

Supporting Information for:

Mechanistic elucidation of O₂ production from ^tBuOOH in water using [Mn₂(mcbpen)₂(H₂O)₂]²⁺ (Mn(II)) as the catalyst: a DFT study

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Table S1. Cartesian coordinates of all structures optimized at the SMD/B3LYP-D3/6-31G(d),SDD level of theory in water (page S3).

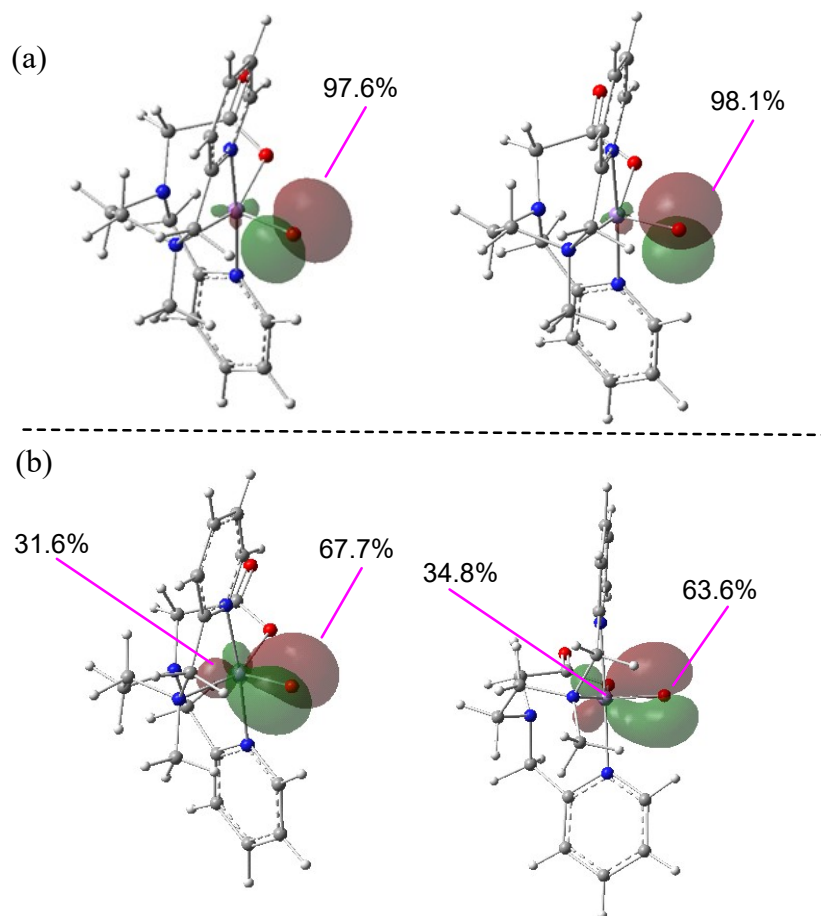


Fig. S1 Spatial plots of two lone pair orbitals with p character for (a) α -spin and (b) β -spin electrons on the oxygen ligand in $[\text{Mn}^{\text{IV}}(^{18}\text{O})(\text{mcbpen})]^+$ (complex **3**), as determined by NLMO calculations.

Table S1. Cartesian coordinates of all structures optimized at the SMD/B3LYP-D3/6-31G(d),SDD level of theory in water.

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Mn	0.98800600	0.94389800	-0.00317400
O	0.82598600	-0.81645400	0.22510200
N	1.03259000	1.54729200	2.00146000
N	3.12538800	0.84590500	0.28791000
N	5.79061800	-0.52007200	-1.03807200
N	0.60330600	3.04078500	-0.12647600
C	2.37702700	2.20558300	2.18839300
H	2.37852100	3.15194900	1.64724000
H	2.51687800	2.42312900	3.25243800
C	3.46903000	1.29540300	1.67331500
H	3.55665500	0.41170600	2.30343200
H	4.43467900	1.80888200	1.67908200
C	3.61122000	1.77700400	-0.76128500
H	3.40761700	2.80659800	-0.45042600
H	4.68335100	1.67467000	-0.93330300
C	3.60234100	-0.56372200	0.03334400
H	3.10875500	-1.19090800	0.77435200
H	3.23839600	-0.85542000	-0.95267100
C	5.10388100	-0.73793200	0.10102800
C	5.72620700	-1.13111500	1.29085600
H	5.13201000	-1.31949300	2.17925000
C	7.11214800	-1.28678000	1.31132900
H	7.61835600	-1.59243300	2.22216800
C	7.82884600	-1.04925100	0.13969900
H	8.90784500	-1.15932000	0.10320800
C	7.12253000	-0.67213000	-1.00307100
H	7.64931600	-0.48949800	-1.93688400
C	0.66370800	3.81009300	-1.22901400
H	1.12578900	3.37443000	-2.10476800
C	0.15043700	5.10042200	-1.25113400
H	0.22260600	5.68919000	-2.15851900
C	-0.44808100	5.60649000	-0.09621700
H	-0.85480400	6.61254700	-0.08174500
C	-0.51378400	4.80550500	1.04299700
H	-0.96574400	5.16202200	1.96214700
C	0.01510900	3.52083100	0.99140800
C	-0.04672500	2.56261500	2.14657700
H	-1.00456400	2.03491500	2.13813300
H	0.05729000	3.08185100	3.10574400
C	0.84756900	0.45409000	2.99148900

H	-0.14721100	0.03616000	2.87360400
H	1.58293600	-0.32958700	2.81604000
H	0.97229100	0.86349300	4.00029200
C	2.82524800	1.50863300	-2.03390100
O	3.25735200	1.76140300	-3.15139700
O	1.61379000	1.02339400	-1.83045800
O	-0.82538900	0.81585500	-0.22701800
Mn	-0.98773700	-0.94411800	0.00292000
N	-1.03084800	-1.55179400	-2.00009600
N	-3.12481300	-0.84537400	-0.28967700
N	-5.79065200	0.52369100	1.03198700
N	-0.60456100	-3.04101800	0.13146400
C	-2.37580000	-2.20911500	-2.18699300
H	-2.37854900	-3.15446500	-1.64406800
H	-2.51487600	-2.42853300	-3.25075900
C	-3.46745000	-1.29699300	-1.67464500
H	-3.55347700	-0.41432500	-2.30643900
H	-4.43359000	-1.80954900	-1.68054300
C	-3.61188300	-1.77445900	0.76073200
H	-3.40855400	-2.80471600	0.45188400
H	-4.68409000	-1.67131600	0.93178300
C	-3.60152800	0.56484100	-0.03780300
H	-3.10718500	1.19066500	-0.77945100
H	-3.23825600	0.85806000	0.94800200
C	-5.10297000	0.73936900	-0.10696000
C	-5.72426600	1.13066900	-1.29794100
H	-5.12932800	1.31731200	-2.18620100
C	-7.11014500	1.28671500	-1.31974700
H	-7.61556700	1.59093300	-2.23150300
C	-7.82781700	1.05143300	-0.14826100
H	-8.90681000	1.16188200	-0.11279400
C	-7.12249200	0.67607700	0.99570100
H	-7.65004400	0.49519700	1.92942300
C	-0.66621300	-3.80771900	1.23575100
H	-1.12835700	-3.36963300	2.11026400
C	-0.15409100	-5.09844300	1.26114200
H	-0.22723900	-5.68501700	2.16986700
C	0.44453100	-5.60775200	0.10770800
H	0.85032900	-6.61421400	0.09577800
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H	0.96370800	-5.16852300	-1.95138700
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H	-0.05653700	-3.08984200	-3.10032200
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H	-1.57821500	0.32431100	-2.81847100
H	-0.96753200	-0.87140700	-4.00005300
C	-2.82671300	-1.50399900	2.03340800
O	-3.25963100	-1.75462700	3.15107300
O	-1.61504300	-1.01939000	1.82985400

