

SUPPORTING INFORMATION

Theoretical Studies on the Mechanism of Molybdenum-Catalysed Deoxydehydration of Diols

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Fig. S1. Catalytic profiles, pathways **A** and **B**, for the DODH of ethylene glycol with PMe_3 catalyzed by $[\text{Mo}(\text{O})_2(\text{Q}^{\text{Me}})_2]$ in gas phase (relative ΔG in $\text{kcal}\cdot\text{mol}^{-1}$).

Table S1. Coordinates of optimized compounds.

Table S2. Comparison of selected energies for pathways **A** and **B**, in gas phase, in the $[\text{Mo}(\text{O})_2(\text{Q}^{\text{Me}})_2]$ -catalyzed DODH of ethylene glycol with PMe_3 reductant.

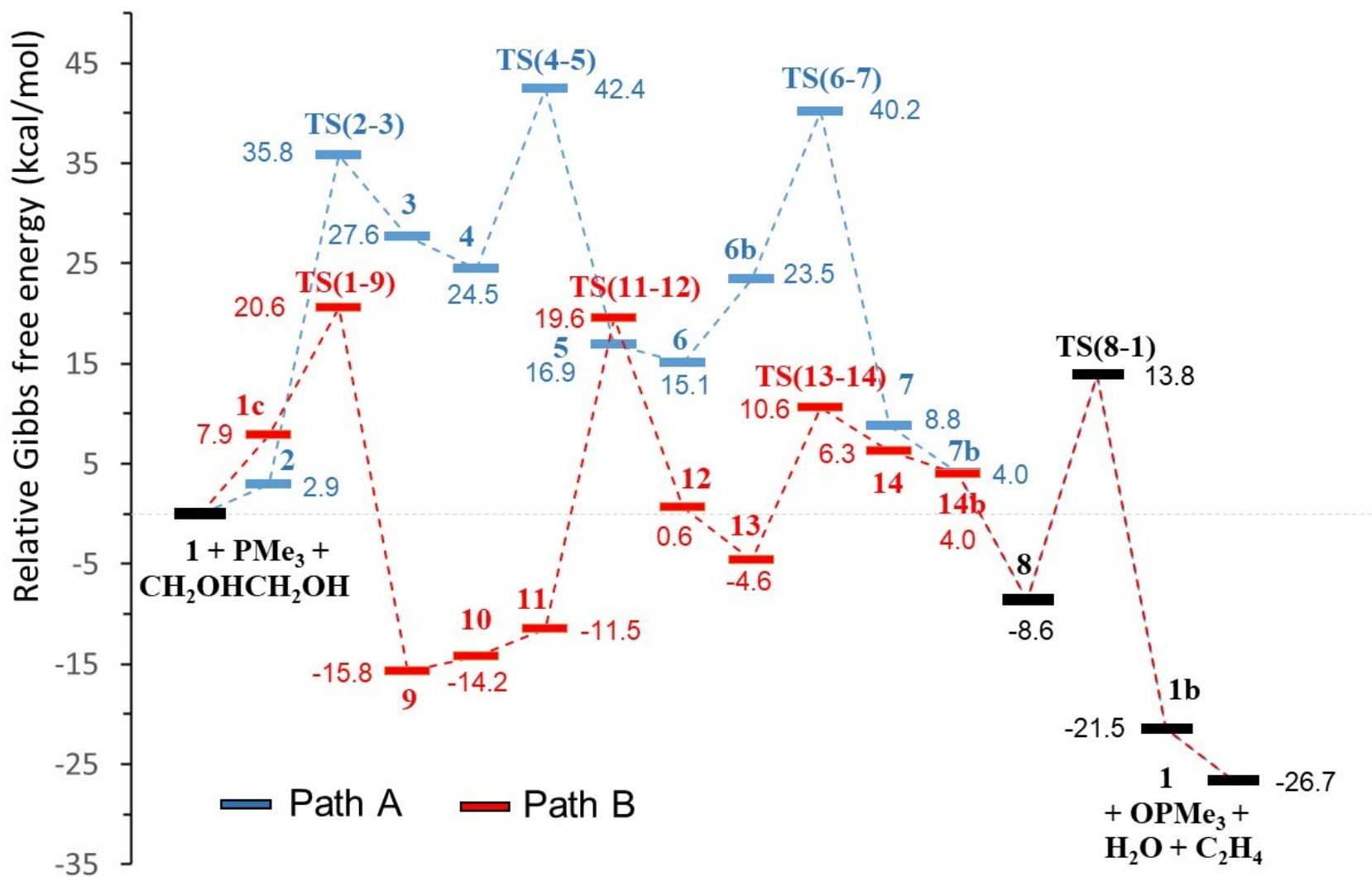


Fig. S1. Catalytic profiles, pathways **A** (blue) and **B** (red), for the DODH of ethylene glycol with PMe₃ catalyzed by [Mo(O)₂(Q^{Me})₂] in gas phase (relative ΔG in kcal·mol⁻¹, common steps in black).

Table S1. Coordinates of optimized compounds.**1**

C	-3.63857500	1.80426200	1.92780900
C	-1.03415800	1.47534700	1.88537800
C	-2.38601400	1.21567000	1.53945500
C	-2.74498000	0.21733300	0.59866400
C	1.03415400	1.47551300	-1.88527700
C	2.38600800	1.21582900	-1.53934300
C	2.74497600	0.21742600	-0.59862100
C	3.63856200	1.80450600	-1.92759300
N	-4.63916600	1.23673800	1.30073200
N	-4.09961700	0.26405500	0.47481000
N	4.09961000	0.26416300	-0.47474300
N	4.63915700	1.23691600	-1.30058300
O	-0.09663900	0.80918800	1.38044300
O	0.09663600	0.80925100	-1.38047500
O	-2.00770100	-0.61318300	-0.05797700
O	2.00771000	-0.61316000	0.05794800
O	0.06731900	-2.02907300	1.35482000
O	-0.06728300	-2.02902400	-1.35491500
Mo	0.00000800	-0.98533900	-0.00002800
C	-0.65931400	2.55773100	2.86631000
H	-1.03631900	3.52979800	2.53968000
H	-1.09348100	2.34941500	3.84762800
H	0.42499400	2.59546000	2.95329900
C	-3.92118200	2.90985500	2.89542100
H	-3.55744200	2.67013600	3.89826100
H	-3.44935700	3.84722500	2.58766500
H	-4.99855600	3.06664800	2.94529100
C	0.65931900	2.55796000	-2.86614000
H	1.03632700	3.53000400	-2.53945000
H	1.09348800	2.34970000	-3.84747000
H	-0.42498900	2.59569600	-2.95313400
C	3.92115500	2.91021800	-2.89507300
H	3.55740200	2.67061800	-3.89793700
H	3.44933200	3.84755000	-2.58719800
H	4.99852800	3.06702100	-2.94493800
C	-4.97565700	-0.53364300	-0.31959200
C	-6.34529900	-0.49647300	-0.03873800
C	-4.49290000	-1.32788200	-1.36494700
C	-7.22491200	-1.25472300	-0.80237300
H	-6.69933500	0.12994800	0.76676900
C	-5.38972400	-2.08353200	-2.11540700
H	-3.43726800	-1.35958800	-1.58508400
C	-6.75436800	-2.05343500	-1.84255000
H	-8.28498200	-1.22055600	-0.57799300
H	-5.00872800	-2.69895100	-2.92225000
H	-7.44369700	-2.64537300	-2.43334600
C	4.97565300	-0.53364300	0.31954700
C	6.34527300	-0.49657300	0.03857600
C	4.49291600	-1.32788500	1.36490800
C	7.22488800	-1.25493500	0.80209800
H	6.69928800	0.12986200	-0.76693000
C	5.38974000	-2.08365400	2.11525000
H	3.43730100	-1.35950800	1.58513700
C	6.75436200	-2.05366200	1.84227200
H	8.28494200	-1.22084800	0.57763100
H	5.00876600	-2.69908000	2.92209700
H	7.44369000	-2.64569300	2.43297600

1b

C	3.61375800	-2.11472600	1.93643200
C	1.01173200	-1.77043300	1.89238900
C	2.36491900	-1.51952900	1.54628700
C	2.73037000	-0.52668700	0.60226800
C	-1.04956600	-1.77610800	-1.87866400
C	-2.40020400	-1.50924100	-1.53457000
C	-2.75577500	-0.50440400	-0.59954200

C	-3.65495800	-2.09496300	-1.92012500
N	4.61750400	-1.55545700	1.30709000
N	4.08430800	-0.58179300	0.47832200
N	-4.11025100	-0.54443000	-0.47597800
N	-4.65322800	-1.51976500	-1.29641100
O	0.07780600	-1.10115000	1.38402600
O	-0.10924700	-1.11130800	-1.37624800
O	1.99685300	0.30568300	-0.05715800
O	-2.01426700	0.32626200	0.05301600
O	0.06698100	1.72664800	-1.36269700
Mo	-0.00672400	0.68708400	-0.00349800
C	0.20377400	5.31830000	-0.66205400
C	0.20663200	5.31986800	0.66613500
O	-0.07025100	1.73746900	1.34787100
H	0.12476000	4.39496900	-1.22615100
H	0.12873200	4.39790100	1.23260000
H	0.28681000	6.24131100	1.23501200
H	0.28111500	6.23845200	-1.23342300
C	3.88976500	-3.21860100	2.90782700
H	3.53117300	-2.97140100	3.91072800
H	3.40900900	-4.15317200	2.60555100
H	4.96589900	-3.38427300	2.95533000
C	0.63033200	-2.84761500	2.87623100
H	0.99085800	-3.82437600	2.54465100
H	1.07618800	-2.64716300	3.85380100
H	-0.45358200	-2.87103800	2.97242300
C	-0.67863500	-2.86491300	-2.85365800
H	-1.05292600	-3.83475400	-2.51718400
H	-1.11841900	-2.66497600	-3.83413700
H	0.40520600	-2.90271000	-2.94604500
C	-3.94173400	-3.20471900	-2.88164700
H	-3.57997300	-2.97036300	-3.88648700
H	-3.47076200	-4.14136500	-2.57051400
H	-5.01948100	-3.35978100	-2.92838100
C	-4.98393400	0.26071100	0.31408100
C	-6.35451900	0.21963800	0.03854300
C	-4.49788500	1.06588200	1.34946600
C	-7.23186000	0.98488600	0.79773800
H	-6.71108700	-0.41471600	-0.75955400
C	-5.39255600	1.82836000	2.09556800
H	-3.44149600	1.10142600	1.56512900
C	-6.75813400	1.79431600	1.82811000
H	-8.29267700	0.94782900	0.57745400
H	-5.00897200	2.45276100	2.89418300
H	-7.44570400	2.39188800	2.41523500
C	4.96610500	0.20607000	-0.32025100
C	6.33737100	0.14505400	-0.05166300
C	4.48721800	1.01388700	-1.35693600
C	7.22248400	0.89295400	-0.81906400
H	6.68825300	-0.49080900	0.74772000
C	5.38974100	1.75873200	-2.11134400
H	3.43045300	1.06491500	-1.56739000
C	6.75600500	1.70472400	-1.85088500
H	8.28373000	0.84044900	-0.60404600
H	5.01164800	2.38534500	-2.91083800
H	7.44966300	2.28875300	-2.44444600

1c

C	3.52300600	0.42354800	2.25054300
C	0.92136900	0.58386400	1.93545700
C	2.25725700	0.23977600	1.59579000
C	2.57825900	-0.45417500	0.40366400
C	-1.46825100	-2.85129500	0.90902000
C	-2.76341700	-2.28918000	0.76873200
C	-2.99191500	-1.09673600	0.03632800
C	-4.06357200	-2.66197100	1.25532700
N	4.49705500	-0.10018900	1.54688400
N	3.92478600	-0.65236300	0.41281600
N	-4.32468200	-0.83311800	0.12238700
N	-4.97429600	-1.80346200	0.86825100

