

Supporting Information for:

Elucidating the Catalytic Mechanisms of O₂ Generation by [Mn₂(μ-O)₂(terpy)₂(OH₂)₂]³⁺ using DFT calculations: A Focus on ClO⁻ as Oxidant

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Computational details. Gaussian 16¹ was used to fully optimize all the structures reported in this paper at the M06-L level of theory, assuming conditions representative of a neutral pH.² The M06-L functional has been confirmed in numerous studies to provide very accurate results for transformations involving transition metal complexes.³ In addition, the M06-L functional has been reported to perform well in modelling water oxidation in various studies⁴ and specifically, benchmark calculations in a recent study clearly indicate that M06-L is more suitable compared to other functionals, including B3LYP, for simulating a water oxidation process.⁵ For all the calculations, solvent effects were considered using the SMD-B solvation model⁶ with water as the solvent. A recent study has suggested that using the SMD-B model with Bondi radii instead of traditional SMD improves the solvation energies of anions in water.⁷ Consequently, we employed the SMD-B model in all our calculations to enhance the accuracy of the results. The SDD basis set with effective core potential (ECP) was chosen to describe Mn. The 6-31G(d) basis set was used for other atoms. This basis set combination will be referred to as BS1. Frequency calculations were carried out at the same level of theory as those for structural optimization. Transition structures were located using the Berny algorithm. Intrinsic reaction coordinate (IRC) calculations were used to confirm the connectivity between transition structures and minima.⁸ To further refine the energies obtained from the SMD-B/M06-L/SDD,6-31G(d) calculations, we carried out single-point energy calculations using the M06-L functional method with SMD-B solvation model in water along with a larger basis set (BS2) for all the optimized structures. BS2 utilizes the 6-311+G(2d,p) on all atoms except for Mn for which SDD basis set with effective core potential (ECP) is used .

In this work, the free energy for each species in solution was calculated using the following formula:

$$G = E(\text{BS2}) + G(\text{BS1}) - E(\text{BS1}) + \Delta G^{1\text{atm} \rightarrow 1\text{M}} \quad (1)$$

where $\Delta G^{1\text{atm} \rightarrow 1\text{M}} = 1.89$ kcal/mol is the free-energy change for compression of 1 mol of an ideal gas from 1 atm to the 1 M solution phase standard state.

An additional correction to Gibbs free energies was made to consider solvent (water) concentration where a $(\text{H}_2\text{O})_n$ is directly involved in transformations. In such a case, the free energy of $(\text{H}_2\text{O})_n$ is described as follows

$$G = E(\text{BS2}) + G(\text{BS1}) - E(\text{BS1}) + \Delta G^{1\text{atm} \rightarrow 1\text{M}} + RT \ln(55.34/n) \quad (2)$$

where the last term corresponds to the free energy required to change the standard state of $(\text{H}_2\text{O})_n$ from 55.34/n M to 1 M.

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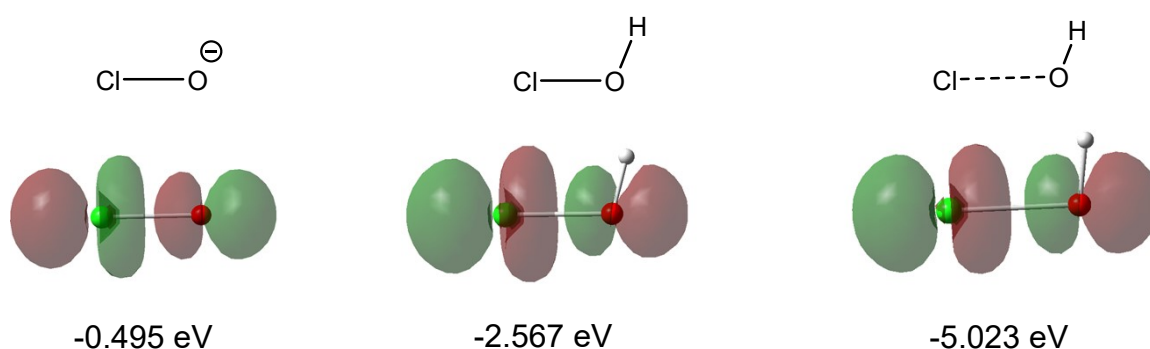


Fig. S1 LUMO energies for ClO^- , HClO , and $\text{HCl}\cdots\text{O}$ (the $\text{HCl}\cdots\text{O}$ species is a deformed HOCl with geometry in transition structure $\text{TS}_{9,10}$).

Benchmark calculations. Our benchmark calculations reveal that among the B3LYP, M06, and M06L functionals, only M06L produces results aligning with experimental data. According to Table S1, B3LYP and M06 predict relatively high activation energies for Mn(III) oxidation via transition structures TS_{20-21} and TS_{20-22} . Additionally, they indicate that ligand oxidation through transition structure TS takes place considerably faster than Mn(III) oxidation, a finding that conflicts with existing experimental data. In contrast, M06L accurately forecasts a lower activation energy for Mn(III) oxidation and correctly indicates that metal oxidation proceeds more rapidly than ligand oxidation.

Table S1. Comparison of calculated free energies for Mn(III) oxidation via transition structures TS_{20-21} and TS_{20-22} , and ligand oxidation through transition structure TS at the SMD-B/Method-D3/6-311+G(2d,p), SDD//SMD-B/B3LYP-D3/6-31G(d),SDD levels of theory, with relative energies in kcal/mol

Method	1	TS_{20-21}	TS_{20-22}	TS
B3LYP	0.0	23.1	24.2	15.8
M06	0.0	26.5	26.3	20.9
M06L	0.0	9.2	6.8	12.5

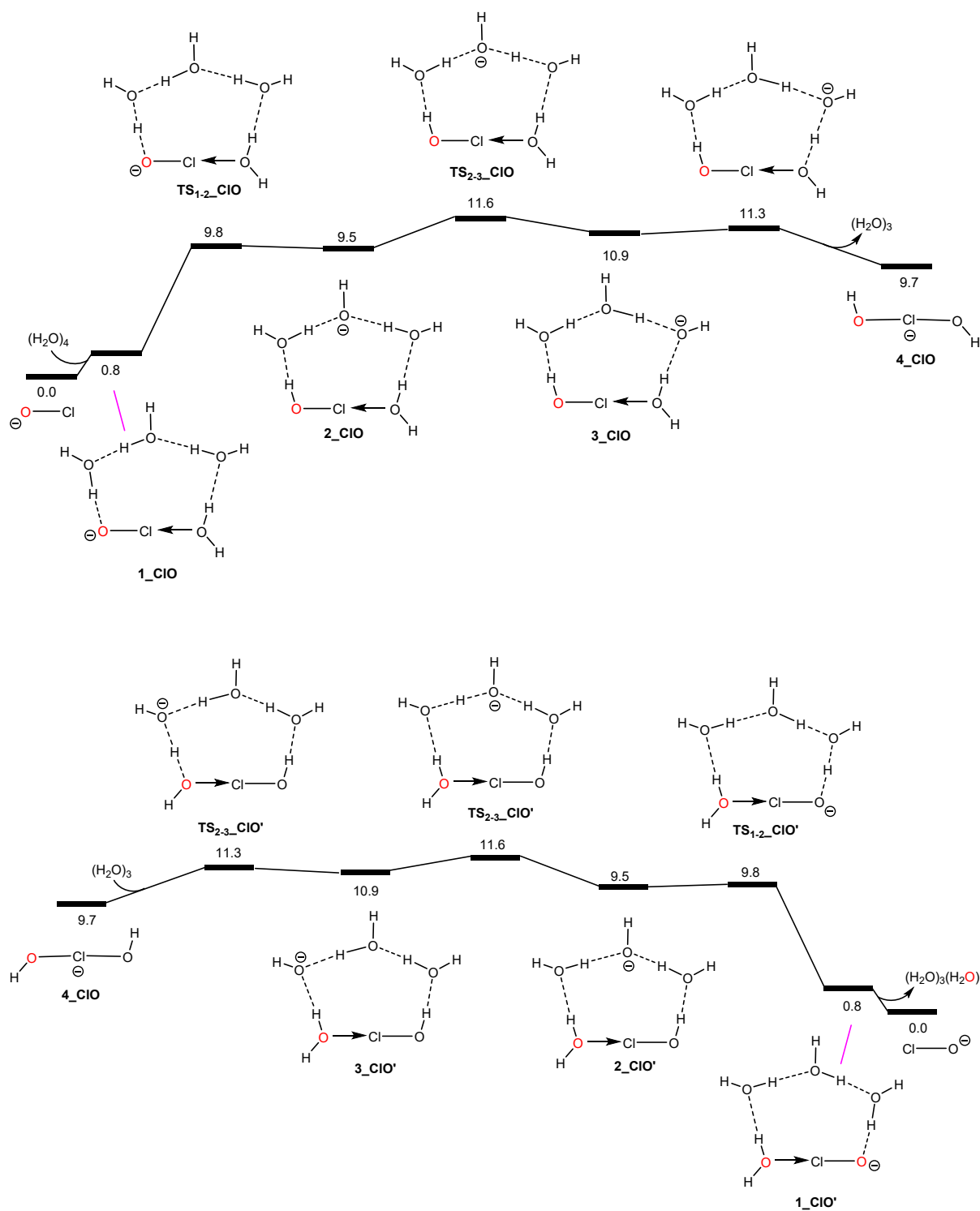


Fig. S2 Free energy profiles depicting the mechanism for exchanging the ClO⁻ oxygen atom with water, involving ClO⁻ hydrolysis to yield **4_CIO** (top profile), followed by **4_CIO** condensation, recreating ClO⁻ with its oxygen derived from water (bottom profile). The relative free energy values are in kcal/mol.

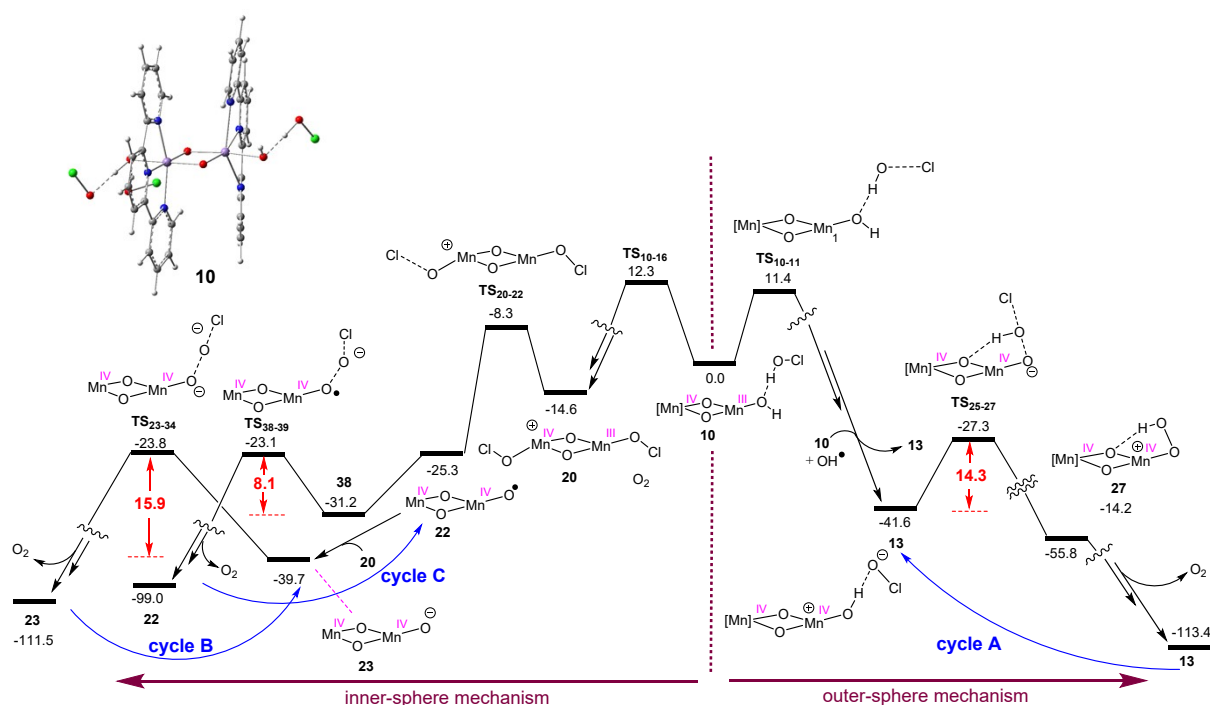


Fig S3. A simplified energy profile for the generation of O₂ from ClO⁻, using complex **10** as the catalyst. The relative Free energy values are in kcal/mol.

Comments to Fig S3

- Oxidation of complex **10** through an outer-sphere mechanism produces complex **13** as the active catalyst, while oxidation through an inner-sphere mechanism results in two active catalysts, **22** and **23**.
- Given that the energy levels of the two transition structures, **TS₁₀₋₁₁** and **TS₁₀₋₁₆**, are very similar, it is anticipated that the inner- and outer-sphere mechanisms will be competitive.
- According to our calculations, the concentration of active catalyst **22** is expected to be significantly lower than that of active catalysts **13** and **23**. Drawing from experimental findings (ref 6a), we can estimate that its concentration should be around 2% of the Mn catalyst used.
- Although the concentration of catalyst **22** is much lower than that of **13** and **23**, it is significantly more reactive than both, outperforming them in catalytic activity. This advantage is evidenced by a substantially lower energy barrier for O-O coupling from **22** (8.1 kcal/mol) compared to **13** (14.3 kcal/mol) and **23** (15.9 kcal/mol)
- Our conclusion that complex **22** serves as the active catalyst for O₂ generation aligns with the kinetic data presented in ref 4b.

Table S2. Cartesian coordinates of all structures optimized at the SMD-B/M06-L-D3/6-31G(d),SDD level of theory in water.

2_c1o

O	1.53571800	-1.69489500	0.01240800
Cl	-0.16014600	-1.35634800	-0.09766400
O	-2.67979500	-0.43307600	-0.17985800
H	-2.20809500	0.38865700	0.12557500
H	-2.88138000	-0.88454500	0.65272700
O	0.60399300	1.84462000	-1.10382800
H	1.57138300	1.25398800	-0.17311500
O	-1.25159700	1.74626600	0.70564200
H	-0.79834000	1.26177200	1.41082100
H	-0.52233400	1.80508500	-0.03012900
O	2.23584200	0.79298300	0.52500800
H	1.88964200	-0.75948400	0.21573400
H	0.34881700	1.04448200	-1.58367700
H	1.76952100	0.90077600	1.36738300

TS2-3_c1o

O	-1.87736200	-1.40074200	-0.00566400
Cl	-0.13978900	-1.35175200	0.09613100
O	2.43666900	-0.91497900	0.16706400
H	2.15546900	-0.00477400	-0.18662700
H	2.58504100	-1.42457800	-0.64280800
O	0.01560700	1.92261900	1.05000400
H	-1.29034400	1.52265300	0.16035200
O	1.58907400	1.42948500	-0.75332000
H	0.98854000	1.05899900	-1.41537700
H	0.80066100	1.69068000	0.17251100
O	-2.06497600	1.23713200	-0.43632300
H	-2.06196900	-0.42103300	-0.16407500
H	0.07391900	1.12011900	1.58778100
H	-1.66699800	1.24960300	-1.32005900

3_c1o

O	-1.95655300	-1.32043300	-0.00159100
Cl	-0.20768500	-1.31530500	0.10091300
O	2.31906000	-1.02520800	0.18222600
H	2.12866200	-0.08150300	-0.22233500
H	2.46654400	-1.57303000	-0.60244100
O	0.13069900	1.91623600	1.09218100
H	-1.25777300	1.58366500	0.12786500
O	1.75867000	1.29526200	-0.80013400
H	1.07709700	0.99036800	-1.41515400
H	0.81747000	1.68473800	0.33680000
O	-2.01758400	1.34396600	-0.47804200
H	-2.11086500	-0.34371500	-0.17386800
H	0.12674100	1.10740800	1.62495800
H	-1.59157100	1.31366900	-1.34844900

TS3-4_c1o

O	-1.99191600	-1.29652100	0.02894200
Cl	-0.21351600	-1.29126400	0.11380900
O	2.20296300	-1.06960300	0.17766800
H	2.06606500	-0.02640000	-0.28098400
H	2.35475900	-1.63044600	-0.59712800
O	0.16376100	1.95900200	1.08277100
H	-1.23262500	1.61935900	0.08114300
O	1.84822900	1.17087300	-0.77375600

H	1.16229600	0.97481500	-1.42756600
H	0.84923400	1.67480200	0.37677400
O	-1.97721000	1.38648800	-0.53924800
H	-2.13645600	-0.32894000	-0.16756500
H	0.11854800	1.18039300	1.65700600
H	-1.51867200	1.28599100	-1.38745300
(H₂O)₃			
O	-1.11579700	-1.18065900	-0.11101700
H	-1.34089400	-1.36176700	0.81385800
H	0.74093600	-0.89688500	0.05139400
O	1.57578800	-0.38007200	0.12376800
H	1.92168100	-0.39968700	-0.78118800
H	0.40748600	1.08340700	-0.00822600
O	-0.44970200	1.55862800	-0.10437400
H	-0.67095400	1.78930100	0.81035900
H	-1.14056800	-0.19754800	-0.15320900
4 ClO			
O	2.04176900	-0.08903700	-0.03779300
Cl	0.00015800	-0.00046400	-0.02905600
O	-2.04186600	0.08970200	-0.03810700
H	-2.19588700	-0.66380100	0.55149100
H	2.19396800	0.66637000	0.54966000
10			
Mn	-1.24621500	0.08110900	-0.83464100
O	-0.31844100	-0.27135900	0.76281000
N	-2.09113900	-2.08243300	-0.83621300
N	-3.04543400	0.01193700	0.46790100
N	-1.92948500	2.25942400	-0.38058800
C	-1.53572000	-3.08477600	-1.51928900
H	-0.88666400	-2.79392100	-2.34575100
C	-1.75168500	-4.42238900	-1.20441400
H	-1.27975200	-5.20600600	-1.79027100
C	-2.56901600	-4.71628900	-0.11832700
H	-2.75153900	-5.74706400	0.17484300
C	-3.15542200	-3.67642000	0.59501200
H	-3.79047400	-3.89125100	1.44945600
C	-2.90228300	-2.36084600	0.20405800
C	-3.49556100	-1.18658000	0.87724100
C	-4.47954000	-1.28940500	1.86278100
H	-4.85330800	-2.25818100	2.17901100
C	-4.98422200	-0.12433300	2.42486600
H	-5.74867800	-0.17682100	3.19550100
C	-4.50881800	1.10887200	1.99886700
H	-4.88877500	2.02510700	2.43944000
C	-3.52780200	1.14551700	1.00543900
C	-2.96221300	2.40294400	0.47235700
C	-3.46984700	3.66421800	0.79123500
H	-4.30590200	3.77157500	1.47589000
C	-2.90423900	4.78769200	0.19899700
H	-3.28995100	5.77704300	0.43202100
C	-1.85210800	4.62982700	-0.69713400
H	-1.38596400	5.48163500	-1.18415400
C	-1.39588700	3.34107900	-0.95100600
H	-0.56146500	3.15968400	-1.62991100
Mn	1.31507300	0.06727200	0.14070600
O	2.10019100	-0.30406200	1.86415200
O	0.48220600	0.38630500	-1.46208000
N	1.45941400	2.07809000	0.58920800
C	0.62037400	2.72585500	1.39998200
H	-0.17127600	2.12635700	1.84320100

