

**Electronic Supplementary Information to:**

**How does Mo-dependent perchlorate reductase work in the decomposition of oxyanions?**

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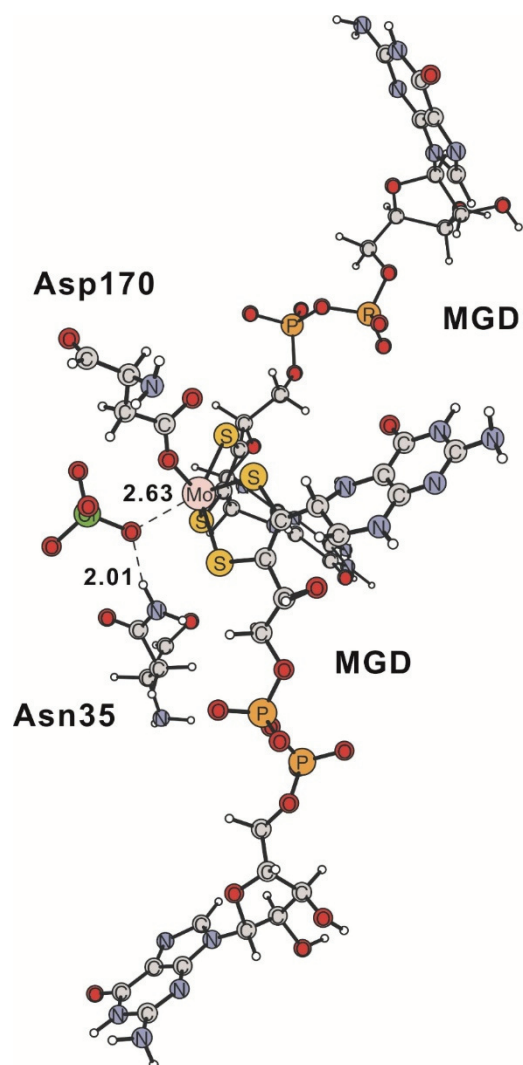
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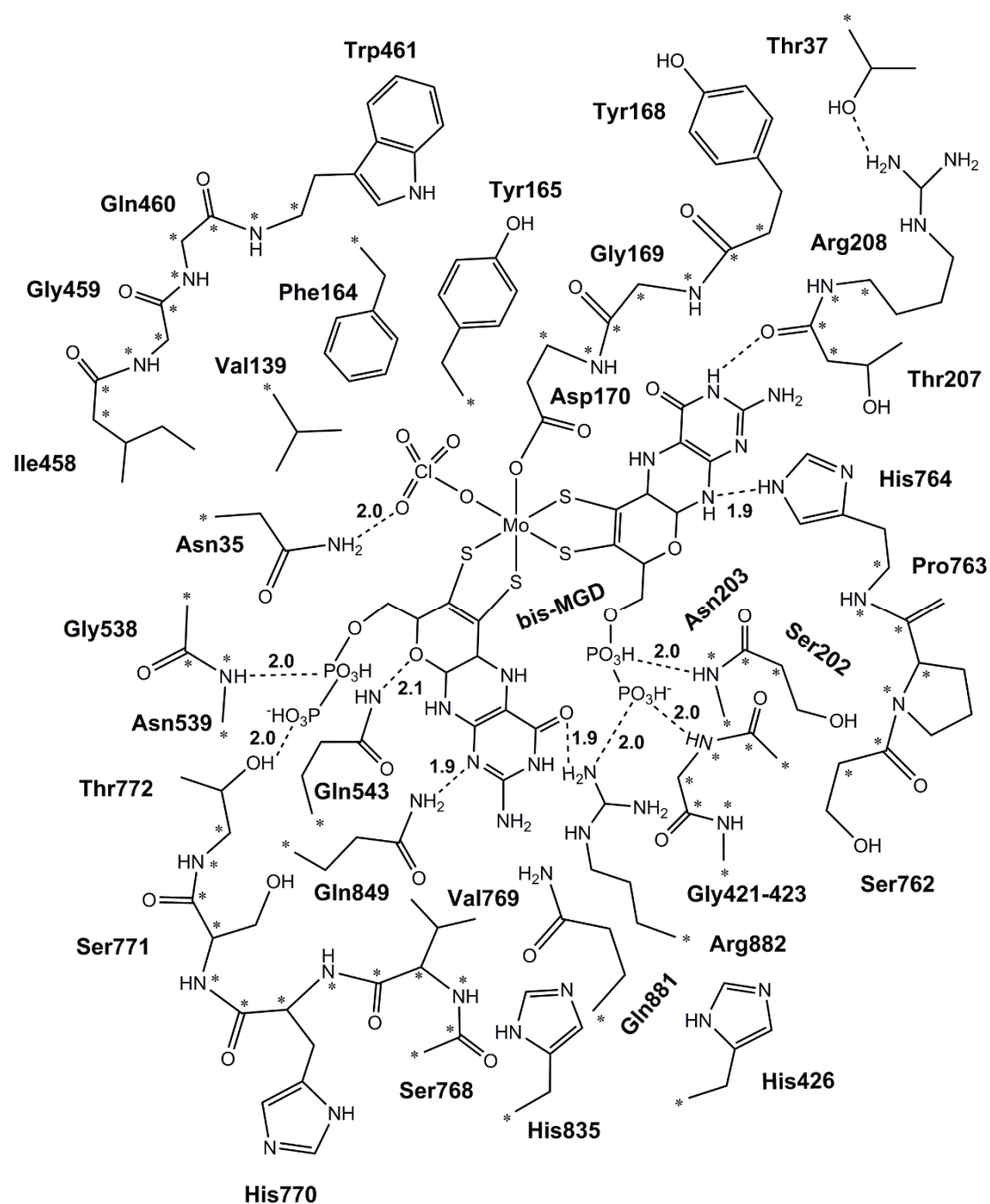
**Contents:**