O	-0.03152300	0.30213200	1.16527400
O	-0.46608500	-2.31026500	0.37860500
O	1.81624000	-0.85585200	-0.56030900
O	-2.16737600	-0.34818700	-0.61406200
O	-0.04650900	1.09759600	-1.54864000
O	-0.15468000	-1.50613300	-2.32855600
Mo	-0.15424600	-0.50420900	-0.94065000
P	1.33629600	4.36170200	0.43866200
C	-0.32794100	4.60132600	-0.35511000
H	-0.28699800	5.29949900	-1.19715700
H	-0.68406200	3.63389200	-0.71540200
H	-1.04062800	4.97822500	0.38244400
C	2.32538100	3.89517400	-1.06495900
H	2.23557100	4.63680000	-1.86502700
H	3.37962900	3.78926000	-0.79852000
H	1.96755800	2.93308200	-1.43776300
C	1.86275700	6.13817000	0.63392100
H	1.76618100	6.70690500	-0.29653000
H	1.25374400	6.61849600	1.40377800
H	2.90432000	6.17745200	0.96230100
C	-1.23080500	-4.11558400	1.69579700
H	-1.55965400	-3.99689900	2.73112900
H	-1.79425100	-4.94703700	1.26487300
H	-0.16817800	-4.35015500	1.67484500
C	-4.47669700	-3.82979700	2.09415700
H	-4.24182100	-4.77956600	1.60600900
H	-3.97760200	-3.82546100	3.06712900
H	-5.55306800	-3.78150800	2.25810700
C	0.58483800	1.30678100	3.21070500
H	1.08508100	0.86610700	4.07414900
H	0.91210600	2.34724800	3.11706300
H	-0.49445600	1.28886300	3.35318700
C	3.84483300	1.10523600	3.54237600
H	3.49077600	2.13929500	3.54530600
H	3.38757600	0.59400400	4.39441800
H	4.92588000	1.10328200	3.68148700
C	-5.08910300	0.22461000	-0.45286300
C	-6.48237000	0.10328700	-0.47173900
C	-4.47526200	1.36596000	-0.97927200
C	-7.25431300	1.12153200	-1.01866900
H	-6.93791400	-0.78188700	-0.05281900
C	-5.26575500	2.37282000	-1.52679900
H	-3.40100500	1.46341900	-0.96626200
C	-6.65294400	2.26005500	-1.55097000
H	-8.33351600	1.01931800	-1.02975500
H	-4.78349400	3.25338900	-1.93535500
H	-7.25882400	3.05001100	-1.97929600
C	4.76713800	-1.27269400	-0.55640500
C	6.14887700	-1.07903300	-0.45675300
C	4.24033600	-2.06634600	-1.58087500
C	6.99604000	-1.67627900	-1.38271800
H	6.53647300	-0.47026800	0.34681200
C	5.10529900	-2.65203400	-2.50138000
H	3.17546300	-2.21916300	-1.66125000
C	6.48145900	-2.46328600	-2.41092000
H	8.06561000	-1.52074300	-1.29838500
H	4.69015700	-3.26314600	-3.29456900
H	7.14561800	-2.92424400	-3.13275100

2

C	3.53973400	0.31564500	2.43480500
C	0.92936900	0.40861200	2.13560200
C	2.28147200	0.19367200	1.75149700
C	2.63060200	-0.29051500	0.46598000
C	-1.34987900	-2.91858500	0.38251100
C	-2.65969600	-2.38143600	0.35265400
C	-2.92092100	-1.06712200	-0.11177900
C	-3.95050100	-2.88654200	0.73501900
N	4.53171600	-0.05656300	1.66300200
N	3.98346600	-0.43592300	0.45010200

N	-4.25956200	-0.86495700	0.01559000
N	-4.88367900	-1.99056400	0.53039500
O	-0.00890900	0.14993000	1.33835100
O	-0.36337300	-2.24192200	-0.01025200
O	1.88364000	-0.56360700	-0.55506300
O	-2.11276600	-0.17865100	-0.58129000
O	-0.03221700	-0.84732200	-2.46704600
Mo	-0.09018300	-0.20843900	-0.88208300
O	-0.02897300	1.50625500	-1.08069900
O	0.45044600	3.38466200	1.09453500
C	1.39849100	4.28844000	0.54239000
H	1.80355000	4.86292600	1.38283700
H	2.23614600	3.76419700	0.06473800
C	0.76316000	5.24439200	-0.46822900
H	0.38478200	4.67653400	-1.32151500
H	0.15374500	2.79655800	0.38271600
H	-0.08949300	5.75264000	0.00218900
O	1.70962300	6.16804400	-0.99769500
H	1.98226200	6.75245400	-0.28369900
C	0.54371400	0.97856500	3.46954800
H	1.22974500	0.70909700	4.26998800
H	0.53870800	2.06764900	3.35059000
H	-0.46951800	0.65979200	3.71245900
C	3.84517500	0.78997500	3.82066400
H	3.45235800	1.79437400	3.99660100
H	3.41779100	0.12611600	4.57785300
H	4.92682900	0.80870100	3.95355200
C	-4.33020200	-4.21771600	1.30182800
H	-4.06258200	-5.03449200	0.62584900
H	-3.83556300	-4.40497600	2.25901700
H	-5.40821600	-4.23823600	1.46050300
C	-1.06849200	-4.31223700	0.88113500
H	-1.39257000	-4.42420400	1.91880300
H	-1.61188200	-5.04970500	0.28527500
H	0.00020800	-4.50525300	0.80978100
C	4.85025600	-0.90391200	-0.58278500
C	6.19402700	-1.13050200	-0.26555700
C	4.38816700	-1.13163000	-1.88359600
C	7.06664800	-1.58360400	-1.24759300
H	6.53405300	-0.94320300	0.74211100
C	5.27805400	-1.58802200	-2.85243500
H	3.35402500	-0.95900600	-2.13577000
C	6.61612600	-1.81663000	-2.54522700
H	8.10617400	-1.75530800	-0.99231800
H	4.91222800	-1.76106600	-3.85795800
H	7.30029700	-2.17020100	-3.30774900
C	-5.05127900	0.27101200	-0.32770000
C	-6.43714600	0.11094800	-0.42272800
C	-4.46905200	1.52226100	-0.55327800
C	-7.23420000	1.20278500	-0.74609700
H	-6.86806300	-0.86156400	-0.23487400
C	-5.28377800	2.60244100	-0.88124900
H	-3.40047000	1.64999200	-0.47748900
C	-6.66420100	2.45247100	-0.97987100
H	-8.30785500	1.07138800	-0.81787100
H	-4.82676600	3.56945800	-1.05666800
H	-7.28949800	3.30012500	-1.23486100

TS(2-3)

C	3.53111300	-0.99602300	2.62521300
C	1.03655500	-0.21358100	2.68749800
C	2.27586200	-0.52601900	2.09810900
C	2.49921300	-0.40100000	0.69483700
C	-1.22130100	-2.37531100	-0.42510900
C	-2.58106200	-2.05518900	-0.54802800
C	-3.02760700	-0.73444100	-0.27693000
C	-3.78297400	-2.79989800	-0.81102000
N	4.41478400	-1.14567100	1.67402500
N	3.79372000	-0.78864400	0.48285000
N	-4.38709500	-0.75677300	-0.38256600

N	-4.83518200	-2.02842900	-0.71738400
O	0.07850300	0.22630200	1.99003900
O	-0.35197900	-1.48486100	-0.18169800
O	1.72376900	-0.02943100	-0.24738000
O	-2.34998200	0.29822500	0.04562200
O	-0.23081300	0.80806300	-1.81624200
Mo	-0.27661700	0.72054400	-0.11230600
O	-1.04490900	2.29833900	0.42850200
O	1.14823100	2.42401100	0.13068800
C	2.02340300	2.91064000	-0.87218400
H	2.63956600	2.07984300	-1.23212300
H	1.46068200	3.30818000	-1.72606200
C	2.92486100	3.99907900	-0.28493000
H	2.31855700	4.84070200	0.05599200
H	0.00475400	2.82599300	0.34724800
H	3.45967500	3.59559000	0.58474000
O	3.81321800	4.51996400	-1.26553500
H	4.42743900	3.82066400	-1.51064100
C	0.77739900	-0.37421300	4.16368100
H	1.00539100	-1.38920800	4.49602100
H	1.40856200	0.31065600	4.73649900
H	-0.26783500	-0.14698400	4.36494800
C	3.91754100	-1.31106400	4.03578300
H	3.79976200	-0.44193300	4.68868200
H	3.30900000	-2.11990800	4.45009300
H	4.96223800	-1.62106600	4.05427000
C	-3.95451900	-4.24189900	-1.16777400
H	-3.42087400	-4.49279800	-2.08902700
H	-3.57899300	-4.89944500	-0.37867300
H	-5.01470500	-4.44748600	-1.31431700
C	-0.70773600	-3.78694900	-0.55198300
H	-1.17324500	-4.43635500	0.19356000
H	-0.95015300	-4.18968300	-1.53860600
H	0.37204500	-3.79042000	-0.41667200
C	4.54381300	-0.82933300	-0.72534900
C	5.93727100	-0.93249100	-0.64394000
C	3.91704100	-0.77741100	-1.97623200
C	6.69484700	-0.97545200	-1.80856600
H	6.40287400	-0.98585800	0.32936200
C	4.69465700	-0.81531200	-3.13133000
H	2.84236600	-0.70688300	-2.04256900
C	6.08128800	-0.91334400	-3.05837600
H	7.77354300	-1.05566300	-1.73488000
H	4.20185200	-0.77241400	-4.09599100
H	6.67675400	-0.94413600	-3.96337800
C	-5.33683400	0.29321000	-0.20854300
C	-6.68920000	0.01040000	-0.42956400
C	-4.93862200	1.58003500	0.17319800
C	-7.63731000	1.01400700	-0.26909700
H	-6.97638500	-0.98842600	-0.72290300
C	-5.90575900	2.56994600	0.32719700
H	-3.89671900	1.80452600	0.34359900
C	-7.25362400	2.29867700	0.10951900
H	-8.68285500	0.78600400	-0.44322700
H	-5.59078600	3.56458700	0.62139700
H	-7.99637700	3.07839200	0.23260300

3

C	3.57789600	-1.06514100	2.60319900
C	1.15487500	-0.10812900	2.80612200
C	2.34406600	-0.47337500	2.15173200
C	2.52999700	-0.27726100	0.74930900
C	-0.86917600	-2.27839400	-0.34804700
C	-2.22185300	-2.04649500	-0.64413600
C	-2.82480800	-0.83023200	-0.23173700
C	-3.30927400	-2.84353300	-1.14209200
N	4.41573800	-1.22052400	1.61268800
N	3.78445900	-0.74611400	0.46816900
N	-4.16003200	-0.95570000	-0.48465500
N	-4.44052800	-2.19163100	-1.05277100

