	-1.68167200	0.42008900
N	-0.25040700	-0.28414700	-1.09217600
H	-1.31313000	2.22580300	0.51711000

TS_D

O	1.68576600	1.07233500	2.25201700
C	1.42882700	0.96740500	1.00807100
C	0.48921200	2.41769700	-0.96939100
C	1.26282600	2.36663400	0.32667800
H	0.56514000	3.42703700	-1.39291200
H	2.29306500	2.72651400	0.20450000
H	0.78730400	3.00114800	1.08513100
C	2.23461100	-0.07879600	0.26088300
C	2.24645100	-1.37270400	0.79208900
C	3.02069200	0.19798900	-0.85706100
C	3.00653600	-2.37535100	0.20571600
H	1.64319200	-1.58305200	1.67528400
C	3.79449800	-0.80489300	-1.44034100
H	3.05299400	1.20107300	-1.27771400
C	3.78508200	-2.09251700	-0.91657500
H	2.99691600	-3.37976800	0.62430200
H	4.40795300	-0.57301300	-2.30866800
H	4.38395200	-2.87507100	-1.37779200
H	0.91332100	1.72964800	-1.71212000
C	-0.96414700	2.07637400	-0.73425400
H	-1.51618500	1.95341100	-1.67223900
C	-1.07777500	0.79981100	0.06588800

C	-2.32951600	0.00065700	-0.02546300
C	-3.53000300	0.60556300	-0.40900700
C	-2.31219000	-1.36337400	0.28950500
C	-4.69939100	-0.14536300	-0.46713500
H	-3.56107000	1.66589300	-0.64976700
C	-3.47956700	-2.11010400	0.21793100
H	-1.37251300	-1.83334500	0.57401800
C	-4.67607600	-1.50182200	-0.15767500
H	-5.63142800	0.33323700	-0.75876900
H	-3.45681800	-3.17178300	0.45274200
H	-5.59071200	-2.08803800	-0.21225400
N	-0.16162200	0.35642200	0.82198900
H	-1.47032100	2.86922800	-0.16294800

E1

O	1.64845700	0.47854000	2.20986700
C	1.15664900	0.72673500	0.95534900
C	0.58918900	2.43189100	-0.75647100
C	1.19275800	2.21235900	0.61691200
H	0.63373100	3.48944700	-1.03964800
H	2.21175400	2.60162700	0.70564400
H	0.59016100	2.72364200	1.38166300
C	2.20187900	-0.14217000	0.22266500
C	2.01734200	-1.53243900	0.21306300
C	3.36918700	0.40088000	-0.32778500
C	2.94823500	-2.35669300	-0.40450400
H	1.12861800	-1.95315400	0.67572900
C	4.29299700	-0.42882100	-0.94935300
H	3.55221100	1.47173500	-0.29622200
C	4.08606600	-1.80712100	-0.99068300
H	2.78835600	-3.43231400	-0.42299800
H	5.18345100	0.00272800	-1.40078500
H	4.81738500	-2.45215900	-1.47270700
H	1.16983000	1.87912000	-1.50874200
C	-0.85076100	1.94731100	-0.75596700
H	-1.22021700	1.79626300	-1.77806000
C	-1.04571500	0.68025300	0.03656800
C	-2.37758400	0.02018800	-0.04947800
C	-3.46414500	0.64396500	-0.67397500
C	-2.56612800	-1.25316000	0.50414800
C	-4.70402900	0.01545800	-0.73695300
H	-3.35499000	1.63335300	-1.11144900
C	-3.80051000	-1.88293300	0.43562900
H	-1.72402800	-1.74334300	0.98707300

C	-4.87629700	-1.24948600	-0.18494700
H	-5.53791100	0.51860500	-1.22165900
H	-3.92589600	-2.87434200	0.86601300
H	-5.84443400	-1.74288300	-0.23916200
N	-0.16613300	0.14059300	0.79749600
H	-1.50753500	2.71189400	-0.31141800
F			
Mn	-0.15331800	1.10918500	0.44397900
O	-1.64954800	0.75256200	1.67537300
O	-1.50395500	1.55098700	-0.92450400
O	-0.06223100	3.21937300	0.84987800
O	1.11709300	0.56833300	1.83915600
C	-1.52371000	2.63037200	-1.62585100
C	-0.23617900	4.07922200	-0.06574500
C	-0.89743900	3.82723500	-1.28810700
H	-0.99988500	4.65553300	-1.98391700
C	0.28339400	5.45879900	0.20158200
H	1.36304500	5.40450900	0.38673700
H	-0.17719900	5.84822900	1.11740000
H	0.09447900	6.15433600	-0.62016600
C	-2.32497000	2.53736400	-2.88538500
H	-1.95982100	1.69564500	-3.48698100
H	-2.28413900	3.45457100	-3.47825300
H	-3.37063600	2.32031200	-2.63461800
C	0.85298400	-0.12179500	2.88566200
C	-1.60015000	0.10069100	2.77606600
C	-0.43189000	-0.40071700	3.35981900
H	-0.52429300	-0.96624400	4.28218600
C	-2.91490700	-0.09312400	3.45727900
H	-2.84741200	-0.77244100	4.31071000
H	-3.64940400	-0.47144800	2.73685500
H	-3.27913700	0.88122900	3.80695800
C	2.05227700	-0.61335700	3.62713000
H	1.79061200	-1.24940800	4.47598900
H	2.63158300	0.24627400	3.98541700
H	2.69913400	-1.16769100	2.93405100
O	1.24790500	1.14408500	-0.80928300
C	1.38644800	-0.17624500	-1.28509600
C	1.17016800	-1.55416000	-3.35484700
C	1.45050800	-0.16480700	-2.80992500
H	1.25217300	-1.57042700	-4.44708500
H	2.42549600	0.21909900	-3.13456600
H	0.67951300	0.53865200	-3.16297700