1. Supplementary figures and scheme.
2. Cartesian coordinates of optimized structures

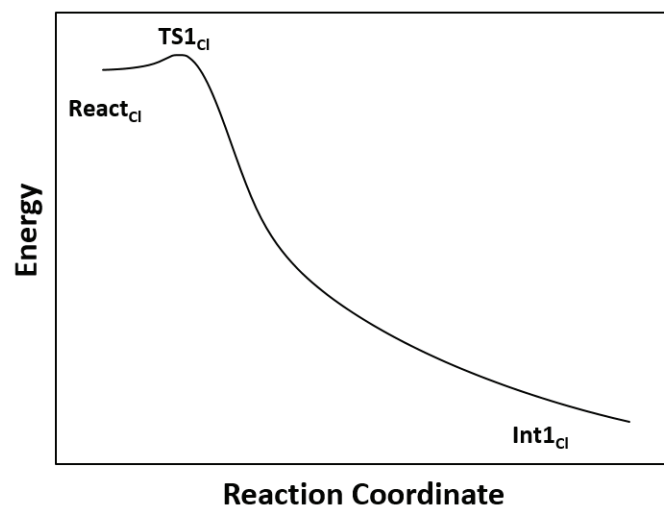
## 1. Supplementary figures and scheme



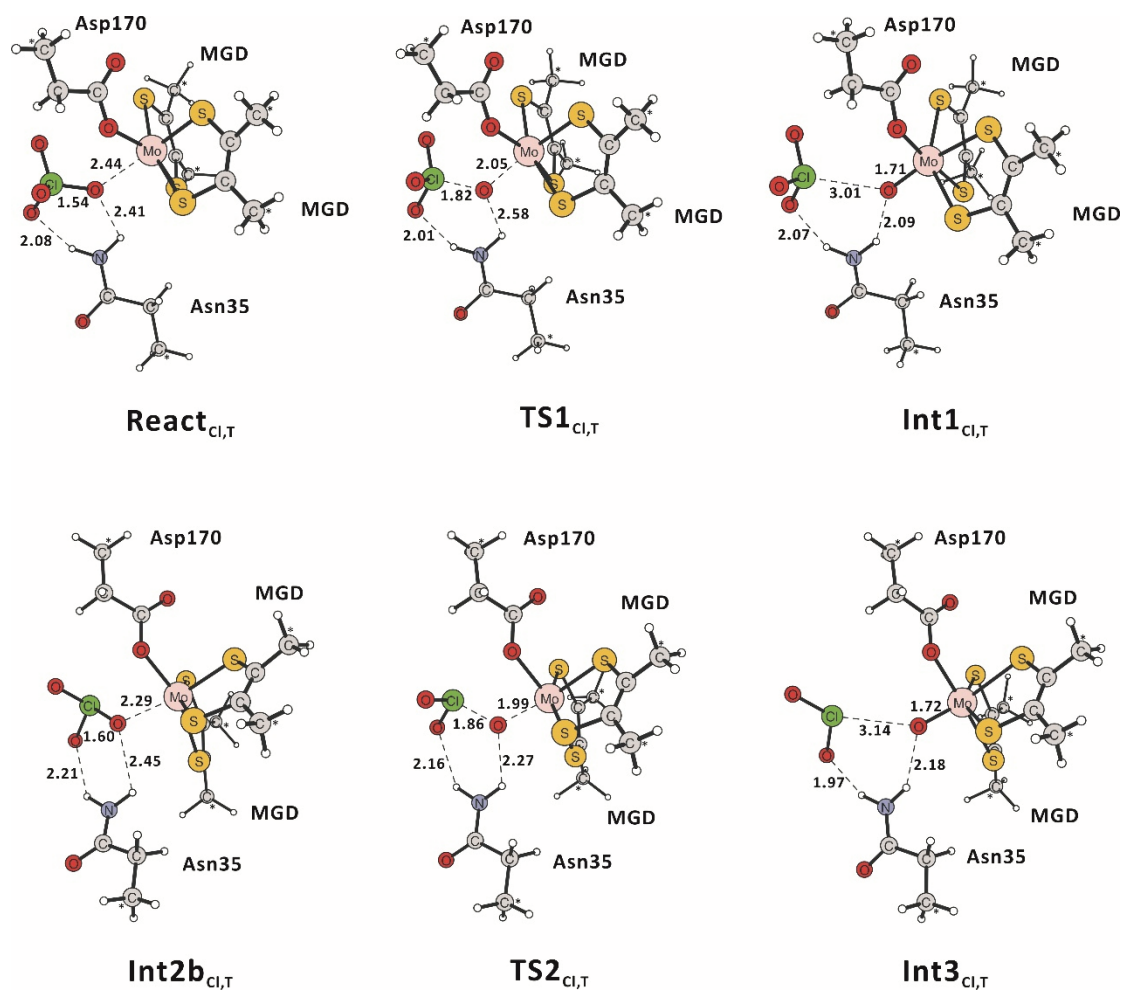
**Fig. S1** The binding of perchlorate in the PcrAB active site predicted by the docking simulation. Some important distances are tagged in angstrom (Å).



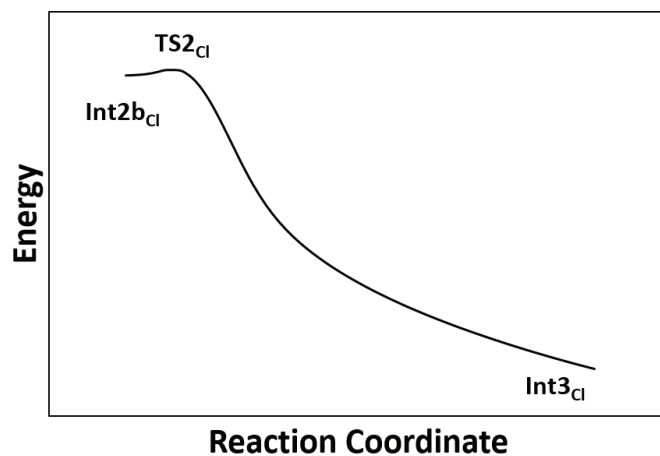
**Fig. S2** A bigger model (537 atoms) of the PcrAB active site used in this work. For clarity, 2-D schematic structure is shown. Asterisks indicate the atoms which are fixed to their X-ray positions. The distances optimized are in angstroms (Å).