C	0.74766200	4.08654100	1.65211800
H	0.04047100	4.57852700	2.31315800
C	1.77541800	4.78526600	1.02960100
H	1.89542100	5.85289100	1.19253400
C	2.66491200	4.10397600	0.20509300
H	3.49034000	4.62502100	-0.27055700
C	2.49654100	2.73689700	0.00746600
C	3.40341900	1.88663200	-0.77475000
N	3.07876400	0.58541100	-0.73511800
N	2.03860400	-1.75817200	-0.53703200
C	3.21163300	-1.70796000	-1.22314200
C	3.77573100	-0.35993600	-1.38125000
C	4.90775200	-0.00545400	-2.11462700
C	5.26945700	1.33830900	-2.16502000
C	4.51874800	2.30359600	-1.50032800
H	4.79650800	3.35203200	-1.54588900
H	6.14431700	1.63685500	-2.73601500
H	5.48685600	-0.75657000	-2.64293700
C	3.80073300	-2.87273100	-1.70493900
H	4.73962900	-2.82165900	-2.24837600
C	3.18199000	-4.09513300	-1.46594300
H	3.63361300	-5.01308500	-1.83234900
C	1.99010200	-4.13002300	-0.75173400
H	1.47854800	-5.06401100	-0.53896700
C	1.44920000	-2.93177600	-0.30024600
H	0.52110300	-2.89412700	0.26500700
H	3.06898600	-0.55126600	1.72789100
H	1.63926800	-1.67182000	2.40476200
O	1.53312100	-2.62773500	2.80104300
Cl	-0.16132200	-2.86770200	2.91956200
O	-2.07292600	0.33402500	-2.59603000
H	-1.65513900	1.14252700	-2.93534700
H	-3.50841600	0.81034500	-2.32063200
O	4.63071000	-1.09826400	1.56095000
O	-4.46318000	1.18478500	-2.15008600
Cl	-5.43140200	-0.22539300	-2.03325900
Cl	5.52192500	0.37593600	1.63933500

TS10-11

Mn	-0.88059100	0.05804400	-0.50370700
O	-1.28587500	0.44532400	-2.32851600
O	-0.41903800	-0.44547300	1.21065400
N	-1.56420200	-1.89373800	-0.82645500
N	-2.81753200	0.12070300	0.14678100
N	-1.12371500	2.04468800	-0.03592300
C	-0.82876600	-2.84986400	-1.39511700
H	0.12937600	-2.53613500	-1.80254300
C	-1.26469400	-4.16842300	-1.46154100
H	-0.63298100	-4.92095000	-1.92410800
C	-2.50355400	-4.48711400	-0.91799600
H	-2.87153800	-5.50913900	-0.94377700
C	-3.27852800	-3.48424600	-0.34478200
H	-4.25410100	-3.71001000	0.07550600
C	-2.78659100	-2.18307700	-0.31239200
C	-3.49963400	-1.03035600	0.25171100
C	-4.75424700	-1.04418100	0.85924100
H	-5.31832900	-1.96653700	0.95525200
C	-5.26533800	0.15511300	1.34664900
H	-6.24244800	0.16955500	1.82125100
C	-4.53076300	1.33308800	1.24630000
H	-4.91885100	2.26626800	1.64305000
C	-3.27613300	1.28053500	0.64039700
C	-2.33306300	2.39306100	0.47836200

C	-2.61277500	3.71888200	0.79281900
H	-3.58019100	3.98529000	1.20782600
C	-1.64987600	4.69283200	0.54906100
H	-1.85908000	5.73298300	0.78392900
C	-0.42780100	4.32267000	0.00115000
H	0.35118200	5.05071700	-0.20485400
C	-0.19850700	2.97937600	-0.27385400
H	0.74749100	2.62362300	-0.67334300
Mn	1.38509600	-0.54590000	0.91922500
O	1.65967600	-1.34792500	2.64964500
O	0.86992300	-0.00315800	-0.81282900
N	1.71451400	1.51026100	1.74843800
C	0.86073800	2.11009000	2.57960800
H	0.00923000	1.51115800	2.89993000
C	1.03497100	3.42249300	3.00291200
H	0.31683100	3.87532900	3.68028100
C	2.13226200	4.13038400	2.52284800
H	2.29666300	5.16336200	2.81873300
C	3.02476800	3.50490900	1.65958200
H	3.89434700	4.03714000	1.28558300
C	2.79517700	2.17793400	1.29495300
C	3.68622900	1.40065000	0.41804000
N	3.38042500	0.09540300	0.29949900
N	2.43315600	-2.33109200	0.03784700
C	3.60232200	-2.09082000	-0.59528100
C	4.08736100	-0.70458200	-0.51600100
C	5.18390900	-0.21793600	-1.22901700
C	5.52404400	1.12210000	-1.09437900
C	4.77184100	1.94710000	-0.26795500
H	5.01411200	3.00118200	-0.17374100
H	6.36805100	1.52822300	-1.64507200
H	5.75093700	-0.86808800	-1.88774900
C	4.28454900	-3.11454300	-1.25069400
H	5.22625400	-2.91555400	-1.75317500
C	3.75216600	-4.39878400	-1.23995300
H	4.27176300	-5.20738500	-1.74745400
C	2.56056700	-4.63654500	-0.56464300
H	2.11465800	-5.62578900	-0.52166400
C	1.93726700	-3.56343200	0.06360200
H	0.99662200	-3.69036600	0.61131700
H	-0.57947500	1.09779100	-2.63658300
H	-2.54787400	1.29088500	-2.40006900
H	2.46288800	-1.88810500	2.57162700
O	-0.24638600	-3.31335700	2.08831600
H	0.36828400	-2.56280700	2.33644200
Cl	-1.74597900	-2.83650500	3.33305800
O	0.33294800	2.35742900	-3.27426800
O	-3.39462100	1.89468600	-2.46934900
Cl	-4.66631700	0.75494400	-2.62396800
Cl	2.02492200	2.22486200	-2.96361100

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Mn	0.80013500	0.07993900	-0.62054300
O	1.13015600	0.01390400	-2.46516800
O	0.32728000	0.28645600	1.19843800
N	1.37777700	2.08039500	-0.64784700
N	2.70632500	0.01343800	0.09794300
N	1.16996100	-1.93490300	-0.52479400
C	0.64191400	3.05914100	-1.17599000
H	-0.29800800	2.75844300	-1.63492800
C	1.05666900	4.38578300	-1.13635100
H	0.42999200	5.15773500	-1.57222700
C	2.26891000	4.68706700	-0.52707400

H	2.62030300	5.71385700	-0.47523700
C	3.04165800	3.66136100	0.00801200
H	4.00065800	3.87228200	0.47169100
C	2.57684600	2.35265800	-0.06984500
C	3.30731400	1.17256200	0.40833500
C	4.50747400	1.16330700	1.11802900
H	5.00943900	2.09019900	1.37692900
C	5.04150700	-0.06478500	1.49747200
H	5.97363800	-0.09646600	2.05450900
C	4.38517500	-1.25244800	1.18787800
H	4.78881400	-2.20955100	1.50316600
C	3.18723000	-1.18017300	0.47930300
C	2.33682400	-2.30241600	0.06655400
C	2.66499300	-3.64821200	0.19839000
H	3.59659900	-3.93672000	0.67583700
C	1.80065000	-4.60955200	-0.31521000
H	2.04656700	-5.66403900	-0.22328200
C	0.63468900	-4.20988300	-0.95878000
H	-0.05731900	-4.93007700	-1.38459800
C	0.34711100	-2.85276600	-1.03901700
H	-0.54438800	-2.46723500	-1.53322800
Mn	-1.42565500	0.14687100	1.01097900
O	-1.71138200	0.37465700	2.86975000
O	-0.97315400	0.06330600	-0.81462500
N	-1.64813200	-1.88578000	1.25516500
C	-0.76232200	-2.64880200	1.90092200
H	0.12274700	-2.13981300	2.27738500
C	-0.96422700	-4.01291900	2.06918800
H	-0.22286900	-4.60348900	2.59849900
C	-2.11256100	-4.58828300	1.53565200
H	-2.29527500	-5.65438000	1.63904200
C	-3.03948100	-3.78742100	0.87690500
H	-3.95518000	-4.21084000	0.47524400
C	-2.79460600	-2.42245300	0.76031400
C	-3.71701900	-1.44910300	0.16142300
N	-3.33842500	-0.17608100	0.35609500
N	-2.14926400	2.07167100	0.71962300
C	-3.36134800	2.15887500	0.11116700
C	-4.00254400	0.86759900	-0.16412600
C	-5.17020600	0.65370600	-0.89430800
C	-5.60117000	-0.65691000	-1.08060500
C	-4.87800300	-1.72587800	-0.55896600
H	-5.20108200	-2.74906900	-0.72409900
H	-6.50436800	-0.84792000	-1.65319300
H	-5.71953500	1.48610900	-1.32311300
C	-3.91398700	3.40021400	-0.18489100
H	-4.88350000	3.46084000	-0.67028000
C	-3.21733400	4.55305400	0.16425800
H	-3.63708200	5.52966800	-0.06089600
C	-1.99275400	4.44348600	0.81196500
H	-1.42287600	5.31885600	1.10827900
C	-1.48669700	3.17485100	1.07293300
H	-0.53251000	3.02072600	1.57724200
H	0.36471900	-0.53109000	-2.86197600
H	2.46951100	-0.75557900	-2.67608600
H	-2.52302300	0.90024000	2.96722800
O	0.41548200	2.18844200	3.47822800
H	-0.23999500	1.48806700	3.22704800
Cl	2.02352700	0.08092600	4.14291400
O	-0.88072100	-1.36470000	-3.49825000
O	3.37360000	-1.23421500	-2.80508400
Cl	4.48643700	0.07059100	-2.82047900
Cl	-1.96490400	-0.11651400	-3.99070900

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Mn	-1.14882400	0.15520300	0.24077900
O	-1.86463200	0.08088600	1.97032400
O	-0.31711600	0.18900200	-1.47351600
N	-1.33664500	2.21658300	0.32723700
N	-2.87219500	0.50102400	-0.78784700
N	-1.85648200	-1.75040400	-0.09897100
C	-0.54875700	2.99281100	1.07490500
H	0.24782800	2.48768200	1.61756800
C	-0.73476300	4.36797000	1.14742100
H	-0.07013100	4.96701400	1.76236600
C	-1.76778700	4.94009200	0.41477200
H	-1.93678400	6.01298500	0.44335500
C	-2.60023400	4.12657400	-0.34678300
H	-3.42945000	4.54994700	-0.90513300
C	-2.37349000	2.75394500	-0.36625500
C	-3.21279300	1.77014500	-1.06109400
C	-4.27162300	2.03589000	-1.92822100
H	-4.55962400	3.05762800	-2.15642300
C	-4.94297400	0.95960000	-2.50032100
H	-5.77017200	1.14210300	-3.18038100
C	-4.55929900	-0.34817100	-2.21792800
H	-5.07360800	-1.18909100	-2.67250900
C	-3.49215900	-0.55135200	-1.34432600
C	-2.94007100	-1.84152300	-0.91457600
C	-3.48334000	-3.08253800	-1.22959500
H	-4.34133500	-3.14806600	-1.89192000
C	-2.93425200	-4.22685000	-0.66005700
H	-3.35295700	-5.20236000	-0.89220000
C	-1.86772000	-4.10684500	0.22243200
H	-1.42519200	-4.97364200	0.70385600
C	-1.34609900	-2.84264900	0.47389200
H	-0.51262500	-2.67867500	1.15724200
Mn	1.35595200	-0.10473400	-0.91587600
O	2.13137600	-0.00198400	-2.60990800
O	0.52402900	-0.12593800	0.77349700
N	1.48350000	-2.16446900	-1.01050500
C	0.70873000	-2.90956600	-1.80209000
H	-0.03428800	-2.37361400	-2.38823300
C	0.83768600	-4.29188800	-1.85746600
H	0.18733000	-4.86528100	-2.51089000
C	1.78866800	-4.90532300	-1.05051400
H	1.90544600	-5.98549000	-1.05837000
C	2.60578300	-4.12461200	-0.23974000
H	3.37273100	-4.58064800	0.37878100
C	2.44816600	-2.74206200	-0.24859200
C	3.29043400	-1.79158800	0.48647700
N	3.03098700	-0.51073500	0.18117300
N	2.10448600	1.78093800	-0.51106600
C	3.15049100	1.82787300	0.35367100
C	3.64171400	0.51626400	0.79191000
C	4.63606700	0.27333600	1.73761600
C	4.95137400	-1.04811300	2.03967200
C	4.27618000	-2.09759400	1.42389400
H	4.50320700	-3.12922700	1.67473900
H	5.72149900	-1.26306300	2.77503000
H	5.14486200	1.09416900	2.23343900
C	3.70705800	3.04787200	0.72347800
H	4.53628400	3.07631300	1.42407300
C	3.20744100	4.21831900	0.16264800
H	3.63713300	5.17783900	0.43713000
C	2.17147100	4.14603100	-0.76116700

H	1.76242400	5.03519100	-1.23093100
C	1.63782100	2.89990000	-1.06800700
H	0.80946900	2.78109400	-1.76287900
H	-1.30527600	-0.61879100	2.46242300
H	-3.30864600	-0.49268500	1.86511800
H	3.03203800	0.37215100	-2.50591100
Cl	5.19473400	1.29104500	-2.46773400
O	-0.39231700	-1.72172900	3.21418300
O	-4.27022600	-0.86081400	1.79992100
Cl	-5.21554100	0.56825800	1.73361800
Cl	0.77462000	-0.75911600	4.04385700

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Mn	0.82655800	-0.11545000	-0.54422500
O	1.39305100	-0.56874300	-2.28315200
O	0.22796200	0.29886400	1.20485000
N	1.21484300	1.84867900	-1.04736500
N	2.69983500	0.17204000	0.20634900
N	1.34510600	-2.00720200	0.09870700
C	0.43288100	2.57728100	-1.84720000
H	-0.46273400	2.08367100	-2.21726400
C	0.74295500	3.89203600	-2.17114900
H	0.08078100	4.45559300	-2.82124000
C	1.89370800	4.45734700	-1.63297600
H	2.15810300	5.48796000	-1.85366100
C	2.71770100	3.68909600	-0.81739800
H	3.63395200	4.10312200	-0.40751400
C	2.36623600	2.36984800	-0.54844500
C	3.18482600	1.42267500	0.22006500
C	4.36672200	1.70122300	0.90459900
H	4.77392500	2.70716300	0.93033100
C	5.01222800	0.65407900	1.55615500
H	5.93727800	0.84443600	2.09314500
C	4.48151300	-0.63278000	1.53842700
H	4.98131200	-1.44508200	2.05667500
C	3.28584800	-0.84546300	0.85339600
C	2.54060000	-2.10661400	0.74236500
C	2.98719500	-3.33546000	1.21505900
H	3.93802400	-3.40515700	1.73496200
C	2.21219200	-4.47056200	0.99579300
H	2.55380800	-5.43774900	1.35438000
C	1.00944900	-4.35487500	0.31187100
H	0.37646800	-5.21543400	0.11723100
C	0.60534800	-3.09600200	-0.12116700
H	-0.33783200	-2.93890000	-0.63833700
Mn	-1.51747500	0.29939200	0.86672900
O	-2.04626200	0.61559500	2.59559700
O	-0.90745900	-0.18509900	-0.89941400
N	-2.24237400	-1.65580600	1.08510400
C	-1.64901200	-2.59573800	1.82186200
H	-0.76060000	-2.28675900	2.36910600
C	-2.13230000	-3.89858100	1.87331500
H	-1.61731900	-4.63950800	2.47709100
C	-3.26046900	-4.22059900	1.12803200
H	-3.65583100	-5.23263800	1.13343300
C	-3.89505600	-3.23110200	0.38360300
H	-4.79248400	-3.45324400	-0.18615500
C	-3.37197300	-1.94182700	0.38788400
C	-3.97263600	-0.79409100	-0.30288100
N	-3.35274900	0.36817700	-0.04545900
N	-1.73132900	2.29816300	0.43647100
C	-2.82964100	2.64482300	-0.28404100
C	-3.70152400	1.51966200	-0.64187100

C	-4.79165600	1.55232900	-1.51021600
C	-5.47659200	0.36626500	-1.75700500
C	-5.06990900	-0.82414000	-1.16191300
H	-5.58663000	-1.75563800	-1.37232200
H	-6.32556400	0.36663100	-2.43479700
H	-5.08732400	2.47657500	-1.99692700
C	-3.07648000	3.97988100	-0.59185500
H	-3.95612600	4.25099900	-1.16803000
C	-2.20166600	4.95565900	-0.12607300
H	-2.38717300	6.00208800	-0.35273700
C	-1.10312100	4.58248800	0.64053000
H	-0.40387800	5.31589100	1.03034900
C	-0.89710100	3.23357000	0.89897200
H	-0.06005100	2.87195400	1.49361100
H	0.87445900	-1.39358500	-2.58117700
H	2.81998400	-1.17239600	-2.22422600
O	-0.07624200	1.93565300	3.77813100
H	-1.28834500	1.12793000	3.04128000
O	0.30121900	-2.78900800	-3.18469400
O	3.75417500	-1.61483400	-2.20516500
Cl	4.81179700	-0.27914500	-2.39758100
Cl	-1.41442800	-2.77189700	-3.02976100
Cl	0.87911500	0.66711100	4.45251200

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Mn	-1.23305100	0.02858900	-0.79959000
O	-2.12532300	0.03989100	-2.50940900
O	-0.36652300	-0.05672200	0.83914200
N	-1.69967200	-1.98622900	-0.73991800
N	-2.94043500	-0.00600200	0.32597800
N	-1.68348800	2.02351900	-0.60799800
C	-1.07832900	-2.91580700	-1.46775400
H	-0.27764300	-2.56452900	-2.11460600
C	-1.42977400	-4.25864400	-1.39073200
H	-0.89766100	-4.98694500	-1.99487700
C	-2.44842200	-4.63291300	-0.52318100
H	-2.73912800	-5.67568100	-0.43072100
C	-3.10901100	-3.65889400	0.21917500
H	-3.92476800	-3.92494400	0.88468200
C	-2.72707700	-2.32898200	0.08298900
C	-3.39198900	-1.19745100	0.74106400
C	-4.40892000	-1.25916900	1.69228900
H	-4.79373300	-2.21289000	2.03948000
C	-4.91705400	-0.06215300	2.18948000
H	-5.71052300	-0.08358000	2.93121700
C	-4.41484300	1.16281300	1.75708200
H	-4.80343700	2.09455200	2.15608600
C	-3.39198000	1.15893800	0.81033100
C	-2.71373700	2.32359100	0.22899400
C	-3.08042000	3.64661000	0.44877400
H	-3.89744300	3.87674200	1.12601100
C	-2.40670000	4.65908800	-0.22626900
H	-2.68587100	5.69678100	-0.06568000
C	-1.38859000	4.33049800	-1.11368100
H	-0.84541200	5.09032500	-1.66690600
C	-1.04854600	2.99262000	-1.27242800
H	-0.24289500	2.67423400	-1.93000200
Mn	1.31380600	0.01435400	0.23664900
O	2.04099600	-0.14474900	1.94043000
O	0.42034000	0.08180200	-1.45009500
N	1.62624700	2.04694400	0.30622300
C	0.91847200	2.87075800	1.08305300
H	0.11207300	2.41475900	1.65342500

C	1.19420800	4.23062200	1.14533500
H	0.59442100	4.87056700	1.78511200
C	2.22846700	4.73713600	0.36674100
H	2.46228500	5.79805500	0.38230500
C	2.97934500	3.87247500	-0.42248200
H	3.81116800	4.24143000	-1.01484800
C	2.67237100	2.51525500	-0.42334000
C	3.43537200	1.47672700	-1.12613200
N	3.02366400	0.23307100	-0.83532800
N	1.85910200	-1.93875300	-0.12638300
C	2.93340900	-2.11001600	-0.94217700
C	3.56943100	-0.86282500	-1.38385200
C	4.63902900	-0.73487700	-2.26844300
C	5.09715500	0.54450100	-2.57196100
C	4.49716800	1.66690600	-2.00970900
H	4.84488600	2.66608400	-2.25372300
H	5.92759000	0.66782900	-3.26134000
H	5.09894000	-1.61090400	-2.71497000
C	3.37787000	-3.38767700	-1.26482500
H	4.22719600	-3.51641000	-1.92887900
C	2.73925200	-4.48905100	-0.70411700
H	3.08063500	-5.49289600	-0.94151100
C	1.67794900	-4.29235400	0.17059800
H	1.16236200	-5.12458900	0.63973900
C	1.26000100	-2.99210500	0.43133000
H	0.42222700	-2.77552900	1.09072300
H	-1.70758600	0.76890900	-2.99988700
H	-3.58293800	0.64677400	-2.30644400
H	2.97115200	-0.56846500	1.85798900
O	0.38411700	-1.65904000	3.30427200
H	1.02850800	-1.07270200	2.76795400
Cl	-0.61559700	-0.51182300	4.09657800
O	4.42433800	-1.17800700	1.68645400
O	-4.50746000	1.07691100	-2.21059000
Cl	-5.51566900	-0.26113000	-1.84805400
Cl	5.38422400	0.24984600	1.62127900