C	2.62385100	-0.83053100	-0.67194600
C	2.60923900	-2.12201700	-0.14294400
C	3.81581300	-0.10147600	-0.63463800
C	3.76310100	-2.67395700	0.41311500
H	1.68930100	-2.70503400	-0.15490800
C	4.96603800	-0.64935600	-0.07863000
H	3.83669000	0.90902600	-1.04028900
C	4.94349000	-1.93914600	0.44954200
H	3.73348700	-3.68232000	0.82155300
H	5.88500400	-0.06691600	-0.05590800
H	5.84293800	-2.36808900	0.88633900
H	1.91709800	-2.26375000	-2.97074500
C	-0.22406300	-1.98766000	-2.93037100
H	-0.38770400	-3.06325900	-3.07488500
C	-0.53491500	-1.62903000	-1.50427000
C	-1.75886200	-2.18640600	-0.88287900
C	-2.88172900	-2.51635500	-1.64983300
C	-1.79894300	-2.38861700	0.50227300
C	-4.03013000	-3.00760600	-1.03734600
H	-2.87135000	-2.37081800	-2.72809100
C	-2.94035500	-2.89539900	1.10985000
H	-0.91565600	-2.16028300	1.09772300
C	-4.06282700	-3.19871000	0.34126500
H	-4.90321500	-3.24453200	-1.64129000
H	-2.95074400	-3.05961100	2.18620400
H	-4.95943400	-3.59155000	0.81584800
N	0.18858800	-0.85449500	-0.78177100
H	-0.97926400	-1.48374700	-3.55594700

F1

O	1.52344400	1.03921400	2.17157400
C	1.16500000	0.84549300	0.81223900
C	0.66454700	2.04064300	-1.32075700
C	1.24684400	2.17948200	0.07131200
H	0.72627300	2.98744800	-1.86873900
H	2.28909700	2.52110800	0.05318100
H	0.66533600	2.91775700	0.64672100
C	2.17316100	-0.15092000	0.25214300
C	1.80881000	-1.14789400	-0.65287900
C	3.51726400	-0.03501000	0.61932000
C	2.76669800	-2.01086400	-1.18137800
H	0.76694700	-1.26139600	-0.94614600
C	4.47342700	-0.89716800	0.09441300
H	3.81365600	0.73747800	1.32599000

C	4.10108000	-1.88980200	-0.80923400
H	2.46330700	-2.78392300	-1.88458400
H	5.51466000	-0.79351400	0.39343500
H	4.84845200	-2.56556900	-1.21985700
H	1.25081100	1.30824200	-1.89337300
C	-0.78330800	1.58685900	-1.22088500
H	-1.12586500	1.14223700	-2.16441200
C	-1.02876000	0.60920700	-0.09964500
C	-2.38402300	-0.00407700	-0.01463400
C	-3.43779000	0.42548000	-0.82990900
C	-2.62758100	-1.03469500	0.90303900
C	-4.69868600	-0.15442200	-0.72567000
H	-3.28658800	1.22420900	-1.55205400
C	-3.88303900	-1.61646400	1.00368800
H	-1.81010500	-1.37403100	1.53420100
C	-4.92572900	-1.17698900	0.18925700
H	-5.50608300	0.19639500	-1.36489100
H	-4.05087300	-2.41872900	1.71928900
H	-5.91071400	-1.63235800	0.26757400
N	-0.17163900	0.27328300	0.79294300
H	-1.44082600	2.45299200	-1.04539000
H	0.91894100	1.70181400	2.53334300

A1

Mn	-0.45600800	-0.52415900	-0.13772800
O	0.82085900	-1.26555300	-1.43765500
O	-2.15475200	-1.59483700	-0.83227700
O	-1.56908400	0.20288100	1.27762500
O	0.30767400	-1.71611600	1.24779500
C	-3.33420000	-1.15796300	-0.66538400
C	-2.84216800	0.39797900	1.21330000
C	-3.70001600	-0.17058800	0.27648000
H	-4.75160300	0.09463200	0.34169700
C	-3.38725500	1.28386200	2.28650300
H	-3.28411000	0.77777700	3.25478100
H	-4.44046300	1.52915400	2.12860800
H	-2.79605200	2.20569800	2.34263200
C	-4.40005400	-1.77133600	-1.51938100
H	-4.14388000	-1.61951000	-2.57487100
H	-5.39325500	-1.35813200	-1.32662000
H	-4.41981800	-2.85448100	-1.34941200
C	1.48301600	-2.22561600	1.22940300
C	1.94141000	-1.82427100	-1.15985500
C	2.32583400	-2.25282200	0.11340000

H	3.30192500	-2.71582800	0.22236500
C	2.85579600	-2.02260700	-2.32340900
H	2.36538900	-2.66696700	-3.06310700
H	3.80966400	-2.46924700	-2.03315100
H	3.03602900	-1.05693700	-2.81137000
C	1.93766100	-2.82709500	2.51816600
H	2.91614400	-3.30576900	2.43544300
H	1.19813000	-3.56050100	2.85972700
H	1.98402300	-2.03926600	3.28059100
O	-0.68253900	0.96970500	-1.24041300
C	-0.14932400	2.15565200	-0.74671400
C	-0.49220200	3.39225000	-1.52529600
C	-1.08994400	3.16399100	-0.16067600
H	-1.14403100	3.25947100	-2.38617000
H	0.27970900	4.15190800	-1.63533500
H	-0.74918100	3.78617200	0.66556800
H	-2.14079600	2.87912800	-0.12611200
C	1.23204700	1.98751900	-0.18334100
C	2.30941900	1.79358600	-1.05414600
C	1.44654700	1.87566400	1.19354400
C	3.57367100	1.49094800	-0.56038200
H	2.14199300	1.87517900	-2.12882300
C	2.71354200	1.57305400	1.69107000
H	0.61122200	2.02305700	1.87834200
C	3.77681800	1.37541600	0.81483900
H	4.40454500	1.34439200	-1.24804800
H	2.86796800	1.49108100	2.76532800
H	4.76578100	1.13859500	1.20180500

TS_{A1}

Mn	-0.98289800	0.38628600	-0.35613600
O	-0.72436300	2.49327600	-0.35213300
O	-2.82211800	0.68352800	0.67849700
O	-2.04660000	-1.01235000	-1.51651300
O	0.64449500	0.39830900	-1.70925800
C	-3.73824900	-0.19380800	0.78536800
C	-3.06169100	-1.67301200	-1.11744500
C	-3.87055200	-1.33935300	-0.01940600
H	-4.71027400	-1.99668600	0.19179200
C	-3.40170000	-2.89501500	-1.91856400
H	-3.58156000	-2.60586300	-2.96131600
H	-4.27813500	-3.42721600	-1.53932200
H	-2.54126900	-3.57537400	-1.92224900
C	-4.76152100	0.05130500	1.85572100