O	0.19289700	0.41566900	2.17181700
O	-0.11908900	-1.35690800	0.08922600
O	1.76320000	0.22693100	-0.13318900
O	-2.29221000	0.18356800	0.33273700
O	-0.41503500	0.79277600	-1.59677700
Mo	-0.28821600	0.88750300	0.10128200
O	-1.43643500	2.28654200	0.79953600
O	0.77755900	2.56530400	0.05749800
C	1.73574200	2.89605400	-0.92495800
H	2.66511600	2.33568100	-0.76821200
H	1.35963600	2.62978100	-1.92291300
C	2.01197000	4.39849700	-0.84966600
H	1.10138100	4.95523700	-1.07718200
H	-0.90160300	3.09278600	0.84308400
H	2.32409400	4.66095100	0.16991100
O	2.97477700	4.79161200	-1.81960500
H	3.81318500	4.37795900	-1.59119600
C	0.94918400	-0.30909700	4.28607000
H	0.99819400	-1.37132700	4.53952700
H	1.72426100	0.20302700	4.86068200
H	-0.02771600	0.08296500	4.56252100
C	3.98534100	-1.49867300	3.97606300
H	3.99356400	-0.65991900	4.67793800
H	3.30882900	-2.25801900	4.37784800
H	4.98960400	-1.91957100	3.92859300
C	-3.29215000	-4.21499900	-1.73789500
H	-2.61649800	-4.26824200	-2.59631900
H	-2.96542600	-4.96627600	-1.01312900
H	-4.29804200	-4.47121100	-2.07011300
C	-0.23387000	-3.63844900	-0.49469300
H	-0.80522700	-4.40045700	0.03939900
H	-0.20812300	-3.92185600	-1.55080800
H	0.78467000	-3.60406100	-0.11278100
C	4.48753000	-0.77122400	-0.76837900
C	5.87511100	-0.95094500	-0.74572100
C	3.81786600	-0.63364400	-1.98977500
C	6.58508900	-0.98608200	-1.94026800
H	6.37278100	-1.06944800	0.20580200
C	4.54785400	-0.66521800	-3.17534500
H	2.74718800	-0.50104100	-2.00897200
C	5.92896100	-0.84016500	-3.16101100
H	7.65984000	-1.12616800	-1.91304100
H	4.02291500	-0.55508300	-4.11744300
H	6.48740400	-0.86478500	-4.08951000
C	-5.22600300	-0.03869400	-0.24803200
C	-6.53156700	-0.44515300	-0.54473300
C	-4.98450400	1.24297500	0.26176500
C	-7.59010000	0.43035000	-0.33256000
H	-6.69604900	-1.43671600	-0.93968900
C	-6.06065500	2.10267500	0.46644900
H	-3.97952900	1.56141200	0.49524000
C	-7.36325400	1.70833000	0.17364200
H	-8.59830600	0.10722500	-0.56634900
H	-5.86773800	3.09409400	0.86039300
H	-8.19172100	2.38788800	0.33711600

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C	-2.69619400	-2.47561200	-2.15732300
C	-0.28338400	-1.76059200	-1.43823300
C	-1.68403100	-1.71461500	-1.46785000
C	-2.41012800	-0.87317800	-0.57515100
C	0.81121400	-0.97157600	2.47884700
C	2.10177400	-1.16339800	1.93461200
C	2.58516200	-0.32741000	0.89570300
C	3.19866300	-2.04105300	2.23587800
N	-3.89160600	-2.14975800	-1.73940200
N	-3.72585300	-1.18347300	-0.75401600
N	3.86874900	-0.72414700	0.65004500
N	4.23037100	-1.78303400	1.47048500
O	0.40930600	-0.94073200	-0.75801100

O	0.00339900	-0.14785900	1.97632200
O	-1.97791000	-0.01742900	0.26318400
O	2.01971100	0.65659100	0.30098400
O	-0.60040000	1.32533700	-1.56239800
Mo	-0.05219500	1.06820400	0.03587200
O	-1.23036400	2.12273500	1.19173800
H	-2.00055600	1.57726000	1.40768100
O	0.85151100	2.74546300	-0.02009400
C	0.62068400	3.88717500	-0.82804200
H	1.60903400	4.25944200	-1.12541200
H	0.05541500	3.58293900	-1.71973500
C	-0.13092500	4.98100400	-0.07039700
H	-0.08812800	5.89362700	-0.67436700
H	0.40015400	5.17671600	0.87255700
O	-1.49113900	4.68248400	0.13559800
H	-1.52900900	3.85671600	0.64776500
C	0.34244100	-1.73119700	3.69623000
H	0.23719800	-2.79402600	3.45944100
H	1.05854800	-1.64521200	4.51592700
H	-0.62359200	-1.33899000	4.00880300
C	3.29396600	-3.14697800	3.23928700
H	3.18815200	-2.77422500	4.26206100
H	2.51841100	-3.90205700	3.08227600
H	4.26919800	-3.62492100	3.14692800
C	0.50644000	-2.79776100	-2.19630600
H	0.09797500	-3.79931000	-2.05546300
H	0.47164900	-2.56856700	-3.26585300
H	1.54377800	-2.76818400	-1.86824700
C	-2.55256100	-3.50078600	-3.23689000
H	-1.99198700	-3.10802300	-4.08962200
H	-2.03124700	-4.39409400	-2.88112300
H	-3.54498300	-3.79623100	-3.57700300
C	4.80594400	-0.23082700	-0.29989000
C	5.91100000	-1.02485500	-0.62461100
C	4.64347500	1.02504200	-0.89470500
C	6.84355500	-0.56299500	-1.54615100
H	6.02653600	-1.98488400	-0.14271100
C	5.58513300	1.46696100	-1.82030200
H	3.79527300	1.64010100	-0.63555800
C	6.68586900	0.68185600	-2.15229800
H	7.69811500	-1.18370800	-1.79100600
H	5.45449400	2.44084800	-2.27842700
H	7.41473100	1.03683900	-2.87163700
C	-4.87000500	-0.63512800	-0.11382200
C	-4.80064000	-0.18040500	1.20543400
C	-6.07397300	-0.57351100	-0.81952100
C	-5.93658500	0.35851100	1.80344900
H	-3.87322500	-0.25706200	1.75446600
C	-7.20230800	-0.04306700	-0.20449200
H	-6.10980900	-0.94881700	-1.83269200
C	-7.13871800	0.43127900	1.10462700
H	-5.87942700	0.71363800	2.82600800
H	-8.13459400	0.00459100	-0.75546500
H	-8.01966800	0.84989000	1.57693400

TS(4-5)

C	2.82958800	2.86618400	-1.44711200
C	0.38223000	2.34239200	-0.64178400
C	1.77660200	2.10909600	-0.83739700
C	2.42729500	1.00198900	-0.24677600
C	-1.37087500	0.51445800	2.64120900
C	-2.61746200	0.56838600	1.98971200
C	-2.78528600	0.03573400	0.68449900
C	-3.91266100	1.08485200	2.34146200
N	3.99388700	2.29023800	-1.25665700
N	3.76014500	1.14962300	-0.51195200
N	-4.08767300	0.26288000	0.34306700
N	-4.77060400	0.90037700	1.36988100
O	-0.35825400	1.48305200	-0.12433700
O	-0.36238600	-0.01296300	2.09586300

O	1.93774900	0.04152400	0.46438500
O	-1.95792800	-0.57190800	-0.07418400
O	0.31472300	-0.63805800	-1.56282500
Mo	0.11084200	-0.92939300	0.10060900
O	1.14048100	-2.00621000	1.78835000
H	1.55601600	-1.32823400	2.33106900
O	-0.61112600	-2.68771800	-0.09276000
C	-0.07636200	-3.56755800	-1.05595700
H	-0.62525500	-4.51255100	-1.00971800
H	-0.19216700	-3.11673800	-2.05080400
C	1.41703000	-3.71955500	-0.71910700
H	1.96693100	-4.08199100	-1.59421800
H	1.53706900	-4.43462100	0.10383300
O	1.89079200	-2.44822200	-0.33946700
H	1.80416200	-2.35653800	0.84712000
C	-1.16781000	1.07772000	4.02631200
H	-1.40815600	2.14357500	4.04661500
H	-1.82111200	0.57715200	4.74516100
H	-0.12998400	0.93539700	4.32158100
C	-4.36434400	1.76665600	3.59418100
H	-4.24208900	1.12301900	4.46995800
H	-3.80139400	2.68595600	3.77909100
H	-5.41955000	2.02145800	3.49612900
C	-0.24737000	3.66128400	-1.03087700
H	0.25824700	4.49872300	-0.54439800
H	-0.16868200	3.81033200	-2.11123100
H	-1.29838500	3.64968400	-0.74762100
C	2.76951300	4.13190400	-2.24338200
H	2.11688600	4.02578000	-3.11449800
H	2.39406400	4.96948800	-1.64917000
H	3.77337400	4.37814900	-2.58941200
C	-4.78491700	-0.08143000	-0.84785000
C	-6.18100300	-0.14953000	-0.81119600
C	-4.09897800	-0.33015600	-2.04113400
C	-6.88472700	-0.47099600	-1.96621700
H	-6.69227400	0.05997300	0.11741200
C	-4.82054500	-0.65714200	-3.18593600
H	-3.02150600	-0.27109400	-2.06966300
C	-6.21082300	-0.73026300	-3.15798000
H	-7.96713400	-0.52150000	-1.93044400
H	-4.28404600	-0.84988500	-4.10809700
H	-6.76348000	-0.98347000	-4.05532000
C	4.86810500	0.33071500	-0.15259700
C	4.78672300	-0.58897000	0.89634200
C	6.06320500	0.47677400	-0.86451300
C	5.89815200	-1.36327100	1.21645700
H	3.86463100	-0.70457600	1.44224300
C	7.16557200	-0.29965800	-0.52723300
H	6.11096700	1.20124500	-1.66428900
C	7.09072300	-1.22524300	0.51175500
H	5.82576900	-2.07741400	2.02891500
H	8.08761000	-0.18004100	-1.08485400
H	7.95195600	-1.83081700	0.76918000

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C	3.13102300	3.06544300	1.16787000
C	0.65078900	2.19945900	1.28256200
C	2.01881300	2.18448700	0.94501000
C	2.59204000	1.00173900	0.41544300
C	-1.38905000	-2.00579500	1.61832400
C	-2.65100800	-1.49639000	1.26424300
C	-2.81148900	-0.41961300	0.33340100
C	-3.99151600	-1.78024200	1.71375400
N	4.25537500	2.49233400	0.81368500
N	3.93618500	1.21747700	0.37167900
N	-4.15019600	-0.15258000	0.28626100
N	-4.85734000	-0.98844600	1.13920100
O	-0.12512300	1.27480800	0.91922700
O	-0.32691300	-1.57835800	1.06845500
O	2.02585300	-0.09843600	0.06938500

O	-1.94418100	0.24630800	-0.31927600
O	0.27137200	0.96397200	-1.80326700
Mo	0.05974900	-0.32710400	-0.71295500
O	2.27633000	-3.07143300	1.01110800
H	1.63580200	-2.51383400	1.46951600
O	-1.12515600	-1.49034200	-1.76148600
C	-0.58350600	-2.37710600	-2.71528000
H	-1.31078100	-3.17123900	-2.91309200
H	-0.37671700	-1.83590000	-3.64786200
C	0.70037900	-2.87796700	-2.07895800
H	1.43510900	-3.23761800	-2.80640100
H	0.50213300	-3.66717700	-1.34382200
O	1.23262300	-1.74473300	-1.41520900
H	2.25848300	-2.67001800	0.13037800
C	-1.19299300	-3.05696900	2.67993900
H	-1.01192900	-2.56516800	3.64171700
H	-2.05244900	-3.71375800	2.79046600
H	-0.30850600	-3.64438600	2.43058400
C	-4.49277700	-2.80255700	2.68543200
H	-4.27752100	-3.82024900	2.34676800
H	-4.04455200	-2.67698100	3.67450500
H	-5.57335200	-2.69403300	2.77772400
C	0.04588000	3.29173600	2.12957900
H	0.56734600	3.37949500	3.08555900
H	0.13301900	4.25255900	1.61497500
H	-1.00606400	3.07151600	2.30073000
C	3.15065900	4.46661500	1.69074400
H	2.52157900	5.12709500	1.08699100
H	2.79077400	4.51881400	2.72216300
H	4.17421900	4.84037600	1.66426100
C	-4.86226000	0.83377100	-0.45547300
C	-6.23537700	0.97822000	-0.22501400
C	-4.22278100	1.64326100	-1.40176200
C	-6.95898600	1.92664000	-0.93839300
H	-6.71428200	0.34315800	0.50529600
C	-4.96599800	2.58743800	-2.10515200
H	-3.16518500	1.53687100	-1.58267900
C	-6.33164300	2.73754600	-1.88159100
H	-8.02208500	2.02944700	-0.75197200
H	-4.46267100	3.20899500	-2.83703000
H	-6.90011700	3.47583200	-2.43516100
C	4.97913500	0.35394600	-0.07153100
C	4.89829300	-1.02403600	0.13290500
C	6.09629300	0.91900600	-0.69090400
C	5.93960800	-1.83588500	-0.31008300
H	4.04401100	-1.46344200	0.62877100
C	7.13169300	0.09495800	-1.11736400
H	6.14320400	1.99176900	-0.81830600
C	7.05598900	-1.28502400	-0.93438000
H	5.87431100	-2.90583100	-0.14905500
H	7.99866900	0.53455200	-1.59738600
H	7.86423700	-1.92436600	-1.27072300