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Mn	-1.55410600	0.16649700	-0.91954200
O	-0.73950500	-0.26513500	0.73032900
N	-2.26089100	-1.92785100	-1.35178500
N	-3.50233400	0.04974900	-0.19686700
N	-2.29787800	2.20748800	-1.00530700
C	-1.53787900	-2.88556700	-1.93824200
H	-0.72735300	-2.54595900	-2.58071900
C	-1.78936100	-4.24071100	-1.75006100
H	-1.17601100	-4.98118800	-2.25517900
C	-2.81996200	-4.60988900	-0.89407400
H	-3.03500100	-5.65815400	-0.70404300
C	-3.58060400	-3.62066600	-0.27906900
H	-4.38905700	-3.88670700	0.39574200
C	-3.28422700	-2.28416700	-0.53429600
C	-4.04962800	-1.15666700	0.02507600
C	-5.27182000	-1.25767800	0.69019700
H	-5.72936600	-2.22537500	0.87090000
C	-5.90647200	-0.08875800	1.09710800
H	-6.86059900	-0.14510600	1.61380800
C	-5.34141600	1.15245000	0.82296200
H	-5.84966900	2.06751400	1.11085900
C	-4.11606000	1.19226300	0.15881700
C	-3.40601400	2.41608600	-0.24889300
C	-3.82146300	3.70366600	0.08109800
H	-4.70084900	3.85467100	0.70019600

C	-3.09586700	4.79106500	-0.39388800
H	-3.40834800	5.80248500	-0.14767500
C	-1.97014900	4.56923600	-1.17927500
H	-1.37513900	5.39061900	-1.56731200
C	-1.59817400	3.25747100	-1.44727200
H	-0.71125700	3.02642900	-2.03439500
Mn	0.91642200	0.06221100	0.18956100
O	1.63387800	-0.23936900	1.90828300
O	0.12349400	0.35215700	-1.51391700
N	1.00709200	2.09427100	0.54668800
C	0.09799700	2.76938900	1.25352900
H	-0.72169000	2.18165000	1.66090100
C	0.19729900	4.14121400	1.45208700
H	-0.56208900	4.65602900	2.03268900
C	1.26716900	4.82148500	0.88181000
H	1.36903900	5.89585400	1.00817600
C	2.21549000	4.11530200	0.14961700
H	3.06553800	4.62452800	-0.29465000
C	2.07063600	2.73941300	-0.00050500
C	3.01728200	1.86929100	-0.70881300
N	2.68947800	0.56948200	-0.65217000
N	1.65579600	-1.77302200	-0.41553900
C	2.85112300	-1.73818800	-1.06298600
C	3.41654500	-0.39330500	-1.23866500
C	4.57865300	-0.05684800	-1.93157600
C	4.94237000	1.28550800	-2.00136400
C	4.16488300	2.26686300	-1.39391600
H	4.44542400	3.31388500	-1.45170400
H	5.84179100	1.56957000	-2.54055700
H	5.18024200	-0.82149700	-2.41314200
C	3.45724100	-2.91430200	-1.49221900
H	4.41317400	-2.87697300	-2.00604600
C	2.83306800	-4.13100900	-1.23720600
H	3.29827400	-5.05802400	-1.56115100
C	1.61807000	-4.14886900	-0.56303800
H	1.09980200	-5.07729600	-0.34269000
C	1.05796700	-2.93972500	-0.16693500
H	0.10752100	-2.88873300	0.35932700
H	2.61496800	-0.49179100	1.82122200
H	1.15923600	-1.62542200	2.49571000
O	1.04916700	-2.55948600	2.91437600
Cl	-0.64763400	-2.78746900	3.00853800
O	4.14225200	-1.03951100	1.76382100
Cl	5.04176500	0.42894500	1.83151800

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Mn	-1.37634200	0.28113800	-1.01103400
O	-0.56342900	0.13686200	0.66917600
N	-2.02398000	-1.94728300	-1.17241900
N	-3.21277900	-0.10069400	0.28067400
N	-2.40689300	2.29360300	-0.47602100
C	-1.43521400	-2.81235600	-2.00031300
H	-0.76760800	-2.37949000	-2.74573400
C	-1.63865400	-4.18587000	-1.92449900
H	-1.13904000	-4.85275300	-2.62132000
C	-2.47675900	-4.67016300	-0.92550400
H	-2.65322500	-5.73765800	-0.81965900
C	-3.09521400	-3.77397300	-0.06074700
H	-3.76040500	-4.13706000	0.71730400
C	-2.85740900	-2.40676400	-0.21820100
C	-3.49199600	-1.36869800	0.62094200
C	-4.32360100	-1.65832900	1.70608800
H	-4.54848300	-2.68476200	1.97924900

C	-4.84726600	-0.60415100	2.44312300
H	-5.49003600	-0.80221300	3.29670700
C	-4.53834500	0.70422500	2.09293700
H	-4.93135900	1.53339600	2.67278400
C	-3.70336000	0.92472800	0.99495300
C	-3.29168300	2.27003200	0.54086500
C	-3.77800400	3.45115400	1.10407300
H	-4.49309000	3.42523700	1.92082900
C	-3.34189600	4.67027900	0.59720100
H	-3.70988800	5.59935800	1.02523100
C	-2.44036300	4.68558300	-0.46168000
H	-2.07739300	5.61676300	-0.88719900
C	-1.99739000	3.46617700	-0.96273700
H	-1.27790100	3.41626500	-1.78056200
Mn	1.11921300	0.18490100	0.10752200
O	1.73677400	-0.00095100	1.92124600
O	0.39292100	0.32883100	-1.58452600
N	1.48600100	2.22725800	0.22101900
C	0.66346800	3.10239900	0.80426500
H	-0.25259400	2.69074200	1.22204800
C	0.96442900	4.45747500	0.87646700
H	0.26810900	5.13674700	1.35883800
C	2.15829400	4.90586400	0.32436100
H	2.42332500	5.95893600	0.36143300
C	3.02253200	3.99142100	-0.26790900
H	3.96969000	4.31458200	-0.68971400
C	2.66857000	2.64656800	-0.30224600
C	3.51456900	1.57781600	-0.84625400
N	3.00029600	0.35243800	-0.67013800
N	1.64960500	-1.79185600	-0.21675300
C	2.87193700	-1.98905400	-0.78035900
C	3.62188600	-0.76242500	-1.07889300
C	4.86162700	-0.67499000	-1.71071800
C	5.41485300	0.58765500	-1.90740800
C	4.74703300	1.73141400	-1.48000700
H	5.17720800	2.71668400	-1.63097200
H	6.37805100	0.68094800	-2.40132200
H	5.38037500	-1.56736700	-2.04731000
C	3.34776700	-3.27475900	-1.01456600
H	4.32551300	-3.41822500	-1.46484700
C	2.56671900	-4.36491000	-0.64624800
H	2.92890600	-5.37518000	-0.81634700
C	1.32688500	-4.14761200	-0.05754300
H	0.68595100	-4.96996900	0.24619700
C	0.90074600	-2.83887000	0.13826600
H	-0.06441800	-2.60825000	0.58389700
H	2.65918000	-0.41101000	1.92052700
H	0.97121400	-1.16935700	2.62839500
O	0.68038600	-2.00418900	3.16830900
Cl	-1.03593000	-2.01080200	3.10914100
O	4.13342400	-1.17672100	2.01082700
O	-1.93104000	0.52405100	-2.88967600
Cl	-3.64130500	0.41833900	-3.05274100
Cl	5.20800700	0.17105800	1.99334600

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Mn	-0.95816600	0.30173500	-0.96122100
O	-0.31684500	0.11368600	0.80217600
N	-1.49791200	-1.95702200	-1.30730800
N	-2.92687200	-0.21493700	0.05242400
N	-2.12066000	2.23251800	-0.49363600
C	-0.78171900	-2.76569600	-2.09027600
H	-0.04796000	-2.27947700	-2.73329300

C	-0.93948500	-4.14738400	-2.09141500
H	-0.33441900	-4.76696300	-2.74711300
C	-1.87416100	-4.70139400	-1.22299200
H	-2.02313900	-5.77750000	-1.18257400
C	-2.62449500	-3.86425900	-0.40463600
H	-3.36686200	-4.28257900	0.26868800
C	-2.41833400	-2.48509100	-0.47654500
C	-3.18410100	-1.50504900	0.32107500
C	-4.11833400	-1.86634800	1.29510900
H	-4.31887000	-2.90999000	1.51676400
C	-4.77843900	-0.86181000	1.99093200
H	-5.50361700	-1.11748800	2.75885000
C	-4.50426400	0.46997900	1.70698300
H	-5.00617800	1.26332800	2.25197100
C	-3.55673800	0.76267000	0.72367900
C	-3.16825000	2.13810400	0.34864600
C	-3.83356400	3.27667100	0.80633400
H	-4.68059400	3.19171800	1.48073200
C	-3.40587900	4.52700400	0.37443100
H	-3.91252900	5.42434200	0.72054200
C	-2.33283000	4.61429100	-0.50638400
H	-1.97084200	5.57159500	-0.87018900
C	-1.71998200	3.43413000	-0.91247200
H	-0.86756500	3.44130300	-1.59214400
Mn	1.41272900	0.20672200	0.40619000
O	1.86418600	0.02797100	2.30729400
O	0.87125700	0.36503000	-1.33157600
N	1.75380800	2.23787100	0.54083100
C	0.84349400	3.11550800	0.96867600
H	-0.11530400	2.69964200	1.26827500
C	1.11044800	4.47809500	1.03045000
H	0.34150900	5.15983800	1.38101200
C	2.36449600	4.92965000	0.63826900
H	2.60596600	5.98847800	0.67057900
C	3.31971500	4.01184300	0.21411400
H	4.31175500	4.34141500	-0.07933500
C	2.99515300	2.65959900	0.17880100
C	3.92441700	1.58629700	-0.19603400
N	3.38314900	0.36215500	-0.10466300
N	1.97628800	-1.78065500	0.15177900
C	3.27293600	-1.98167800	-0.20837600
C	4.06438800	-0.75829100	-0.38458900
C	5.39608300	-0.67932700	-0.78914300
C	5.97980400	0.57984200	-0.89345400
C	5.25214900	1.72919000	-0.59727600
H	5.70966400	2.71064500	-0.67408800
H	7.01627800	0.66720100	-1.20691100
H	5.96307100	-1.57666700	-1.01672100
C	3.77768900	-3.26854400	-0.35883400
H	4.81347600	-3.41448000	-0.65030400
C	2.94599500	-4.35686200	-0.11565900
H	3.32911000	-5.36799300	-0.22261100
C	1.63041400	-4.13575300	0.27128300
H	0.94982400	-4.95619000	0.47823700
C	1.18065000	-2.82514200	0.39116600
H	0.15955300	-2.59158600	0.68313800
H	2.78004700	-0.29433100	2.34157300
H	1.03774300	-1.20769600	2.91978400
O	0.70267500	-2.04987000	3.40053600
Cl	-0.99717300	-2.06160400	3.16361600
O	-1.23306200	0.64727200	-2.87231600
Cl	-2.89800300	0.63326900	-3.29803700

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Mn	-0.99659800	-0.02178100	-0.60857900
O	-0.20736300	-0.04804300	1.12771900
N	-1.55913900	-2.23698200	-0.63225700
N	-2.92320200	-0.25255300	0.42532800
N	-1.93008900	2.04822600	-0.39373400
C	-0.83463600	-3.17859000	-1.23915900
H	-0.04925300	-2.82120600	-1.90515000
C	-1.05060500	-4.53738700	-1.03666600
H	-0.43727500	-5.27086400	-1.55202500
C	-2.05205400	-4.91846900	-0.15025600
H	-2.24528300	-5.96953000	0.04888300
C	-2.81311600	-3.94088900	0.48101700
H	-3.60195200	-4.22379300	1.17134400
C	-2.54684000	-2.59804500	0.21178400
C	-3.31681600	-1.48205400	0.79691500
C	-4.39912100	-1.65448000	1.66194400
H	-4.72595500	-2.64740100	1.95466400
C	-5.05500400	-0.52855800	2.14314000
H	-5.89491500	-0.63781200	2.82389100
C	-4.63917100	0.73698600	1.74988600
H	-5.14375400	1.62235900	2.12333600
C	-3.55758600	0.84366000	0.87362200
C	-3.04637500	2.12935700	0.35678200
C	-3.67986000	3.35281400	0.57951300
H	-4.58251000	3.41017800	1.18050800
C	-3.15097500	4.50066700	0.00037600
H	-3.63298600	5.46165900	0.16067600
C	-2.01273400	4.40308000	-0.79290000
H	-1.57442400	5.27480100	-1.27012600
C	-1.43545900	3.14963800	-0.96130000
H	-0.53771400	3.01317900	-1.56438500
Mn	1.45959200	0.09457500	0.57180400
O	0.87046000	0.11310500	-1.05790800
N	1.79546500	2.11614500	0.68201400
C	0.88806800	3.00494100	1.09704000
H	-0.05744200	2.59579500	1.44170600
C	1.14163800	4.37129300	1.08593900
H	0.37652000	5.06006200	1.43043100
C	2.37205100	4.81708500	0.62164400
H	2.59901000	5.87902600	0.58858300
C	3.32543800	3.89037200	0.21078300
H	4.30236000	4.21725400	-0.13220300
C	3.02143900	2.53540000	0.25856200
C	3.95936500	1.45418800	-0.06442400
N	3.43909500	0.23157000	0.13177900
N	2.10447600	-1.89472200	0.66680200
C	3.39255800	-2.11163500	0.28243400
C	4.14709900	-0.89617300	-0.04286400
C	5.47481900	-0.82455400	-0.45904900
C	6.02941200	0.43136800	-0.68749400
C	5.28027200	1.58747700	-0.48823500
H	5.71685100	2.56760700	-0.65215700
H	7.06172800	0.51041900	-1.01619000
H	6.06415500	-1.72504700	-0.59997400
C	3.91599100	-3.39861700	0.25604400
H	4.94319200	-3.56213900	-0.05598300
C	3.11350900	-4.46654100	0.64685800
H	3.51209900	-5.47716100	0.63406100
C	1.80894300	-4.22656000	1.05912100
H	1.15340100	-5.03079500	1.37895600
C	1.33582800	-2.91954000	1.04813500
H	0.32077500	-2.67056300	1.34802700

O	-1.29812400	0.08563100	-2.52707100
Cl	-2.95552800	0.00937500	-2.94788800

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Mn	-1.18795000	0.01975400	-0.69454100
O	-0.38298800	0.00426800	1.01796400
N	-1.73133100	-2.24252900	-0.74265300
N	-3.10316400	-0.29021800	0.39546500
N	-2.18860700	2.07689800	-0.37621000
C	-1.00868900	-3.16759200	-1.37720100
H	-0.26358700	-2.79236400	-2.07905800
C	-1.17616300	-4.53158200	-1.16329000
H	-0.56530100	-5.24896300	-1.70390600
C	-2.12384300	-4.93741700	-0.23016500
H	-2.27681800	-5.99266500	-0.01814000
C	-2.88103500	-3.97869700	0.43367200
H	-3.62565300	-4.28287700	1.16293100
C	-2.66779500	-2.62904000	0.14705200
C	-3.44380000	-1.53583900	0.76892500
C	-4.48178100	-1.75338800	1.67774200
H	-4.76475400	-2.75933100	1.97121900
C	-5.15141200	-0.65615800	2.20255100
H	-5.95683200	-0.80055600	2.91762800
C	-4.79048300	0.62595700	1.81012000
H	-5.30350500	1.48962700	2.22118900
C	-3.75094600	0.77877600	0.88988100
C	-3.29582600	2.09447800	0.39218100
C	-3.96749600	3.28767400	0.66420800
H	-4.86527000	3.29386200	1.27497000
C	-3.48191900	4.47344000	0.12513300
H	-3.99468300	5.41088400	0.32500400
C	-2.34596400	4.44392300	-0.67657900
H	-1.93877800	5.34736600	-1.12144500
C	-1.73373500	3.21581800	-0.90100500
H	-0.84131400	3.13125000	-1.52150700
Mn	1.30323400	0.10517900	0.44904000
O	0.59299500	0.10345900	-1.22366800
N	1.68616600	2.13359000	0.38963700
C	0.87169300	3.05930700	0.90126400
H	-0.02657300	2.68749800	1.38793400
C	1.15602500	4.41695500	0.80905900
H	0.46432600	5.13991800	1.23055500
C	2.32454000	4.81098800	0.16845400
H	2.57500400	5.86414400	0.07519700
C	3.18300100	3.84446600	-0.34570400
H	4.11247100	4.12895600	-0.82980600
C	2.84535300	2.50092500	-0.21876900
C	3.67729500	1.37962900	-0.67362700
N	3.16990200	0.18007900	-0.35323700
N	1.85157900	-1.88659400	0.39975100
C	3.05981800	-2.15536900	-0.16361900
C	3.78646400	-0.97451700	-0.64540600
C	5.00439600	-0.95823000	-1.32413200
C	5.54603800	0.27438600	-1.67769200
C	4.89121300	1.45945200	-1.35437300
H	5.31506600	2.42057300	-1.62837500
H	6.49194800	0.31232800	-2.21062400
H	5.51794100	-1.88167700	-1.57266500
C	3.54393200	-3.45845900	-0.21498600
H	4.51009100	-3.66261800	-0.66664400
C	2.78472500	-4.48625300	0.33431600
H	3.15316600	-5.50800400	0.30638600
C	1.56266100	-4.19134100	0.92600500

H	0.94325100	-4.96370300	1.37185600
C	1.12677200	-2.87139200	0.93610300
H	0.17740400	-2.57872900	1.37937300
O	-1.57936800	0.15368600	-2.62979700
Cl	-3.26244200	0.11246400	-2.98666700
O	1.76626000	0.11352600	2.37092700
Cl	3.43509100	0.18390400	2.76737600

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Mn	-1.27920100	0.03949800	-0.59621300
O	-0.49054700	0.04580800	1.16595100
N	-1.87067100	-2.06860800	-0.48713800
N	-3.16027500	0.03629300	0.34631800
N	-1.91551500	2.11082300	-0.61631100
C	-1.16132500	-3.08692300	-0.97856900
H	-0.30159400	-2.82199800	-1.59158900
C	-1.48315400	-4.41464600	-0.71872700
H	-0.87582600	-5.21023700	-1.14020500
C	-2.57202300	-4.68414400	0.10166100
H	-2.84502500	-5.70835000	0.34178600
C	-3.31482100	-3.62694000	0.61531900
H	-4.17241200	-3.81356800	1.25509200
C	-2.94713000	-2.32156200	0.29584800
C	-3.68504000	-1.13146600	0.74782200
C	-4.84965700	-1.15175300	1.51667400
H	-5.28501600	-2.09166400	1.84123400
C	-5.44222000	0.05854200	1.85719000
H	-6.34881100	0.06734000	2.45590900
C	-4.88193700	1.25900500	1.43302800
H	-5.34427600	2.20585900	1.69377100
C	-3.71785900	1.21588400	0.66601600
C	-3.01481300	2.38964400	0.12372800
C	-3.43216300	3.70679000	0.30221300
H	-4.30776100	3.92909600	0.90441500
C	-2.72017800	4.73237100	-0.31057700
H	-3.03764500	5.76382500	-0.18341600
C	-1.61102100	4.42495700	-1.09063100
H	-1.03304200	5.19645100	-1.59043200
C	-1.23759900	3.09217900	-1.21387400
H	-0.37135900	2.78921000	-1.79966100
Mn	1.18303700	0.05402900	0.59732000
O	1.66736200	0.07957100	2.49716200
O	0.45574900	0.02128100	-1.10227800
N	1.61637800	2.06929100	0.50744100
C	0.86416100	3.01571100	1.07408800
H	-0.01429000	2.66924400	1.61422900
C	1.18149700	4.36467500	0.96537500
H	0.54266900	5.10564500	1.43614300
C	2.30605500	4.72822000	0.23433900
H	2.57496300	5.77454500	0.11831500
C	3.09710000	3.73949400	-0.34234500
H	3.99289900	3.99899300	-0.89860900
C	2.73927700	2.40489300	-0.18202600
C	3.51916200	1.26110200	-0.66946500
N	3.01725900	0.07873900	-0.28320000
N	1.69917500	-1.94676100	0.57160500
C	2.85887600	-2.25093200	-0.06926600
C	3.57895800	-1.09365900	-0.61221700
C	4.74393000	-1.11547500	-1.37746000
C	5.28676100	0.09940900	-1.78685100
C	4.68136400	1.30362400	-1.43814500
H	5.10248800	2.25034100	-1.76153400
H	6.19158600	0.10806400	-2.38802300