H	-4.25739100	0.15543000	2.82407600
H	-5.51136900	-0.74148300	1.92389600
H	-5.26799100	1.00412300	1.65742800
C	1.58589000	1.25649000	-1.72202000
C	0.38044400	3.09790800	-0.54540100
C	1.51124000	2.54585300	-1.16877200
H	2.38771500	3.18175600	-1.26481000
C	0.45671700	4.50517500	-0.03140200
H	-0.40491600	5.07749600	-0.39455800
H	1.37957100	5.01783800	-0.31612800
H	0.38663300	4.48564600	1.06462300
C	2.86141100	0.82787100	-2.38488100
H	3.61335900	1.62071500	-2.42296500
H	2.64636600	0.48406800	-3.40375800
H	3.27612500	-0.03344800	-1.84200300
O	-0.27388300	-0.92489000	1.16079700
C	0.86891500	-0.69236000	1.67644500
C	1.03401900	1.11045100	2.15838200
C	0.91211900	-0.03633300	3.04502600
H	0.13935100	1.62422300	1.80652500
H	2.00449400	1.52048300	1.88927400
H	1.78402100	-0.28837600	3.64841000
H	-0.04085500	-0.14798900	3.56122800
C	2.10063900	-1.21384500	1.04604200
C	1.96722400	-2.07187600	-0.05506100
C	3.38527500	-0.91910600	1.52545000
C	3.08977000	-2.62202500	-0.65954500
H	0.97200500	-2.30753800	-0.42689400
C	4.50519600	-1.46548400	0.91315900
H	3.52287400	-0.25742900	2.37840700
C	4.36227500	-2.31983800	-0.17850600
H	2.97173800	-3.29093400	-1.50896700
H	5.49556900	-1.22629600	1.29349600
H	5.24161600	-2.75126700	-0.65144100

B1

Mn	-0.19231000	-1.12066900	-0.20740000
O	-1.61228200	-1.77251900	1.21860700
O	1.12387500	-2.77347500	-0.02109700
O	1.20388600	-0.39465100	-1.62314300
O	-1.84218200	-0.78232000	-1.47175200
C	2.38787800	-2.67760300	-0.15250200
C	2.46028100	-0.56705600	-1.49363800
C	3.06501900	-1.62537400	-0.79550100

H	4.15149100	-1.66733500	-0.80325200
C	3.33514600	0.44945600	-2.16751100
H	3.16069200	0.42074600	-3.25044900
H	4.40059600	0.29609700	-1.97517800
H	3.04609500	1.45353600	-1.82880300
C	3.19607000	-3.79923200	0.43053100
H	2.94743800	-3.91488900	1.49232300
H	4.27420500	-3.65000800	0.32662100
H	2.91789500	-4.73782800	-0.06484700
C	-3.06065100	-0.65624600	-1.12002000
C	-2.86521900	-1.54687700	1.20983000
C	-3.58554000	-0.98735900	0.13969400
H	-4.65318900	-0.84205100	0.28426300
C	-3.61027800	-1.92890200	2.45508400
H	-3.50012900	-3.00760000	2.62228500
H	-4.67482500	-1.68392400	2.41081700
H	-3.15907000	-1.42666600	3.31928700
C	-3.98736000	-0.10921800	-2.16577600
H	-5.01996300	-0.01540300	-1.81884900
H	-3.96376100	-0.75996300	-3.04862000
H	-3.62489500	0.87501300	-2.48835700
O	0.91403000	0.06749800	1.37414600
C	1.25600900	1.24323000	1.19955300
C	2.66223300	2.95423800	2.38112600
C	2.63455600	1.68301100	1.61628000
H	1.95198200	3.12223600	3.18708700
H	3.47069900	3.66682400	2.24993800
H	3.22746800	1.77368000	0.69047000
H	3.07433200	0.83898500	2.17202900
C	0.33290500	2.20804000	0.56552300
C	-1.03621800	1.91025200	0.53026700
C	0.79317500	3.39592400	-0.01893000
C	-1.92973000	2.77648800	-0.08277200
H	-1.39261800	0.99328900	1.00136600
C	-0.10203000	4.25384500	-0.64591400
H	1.85267800	3.64437400	-0.00089600
C	-1.46094500	3.94768800	-0.67573900
H	-2.99204000	2.54074700	-0.09367500
H	0.26101200	5.16715200	-1.11069000
H	-2.15876600	4.62760800	-1.15946900

B2 (Quintet)

Mn	1.05900900	0.13213800	-0.06996000
O	1.72718500	-1.34953500	1.21740600

O	1.22350400	1.58102400	1.40630900
O	0.40203500	1.59494000	-1.33783300
O	3.03506400	0.11148500	-0.84845000
C	0.64355400	2.71480000	1.39801800
C	-0.10707600	2.71168400	-0.98027400
C	-0.04563400	3.26558400	0.30439900
H	-0.50566300	4.23976600	0.44639600
C	-0.80192500	3.47319300	-2.06756800
H	-0.09608600	3.66560700	-2.88468000
H	-1.22022200	4.42261800	-1.72375700
H	-1.60692000	2.85314700	-2.48176600
C	0.74035600	3.50762800	2.66559400
H	0.36654800	2.90468100	3.50157000
H	0.18861700	4.45023300	2.62354700
H	1.79597900	3.72114400	2.87425500
C	3.86173100	-0.85265900	-0.76993500
C	2.72953200	-2.12339900	1.05325600
C	3.74277800	-1.95011000	0.10088600
H	4.53350000	-2.69544000	0.07448100
C	2.79964700	-3.29766800	1.98235000
H	2.81599500	-2.93892100	3.01867200
H	3.67612900	-3.92734300	1.80833500
H	1.89226700	-3.90359200	1.86996300
C	5.05440500	-0.77393900	-1.67558500
H	5.73018400	-1.62673900	-1.56990300
H	5.60735500	0.14976000	-1.46565300
H	4.71410000	-0.71069400	-2.71631400
O	-1.07913400	-0.30992200	0.62451800
C	-1.78565200	-0.77259900	-0.28292200
C	0.35778000	-1.27397600	-1.47018900
C	-1.13980100	-1.13921200	-1.58808000
H	0.91124000	-1.03568700	-2.38286600
H	-1.41385600	-0.34126400	-2.29666600
H	-1.59320900	-2.05753100	-1.98979200
C	-3.23955200	-0.91413700	-0.08939400
C	-3.78501300	-0.61995600	1.16795100
C	-4.08566200	-1.31895500	-1.12993400
C	-5.14974600	-0.73484100	1.38227500
H	-3.12392600	-0.30620700	1.97207700
C	-5.45354900	-1.42487000	-0.91385200
H	-3.68185100	-1.54359000	-2.11429900
C	-5.98499500	-1.13664400	0.34065600
H	-5.56695100	-0.51078600	2.36110600
H	-6.10699300	-1.73487800	-1.72556900

H	-7.05610800	-1.22544100	0.50879900
H	0.68835900	-2.21577000	-1.02043200

B2 (Triplet)