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Mn	1.28402700	-0.00144400	0.14851700
O	-0.43523600	0.21633700	-0.12748600
N	1.34276400	1.17725500	1.84741500
N	3.37751600	-0.02783400	0.35818800
N	6.23411500	1.43025800	-0.35163300
N	0.63773700	-1.36766200	1.68571400
C	2.61871500	0.80198700	2.55394100
H	2.47238100	-0.17369400	3.01810700
H	2.81482400	1.53002800	3.34787600
C	3.77348700	0.75259500	1.57502500
H	4.04794100	1.75331600	1.24570300
H	4.65208000	0.30242600	2.04502300
C	3.63605000	-1.48731500	0.45928400
H	3.28973500	-1.84615400	1.43280000
H	4.69831400	-1.72318300	0.37128400
C	4.02574600	0.54295600	-0.88453700
H	3.72887000	1.59055400	-0.93583100
H	3.59418100	0.02251500	-1.73969800
C	5.53311600	0.42794700	-0.91481700
C	6.14473500	-0.67135600	-1.52863700
H	5.53364300	-1.45183400	-1.97252900
C	7.53730900	-0.74613400	-1.54987100
H	8.03706300	-1.58846900	-2.01878600
C	8.26899100	0.28440100	-0.96195500
H	9.35419600	0.27595600	-0.95528100
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H	8.11397300	2.16765100	0.08007700
C	0.49677400	-2.70220300	1.58702400
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C	-0.24887700	-3.43422000	2.50213400
H	-0.33847700	-4.50786300	2.38217600
C	-0.86937200	-2.76058800	3.55607000

H	-1.45839400	-3.30353100	4.28831100
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C	0.17665200	0.78412000	2.68549300
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H	0.39043700	2.83816500	0.97179200
H	2.16054500	2.93407500	0.99029100
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C	2.82220500	-2.17359000	-0.63491300
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Mn	-2.23460100	0.17576700	-0.29332600
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N	-4.26231300	-0.12901000	-0.58301700
N	-2.32527100	-2.01103000	-0.80335800
N	-2.15729500	2.55383700	-0.20830800
C	-3.71897600	1.20646600	-2.59691200
H	-3.92592500	2.16880400	-2.12682800
H	-3.89054100	1.31081700	-3.67437600
C	-4.61807100	0.13176600	-2.02043800
H	-4.49346900	-0.80819600	-2.55989800
H	-5.67141500	0.42160100	-2.08392000
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H	-4.86224000	1.82334400	-0.02412900
H	-5.96530800	0.54120600	0.51761000
C	-4.61113900	-1.53896500	-0.21062800
H	-4.64966100	-1.60135900	0.88063400
H	-5.60928200	-1.77315100	-0.59348800
C	-3.57217000	-2.50758200	-0.70653000
C	-3.85376800	-3.84241100	-0.98553400
H	-4.87173900	-4.20909700	-0.90809500
C	-2.80263300	-4.68111900	-1.35709400
H	-2.99181100	-5.72760600	-1.57519600
C	-1.51030700	-4.15996300	-1.45160900
H	-0.66855900	-4.78036700	-1.73904900
C	-1.31245800	-2.81243300	-1.17270500
H	-0.33617000	-2.34848000	-1.23945800
C	-2.28845000	3.36230200	0.85881000
H	-2.72865100	2.92250800	1.74641800
C	-1.88255500	4.69175200	0.84317300

H	-2.00778500	5.30768500	1.72687500
C	-1.31307900	5.20086000	-0.32693000
H	-0.98289500	6.23383300	-0.37673800
C	-1.17927400	4.36620200	-1.43387900
H	-0.74773200	4.72368000	-2.36333400
C	-1.61155600	3.04275600	-1.33332500
C	-1.43106200	2.07565200	-2.47726500
H	-0.38973100	1.74350700	-2.48968400
H	-1.64123600	2.56638700	-3.43564000
C	-1.78553700	-0.17114500	-3.28220700
H	-0.78533000	-0.47646100	-2.96990400
H	-2.44159700	-1.03964300	-3.26443500
H	-1.75039400	0.23620000	-4.29954600
C	-4.14099700	0.76910900	1.69402300
O	-4.65218900	1.16316900	2.74125500
O	-2.91254800	0.33133900	1.59249200
O	1.40763800	1.29587100	-1.02186500

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Mn	1.24883600	0.22107500	0.04833400
O	-0.48668200	0.25205000	-0.07956200
N	1.39486600	1.16112700	1.88826400
N	3.39415700	0.05624500	0.21720400
N	6.34885800	1.30148000	-0.38854000
N	0.72037200	-1.36631300	1.55079400
C	2.69684300	0.70098400	2.49832200
H	2.55135600	-0.30903900	2.87875000
H	2.92970500	1.35412300	3.34562500
C	3.82047400	0.72691500	1.48273100
H	4.08844700	1.75124200	1.22835100
H	4.70809400	0.24120800	1.89813500
C	3.56621100	-1.41367700	0.18804900
H	3.23602000	-1.84141000	1.13767700
H	4.60566100	-1.70974500	0.03295800
C	4.06708800	0.68239700	-0.98037600
H	3.86422900	1.74927400	-0.93205200
H	3.57447300	0.28577700	-1.87004100
C	5.55858400	0.44238500	-1.06015600
C	6.06837500	-0.61501700	-1.82259900
H	5.38740000	-1.28033700	-2.34538800
C	7.44938000	-0.79973200	-1.88620200
H	7.87081500	-1.61240200	-2.47032600
C	8.27262400	0.08197700	-1.18761200

H	9.35321000	-0.01646700	-1.20677100
C	7.67438500	1.11014500	-0.45761900
H	8.28921600	1.81853900	0.09310500
C	0.59097700	-2.68980600	1.35418700
H	1.07857400	-3.11108700	0.48493100
C	-0.14240700	-3.49987900	2.21326700
H	-0.22328100	-4.56135400	2.00807500
C	-0.76039700	-2.91809200	3.32102900
H	-1.33990300	-3.52184400	4.01211900
C	-0.61822100	-1.54756700	3.53158800
H	-1.07638500	-1.05207600	4.38066700
C	0.12183700	-0.80267800	2.61840800
C	0.25419400	0.68867700	2.72204400
H	-0.65692100	1.15956100	2.34585600
H	0.41017700	1.00860100	3.75853500
C	1.34078000	2.64606000	1.77490000
H	0.42846900	2.92532900	1.25021200
H	2.20779300	2.99988100	1.21738700
H	1.34248600	3.08209000	2.77954600
C	2.67811800	-1.94530000	-0.93336400
O	2.92109600	-2.97568800	-1.54704400
O	1.59570200	-1.21645000	-1.17137300
Mn	-2.26273400	0.14910200	-0.18019800
N	-2.35412700	0.94942900	-2.21874900
N	-4.30672500	-0.10186100	-0.44500100
N	-2.38489800	-1.96590200	-0.76708300
N	-2.20714900	2.53490500	-0.00895400
C	-3.79040800	1.31185500	-2.42137200
H	-3.97856500	2.25595600	-1.90795400
H	-3.99664000	1.46084200	-3.48817800
C	-4.68635400	0.22110900	-1.86253100
H	-4.58020100	-0.69700300	-2.44259300
H	-5.73854000	0.52040000	-1.89642500
C	-4.93587100	0.79615600	0.55940000
H	-4.87834300	1.82760100	0.20364600
H	-5.98879000	0.53570800	0.70299400
C	-4.65869700	-1.52334600	-0.12615500
H	-4.66807400	-1.63505600	0.96193700
H	-5.66679100	-1.73922100	-0.49383700
C	-3.63365200	-2.46527600	-0.69438300
C	-3.92142400	-3.77302600	-1.07430800
H	-4.93947000	-4.14239700	-1.01370800
C	-2.87834500	-4.58046300	-1.52940800