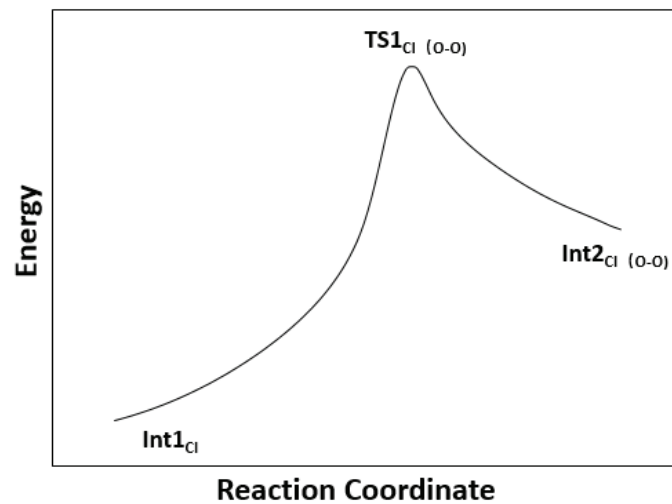
**Fig. S3** Schematic potential energy surface obtained by the IRC (intrinsic reaction coordinate) calculations with the **TS1<sub>cl</sub>** structure as the starting point.



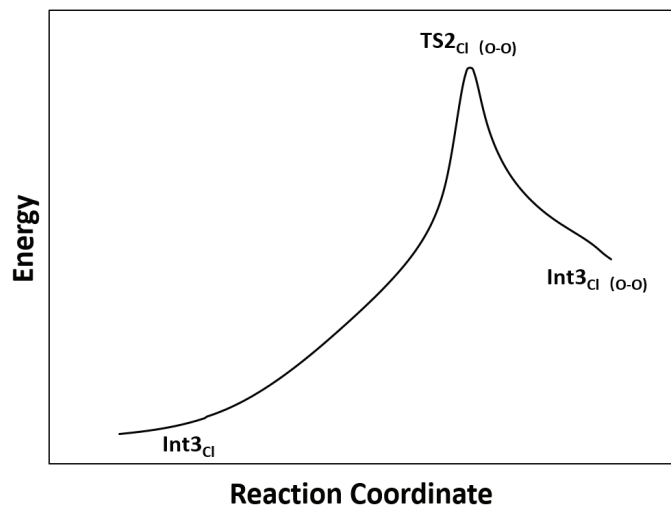
**Fig. S4** Optimized structures of stationary points for the PcrAB-catalyzed decomposition of perchlorate in the triplet state. Some important distances are tagged in angstrom (Å). Asterisks indicate the atoms that are fixed at their crystal positions.



**Fig. S5** Schematic potential energy surface obtained by the IRC (intrinsic reaction coordinate) calculations with the **TS2<sub>Cl</sub>** structure as the starting point.

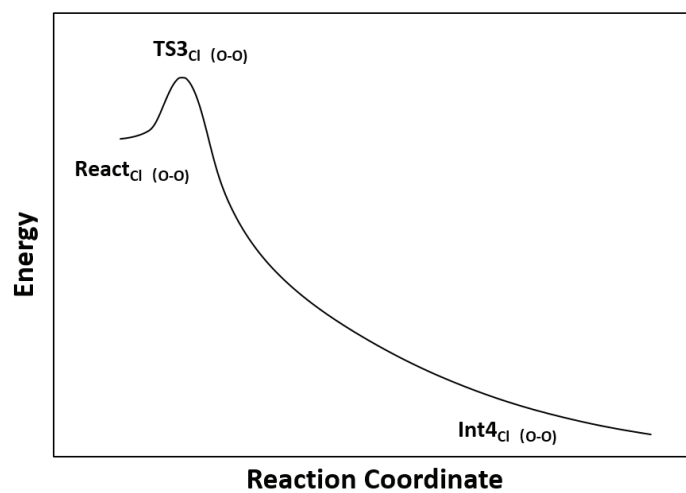


**Fig. S6** Schematic potential energy surface obtained by the IRC (intrinsic reaction coordinate) calculations with the **TS1<sub>Cl(0-0)</sub>** structure as the starting point.

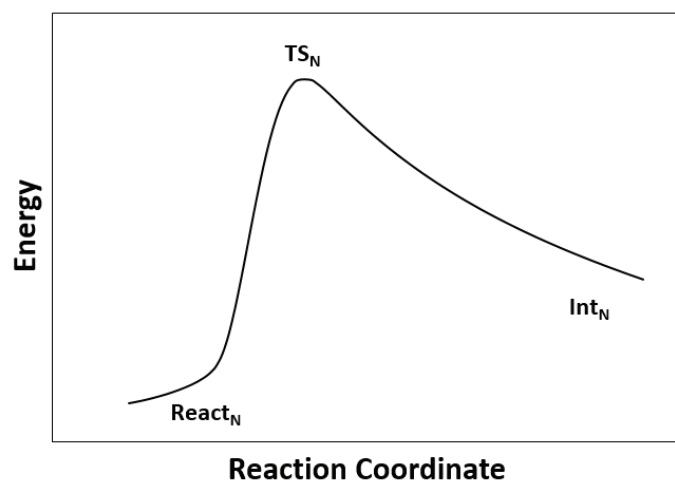


**Fig. S7** Schematic potential energy surface obtained by the IRC (intrinsic reaction coordinate) calculations with the **TS2<sub>Cl(0-0)</sub>** structure as the starting point.