Mn	0.92908000	-0.07171100	-0.22822800
O	1.37755600	-1.61905800	0.90271400
O	1.34182800	1.14180400	1.39602100
O	0.41874400	1.49679500	-1.28938100
O	2.72044700	0.05454500	-1.00265200
C	0.92700800	2.34138900	1.51055000
C	0.12917700	2.65423700	-0.83095700
C	0.30813900	3.08190900	0.49069200
H	0.01286100	4.10132500	0.72419500
C	-0.42274400	3.61209400	-1.84193800
H	0.32235400	3.77841000	-2.62958300
H	-0.69683000	4.57550200	-1.40472400
H	-1.30316300	3.16914900	-2.32298400
C	1.15151500	2.98802300	2.84335800
H	0.67239400	2.38595900	3.62477400
H	0.76770100	4.01041100	2.89105000
H	2.22604400	2.99833300	3.06348400
C	3.69677500	-0.71572700	-0.70035900
C	2.53467700	-2.15410500	0.96836800
C	3.65628200	-1.76469600	0.22486400
H	4.57363400	-2.32579600	0.37880900
C	2.65360800	-3.29551600	1.92822500
H	2.37090600	-2.95527000	2.93155600
H	3.66101700	-3.71716000	1.96193100
H	1.94251900	-4.08131500	1.64613200
C	4.97335200	-0.43039900	-1.42565800
H	5.78752500	-1.09288200	-1.12217000
H	5.26753500	0.61060700	-1.24680400
H	4.80774200	-0.53442400	-2.50472800
O	-0.99193200	-0.24906300	0.40272600
C	-1.80932800	-0.69165000	-0.43176700
C	0.22844000	-1.25367200	-1.73271000
C	-1.28265800	-1.10828700	-1.76614700
H	0.71338100	-0.92454500	-2.65751300
H	-1.59016200	-0.31101100	-2.46304000
H	-1.79764800	-2.01444700	-2.11484500
C	-3.23749500	-0.72917200	-0.10134700
C	-3.65940000	-0.33024600	1.17562000
C	-4.19016300	-1.12707800	-1.04957700
C	-5.00765900	-0.33065600	1.49646900

H	-2.91882400	-0.02219700	1.90939000
C	-5.54000900	-1.12005900	-0.72520200
H	-3.88187500	-1.43462000	-2.04593100
C	-5.94894300	-0.72386800	0.54574700
H	-5.32971400	-0.02218800	2.48809800
H	-6.27548800	-1.42493400	-1.46545900
H	-7.00717400	-0.72095500	0.79756700
H	0.55166000	-2.27050100	-1.47831400

B2 (Singlet)

Mn	1.02969600	-0.05592500	-0.20486200
O	1.30376900	-1.74056600	0.63324100
O	1.05372300	0.95598200	1.47056400
O	0.71485600	1.78323900	-1.08655300
O	2.85529700	0.16232600	-0.73218500
C	0.61684500	2.11727200	1.77375900
C	0.25953200	2.83539700	-0.54128700
C	0.13202700	3.03510700	0.84325100
H	-0.24491700	3.98880300	1.20114600
C	-0.12643800	3.94056500	-1.47795700
H	0.74980900	4.24769600	-2.06155300
H	-0.53134700	4.81305500	-0.95824600
H	-0.87152100	3.56783700	-2.19152100
C	0.67601100	2.47013700	3.22617900
H	0.14161200	1.71390700	3.81303000
H	0.25140600	3.45606300	3.43253700
H	1.72079800	2.45589700	3.56020700
C	3.78138200	-0.70595000	-0.56376500
C	2.42010500	-2.38020200	0.65970100
C	3.61511500	-1.93109900	0.09485700
H	4.48411100	-2.57800400	0.17814800
C	2.37431600	-3.70212800	1.35525700
H	2.06148700	-3.55643500	2.39627800
H	3.33821000	-4.21674400	1.34063500
H	1.61875300	-4.33994800	0.88091800
C	5.11597700	-0.33717500	-1.12763800
H	5.86596100	-1.11672600	-0.97279000
H	5.46523800	0.59338700	-0.66421500
H	5.01734000	-0.14158700	-2.20214800
O	-0.95195700	-0.32454000	0.33748200
C	-1.77873400	-0.50224000	-0.57457200
C	0.24809600	-0.59894700	-1.95045300
C	-1.26099100	-0.48863800	-1.97421700
H	0.72564100	-0.07444700	-2.78427000

H	-1.57818900	0.47521900	-2.40647300
H	-1.75652900	-1.25948600	-2.58113800
C	-3.20169600	-0.67511000	-0.25347500
C	-3.59944600	-0.75074900	1.08914800
C	-4.16807200	-0.75238700	-1.26480800
C	-4.93849100	-0.90561700	1.41241100
H	-2.84651600	-0.69224200	1.87131800
C	-5.50922000	-0.89993900	-0.93618400
H	-3.87729500	-0.68922400	-2.31077800
C	-5.89430300	-0.97942000	0.39978500
H	-5.24146800	-0.96925600	2.45476500
H	-6.25657600	-0.95522800	-1.72385500
H	-6.94497800	-1.10003200	0.65463200
H	0.58898400	-1.64916400	-1.92542400

TS_{B2}

Mn	0.54190000	1.42257100	0.09229700
O	-0.62179200	1.81107000	-1.61428400
O	1.88044600	3.05411200	-0.16103100
O	1.70260400	0.98480000	1.81220600
O	-1.20826500	1.88621800	1.21391100
C	3.10389600	3.02957500	0.19465700
C	2.95797300	1.19258000	1.88486800
C	3.66607800	2.14098000	1.12839800
H	4.73306200	2.23055500	1.31690100
C	3.70790500	0.34544100	2.87003800
H	3.27666000	0.47702300	3.86990500
H	4.77706500	0.57111200	2.90755600
H	3.57423900	-0.71135400	2.60396100
C	3.99626300	4.04737000	-0.45325600
H	3.98457800	3.89753800	-1.54002200
H	5.02917200	4.00199000	-0.09767700
H	3.59619500	5.05151200	-0.26736700
C	-2.40242000	1.88499000	0.77062800
C	-1.89460500	1.81626400	-1.68223100
C	-2.77133200	1.84003900	-0.58555100
H	-3.83660200	1.84034000	-0.80643400
C	-2.47309100	1.78881300	-3.06677100
H	-2.05122700	2.61337000	-3.65406600
H	-3.56463800	1.85744100	-3.07944400
H	-2.16914100	0.85732200	-3.56255500
C	-3.48607100	1.93277300	1.80832400
H	-4.48961000	2.01074700	1.38002600
H	-3.31047500	2.78316400	2.47825800