H	-3.07378600	-5.60524800	-1.82947400
C	-1.58687100	-4.05457500	-1.60565700
H	-0.75250200	-4.64899300	-1.96129700
C	-1.38096000	-2.73478900	-1.22155800
H	-0.40811100	-2.26249900	-1.27737700
C	-2.31794300	3.29898400	1.09234700
H	-2.77191300	2.83389200	1.95966700
C	-1.87795800	4.61733700	1.13785900
H	-1.98954600	5.19477300	2.04906300
C	-1.29277200	5.16408800	-0.00696700
H	-0.93542800	6.18916700	-0.00984800
C	-1.17896100	4.37566000	-1.14954300
H	-0.73659600	4.76248400	-2.06206600
C	-1.64540200	3.06021500	-1.10921400
C	-1.48499800	2.14477500	-2.29772400
H	-0.44874400	1.79461000	-2.32257000
H	-1.67922900	2.68980200	-3.23060100
C	-1.89362100	-0.04381000	-3.21903100
H	-0.88849100	-0.37433300	-2.95052200
H	-2.55793900	-0.90682600	-3.22408100
H	-1.88001700	0.40647600	-4.21961900
C	-4.15528500	0.70326100	1.87478400
O	-4.67395100	1.06643200	2.93350100
O	-2.93282200	0.26787600	1.76086600
O	1.51138700	1.66630000	-0.79249300

¹TS₅

Mn	1.17570600	-0.16846700	-0.11680200
O	-0.44772600	0.68196100	-0.30160200
N	1.24668700	-0.33013400	-2.27477000
N	3.40004500	-0.10034600	-0.44184800
N	6.20093900	0.77460800	1.02273900
N	0.75022300	-2.45011300	-0.62429100
C	2.61906200	-0.75896400	-2.67611700
H	2.71726200	-1.82442800	-2.46147300
H	2.74778700	-0.62139200	-3.75621600
C	3.65138600	0.03855400	-1.90596900
H	3.58244600	1.09625500	-2.16202200
H	4.66280300	-0.29711800	-2.15947100
C	3.96829100	-1.36428200	0.08227500
H	3.68995400	-2.17660800	-0.59583100
H	5.05882700	-1.32060600	0.12929900
C	3.89439000	1.09700400	0.31490000

H	3.29261400	1.94627500	-0.01854000
H	3.68961000	0.91620500	1.36830200
C	5.37102000	1.39442100	0.15987000
C	5.83180300	2.27793100	-0.82213100
H	5.12565900	2.77019900	-1.48317000
C	7.20137500	2.51853800	-0.92958400
H	7.58341000	3.20233400	-1.68181700
C	8.06543000	1.86931500	-0.04882900
H	9.13870000	2.02484700	-0.08977700
C	7.51566800	1.01266600	0.90521100
H	8.15985000	0.49789400	1.61461200
C	0.89791500	-3.53706400	0.14919800
H	1.17058700	-3.35204800	1.18076700
C	0.71745600	-4.82964100	-0.33672800
H	0.84879800	-5.67843000	0.32533000
C	0.36641200	-4.99737400	-1.67623100
H	0.22336400	-5.99057100	-2.09057900
C	0.20443000	-3.86885700	-2.48020300
H	-0.06119100	-3.95409500	-3.52865600
C	0.40280000	-2.61123600	-1.91541300
C	0.23775300	-1.33533900	-2.69935000
H	-0.75094900	-0.91201400	-2.49964400
H	0.32412900	-1.51938800	-3.77659300
C	0.91157500	0.99560300	-2.85759100
H	1.56684300	1.76085600	-2.43899500
H	1.03357200	0.96312900	-3.94706400
H	-0.11781400	1.24382000	-2.60465500
C	3.39119900	-1.71037800	1.45236800
O	4.04324600	-2.41385400	2.23386200
O	2.19495100	-1.26051300	1.66608200
Mn	-2.24244100	0.72228600	-0.04203900
N	-2.66818200	0.59159200	2.27820300
N	-4.32774200	1.19679900	0.02313700
N	-2.19222000	2.82782600	0.00977500
N	-2.32512100	-1.41195400	0.46598900
C	-4.13461900	0.37875800	2.36379600
H	-4.35350300	-0.65508800	2.08761400
H	-4.49344900	0.52976700	3.39072600
C	-4.85442400	1.32461400	1.42168100
H	-4.70081700	2.35849100	1.73561300
H	-5.93244300	1.13367000	1.42138600
C	-5.01300100	0.13869100	-0.75918800
H	-5.06705200	-0.76918300	-0.15206300

H	-6.03263600	0.44605000	-1.01361100
C	-4.46846500	2.51116500	-0.68064100
H	-4.37006400	2.34055900	-1.75619400
H	-5.46231600	2.93046100	-0.49468600
C	-3.37160500	3.43619200	-0.24226000
C	-3.51474300	4.81474500	-0.12992800
H	-4.47732200	5.27329800	-0.32810300
C	-2.40706200	5.57603500	0.24430600
H	-2.49466200	6.65340600	0.34323800
C	-1.19163600	4.93816000	0.49871700
H	-0.31091200	5.49584700	0.79695700
C	-1.12198800	3.55628200	0.37451000
H	-0.21759600	2.99585200	0.57303700
C	-2.48598000	-2.39206500	-0.44479400
H	-2.59558700	-2.07746800	-1.47310000
C	-2.50724900	-3.73586900	-0.09811900
H	-2.64366500	-4.48606500	-0.86785600
C	-2.32398600	-4.08361000	1.24046400
H	-2.32742900	-5.12463300	1.54729300
C	-2.13479400	-3.07262700	2.17952500
H	-1.99464000	-3.29811700	3.23137000
C	-2.14114700	-1.74291700	1.76120300
C	-1.93970700	-0.60637700	2.72972300
H	-0.87580400	-0.35564600	2.76071100
H	-2.25141800	-0.90871900	3.73892900
C	-2.24108500	1.77182600	3.05355100
H	-1.17636400	1.93918300	2.88792100
H	-2.78757400	2.65544600	2.72099200
H	-2.42598400	1.62224600	4.12708100
C	-4.20718100	-0.18015300	-2.02396000
O	-4.75466400	-0.77450900	-2.96084600
O	-2.96216200	0.17671400	-1.98671300
O	0.52700000	0.91799100	1.37991300
O	1.49139700	0.86532600	2.87402800
H	2.15182500	1.55943100	2.68402900
H	1.92502700	-0.01254300	2.60919300

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Mn	-1.23025600	-0.10516200	-0.17463100
O	0.53972400	-0.29005500	-0.02855600
N	-1.39560000	-0.63510400	-2.15738800
N	-3.40522900	0.01882500	-0.28336600
N	-6.30465700	0.14754300	1.06412800

N	-0.73457500	1.70105300	-1.14203300
C	-2.67816500	-0.02287300	-2.65623100
H	-2.51658100	1.04752600	-2.78019600
H	-2.91695300	-0.44010600	-3.64102500
C	-3.81974600	-0.26279100	-1.69129900
H	-4.11844000	-1.31086300	-1.73312500
H	-4.68767500	0.34146000	-1.97416700
C	-3.59118300	1.41208300	0.19112700
H	-3.24615200	2.10814900	-0.57762600
H	-4.63722500	1.63162200	0.40958800
C	-4.14283900	-0.92702900	0.63065600
H	-3.77707200	-1.92510500	0.40066500
H	-3.85738400	-0.69324100	1.65753900
C	-5.65335000	-0.89561900	0.51184500
C	-6.32716900	-1.94888300	-0.11653300
H	-5.76493100	-2.77444700	-0.54151900
C	-7.71993800	-1.92014200	-0.18824700
H	-8.26348700	-2.72823400	-0.66874500
C	-8.39545600	-0.83606400	0.36934900
H	-9.47805600	-0.76599100	0.34102000
C	-7.64246700	0.16776900	0.97938400
H	-8.13684700	1.02529500	1.43043100
C	-0.69615200	2.94500500	-0.63377500
H	-1.09963800	3.08242800	0.36142300
C	-0.16385000	4.01780200	-1.33893000
H	-0.16415400	5.00439800	-0.89123600
C	0.38449800	3.78738700	-2.60045000
H	0.81630500	4.60206400	-3.17296200
C	0.37318900	2.49218900	-3.11544000
H	0.78668300	2.26712900	-4.09260200
C	-0.19808400	1.47228800	-2.36162900
C	-0.26250200	0.04612700	-2.83936000
H	0.66020900	-0.47142100	-2.56812500
H	-0.38597600	-0.00134500	-3.92769300
C	-1.35305900	-2.09507000	-2.39813700
H	-0.39733100	-2.48233000	-2.04084100
H	-2.16031500	-2.57626400	-1.84361100
H	-1.46298400	-2.31093600	-3.46807000
C	-2.74957800	1.59845300	1.46302400
O	-3.04158700	2.44842100	2.29996800
O	-1.69538000	0.81188100	1.56047800
Mn	2.29343800	-0.36852600	0.01898100
N	2.49064600	-0.36192400	2.21624300