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C	3.21816800	3.04711700	0.77426200
C	0.72285200	2.23244100	0.95228500
C	2.09863400	2.15764700	0.64830700
C	2.66442200	0.91480500	0.27534200
C	-1.35289800	-1.61747400	2.05145000
C	-2.59833800	-1.13239400	1.61188100
C	-2.74806900	-0.34919000	0.42462200
C	-3.92953600	-1.22179500	2.15401200
N	4.33918900	2.42686600	0.49995300
N	4.01464400	1.11230400	0.19825600
N	-4.08028000	-0.04989800	0.33492000
N	-4.78842700	-0.58602700	1.40195900
O	-0.05755800	1.27409600	0.71158500
O	-0.29947100	-1.45088800	1.36961600
O	2.09445400	-0.21760900	0.09714300
O	-1.88074700	0.07515800	-0.40372700

O	0.32124100	0.44635200	-1.92730700
Mo	0.12940900	-0.61326500	-0.60677200
O	-1.06615600	-1.97759400	-1.37023400
C	-0.53263200	-3.06826400	-2.08560700
H	-1.24961800	-3.89571500	-2.06110500
H	-0.35423900	-2.77501400	-3.12858100
C	0.77681900	-3.38095600	-1.37920000
H	1.49710400	-3.91058700	-2.01142200
H	0.60414400	-3.96058900	-0.46332400
O	1.30221700	-2.11465300	-1.04509200
C	3.24868900	4.50133000	1.12263300
H	2.62802900	5.08807600	0.43947100
H	2.88396300	4.68179900	2.13795400
H	4.27533600	4.86119900	1.05577700
C	0.11723300	3.44583900	1.61521400
H	0.61758400	3.66477400	2.56152300
H	0.23240600	4.32042000	0.96926100
H	-0.94197300	3.26723900	1.79010900
C	-1.19255300	-2.36024400	3.35501000
H	-1.54269300	-1.75539500	4.19457500
H	-1.77673800	-3.28394800	3.34830300
H	-0.14018800	-2.60074000	3.49459000
C	-4.42007000	-1.92175700	3.38239500
H	-4.20387400	-2.99325300	3.34915700
H	-3.95902300	-1.52014500	4.28907700
H	-5.49938000	-1.78855900	3.45487100
C	-4.77937400	0.72165700	-0.63641000
C	-6.12341800	1.03311800	-0.40002200
C	-4.15669700	1.15731600	-1.81217200
C	-6.83495600	1.77524800	-1.33541500
H	-6.59062800	0.68333700	0.50859500
C	-4.88680400	1.90114800	-2.73528800
H	-3.12152900	0.91908000	-1.99836500
C	-6.22363300	2.21541600	-2.50740400
H	-7.87580600	2.00989300	-1.14243200
H	-4.39660200	2.23363200	-3.64333600
H	-6.78241100	2.79454300	-3.23346200
C	5.05754600	0.19379700	-0.11442500
C	6.38360800	0.61613400	0.03193500
C	4.77705000	-1.10069000	-0.56850700
C	7.42248200	-0.25443800	-0.27607900
H	6.57874800	1.62039600	0.37800900
C	5.83377300	-1.95653500	-0.86848700
H	3.75528800	-1.43091400	-0.68110700
C	7.15634600	-1.54554300	-0.72676000
H	8.44654000	0.08270300	-0.16090200
H	5.61125400	-2.95778900	-1.22022800
H	7.96952000	-2.22135000	-0.96546300

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C	-3.93787600	-2.05827900	-2.31523700
C	-1.40175700	-2.23038400	-1.62909000
C	-2.72113800	-1.72541700	-1.63035600
C	-3.09769500	-0.74655600	-0.68229800
C	0.60617300	-1.97533400	2.38464100
C	1.90620600	-2.01213800	1.85105600
C	2.26468800	-1.34426300	0.63602800
C	3.10954000	-2.69419700	2.25630100
N	-4.94221600	-1.35707300	-1.84881000
N	-4.43946500	-0.54852100	-0.84070200
N	3.57743200	-1.65787700	0.41018800
N	4.08077700	-2.48090900	1.40879200
O	-0.50586500	-1.72000900	-0.91029200
O	-0.30820000	-1.26764900	1.86542300
O	-2.39560800	-0.16117600	0.21697400
O	1.57530000	-0.62815700	-0.15491200
O	-0.18317300	1.00932800	-1.21658000
Mo	-0.34047700	0.25863300	0.30620800
O	1.03023300	1.17230000	1.38437600
C	0.66229200	2.06767500	2.41391300

H	0.51569800	1.51095400	3.34837900
H	1.46188200	2.80290600	2.54507600
C	-0.63875600	2.68825400	1.93559700
H	-0.44513600	3.49024300	1.21310100
H	-1.26222900	3.07180100	2.74967500
O	-1.31876000	1.62268900	1.30280300
P	2.33597000	4.55848600	-0.29744400
C	3.62113300	3.24938300	0.00762900
H	3.12047700	2.30241100	0.22105600
H	4.29254900	3.11418000	-0.84581700
H	4.21691200	3.52141400	0.88302200
C	1.71881400	4.02057300	-1.96719100
H	1.15728300	3.08900500	-1.86707400
H	1.04116600	4.77948900	-2.36640800
H	2.53631000	3.86753800	-2.67916800
C	3.43193700	5.97586300	-0.80773000
H	3.99399600	6.33430400	0.05815100
H	4.13905000	5.69533800	-1.59501500
H	2.81468400	6.80250500	-1.16801100
C	-1.00585800	-3.42511200	-2.46289700
H	-1.61853000	-4.29454600	-2.21232100
H	-1.15653400	-3.20926600	-3.52396700
H	0.04401200	-3.65193300	-2.28739500
C	-4.17195300	-3.01991600	-3.43676200
H	-3.54841600	-2.78316300	-4.30357700
H	-3.94846700	-4.04863300	-3.14005900
H	-5.21841000	-2.96662200	-3.73694000
C	0.20763700	-2.78557500	3.59374100
H	0.26704300	-3.85493800	3.37354800
H	0.86980600	-2.58570000	4.43833700
H	-0.81594300	-2.53299800	3.86456500
C	3.37132500	-3.55116200	3.45490000
H	3.22899700	-2.99481000	4.38601100
H	2.71011100	-4.42126000	3.48569000
H	4.40292500	-3.90084500	3.41644100
C	-5.32700700	0.30926300	-0.12907500
C	-6.70410600	0.12538700	-0.29281300
C	-4.84463800	1.32469200	0.70499900
C	-7.59445300	0.95696800	0.37643600
H	-7.05433700	-0.65868700	-0.94804700
C	-5.75477700	2.14340000	1.36876400
H	-3.78226200	1.46664900	0.83771300
C	-7.12721400	1.96936400	1.21178500
H	-8.66010800	0.80869900	0.24249700
H	-5.37746800	2.92954500	2.01313300
H	-7.82471400	2.61558400	1.73220800
C	4.43013000	-1.27422400	-0.66186700
C	5.81002400	-1.45597400	-0.51580100
C	3.91496600	-0.73844400	-1.84772000
C	6.66589800	-1.09888600	-1.55096100
H	6.18851000	-1.88125500	0.40223300
C	4.78960000	-0.38250000	-2.87126100
H	2.85111900	-0.59954400	-1.96177500
C	6.16371300	-0.55837800	-2.73319500
H	7.73346300	-1.24339000	-1.42848000
H	4.38340600	0.03269300	-3.78672500
H	6.83542100	-0.27995300	-3.53699300

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C	-2.89162800	-2.18382200	-2.53695400
C	-0.40693100	-1.45274400	-2.04942100
C	-1.80512600	-1.51973100	-1.87028500
C	-2.42232100	-0.72892300	-0.86768700
C	1.86990600	-2.58374900	1.04058700
C	3.04218600	-1.91402600	0.63911500
C	3.05281100	-0.53822400	0.24540200
C	4.41020900	-2.34355800	0.49234400
N	-4.04332900	-1.85875900	-2.00042400
N	-3.76472900	-0.97283300	-0.96779300
N	4.35603800	-0.25596300	-0.08717800

N	5.17066600	-1.37043900	0.06537800
O	0.33275200	-0.83077400	-1.24029700
O	0.74803000	-2.00540000	1.11344300
O	-1.90138600	0.12225600	-0.07524300
O	2.11625900	0.30886900	0.16368000
O	-0.03172700	1.83081600	0.39788700
Mo	0.07885500	0.08889700	0.82346500
O	1.04205000	0.48409200	2.51499200
C	0.61850200	-0.21456200	3.65708300
H	0.95489000	-1.26038700	3.63622400
H	1.02590500	0.27179100	4.55101400
C	-0.90436600	-0.16163500	3.59354400
H	-1.27217400	0.82017900	3.92485100
H	-1.38698100	-0.94287000	4.19206700
O	-1.22502000	-0.34796700	2.23118900
P	-1.55549000	2.88165100	-0.48378100
C	-2.99416400	2.97527500	-1.66545400
H	-3.78663200	2.31356700	-1.31455500
H	-3.38033600	3.99794900	-1.73985000
H	-2.67468500	2.64129600	-2.65413600
C	-2.26916900	3.51043600	1.08228300
H	-2.99513700	2.78719700	1.45692600
H	-1.46797200	3.61400400	1.81446000
H	-2.76259500	4.47549000	0.93754200
C	-0.45861900	4.23011200	-1.07371900
H	-0.09096100	3.98921600	-2.07325900
H	-0.98314800	5.18908400	-1.10941500
H	0.39637400	4.30324900	-0.40189000
C	0.27765300	-2.11076600	-3.22384800
H	0.15869200	-3.19672700	-3.16889900
H	-0.15925200	-1.78048300	-4.16909600
H	1.33781000	-1.86475600	-3.20355400
C	-2.86145100	-3.15945300	-3.67093500
H	-2.43695200	-2.71541500	-4.57604400
H	-2.26123300	-4.04012300	-3.42460100
H	-3.87935100	-3.48353100	-3.88805100
C	1.87984600	-4.04999200	1.41159500
H	2.21504700	-4.66362900	0.57171400
H	2.55894100	-4.23769300	2.24669200
H	0.87072800	-4.34578300	1.69361600
C	5.03501200	-3.67689600	0.76326400
H	4.91309100	-3.97570600	1.80821800
H	4.59896900	-4.46479300	0.14265600
H	6.10106400	-3.61392800	0.54444900
C	-4.82395900	-0.43345400	-0.19286300
C	-6.09612300	-0.32837900	-0.76191100
C	-4.60309700	-0.03385000	1.13037300
C	-7.14602200	0.18610400	-0.00786300
H	-6.24583800	-0.66640500	-1.77804800
C	-5.66464900	0.48843300	1.86517300
H	-3.61958900	-0.13997600	1.56975400
C	-6.93580800	0.60295500	1.30500100
H	-8.13224200	0.26155500	-0.45195200
H	-5.49504200	0.79315300	2.89197400
H	-7.75628400	1.00398100	1.88887800
C	4.92730700	0.95394000	-0.56200000
C	6.23514100	0.92786200	-1.06208300
C	4.21780700	2.16136000	-0.52763600
C	6.82288200	2.09932000	-1.52494900
H	6.77173600	-0.00945700	-1.07115100
C	4.82446600	3.32286100	-0.99835000
H	3.21136100	2.18279400	-0.13957400
C	6.12342900	3.30413200	-1.49907200
H	7.83664700	2.06624000	-1.90867100
H	4.26919000	4.25389100	-0.96548800
H	6.58589600	4.21525800	-1.86113200