H	-3.43216700	1.02420800	2.42364300
O	1.98894900	0.03538700	-1.06349100
C	2.13676400	-1.14759600	-0.73773100
C	-0.25180200	-1.13200900	0.06946300
C	0.99561500	-1.92118900	-0.11775900
H	-0.49261900	-0.71312300	1.04448600
H	1.34981900	-2.33558100	0.83750200
H	0.81545400	-2.79367800	-0.76788600
C	3.43779100	-1.81651700	-0.93529000
C	4.52973200	-1.05274000	-1.37043300
C	3.61114900	-3.18369600	-0.68262900
C	5.77034000	-1.64595200	-1.55044300
H	4.39279000	0.00978400	-1.55882400
C	4.85352100	-3.77517700	-0.86943300
H	2.77736400	-3.79439400	-0.34527800
C	5.93239000	-3.00798000	-1.30178800
H	6.61494900	-1.04813800	-1.88450400
H	4.98107000	-4.83752700	-0.67626800
H	6.90520000	-3.47343100	-1.44463600
H	-0.79243300	-0.75326900	-0.79648800
C	-1.92098300	-2.79016000	0.39781500
H	-1.28245100	-3.26110700	1.14232500
C	-3.01599100	-2.06771000	0.76483700
C	-4.00883400	-1.50574100	-0.15273200
C	-3.80817300	-1.54431200	-1.54278900
C	-5.17079500	-0.88746900	0.33403100
C	-4.74217900	-0.99351900	-2.40965800
H	-2.90749700	-1.99627300	-1.95429300
C	-6.10062600	-0.33261700	-0.53756500
H	-5.34655600	-0.84510800	1.40641400
C	-5.89260700	-0.38151500	-1.91353000
H	-4.56508900	-1.03344900	-3.48269100
H	-6.99475000	0.14033000	-0.13655100
H	-6.62007600	0.05343400	-2.59531600
N	-3.23754200	-1.68495400	2.11775200
N	-2.39561300	-1.99722800	2.95470600
N	-1.67715200	-2.23165200	3.80896100
H	-1.82263200	-3.16110200	-0.61736900
C1			
Mn	-0.67489100	-1.49133400	-0.21773000
O	0.82852300	-1.45554800	-1.68734300
O	-2.13586500	-2.79549400	-0.95447000
O	-2.07465600	-0.91227000	1.25666900

O	0.74137800	-2.34162100	1.07298000
C	-3.39203700	-2.66173800	-0.77070500
C	-3.33694500	-1.00533700	1.11387800
C	-3.99697100	-1.81332300	0.17077200
H	-5.08421100	-1.79428100	0.18623200
C	-4.16579100	-0.18408500	2.05825800
H	-4.02070300	-0.55219700	3.08193000
H	-5.23408100	-0.20551300	1.82416000
H	-3.80989400	0.85476400	2.03896300
C	-4.27098300	-3.49646300	-1.65400600
H	-4.07298600	-3.24410900	-2.70316200
H	-5.33657200	-3.36305100	-1.44941500
H	-4.01069600	-4.55444800	-1.52804800
C	2.00469200	-2.36719000	0.89854700
C	2.08144800	-1.53535600	-1.46525600
C	2.67634200	-1.97041200	-0.26936100
H	3.76301900	-2.00793800	-0.24756200
C	2.97379700	-1.11088000	-2.59497300
H	2.70866400	-1.66565600	-3.50304200
H	4.03729600	-1.25274800	-2.38060700
H	2.79510800	-0.04787200	-2.80848600
C	2.81539800	-2.88458100	2.05116200
H	3.88949200	-2.72046300	1.92650600
H	2.63722500	-3.96307400	2.15378000
H	2.47673200	-2.42089700	2.98627500
O	-1.45558600	0.55243300	-1.25828200
C	-1.70849600	1.54379500	-0.56576300
C	0.69275300	1.48374700	0.22812600
C	-0.63615500	2.20920900	0.25164000
H	0.56682300	0.49316900	0.69364100
H	-0.99956000	2.30604300	1.28650800
H	-0.52756100	3.24248100	-0.11575100
C	-3.08652600	2.08253000	-0.51014900
C	-4.09843700	1.41945700	-1.21723700
C	-3.41502300	3.19919300	0.27053700
C	-5.41457000	1.84973700	-1.12886600
H	-3.84024500	0.55918800	-1.83009900
C	-4.73274300	3.63044300	0.35420600
H	-2.64632800	3.73508800	0.82187500
C	-5.73332000	2.95268800	-0.33853600
H	-6.19543800	1.32542800	-1.67483500
H	-4.98088900	4.49542900	0.96455100
H	-6.76565500	3.28781800	-0.26495500
H	1.02015000	1.30741900	-0.80592300

C	1.79211300	2.23238300	0.98641800
H	1.43872700	2.47752600	1.99982600
C	3.03645300	1.41201500	1.07575400
C	4.08355200	1.41186500	0.10407200
C	4.01788400	2.25346000	-1.03237300
C	5.20639600	0.55495100	0.22212800
C	5.01979400	2.23626800	-1.99031300
H	3.16902900	2.92021700	-1.16720100
C	6.19991000	0.54651900	-0.74201200
H	5.28508200	-0.10204100	1.08578000
C	6.11727900	1.38461900	-1.85737200
H	4.94272600	2.89336000	-2.85424100
H	7.05177700	-0.12066700	-0.62573100
H	6.90007200	1.37369300	-2.61234800
N	3.15354400	0.47457500	2.09503700
N	2.24593400	0.33063300	2.91474500
N	1.47301700	0.08226000	3.72401300
H	1.99849100	3.19334300	0.50016100

TS_{c1}

Mn	-1.54384500	0.83684100	-0.01767600
O	-1.35282800	1.32933500	2.02790300
O	-3.04090300	-0.59813000	0.49949500
O	-2.63384800	1.01249000	-1.84459000
O	-1.04653900	2.87757300	-0.35666300
C	-3.72877100	-1.28316400	-0.32479200
C	-3.35068700	0.10192600	-2.37162900
C	-3.87314900	-1.01256000	-1.69644300
H	-4.49257900	-1.69560200	-2.27256700
C	-3.66397100	0.27389800	-3.82979600
H	-4.17453300	1.23304600	-3.98024200
H	-4.28641200	-0.52898500	-4.23420700
H	-2.72671600	0.32152600	-4.39783100
C	-4.44128000	-2.47868000	0.23962400
H	-3.70280600	-3.24752400	0.50327200
H	-5.16231400	-2.91445200	-0.45747800
H	-4.95339200	-2.19719700	1.16716500
C	-0.53706400	3.70575500	0.46406300
C	-0.80714300	2.35619700	2.54750600
C	-0.41106700	3.50789500	1.84966600
H	0.04020700	4.31014800	2.42837300
C	-0.55868500	2.28791300	4.02615000
H	-1.46003200	1.92852600	4.53595900
H	-0.25357300	3.24659800	4.45473700