N	4.36366800	-0.72039300	0.11165000
N	2.41609200	-2.58718000	-0.18267800
N	2.37515000	1.94714900	0.77796200
C	3.93744500	-0.09367900	2.47877800
H	4.12341100	0.96997400	2.32843700
H	4.18503000	-0.33389300	3.52010000
C	4.80154600	-0.91088700	1.53440400
H	4.71057200	-1.97469300	1.76081200
H	5.85691400	-0.63691500	1.63411600
C	4.97462700	0.46138700	-0.54767100
H	4.98311600	1.29878200	0.15464700
H	6.00684500	0.25013500	-0.84458700
C	4.67508500	-1.94731900	-0.68738000
H	4.61919800	-1.68296600	-1.74767100
H	5.69845800	-2.27448300	-0.47676800
C	3.66731200	-3.02950400	-0.41087400
C	3.97219000	-4.38784300	-0.42864700
H	4.99269700	-4.71196900	-0.60257700
C	2.94283900	-5.30550000	-0.21389500
H	3.15256900	-6.37063500	-0.22040900
C	1.64682800	-4.83990900	0.01748200
H	0.82342800	-5.52356800	0.19325500
C	1.42380300	-3.46702700	0.03189200
H	0.44516200	-3.04010600	0.22186100
C	2.62669700	3.08033900	0.10377900
H	3.02641900	2.97079300	-0.89785700
C	2.39512600	4.34297200	0.64148500
H	2.62239100	5.22893500	0.05892400
C	1.85016200	4.43090700	1.92279100
H	1.64448000	5.39759200	2.37218600
C	1.58472800	3.25639000	2.62528400
H	1.17982500	3.27967200	3.63198000
C	1.87140100	2.03148100	2.02171900
C	1.63507600	0.72705500	2.74344200
H	0.59422500	0.42139300	2.60279600
H	1.80864100	0.85567700	3.81996600
C	2.06223600	-1.64312200	2.82529200
H	1.03555300	-1.85176600	2.52452800
H	2.70051900	-2.45623000	2.48129200
H	2.11946300	-1.58005600	3.91992000
C	4.13125100	0.86824200	-1.76274300
O	4.61444100	1.60595400	-2.62739500
O	2.90811200	0.42260300	-1.77130800

O	-1.48819100	-1.82355800	0.55898100
O	-1.38380000	-1.71320400	2.09425800
H	-2.18098600	-2.19565100	2.41152600
H	-1.55951500	-0.72141900	2.23967500

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Mn	-0.00374000	-0.03937500	-0.55597500
O	0.15924700	-0.88072600	-1.98608600
N	0.25880500	-1.63333500	0.78055100
N	-0.59538200	1.01822700	1.25825000
N	-2.04650700	-0.18512700	-0.63061400
N	2.07555000	-0.09478100	-0.36090400
C	0.50744100	-1.00575500	2.13035300
H	1.51579500	-0.58952800	2.12576700
H	0.46677700	-1.78501900	2.89910600
C	-0.49893400	0.09017700	2.42095800
H	-1.48967000	-0.33926200	2.58051200
H	-0.22000000	0.63332000	3.32998400
C	0.33554600	2.16143800	1.24880000
H	1.33350100	1.82072000	1.54214800
H	0.02553200	2.95937000	1.93144700
C	-1.99070500	1.50169200	1.08773000
H	-1.97767100	2.45416100	0.54836400
H	-2.46200000	1.68885000	2.05752900
C	-2.76979700	0.51993300	0.26705600
C	-4.14984400	0.37301100	0.36193600
H	-4.69612600	0.94701600	1.10234800
C	-4.79649200	-0.51166100	-0.49883500
H	-5.87188200	-0.64554700	-0.43882700
C	-4.04349200	-1.22476500	-1.43360500
H	-4.50600900	-1.92310200	-2.12178300
C	-2.66915000	-1.03915900	-1.46780900
H	-2.02594700	-1.57006500	-2.15756800
C	2.94522400	0.86598000	-0.72628200
H	2.52991200	1.81129700	-1.04652900
C	4.31871700	0.65951500	-0.70895300
H	4.98080900	1.46398300	-1.00816100
C	4.81018700	-0.58150300	-0.30457400
H	5.87831300	-0.77106400	-0.27470700
C	3.90791600	-1.57763300	0.06347700
H	4.24351000	-2.55677600	0.38726900
C	2.54547900	-1.30596600	0.01320600
C	1.49691100	-2.32763000	0.33451900

H	1.25502100	-2.89735300	-0.56710400
H	1.83820100	-3.02572100	1.10671000
C	-0.86017000	-2.60946200	0.82883900
H	-1.04089000	-2.98594300	-0.17860300
H	-1.76366300	-2.12743200	1.19999900
H	-0.59101000	-3.43963400	1.49155100
O	0.11102800	1.79800400	-1.13167100
C	0.39811900	2.68740400	-0.18939100
O	0.71747400	3.84191000	-0.44544500

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Mn	-0.68217900	0.01643500	0.01984900
O	0.36467100	1.22140800	-0.49509800
N	-1.06031000	-0.84353600	-1.84736400
N	-2.30254700	-1.28705200	0.64718300
N	-2.28276800	1.29551100	-0.02692800
N	0.90071800	-1.33974400	-0.16088500
C	-1.68788600	-2.18701700	-1.56657100
H	-0.90395900	-2.85472200	-1.20796100
H	-2.08127600	-2.59767900	-2.50241800
C	-2.78432700	-2.07531300	-0.52543100
H	-3.64850400	-1.55363600	-0.93969600
H	-3.11432700	-3.07116600	-0.21253300
C	-1.65861400	-2.05171500	1.73296700
H	-0.97892700	-2.79392100	1.30243400
H	-2.38623600	-2.57230600	2.36365200
C	-3.39829000	-0.44847200	1.20392400
H	-3.18764300	-0.23834200	2.25751300
H	-4.35367800	-0.98047000	1.16744600
C	-3.45778900	0.86098000	0.47826600
C	-4.61488400	1.62650100	0.38008500
H	-5.54341100	1.24182800	0.78730900
C	-4.54992300	2.87310700	-0.23912500
H	-5.44095000	3.48637500	-0.32803700
C	-3.32735500	3.32039700	-0.74414400
H	-3.23280800	4.28407300	-1.23157700
C	-2.21386700	2.50191200	-0.62490800
H	-1.23998000	2.78125300	-1.00548100
C	1.72442400	-1.74659900	0.82266900
H	1.46740800	-1.46124700	1.83261900
C	2.86447400	-2.49686600	0.56135800
H	3.49678300	-2.80594800	1.38564200
C	3.16635300	-2.82983200	-0.75876200