H	5.21375900	-2.05449100	-1.65229000
C	3.31107200	-3.56487800	-0.12939400
H	4.23605000	-3.79793100	-0.64850300
C	2.57838100	-4.56341200	0.50417400
H	2.92349200	-5.59316400	0.47246600
C	1.41599700	-4.22872700	1.18809900
H	0.82190500	-4.97666900	1.70423700
C	1.00383800	-2.90121100	1.19378400
H	0.09414300	-2.58065400	1.69712700
O	-2.03599600	0.24468900	-2.33063700
Cl	-1.60335700	-1.14247800	-3.77135300
Cl	3.34437400	0.04824600	2.86431800

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Mn	-1.37597600	-0.00002200	-0.78577600
O	-0.66676600	-0.00004100	0.95210900
N	-1.86335200	-1.98920500	-0.80163600
N	-3.21620600	0.00004200	0.05951200
N	-1.86336200	1.98917200	-0.80185900
C	-1.12806600	-2.92587900	-1.40778700
H	-0.24429500	-2.57524500	-1.93499100
C	-1.47307100	-4.27028600	-1.34623400
H	-0.85174900	-5.00606200	-1.84710100
C	-2.60210800	-4.63697000	-0.62335100
H	-2.89153700	-5.68123900	-0.54585400
C	-3.37350900	-3.65595100	-0.00709100
H	-4.27139600	-3.91838900	0.54420000
C	-2.99494600	-2.32337600	-0.12167200
C	-3.75368000	-1.18077300	0.39701700
C	-4.93459500	-1.21177300	1.13759600
H	-5.39111400	-2.15502000	1.42020300
C	-5.51398200	0.00011700	1.50525100
H	-6.43307100	0.00015200	2.08418300
C	-4.93458800	1.21196800	1.13748100
H	-5.39112800	2.15523800	1.41997200
C	-3.75366700	1.18089500	0.39691400
C	-2.99490600	2.32344100	-0.12186100
C	-3.37337100	3.65604500	-0.00730200
H	-4.27121600	3.91856600	0.54401600
C	-2.60190000	4.63699400	-0.62358600
H	-2.89123500	5.68129000	-0.54608200
C	-1.47291000	4.27021400	-1.34649500
H	-0.85154900	5.00593700	-1.84739300
C	-1.12802000	2.92577900	-1.40804900
H	-0.24431200	2.57506800	-1.93530500
Mn	1.05324500	-0.00008200	0.49044400
O	1.44486100	-0.00003600	2.39733700
O	0.36863200	-0.00021900	-1.23318600
N	1.52898800	2.00280200	0.45002400
C	0.77209600	2.94681600	1.01440600
H	-0.13826500	2.60499300	1.50163800
C	1.12765200	4.28952000	0.96641800
H	0.48530800	5.03063500	1.43194000
C	2.29605100	4.64691200	0.30419200
H	2.59703600	5.68884300	0.24021900
C	3.09022900	3.65835500	-0.26831800
H	4.01939700	3.91252000	-0.76942700
C	2.69192000	2.32907800	-0.17281600
C	3.46334100	1.17968100	-0.65668100
N	2.91289000	-0.00006400	-0.33084500
N	1.52904600	-2.00294200	0.45005300
C	2.69193500	-2.32921400	-0.17287100
C	3.46334000	-1.17980000	-0.65672700

C	4.66410500	-1.21059700	-1.36384700
C	5.25599200	-0.00003800	-1.71359400
C	4.66411000	1.21050700	-1.36379500
H	5.12603000	2.15427500	-1.63554700
H	6.19157300	-0.00003200	-2.26552700
H	5.12602300	-2.15435200	-1.63564500
C	3.09022400	-3.65849300	-0.26842600
H	4.01936200	-3.91265500	-0.76959400
C	2.29607700	-4.64705500	0.30412000
H	2.59704500	-5.68898800	0.24010100
C	1.12773500	-4.28966500	0.96644700
H	0.48542600	-5.03078100	1.43201600
C	0.77219000	-2.94695900	1.01448000
H	-0.13812700	-2.60513700	1.50179300
O	-2.02194800	0.00006100	-2.54364100
Cl	3.09610200	0.00054400	2.82558000

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Mn	-1.40322100	-0.00000200	-0.96806600
O	-0.67369000	-0.00002700	0.97697900
N	-1.84545200	-2.02105400	-0.80821000
N	-3.22423600	0.00016100	-0.03039000
N	-1.84514800	2.02111500	-0.80836000
C	-1.11412900	-2.98589100	-1.37125500
H	-0.22740100	-2.66005900	-1.91129900
C	-1.45778500	-4.32802200	-1.26286600
H	-0.83312200	-5.08273400	-1.73110200
C	-2.59303200	-4.66794400	-0.53613300
H	-2.88573600	-5.70818300	-0.42223800
C	-3.36401200	-3.66183600	0.03633700
H	-4.26720900	-3.90282000	0.58901600
C	-2.97661300	-2.33454500	-0.12494600
C	-3.73288800	-1.17661100	0.36754600
C	-4.87172000	-1.20847700	1.17145400
H	-5.29973000	-2.15198300	1.49543300
C	-5.44064800	0.00038500	1.56089400
H	-6.32810100	0.00047700	2.18756900
C	-4.87154100	1.20913200	1.17136000
H	-5.29941500	2.15272600	1.49526500
C	-3.73271100	1.17704000	0.36745900
C	-2.97625700	2.33482500	-0.12511200
C	-3.36344900	3.66218700	0.03608600
H	-4.26660400	3.90334600	0.58875700
C	-2.59231400	4.66813600	-0.53645500
H	-2.88485300	5.70842900	-0.42262500
C	-1.45712600	4.32799000	-1.26317600
H	-0.83234900	5.08257500	-1.73146500
C	-1.11367700	2.98580000	-1.37147700
H	-0.22700100	2.65979100	-1.91149700
Mn	0.99395700	-0.00009000	0.47955200
O	1.43367700	-0.00008100	2.40598700
O	0.38721100	-0.00010600	-1.26820700
N	1.49934400	2.01332000	0.45638200
C	0.76889800	2.96710700	1.03911000
H	-0.14880600	2.63778300	1.52210300
C	1.15141800	4.30308700	1.01533700
H	0.52747900	5.04904200	1.49820700
C	2.32200100	4.64860100	0.35100400
H	2.64389100	5.68523100	0.30149800
C	3.09188300	3.65243900	-0.24069800
H	4.02366200	3.89600000	-0.74253300
C	2.66827500	2.32935500	-0.16179300
C	3.43240000	1.17723400	-0.65919600

N	2.88735300	-0.00012300	-0.32496300
N	1.49928300	-2.01352300	0.45636400
C	2.66818000	-2.32959500	-0.16186000
C	3.43235100	-1.17749100	-0.65923100
C	4.62378800	-1.21095000	-1.38346700
C	5.21065000	-0.00014900	-1.74180100
C	4.62383900	1.21066600	-1.38343000
H	5.08269300	2.15364900	-1.66366700
H	6.13775200	-0.00016000	-2.30824700
H	5.08260200	-2.15394300	-1.66373400
C	3.09171100	-3.65269900	-0.24084000
H	4.02346500	-3.89628700	-0.74270800
C	2.32178700	-4.64884900	0.35082900
H	2.64361600	-5.68549400	0.30126200
C	1.15123900	-4.30330200	1.01520500
H	0.52726800	-5.04924600	1.49804900
C	0.76879600	-2.96730000	1.03905600
H	-0.14887800	-2.63795300	1.52209100
O	-1.94347600	-0.00001900	-2.59051500
Cl	3.10263000	0.00016200	2.81749200

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Mn	-1.25130200	0.00057900	-0.56015300
O	-0.44713300	0.00142000	1.12176500
N	-1.71696200	-2.00080300	-0.49220500
N	-3.03522000	0.00275400	0.39122400
N	-1.71347800	2.00264100	-0.49496000
C	-1.02050600	-2.94674900	-1.12588000
H	-0.16113100	-2.60814200	-1.69998700
C	-1.37196200	-4.28880500	-1.04064600
H	-0.77975900	-5.03138600	-1.56635700
C	-2.46738200	-4.64458100	-0.26302700
H	-2.75907400	-5.68648700	-0.16442200
C	-3.20201200	-3.65370700	0.38073000
H	-4.07696700	-3.90429000	0.97302300
C	-2.81604500	-2.32567700	0.23884200
C	-3.54139700	-1.17591900	0.78614600
C	-4.65986500	-1.20548400	1.61632400
H	-5.08576300	-2.14878000	1.94299000
C	-5.21162200	0.00579400	2.02459900
H	-6.08067600	0.00703300	2.67632100
C	-4.65768100	1.21553700	1.61472300
H	-5.08192800	2.16003000	1.94005500
C	-3.53919400	1.18286000	0.78471300
C	-2.81153500	2.33056300	0.23618300
C	-3.19439900	3.65957800	0.37720000
H	-4.06851800	3.91265200	0.96967700
C	-2.45771300	4.64824700	-0.26760000
H	-2.74694000	5.69090800	-0.16970600
C	-1.36343000	4.28935400	-1.04541000
H	-0.76978300	5.03017300	-1.57198000
C	-1.01506900	2.94644300	-1.12971300
H	-0.15672000	2.60540800	-1.70389800
Mn	1.25130600	-0.00214500	0.56018000
O	0.44713100	-0.00331700	-1.12174300
N	1.71722000	1.99908300	0.49195700
C	1.02104200	2.94514400	1.12576400
H	0.16144700	2.60674900	1.69966700
C	1.37305100	4.28707900	1.04090500
H	0.78105500	5.02977600	1.56668200
C	2.46880400	4.64258700	0.26362700
H	2.76095900	5.68439500	0.16535900
C	3.20318600	3.65156800	-0.38018600

H	4.07841900	3.90192200	-0.97216600
C	2.81662400	2.32366100	-0.23872200
C	3.54168000	1.17374400	-0.78609300
N	3.03522000	-0.00483000	-0.39122700
N	1.71325000	-2.00435200	0.49526700
C	2.81095700	-2.33257300	-0.23628600
C	3.53888500	-1.18503500	-0.78479600
C	4.65735200	-1.21793600	-1.61483600
C	5.21157700	-0.00830900	-2.02465500
C	4.66012700	1.20308600	-1.61629700
H	5.08623100	2.14629700	-1.94293800
H	6.08061500	-0.00972600	-2.67639800
H	5.08137800	-2.16251100	-1.94021400
C	3.19322000	-3.66171000	-0.37773400
H	4.06703400	-3.91501500	-0.97056100
C	2.45631500	-4.65022900	0.26705100
H	2.74507400	-5.69298800	0.16881200
C	1.36240500	-4.29106500	1.04525200
H	0.76857900	-5.03176100	1.57179300
C	1.01459800	-2.94803300	1.12993300
H	0.15649500	-2.60678500	1.70435900
O	-1.71176900	0.00013600	-2.44333400
Cl	-3.38327700	0.00374000	-2.78796600
O	1.71177200	-0.00038400	2.44335000
Cl	3.38325300	0.01395400	2.78784000

TS₂₀₋₂₂

Mn	-1.27429300	0.02078800	-0.57773100
O	-0.52256500	0.02745500	1.14225100
N	-1.82886700	-2.08619900	-0.48198900
N	-3.19916000	-0.01497200	0.31574400
N	-1.95258700	2.11138800	-0.52390800
C	-1.10318000	-3.08170400	-0.99621600
H	-0.22151700	-2.78961200	-1.56427200
C	-1.43591800	-4.41907400	-0.81084700
H	-0.81506300	-5.19620000	-1.24683500
C	-2.55477900	-4.72205800	-0.04454300
H	-2.83934200	-5.75522300	0.13643200
C	-3.31471700	-3.68744000	0.49034200
H	-4.19798600	-3.90360300	1.08370000
C	-2.93445500	-2.36937500	0.24684500
C	-3.69304000	-1.19844500	0.71540200
C	-4.84659200	-1.25544500	1.49822900
H	-5.25381300	-2.20842200	1.82129400
C	-5.46181500	-0.06389600	1.86342500
H	-6.35693100	-0.08364900	2.47895100
C	-4.93375700	1.15299800	1.44698300
H	-5.40597300	2.08644400	1.73669300
C	-3.78138200	1.14550100	0.66056800
C	-3.11334700	2.34534100	0.12966500
C	-3.62997400	3.63555800	0.23282300
H	-4.56476800	3.81717000	0.75423800
C	-2.94215300	4.68827600	-0.36118600
H	-3.33448400	5.69944900	-0.29287300
C	-1.76277500	4.43128000	-1.05063600
H	-1.20034900	5.22435600	-1.53437600
C	-1.30219000	3.12057400	-1.10555600
H	-0.38101900	2.86069700	-1.62558200
Mn	1.20584800	0.05866500	0.61529500
O	1.59692200	0.10770300	2.42064100
O	0.44694700	0.02506500	-1.09569400
N	1.63050200	2.07815300	0.50566200
C	0.88525300	3.02568700	1.07884800

H	0.01289900	2.68135600	1.62953700
C	1.20250900	4.37432200	0.96620500
H	0.56865000	5.11649500	1.44176500
C	2.32321400	4.73600900	0.22799600
H	2.59332200	5.78187800	0.11061400
C	3.10975100	3.74579100	-0.35187200
H	4.00358300	4.00347700	-0.91210400
C	2.74901700	2.41196000	-0.18900200
C	3.52113200	1.26503300	-0.67780200
N	3.01780000	0.08349500	-0.28581500
N	1.71036800	-1.94243600	0.57557200
C	2.85523300	-2.24880300	-0.08919000
C	3.57315900	-1.08971300	-0.62861000
C	4.73124200	-1.11202000	-1.40395500
C	5.27729400	0.10141000	-1.81225700
C	4.67748700	1.30541000	-1.45490900
H	5.09780600	2.25238900	-1.77857200
H	6.17772600	0.10895600	-2.41994800
H	5.19389800	-2.05211100	-1.68714900
C	3.29539400	-3.56570100	-0.17362000
H	4.20882200	-3.80081000	-0.71177000
C	2.56500700	-4.56569300	0.46022000
H	2.89960200	-5.59811600	0.40852300
C	1.41888600	-4.22909000	1.17041200
H	0.82790000	-4.97829500	1.68824800
C	1.01894600	-2.89812700	1.20008200
H	0.12190700	-2.57621100	1.72464300
O	-1.98450400	0.25786200	-2.43242300
Cl	-1.47249500	-0.93649500	-3.55619200
Cl	3.48865700	0.14244800	2.93134600

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Mn	-1.38136800	0.00002200	-0.88136100
O	-0.68457900	-0.00000100	0.90744800
N	-1.85048900	-2.00762200	-0.79741400
N	-3.21727100	0.00007600	0.02244100
N	-1.85037700	2.00768000	-0.79744500
C	-1.11315000	-2.95185400	-1.38645500
H	-0.22828900	-2.60995700	-1.91766800
C	-1.45814000	-4.29561000	-1.30564200
H	-0.83445400	-5.03846700	-1.79307200
C	-2.59053200	-4.65099900	-0.58280000
H	-2.88122400	-5.69377200	-0.49114500
C	-3.36372500	-3.66016600	0.01425900
H	-4.26558100	-3.91375400	0.56316800
C	-2.98310400	-2.32898500	-0.11817500
C	-3.74336500	-1.17937500	0.38293100
C	-4.91188500	-1.21054200	1.14275500
H	-5.35843300	-2.15410200	1.43986400
C	-5.48992600	0.00015100	1.51443100
H	-6.40090300	0.00018300	2.10604500
C	-4.91182300	1.21080600	1.14272500
H	-5.35832500	2.15439600	1.43981200
C	-3.74330500	1.17956200	0.38290400
C	-2.98297900	2.32912100	-0.11822100
C	-3.36352100	3.66032800	0.01418600
H	-4.26536700	3.91397900	0.56308200
C	-2.59026200	4.65110300	-0.58288300
H	-2.88089200	5.69389600	-0.49124900
C	-1.45788500	4.29563500	-1.30570900
H	-0.83414800	5.03844600	-1.79314500
C	-1.11297500	2.95185700	-1.38649600
H	-0.22813000	2.60989600	-1.91769400

Mn	1.02936600	-0.00003400	0.47110100
O	1.41081400	-0.00003600	2.37366600
O	0.36264500	-0.00001800	-1.27691500
N	1.51428800	2.00321700	0.44341200
C	0.76668600	2.94539100	1.02295700
H	-0.14794800	2.60469200	1.50278600
C	1.13565500	4.28502300	0.99930900
H	0.50030100	5.02414700	1.47745400
C	2.30815300	4.64218000	0.34449600
H	2.61952100	5.68204600	0.29870700
C	3.09444600	3.65531100	-0.24154900
H	4.02846700	3.90850700	-0.73407200
C	2.68403600	2.32830600	-0.16768200
C	3.45555100	1.17948500	-0.65444800
N	2.90013000	-0.00008300	-0.33844400
N	1.51419500	-2.00330300	0.44343100
C	2.68391600	-2.32846000	-0.16767700
C	3.45549000	-1.17968000	-0.65444600
C	4.66566300	-1.21098100	-1.34546400
C	5.26151800	-0.00014500	-1.68781900
C	4.66572700	1.21072300	-1.34546500
H	5.13357700	2.15419800	-1.60798900
H	6.20538200	-0.00017100	-2.22550200
H	5.13346300	-2.15448100	-1.60798800
C	3.09424600	-3.65548900	-0.24155000
H	4.02824800	-3.90874100	-0.73408100
C	2.30790200	-4.64231300	0.34450500
H	2.61920600	-5.68219700	0.29871200
C	1.13543400	-4.28508600	0.99933500
H	0.50004200	-5.02417200	1.47748800
C	0.76654500	-2.94543200	1.02298600
H	-0.14806400	-2.60467900	1.50282600
O	-1.98889100	0.00002400	-2.50192100
Cl	3.05905900	0.00010200	2.81401700

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Mn	0.82002500	0.05473900	-0.58710100
O	1.40428300	-0.28608900	-2.37901800
O	0.28947200	0.53117200	1.14661200
N	1.44504600	2.04077000	-0.89440100
N	2.71921000	0.08659500	0.19676500
N	1.13845900	-1.91617800	-0.12033400
C	0.76191400	2.94338800	-1.60009200
H	-0.17737900	2.60260700	-2.03121800
C	1.21923600	4.24597900	-1.76753700
H	0.62986600	4.95253700	-2.34408500
C	2.42382700	4.60966600	-1.17799100
H	2.80748000	5.62086400	-1.28278300
C	3.14833500	3.66161000	-0.46299000
H	4.10471300	3.91443700	-0.01459400
C	2.64168200	2.37137900	-0.34225100
C	3.33736700	1.26742400	0.33362300
C	4.52424400	1.35213400	1.06043900
H	5.03909800	2.30041500	1.17934400
C	5.02681800	0.19048100	1.64003400
H	5.94805600	0.23230100	2.21442900
C	4.35611400	-1.02149400	1.50155700
H	4.73932800	-1.92481100	1.96630800
C	3.17341700	-1.03975500	0.76278800
C	2.31046700	-2.20110800	0.50927100
C	2.64281800	-3.51421300	0.82608600
H	3.57744200	-3.72954500	1.33544500
C	1.78089700	-4.54187600	0.45686200