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C	-3.03606900	-2.29605400	-2.25448000
C	-0.50568600	-1.65542800	-1.89079700

C	-1.91081800	-1.60089800	-1.69465200
C	-2.47722300	-0.60094500	-0.85657400
C	1.66117200	-2.64772300	1.09651000
C	2.83081800	-2.04731300	0.59426800
C	2.88481000	-0.65532400	0.30791500
C	4.15736700	-2.52781300	0.30600800
N	-4.16880800	-1.80664200	-1.80823400
N	-3.83634900	-0.77226600	-0.94424400
N	4.17323100	-0.39791300	-0.08947500
N	4.93584400	-1.55681800	-0.10204600
O	0.28013100	-0.97569700	-1.18884500
O	0.58570100	-1.98576000	1.24854500
O	-1.90157800	0.35078100	-0.23472900
O	1.96799400	0.22107200	0.38110800
O	-0.04545100	2.07264500	0.57137000
Mo	-0.03630000	-0.00815200	0.97979400
O	0.56818100	0.55186500	2.76693400
C	0.07528500	-0.26729800	3.80208500
H	0.56499600	-1.25115500	3.79109300
H	0.26171300	0.20688300	4.77278700
C	-1.41871700	-0.43511800	3.51128200
H	-1.99285300	0.42902300	3.87424400
H	-1.83753900	-1.34202800	3.96245900
O	-1.55470200	-0.49899400	2.10152000
P	-0.48911900	3.00180000	-0.56509700
C	-0.34666900	2.28635700	-2.22741000
H	-1.09276200	1.50299100	-2.34246500
H	-0.48689900	3.05984300	-2.98601100
H	0.64507700	1.84270200	-2.32953900
C	-2.18735000	3.59880800	-0.34447700
H	-2.85421500	2.73714000	-0.32595300
H	-2.25738900	4.12203800	0.61099000
H	-2.47025200	4.27838100	-1.15165500
C	0.59184700	4.46254500	-0.54506500
H	1.61548200	4.14828800	-0.75594000
H	0.27631500	5.19754600	-1.28876400
H	0.56084300	4.91213400	0.44864000
C	0.10017400	-2.51282000	-2.98217700
H	1.18280200	-2.39708500	-2.96505900
H	-0.15375700	-3.56514800	-2.82875900
H	-0.28282100	-2.22607800	-3.96526600
C	-3.07137800	-3.46151700	-3.19349400
H	-2.61172300	-3.22268800	-4.15695200
H	-2.54000000	-4.32449200	-2.78122700
H	-4.10989700	-3.74525300	-3.36569300
C	1.60630500	-4.09465600	1.51878000
H	1.89283100	-4.75540800	0.69698800
H	2.29419300	-4.28395500	2.34788200
H	0.59183000	-4.33379000	1.83397100
C	4.71443600	-3.91327900	0.40547000
H	4.65938000	-4.29963700	1.42708100
H	4.17431700	-4.61215900	-0.24017700
H	5.76034500	-3.89589800	0.09853300
C	-4.86316100	-0.02223300	-0.31931500
C	-6.10457800	0.09534100	-0.95091500
C	-4.64513200	0.57437500	0.92771100
C	-7.12221400	0.81993000	-0.33895100
H	-6.25715000	-0.39754000	-1.90123300
C	-5.67132300	1.30671100	1.51886900
H	-3.69110400	0.44230200	1.42058000
C	-6.91006900	1.43607600	0.89306100
H	-8.08510500	0.90367700	-0.83064600
H	-5.50294400	1.76435600	2.48765300
H	-7.70537400	2.00116700	1.36570600
C	4.76068200	0.82987300	-0.47949500
C	5.91256900	0.80950600	-1.27310000
C	4.22045000	2.05180800	-0.05995200
C	6.51350100	2.00552800	-1.64959400
H	6.32598200	-0.14429600	-1.56892100
C	4.83495200	3.23921900	-0.44999100
H	3.34114200	2.06324600	0.56760100

C	5.97841300	3.22724500	-1.24571500
H	7.40708300	1.97929800	-2.26328900
H	4.42281000	4.18276100	-0.10833300
H	6.45203500	4.15696800	-1.53929000

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C	-3.36206500	1.09879600	2.65985200
C	-0.80915000	0.79044900	2.18674900
C	-2.18751200	0.78308600	1.88661200
C	-2.69630700	0.44876700	0.59633800
C	0.82366000	2.80136000	-0.71175300
C	2.17312900	2.46124300	-0.46133900
C	2.63310400	1.11410200	-0.34433100
C	3.35671400	3.26450600	-0.28160300
N	-4.45156700	0.96797100	1.94818700
N	-4.06055200	0.57814000	0.67500900
N	3.98839200	1.20041500	-0.13971400
N	4.41511700	2.51934800	-0.08981200
O	0.07172900	0.41452000	1.35932900
O	-0.08966900	1.94176700	-0.84802600
O	-2.07478700	0.12925800	-0.46507000
O	2.01725100	0.00165900	-0.40498700
O	-0.86121000	-1.91960300	0.56108400
Mo	-0.07260600	-0.23320300	-0.76459800
O	0.73877700	-1.91334200	-1.53624100
C	0.45095600	-2.20349600	-2.88694700
H	1.21835900	-2.87508400	-3.29326500
H	-0.53130200	-2.69363700	-2.98437400
C	0.43237700	-0.85753300	-3.59044500
H	-0.12591600	-0.86286100	-4.53261900
H	1.45159300	-0.49671600	-3.78453200
O	-0.20222000	0.01810400	-2.67362600
P	-0.08881300	-3.12244600	1.09511100
C	-0.84467800	-3.65807500	2.66446100
H	-1.89864200	-3.88444800	2.49469000
H	-0.34296800	-4.54221700	3.06393200
H	-0.77668800	-2.84540000	3.38920500
C	-0.16161600	-4.57249800	-0.00056100
H	-1.20611100	-4.79385800	-0.22770400
H	0.35996500	-4.32401100	-0.92315800
H	0.30024300	-5.44316400	0.47080900
C	1.66016300	-2.79248900	1.43442000
H	1.73619600	-1.96751800	2.14367700
H	2.15341200	-3.67967600	1.83795100
H	2.13037100	-2.48139600	0.50265200
C	-0.29559800	1.26399100	3.52947900
H	-0.64004700	2.27682000	3.75068600
H	-0.65052800	0.61561600	4.33536000
H	0.79315200	1.25003900	3.51255200
C	-3.48622900	1.52073000	4.09121700
H	-3.05799500	0.77925400	4.77199100
H	-2.97945500	2.47125800	4.28055000
H	-4.54311300	1.64075600	4.32991800
C	0.38169000	4.24146300	-0.83633300
H	0.69385100	4.83172900	0.02733700
H	0.82121400	4.69919200	-1.72689000
H	-0.70287300	4.26573400	-0.92559000
C	3.52425900	4.75240700	-0.29055800
H	3.19496400	5.19254600	-1.23558900
H	2.95450700	5.23085900	0.51126700
H	4.58003100	4.98439000	-0.14937700
C	-5.05038700	0.36419300	-0.31875700
C	-6.39389900	0.30674900	0.07201500
C	-4.71087500	0.22320300	-1.67032200
C	-7.38412200	0.10691600	-0.88255100
H	-6.63936300	0.42851600	1.11689100
C	-5.71804900	0.02060200	-2.61034200
H	-3.67772100	0.27336600	-1.97800100
C	-7.05550100	-0.03988700	-2.22889500
H	-8.42099900	0.06534800	-0.56746200

H	-5.44505400	-0.08498200	-3.65449000
H	-7.83140300	-0.19602900	-2.96955400
C	4.93903800	0.16085400	0.02002800
C	6.14197200	0.44243400	0.67694400
C	4.70409400	-1.12156900	-0.48988600
C	7.09763600	-0.55594600	0.82718400
H	6.31368000	1.44384200	1.04539900
C	5.67025500	-2.11077000	-0.32368600
H	3.77931800	-1.33311600	-1.00613100
C	6.86773100	-1.83885100	0.33327100
H	8.02771700	-0.32720100	1.33555500
H	5.48400900	-3.10102900	-0.72489900
H	7.61580500	-2.61417700	0.45269500

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C	-3.66810400	-2.02366300	-1.93288600
C	-1.06322900	-1.66798900	-1.93623900
C	-2.41354200	-1.43424300	-1.55653300
C	-2.76203700	-0.43834200	-0.61088300
C	1.06322800	-1.66798700	1.93623900
C	2.41354100	-1.43424200	1.55653300
C	2.76203700	-0.43834200	0.61088300
C	3.66810300	-2.02366200	1.93288800
N	-4.66503000	-1.45960800	-1.29465300
N	-4.11789100	-0.48698300	-0.47470300
N	4.11789100	-0.48698400	0.47470400
N	4.66503000	-1.45960700	1.29465500
O	-0.13389600	-0.98020100	-1.44918000
O	0.13389600	-0.98020000	1.44918000
O	-2.01888300	0.39718300	0.03163800
O	2.01888300	0.39718200	-0.03164000
O	-0.12260600	1.96717200	1.27114900
Mo	0.00000000	0.70954800	0.00000000
C	-0.06219600	3.72061900	0.70489900
C	0.06220000	3.72061900	-0.70490000
O	0.12260700	1.96717200	-1.27115000
H	0.79979500	3.98775400	1.30388300
H	1.01395200	3.99113000	-1.14445000
H	-0.79979000	3.98775500	-1.30388400
H	-1.01394800	3.99113200	1.14444900
C	-3.95728000	-3.13053200	-2.89744600
H	-3.60818400	-2.88878600	-3.90507800
H	-3.47565100	-4.06519500	-2.59650600
H	-5.03432700	-3.29394000	-2.93328100
C	-0.68959200	-2.73642000	-2.93312700
H	-1.05561500	-3.71565300	-2.61552700
H	-1.13354000	-2.52026100	-3.90869900
H	0.39420100	-2.76473600	-3.03148000
C	0.68959100	-2.73641700	2.93312900
H	1.05562100	-3.71564900	2.61553500
H	1.13353200	-2.52025300	3.90870200
H	-0.39420300	-2.76473800	3.03147500
C	3.95728000	-3.13052900	2.89745000
H	3.60818000	-2.88878300	3.90508000
H	3.47565300	-4.06519300	2.59650800
H	5.03432700	-3.29393500	2.93328700
C	4.98328900	0.31024500	-0.32811200
C	6.35205200	0.30449400	-0.04015300
C	4.49200000	1.07455900	-1.39212700
C	7.22193400	1.06369300	-0.81407500
H	6.71265300	-0.30104700	0.77851500
C	5.37902400	1.83174600	-2.15282900
H	3.43671000	1.07969500	-1.61756600
C	6.74264200	1.83309800	-1.87228900
H	8.28137300	1.05308500	-0.58407100
H	4.99222200	2.42160300	-2.97608300

H	7.42441500	2.42509200	-2.47182900
C	-4.98328900	0.31024600	0.32811200
C	-6.35205200	0.30449400	0.04015300
C	-4.49200000	1.07456100	1.39212600
C	-7.22193400	1.06369400	0.81407500
H	-6.71265400	-0.30104800	-0.77851400
C	-5.37902400	1.83174900	2.15282800
H	-3.43671000	1.07969700	1.61756400
C	-6.74264200	1.83310000	1.87228700
H	-8.28137300	1.05308600	0.58407100
H	-4.99222100	2.42160700	2.97608000
H	-7.42441400	2.42509500	2.47182700

TS(1-9)