H	4.04792800	-3.41753500	-0.99303700
C	2.32062300	-2.39245400	-1.77652200
H	2.51780700	-2.62124900	-2.81800000
C	1.20372900	-1.63455700	-1.44514300
C	0.27621600	-1.05327800	-2.46772000
H	0.65568200	-0.07783400	-2.78487700
H	0.18669500	-1.69906200	-3.34797500
C	-1.90296800	-0.02658800	-2.75782500
H	-1.44357800	0.95534600	-2.87557200
H	-2.90190500	0.08936700	-2.33984900
H	-1.97043900	-0.52276200	-3.73237600
O	-0.44859500	0.03452000	1.92741300
C	-0.84229200	-1.05976800	2.56924200
O	-0.55142400	-1.27921400	3.73769100
O	2.32315600	1.33377500	1.35917900
H	1.61469700	1.29730800	0.65505100
O	3.21334900	2.35982700	0.83557700
C	4.30714900	1.75181600	0.08797700
C	5.15500600	2.97468300	-0.27177600
H	5.50832700	3.48219600	0.63220200
H	6.02544500	2.65745400	-0.85477900
H	4.57708700	3.68595000	-0.87178800
C	3.77144000	1.06019900	-1.16631200
H	3.13345500	0.21580000	-0.90097200
H	3.19148600	1.76178500	-1.77576300
H	4.60186300	0.67855000	-1.77011200
C	5.08425600	0.78064800	0.97793300
H	5.41195700	1.28121000	1.89573700
H	4.46829400	-0.08197900	1.24732600
H	5.96943700	0.41500700	0.44641500

TBHP

O	-1.98889500	0.12492000	-0.17020900
H	-2.23724600	-0.81475900	-0.07774100
O	-0.73194600	0.01615200	-0.89674400
C	0.38980200	-0.00143700	0.03706800
C	1.58289300	-0.09968800	-0.91699300
H	1.61122800	0.76089100	-1.59385000
H	2.51120100	-0.11513600	-0.33717200
H	1.53113100	-1.01652300	-1.51382300
C	0.29995300	-1.23041300	0.94252400
H	-0.57743500	-1.17374800	1.59449600
H	0.23342700	-2.14441800	0.34178100

H	1.19028400	-1.29564600	1.57659500
C	0.42545700	1.29857200	0.84046400
H	0.46272100	2.16271300	0.16810800
H	-0.45991500	1.38728300	1.47661100
H	1.31270100	1.31855600	1.48224900

TS₈₋₉

Mn	-0.62866500	-0.11628700	-0.22313000
O	0.30755100	-1.49814600	0.18628800
N	-0.85803200	0.54575100	1.99662600
N	-2.17377500	1.41029500	-0.37618900
N	-2.42945800	-1.27432500	-0.19499400
N	1.15059100	1.17108100	0.24981200
C	-1.48362200	1.89203600	1.95635200
H	-0.72099800	2.61546400	1.66010500
H	-1.84699500	2.18248600	2.95108000
C	-2.62822800	1.90501900	0.96066900
H	-3.43013200	1.24706000	1.29989200
H	-3.04700600	2.91193700	0.85894200
C	-1.58054600	2.47576900	-1.21597700
H	-0.88782900	3.06433500	-0.60743600
H	-2.35011900	3.14645400	-1.61189100
C	-3.31671600	0.77284200	-1.09452600
H	-3.05941900	0.69229000	-2.15467500
H	-4.21170900	1.39810000	-1.01376400
C	-3.54841100	-0.61042400	-0.55575900
C	-4.80436500	-1.20049700	-0.45799300
H	-5.68588300	-0.63752200	-0.74444400
C	-4.89707900	-2.50912700	0.01682700
H	-5.86631700	-2.98942900	0.10623400
C	-3.73394400	-3.18859200	0.38342100
H	-3.76587700	-4.20431100	0.76121200
C	-2.51419000	-2.53364400	0.26692200
H	-1.57500300	-2.99775200	0.54285800
C	1.98409800	1.70031400	-0.66364700
H	1.72283900	1.54016200	-1.70132000
C	3.12496200	2.41105600	-0.30927000
H	3.76370300	2.82310700	-1.08251900
C	3.41816300	2.57118600	1.04536300
H	4.29808800	3.12330700	1.36028000
C	2.56238000	2.01030600	1.99132600
H	2.75288000	2.11028900	3.05471700
C	1.43899900	1.30751700	1.55826900

C	0.51373300	0.61772700	2.52814400
H	0.86960000	-0.40859500	2.67118000
H	0.53646000	1.12082500	3.50391200
C	-1.65456800	-0.41226000	2.78884700
H	-1.21630400	-1.40745700	2.68676300
H	-2.67943800	-0.44637600	2.41801300
H	-1.66748400	-0.12554000	3.84953000
O	-0.41364700	0.60226500	-2.12915900
C	-0.77976600	1.83624100	-2.34943000
O	-0.48914500	2.47805900	-3.36022100
O	1.99582200	-2.07238700	-1.42686900
O	3.10585400	-1.24382300	-1.25521200
C	4.08038900	-1.80169200	-0.29548900
C	5.22263000	-0.79157500	-0.38857200
H	6.02943100	-1.10085300	0.28319600
H	5.61873300	-0.74453500	-1.40823000
H	4.88593000	0.20614900	-0.09119500
C	4.50806300	-3.19094500	-0.76293200
H	5.29861200	-3.56639400	-0.10530200
H	3.66914700	-3.89114600	-0.72887200
H	4.89574600	-3.14948600	-1.78620100
C	3.46574100	-1.82798600	1.10370100
H	3.14514100	-0.82630200	1.40402800
H	2.60882400	-2.50538700	1.14630300
H	4.21737300	-2.18065000	1.81755700
H	1.27152700	-1.79003800	-0.64459400

tBuOO•

O	1.98141500	-0.00006200	-0.18724100
O	0.84135100	-0.00166900	-0.84859100
C	-0.37127100	0.00009800	0.04934300
C	-1.51787900	-0.00163800	-0.95263000
H	-1.48163100	-0.89372600	-1.58648500
H	-2.46827300	-0.00123200	-0.40992900
H	-1.48217900	0.88879900	-1.58880700
C	-0.32444700	1.27108500	0.88781800
H	0.56243100	1.27902900	1.52752300
H	-0.31058700	2.15831900	0.24637900
H	-1.21386000	1.31472800	1.52430400
C	-0.32424700	-1.26807300	0.89208100
H	-0.30574500	-2.15726500	0.25346100
H	0.56047400	-1.27158900	1.53484900
H	-1.21569200	-1.31204500	1.52568200

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Mn	-0.08705500	-0.05311100	0.66817900
O	0.06606900	0.90196800	2.21854300
N	0.24019700	1.64675000	-0.82357700
N	-0.62494500	-1.05581900	-1.11033700
N	-2.23654100	0.19481400	0.66910300
N	2.20525100	0.18338000	0.38760800
C	0.40472100	0.96076700	-2.13517000
H	1.40619600	0.52706000	-2.17005100
H	0.32363400	1.68000700	-2.96040800
C	-0.63688000	-0.13156400	-2.29245300
H	-1.63667500	0.30052400	-2.35757400
H	-0.46400000	-0.70865900	-3.20643400
C	0.36305600	-2.15720000	-1.23989100
H	1.30136500	-1.74391300	-1.62068400
H	0.00883000	-2.91783800	-1.94250100
C	-1.99459200	-1.61810200	-0.89306700
H	-1.90694300	-2.48763000	-0.23509300
H	-2.41299000	-1.95711800	-1.84582500
C	-2.87078300	-0.59624900	-0.22185200
C	-4.23850900	-0.48395000	-0.44921700
H	-4.71806200	-1.12421900	-1.18150300
C	-4.96241400	0.46190500	0.27803800
H	-6.03061600	0.57042100	0.11861300
C	-4.30019100	1.26928600	1.20488000
H	-4.82980300	2.01558100	1.78625000
C	-2.92905700	1.10906300	1.36752200
H	-2.35289800	1.71281600	2.05931100
C	3.14686000	-0.70482500	0.75507300
H	2.78771400	-1.64482300	1.15595800
C	4.50708300	-0.44286200	0.63569900
H	5.23030700	-1.19073600	0.94170900
C	4.90594400	0.78872400	0.11328900
H	5.95917300	1.02584900	-0.00141500
C	3.93175100	1.71029300	-0.26525300
H	4.19859300	2.67664700	-0.68054000
C	2.58761800	1.37575100	-0.10558300
C	1.48327500	2.34688800	-0.44046200
H	1.26209100	2.94768500	0.44841600
H	1.80467200	3.03276500	-1.23524200
C	-0.87795200	2.61551100	-0.84235200
H	-1.02845500	3.00053300	0.16833700