H	2.03379300	-5.57267900	0.69010000
C	0.60406300	-4.23660100	-0.21548900
H	-0.09567200	-5.00795900	-0.52318600
C	0.31226800	-2.90356200	-0.47910900
H	-0.61196300	-2.59821200	-0.96261900
Mn	-1.49365100	0.41602800	0.93301000
O	-1.97011000	0.87478800	2.54023500
O	-0.88197600	0.03495300	-0.96656300
N	-1.79512500	-1.56750800	1.39898800
C	-1.01603800	-2.25559600	2.23801300
H	-0.16156100	-1.71793100	2.64463100
C	-1.27673500	-3.58127000	2.55914700
H	-0.61891200	-4.10855400	3.24329100
C	-2.37418500	-4.20533300	1.97482500
H	-2.59959000	-5.24544400	2.19440600
C	-3.19440900	-3.48334900	1.11474500
H	-4.07083900	-3.94251500	0.66732800
C	-2.89494300	-2.14898200	0.85442500
C	-3.71813300	-1.25003300	0.03529700
N	-3.32838900	0.03277800	0.10088400
N	-2.09175300	2.28076000	0.23252400
C	-3.24337400	2.30506700	-0.48756200
C	-3.89721200	0.99774300	-0.63757800
C	-4.98487000	0.69871100	-1.45775900
C	-5.43526400	-0.61750700	-1.50509500
C	-4.80079400	-1.61118700	-0.76502500
H	-5.12989600	-2.64420600	-0.82360200
H	-6.27759900	-0.87493100	-2.14108800
H	-5.45763400	1.46880100	-2.05962300
C	-3.73573700	3.50127300	-1.00119500
H	-4.65933900	3.50849000	-1.57265400
C	-3.04175200	4.68117000	-0.75481900
H	-3.41482000	5.62308300	-1.14770600
C	-1.87963600	4.64310800	0.00676400
H	-1.31242200	5.54240700	0.22696100
C	-1.43621700	3.41534300	0.48473400
H	-0.52973800	3.32167900	1.07977100
H	0.75824300	-0.96237700	-2.76102700
H	2.67416900	-1.11801400	-2.35549900
O	-0.11989000	2.25097700	3.62597500
H	-0.85066200	1.65439700	3.16825200
O	-0.01661600	-2.24886400	-3.50118200
O	3.51321900	-1.73777400	-2.36174000
Cl	4.81931700	-0.62649000	-2.37508800
Cl	-1.73288700	-2.17396800	-3.33339000
Cl	0.92135400	1.10907700	4.37326900

TS₂₅

Mn	-1.24711600	0.11389000	0.22630000
O	-2.09974900	0.06827700	1.92513800
O	-0.41811300	0.16287900	-1.47176900
N	-1.39984500	2.18493000	0.33481300
N	-2.95808000	0.51615200	-0.83028900
N	-2.00046200	-1.77634700	-0.16175000
C	-0.63119100	2.93755800	1.12546200
H	0.13624100	2.41068300	1.68918100
C	-0.79611400	4.31451500	1.21332100
H	-0.14728400	4.89253200	1.86433500
C	-1.78516700	4.91684500	0.44475500
H	-1.93380300	5.99265300	0.47931700
C	-2.60222800	4.12857400	-0.35863500
H	-3.40158200	4.57466300	-0.94257700
C	-2.40291100	2.75137700	-0.38482500

C	-3.25293800	1.79451300	-1.10680500
C	-4.28803600	2.09654100	-1.99119700
H	-4.53973000	3.12665900	-2.22450200
C	-4.98666600	1.04276600	-2.57301400
H	-5.79724700	1.25257100	-3.26526900
C	-4.65121600	-0.27710200	-2.28509500
H	-5.18768100	-1.09974900	-2.74781700
C	-3.60258100	-0.51378600	-1.39711800
C	-3.09059500	-1.82369000	-0.97286700
C	-3.67152500	-3.04264200	-1.30678900
H	-4.53692700	-3.07039300	-1.96219400
C	-3.14751100	-4.21442300	-0.77077700
H	-3.59600400	-5.17276400	-1.01830700
C	-2.06131000	-4.14347100	0.09256100
H	-1.62950200	-5.03273700	0.54175500
C	-1.50776600	-2.89811900	0.36785000
H	-0.65281300	-2.77720400	1.03103600
Mn	1.28172800	-0.10811800	-0.94646200
O	2.02051100	-0.03045300	-2.51154000
O	0.35825200	-0.20851100	0.83533300
N	1.46644400	-2.17795400	-0.93611000
C	0.73524900	-2.98521400	-1.70732200
H	0.00160500	-2.49943200	-2.34750900
C	0.89297900	-4.36582400	-1.68321900
H	0.27455400	-4.98850400	-2.32245200
C	1.83434600	-4.91354700	-0.81974900
H	1.97716800	-5.98940300	-0.76789100
C	2.60602100	-4.07093600	-0.02698100
H	3.36113600	-4.47370200	0.64149700
C	2.41369700	-2.69476600	-0.11089500
C	3.19435500	-1.69395700	0.62816500
N	2.92051000	-0.43082200	0.26459300
N	1.93390800	1.81288300	-0.50877500
C	2.96244900	1.91472600	0.37168700
C	3.46406300	0.63169000	0.88020000
C	4.40709900	0.44666500	1.88997200
C	4.74311400	-0.85536300	2.24884800
C	4.13279900	-1.94198500	1.62948300
H	4.37246800	-2.95860800	1.92607900
H	5.47623200	-1.02544100	3.03226600
H	4.86364400	1.29669600	2.38773700
C	3.49373100	3.15776000	0.70270900
H	4.31066700	3.22771400	1.41473400
C	2.98191300	4.29757300	0.09203600
H	3.39061900	5.27449600	0.33578900
C	1.95924100	4.17132300	-0.84098700
H	1.53911500	5.03509500	-1.34724800
C	1.45629100	2.90417200	-1.11065700
H	0.64227600	2.74486200	-1.81465900
H	-1.57494300	-0.61592600	2.45977300
H	-3.51086700	-0.47764800	1.77692900
H	3.84734900	-0.08303800	-1.66051600
O	4.17226600	0.56041000	-2.31885400
O	-4.48265400	-0.84192000	1.68351700
Cl	-5.41899700	0.59250400	1.60175600
Cl	6.00035700	0.75953800	-1.67006700
O	-0.71089400	-1.74795400	3.30107500
Cl	0.48912000	-0.80749600	4.11085600
TS ₂₅₋₂₇			
Mn	-0.74019000	0.23846000	0.58001900
O	-1.17199200	0.42010700	2.40638200
O	-0.31978100	0.10195400	-1.26759800

N	-0.98588700	2.27827500	0.41664000
N	-2.65703000	0.40524800	-0.13171800
N	-1.43958700	-1.72011500	0.64860600
C	-0.11701200	3.16744500	0.90264100
H	0.77767700	2.75720400	1.36695800
C	-0.34118000	4.53580100	0.81005800
H	0.39166800	5.22839300	1.21251000
C	-1.49988600	4.98023700	0.18383400
H	-1.70159500	6.04341600	0.08545500
C	-2.41542600	4.05225900	-0.30153300
H	-3.34277700	4.37692600	-0.76410000
C	-2.14513500	2.69489200	-0.15942800
C	-3.05912500	1.61315200	-0.55236500
C	-4.23715200	1.73838600	-1.28730100
H	-4.57715900	2.70782700	-1.63830700
C	-4.96060800	0.58410300	-1.57475500
H	-5.87989000	0.65583200	-2.14928300
C	-4.50819800	-0.66275500	-1.15288500
H	-5.05836800	-1.56565300	-1.40012300
C	-3.31785500	-0.72254000	-0.42818600
C	-2.65326300	-1.93276700	0.07410700
C	-3.20113700	-3.21084100	0.03142000
H	-4.16428200	-3.37503800	-0.44238400
C	-2.51362500	-4.26409200	0.62585700
H	-2.93346000	-5.26613700	0.60543900
C	-1.30073300	-4.01774800	1.25697300
H	-0.73948000	-4.80944400	1.74401600
C	-0.78821900	-2.72540100	1.23707900
H	0.16235500	-2.47004900	1.70456600
Mn	1.46588400	-0.09003900	-1.14127100
O	1.76637900	-0.27353700	-2.83174500
O	0.98459700	0.06303300	0.80652300
N	1.73855000	-2.11344700	-0.84320700
C	0.89396100	-3.05045900	-1.27993900
H	0.00069100	-2.69086100	-1.78722000
C	1.14219900	-4.40493900	-1.09131100
H	0.42869100	-5.13653000	-1.45798300
C	2.29674500	-4.78459800	-0.41766400
H	2.51725700	-5.83473200	-0.24645400
C	3.18076500	-3.80779800	0.02835800
H	4.10041900	-4.08104300	0.53720700
C	2.88624600	-2.46840300	-0.20699800
C	3.75374200	-1.34309800	0.16199700
N	3.35046200	-0.16839300	-0.34873900
N	2.08558600	1.90388200	-1.19777500
C	3.26628400	2.17149900	-0.58503300
C	3.94512400	0.99402000	-0.03111200
C	5.07841400	1.00019800	0.78006500
C	5.54630300	-0.21347600	1.27434200
C	4.87967700	-1.39916400	0.98240100
H	5.21596400	-2.34232000	1.40155700
H	6.42312600	-0.23198600	1.91544800
H	5.57266400	1.93188800	1.03741000
C	3.75664800	3.47313600	-0.52848600
H	4.69598200	3.68115300	-0.02490200
C	3.03639300	4.49432500	-1.13905900
H	3.40815400	5.51488600	-1.10688500
C	1.84858900	4.19546200	-1.79712000
H	1.26120700	4.96378500	-2.29066500
C	1.40058400	2.88014200	-1.79681400
H	0.46693500	2.58684700	-2.27261000
H	-0.50670200	-0.17468300	2.89523100
H	-2.57915100	-0.15328200	2.63721900

H	-0.34768000	-0.59984200	-2.77049500
O	-0.18800700	-1.00052900	-3.67014400
O	-3.53216100	-0.53158800	2.79372300
Cl	-4.52093600	0.86089200	2.64242400
Cl	-2.05806700	-1.54319800	-3.97166400
O	0.57628000	-1.13060200	3.65574200
Cl	1.84838600	-0.03050700	4.04542400

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Mn	0.92442700	0.04782000	0.29494000
O	1.55988400	0.38530900	2.00791600
O	0.17427200	-0.16871700	-1.46863400
N	1.26664900	-1.94853300	0.67345200
N	2.73497700	-0.27541400	-0.58016400
N	1.50108900	1.95658200	-0.27479900
C	0.50086400	-2.67754700	1.48988600
H	-0.35294300	-2.16544400	1.92701000
C	0.77763600	-4.01391000	1.74762700
H	0.13260000	-4.57645500	2.41545600
C	1.87302200	-4.60025700	1.12285400
H	2.10938000	-5.64737600	1.29109900
C	2.67920000	-3.83268900	0.28914500
H	3.55456900	-4.26391600	-0.18685500
C	2.36664300	-2.49127900	0.09112200
C	3.17984000	-1.53866100	-0.67187300
C	4.32785600	-1.81990600	-1.41014700
H	4.70074100	-2.83597500	-1.49381500
C	4.98463200	-0.76432100	-2.03596900
H	5.88199900	-0.95818100	-2.61669500
C	4.50170400	0.53690700	-1.92999700
H	5.00836400	1.36017900	-2.42384600
C	3.34392500	0.75466400	-1.18499700
C	2.67196000	2.03802600	-0.96158200
C	3.16403300	3.26855300	-1.38093600
H	4.10379900	3.32013300	-1.92287300
C	2.44623800	4.42285900	-1.08308800
H	2.81953400	5.39181600	-1.40311800
C	1.25710600	4.32285700	-0.37238500
H	0.66639200	5.19815900	-0.11959700
C	0.81571500	3.06308300	0.01997900
H	-0.11145600	2.92075000	0.56872000
Mn	-1.52553700	-0.20962800	-0.92846000
O	-2.16545700	-0.36075600	-2.73145800
O	-0.80043200	0.10557000	0.77230100
N	-2.26090200	1.75091800	-1.02435400
C	-1.68032800	2.73066900	-1.71831900
H	-0.80893200	2.45141200	-2.30624300
C	-2.16114900	4.03483500	-1.68290200
H	-1.66053200	4.80845700	-2.25684200
C	-3.27194700	4.31285600	-0.89519000
H	-3.66688200	5.32324700	-0.83510000
C	-3.89116700	3.28338700	-0.19242400
H	-4.77386900	3.47543800	0.41001800
C	-3.37132800	1.99622000	-0.28192100
C	-3.95979700	0.80512800	0.34374100
N	-3.32848100	-0.33311800	0.01532100
N	-1.75561900	-2.23520100	-0.69750600
C	-2.84300800	-2.62955400	0.01965900
C	-3.69837500	-1.53365800	0.48794900
C	-4.80163000	-1.63631600	1.33418400
C	-5.48043500	-0.47142400	1.67836900
C	-5.06697100	0.76438100	1.18861900
H	-5.59186300	1.67422600	1.46250300

H	-6.33913800	-0.52651400	2.34141800
H	-5.11787500	-2.59843300	1.72476700
C	-3.09337000	-3.98100600	0.23344200
H	-3.96232200	-4.28718400	0.80829800
C	-2.23167200	-4.92598600	-0.31448700
H	-2.41868400	-5.98487700	-0.15825800
C	-1.13784200	-4.50428600	-1.06118600
H	-0.44042500	-5.21057800	-1.50083500
C	-0.92559500	-3.14059800	-1.22344500
H	-0.06883400	-2.74811700	-1.76380400
H	1.09202500	1.22225700	2.37812000
H	3.03161300	0.94320500	1.91070900
O	-1.28041200	-1.19825800	-3.51074200
H	-0.40919900	-0.95621700	-3.11615800
O	0.62863200	2.56759000	3.07275300
O	3.97690100	1.34346200	1.88278500
Cl	4.97754500	-0.04668000	1.95626200
Cl	-1.08671900	2.65119700	2.97588800

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Mn	-0.96512200	0.00046500	0.33539900
O	-1.51025600	-0.28855300	2.03821200
O	-0.20904000	0.25530800	-1.57110400
N	-1.45817300	2.01884800	0.53555400
N	-2.79724300	0.11843600	-0.54953500
N	-1.33232800	-1.95834500	-0.14086100
C	-0.74490300	2.89342900	1.24769300
H	0.14656000	2.50205800	1.73324500
C	-1.11749700	4.22855800	1.35128600
H	-0.51091700	4.91113100	1.93849200
C	-2.25426800	4.65735000	0.67636400
H	-2.56433900	5.69767300	0.72268600
C	-3.00621500	3.74023100	-0.05091600
H	-3.91207200	4.04691800	-0.56547000
C	-2.59686800	2.41163800	-0.09384900
C	-3.33937100	1.32868700	-0.74973400
C	-4.50492400	1.45062900	-1.50417600
H	-4.95710100	2.42206800	-1.67764600
C	-5.07292100	0.29528900	-2.03328200
H	-5.98214800	0.36620800	-2.62353300
C	-4.48213900	-0.94811800	-1.82610300
H	-4.91386100	-1.84740400	-2.25435100
C	-3.31054600	-1.00464500	-1.07306300
C	-2.51209600	-2.20045800	-0.77647200
C	-2.89167800	-3.50128900	-1.08511800
H	-3.83396200	-3.68671500	-1.59180000
C	-2.06068100	-4.55654100	-0.71976800
H	-2.34876800	-5.57849500	-0.95043200
C	-0.86932500	-4.29104700	-0.05797300
H	-0.19221800	-5.08491500	0.24252300
C	-0.53575700	-2.96917800	0.21571800
H	0.39159300	-2.69744300	0.71356400
Mn	1.58737900	0.31183400	-1.03742900
O	1.97309000	0.66940800	-2.82119300
O	0.75327900	-0.00692700	0.68841900
N	2.17015400	-1.68503900	-1.25031700
C	1.54055700	-2.58070800	-2.01258800
H	0.71548500	-2.20476000	-2.61359500
C	1.91286900	-3.92016900	-2.02427400
H	1.37645800	-4.62207000	-2.65522800
C	2.95617800	-4.32924400	-1.20173800
H	3.25942500	-5.37226100	-1.17297500
C	3.62141300	-3.39079400	-0.41862500

H	4.45006500	-3.68492900	0.21876300
C	3.21772700	-2.06108500	-0.47410400
C	3.85922000	-0.95547400	0.24346700
N	3.33245100	0.24988100	-0.04408700
N	1.92380400	2.28755200	-0.64610600
C	2.99162800	2.56262200	0.15038600
C	3.75345800	1.38054200	0.55357700
C	4.80900500	1.33653200	1.46266300
C	5.38624600	0.10480900	1.75105400
C	4.91302400	-1.05711300	1.14759900
H	5.34951300	-2.02291100	1.38245100
H	6.20563800	0.04734600	2.46182900
H	5.16041900	2.24358700	1.94458800
C	3.30174300	3.87457700	0.48953700
H	4.15446700	4.08331800	1.12865600
C	2.52201400	4.90820900	-0.02047800
H	2.75537600	5.93896500	0.23181400
C	1.45400500	4.60996000	-0.85817800
H	0.82366700	5.38838500	-1.27725100
C	1.17537900	3.27732700	-1.13977900
H	0.34399200	2.97724500	-1.77300100
H	-0.94127900	-1.05065800	2.46613200
H	-2.97971200	-0.95141800	2.01579500
O	1.01186600	1.38509100	-3.49313600
H	-0.21306000	0.85919900	-2.37357000
O	-0.36014600	-2.25837200	3.20252200
O	-3.90549700	-1.37593800	2.03713500
Cl	-4.93885600	-0.00792900	2.06072500
Cl	1.35483600	-2.13996500	3.16780200

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Mn	1.28874100	-0.05562200	0.25641400
O	2.23717500	0.24299000	1.85827700
O	0.26692500	-0.21687800	-1.34396700
N	1.21497200	-2.05474900	0.80288100
N	2.86099400	-0.86308300	-0.75507800
N	2.20218800	1.61085200	-0.55765100
C	0.40976800	-2.52326400	1.75976800
H	-0.26757300	-1.79916700	2.20683900
C	0.43253200	-3.85765500	2.14408400
H	-0.23797600	-4.20285800	2.92505200
C	1.31260200	-4.72144700	1.50098400
H	1.34789200	-5.77392600	1.76861400
C	2.16340100	-4.22610800	0.51898100
H	2.87745600	-4.87658100	0.02280300
C	2.11076700	-2.87338500	0.19544600
C	3.01459700	-2.19628700	-0.74195200
C	3.98663400	-2.79378700	-1.54262600
H	4.12392700	-3.87049800	-1.54173000
C	4.77899600	-1.97370800	-2.33992500
H	5.54566000	-2.41507800	-2.97047000
C	4.59962300	-0.59352200	-2.33957800
H	5.21667100	0.04408000	-2.96470000
C	3.60485700	-0.05417700	-1.52479400
C	3.25667000	1.36443100	-1.38100600
C	3.93655500	2.41307000	-1.99077800
H	4.77568700	2.20954000	-2.64872500
C	3.53696000	3.72139200	-1.73532200
H	4.06031200	4.54974200	-2.20495500
C	2.47368900	3.95490700	-0.87345000
H	2.13322800	4.96012700	-0.64363400
C	1.82808500	2.86526700	-0.29824800
H	0.98224700	2.98487800	0.37247800

Mn	-1.31958600	0.18097700	-0.62071400
O	-2.32295100	0.29476100	-2.23236900
O	-0.27568100	0.41440000	0.94702000
N	-1.58977000	2.25466700	-0.70652000
C	-0.93438400	3.05811400	-1.54509300
H	-0.23357500	2.57497300	-2.22166700
C	-1.13075100	4.43440300	-1.54512000
H	-0.57235600	5.05685400	-2.23745100
C	-2.03989400	4.97615400	-0.64448400
H	-2.21192400	6.04841700	-0.61116200
C	-2.74961900	4.13230500	0.20380000
H	-3.48770100	4.53044200	0.89368700
C	-2.51795500	2.76167600	0.14660700
C	-3.25104200	1.75581500	0.92754600
N	-2.92675700	0.49311300	0.61200100
N	-1.92680300	-1.73525400	-0.16468500
C	-2.93209600	-1.84919600	0.74160500
C	-3.46706000	-0.57088100	1.22358800
C	-4.44086800	-0.38838000	2.20494400
C	-4.80999000	0.91200200	2.53492500
C	-4.21570100	2.00105300	1.90402600
H	-4.49350000	3.01702900	2.16750600
H	-5.56446800	1.07945000	3.29833900
H	-4.89439400	-1.23935000	2.70359900
C	-3.40458200	-3.10248200	1.12034900
H	-4.20479600	-3.18378600	1.84970500
C	-2.85714800	-4.23808800	0.53388600
H	-3.21924100	-5.22297900	0.81646000
C	-1.85524100	-4.10051800	-0.42069500
H	-1.40653100	-4.96228400	-0.90521400
C	-1.41015500	-2.82413200	-0.74040300
H	-0.61183600	-2.65121500	-1.45757100
H	2.00900300	1.18428700	2.18018100
H	3.74134000	0.45993800	1.54005300
O	-2.26244000	-0.90619100	-3.01371400
H	-3.10905800	-1.41270300	-2.67866100
O	1.93365000	2.69275500	2.76292400
O	4.74221300	0.64363800	1.36032200
Cl	5.44517000	-0.91369000	1.50454700
Cl	0.27260700	3.13089800	2.87338700
O	-4.31963700	-2.17618000	-2.14623300
Cl	-5.53781800	-0.97355000	-1.94787400