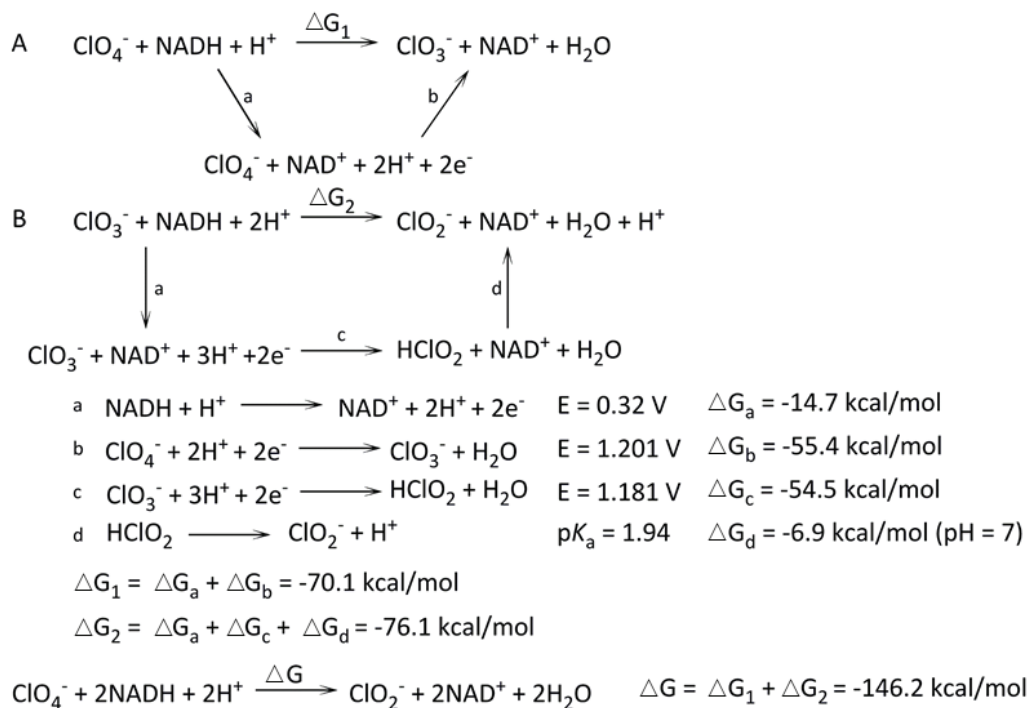




**Fig. S8** Schematic potential energy surface obtained by the IRC (intrinsic reaction coordinate) calculations with the **TS3<sub>Cl(0-0)</sub>** structure as the starting point.



**Fig. S9** Schematic potential energy surface obtained by the IRC (intrinsic reaction coordinate) calculations with the **TS<sub>N</sub>** structure as the starting point.



**Scheme S1** The thermochemical cycle for the uncatalyzed reduction of  $\text{ClO}_4^-$  to  $\text{ClO}_2^-$  via  $\text{ClO}_3^-$  by NADH. The reduction potentials for the reactions of a, b, and c are obtained from Refs. 72, 73, and 74 (given in the text), respectively. The  $\text{p}K_a$  of reaction d is taken from Refs. 75 and 76.

## 2. Cartesian coordinates of optimized structures

The abbreviations used here are consistent with those in the text.

### React1

C	257.8290000000	191.8650000000	391.3050000000
C	258.0021737897	190.7011002278	392.2837700954
C	257.3431771609	189.4362235749	391.7178649005
O	257.4402230429	189.1612146440	390.5163086866
N	256.6845763816	188.6815486942	392.6122901510
C	251.9230000000	184.0210000000	398.3810000000
C	252.6231875939	184.8670207252	397.3250814532
C	253.4465894810	186.0013227554	397.9394804719
O	253.4433560237	186.2290336052	399.1448530840
O	254.1061739460	186.6463863492	397.0143959225
Mo	255.5042595714	188.1382225588	397.0608762780
C	253.4590000000	191.9940000000	399.2530000000
C	254.1526237920	191.0325439174	398.3000855722
S	254.1258631582	189.3119883251	398.6621391622
C	254.8566251975	191.4753695164	397.2297247584
S	255.6831635179	190.3523281362	396.1611746652
C	255.0790000000	192.9360000000	396.9760000000
C	260.3070000000	187.3170000000	397.1300000000
C	258.8366646394	187.3641910715	397.5552448156
S	257.7673640234	187.9242253805	396.2532621969
C	258.2733785254	187.0851260130	398.7635744637
S	256.5209718051	187.2684494790	398.9935083598
C	258.9150000000	186.6290000000	400.0610000000
O	254.5790542204	186.6229373865	392.6101528668
O	255.1054947163	187.5993403174	394.7777986846
O	254.7044059805	185.1369721831	394.5525632645
H	257.6024064416	190.9454696828	393.2740381867
H	259.0699545026	190.4805290538	392.4158805877
H	256.5679551383	188.9416909348	393.5814244139
H	256.1541358848	187.8674308124	392.3213621372
H	258.1523728221	191.5527189802	390.3081295280
H	251.2758048783	184.6431540739	399.0070569102
H	251.9125249541	185.3246322216	396.6265416021
H	253.2958519899	184.2755137702	396.6947188951
H	254.1736116018	192.6838034015	399.7252862077
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H	258.7382837531	187.3602168902	400.8593673932

H	260.0004073642	186.4895406002	399.9628781045
H	255.8200591885	193.3554733037	397.6743070485
H	254.1598952288	193.5259110984	397.0993017379
H	252.9453597256	191.4492584965	400.0507539674
H	256.7755442390	192.1598635307	391.2356907593
H	258.4064183498	192.7441249630	391.6158377457
H	260.6539415296	188.3152920237	396.8382511713
H	260.9544381938	186.9484863017	397.9357211106
H	251.3147361381	183.2286849047	397.9245763109
H	252.6527155820	183.5541357883	399.0507705638
Cl	254.2767728401	186.4867926648	394.0852779775
O	252.8180852469	186.7028002184	394.3115035156
H	252.7133321642	192.6110524059	398.7320286770
H	255.4532887563	193.1151134139	395.9629850870