C	3.28317100	-1.77281800	2.36293800
C	0.71682200	-1.27037200	2.13884100
C	2.07958800	-1.29132700	1.73922000
C	2.51664500	-0.73968700	0.50337000
C	-1.72633400	-2.64167300	-1.00346200
C	-2.97820500	-2.03074000	-0.75365500
C	-3.12177600	-0.64399200	-0.45114100
C	-4.32041000	-2.54947800	-0.70575200
N	4.33189500	-1.54820500	1.61074200
N	3.87189200	-0.92107200	0.46169100
N	-4.45848900	-0.43666200	-0.24667100
N	-5.18103000	-1.60994600	-0.41061200
O	-0.17282900	-0.77701500	1.40455600
O	-0.64618200	-1.99297400	-0.98459500
O	1.85898400	-0.15948200	-0.43117100
O	-2.25249300	0.29195300	-0.36482000
O	-0.00132600	1.81920900	0.02121200
O	-0.06862100	0.41073100	-2.36741700
Mo	-0.18394800	0.15251300	-0.68957300
P	1.67354000	2.93287400	0.41499500
C	1.69325100	3.78663700	-1.20965900
H	2.26553600	3.18814500	-1.92085500
H	0.67051300	3.86662200	-1.57788000
H	2.14094000	4.78186600	-1.13735700
C	3.44876700	3.12368600	0.97743200
H	3.55906800	2.70772200	1.98050000
H	4.10099800	2.56819000	0.30179600
H	3.75254200	4.17657400	0.99031000
C	0.79067100	4.08415300	1.53957500
H	-0.26382800	4.09849900	1.26598000
H	0.87694600	3.72644200	2.56768700
H	1.20183200	5.09574800	1.48126300
C	-1.61254500	-4.11696500	-1.30655200
H	-2.03368000	-4.71765000	-0.49707400
H	-2.15795100	-4.36624800	-2.22017300
H	-0.56115300	-4.36669800	-1.43685600
C	-4.82574100	-3.93937700	-0.93701900
H	-4.57674200	-4.29910700	-1.93912300
H	-4.40619600	-4.64880700	-0.21815000
H	-5.91031000	-3.93927500	-0.82841000
C	3.47388900	-2.46423600	3.67678600
H	4.53128300	-2.69848600	3.80000400
H	3.15719600	-1.83688800	4.51479900
H	2.90362800	-3.39575100	3.72906000
C	0.27515900	-1.83670100	3.46834300
H	0.49630600	-2.90584400	3.52444100
H	0.79728900	-1.35037200	4.29574800
H	-0.79719800	-1.68323800	3.57563700
C	4.80710500	-0.51280200	-0.52733900
C	6.15796700	-0.41896600	-0.17375300
C	4.40274300	-0.21777500	-1.83491800
C	7.09410200	-0.02558500	-1.12327300
H	6.45240000	-0.66758800	0.83565600
C	5.35491900	0.18021600	-2.77030500
H	3.36304700	-0.29823200	-2.11322400
C	6.69995900	0.28047300	-2.42456900

H	8.13862300	0.04214300	-0.84049800
H	5.03447100	0.40473500	-3.78139300
H	7.43327400	0.58791200	-3.16106600
C	-5.15902500	0.76123800	0.07130600
C	-6.55879600	0.73642600	0.06272400
C	-4.48338200	1.94403200	0.39603100
C	-7.27281200	1.88710400	0.37527100
H	-7.06365400	-0.18556600	-0.18456900
C	-5.21805300	3.08619200	0.70385000
H	-3.40508700	1.96558200	0.40201700
C	-6.60983900	3.06961600	0.69664600
H	-8.35661300	1.85548300	0.36471100
H	-4.68713400	3.99837100	0.95262600
H	-7.17081300	3.96521900	0.93775400

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C	3.45051500	-0.84133600	2.83935400
C	0.87205800	-0.73692300	2.41190100
C	2.24082300	-0.70615900	2.06937900
C	2.69048300	-0.55089300	0.71920300
C	-1.41109500	-2.79375100	-1.01380400
C	-2.68418300	-2.24381100	-0.75025300
C	-2.92014200	-0.88088900	-0.36601900
C	-3.99721000	-2.84739900	-0.74480900
N	4.51221000	-0.77420300	2.07940700
N	4.06711200	-0.60274800	0.77377300
N	-4.26983200	-0.78292600	-0.15339600
N	-4.91749300	-1.98646800	-0.40077400
O	-0.03453100	-0.58286500	1.54494100
O	-0.32790600	-2.13228200	-0.97185800
O	2.02838400	-0.40779600	-0.35045000
O	-2.12558300	0.10324800	-0.22571900
O	0.32548900	1.96910800	0.24765700
O	-0.03620900	0.57698900	-2.21789500
Mo	-0.04589700	-0.03935100	-0.62849300
P	0.55472100	3.27323600	-0.50932300
C	-0.88959100	3.77338800	-1.49188200
H	-1.08059200	2.99557900	-2.23298000
H	-1.75997800	3.85418600	-0.83852800
H	-0.71521800	4.72821200	-1.99286400
C	1.96104300	3.19996100	-1.65762300
H	2.86174800	2.91676800	-1.11069700
H	1.74997100	2.43283900	-2.40392800
H	2.11664800	4.16313500	-2.14899400
C	0.89456800	4.60792600	0.67625900
H	0.05206400	4.69881700	1.36373700
H	1.78839800	4.35635000	1.24945500
H	1.04922200	5.55981200	0.16383900
C	-1.24331400	-4.25427400	-1.36335000
H	-1.64151300	-4.89607800	-0.57454000
H	-1.77385000	-4.49714400	-2.28710500
H	-0.18231200	-4.45715500	-1.49504500
C	-4.42125600	-4.24788300	-1.06267600
H	-4.14739800	-4.53477800	-2.08164100
H	-3.96854400	-4.97482000	-0.38285500
H	-5.50488200	-4.31198600	-0.96368300
C	3.63283900	-1.03487100	4.31274600
H	4.69958300	-1.09359100	4.52976100
H	3.20619200	-0.20657100	4.88584300
H	3.15620400	-1.95505400	4.66191900
C	0.41415900	-0.97063400	3.83416700
H	0.74790100	-1.94586100	4.19832700
H	0.82052300	-0.21199000	4.50734100
H	-0.67344900	-0.92957600	3.86042900
C	5.02011200	-0.47051600	-0.26603700
C	6.37483900	-0.34851800	0.07195900
C	4.63928000	-0.46550900	-1.61522200
C	7.33048200	-0.21867400	-0.92856400
H	6.65469800	-0.36524200	1.11501900
C	5.61276500	-0.33019400	-2.60218100

H	3.59931500	-0.57168600	-1.88127800
C	6.95927300	-0.20521100	-2.27194300
H	8.37510300	-0.12724300	-0.65174400
H	5.30607500	-0.33087500	-3.64246900
H	7.70874000	-0.10374600	-3.04842500
C	-5.03994000	0.34499300	0.23484900
C	-6.42210100	0.32135700	0.01703900
C	-4.44721200	1.45726200	0.84486700
C	-7.20133700	1.40644100	0.40178200
H	-6.86395400	-0.55212500	-0.44010900
C	-5.24441600	2.53557500	1.21995700
H	-3.38213200	1.46855500	1.01804300
C	-6.61974600	2.52135500	1.00193700
H	-8.27136600	1.37735700	0.22877200
H	-4.78023900	3.39141200	1.69803100
H	-7.23143400	3.36505600	1.30021500

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C	3.59359000	-2.79145200	-0.47917100
C	1.10353100	-2.76086500	0.29460200
C	2.35673000	-2.20083100	-0.02742300
C	2.62413400	-0.79645200	-0.00747800
C	-1.10358500	2.76080100	0.29513700
C	-2.35673400	2.20084100	-0.02720900
C	-2.62414000	0.79645700	-0.00762400
C	-3.59352700	2.79156300	-0.47901000
N	4.49759200	-1.87628400	-0.70589500
N	3.91272000	-0.64725200	-0.42584700
N	-3.91266400	0.64735100	-0.42621900
O	-4.49749300	1.87644600	-0.70608000
O	0.11245600	-2.06510800	0.68136100
O	-0.11256100	2.06495400	0.68186400
O	1.86231200	0.19127700	0.29755400
O	-1.86236300	-0.19134000	0.29729600
O	-0.00016700	-0.00035200	2.91434700
Mo	-0.00007900	-0.00014400	1.23023800
C	-0.84354500	4.24256200	0.18368700
H	-0.92890900	4.57198300	-0.85516800
H	-1.56539800	4.81318200	0.77131400
H	0.16239200	4.44793700	0.54444500
C	-3.95268200	4.22772400	-0.69748300
H	-3.86881700	4.80868000	0.22525700
H	-3.30803100	4.69827400	-1.44455800
H	-4.98375600	4.28058600	-1.04651200
C	0.84350200	-4.24259600	0.18274800
H	0.92914700	-4.57179500	-0.85615300
H	1.56519100	-4.81335000	0.77045000
H	-0.16253200	-4.44804000	0.54319500
C	3.95277700	-4.22756500	-0.69790500
H	3.86874300	-4.80872800	0.22469000
H	3.30825300	-4.69794200	-1.44519900
H	4.98391100	-4.28035400	-1.04676500
C	-4.69244300	-0.53533100	-0.58617100
C	-6.05385900	-0.39893000	-0.88071100
C	-4.12667400	-1.80967600	-0.46082500
C	-6.84072800	-1.53243800	-1.04700700
H	-6.47266500	0.59158900	-0.97824600
C	-4.93376500	-2.93195100	-0.62871400
H	-3.07809700	-1.91616400	-0.23159700
C	-6.28850300	-2.80534000	-0.92179300
H	-7.89419500	-1.41532700	-1.27490900
H	-4.48937000	-3.91580700	-0.52819300
H	-6.90649600	-3.68628800	-1.05104400
C	4.69252300	0.53546700	-0.58541200
C	6.05399700	0.39913300	-0.87971800
C	4.12672100	1.80978200	-0.45992100
C	6.84089000	1.53267900	-1.04563800
H	6.47282700	-0.59136300	-0.97737200
C	4.93383500	2.93209600	-0.62743200
H	3.07809900	1.91621600	-0.23087100

C	6.28863100	2.80555300	-0.92027700
H	7.89440100	1.41562100	-1.27336200
H	4.48941500	3.91592900	-0.52680000
H	6.90664200	3.68653100	-1.04923400

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C	3.47974400	-1.38439400	-2.22701700
C	1.08554700	-2.01693200	-1.39186600
C	2.23009300	-1.20535900	-1.52548200
C	2.33700400	0.10028800	-0.95207600
C	-1.61320000	2.59974200	1.26095600
C	-2.84618500	2.08961700	0.80802900
C	-2.99035300	0.81323600	0.18074600
C	-4.17846800	2.64436800	0.79317800
N	4.23981400	-0.32831400	-2.11173000
N	3.54636400	0.59274500	-1.33601400
N	-4.30625800	0.69502600	-0.14947600
N	-5.02470800	1.82096200	0.23472600
O	0.04173300	-1.63429900	-0.76619200
O	-0.52461700	1.94544800	1.18707000
O	1.51428500	0.75545300	-0.20985500
O	-2.11157500	-0.08614400	-0.08372900
O	0.09335800	-0.92836700	2.12787500
Mo	-0.16761400	-0.09745500	0.67114800
C	2.74124600	-3.40567800	2.25606900
H	3.46335100	-4.08055700	1.79139600
H	3.17708100	-2.39918500	2.26276700
O	1.55565500	-3.46292500	1.47220500
H	0.95742800	-2.77006900	1.78568500
C	2.49236600	-3.85417400	3.69023400
H	1.77117600	-3.17129000	4.16244800
H	2.05246200	-4.86055400	3.67634800
O	3.74859400	-3.83314600	4.36327800
H	3.60241500	-4.08011400	5.28006500
C	-1.49517000	3.97923100	1.85861600
H	-1.77395700	4.74313500	1.12833100
H	-2.15719800	4.08926800	2.72023600
H	-0.46482400	4.13783500	2.17071400
C	-4.68309500	3.95452100	1.31072200
H	-4.52265500	4.05108200	2.38816100
H	-4.18859200	4.80020900	0.82544300
H	-5.75302200	4.01911000	1.11379100
C	1.00030500	-3.41110700	-1.93974400
H	1.66636600	-3.59635800	-2.77761700
H	1.26227000	-4.08103500	-1.11291600
H	-0.03180300	-3.61714900	-2.22310800
C	3.99269800	-2.54639800	-3.01899000
H	4.01229300	-3.46245900	-2.42345600
H	3.37907000	-2.73439000	-3.90485200
H	5.00727900	-2.32119300	-3.34745200
C	-4.99987800	-0.37918600	-0.78165600
C	-6.39262200	-0.29667800	-0.89171000
C	-4.32105900	-1.49477400	-1.28623500
C	-7.09841300	-1.32717800	-1.50124900
H	-6.89935400	0.57283900	-0.50045900
C	-5.04819600	-2.51709600	-1.89050100
H	-3.24764200	-1.56019100	-1.20351100
C	-6.43348300	-2.44376700	-2.00320400
H	-8.17712400	-1.25352400	-1.58092900
H	-4.51634500	-3.37926200	-2.27669600
H	-6.98843400	-3.24573700	-2.47600700
C	4.16474300	1.84323100	-1.04107300
C	5.48080700	2.05037500	-1.46991700
C	3.48733200	2.85248300	-0.34636400
C	6.11154400	3.25957900	-1.20242600
H	5.98718400	1.26248300	-2.00716700
C	4.13891300	4.05549600	-0.08701200
H	2.47412300	2.69391600	-0.01249500
C	5.44746800	4.26958000	-0.50983100
H	7.13127900	3.40897300	-1.53889100