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Mn	1.28356700	-0.07404900	0.26991300
O	2.28432100	0.20310800	1.86641300
O	0.27109500	-0.25183600	-1.32504900
N	1.18362300	-2.07276800	0.81526700
N	2.85328200	-0.90495400	-0.74184800
N	2.21431100	1.57911000	-0.56608400
C	0.36542500	-2.53317300	1.76486200
H	-0.31066300	-1.80234000	2.20308800
C	0.37403400	-3.86614700	2.15508400
H	-0.30680800	-4.20321200	2.93073100
C	1.25535500	-4.73849400	1.52562400
H	1.28191800	-5.78973300	1.79923600
C	2.11878000	-4.25290500	0.54973300
H	2.83374000	-4.91015200	0.06378000
C	2.07819900	-2.90147000	0.21892200
C	2.99223600	-2.23893600	-0.72042100
C	3.95436300	-2.85326400	-1.52065400
H	4.07930700	-3.93155200	-1.51363700
C	4.75103100	-2.04719100	-2.32813100

H	5.50990800	-2.50124800	-2.95918900
C	4.58459900	-0.66522600	-2.33877300
H	5.20369400	-0.03932800	-2.97376600
C	3.59960600	-0.11008000	-1.52217800
C	3.26328800	1.31350000	-1.39080600
C	3.95048800	2.34763200	-2.01720100
H	4.78449900	2.12706100	-2.67625900
C	3.56392100	3.66290000	-1.77841700
H	4.09245500	4.48006100	-2.26174300
C	2.50602700	3.91728800	-0.91568400
H	2.17492500	4.92854200	-0.69890800
C	1.85338500	2.84086700	-0.32368800
H	1.01019300	2.97698300	0.34754600
Mn	-1.32225900	0.17481400	-0.62606700
O	-2.29674100	0.26149700	-2.23176400
O	-0.24320100	0.43339700	0.97664500
N	-1.56572700	2.28298200	-0.72743500
C	-0.90895300	3.07070400	-1.57948700
H	-0.22354700	2.57139300	-2.26100300
C	-1.08241800	4.45025500	-1.59022500
H	-0.52369200	5.05823000	-2.29529300
C	-1.97084000	5.01428000	-0.68212900
H	-2.12551800	6.08947800	-0.65596200
C	-2.68231700	4.18852500	0.18225500
H	-3.40482200	4.60428000	0.87835700
C	-2.47204300	2.81351900	0.13136000
C	-3.21390100	1.82735200	0.92974800
N	-2.92913200	0.55352300	0.61615700
N	-2.01407600	-1.72834000	-0.13494300
C	-3.00987200	-1.78983800	0.78479500
C	-3.49295000	-0.48532300	1.25208800
C	-4.44576300	-0.26544000	2.24639500
C	-4.77183300	1.04718600	2.57111600
C	-4.15437900	2.11040000	1.91936200
H	-4.39699100	3.13679700	2.17710700
H	-5.50845200	1.24454900	3.34483600
H	-4.91604800	-1.09825200	2.76011600
C	-3.52452300	-3.01762000	1.19301900
H	-4.31999500	-3.05626300	1.93136200
C	-3.01983700	-4.18437300	0.62941600
H	-3.41179100	-5.14980500	0.93824900
C	-2.01994500	-4.10186800	-0.33389800
H	-1.60218700	-4.98943200	-0.79940900
C	-1.53998600	-2.84730700	-0.68863800
H	-0.74736600	-2.71828400	-1.42203700
H	2.04718200	1.13528600	2.19172200
H	3.76180200	0.42901900	1.53239200
O	-2.20906600	-0.89783400	-3.01177700
H	-3.42343000	-1.61095700	-2.58305400
O	1.98407800	2.67854800	2.75751500
O	4.76445100	0.62171100	1.33775600
Cl	5.48212800	-0.93023100	1.46802300
Cl	0.33963700	3.18012400	2.87423100
O	-4.26049800	-2.16918400	-2.24647200
Cl	-5.50115000	-0.99912200	-2.03925600

TS₃₀₋₃₁

Mn	1.30581900	-0.09429800	0.27038700
O	2.28377300	0.16400300	1.87224400
O	0.29983900	-0.25425800	-1.34257600
N	1.17634400	-2.09158000	0.79588100
N	2.87670600	-0.93008800	-0.73101000
N	2.25519800	1.55552200	-0.54494400

C	0.33243100	-2.55161700	1.72301900
H	-0.33778600	-1.81589600	2.16159900
C	0.30929400	-3.89084900	2.09042800
H	-0.39237200	-4.22798800	2.84724300
C	1.18629700	-4.76874200	1.46275900
H	1.18857400	-5.82464700	1.71908700
C	2.07620400	-4.28363800	0.51066200
H	2.78717900	-4.94668300	0.02659600
C	2.06585300	-2.92672300	0.20027000
C	3.00263900	-2.26583700	-0.71779800
C	3.97147400	-2.88176300	-1.50869000
H	4.08664100	-3.96103100	-1.50996900
C	4.78796800	-2.07634900	-2.29678900
H	5.55236300	-2.53246500	-2.91961300
C	4.63491400	-0.69285700	-2.29828800
H	5.26988500	-0.06749800	-2.91791100
C	3.64253400	-0.13537900	-1.49246100
C	3.31664800	1.28949600	-1.35333400
C	4.02427400	2.32414600	-1.95552500
H	4.86883700	2.10331900	-2.60087600
C	3.64472100	3.64003600	-1.70917300
H	4.18970200	4.45770700	-2.17293500
C	2.57285000	3.89439700	-0.86381000
H	2.24670400	4.90609700	-0.64172100
C	1.90046400	2.81755900	-0.29530300
H	1.04700900	2.95354800	0.36295200
Mn	-1.28180400	0.19446500	-0.64982300
O	-2.26764600	0.28613000	-2.29529600
O	-0.22491900	0.43544500	0.95607900
N	-1.51779800	2.30602000	-0.76400800
C	-0.83509200	3.08747000	-1.60150300
H	-0.13952000	2.58204000	-2.26801000
C	-0.99606300	4.46842300	-1.61611800
H	-0.41639300	5.07158400	-2.30828500
C	-1.90057100	5.03966600	-0.72879800
H	-2.04722700	6.11605800	-0.70638800
C	-2.63783800	4.22061700	0.12033600
H	-3.37154400	4.64471200	0.79926100
C	-2.43729700	2.84382300	0.07603400
C	-3.20052800	1.86226700	0.86073100
N	-2.90642000	0.58642100	0.56383700
N	-2.01328900	-1.70498100	-0.19365100
C	-3.02058300	-1.75859100	0.71324000
C	-3.49535200	-0.45021200	1.18007600
C	-4.47411700	-0.22574300	2.14754900
C	-4.80467000	1.08838200	2.46046700
C	-4.16868000	2.14902600	1.82242600
H	-4.41934900	3.17597300	2.06990700
H	-5.56287900	1.28958200	3.21200900
H	-4.96467700	-1.05622200	2.64590200
C	-3.56114000	-2.98150400	1.10087100
H	-4.36779100	-3.01528300	1.82737400
C	-3.06982300	-4.15031600	0.52913200
H	-3.48237300	-5.11216000	0.82184000
C	-2.05915900	-4.07448100	-0.42317500
H	-1.65360600	-4.96360000	-0.89637300
C	-1.55378900	-2.82412100	-0.75776700
H	-0.75187000	-2.69971300	-1.48210000
H	2.05071000	1.09646000	2.20595300
H	3.77583900	0.38602100	1.55873100
O	-2.21405500	-0.82989600	-3.06277600
H	-3.69073300	-1.41015800	-2.59517300
O	2.00664100	2.62316400	2.78517400

O	4.77963000	0.57442300	1.38149400
Cl	5.48566900	-0.98331800	1.50547400
Cl	0.37377500	3.16288100	2.88377500
O	-4.36572800	-2.07345800	-2.26564200
Cl	-5.80440600	-0.99292200	-1.57409000

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Mn	1.33145200	-0.01996800	0.25634900
O	2.26701600	0.27246000	1.85446400
O	0.29481800	-0.16677500	-1.36048700
N	1.26161600	-2.02664000	0.77514500
N	2.90891400	-0.80322900	-0.75354700
N	2.21380200	1.65955800	-0.54209000
C	0.43918200	-2.51736700	1.70586500
H	-0.23437800	-1.80113100	2.17041300
C	0.44074400	-3.86460100	2.04324600
H	-0.24410700	-4.22833500	2.80310100
C	1.31691900	-4.71683700	1.37971000
H	1.33351200	-5.77889500	1.60858600
C	2.18721600	-4.19860300	0.42694200
H	2.89799600	-4.84129700	-0.08427800
C	2.15622600	-2.83449700	0.15095100
C	3.07747200	-2.13505000	-0.75259300
C	4.08185300	-2.70802800	-1.53068100
H	4.23309200	-3.78266200	-1.54105500
C	4.89157300	-1.86707300	-2.28778100
H	5.68483600	-2.29084400	-2.89706700
C	4.69699500	-0.48905900	-2.27306300
H	5.32840000	0.16517600	-2.86571600
C	3.66830900	0.02642400	-1.48576200
C	3.29381500	1.43810300	-1.33858100
C	3.96570000	2.50480300	-1.92550800
H	4.82819500	2.32389200	-2.55952600
C	3.52666900	3.80222000	-1.67934500
H	4.04467400	4.64404100	-2.13051900
C	2.42972400	4.00862900	-0.85297000
H	2.05722800	5.00490300	-0.63445100
C	1.79615800	2.90307600	-0.29594300
H	0.92893200	2.99887800	0.35163000
Mn	-1.27162100	0.14145400	-0.58434300
O	-2.37053800	0.05065600	-2.29884000
O	-0.23933000	0.43929900	0.95018600
N	-1.68443700	2.18170900	-0.74923600
C	-1.04001800	3.00866200	-1.57495900
H	-0.31560700	2.54991600	-2.24382900
C	-1.27480400	4.37873400	-1.57096600
H	-0.72645100	5.02027000	-2.25378300
C	-2.20725500	4.89066900	-0.67663500
H	-2.40842500	5.95772800	-0.63948300
C	-2.89622700	4.02455400	0.16644500
H	-3.64399900	4.40025700	0.85847700
C	-2.62403800	2.66186300	0.10725600
C	-3.31053100	1.63243200	0.89874600
N	-2.91136200	0.38539100	0.60903100
N	-1.85604200	-1.80145400	-0.20685500
C	-2.86182000	-1.95863400	0.69360500
C	-3.42473200	-0.70216900	1.20319500
C	-4.41864200	-0.55897200	2.17050800
C	-4.84992700	0.72520300	2.48960300
C	-4.30340900	1.83750400	1.85562700
H	-4.64167900	2.84005000	2.09893100
H	-5.62411600	0.86075600	3.23943400
H	-4.84712800	-1.42842300	2.65934000

C	-3.32380600	-3.22947300	1.02138700
H	-4.12511200	-3.34712200	1.74456200
C	-2.76913700	-4.33592900	0.38640500
H	-3.12418600	-5.33412000	0.62812500
C	-1.77373300	-4.15241000	-0.56680500
H	-1.32508600	-4.98999600	-1.09198200
C	-1.33676000	-2.86008000	-0.83267800
H	-0.54300700	-2.65120000	-1.54625400
H	2.02469300	1.21036200	2.18605300
H	3.78343700	0.50143000	1.56112700
O	-2.03966600	-0.89461700	-3.10304700
H	-3.90520700	-1.87251400	-2.73639800
O	1.92975800	2.70199200	2.76667400
O	4.78507200	0.68625400	1.40408700
Cl	5.48194800	-0.87441100	1.54105900
Cl	0.26646900	3.12396000	2.89663900
O	-4.40237000	-2.54223100	-2.22921800
Cl	-5.84136600	-0.42581300	-1.53267400

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Mn	1.32735600	-0.02120100	0.25447200
O	2.26390800	0.27194700	1.85237400
O	0.29030000	-0.16658100	-1.36206400
N	1.25431900	-2.02679800	0.77666100
N	2.90386800	-0.80904100	-0.75391200
N	2.21360200	1.65553300	-0.54578100
C	0.43197800	-2.51411200	1.70928200
H	-0.24068500	-1.79591100	2.17216200
C	0.43269400	-3.86029400	2.05077300
H	-0.25182700	-4.22115300	2.81229500
C	1.30750600	-4.71531500	1.38900300
H	1.32326700	-5.77670900	1.62100400
C	2.17738700	-4.20070500	0.43391000
H	2.88719000	-4.84552500	-0.07599300
C	2.14762200	-2.83733600	0.15410600
C	3.06973400	-2.14118400	-0.75121200
C	4.07270600	-2.71727900	-1.52880800
H	4.22163300	-3.79224400	-1.53791000
C	4.88411600	-1.87891600	-2.28697500
H	5.67645000	-2.30511400	-2.89577900
C	4.69262000	-0.50044600	-2.27374500
H	5.32558000	0.15168400	-2.86705900
C	3.66508300	0.01815400	-1.48697700
C	3.29386800	1.43082800	-1.34104200
C	3.96917200	2.49543200	-1.92783300
H	4.83201300	2.31195000	-2.56062000
C	3.53309300	3.79411500	-1.68308800
H	4.05390400	4.63433600	-2.13400700
C	2.43549800	4.00381400	-0.85839200
H	2.06521800	5.00115000	-0.64096500
C	1.79863400	2.90022100	-0.30125500
H	0.93107100	2.99854000	0.34551700
Mn	-1.27644600	0.14807400	-0.58701600
O	-2.37504200	0.06995600	-2.29965200
O	-0.24168600	0.44308400	0.94754100
N	-1.68209600	2.18923400	-0.75123100
C	-1.03761000	3.01332600	-1.57976100
H	-0.31638500	2.55169300	-2.25007000
C	-1.26838200	4.38405900	-1.57662100
H	-0.72010900	5.02322700	-2.26171600
C	-2.19671900	4.89966100	-0.68011300
H	-2.39461200	5.96734800	-0.64346900
C	-2.88604600	4.03642900	0.16564800

H	-3.63093200	4.41508500	0.85915900
C	-2.61812600	2.67284600	0.10718000
C	-3.30620100	1.64629600	0.90107100
N	-2.91120700	0.39767900	0.61268300
N	-1.86635100	-1.79371300	-0.20409400
C	-2.86873200	-1.94648700	0.70072400
C	-3.42653300	-0.68738500	1.20949400
C	-4.41857400	-0.53986500	2.17799700
C	-4.84630500	0.74596500	2.49515700
C	-4.29757500	1.85566700	1.85861900
H	-4.63301200	2.85952600	2.10043700
H	-5.61942100	0.88490400	3.24547700
H	-4.84871400	-1.40727700	2.66897500
C	-3.33087600	-3.21555800	1.03517000
H	-4.13026300	-3.32943100	1.76106200
C	-2.77791000	-4.32527300	0.40435500
H	-3.13248000	-5.32221300	0.65191200
C	-1.78447400	-4.14662500	-0.55180800
H	-1.33650200	-4.98690300	-1.07326600
C	-1.34869100	-2.85558400	-0.82580500
H	-0.55661200	-2.65054700	-1.54230100
H	2.02444200	1.21083500	2.18215500
H	3.78039000	0.49364300	1.56051800
O	-2.08498300	-0.90296000	-3.08688300
H	-3.85157700	-1.96189700	-2.72726100
O	1.93405700	2.70511500	2.76035400
O	4.78300200	0.67537400	1.40407600
Cl	5.47560600	-0.88694100	1.54400500
Cl	0.27152500	3.12998500	2.89134800
O	-4.40134400	-2.60634300	-2.23974200
Cl	-5.77390400	-0.44154400	-1.55531300

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Mn	1.31956400	-0.04461400	0.28400700
O	2.24239900	0.25722200	1.86845200
O	0.23035600	-0.17454900	-1.29576900
N	1.21607300	-2.03546900	0.83620000
N	2.84160700	-0.88138300	-0.75889900
N	2.23071100	1.60076900	-0.55963800
C	0.42529500	-2.48178000	1.81567100
H	-0.20203400	-1.73641800	2.29855900
C	0.40367100	-3.82218300	2.17841900
H	-0.25366700	-4.15092100	2.97742900
C	1.22168500	-4.71244900	1.49072400
H	1.21822400	-5.77004600	1.73976700
C	2.06071000	-4.23873600	0.48797400
H	2.72824700	-4.91124100	-0.04234200
C	2.05642200	-2.87994200	0.18724300
C	2.95653800	-2.22005900	-0.76298700
C	3.89208800	-2.83573700	-1.59181200
H	3.99500400	-3.91607700	-1.60551500
C	4.69166500	-2.03100300	-2.39719700
H	5.43051400	-2.48792700	-3.04934800
C	4.55273700	-0.64639400	-2.37880000
H	5.17273400	-0.01942700	-3.01163300
C	3.59080700	-0.08617600	-1.53951400
C	3.27446500	1.33770100	-1.39043700
C	3.96164700	2.37558800	-2.00973700
H	4.79470900	2.15912100	-2.67116000
C	3.57370600	3.68867500	-1.76110400
H	4.10320400	4.50934100	-2.23713200
C	2.51213800	3.93779900	-0.90099700
H	2.17959800	4.94761200	-0.68050400

C	1.86109800	2.85875100	-0.31233900
H	1.01758000	2.98877200	0.35986700
Mn	-1.30404100	0.19688000	-0.48828800
O	-2.45158600	0.10971200	-2.18475400
O	-0.25912800	0.45135700	0.99037500
N	-1.63196100	2.23126000	-0.68126700
C	-0.97619400	3.01245200	-1.54226600
H	-0.28720600	2.51005500	-2.21661200
C	-1.15816000	4.39021700	-1.56169800
H	-0.60293700	4.99434800	-2.27240700
C	-2.04368500	4.95723200	-0.65328300
H	-2.19906900	6.03225700	-0.63195300
C	-2.74732700	4.13719000	0.22343900
H	-3.46087500	4.55789800	0.92527800
C	-2.53533200	2.76354300	0.18621200
C	-3.24759600	1.77867700	1.01065600
N	-2.91374300	0.51005800	0.72904800
N	-1.93235700	-1.72225000	-0.04839400
C	-2.91973200	-1.82813400	0.87976000
C	-3.43919000	-0.54534000	1.36686800
C	-4.40064900	-0.34675800	2.35658300
C	-4.77433600	0.95921400	2.65990500
C	-4.20244700	2.03888400	1.99217000
H	-4.49237000	3.05759800	2.23042400
H	-5.52031900	1.13937800	3.42869100
H	-4.84494500	-1.18936300	2.87725500
C	-3.40701100	-3.07684600	1.25143200
H	-4.19190500	-3.15207000	1.99798100
C	-2.90075900	-4.21352500	0.63008200
H	-3.27910600	-5.19469800	0.90374100
C	-1.92147700	-4.08198900	-0.34836400
H	-1.50821100	-4.94481200	-0.86142900
C	-1.45127300	-2.81103400	-0.65481300
H	-0.66397000	-2.64286800	-1.38518300
H	2.05169300	1.21872000	2.18339900
H	3.77825400	0.42015000	1.52165600
O	-2.20031900	-0.89744900	-2.93323900
H	-4.39939100	-0.96747500	-3.64010100
O	2.01359100	2.69252000	2.74549800
O	4.77479600	0.57095200	1.33178800
Cl	5.42927000	-1.00813500	1.46256700
Cl	0.35999900	3.14006900	2.88502600
O	-3.90123300	-0.82001200	-4.46778200
Cl	-5.59351300	-1.48278900	-1.55690800