H	0.23423200	1.55264400	4.21955800
C	-0.02426000	4.98600300	-0.12761700
H	0.37682300	5.67532600	0.62059100
H	-0.83020400	5.48297700	-0.68102200
H	0.76350900	4.75145000	-0.85571400
O	-0.19162100	-0.70094200	-0.93274700
C	0.92359100	-0.64038000	-1.46411100
C	2.76921200	-2.36606900	-1.93888700
C	1.39986800	-1.78949100	-2.30730200
H	3.08325800	-3.03218500	-2.75036700
H	1.44512400	-1.42220100	-3.34350300
H	0.62347200	-2.56352800	-2.27698900
C	1.79445100	0.53752400	-1.26912500
C	1.72237400	1.23823400	-0.05862900
C	2.70430800	0.94800000	-2.25235500
C	2.54930700	2.33082600	0.16757400
H	1.02763400	0.90122900	0.71178700
C	3.50878200	2.05965100	-2.03386100
H	2.76580700	0.41691100	-3.20017800
C	3.43627000	2.74696500	-0.82403100
H	2.49607200	2.86306200	1.11504200
H	4.19807100	2.38823200	-2.80776800
H	4.07794800	3.60795800	-0.65012000
H	3.51386400	-1.56195200	-1.89743000
C	2.80649600	-3.18473400	-0.64218900
H	3.83487400	-3.53470400	-0.48946000
C	2.40397800	-2.40942900	0.58446600
C	1.06928600	-2.59935600	1.20673400
C	0.21327400	-3.63473100	0.81272200
C	0.62831100	-1.70585100	2.19847000
C	-1.04051700	-3.77909500	1.39825100
H	0.51134400	-4.34801700	0.05016300
C	-0.62233800	-1.85115200	2.77846400
H	1.27551000	-0.88724600	2.50663800
C	-1.46369300	-2.88931300	2.37913900
H	-1.68612500	-4.59669000	1.08419300
H	-0.94944200	-1.14541800	3.53931700
H	-2.44758400	-2.99921100	2.83096300
N	3.14505700	-1.50932000	1.13837600
N	4.51794100	-1.39912200	0.45238000
N	5.04497600	-0.37088000	0.33937000
H	2.18288000	-4.07378600	-0.76140000

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O	1.92634100	2.29995900	1.45196300
C	2.34654600	2.35990400	0.29890900
C	1.12954100	3.63412200	-1.59708400
C	2.19146000	3.63734300	-0.48875100
H	1.22035500	4.59367800	-2.11978300
H	3.16043800	3.89872500	-0.93414500
H	1.94370500	4.41962700	0.23967700
C	3.03114100	1.19070100	-0.31729400
C	3.09347000	-0.00623600	0.40726100
C	3.56957900	1.23356400	-1.60792600
C	3.66080700	-1.14185700	-0.15500000
H	2.68586800	-0.03615800	1.41735900
C	4.13800700	0.09573300	-2.17035300
H	3.54838300	2.15506300	-2.18546100
C	4.17818000	-1.09446200	-1.44864300
H	3.70008800	-2.06814200	0.41511300
H	4.55171100	0.13904300	-3.17519500
H	4.62040400	-1.98459300	-1.89101800
H	1.34468800	2.85665200	-2.34139200
C	-0.31096600	3.50448600	-1.12210500
H	-0.99986200	3.90503600	-1.87924000
C	-0.78817100	2.10511200	-0.80498600
C	-2.23610600	1.93358300	-0.49579700
C	-2.85747100	2.69952500	0.49432800
C	-2.97858300	0.99750100	-1.22043600
C	-4.20830600	2.51216200	0.76776200
H	-2.28018500	3.42550600	1.06463500
C	-4.33350500	0.82910000	-0.95684800
H	-2.48942900	0.40874300	-1.99624400
C	-4.94788700	1.58164300	0.04086100
H	-4.68668200	3.09878700	1.54885100
H	-4.90992300	0.10855600	-1.53376600
H	-6.00654800	1.44560300	0.25083300
N	0.01448500	1.12779100	-0.83694100
H	-0.47984900	4.11499200	-0.21992200
Mn	-0.13798300	-0.64940400	0.08302300
O	-0.38376700	0.29961100	1.87998100
O	0.18860000	-1.57128900	-1.70957100
O	-2.04188000	-1.59157500	0.15696700
O	0.76637500	-2.23378200	1.10111200
C	0.11178000	-0.04647300	3.00465500
C	1.09868900	-2.24367400	2.33113200
C	0.82976500	-1.22321800	3.25900800
H	1.17999800	-1.37524000	4.27649900

C	-0.11247400	0.92443400	4.12310300
H	0.27283700	0.56828400	5.08186200
H	-1.18547100	1.13040000	4.21599900
H	0.37473600	1.87467400	3.87014200
C	1.84161000	-3.46023500	2.79434400
H	1.24665100	-4.35437200	2.57301800
H	2.07550400	-3.43817300	3.86177400
H	2.77550000	-3.55197100	2.22509700
C	-2.41218500	-2.54442800	-0.59667300
C	-0.47824600	-2.55023900	-2.19334100
C	-1.69355500	-3.04124000	-1.70190700
H	-2.14008600	-3.87051500	-2.24431800
C	0.12338000	-3.18858700	-3.40880900
H	0.20732000	-2.44057600	-4.20681600
H	-0.45622000	-4.03951300	-3.77604600
H	1.14280900	-3.51891500	-3.17477100
C	-3.73439400	-3.16837800	-0.26228100
H	-4.01732000	-3.97168600	-0.94753600
H	-4.51008200	-2.39226400	-0.27492100
H	-3.69913400	-3.56338300	0.76032100

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Mn	-0.32692200	1.32952900	0.70541000
O	-0.35867400	-0.44742600	1.84449200
O	-2.40834000	1.45506500	0.38895800
O	-0.28811900	3.33595200	-0.06220800
O	1.03224400	2.02795700	2.19328100
C	-2.97018100	2.16268500	-0.51088800
C	-1.12034100	3.79835500	-0.90544700
C	-2.38957700	3.25499600	-1.17473000
H	-3.00016400	3.76528400	-1.91555900
C	-0.69645100	5.03505900	-1.64323300
H	0.23747800	4.83348600	-2.18200300
H	-0.47998200	5.83085400	-0.92000400
H	-1.44864000	5.39247600	-2.35171200
C	-4.37957900	1.77998000	-0.86060500
H	-4.39089600	0.76051200	-1.26928800
H	-4.83893600	2.45515200	-1.58773900
H	-4.98942200	1.76506000	0.05102600
C	1.75328700	1.30667000	2.95577100
C	0.57218100	-0.86776400	2.60647100
C	1.58176200	-0.07041300	3.17221200
H	2.29335200	-0.56292700	3.83049500
C	0.58120600	-2.34029200	2.88946900