H	3.60884800	4.83172400	0.45344300
H	5.94405700	5.21036000	-0.30242000

TS(11-12)

C	-3.93020900	-2.91053700	0.47901300
C	-1.34194300	-2.85849500	0.21390500
C	-2.63573700	-2.32123700	0.21857300
C	-2.92495400	-0.93784200	-0.03884600
C	0.94418800	1.05570400	2.02018100
C	2.28626700	0.79357700	1.73321700
C	2.67672100	0.00407100	0.60195600
C	3.53128000	1.10389800	2.39739000
N	-4.87834000	-2.01898400	0.39187500
N	-4.27739400	-0.80455900	0.07784600
N	4.03497200	-0.11072200	0.66500000
N	4.54213800	0.57661700	1.76332900
O	-2.14018300	0.02764500	-0.30924200
O	-0.00370700	0.66195500	1.24922200
O	-0.29317500	-2.16297400	-0.03636800
O	1.94244400	-0.53678600	-0.28517400
O	-0.06491700	0.02186500	-2.47931500
Mo	-0.08271300	-0.15682100	-0.66382400
C	1.10695000	2.84489800	-0.97042600
H	1.15943300	3.07094400	0.10412600
H	2.08596600	2.43020800	-1.26182500
O	0.04513800	1.97560300	-1.25785700
H	0.01470600	1.07911800	-2.43533800
C	0.89573700	4.16242500	-1.70671400
H	0.91209900	3.97925800	-2.79020400
H	-0.09516600	4.55472100	-1.44175100
O	1.94035500	5.05122100	-1.31033300
H	1.83622600	5.87032200	-1.80133000
C	-1.07604700	-4.31338000	0.50654700
H	-1.54014500	-4.62498200	1.44375300
H	-1.48472500	-4.94155300	-0.28996500
H	0.00000700	-4.46674800	0.56072100
C	-4.29590700	-4.32285300	0.81147600
H	-3.96551300	-5.01962200	0.03658400
H	-3.84993900	-4.64360900	1.75716200
H	-5.37987400	-4.39111900	0.90136900
C	3.79129600	1.91638400	3.62642200
H	3.35926200	2.91701300	3.54477000
H	3.37384600	1.44218500	4.51972700
H	4.86857900	2.01070500	3.76208000
C	0.48203900	1.79962700	3.24131300
H	1.19170500	1.75641100	4.06389600
H	0.32266400	2.84931500	2.97213800
H	-0.48085200	1.39370600	3.55310800
C	-5.09804300	0.35078600	-0.07720100
C	-6.48018500	0.21276300	0.09617900
C	-4.55185700	1.60066500	-0.39470800
C	-7.30752200	1.32007900	-0.04884300
H	-6.88458700	-0.75827100	0.34007800
C	-5.39959200	2.69651100	-0.53450000
H	-3.48740800	1.71247000	-0.52931900
C	-6.77510300	2.56814400	-0.36460500
H	-8.37675200	1.20175300	0.08633600
H	-4.96929900	3.66037200	-0.78166100
H	-7.42445200	3.42851100	-0.47803400
C	4.93864800	-0.78842900	-0.20162800
C	6.30810000	-0.73156700	0.08183300
C	4.48315600	-1.50252100	-1.31621000
C	7.21119900	-1.38599100	-0.74755700
H	6.64304600	-0.17550100	0.94473100
C	5.40475500	-2.15112200	-2.13388000
H	3.42878100	-1.54757500	-1.53770200
C	6.76819800	-2.09962200	-1.85917000
H	8.26993600	-1.33438700	-0.51978600
H	5.04358900	-2.70036800	-2.99597900
H	7.47693600	-2.60709300	-2.50318400

C	-3.93378000	-2.70641600	-0.73732000
C	-1.33128900	-2.61467800	-0.99608600
C	-2.62929300	-2.09958900	-0.74314200
C	-2.87348700	-0.74126700	-0.39663700
C	0.85652100	-0.55139900	2.41714900
C	2.22854400	-0.58384700	2.06593900
C	2.65724200	-0.37285200	0.73235500
C	3.44524800	-0.82528600	2.79214400
N	-4.86065300	-1.83444100	-0.42762300
N	-4.22216500	-0.62446200	-0.21274400
N	4.01724900	-0.49163800	0.72666800
N	4.48730000	-0.76310200	1.99865300
O	-2.06093000	0.24732400	-0.26773600
O	-0.01793500	-0.28177900	1.54289100
O	-0.30685500	-1.87978200	-0.96293500
O	1.94328500	-0.12108000	-0.31173900
O	-0.16784600	0.53486300	-2.42282700
Mo	-0.02610900	0.22252600	-0.53106400
C	0.83949300	3.06262100	-0.87833900
H	1.84481100	2.67755200	-1.09361500
H	0.36240100	3.28647200	-1.84553800
O	0.07173900	2.12941600	-0.14740100
H	-0.44378300	1.42024400	-2.69913400
C	0.93704900	4.35564000	-0.08185800
H	-0.07798500	4.70752700	0.14479700
H	1.44923900	4.15262000	0.86813500
O	1.65710400	5.28790500	-0.88314600
H	1.75298700	6.10244600	-0.38288200
C	-1.10279200	-4.07130500	-1.31497600
H	-1.54854200	-4.72065900	-0.55869200
H	-1.55573500	-4.32600600	-2.27727300
H	-0.03085600	-4.25280200	-1.37045100
C	-4.34050400	-4.11896600	-1.01929400
H	-4.03851700	-4.43520500	-2.02140900
H	-3.89736500	-4.81850800	-0.30488500
H	-5.42542300	-4.19222400	-0.94442100
C	3.64761700	-1.11751200	4.24529200
H	3.25517400	-0.31445800	4.87527700
H	3.14919400	-2.04429900	4.54319700
H	4.71493600	-1.22188700	4.43999200
C	0.36880100	-0.83783200	3.81301100
H	0.70773200	-1.81781400	4.15825200
H	0.75160200	-0.09166400	4.51499100
H	-0.71942200	-0.80580200	3.82020600
C	-5.00354300	0.51536100	0.13356300
C	-6.39812800	0.40083300	0.09739000
C	-4.41028800	1.72596100	0.51205800
C	-7.18983600	1.49152700	0.43665200
H	-6.83844000	-0.54188000	-0.19174900
C	-5.22211100	2.80660400	0.84706900
H	-3.33597200	1.81982300	0.53978800
C	-6.60962400	2.70114700	0.81253300
H	-8.26896900	1.39133600	0.40446300
H	-4.75486200	3.74044200	1.13889900
H	-7.23111500	3.54958400	1.07466100
C	4.94467300	-0.34745600	-0.34391100
C	6.30416200	-0.22399600	-0.03810200
C	4.52107900	-0.33912600	-1.67739200
C	7.23121800	-0.08978700	-1.06480400
H	6.61271100	-0.24226600	0.99692000
C	5.46506300	-0.19825000	-2.69129900
H	3.47424600	-0.43982200	-1.91922900
C	6.81958700	-0.07309200	-2.39595200
H	8.28274800	0.00526500	-0.81852900
H	5.12940300	-0.19091900	-3.72201000
H	7.54603100	0.03514800	-3.19288800

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C	-3.55123300	-2.41860100	-1.69827800
C	-0.97741500	-2.04648700	-1.39387700
C	-2.34531000	-1.76032500	-1.26276400
C	-2.81077300	-0.63367200	-0.52428700
C	0.99021100	-1.18384900	2.40330100
C	2.29391700	-1.09570200	1.84104100
C	2.64066100	-0.36589800	0.65942800
C	3.54536700	-1.67702600	2.26794800
N	-4.61185800	-1.77796800	-1.28201200
N	-4.17660200	-0.68131900	-0.55211600
N	3.98167900	-0.53836600	0.48194600
N	4.52535000	-1.34718600	1.46582600
O	-0.09121900	-1.27576500	-0.89002500
O	-0.02531800	-0.61290800	1.91639100
O	-2.11562500	0.24697300	0.08613200
O	1.93289600	0.33832300	-0.14924300
O	-0.26303200	1.47775600	-1.70197700
O	0.24709100	2.14414600	1.03532100
Mo	-0.11241900	0.59072600	0.07558800
H	0.45068900	1.17786300	-2.28127600
C	1.03612300	3.31375200	1.16341800
H	2.08981500	3.02127800	1.09009400
H	0.84802100	3.73155800	2.15903400
C	0.70116800	4.33357400	0.07815500
H	-0.36984700	4.57356300	0.13578400
H	1.26098300	5.25053500	0.29167900
O	1.07600700	3.89628100	-1.20878900
H	0.47072200	3.17727500	-1.46899300
C	-3.71890100	-3.65705900	-2.52020700
H	-3.22660000	-3.56448200	-3.49211000
H	-3.29848300	-4.53340600	-2.01874500
H	-4.78225600	-3.83088100	-2.68426400
C	-0.46324200	-3.26401300	-2.11625700
H	-0.89920700	-4.17979200	-1.71060500
H	-0.72125400	-3.21847100	-3.17799200
H	0.62016000	-3.30249500	-2.01654700
C	3.86066000	-2.55247300	3.44151400
H	3.61778900	-2.06639400	4.39005100
H	3.31188900	-3.49742800	3.40507800
H	4.92809600	-2.77251600	3.42980200
C	0.73844900	-1.99144900	3.65622200
H	1.03208300	-3.03460400	3.52016300
H	1.31180500	-1.59505200	4.49756200
H	-0.32307000	-1.94017800	3.89056400
C	4.82726200	-0.03763700	-0.54879200
C	6.04282800	-0.68906600	-0.78361800
C	4.47617400	1.08750900	-1.30374100
C	6.89779200	-0.21897200	-1.77340000
H	6.30330100	-1.54588200	-0.17906900
C	5.34373300	1.53982600	-2.29494200
H	3.54350400	1.60088000	-1.12650200
C	6.55310700	0.89446000	-2.53727200
H	7.83812100	-0.72974700	-1.94771000
H	5.06566200	2.41267800	-2.87457300
H	7.22190600	1.25719900	-3.30922500
C	-5.13826900	0.19680700	0.02009400
C	-6.49674500	-0.07383500	-0.18148900
C	-4.75192400	1.31159200	0.77314600
C	-7.45633100	0.76816000	0.36760600
H	-6.77825500	-0.93771300	-0.76505000
C	-5.72920100	2.14257400	1.31453900
H	-3.70694700	1.52589400	0.93178000
C	-7.08189100	1.88067500	1.11833100
H	-8.50566000	0.54956300	0.20433900
H	-5.42046200	3.00420800	1.89560400
H	-7.83457400	2.53428100	1.54351500