TS₃₂₋₃₃

Mn	-1.26849800	0.22773200	0.37039000
O	-2.03854000	0.05216200	2.02440900
O	-0.19683600	0.41299600	-1.22321600
N	-1.42207900	2.27300000	0.57949200
N	-2.86869300	0.66530200	-0.77227600
N	-1.95006800	-1.64437600	-0.15181000
C	-0.67869600	2.98222400	1.43027700
H	0.02939300	2.42087700	2.03519300
C	-0.80399500	4.36341900	1.52555400
H	-0.17982900	4.91066700	2.22506300
C	-1.72532500	5.00825200	0.70912600
H	-1.84114100	6.08750500	0.75355500
C	-2.51479900	4.26117900	-0.15963900
H	-3.25737000	4.74159700	-0.78923300
C	-2.35359100	2.88070500	-0.20000500
C	-3.15874100	1.95724200	-1.00284200
C	-4.15642700	2.29064400	-1.91616700

H	-4.40321700	3.32935800	-2.11213700
C	-4.82687000	1.26212400	-2.57104000
H	-5.60776400	1.50056000	-3.28740600
C	-4.50408900	-0.06799500	-2.32097900
H	-5.02098100	-0.87325800	-2.83332400
C	-3.49336500	-0.34354800	-1.40278100
C	-3.00458900	-1.66618100	-1.00854000
C	-3.55857300	-2.87445700	-1.41527200
H	-4.39535800	-2.88275900	-2.10709500
C	-3.04067600	-4.06198400	-0.90687200
H	-3.46785600	-5.01348600	-1.21151700
C	-1.98132300	-4.01814100	-0.00955000
H	-1.54799000	-4.92169300	0.40861300
C	-1.45224100	-2.78099400	0.34185800
H	-0.59796000	-2.68356200	1.00552100
Mn	1.32072000	-0.06230700	-0.47263500
O	3.06290700	-0.44185000	-2.47529800
O	0.38234700	-0.18820700	1.03566500
N	1.25560100	-2.05136200	-1.02819600
C	0.47342200	-2.52070300	-2.00357400
H	-0.18684500	-1.79622700	-2.47460600
C	0.49566200	-3.85972800	-2.37286500
H	-0.15404300	-4.20672300	-3.17029000
C	1.33950600	-4.72584900	-1.68695800
H	1.36612200	-5.78309200	-1.93594100
C	2.16959100	-4.22805700	-0.68731000
H	2.86089000	-4.88096000	-0.16332400
C	2.13342500	-2.86991200	-0.39045700
C	3.03724100	-2.18535700	0.54177600
N	2.93262800	-0.84823600	0.49086700
N	2.29917200	1.61158700	0.19432800
C	3.31595000	1.38786100	1.07319700
C	3.64719400	-0.02712300	1.27570500
C	4.57933100	-0.55964300	2.16445900
C	4.72315300	-1.94369800	2.21949800
C	3.95404100	-2.77514700	1.41045700
H	4.05839300	-3.85430300	1.46249000
H	5.43980800	-2.37982000	2.90954200
H	5.17096900	0.08522400	2.80635600
C	3.96830500	2.45288400	1.68318200
H	4.77495500	2.26582900	2.38524000
C	3.58590700	3.75364400	1.36983900
H	4.08825900	4.59446400	1.84003900
C	2.57185100	3.96383200	0.44463500
H	2.25236400	4.96262100	0.16361800
C	1.94492000	2.86048500	-0.12280700
H	1.14535200	2.95942000	-0.85265200
H	-1.73137100	-0.81926600	2.49864200
H	-3.57712300	-0.32274800	1.76244400
O	2.64922000	-0.04298500	-3.58587100
H	2.29697800	2.00159700	-2.65289100
O	-1.51524700	-2.11458700	3.30386500
O	-4.55229700	-0.59150200	1.63087900
Cl	-5.35404100	0.92281400	1.57818100
Cl	0.17694300	-2.35413800	3.46216500
O	1.50762800	2.11997700	-3.20050600
Cl	5.23258300	2.32763400	-1.94902000
O ₂			
O	0.00000000	0.00000000	0.60819000
O	0.00000000	0.00000000	-0.60819000

Mn	1.37112200	0.10823300	-0.68964400
O	1.89097600	0.40833800	-2.29958000
O	0.69975800	-0.22867600	1.25838500
N	1.81378300	2.05496400	-0.08834000
N	3.22646800	-0.08777200	0.15861400
N	1.81189300	-1.90628500	-0.96236500
C	1.03737300	3.11436200	-0.32886700
H	0.12004000	2.91466600	-0.87527900
C	1.39079900	4.39516500	0.08361300
H	0.72655800	5.22768500	-0.12951300
C	2.58480900	4.57074400	0.77106600
H	2.88886400	5.55705400	1.11145400
C	3.39613500	3.46805300	1.01813300
H	4.33963100	3.57871500	1.54444000
C	2.99166100	2.21485000	0.57026200
C	3.77014200	0.98485800	0.75327300
C	4.95437800	0.85840000	1.47882100
H	5.40844200	1.72189200	1.95541000
C	5.53124100	-0.40262900	1.58872200
H	6.45214700	-0.52747100	2.15138800
C	4.92838900	-1.50973500	0.99895600
H	5.36340500	-2.49930000	1.10221900
C	3.74845000	-1.31928900	0.28131400
C	2.96346900	-2.35461000	-0.40279100
C	3.34190300	-3.68840200	-0.53172900
H	4.25980400	-4.04288100	-0.07263900
C	2.54431300	-4.54933700	-1.27758000
H	2.82958900	-5.59170700	-1.39134600
C	1.39368500	-4.06088600	-1.88727200
H	0.75184400	-4.69800700	-2.48820500
C	1.05691700	-2.72648900	-1.69760300
H	0.15913800	-2.28774400	-2.12827500
Mn	-0.97682200	-0.28887200	0.78827000
O	-1.36827400	-0.58691300	2.69234800
O	-0.42111700	0.04691800	-0.93844200
N	-1.25131500	-2.31556700	0.48043500
C	-0.42584900	-3.25045900	0.95891500
H	0.45282800	-2.88453500	1.48526700
C	-0.66935000	-4.60604500	0.77786000
H	0.02826700	-5.33534400	1.17811100
C	-1.79975100	-4.99025600	0.06581000
H	-2.01471300	-6.04163500	-0.10509300
C	-2.66781600	-4.01700800	-0.41787200
H	-3.57222000	-4.29493100	-0.95097200
C	-2.38193600	-2.67504700	-0.18391900
C	-3.25516500	-1.55389100	-0.55871000
N	-2.85854400	-0.38392000	-0.03974500
N	-1.70702600	1.65272400	1.02135600
C	-2.87505000	1.92427600	0.38168500
C	-3.50182000	0.76802500	-0.27254400
C	-4.65493100	0.77671100	-1.05621700
C	-5.09504500	-0.42944900	-1.59366500
C	-4.39899600	-1.61113600	-1.35418100
H	-4.73343400	-2.54944100	-1.78578700
H	-5.98717300	-0.44779000	-2.21341300
H	-5.19222100	1.70029800	-1.24889100
C	-3.41974200	3.20399500	0.41330400
H	-4.34713000	3.41397600	-0.11109800
C	-2.77319800	4.19841600	1.14054200
H	-3.18838700	5.20188000	1.17614100
C	-1.60730300	3.89071300	1.83086700
H	-1.08016200	4.63411000	2.42104700
C	-1.10017400	2.59962400	1.73939500

H	-0.17882500	2.30596100	2.23780900
O	0.60546100	1.92678300	-3.03402700
Cl	-0.61528700	3.41390000	-3.71801600
Cl	-3.02531600	-0.79691200	3.10124600

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Mn	-1.26455300	0.00673600	-0.74638600
O	-1.85983400	0.14483600	-2.65438700
O	-0.51494500	0.00965300	1.01506700
N	-2.04462900	-2.14058800	-0.70307900
N	-3.31419300	0.01144900	0.12136300
N	-2.06993200	2.16257400	-0.73692600
C	-1.36469400	-3.17835700	-1.19559200
H	-0.48114400	-2.93497400	-1.78538800
C	-1.74045100	-4.49914600	-0.97490000
H	-1.15356500	-5.31075900	-1.39533600
C	-2.86566300	-4.73992200	-0.19505100
H	-3.18844600	-5.75663100	0.01417300
C	-3.58260400	-3.66386300	0.31604300
H	-4.46747200	-3.83712500	0.92110900
C	-3.15019700	-2.36673800	0.03715300
C	-3.86044000	-1.15689700	0.49800500
C	-5.02872900	-1.19012800	1.26244900
H	-5.47234400	-2.13434900	1.56210800
C	-5.61601900	0.01174000	1.63594600
H	-6.52515300	0.01173100	2.23125600
C	-5.03808700	1.21368800	1.24798600
H	-5.48912500	2.15839700	1.53495000
C	-3.86960900	1.18017300	0.48438400
C	-3.17029300	2.39075300	0.00834900
C	-3.60721400	3.68898700	0.27547000
H	-4.48737100	3.86592200	0.88637400
C	-2.89960900	4.76175600	-0.25565500
H	-3.22555000	5.77948100	-0.05648000
C	-1.78110200	4.51740300	-1.04459300
H	-1.20451100	5.32707000	-1.48271600
C	-1.40078500	3.19573900	-1.25145700
H	-0.52353900	2.94663500	-1.84933600
Mn	1.18397400	0.02130300	0.47662500
O	1.62286800	0.02473400	2.40723400
O	0.54939700	0.02335700	-1.22122700
N	1.65839700	2.03510100	0.42195500
C	0.87531500	2.99596100	0.91848200
H	-0.05701800	2.66630200	1.37192700
C	1.23095400	4.33832400	0.85453600
H	0.56434700	5.08982400	1.26646300
C	2.43539000	4.68152500	0.25261400
H	2.74121500	5.72170700	0.18194400
C	3.25666000	3.67920800	-0.25272000
H	4.21110700	3.92246400	-0.71001300
C	2.84992000	2.35252900	-0.15102500
C	3.64084100	1.19860700	-0.59565600
N	3.07748200	0.02153800	-0.28711400
N	1.66709500	-1.99048300	0.44373800
C	2.86525900	-2.30845700	-0.11423700
C	3.64848300	-1.15669700	-0.57712400
C	4.87560600	-1.19018900	-1.23837400
C	5.47577100	0.01897500	-1.57792100
C	4.86746000	1.22937300	-1.25832800
H	5.33618700	2.17253800	-1.52110600
H	6.43038800	0.01785300	-2.09647600
H	5.35145300	-2.13420700	-1.48465000
C	3.28649200	-3.63277800	-0.18214600

H	4.24584200	-3.87697900	-0.62845800
C	2.47363600	-4.63129400	0.34392700
H	2.79109200	-5.66949800	0.30048600
C	1.26317000	-4.28662700	0.93272000
H	0.60304900	-5.03481500	1.36085100
C	0.89293700	-2.94707900	0.96195700
H	-0.04413200	-2.61590600	1.40434000
O	-1.35079800	-0.76257300	-3.44342900
Cl	3.28774800	-0.01954500	2.82829000

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Mn	-1.27263600	0.00234200	-0.72136500
O	-1.82183600	0.09777300	-2.73162900
O	-0.52775500	0.01440600	1.02523300
N	-2.10555300	-2.13242300	-0.66180700
N	-3.28531500	0.09424000	0.11418000
N	-1.97408200	2.18588600	-0.81082800
C	-1.45914600	-3.20992500	-1.11193900
H	-0.56634800	-3.01777500	-1.70644500
C	-1.88125100	-4.50814700	-0.84573000
H	-1.32168400	-5.35390100	-1.23504400
C	-3.01717100	-4.68226200	-0.06349400
H	-3.37539300	-5.67924400	0.18015100
C	-3.69887900	-3.56483400	0.40524200
H	-4.58982500	-3.68632600	1.01397600
C	-3.22160700	-2.29437100	0.07952800
C	-3.89199600	-1.04548000	0.49263300
C	-5.08490100	-1.01430400	1.21747100
H	-5.58044300	-1.93286400	1.51447300
C	-5.63236600	0.21735400	1.55155600
H	-6.56048500	0.26620900	2.11454400
C	-4.99234800	1.38695400	1.16314600
H	-5.41486100	2.35387300	1.41702800
C	-3.80312500	1.29358700	0.43772800
C	-3.04524500	2.46736900	-0.04027900
C	-3.40286400	3.78478400	0.24944200
H	-4.25570000	4.00282900	0.88534900
C	-2.65012500	4.82229800	-0.28970800
H	-2.91375500	5.85429200	-0.07260200
C	-1.56657000	4.52429200	-1.10840500
H	-0.95688700	5.30552000	-1.55335400
C	-1.26070300	3.18609800	-1.33145800
H	-0.40903900	2.89578800	-1.94724700
Mn	1.17296000	-0.01219700	0.48684400
O	1.61306800	-0.01511200	2.41210700
O	0.51351400	-0.01786200	-1.20850200
N	1.65480200	1.99856600	0.44204900
C	0.88358100	2.95768800	0.96002500
H	-0.05163700	2.62935600	1.40863500
C	1.25486800	4.29677500	0.92318300
H	0.59843500	5.04697700	1.35349100
C	2.46038000	4.63862900	0.32278700
H	2.77785500	5.67650000	0.27247200
C	3.26810900	3.63781100	-0.20694500
H	4.22300600	3.87985200	-0.66385500
C	2.84794100	2.31385500	-0.12853100
C	3.62638600	1.15981400	-0.59297900
N	3.05722000	-0.01692800	-0.29287800
N	1.64562300	-2.02499900	0.44070700
C	2.82941600	-2.34709300	-0.14496300
C	3.61595500	-1.19602600	-0.60353700
C	4.83565600	-1.23039000	-1.27826400
C	5.44245700	-0.02172700	-1.60748800

C	4.84730800	1.18928500	-1.26598100
H	5.32186200	2.13184700	-1.52005600
H	6.39187900	-0.02362300	-2.13547900
H	5.30041400	-2.17501300	-1.54271700
C	3.23341900	-3.67484500	-0.24251800
H	4.18078600	-3.92267600	-0.71186800
C	2.41852500	-4.67227700	0.28282600
H	2.72205700	-5.71333300	0.21521100
C	1.22434400	-4.32335900	0.90165100
H	0.56419600	-5.07092400	1.33072900
C	0.87034100	-2.98021500	0.95930000
H	-0.05440800	-2.64561200	1.42421200
O	-1.34125600	-0.91851700	-3.41979900
Cl	3.27792800	-0.07407700	2.82802000

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Mn	-1.29240900	0.06375600	-0.61113500
O	-1.94828800	0.19676200	-2.50995400
O	-0.66952100	0.14807000	1.13685000
N	-2.03486100	-2.16467200	-0.46344500
N	-3.37982800	0.02688700	0.21232500
N	-2.16174900	2.22581700	-0.63374400
C	-1.30042900	-3.22048900	-0.82159400
H	-0.38178700	-2.99951400	-1.36629100
C	-1.66265500	-4.53075900	-0.52785800
H	-1.03144500	-5.35664700	-0.84393700
C	-2.84056900	-4.74152400	0.18015800
H	-3.16038900	-5.74796300	0.43849100
C	-3.61150700	-3.64815200	0.55749100
H	-4.53353900	-3.80042600	1.11032000
C	-3.18341300	-2.36325500	0.21445500
C	-3.94409600	-1.14411100	0.56058100
C	-5.17791400	-1.18383000	1.21519000
H	-5.63431900	-2.12900700	1.49005600
C	-5.81815400	0.01076800	1.51270200
H	-6.77953500	0.00360600	2.01936900
C	-5.22394300	1.21443400	1.16018600
H	-5.71666700	2.15405300	1.38796800
C	-3.98999100	1.18993400	0.50632700
C	-3.27772600	2.41821800	0.09673900
C	-3.71244000	3.70276500	0.43065600
H	-4.60591000	3.85077100	1.02999500
C	-2.98186300	4.79943900	-0.01259100
H	-3.30533100	5.80609300	0.24021700
C	-1.83978100	4.59305500	-0.77881100
H	-1.24275100	5.42258100	-1.14714700
C	-1.46729100	3.28275100	-1.05930500
H	-0.57544600	3.06058800	-1.64652400
Mn	1.12362600	0.04198700	0.67458700
O	1.48912900	0.13346500	2.64404000
O	0.49411800	-0.05008600	-1.06668300
N	1.88047400	2.26026000	0.49330800
C	1.16276600	3.31923000	0.87265000
H	0.25678000	3.10173700	1.44004300
C	1.52873500	4.62729400	0.57307500
H	0.91249700	5.45822400	0.90508200
C	2.69188400	4.82916100	-0.16189800
H	3.01304000	5.83349300	-0.42673200
C	3.44812200	3.73096200	-0.55553500
H	4.36037200	3.87737500	-1.12609500
C	3.01761700	2.44917000	-0.20425900
C	3.76266300	1.22145800	-0.55538200
N	3.19282900	0.05758900	-0.19296000

N	1.96532100	-2.12496400	0.68022200
C	3.08446900	-2.33184500	-0.04139300
C	3.79626100	-1.11125300	-0.47563600
C	5.02641400	-1.14905900	-1.13677400
C	5.62343500	0.04715600	-1.50915700
C	4.99113900	1.24823000	-1.22053800
H	5.45029800	2.18838800	-1.50799700
H	6.58133400	0.04343500	-2.02244500
H	5.51487000	-2.09346900	-1.35382900
C	3.52450500	-3.62298800	-0.34232600
H	4.41856000	-3.78357700	-0.93757800
C	2.79847100	-4.71097100	0.12890300
H	3.12645600	-5.72238900	-0.09775800
C	1.65525300	-4.48959100	0.88900900
H	1.06161300	-5.31171400	1.27885300
C	1.27584600	-3.17374700	1.13256800
H	0.38083000	-2.94059000	1.71092900
Cl	3.16472700	0.07971400	3.06003400
Cl	-1.35199700	-1.05179800	-3.54421400

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Mn	-1.37562600	0.19204500	-0.79137300
O	-0.85838600	-0.08114700	1.18958700
N	-2.00730000	-1.78884200	-0.92234300
N	-3.25204000	0.25490300	0.01255100
N	-1.62312400	2.20413500	-0.37857900
C	-1.31908100	-2.74165900	-1.55382900
H	-0.37228700	-2.43611500	-1.99369300
C	-1.78375900	-4.04909600	-1.62990800
H	-1.19413200	-4.79965800	-2.14746200
C	-2.99146000	-4.36326100	-1.01723800
H	-3.37638400	-5.37900900	-1.04437800
C	-3.71657300	-3.36320600	-0.37769300
H	-4.67269300	-3.58257500	0.08795500
C	-3.20936100	-2.06739200	-0.35806800
C	-3.89687000	-0.90532900	0.21635300
C	-5.09914600	-0.91667100	0.92132200
H	-5.63616100	-1.84453000	1.09024900
C	-5.59010100	0.28884200	1.41364100
H	-6.52596000	0.30321400	1.96500700
C	-4.88594600	1.47287600	1.22014000
H	-5.25620000	2.41269500	1.61824400
C	-3.68620800	1.42279800	0.51175900
C	-2.78422400	2.54690300	0.23728600
C	-3.06068600	3.87734900	0.53505200
H	-3.98547500	4.14007100	1.03985900
C	-2.14867500	4.85924800	0.16226800
H	-2.35542700	5.90301300	0.38221300
C	-0.98400500	4.49341700	-0.50101200
H	-0.24982800	5.22910500	-0.81477600
C	-0.75294300	3.14519400	-0.74938400
H	0.14850600	2.79473800	-1.24780300
Mn	0.84284500	-0.28425400	0.85629700
O	1.13101900	-0.52106100	2.75806200
O	0.37707500	-0.04595500	-0.92763200
N	1.62026600	1.64023300	1.00595400
C	1.01608800	2.63960500	1.65258700
H	0.06060100	2.40269000	2.11596900
C	1.56740300	3.91390200	1.71303500
H	1.04232300	4.70110500	2.24521700
C	2.77266600	4.14944200	1.06298200
H	3.22261500	5.13837200	1.07368700
C	3.41202400	3.10261000	0.40698200