H	-1.79660700	2.12836900	-1.16808900
H	-0.65510700	3.44879500	-1.52221000
O	0.37228800	-2.00202200	1.15286300
C	0.64704900	-2.77014700	0.13613700
O	1.14337700	-3.89672500	0.21751400
H	0.98247900	0.82627900	2.54152700
TS₉₋₁₀			
Mn	-0.53664200	0.12480200	-0.46840400
O	1.21973700	-0.13227400	-1.53895800
N	-0.49306300	0.32390600	1.94667800
N	-2.75638600	-0.21324700	0.14135200
N	-0.78921800	-2.11402400	-0.30145200
N	0.09891400	2.24776900	0.04293200
C	-1.88345100	0.73914200	2.26123400
H	-2.01522600	1.75989500	1.89054700
H	-2.04180200	0.76075400	3.35007700
C	-2.91952000	-0.17393600	1.61575600
H	-2.81569400	-1.19194300	1.99651300
H	-3.92831000	0.16544700	1.88451900
C	-3.47346300	0.88000200	-0.53763000
H	-3.37319700	1.78857200	0.06511800
H	-4.54520300	0.66475200	-0.63615800
C	-3.13157600	-1.53062000	-0.41392000
H	-3.22199900	-1.42402100	-1.50048400
H	-4.10393300	-1.86513000	-0.03016000
C	-2.05408100	-2.54791700	-0.12510000
C	-2.32688600	-3.85235000	0.27995700
H	-3.35491900	-4.16755300	0.42447500
C	-1.26246100	-4.72800700	0.50203600
H	-1.45186000	-5.74708200	0.82522800
C	0.04336100	-4.27566000	0.30993300
H	0.89862900	-4.92228100	0.47350700
C	0.23430500	-2.95684300	-0.09091200
H	1.22492100	-2.54799300	-0.25424500
C	0.12224600	3.21397000	-0.89345500
H	-0.17968000	2.90961100	-1.88989200
C	0.49915100	4.52018800	-0.60643900
H	0.50735600	5.26902600	-1.39096000
C	0.85317900	4.83385600	0.70825700
H	1.14655600	5.84487500	0.97401800
C	0.81525100	3.83529300	1.67894900
H	1.07225700	4.04506600	2.71227600
C	0.43774400	2.54233700	1.31013900

C	0.44367500	1.40577000	2.30608000
H	1.45253100	0.98345100	2.33169400
H	0.23547400	1.79305900	3.31412900
C	-0.12036500	-0.90661900	2.67185300
H	0.88878900	-1.20554200	2.38065300
H	-0.79997900	-1.71951400	2.41534200
H	-0.14864800	-0.75129300	3.76118100
O	-1.66271800	0.83296100	-2.13094000
C	-2.88231000	1.20482000	-1.91719400
O	-3.58390700	1.83366500	-2.72638000
O	2.63222300	-1.14822400	-1.92443200
H	1.09889500	0.23042600	-2.44011200
O	3.74944800	-0.47881400	-1.63214800
C	4.24759200	-0.74029300	-0.24139900
C	5.56666200	0.02431100	-0.23856000
H	5.40060300	1.08893500	-0.43281100
H	6.03543300	-0.07966800	0.74482600
H	6.25208500	-0.37389400	-0.99370100
C	4.44746000	-2.24087300	-0.06654400
H	3.49529800	-2.77595600	-0.11412600
H	5.11735300	-2.63381300	-0.83816100
H	4.89704600	-2.42831000	0.91376500
C	3.24480500	-0.16249900	0.74981500
H	3.10040000	0.90871700	0.58003600
H	2.27927700	-0.66473300	0.66609000
H	3.62570000	-0.30768300	1.76605400

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Mn	-0.47332400	0.18583900	-0.46602400
O	1.55720900	-0.06429700	-1.75834400
N	-0.55134500	0.37683400	1.97694900
N	-2.78679900	0.14073200	0.05368300
N	-1.03851900	-2.02234800	-0.32402700
N	0.49044900	2.17007300	0.10666500
C	-1.88288500	0.98380900	2.21196500
H	-1.85006100	2.00869400	1.82958900
H	-2.09550000	1.04181200	3.29097100
C	-3.00602700	0.21783400	1.51701400
H	-3.06416100	-0.80027800	1.90831200
H	-3.96760700	0.69814500	1.74373600
C	-3.31114100	1.31040500	-0.66455100
H	-3.12074800	2.20202000	-0.05732600
H	-4.39645400	1.24546200	-0.82088400

C	-3.28501800	-1.12406500	-0.51826400
H	-3.30456500	-1.01424300	-1.60826500
H	-4.30986700	-1.34315700	-0.18952300
C	-2.35758100	-2.26760000	-0.17213800
C	-2.82308800	-3.50262900	0.27480800
H	-3.88903800	-3.66205200	0.39988100
C	-1.90232900	-4.51075200	0.56631000
H	-2.24420600	-5.47772500	0.92276200
C	-0.54107200	-4.25492200	0.40210200
H	0.20976200	-5.00647400	0.62093400
C	-0.15511700	-2.99376400	-0.04230100
H	0.88836600	-2.73634400	-0.17976900
C	0.73453400	3.11620400	-0.81813900
H	0.49422000	2.84703600	-1.84162700
C	1.25313100	4.36414600	-0.49322200
H	1.43811300	5.09686400	-1.27129900
C	1.51480800	4.64195900	0.85060200
H	1.91213300	5.60801400	1.14706000
C	1.25010900	3.66657000	1.80981500
H	1.43230500	3.85127000	2.86369900
C	0.74232200	2.43124300	1.40156000
C	0.51517100	1.30888600	2.38918700
H	1.44710600	0.73869100	2.46280100
H	0.31739800	1.72495200	3.38822300
C	-0.39138900	-0.89590600	2.70475500
H	0.57776800	-1.33352900	2.45290600
H	-1.16664100	-1.60437700	2.41183900
H	-0.44495000	-0.74509900	3.79429100
O	-1.43608100	1.04921700	-2.16962600
C	-2.61519300	1.55132100	-2.01465300
O	-3.20717800	2.24887800	-2.85757000
O	2.26510900	-1.32365500	-1.84113800
H	1.43447900	0.16657300	-2.70214300
O	3.64100700	-1.02462400	-1.64344300
C	4.02834900	-1.27847800	-0.24232100
C	5.45963700	-0.74094200	-0.22588800
H	5.47454800	0.33373600	-0.43423900
H	5.89477800	-0.91159600	0.76378800
H	6.07838900	-1.25569400	-0.96850300
C	3.99119100	-2.78361400	0.01557300
H	2.97196100	-3.17242800	-0.06558500
H	4.62576900	-3.31077400	-0.70452900
H	4.35690500	-2.99730900	1.02530000

C	3.12542800	-0.50886800	0.71920600
H	3.14831000	0.56461700	0.51017800
H	2.09080100	-0.85671400	0.65329000
H	3.47370000	-0.67229400	1.74429500