TS(13-14)

C	3.14324700	3.13308500	-0.46748000
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C	0.63462700	2.34703100	-0.66715300
C	2.01963500	2.23127200	-0.49680000
C	2.59357900	0.94163600	-0.31028500
C	-0.91434500	-0.19530000	2.43278400
C	-2.24056300	0.00185200	2.00750700
C	-2.67741500	-0.04369900	0.63590300
C	-3.44374900	0.28868600	2.75606200
N	4.26140600	2.47676600	-0.29020500
N	3.94450800	1.13020900	-0.19982500
N	-4.02673800	0.21314100	0.66989700
N	-4.47778400	0.40686800	1.96915600
O	-0.11607100	1.31723800	-0.63812800
O	0.04886500	-0.48697200	1.65242800
O	2.02200700	-0.18957500	-0.24750600
O	-2.04067600	-0.25815300	-0.43522600
O	0.32939500	-1.11843100	-2.54153100
O	-0.92241100	-2.44519600	-0.23403600
Mo	0.05241000	-0.81208500	-0.45137000
H	-0.42764100	-1.24069600	-3.12112800
C	-0.48032800	-3.76540500	-0.49662600
H	-0.90488500	-4.06816600	-1.46350900
H	-0.87800600	-4.43628100	0.27235500
C	1.04442500	-3.73304900	-0.53645000
H	1.45950100	-3.82448000	0.47346700
H	1.44897600	-4.54637900	-1.15221400
O	1.40988900	-2.47857500	-1.06126900
H	0.92705200	-2.04713400	-2.13960000
C	-4.96409100	0.27460800	-0.39508200
C	-6.33024700	0.27362100	-0.08773700
C	-4.55183100	0.34953700	-1.73126200
C	-7.26988000	0.34180400	-1.10959900
H	-6.63297100	0.22680200	0.94798800
C	-5.50874800	0.41343500	-2.74074400
H	-3.49939200	0.35570900	-1.96628900
C	-6.86846600	0.40931000	-2.44218500
H	-8.32470200	0.34000600	-0.85819800
H	-5.18003800	0.47177700	-3.77260900
H	-7.60509800	0.46009400	-3.23565400
C	4.97922600	0.17598200	0.00241600
C	6.24113100	0.63052500	0.40014300
C	4.75299300	-1.19069500	-0.20159800
C	7.27168200	-0.28154300	0.59559000
H	6.39686700	1.69033400	0.54106300
C	5.79883800	-2.08691100	0.00528200
H	3.78097300	-1.54662500	-0.51222100
C	7.05791300	-1.64492900	0.40274700
H	8.24702100	0.07931900	0.90249700
H	5.62018700	-3.14444000	-0.15437500
H	7.86393600	-2.35296800	0.55765600
C	-0.52184600	-0.07926000	3.88808900
H	-0.84395000	0.87078700	4.31772500
H	-0.97844600	-0.88078900	4.47491700
H	0.56100900	-0.16367300	3.95920200
C	-3.65010000	0.45749700	4.22962900
H	-3.33599200	-0.42790300	4.78855800
H	-3.09226200	1.31146500	4.62385200
H	-4.71123600	0.62624600	4.41303900
C	3.18793000	4.62206700	-0.60788200
H	2.76981600	4.94882300	-1.56416200
H	2.62665200	5.11867600	0.18921400
H	4.22618700	4.94960000	-0.55392400
C	-0.07621200	3.65127200	-0.90959300
H	0.55868800	4.52077500	-0.75694900
H	-0.45064000	3.66223000	-1.93775800
H	-0.94498200	3.70831400	-0.25044800

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C	3.36998600	2.41522600	-1.65364600
C	0.82022200	1.79685500	-1.62775300
C	2.19581500	1.64263200	-1.34178500

C	2.68815900	0.54995800	-0.57874700
C	-0.84292000	1.17762600	2.13907700
C	-2.19265300	1.16336100	1.74668900
C	-2.67089700	0.32635400	0.69384600
C	-3.36598300	1.85108500	2.22218000
N	4.44608900	1.86724400	-1.14679700
N	4.04264200	0.72327700	-0.47707300
N	-4.01944600	0.55009200	0.61350800
N	-4.42792300	1.48765700	1.55137700
O	-0.02550600	0.94280700	-1.23132800
O	0.03492000	0.44856100	1.57960400
O	2.05600900	-0.44171500	-0.06906700
O	-2.05117600	-0.50414000	-0.04651600
O	0.90560200	-1.39761100	-2.31266200
O	-0.84700100	-2.49655400	-0.93589100
Mo	0.03712600	-0.85473500	-0.07788600
H	0.22668700	-2.10486700	-2.29064200
C	-1.02394100	-3.63387000	-0.12004700
H	-0.98810600	-4.54221300	-0.73492000
H	-2.01259300	-3.58622200	0.35882600
C	0.07935000	-3.61370900	0.92713000
H	-0.18653700	-4.15219100	1.84270600
H	1.01625800	-4.03664000	0.53926400
O	0.30320300	-2.24112600	1.23769200
H	1.75403300	-1.84235200	-2.19778600
C	0.28163400	2.96807600	-2.40878200
H	0.64097700	3.91843700	-2.00915900
H	0.60262100	2.90520500	-3.45289800
H	-0.80641900	2.94337200	-2.37565100
C	3.49891300	3.68650900	-2.43266600
H	3.10288300	3.58096500	-3.44631100
H	2.96145900	4.50963900	-1.95289000
H	4.55327700	3.95564700	-2.49630800
C	-0.33732700	2.04800200	3.26216000
H	-0.66915700	3.08144000	3.14948600
H	-0.71339200	1.68077900	4.22158900
H	0.75051600	2.00839400	3.27485100
C	-3.50925100	2.86426800	3.31409800
H	-3.16275400	2.47497000	4.27532300
H	-2.93724100	3.77183600	3.10005100
H	-4.56117000	3.13421700	3.40698500
C	-4.98396500	-0.01325100	-0.26904400
C	-6.29649400	0.47128400	-0.22037400
C	-4.64523600	-1.03086700	-1.17050600
C	-7.26070000	-0.05975900	-1.06899100
H	-6.54013900	1.25391900	0.48276600
C	-5.62700000	-1.54590600	-2.01336300
H	-3.63372100	-1.40530000	-1.21223000
C	-6.93443800	-1.06998400	-1.97133600
H	-8.27418600	0.32288100	-1.02210100
H	-5.35688700	-2.33216000	-2.70945000
H	-7.68958100	-1.48045200	-2.63179100
C	5.01572300	-0.09137100	0.16235700
C	6.36566100	0.10714000	-0.14877400
C	4.64752000	-1.06756600	1.09607800
C	7.33737600	-0.67165000	0.46861700
H	6.63080600	0.87460700	-0.86142500
C	5.63618000	-1.84094200	1.69931900
H	3.60818600	-1.21752600	1.34656700
C	6.98097800	-1.65205700	1.39270900
H	8.38064200	-0.50961200	0.22170900
H	5.34370500	-2.59409500	2.42235200
H	7.74234400	-2.25815300	1.86987200

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C	3.33044000	2.88691300	-0.78587200
C	0.80272900	2.23670300	-1.00418200
C	2.16858000	2.03385700	-0.76452000
C	2.67766200	0.73831500	-0.44304500
C	-0.83104600	0.46340800	2.28719300

C	-2.18470300	0.48216900	1.90043100
C	-2.66998200	0.15086100	0.58961500
C	-3.37494800	0.83134500	2.64270800
N	4.41620000	2.21267000	-0.51456600
N	4.03655300	0.89056300	-0.30844100
N	-4.02745800	0.33272400	0.63931900
N	-4.44536200	0.73592600	1.90118000
O	-0.05056200	1.30366700	-0.87878100
O	0.12863300	0.09652300	1.53688200
O	2.06674300	-0.35979300	-0.31029200
O	-2.05606800	-0.22314600	-0.45792500
O	0.14441500	-0.76139500	-2.65440800
O	-0.88568100	-2.24242400	0.64559500
Mo	-0.00856200	-0.83989000	-0.37006100
H	-0.72011800	-0.79155200	-3.07986900
C	-0.59075000	-3.62272500	0.53059500
H	-1.42491900	-4.10279000	0.00190300
H	-0.51368700	-4.07057100	1.52731000
C	0.71796700	-3.71475800	-0.25038200
H	1.58391600	-3.72850900	0.42365300
H	0.76318200	-4.60216200	-0.89216600
O	0.77076400	-2.54402600	-1.04267400
H	0.54548600	-1.64587900	-2.73787900
C	-5.00328200	0.12849600	-0.37074400
C	-6.34350400	-0.01289700	0.00715800
C	-4.65377400	0.08695500	-1.72531000
C	-7.31974500	-0.20056300	-0.96433500
H	-6.59869500	0.03677800	1.05572500
C	-5.64449500	-0.10712400	-2.68399000
H	-3.62119400	0.20765900	-2.01265200
C	-6.97886500	-0.25292300	-2.31450200
H	-8.35478400	-0.30867100	-0.65989000
H	-5.36584800	-0.13588400	-3.73173800
H	-7.74361700	-0.40147300	-3.06803800
C	5.02639100	-0.07498600	0.00551700
C	6.29229800	0.36398200	0.41101200
C	4.76171200	-1.44637400	-0.09657400
C	7.28052800	-0.56457400	0.71609900
H	6.48285200	1.42573600	0.47098800
C	5.76395500	-2.36038200	0.21813700
H	3.78819700	-1.78530200	-0.41698200
C	7.02427200	-1.93142400	0.62570100
H	8.25778200	-0.21356400	1.02867100
H	5.55183900	-3.42072000	0.13597300
H	7.79769900	-2.65161600	0.86658300
C	-0.39760700	0.89171700	3.67024100
H	-0.80777300	1.86589200	3.93942300
H	-0.73988000	0.16767000	4.41487000
H	0.68982000	0.93153400	3.69341600
C	-3.53911700	1.25533700	4.06949500
H	-3.13003500	0.51562400	4.76249400
H	-3.04240800	2.20825800	4.27247500
H	-4.60320100	1.37347500	4.27421400
C	3.43567700	4.35437100	-1.05981600
H	3.03793200	4.61091200	-2.04552100
H	2.88599500	4.94285400	-0.31885800
H	4.48539900	4.64572800	-1.02109000
C	0.25143600	3.57311600	-1.44202400
H	0.62926600	4.38713100	-0.82144700
H	0.54543200	3.78115000	-2.47543600
H	-0.83547800	3.54235800	-1.38485100

Table S2. Comparison of selected energies for pathways **A** and **B**, in gas phase, in the $[\text{Mo}(\text{O})_2(\text{Q}^{\text{Me}})_2]$ -catalyzed DODH of ethylene glycol with PMe_3 reductant.

	Path A		Path B	
ΔG (kcal/mol) ^a				
Diol activation	TS(2-3)	32.9 (35.8)	TS(11-12)	31.1 (19.6)
Water formation	TS(4-5)	17.9 (42.4)	TS(13-14)	15.2 (10.6)
Oxo-transfer	TS(6-7)	16.7 (40.2)	TS(1-9)	12.7 (20.6)
Alkene extrusion	TS(8-1)	22.4 (13.8)	TS(8-1)	22.4 (13.8)
Energies (kcal/mol)				
Highest TS relative energy	TS(6-7)	42.4	TS(11-12)	20.6
Highest ΔG difference	TS(2-3)	32.9	TS(11-12)	31.1
Maximum relative ΔG between intermediates		49.1		29.4

^a Difference in the calculated Gibbs energies of the TS and its precedent intermediate. The energetic span value, which is the difference in the calculated Gibbs energies of the TS and the relative zero energy, appears in parentheses.