## TS1Cl

C	257.8290000000	191.8650000000	391.3050000000
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C	252.6765490000	184.8319310000	397.3427290000
C	253.4486130000	185.9941980000	397.9666580000
O	253.4249160000	186.2263430000	399.1706420000
O	254.0927420000	186.6503100000	397.0426650000
Mo	255.4965650000	188.1403620000	397.0063570000
C	253.4590000000	191.9940000000	399.2530000000
C	254.1345830000	191.0324360000	398.2831160000
S	254.0681850000	189.3066100000	398.6129410000
C	254.8433180000	191.4801660000	397.2197920000
S	255.6529810000	190.3754040000	396.1232830000
C	255.0790000000	192.9360000000	396.9760000000
C	260.3070000000	187.3170000000	397.1300000000
C	258.8408200000	187.3789580000	397.5566190000
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C	258.2725760000	187.0951820000	398.7627930000
S	256.5232770000	187.2843940000	398.9737120000
C	258.9150000000	186.6290000000	400.0610000000
O	254.6710710000	186.5573610000	392.7829930000
O	255.2227160000	187.6769190000	394.9608860000
O	254.7780550000	185.0728310000	394.7276320000
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H	260.4285870000	186.6441580000	396.2731710000
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H	252.6113620000	183.6073920000	399.1252920000
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## Int1Cl

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N	256.0036787254	188.7703009134	392.4211206340
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O	254.1498298902	186.7261673953	397.1803165978
Mo	255.4902342329	188.1884251377	396.8946003075
C	253.4590000000	191.9940000000	399.2530000000
C	254.2329768059	191.0620409322	398.3532492972
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C	255.1468928158	191.5345606597	397.4858151574
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C	258.2551871315	187.1066850331	398.7732109669
S	256.5610359635	187.3603812909	399.0356232025
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O	254.5148929381	184.3375464474	394.4527167693
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H	258.4434129836	185.6970400020	400.3887510798
H	258.7859920011	187.3645564848	400.8615609643
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H	253.3201455837	191.5230808944	400.2337199433
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H	251.3791836245	183.2297797083	397.8522973002
H	252.5732379535	183.5589713067	399.1310473374
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H	252.4509468395	192.2279740765	398.8772250361
H	254.7647170721	192.9162817066	395.9233431923

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N	256.5758080676	188.6905812398	392.7389479046

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O	254.1748238001	186.6738972687	397.2090821226
Mo	255.4867280935	188.1689160461	396.8679567311
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S	256.2916264017	190.4821485312	396.6635214848
C	255.0790000000	192.9360000000	396.9760000000
C	260.3070000000	187.3170000000	397.1300000000
C	258.8239832742	187.3195540329	397.5277372072
S	257.7587961703	187.6014737758	396.1680068622
C	258.2561097233	187.1198388689	398.7739799213
S	256.5681962058	187.4214747962	399.0316979656
C	258.9150000000	186.6290000000	400.0610000000
O	255.1583971498	188.0407086744	395.1672376012
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H	256.2643928317	188.9560311177	393.6650480805
H	256.4059031991	187.7330861140	392.4709434763
H	258.5348179361	191.4710160818	390.5693595066
H	251.1574784210	184.6773865749	398.8057925209
H	252.2593422695	185.2246092506	396.5946052011
H	253.5723849744	184.1315721495	396.9662393741
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H	256.8780866914	192.0370947956	390.7886430750
H	258.1943358146	192.8278890949	391.6777374655
H	260.6040416009	188.3170512990	396.7969580575
H	260.9453175574	187.0340143244	397.9737658656
H	251.4214583899	183.1890408097	397.8732962180
H	252.5021379055	183.6230224565	399.2187137423
H	252.4992922373	192.3364940820	398.8402292853
H	254.8376948131	192.9692044518	395.9050369594

**Int2Cl**



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C	256.7746564875	189.8629494585	392.4549994947
O	255.7984072584	189.8745743041	391.7069387435
N	257.1373971624	188.7749503854	393.1872624072
C	251.9230000000	184.0210000000	398.3810000000
C	252.6188209834	184.8147573803	397.2775564822
C	253.4429417837	185.9789675404	397.8350089300
O	253.4605328588	186.2359666811	399.0271468637
O	254.0987215539	186.6307216494	396.8930198755
Mo	255.5366193719	188.1743160144	397.0714186660
C	253.4590000000	191.9940000000	399.2530000000
C	254.1589245821	191.0334737289	398.3057780493
S	254.1514178681	189.3115223700	398.6586623000
C	254.8620612240	191.4813582706	397.2373535729
S	255.7084276916	190.3706369282	396.1797128220
C	255.0790000000	192.9360000000	396.9760000000
C	260.3070000000	187.3170000000	397.1300000000
C	258.8420189877	187.3497769914	397.5604544534
S	257.7689116745	187.9369549058	396.2791661302
C	258.2691525986	187.0627489651	398.7615249397
S	256.5133948327	187.2231454974	398.9805854813
C	258.9150000000	186.6290000000	400.0610000000
O	254.8672079058	187.6548716480	394.7950890678
H	257.2121559380	191.7112606249	393.3860775171
H	258.6596435744	190.7895473848	393.0122750692
H	257.7674770764	188.8732965630	393.9752926913
H	256.4405700486	188.0509509677	393.3152057842
H	258.3824711829	191.2813814874	390.5607170137
H	251.2664173465	184.6720528201	398.9645132848
H	251.8936039310	185.2279302418	396.5637078250
H	253.2911693851	184.1798481594	396.6869115477
H	254.1734464307	192.6848134249	399.7205394952
H	260.4359725716	186.6670299701	396.2569264117
H	258.4815842990	185.6871330060	400.4158672466
H	258.7462705946	187.3789460379	400.8422875538
H	259.9976447064	186.4837603249	399.9577509282
H	255.8248659643	193.3549935297	397.6675842282
H	254.1607740071	193.5233248775	397.1064089431
H	252.9451499157	191.4527874717	400.0524106152
H	256.8393682074	192.0743028329	390.8905267442
H	258.3598816610	192.8100175889	391.4620592856
H	260.6474474791	188.3197838017	396.8481440219