TS₃₋₁₁

Mn	0.60734500	-0.08891900	-0.40401000
O	-0.51378300	0.91713800	-1.27113600
N	0.40948700	-0.02887600	1.94115800
N	2.38413300	-1.19386100	0.22817500
N	2.08686100	1.39730200	-0.43570800
N	-1.00417600	-1.49701600	0.13766600
C	1.25259300	-1.14923100	2.42855300
H	0.71745900	-2.08245300	2.23746100
H	1.40892600	-1.07193300	3.51302700
C	2.58663500	-1.16188100	1.70918000
H	3.15603100	-0.26187300	1.94806800
H	3.18822500	-2.02326600	2.01892000
C	2.22223600	-2.57152000	-0.29052300
H	1.52885600	-3.11373600	0.35871700
H	3.17867000	-3.10545700	-0.29100900
C	3.53220500	-0.52181000	-0.45006800
H	3.52503800	-0.80648800	-1.50625300
H	4.48088400	-0.85560100	-0.01705800
C	3.36511100	0.96791700	-0.35600000
C	4.41972400	1.86515600	-0.22713600
H	5.43560300	1.49277400	-0.15446800
C	4.13936100	3.23148000	-0.18575300
H	4.94603700	3.94998800	-0.08007400
C	2.81455800	3.66384500	-0.27185200
H	2.55830900	4.71673900	-0.23798000
C	1.80987800	2.71258900	-0.39393100
H	0.76100200	2.97677400	-0.45521600
C	-1.54535000	-2.35998600	-0.74586400
H	-1.03984500	-2.44089500	-1.69889700
C	-2.68975700	-3.09382700	-0.46443400
H	-3.08650100	-3.77705500	-1.20707700
C	-3.30417300	-2.92483800	0.77784400
H	-4.20066700	-3.48123900	1.03268400
C	-2.74845800	-2.03032300	1.68806000
H	-3.19273800	-1.86933900	2.66470000
C	-1.59846100	-1.32359200	1.33399200
C	-1.00555400	-0.28937300	2.25630600

H	-1.56017400	0.64331500	2.12460000
H	-1.12746800	-0.59901500	3.30332800
C	0.81827700	1.26860800	2.51778800
H	0.23269400	2.06297500	2.05024200
H	1.87382800	1.45572400	2.31871600
H	0.65242800	1.28362300	3.60420600
O	1.00375000	-1.45241600	-2.02140500
C	1.61979800	-2.54546800	-1.69797600
O	1.71444800	-3.54919500	-2.41650100
O	-1.71931000	1.89576600	0.10099700
O	-2.67510400	2.53915800	-0.52972000
C	-3.97967600	1.77651200	-0.61051000
C	-4.88694600	2.79061000	-1.29414600
H	-5.88147900	2.35109500	-1.41702000
H	-4.98152200	3.70033800	-0.69251000
H	-4.50023200	3.05506600	-2.28362000
C	-4.42299500	1.45229500	0.80998100
H	-5.41447400	0.98994400	0.77234900
H	-3.73570200	0.74813500	1.28582400
H	-4.48555300	2.36265500	1.41462300
C	-3.75113000	0.52981700	-1.45352400
H	-3.36785800	0.79119900	-2.44459800
H	-3.04880100	-0.14538400	-0.96434700
H	-4.70596400	0.00801400	-1.57392700

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Mn	0.53593200	-0.06426300	-0.34157700
O	-0.65897800	1.23428600	-0.92346300
N	0.55149200	-0.21652200	2.01547000
N	2.22777700	-1.33867200	-0.01545100
N	2.11038800	1.32745700	-0.32938000
N	-1.12008700	-1.38859100	0.22285300
C	1.31369300	-1.45949400	2.29001800
H	0.67372300	-2.31326000	2.05529400
H	1.58248400	-1.52712200	3.35280800
C	2.56476900	-1.50537800	1.43582300
H	3.24232400	-0.69581200	1.71176200
H	3.10071800	-2.44960700	1.57617300
C	1.90545500	-2.62638400	-0.67734100
H	1.20596200	-3.17923200	-0.04361700
H	2.80843500	-3.23199600	-0.80640800
C	3.37389600	-0.67556200	-0.71458400
H	3.25394400	-0.82278800	-1.79141600

H	4.31715700	-1.14029100	-0.41139400
C	3.34934500	0.79792400	-0.42586900
C	4.48348500	1.59161700	-0.29604000
H	5.46697800	1.14040800	-0.36634300
C	4.32278800	2.95960300	-0.07045600
H	5.19319300	3.59894200	0.03804600
C	3.03692200	3.49582000	0.02190600
H	2.87501600	4.55286600	0.19991600
C	1.94795000	2.64357800	-0.11074600
H	0.92390200	2.98986600	-0.04112300
C	-1.77929100	-2.15422600	-0.66977100
H	-1.37361500	-2.17115200	-1.67249500
C	-2.91945300	-2.87266200	-0.33588400
H	-3.41416200	-3.47566200	-1.08900700
C	-3.40022500	-2.79425000	0.97216700
H	-4.28733600	-3.34429900	1.27013600
C	-2.72222100	-1.99973900	1.89277700
H	-3.05927100	-1.91184700	2.92025800
C	-1.58725400	-1.29976500	1.48409100
C	-0.85413400	-0.37616000	2.42187800
H	-1.33314500	0.60694000	2.38214400
H	-0.93325000	-0.74200100	3.45491900
C	1.13892700	0.95711400	2.69145400
H	0.59997800	1.85371600	2.37713800
H	2.18687100	1.06912000	2.41127300
H	1.07046400	0.85586700	3.78385500
O	0.68539600	-1.19573300	-2.15287600
C	1.22466000	-2.36825800	-2.02559800
O	1.19142400	-3.26782000	-2.87343800
O	-1.47862700	1.73953400	0.17419300
O	-2.41925400	2.62656700	-0.41397900
C	-3.71491400	1.96454700	-0.64720900
C	-4.56131500	3.14337400	-1.13252000
H	-5.57378900	2.78987800	-1.35161500
H	-4.62316500	3.92319400	-0.36646900
H	-4.14010800	3.57557200	-2.04631800
C	-4.24472200	1.39514200	0.66669300
H	-5.26063700	1.01419800	0.51832000
H	-3.62126000	0.56825600	1.01665800
H	-4.27293800	2.17118200	1.43901700
C	-3.58763800	0.89183400	-1.72611500
H	-3.16128300	1.31200600	-2.64276300
H	-2.95629300	0.06799200	-1.38934500

H	-4.58023000	0.48920600	-1.95597100
TS₁₁			
Mn	0.45257800	0.03667200	-0.32207000
O	-0.83585700	2.16385900	0.81494500
N	0.82096100	-0.57751600	1.94381000
N	2.26497000	-1.43986600	-0.46942200
N	2.30885000	1.35630200	-0.33350600
N	-1.34527100	-1.21502100	0.34692400
C	1.49612700	-1.89707500	1.85472200
H	0.75659500	-2.62640400	1.51292200
H	1.84306500	-2.22029200	2.84765900
C	2.67640000	-1.88150600	0.88474200
H	3.44650900	-1.19454300	1.24314000
H	3.13150600	-2.88033800	0.84958700
C	1.74047300	-2.52519700	-1.31123200
H	1.12325200	-3.18135200	-0.68866300
H	2.54312000	-3.13740000	-1.74394900
C	3.33439500	-0.69007100	-1.15505300
H	3.06257100	-0.60875400	-2.21290600
H	4.29584800	-1.21782500	-1.10164000
C	3.46428000	0.70817100	-0.59472600
C	4.70305600	1.30909400	-0.37812400
H	5.61205500	0.75415000	-0.58557100
C	4.74940300	2.61482800	0.11094600
H	5.70456000	3.09913400	0.28976900
C	3.55354500	3.28278900	0.37479900
H	3.54148300	4.29665700	0.75976100
C	2.35689800	2.61219900	0.14275100
H	1.40058400	3.08262100	0.34395900
C	-2.18296300	-1.82331300	-0.51110000
H	-1.99458700	-1.64064400	-1.56326100
C	-3.22930100	-2.63422900	-0.08585600
H	-3.88324200	-3.10380800	-0.81251700
C	-3.40776600	-2.82014600	1.28641500
H	-4.21349800	-3.44521500	1.65920900
C	-2.52625800	-2.20653100	2.17537100
H	-2.61967100	-2.34754500	3.24732100
C	-1.49775200	-1.41041700	1.66932400
C	-0.50789500	-0.71276700	2.57396200
H	-0.87901300	0.29552900	2.78467100
H	-0.44057400	-1.24287900	3.53484100
C	1.62387400	0.39970900	2.70280700