H	4.36652000	3.25837900	-0.08691000
C	2.82431000	1.84146200	0.40747400
C	3.43248900	0.63617700	-0.17258400
N	2.74244600	-0.48125000	0.09022300
N	1.03945100	-2.32221600	0.63907200
C	2.17036200	-2.75352300	0.01820100
C	3.10100200	-1.68623400	-0.37404200
C	4.25888200	-1.81857300	-1.13894000
C	5.00628100	-0.67429700	-1.40666200
C	4.60239800	0.56896800	-0.92890300
H	5.17807400	1.46291600	-1.14919500
H	5.91019200	-0.75225400	-2.00421100
H	4.56691300	-2.78483500	-1.52637100
C	2.40294200	-4.11343300	-0.16145400
H	3.30836400	-4.44934600	-0.65798800
C	1.48062700	-5.03055600	0.33130600
H	1.65403500	-6.09564900	0.20434800
C	0.35033400	-4.57309300	0.99844300
H	-0.38894000	-5.25663500	1.40447300
C	0.16143600	-3.20256700	1.12655100
H	-0.71342600	-2.78278500	1.61781400
O	-1.74046300	0.45777300	-2.40825900
Cl	2.74523300	-0.82844100	3.23869700
O	0.32192600	1.60037200	-3.60591300
Cl	1.91358000	1.81046100	-3.14247600

TS₃₈₋₃₉

Mn	-1.36014500	0.07495200	-0.64784700
O	-0.72176300	-0.14956700	1.23822500
N	-1.78658400	-1.95495400	-0.84918200
N	-3.22923300	-0.09050900	0.15110100
N	-1.82871900	2.04701900	-0.21807100
C	-1.00744800	-2.81009000	-1.51569800
H	-0.11041400	-2.38922500	-1.96464300
C	-1.32204700	-4.15978400	-1.61482400
H	-0.66271900	-4.82634200	-2.16231100
C	-2.47138700	-4.62368000	-0.98447200
H	-2.73740800	-5.67631500	-1.02712900
C	-3.29119100	-3.72709900	-0.30742300
H	-4.20588300	-4.06287000	0.17193200
C	-2.93646700	-2.38220300	-0.26829700
C	-3.74117800	-1.31731500	0.33963500
C	-4.93133400	-1.47170200	1.04804800
H	-5.36323000	-2.45612300	1.19947300
C	-5.54785000	-0.33535100	1.56313000
H	-6.47471900	-0.43315600	2.12111400
C	-4.98042600	0.92235200	1.38313900
H	-5.44694000	1.80836100	1.80244200
C	-3.78958200	1.01560300	0.66432500
C	-3.02740100	2.23947000	0.39460000
C	-3.46832700	3.52148800	0.70411000
H	-4.42857400	3.66347600	1.19075100
C	-2.67470000	4.61217200	0.36351300
H	-3.00758300	5.62009700	0.59573800
C	-1.46265900	4.39855000	-0.28028900
H	-0.81356900	5.22146800	-0.56364000
C	-1.07138400	3.09275100	-0.55559300
H	-0.13083100	2.86627900	-1.05060600
Mn	0.98280000	-0.16788100	0.82043800
O	1.36001900	-0.33348500	2.72250800
O	0.40843200	0.06398600	-0.92936500
N	1.61362500	1.81955400	0.93184600
C	0.97168800	2.77444300	1.60634400

H	0.06816000	2.46847400	2.12913600
C	1.42359000	4.08920000	1.62272700
H	0.87120900	4.83959000	2.17987400
C	2.56661500	4.40922000	0.90059400
H	2.93750000	5.43022700	0.87750600
C	3.24951000	3.40630600	0.21922300
H	4.16211300	3.62795200	-0.32593400
C	2.76348900	2.10366700	0.26519900
C	3.44200800	0.93855200	-0.31667700
N	2.85486200	-0.22675600	-0.00886600
N	1.33504300	-2.18941100	0.63722500
C	2.47798500	-2.54041300	-0.01133900
C	3.30678700	-1.40952700	-0.44810900
C	4.45811900	-1.46499000	-1.23236100
C	5.09593500	-0.26941500	-1.55180400
C	4.59452300	0.94851200	-1.10087900
H	5.08627300	1.88103700	-1.35947000
H	5.99115800	-0.28652500	-2.16699700
H	4.84208400	-2.41306400	-1.59551300
C	2.80679500	-3.88130900	-0.18422600
H	3.71885400	-4.15311100	-0.70727800
C	1.96939200	-4.85902800	0.34295700
H	2.21770200	-5.90960800	0.21948500
C	0.82550100	-4.48002700	1.03612000
H	0.15045900	-5.21264000	1.46759100
C	0.53733600	-3.12630000	1.15681200
H	-0.35377200	-2.76590800	1.66542300
O	-1.85917700	0.29766500	-2.30910300
Cl	3.01363700	-0.47266000	3.14492800
O	-0.91308200	1.60901500	-3.17383800
Cl	0.84636500	1.88803200	-3.81189300

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Mn	-1.32819100	-0.00627200	-0.65810000
O	-0.58032800	-0.01808300	1.08760800
N	-1.86933400	-2.03794900	-0.68887700
N	-3.19604400	-0.00388500	0.16451700
N	-1.84891400	2.02406000	-0.65610200
C	-1.15530200	-2.99605500	-1.28321200
H	-0.26293300	-2.67121400	-1.81446000
C	-1.52808700	-4.33357000	-1.21571200
H	-0.92338300	-5.08659100	-1.71165500
C	-2.66667700	-4.67034400	-0.49341100
H	-2.97985400	-5.70734900	-0.40939900
C	-3.41661100	-3.66787600	0.11454800
H	-4.32102200	-3.90997600	0.66443100
C	-3.00419700	-2.34499300	-0.00909200
C	-3.74123000	-1.18404400	0.50585800
C	-4.91258900	-1.21372600	1.26067800
H	-5.36927900	-2.15663300	1.54381700
C	-5.48287400	-0.00432100	1.64703800
H	-6.39457200	-0.00461800	2.23766700
C	-4.89738500	1.20523900	1.28548800
H	-5.34114700	2.14834200	1.58807400
C	-3.72657500	1.17582700	0.52983100
C	-2.97471700	2.33604000	0.03625300
C	-3.36434500	3.66281400	0.18692700
H	-4.26367200	3.90867600	0.74352900
C	-2.59890100	4.66433900	-0.40352700
H	-2.89295300	5.70482300	-0.29631400
C	-1.46851600	4.32290700	-1.13609700
H	-0.85010900	5.07562900	-1.61533200
C	-1.11943400	2.98025900	-1.23248500

H	-0.23296100	2.65120600	-1.77099800
Mn	1.11336200	-0.02834200	0.56492700
O	1.55680200	-0.02867000	2.45577400
O	0.38271200	-0.01874000	-1.16517900
N	1.59438500	1.97081100	0.51388000
C	0.86911400	2.92021600	1.10959400
H	-0.03125000	2.58632000	1.62050800
C	1.24209400	4.25831200	1.06402800
H	0.62567700	5.00353600	1.55722800
C	2.39415100	4.60645100	0.36900900
H	2.70766500	5.64475300	0.30572100
C	3.15662000	3.61247500	-0.23629400
H	4.07363700	3.85809600	-0.76342200
C	2.74350400	2.28799100	-0.13895700
C	3.48960900	1.13392600	-0.65090700
N	2.94015100	-0.04201600	-0.31053400
N	1.56339700	-2.03485400	0.50506800
C	2.69922300	-2.36942100	-0.16241300
C	3.46749800	-1.22459900	-0.66281000
C	4.64435600	-1.26282900	-1.40863800
C	5.23672600	-0.05591800	-1.77025500
C	4.66734400	1.15819500	-1.39586300
H	5.12873100	2.09910300	-1.67821600
H	6.15392300	-0.06179400	-2.35227100
H	5.08780500	-2.20915300	-1.70155400
C	3.07771700	-3.70215000	-0.28538800
H	3.98467600	-3.96202300	-0.82295200
C	2.29288400	-4.68713400	0.30617500
H	2.57854300	-5.73190900	0.22106800
C	1.15367800	-4.32250600	1.01385600
H	0.51990800	-5.06076900	1.49541300
C	0.81611000	-2.97624900	1.08650300
H	-0.07319000	-2.62871100	1.60744400
O	-1.98791300	-0.03245200	-2.64631800
Cl	3.22185400	0.06409100	2.83970400
O	-1.36748000	0.76011400	-3.41613500

TS_{22B}

Mn	-1.41339200	-0.07462500	-0.54433600
O	-0.88018600	0.15995800	1.30301300
N	-1.61545700	-2.11030300	-0.27975200
N	-3.32252700	-0.24505500	0.10811100
N	-2.10440700	1.87402300	-0.66044100
C	-0.70012900	-3.00507000	-0.66189000
H	0.21520400	-2.60089800	-1.08884000
C	-0.89843200	-4.37123300	-0.50585900
H	-0.12713200	-5.06467200	-0.82756900
C	-2.07897600	-4.81109800	0.08242700
H	-2.26030400	-5.87177800	0.23351300
C	-3.03845800	-3.88085200	0.46577300
H	-3.97660000	-4.20279100	0.90785900
C	-2.79355400	-2.52632500	0.25698200
C	-3.74767200	-1.44843300	0.53229100
C	-4.98820100	-1.57080000	1.15743900
H	-5.34372800	-2.53857000	1.49813800
C	-5.75301500	-0.42437400	1.34492900
H	-6.72019400	-0.49536200	1.83441300
C	-5.28321300	0.81581200	0.92136700
H	-5.87086900	1.71445800	1.08170000
C	-4.03796600	0.87803200	0.29898900
C	-3.36472200	2.08325300	-0.19696700
C	-3.93230300	3.35330000	-0.23629600
H	-4.93776400	3.51272500	0.14134800

C	-3.20266900	4.40640400	-0.77728900
H	-3.63477100	5.40260900	-0.81578200
C	-1.92722000	4.16884600	-1.27547600
H	-1.32795200	4.96162700	-1.71287000
C	-1.41008000	2.88125400	-1.19516800
H	-0.41237800	2.63734300	-1.55449200
Mn	0.85674800	0.36180900	0.96252600
O	1.10017900	0.59997700	2.88892600
O	0.34407500	0.16508600	-0.82714600
N	1.31023800	2.41924000	0.66428900
C	0.54849800	3.42095300	1.10824800
H	-0.34048100	3.13542200	1.66728800
C	0.86202400	4.75230100	0.85985100
H	0.21258400	5.53808400	1.23342100
C	2.00282200	5.03772000	0.11903300
H	2.27446300	6.06589000	-0.10446100
C	2.80769700	3.99428100	-0.32605700
H	3.71785000	4.19754100	-0.88248200
C	2.44616300	2.68291800	-0.02856300
C	3.24918000	1.50232800	-0.38586900
N	2.81129600	0.36060400	0.16682900
N	1.56905900	-1.67844900	1.18188100
C	2.74341000	-1.96426700	0.57202300
C	3.40154200	-0.81878700	-0.07477800
C	4.53637900	-0.88686100	-0.88470900
C	5.01378100	0.28860800	-1.45442000
C	4.37137600	1.49935200	-1.21420000
H	4.73093200	2.41589600	-1.67146300
H	5.88748800	0.25975500	-2.09958600
H	5.02497200	-1.83697800	-1.08007700
C	3.26867700	-3.25404000	0.60094200
H	4.20209200	-3.47617900	0.09196000
C	2.59357700	-4.24192700	1.31006800
H	2.99260100	-5.25206300	1.34813700
C	1.41654700	-3.92069400	1.97674400
H	0.86576900	-4.66072800	2.54959900
C	0.93045700	-2.62234300	1.87495100
H	-0.00568000	-2.32126500	2.34304500
O	-1.84581800	-0.33138300	-2.26992700
Cl	2.72205100	0.87615500	3.37308600
O	-0.61485100	0.30952700	-3.34713600
H	-0.00760700	0.52875300	-2.60304100
H	0.05845600	-1.15376600	-3.61762000
O	0.51334200	-2.05987300	-3.71376800
Cl	2.04351900	-1.77444700	-2.98791500

TS_{22A}

Mn	-1.42268100	-0.01644100	-0.65717600
O	-0.74858600	0.05790500	1.04798000
N	-1.76169600	-2.04256700	-0.58672400
N	-3.29428800	-0.10317000	0.08758900
N	-1.97870700	1.97413000	-0.61566900
C	-0.93435600	-2.95882100	-1.09601300
H	-0.01610500	-2.58233700	-1.54145000
C	-1.22506400	-4.31701500	-1.04440100
H	-0.52464100	-5.03085900	-1.46676700
C	-2.40547000	-4.72368900	-0.43465200
H	-2.65803500	-5.77829500	-0.36860400
C	-3.27427300	-3.76742300	0.08087000
H	-4.21422100	-4.06110100	0.53838000
C	-2.93829700	-2.42133600	-0.01836800
C	-3.78644000	-1.30905000	0.42090600
C	-4.99088100	-1.39874100	1.11573600

H	-5.40180900	-2.36454000	1.39261000
C	-5.64798800	-0.22065900	1.45930300
H	-6.58542400	-0.26836000	2.00594100
C	-5.11048600	1.01701900	1.11890100
H	-5.61482600	1.93698200	1.39740000
C	-3.90419900	1.04786700	0.42073100
C	-3.17350300	2.23801400	-0.02322000
C	-3.63038300	3.54681100	0.09557500
H	-4.58439800	3.74899100	0.57338300
C	-2.85662000	4.58349000	-0.41525000
H	-3.20102600	5.61038100	-0.33008600
C	-1.65043100	4.29234500	-1.04184700
H	-1.02151700	5.07270600	-1.45923100
C	-1.24163300	2.96619300	-1.12067000
H	-0.30472000	2.67707300	-1.59166000
Mn	1.01715000	0.05455800	0.59817700
O	1.33975700	0.05161900	2.52988900
O	0.31015100	0.04329000	-1.17269700
N	1.59376300	2.17272600	0.55762000
C	0.88277900	3.14413800	1.13126400
H	-0.00553500	2.82904300	1.67748600
C	1.24296400	4.48360200	1.03358400
H	0.63655900	5.24526300	1.51473400
C	2.37792000	4.80942100	0.29990100
H	2.68722000	5.84558200	0.19129700
C	3.12672800	3.79585500	-0.28920700
H	4.02606900	4.03409100	-0.84886300
C	2.71512700	2.47311100	-0.13484000
C	3.45858200	1.30971500	-0.64849500
N	2.96666300	0.11931100	-0.26668600
N	1.74736600	-2.02313700	0.57476800
C	2.90122900	-2.24263900	-0.09427900
C	3.54895200	-1.03430300	-0.63210300
C	4.69149400	-1.02927600	-1.43296700
C	5.21130200	0.19421600	-1.83974800
C	4.60177800	1.37977200	-1.44533900
H	5.00635700	2.33707200	-1.75871000
H	6.09720400	0.22465300	-2.46805300
H	5.16272100	-1.95797800	-1.73920100
C	3.43586800	-3.52550800	-0.19986800
H	4.36426200	-3.69491600	-0.73671900
C	2.77551200	-4.58473500	0.41320900
H	3.18099000	-5.59054900	0.34229400
C	1.60693100	-4.34063900	1.12559800
H	1.06694800	-5.13888800	1.62594700
C	1.12470200	-3.03742900	1.17694800
H	0.20641200	-2.78995100	1.70788500
O	-2.02346100	-0.05039400	-2.47262100
Cl	2.99413900	0.02466900	2.96870300
O	-0.71505000	-0.45581300	-3.39493400
H	-0.01959900	-0.32648000	-2.63270900
H	-0.85023400	-1.42559000	-3.46306500

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O	-2.22823900	-0.95028100	-0.06101600
Cl	-0.56385000	-1.39562000	0.03927400
O	2.64488800	-1.01097400	0.30364800
H	2.33133200	-0.30785600	-0.30715700
H	2.27818900	-1.81370600	-0.09241400
O	0.55224800	1.64669800	1.28115900
H	-0.34560500	1.64927300	0.85354200
O	1.52200200	1.07423800	-1.26470500
H	0.77051600	0.50970200	-1.50612200

H	1.23995000	1.41921900	-0.38229000
O	-1.75809400	1.64050800	-0.20193100
H	-1.98839100	0.64970300	-0.15768500
H	0.68724400	0.70921100	1.49132700
H	-1.25022800	1.70847900	-1.02409800

TS1-2_C1O

O	-1.46006200	-1.73201000	0.00836700
Cl	0.22554000	-1.34808300	0.10069100
O	2.73167900	-0.33927800	0.15897700
H	2.21557000	0.47006900	-0.09795000
H	2.91789600	-0.75214200	-0.69683200
O	-0.79525500	1.79424100	1.07679200
H	-1.60192400	1.19779700	0.17289100
O	1.20058500	1.82360100	-0.62024100
H	0.79948100	1.36502500	-1.37296100
H	0.43742200	1.82909300	0.06706500
O	-2.24030800	0.67730600	-0.59120100
H	-1.84160100	-0.80672300	-0.23730500
H	-0.52063800	1.02831300	1.59996900
H	-1.73350200	0.79510600	-1.40817400

TS22C

Mn	-1.39297600	0.00651100	0.58290000
O	-0.78146300	0.20164900	-1.14348500
N	-2.06644600	1.97985000	0.57031000
N	-3.25892100	-0.15857000	-0.18655200
N	-1.62622500	-2.02175500	0.48181800
C	-1.37292100	3.01010000	1.06143000
H	-0.42029500	2.76938000	1.52829300
C	-1.84360800	4.31480800	0.97502500
H	-1.24816700	5.12747400	1.37965600
C	-3.06921600	4.54306700	0.35998800
H	-3.46459000	5.55127600	0.27260000
C	-3.79487200	3.46745100	-0.14083300
H	-4.75830200	3.62234700	-0.61711900
C	-3.27319700	2.18277500	-0.02243300
C	-3.93731600	0.95974000	-0.48701400
C	-5.14300400	0.87294000	-1.18336200
H	-5.70718900	1.76557600	-1.43512600
C	-5.60221100	-0.38628800	-1.55668900
H	-6.53594900	-0.47731200	-2.10425300
C	-4.87546200	-1.53112400	-1.24118600
H	-5.22946300	-2.51364400	-1.53769000
C	-3.67906500	-1.38314200	-0.54262400
C	-2.77455700	-2.45350600	-0.10764000
C	-3.04254500	-3.81339100	-0.21820900
H	-3.95952700	-4.14973700	-0.69262800
C	-2.13907300	-4.72915900	0.31191400
H	-2.34046600	-5.79430700	0.23869900
C	-0.99245700	-4.26904100	0.94727800
H	-0.26735800	-4.94959000	1.38281900
C	-0.76709500	-2.89902200	1.00628300
H	0.12114200	-2.47980900	1.47219500
Mn	0.99771500	0.13407300	-0.75433200
O	1.29464200	0.18330800	-2.69580700
O	0.34894200	0.14207700	1.00767800
N	1.72945600	-1.93581200	-0.77241100
C	1.11499900	-2.93375000	-1.40967800
H	0.21148700	-2.67043000	-1.95788100
C	1.58610400	-4.24127200	-1.36800500
H	1.05435800	-5.02641300	-1.89712000
C	2.72896900	-4.50818700	-0.62264000

H	3.12191600	-5.51917700	-0.55448000
C	3.37998800	-3.46529700	0.02767600
H	4.28925200	-3.65147300	0.59114500
C	2.86252500	-2.17505300	-0.07540900
C	3.50801200	-0.98097900	0.49695500
N	2.94982800	0.18605900	0.13419100
N	1.59283300	2.27752500	-0.63406600
C	2.69577300	2.54617400	0.09816600
C	3.43280700	1.36066400	0.57119200
C	4.55327200	1.40144700	1.40220900
C	5.14425400	0.20233600	1.78279300
C	4.62510000	-1.00589800	1.33266100
H	5.07625700	-1.94629800	1.63364300
H	6.01161200	0.20963600	2.43715200
H	4.95305200	2.34745200	1.75375100
C	3.08643000	3.86052100	0.34964700
H	3.97055500	4.07201000	0.94333200
C	2.33185200	4.90219100	-0.17982700
H	2.62422000	5.93248900	0.00525800
C	1.20993700	4.61219900	-0.94791400
H	0.59705200	5.39697200	-1.38153100
C	0.87313900	3.27715100	-1.14355600
H	-0.00391500	2.98839000	-1.72249100
O	-2.07695200	0.07591800	2.34480600
Cl	2.94742800	0.11777000	-3.14391600
O	-1.54479000	-1.15999600	3.33679500
H	-0.51200500	-0.97468700	3.42666400
H	-1.94277500	-0.83091600	4.16903500
O	0.98652700	-0.77351900	3.39239200
H	1.16514700	-0.01496600	3.97238100
H	0.95089900	-0.37825400	2.47680900