H	260.9578474039	186.9461994241	397.9302435678
H	251.3279564279	183.1987835614	397.9658141536
H	252.6584454990	183.6054842223	399.0755655418
H	252.7144759381	192.6043745536	398.7250450092
H	255.4446471485	193.1150057032	395.9601817887
H	254.2300239878	187.0210307058	395.1992064335
H	254.3837801215	188.4538516329	394.5382019025

## Int2bCl

C	257.8290000000	191.8650000000	391.3050000000
C	257.5184926313	190.6714357155	392.2110648773
C	256.4629990906	189.7556170378	391.5737893819
O	256.3073896077	189.7217776001	390.3466084340
N	255.7628812838	189.0045397686	392.4398203745
C	251.9230000000	184.0210000000	398.3810000000
C	252.4218789234	185.0335802207	397.3651357534
C	253.3829826903	186.0499656590	397.9933155646
O	253.4587904366	186.2055417693	399.2072329917
O	254.0432399821	186.6827624460	397.0661057627
Mo	255.5163314696	188.1503228862	397.0489961659
C	253.4590000000	191.9940000000	399.2530000000
C	254.1704007048	191.0374053008	398.3114510056
S	254.1456430039	189.3175720261	398.6672519975
C	254.8887441606	191.4811411877	397.2528277557
S	255.7563680953	190.3778406236	396.2044858801
C	255.0790000000	192.9360000000	396.9760000000
C	260.3070000000	187.3170000000	397.1300000000
C	258.8355876815	187.3485539641	397.5486024926
S	257.7715429965	187.8971124563	396.2365028806
C	258.2695790100	187.0551323620	398.7532949385
S	256.5143286323	187.1930153933	398.9722177262
C	258.9150000000	186.6290000000	400.0610000000
O	253.3076292824	187.5896731726	393.1564714927
O	255.0497735383	187.6981523425	394.9437040856
O	253.9674734108	185.4605356695	394.2825231023
H	257.1900704919	190.9916059033	393.2066474842
H	258.4242176055	190.0704242912	392.3701981074
H	255.8612779950	189.0375153418	393.4481110879
H	255.0205486010	188.3909610799	392.1254734301
H	258.0770631375	191.5127271160	390.3002168062
H	251.4709351444	184.5305293613	399.2371429092
H	251.5852036463	185.6029607886	396.9356043318
H	252.9289103490	184.5643624253	396.5162382615

H	254.1635507803	192.6788246237	399.7476012886
H	260.4465740386	186.6520644948	396.2691182855
H	258.4930061493	185.6791277620	400.4107912295
H	258.7272300495	187.3736650751	400.8441506121
H	260.0026482453	186.5007784718	399.9688614769
H	255.8512149841	193.3750721673	397.6280529957
H	254.1609305718	193.5170811119	397.1404264359
H	252.9255634546	191.4453845367	400.0352959832
H	256.9555892032	192.5201684351	391.2118764421
H	258.6613122898	192.4600650645	391.6991251106
H	260.6431435418	188.3160762889	396.8280247360
H	260.9577628604	186.9658503408	397.9415080111
H	251.1853027407	183.3344604464	397.9444688243
H	252.7539421914	183.4238478460	398.7723240134
Cl	253.6603532563	186.9362329817	394.5048332648
H	252.7256987414	192.6173705698	398.7213796320
H	255.3974166465	193.1102375811	395.9428832086

## TS<sub>2Cl</sub>

C	257.8281960000	191.8641050000	391.3057130000
C	257.3880820000	190.7625400000	392.2692790000
C	256.4351920000	189.7679330000	391.5921360000
O	256.2157080000	189.8171040000	390.3753270000
N	255.8980230000	188.8524460000	392.4167460000
C	251.9235630000	184.0217280000	398.3807150000
C	252.5088160000	184.9468930000	397.3300940000
C	253.4019220000	186.0244810000	397.9541290000
O	253.4386950000	186.2103910000	399.1647720000
O	254.0529770000	186.6631080000	397.0255020000
Mo	255.5092740000	188.1501720000	396.9881910000
C	253.4589030000	191.9933110000	399.2523550000
C	254.1397680000	191.0343980000	398.2838110000
S	254.0746230000	189.3062580000	398.6048750000
C	254.8588470000	191.4834840000	397.2293580000
S	255.6959680000	190.3923340000	396.1416710000
C	255.0794330000	192.9368540000	396.9763790000
C	260.3074000000	187.3173200000	397.1302730000
C	258.8412010000	187.3746060000	397.5533450000
S	257.7978560000	187.9316430000	396.2356520000
C	258.2692590000	187.0757140000	398.7547250000
S	256.5146230000	187.2293530000	398.9514100000
C	258.9145050000	186.6286820000	400.0605640000
O	253.7446400000	187.0012510000	392.9924320000