H	1.12828600	1.37291400	2.66772700
H	2.61275200	0.50567700	2.25564600
H	1.74056700	0.09141900	3.75284300
O	0.34571700	-0.81339200	-2.29156200
C	0.82912100	-2.00301800	-2.43687600
O	0.58414400	-2.76090200	-3.39125700
O	-2.01009100	1.96717900	1.12087100
O	-3.11424400	2.89087900	0.09214100
C	-3.73426200	1.97905600	-0.80792600
C	-4.75412900	2.90034000	-1.51849100
H	-5.29193100	2.30146800	-2.26193300
H	-5.47444900	3.30876400	-0.80363200
H	-4.24713100	3.72369100	-2.03057300
C	-4.46522600	0.86821600	-0.04376400
H	-5.00724300	0.22242200	-0.74188400
H	-3.75932100	0.24760100	0.51384900
H	-5.18045100	1.30334100	0.66221400
C	-2.71840400	1.42980200	-1.81567700
H	-2.24649600	2.25096400	-2.36641900
H	-1.93589900	0.86306000	-1.30606600
H	-3.20928700	0.76291600	-2.53218300

tBuO•

O	-0.00098600	0.27496700	-1.43774600
C	0.00015600	-0.02971200	-0.07766100
C	-0.00547400	1.38374300	0.58857700
H	-0.90018900	1.94187100	0.30006100
H	-0.00615000	1.23430800	1.67349500
H	0.88579200	1.94831700	0.30200300
C	1.27858100	-0.78923000	0.31086600
H	1.30810300	-1.75865800	-0.19871200
H	2.16554400	-0.21534400	0.02321900
H	1.30654700	-0.96632600	1.39137100
C	-1.27239500	-0.79916900	0.31077100
H	-2.16375800	-0.23357000	0.02033300
H	-1.29265500	-1.76994200	-0.19672200
H	-1.30055300	-0.97418000	1.39160200

tBu-O-O-O-O-tBu

O	-0.39721800	-0.59522600	-0.42310200
O	-1.37996300	-0.46746300	0.61265200
C	-2.64988100	0.03318000	0.06278800
C	-3.52445500	0.06015700	1.31785000

H	-3.11333400	0.74644400	2.06546600
H	-4.52856600	0.40169800	1.04713000
H	-3.60511000	-0.93862800	1.75926600
C	-3.18032100	-0.95745700	-0.97176100
H	-2.51219000	-1.01289700	-1.83647100
H	-3.27435600	-1.95673000	-0.53356700
H	-4.16678000	-0.63564000	-1.32159200
C	-2.46922600	1.43214100	-0.52252300
H	-2.02623300	2.10762900	0.21588600
H	-1.82889200	1.40969000	-1.40902800
H	-3.44632200	1.82885400	-0.81795600
O	0.39748600	0.59510300	-0.42453400
O	1.38037100	0.47014200	0.61136300
C	2.64976900	-0.03327100	0.06294800
C	3.52515400	-0.05484800	1.31754600
H	3.11664000	-0.74045500	2.06721000
H	4.53001400	-0.39407900	1.04678800
H	3.60327200	0.94526300	1.75643500
C	3.17995200	0.95255200	-0.97629000
H	2.51137100	1.00451000	-1.84087700
H	3.27440600	1.95371300	-0.54250900
H	4.16613300	0.62893800	-1.32516200
C	2.46834900	-1.43467600	-0.51625400
H	2.02583700	-2.10696500	0.22533000
H	1.82742600	-1.41585900	-1.40242500
H	3.44522900	-1.83259900	-0.81077000

2

Mn	-0.00011200	-0.03691400	0.81732900
O	0.07136900	-1.10420800	2.85348000
N	-0.29083800	-1.60430100	-0.92506400
N	0.67661600	1.15663500	-1.13725200
N	2.37159800	-0.13956600	0.67703000
N	-2.31087100	-0.38034600	0.58101900
C	-0.43046300	-0.81663400	-2.17449700
H	-1.41547400	-0.34207100	-2.15778100
H	-0.40098900	-1.47822200	-3.05338300
C	0.65121600	0.25430200	-2.30931100
H	1.63364600	-0.21700400	-2.39022600
H	0.49009100	0.81753400	-3.23936400
C	-0.31828200	2.23590200	-1.20655200
H	-1.24295700	1.83396200	-1.63353200
H	0.00979700	3.06067700	-1.85436600

C	2.02724900	1.68887200	-0.88322200
H	1.93434500	2.51346500	-0.16807600
H	2.47900400	2.09794300	-1.79760700
C	2.92746000	0.63824000	-0.27270200
C	4.26338200	0.49584800	-0.64741600
H	4.67532200	1.13305600	-1.42324500
C	5.04468900	-0.47351000	-0.01781300
H	6.08671800	-0.60196400	-0.29479700
C	4.46526100	-1.28011000	0.96233400
H	5.03283800	-2.05160100	1.47146700
C	3.12275800	-1.08053800	1.27209400
H	2.62180100	-1.69306100	2.01574100
C	-3.25390300	0.49390700	0.96947600
H	-2.91075500	1.31137400	1.59521400
C	-4.58870100	0.37489400	0.59218300
H	-5.31709800	1.10334000	0.93163300
C	-4.95126600	-0.68883800	-0.23522100
H	-5.98024200	-0.81100900	-0.55964600
C	-3.96984600	-1.58675800	-0.65572500
H	-4.21013000	-2.41414000	-1.31549000
C	-2.65600400	-1.40246000	-0.22613400
C	-1.53858500	-2.33864500	-0.62598600
H	-1.32879400	-3.01105900	0.21420000
H	-1.85008500	-2.96005900	-1.47776500
C	0.83741500	-2.55148600	-0.99725400
H	0.95833600	-3.03826800	-0.02573500
H	1.76088300	-2.01886700	-1.22573900
H	0.66874000	-3.31904300	-1.76792700
O	-0.40708100	2.05599700	1.20350600
C	-0.68540700	2.79298200	0.18119600
O	-1.25813800	3.89682200	0.23152900
H	-0.64051600	-0.71424800	3.39168700
H	0.89173500	-0.82953700	3.30055400

tBuOH

O	0.07734300	-0.00529500	1.45729900
C	-0.00771200	0.00011900	0.01177200
C	0.65306400	1.27251800	-0.53046700
H	1.71686300	1.29492100	-0.26245300
H	0.57659400	1.32131100	-1.62269200
H	0.17219700	2.16199400	-0.10801800
C	-1.50333200	-0.01626000	-0.30333300
H	-1.97469900	-0.91149700	0.11804400

H	-1.99493200	0.86606100	0.12215600
H	-1.66661300	-0.01560900	-1.38601200
C	0.68303400	-1.25191800	-0.54030200
H	1.74706400	-1.25100400	-0.27210200
H	0.22350900	-2.15562600	-0.12427800
H	0.60775300	-1.29456800	-1.63281300
H	1.02319900	-0.00037400	1.68376100

O₂

O	0.00000000	0.00000000	0.60662400
O	0.00000000	0.00000000	-0.60662400

H₂O

O	0.00000000	0.00000000	0.12099200
H	0.00000000	-0.75908000	-0.48396800
H	0.00000000	0.75908000	-0.48396800