H	1.32040800	-2.62716500	3.64251700
H	0.80356300	-2.87157700	1.95184800
H	-0.41615800	-2.66477100	3.21001600
C	2.88802100	2.00764900	3.64388700
H	3.44924100	1.35619200	4.31955000
H	2.50123300	2.86530300	4.20725700
H	3.57249700	2.40886100	2.88520300
O	0.27756000	0.54828300	-1.29648900
C	1.12829300	0.00560900	-2.01407200
C	0.37958900	-1.88651100	-3.52788900
C	0.73232600	-0.39629300	-3.40486800
H	0.15337600	-2.07417800	-4.58337700
H	1.53039000	-0.15227200	-4.11436000
H	-0.14712900	0.20208700	-3.67154300
C	2.49294100	-0.27158100	-1.52138100
C	2.78717900	-0.06757600	-0.16685400
C	3.49581000	-0.76278700	-2.36826000
C	4.04982700	-0.34500100	0.33243200
H	2.01255800	0.29679400	0.50183000
C	4.76362100	-1.03371400	-1.86852400
H	3.29655900	-0.93292700	-3.42336200
C	5.04244000	-0.82644700	-0.52043700
H	4.25908300	-0.19264300	1.38991400
H	5.53637700	-1.41031200	-2.53419100
H	6.03497100	-1.04357800	-0.13183000
H	1.24782100	-2.51065600	-3.27712400
C	-0.82594300	-2.29834300	-2.69460100
H	-1.27342600	-3.21839800	-3.09759000
C	-0.54799400	-2.59269900	-1.23570100
C	-1.69810000	-2.69030100	-0.29257900
C	-2.70681300	-1.72408900	-0.30158100
C	-1.72915100	-3.71667900	0.65644400
C	-3.72830600	-1.77679800	0.64121300
H	-2.67621500	-0.90559800	-1.02035700
C	-2.76069400	-3.77445900	1.58597200
H	-0.94385500	-4.47064900	0.65346600
C	-3.75761800	-2.80109700	1.58394300
H	-4.50213500	-1.01151800	0.64076200
H	-2.78549600	-4.58032000	2.31640200
H	-4.56103600	-2.84329700	2.31617000
N	0.61843100	-2.79556800	-0.79915000
H	-1.61516400	-1.53610300	-2.75887800

TS_{D2}

O	-2.01736300	1.06231700	-2.17584300
C	-1.71778300	1.74726600	-1.14973100
C	-0.44624800	3.96278200	-0.59208100
C	-1.49741200	3.24296800	-1.41202400
H	-0.46775400	5.03447800	-0.82465300
H	-2.48162900	3.71876100	-1.28868000
H	-1.23828000	3.31935600	-2.47846500
C	-2.49571500	1.43015400	0.12338000
C	-3.75988500	0.85542900	-0.03659500
C	-2.05097400	1.70422200	1.42040500
C	-4.55788000	0.55635600	1.06388400
H	-4.10934200	0.63673800	-1.04351300
C	-2.84326200	1.39971300	2.52452100
H	-1.06102200	2.12615800	1.58021800
C	-4.10028600	0.82576900	2.35113100
H	-5.53785800	0.10562400	0.91523100
H	-2.47302200	1.60948500	3.52642600
H	-4.71775700	0.58683900	3.21486000
H	-0.65733800	3.87674600	0.48220500
C	0.93249800	3.41490600	-0.89841600
H	1.70002300	3.87780600	-0.26464100
C	1.03197000	1.91911200	-0.74212000
C	2.40824500	1.34715200	-0.73427900
C	2.71888800	0.26422500	-1.56555700
C	3.40451700	1.88374900	0.09006600
C	3.99867200	-0.28072800	-1.55976600
H	1.95011800	-0.14336100	-2.22169500
C	4.67786500	1.32510400	0.10589200
H	3.17864300	2.72587300	0.74209000
C	4.97779800	0.24365900	-0.71914000
H	4.23238400	-1.11448800	-2.21859700
H	5.43873500	1.73734800	0.76511100
H	5.97699800	-0.18656000	-0.71213600
N	-0.01200100	1.18537100	-0.64379300
H	1.22574700	3.65367600	-1.93376300
Mn	0.06424100	-0.72674300	-0.00741000
O	-0.44798100	-1.46198900	-1.71541500
O	0.73363100	-0.07577800	1.68688900
O	1.41056100	-2.29303000	0.12454200
O	-1.53625200	-1.69467200	0.90378800
C	-1.54403800	-2.07522900	-2.00969700
C	-2.47305300	-2.29044600	0.28688300
C	-2.52767900	-2.46905500	-1.11067400
H	-3.39178500	-2.98858000	-1.51559800

C	-1.71266400	-2.34834900	-3.46873800
H	-2.59718500	-2.95332900	-3.68164200
H	-0.82024300	-2.85304600	-3.85602000
H	-1.79663300	-1.39030800	-3.99766000
C	-3.56611300	-2.87822700	1.12318300
H	-3.26937700	-3.88956100	1.43184400
H	-4.50661400	-2.95930400	0.57000700
H	-3.71339900	-2.28160500	2.02886600
C	2.48947200	-2.25539800	0.79824400
C	1.89983100	-0.29838200	2.18973300
C	2.78307600	-1.28987100	1.77761100
H	3.73976100	-1.35650400	2.28801400
C	2.26163600	0.59721500	3.32963200
H	2.05636000	1.63937500	3.05822800
H	3.30938900	0.49054900	3.62291600
H	1.62635600	0.35781500	4.19187100
C	3.47689200	-3.34734100	0.53494400
H	4.46675600	-3.11946600	0.94017200
H	3.54857400	-3.52968300	-0.54261400
H	3.11640500	-4.27517100	0.99757300