O	255.1906850000	187.7020780000	394.9851400000
O	254.6620490000	185.1568430000	394.4300710000
H	256.9016040000	191.1742930000	393.1623570000
H	258.2546960000	190.2025910000	392.6446060000
H	256.0015280000	188.8501230000	393.4266830000
H	255.2013370000	188.1945340000	392.0879950000
H	258.2789600000	191.4292880000	390.4093370000
H	251.3813120000	184.5968710000	399.1368310000
H	251.7159720000	185.4628520000	396.7711030000
H	253.1023050000	184.4082620000	396.5834850000
H	254.1888760000	192.6175520000	399.7868340000
H	260.4323420000	186.6468430000	396.2717890000
H	258.4880080000	185.6765030000	400.3979000000
H	258.7306880000	187.3645040000	400.8526310000
H	260.0006370000	186.4975330000	399.9633340000
H	255.9814810000	193.3043460000	397.4911980000
H	254.2416730000	193.5571320000	397.3185480000
H	252.8861140000	191.4402050000	400.0028490000
H	256.9684000000	192.4540880000	390.9725240000
H	258.5503360000	192.5390920000	391.7801940000
H	260.6608830000	188.3087200000	396.8232250000
H	260.9559850000	186.9579560000	397.9399270000
H	251.2420070000	183.2819810000	397.9399620000
H	252.7190930000	183.4836640000	398.9067200000
Cl	253.9981610000	186.5278740000	394.4342060000
H	252.7660560000	192.6724000000	398.7366090000
H	255.2248040000	193.1415540000	395.9093410000

### **Int3Cl**

C	257.8281960000	191.8641050000	391.3057130000
C	257.0916077694	191.1217958862	392.4293925195
C	255.5900395726	190.9275973861	392.1230219546
O	255.0772096861	191.4755215112	391.1408526502
N	254.9295802011	190.1439680593	392.9962209536
C	251.9235630000	184.0217280000	398.3807150000
C	252.5934278979	184.9619178892	397.3800659374
C	253.4803135386	186.0055566542	398.0585249452
O	253.5533493128	186.1390740697	399.2710697446
O	254.1278315396	186.7126908416	397.1557932333
Mo	255.5044568817	188.1749816046	396.8875649522
C	253.4589030000	191.9933110000	399.2523550000
C	254.2447589295	191.0572256926	398.3586462958
S	253.9262230245	189.3278587437	398.4531374548

C	255.1420736741	191.5308150095	397.4738344823
S	256.3406425446	190.4886902752	396.7148717891
C	255.0794330000	192.9368540000	396.9763790000
C	260.3074000000	187.3173200000	397.1302730000
C	258.8279630701	187.3109068184	397.5301991715
S	257.7752598064	187.6319718857	396.1625895448
C	258.2545646976	187.0694339128	398.7596018563
S	256.5421711904	187.2560569363	399.0067592636
C	258.9145050000	186.6286820000	400.0605640000
O	252.1604185206	189.3234741325	393.5125573502
O	255.1876632465	188.0962756583	395.1897611859
O	251.1608123518	187.0357323045	394.6115914136
H	257.1758535807	191.6681377354	393.3783709643
H	257.5486525345	190.1417907218	392.6174821668
H	255.3866642559	189.7262313662	393.7977426102
H	253.9215612916	189.9495064332	392.9330361111
H	257.8017802409	191.2857909785	390.3766030023
H	251.3153146301	184.5883431692	399.0921865346
H	251.8688744056	185.5067025017	396.7594181964
H	253.2180119944	184.4109605564	396.6668482127
H	254.0260200357	192.9001646033	399.4792935095
H	260.4954856463	186.6249592564	396.3015444148
H	258.4557953558	185.6977229855	400.4097995504
H	258.7690617832	187.3807932196	400.8427940048
H	259.9936596123	186.4579509029	399.9493612165
H	256.0626683645	193.4299366545	396.9442316639
H	254.4091177049	193.5655584341	397.5670729549
H	253.2358997053	191.4967481221	400.2037589633
H	257.3361378495	192.8184545865	391.0987299502
H	258.8752419953	192.0484528781	391.5751251209
H	260.6060273382	188.3183966816	396.7996373102
H	260.9531460038	187.0282220888	397.9682200113
H	251.2785889003	183.2976997443	397.8681417775
H	252.6702946323	183.4723654026	398.9644024641
Cl	252.2391458117	188.2345667749	394.7197113551
H	252.4931501839	192.2893255414	398.8175920276
H	254.7003736137	192.9322677907	395.9455051952

### **TS1Cl(O-O)**

C	257.8290000000	191.8650000000	391.3050000000
C	257.3944859300	190.8121678400	392.3371067400
C	257.4104824900	189.3878758000	391.7606708000
O	257.9848076700	189.1388097300	390.6941065300

N	256.7731371100	188.4517844100	392.4960549200
C	251.8411914600	183.9704919300	398.3534991400
C	252.5552728300	184.8160487600	397.2919645400
C	253.4266553600	185.9475479400	397.8765923900
O	253.3926270800	186.2138557200	399.0740238600
O	254.1313378200	186.5392265700	396.9466163400
Mo	255.4904951500	188.1601576500	396.9890591400
C	253.4590000000	191.9940000000	399.2530000000
C	254.1453007400	191.0291707700	398.2973642100
S	254.0278195300	189.2890529900	398.5849569300
C	254.8737763900	191.4850036400	397.2537516400
S	255.6712760900	190.3992135800	396.1377914400
C	255.0790000000	192.9360000000	396.9760000000
C	260.3070000000	187.3170000000	397.1300000000
C	258.8410522000	187.3845357400	397.5620413300
S	257.7968515800	187.9640391000	396.2612277600
C	258.2654925700	187.0847044700	398.7626095700
S	256.5093554100	187.2419496600	398.9581777700
C	258.9150000000	186.6290000000	400.0610000000
O	256.5964762600	185.2558638700	393.5461301900
O	255.2987940000	187.8733285100	394.9271083600
O	254.5530722300	184.1155187300	394.4759119800
H	256.4031791300	191.0334288500	392.7495706800
H	258.0688169200	190.8202785900	393.2035535300
H	256.3375144800	188.5944980500	393.4086577000
H	256.8613415300	187.4821796700	392.2231320600
H	258.7949770900	191.5899166600	390.8735125900
H	251.2477611500	184.6090943200	399.0148654400
H	251.8289915300	185.2945821100	396.6217116900
H	253.1837541300	184.2022756000	396.6376904000
H	254.1787418900	192.6444141800	399.7686909900
H	260.4205047500	186.6466621500	396.2698488800
H	258.4957900700	185.6709484600	400.3915202700
H	258.7284331700	187.3564223700	400.8605354200
H	260.0019030100	186.5057433600	399.9603061500
H	256.1463000900	193.1987713000	397.0048596900
H	254.5618126700	193.5886142000	397.6863757600
H	252.9093279900	191.4436441900	400.0238545200
H	257.1124134800	191.9222417500	390.4785317300
H	257.9062953300	192.8558660100	391.7668412800
H	260.6653942300	188.3064574100	396.8223177000
H	260.9572078800	186.9517852100	397.9358836100
H	251.1831264600	183.2235101100	397.8909242600
H	252.5674326500	183.4479810500	398.9853120900