TS_{D2'}

O	3.15118000	-3.25069200	0.30865600
C	2.80592100	-2.38463700	-0.50010900
C	0.67652100	-3.71063000	-1.01883000
C	1.55664400	-2.52154800	-1.26725800
H	1.02909600	-4.59744800	-1.56438000
H	1.62638500	-2.20359000	-2.31387900
H	0.77632700	-1.61308300	-0.80522000
C	3.61099000	-1.14715100	-0.67911100
C	4.85870900	-1.06665000	-0.05104900
C	3.13720000	-0.04501100	-1.40288600
C	5.62435800	0.08661100	-0.15132700
H	5.21521300	-1.92237600	0.51813900
C	3.90148100	1.11249100	-1.49597200
H	2.15972000	-0.07489900	-1.88410500
C	5.14579600	1.17843200	-0.87382600
H	6.59499400	0.13888400	0.33663600
H	3.52149700	1.96614600	-2.05303900
H	5.74332500	2.08438100	-0.94939600
H	0.70597900	-3.96443600	0.04973500
C	-0.75534800	-3.40539600	-1.43730500
H	-1.43531900	-4.20860800	-1.13528900
C	-1.25373300	-2.08662300	-0.87261800

C	-2.71441100	-1.88834400	-0.70858600
C	-3.61491200	-2.59575000	-1.51267200
C	-3.20474400	-0.97331900	0.23148700
C	-4.98192400	-2.37396300	-1.39133800
H	-3.25138200	-3.30714500	-2.25065300
C	-4.57147900	-0.76420700	0.35674600
H	-2.51190000	-0.43212700	0.87461800
C	-5.46234700	-1.46039900	-0.45753500
H	-5.67387400	-2.91954800	-2.02860000
H	-4.94332200	-0.05606400	1.09401100
H	-6.53278000	-1.29330500	-0.36048000
N	-0.43842200	-1.14982900	-0.57617000
H	-0.83047400	-3.32547600	-2.53324000
Mn	-0.27009400	0.87389500	0.09838000
O	-1.73320900	1.71699700	-1.15772300
O	1.25649600	0.14249400	1.41998700
O	-1.25526500	1.39017100	1.89514600
O	0.91836900	2.52223300	-0.47190100
C	-1.90448800	2.97878100	-1.23668400
C	0.42407000	3.68122000	-0.66953700
C	-0.92114700	3.94771000	-0.97855300
H	-1.20349700	4.98912500	-1.11062500
C	-3.26644400	3.42672300	-1.67569000
H	-3.46239200	3.04885800	-2.68694800
H	-3.38163600	4.51393600	-1.67466000
H	-4.02213900	2.98020900	-1.01776400
C	1.38477700	4.82880200	-0.57652900
H	0.90686900	5.80068100	-0.72536700
H	2.17397900	4.70080400	-1.32803000
H	1.87533000	4.81319500	0.40412000
C	-1.20902500	0.66730900	2.94709800
C	0.96374100	-0.47664400	2.49111600
C	-0.20541800	-0.26567600	3.24779100
H	-0.30928500	-0.82892200	4.17206000
C	1.93992700	-1.51888800	2.94980300
H	1.82550600	-2.40461800	2.30817000
H	1.78518800	-1.82363900	3.98882100
H	2.96676500	-1.15888000	2.81620400
C	-2.34456000	0.84479800	3.91063600
H	-2.24045900	0.24002000	4.81555600
H	-3.28498300	0.57918800	3.40986500
H	-2.42292000	1.90229300	4.19054500

O	1.27811500	2.02601500	2.61438700
C	1.35805900	0.78635300	2.70125900
C	-0.81801800	0.65436400	4.03817100
C	0.44802800	0.05581000	3.55328800
H	-0.93796800	0.48602800	5.11616900
H	0.63139500	-0.99653500	3.76945200
H	-0.83965800	1.58887900	1.74433200
C	2.35314200	0.04215700	1.88703500
C	3.39203400	0.75988200	1.28172900
C	2.24418700	-1.33546200	1.64998400
C	4.32120900	0.11077300	0.48013300
H	3.46394200	1.83074900	1.45829500
C	3.17226200	-1.98194500	0.84196900
H	1.42061700	-1.90813400	2.07514500
C	4.21427500	-1.26221000	0.26202300
H	5.13183800	0.67419300	0.02305600
H	3.07483000	-3.04939200	0.65415900
H	4.93965300	-1.77133100	-0.37000900
H	-0.81407800	1.73850600	3.87713000
C	-2.00770900	-0.01361700	3.32840700
H	-2.94654900	0.48752500	3.60557000
C	-1.90572900	-0.01758300	1.82759500
C	-2.59324200	-1.08051300	1.06551100
C	-2.55717400	-2.41646200	1.47740400
C	-3.21708200	-0.75172400	-0.14481500
C	-3.11040700	-3.40912500	0.67537600
H	-2.05541000	-2.69245700	2.40338300
C	-3.78512900	-1.74256600	-0.93443600
H	-3.25529800	0.29097900	-0.45558700
C	-3.72474300	-3.07496200	-0.52899900
H	-3.05752900	-4.44892700	0.99033500
H	-4.27556600	-1.47571400	-1.86839700
H	-4.16197900	-3.85341300	-1.15063000
N	-1.24551600	0.85909000	1.15374600
H	-2.11358400	-1.04681400	3.68076600
Mn	-0.00865000	0.49158600	-0.70637400
O	-0.07504100	-1.61353500	-0.75666700
O	0.54696100	2.55038700	-0.48304100
O	-1.27759700	1.20285100	-2.25694000
O	1.78009200	0.22998800	-1.88368700
C	0.60706200	-2.44148900	-1.44268300
C	2.21796800	-0.82372200	-2.44043200
C	1.67853200	-2.11389200	-2.28469900
H	2.17024000	-2.92891300	-2.81011300

C	0.22449700	-3.88418900	-1.28092800
H	0.33532700	-4.16335800	-0.22390700
H	0.82549800	-4.56150600	-1.89411200
H	-0.83639800	-4.01418400	-1.53116500
C	3.42447400	-0.65236800	-3.31847500
H	3.79329200	-1.59458900	-3.73343200
H	4.22582500	-0.17454500	-2.74049200
H	3.18012300	0.02947500	-4.14242300
C	-1.86693900	2.33205300	-2.20010200
C	-0.31399900	3.47914200	-0.60287300
C	-1.47748900	3.41556600	-1.39328500
H	-2.09542500	4.30938700	-1.43408100
C	-0.03409200	4.73575800	0.16862000
H	0.03401100	4.48431600	1.23545700
H	-0.79480100	5.50886400	0.02939000
H	0.94425900	5.13535600	-0.12483700
C	-3.06985000	2.48712600	-3.08396200
H	-3.57285800	3.45039500	-2.96310000
H	-3.78079400	1.67752400	-2.87497300
H	-2.76310700	2.37578800	-4.13157200