Cl	255.5407935100	185.2584001800	394.6349641200
O	254.5206380500	186.7491298900	394.3101392800
H	252.7392153400	192.6426442700	398.7353833100
H	254.7279913400	193.2060864100	395.9691857600

## Int2Cl(O-O)

C	257.8289900000	191.8649720000	391.3050180000
C	257.3721108186	190.7331037694	392.2333735089
C	256.7099192225	189.5773929377	391.4576977969
O	256.8546494811	189.4748797940	390.2350141788
N	256.0062815587	188.7138925856	392.2155124237
C	251.8412840000	183.9705860000	398.3534410000
C	252.7266954342	184.7105432659	397.3410822851
C	253.4791876887	185.9102882853	397.9325336380
O	253.4514377568	186.1724879594	399.1310586381
O	254.1418636691	186.5732326300	397.0081474813
Mo	255.5015593441	188.1304216366	397.0735736915
C	253.4590050000	191.9940430000	399.2530520000
C	254.2294953567	191.0345395780	398.3686031057
S	254.0968257438	189.3188742202	398.7205256007
C	255.0401005723	191.4890000366	397.3815025555
S	256.1724329412	190.4294937829	396.5661033146
C	255.0789740000	192.9358990000	396.9759750000
C	260.3069290000	187.3169980000	397.1300020000
C	258.8251509377	187.3031306217	397.5330698413
S	257.7424130584	187.7229719427	396.2055522794
C	258.2604779424	187.0283678780	398.7506076708
S	256.5180721869	187.1214800683	398.9774699904
C	258.9150090000	186.6289940000	400.0610120000
O	254.4493795828	186.1560434358	391.9746332706
O	255.1665205707	187.9781752264	394.9815786105
O	253.0843581583	184.4197841477	393.5013796682
H	256.6891826627	191.1007401275	393.0089383894
H	258.2315364498	190.3164631605	392.7761989080
H	255.9192609939	188.8090859322	393.2199324218
H	255.5621817364	187.8795826624	391.8297107896
H	258.4602702096	191.4623636790	390.5085005746
H	251.0569086580	184.6300850818	398.7395340611
H	252.1525359066	185.0631176394	396.4777147180
H	253.4795689168	184.0396903963	396.9096374830
H	254.0947872265	192.8161992402	399.6038708132
H	260.4771051271	186.6565873138	396.2725886786
H	258.4854460957	185.6927337210	400.4344456957

H	258.7499998929	187.3945602690	400.8277111069
H	259.9979997004	186.4844847085	399.9547811937
H	255.9468123220	193.4654936596	397.3992460111
H	254.1790118520	193.4752290805	397.2872365560
H	253.0668424960	191.4758241427	400.1332910367
H	256.9702382564	192.3432677820	390.8219194222
H	258.3850711890	192.6301130252	391.8592775806
H	260.6115844706	188.3275838723	396.8365557180
H	260.9521377391	186.9866978585	397.9526382362
H	251.3669243164	183.0978156308	397.8895503952
H	252.4322407150	183.6392890123	399.2130875886
Cl	253.8631347487	185.8138737594	393.4341193553
O	253.9968655793	188.5819661552	395.0930488042
H	252.5998865118	192.4410433948	398.7317811348
H	255.1572268532	193.0263042434	395.8868359221

### **TS2Cl(o-o)**

C	257.8289450000	191.8649240000	391.3050560000
C	257.2732230000	190.7937910000	392.2529620000
C	256.3235940000	189.8240780000	391.5344550000
O	256.1703570000	189.8712710000	390.3081040000
N	255.6960280000	188.9327130000	392.3288270000
C	251.8414800000	183.9707720000	398.3533320000
C	252.6707010000	184.7073310000	397.3052110000
C	253.4385210000	185.9171300000	397.8710360000
O	253.3764790000	186.1998590000	399.0624950000
O	254.1026160000	186.5340390000	396.9332120000
Mo	255.4931440000	188.1133900000	396.9297890000
C	253.4590040000	191.9940900000	399.2530890000
C	254.1567680000	191.0276040000	398.2960590000
S	254.0341490000	189.2846540000	398.5523140000
C	254.9186380000	191.4843070000	397.2771130000
S	255.8174410000	190.4178030000	396.2254280000
C	255.0789620000	192.9357490000	396.9759540000
C	260.3067490000	187.3169860000	397.1300150000
C	258.8341640000	187.3323830000	397.5429990000
S	257.7910290000	187.8198010000	396.2014750000
C	258.2559500000	187.0364730000	398.7447410000
S	256.4965510000	187.1404640000	398.9271190000
C	258.9150510000	186.6289720000	400.0610540000
O	254.0462660000	185.0162980000	392.6806130000
O	255.3047460000	187.8998280000	394.9915320000
H	256.7513830000	191.2401160000	393.1085630000



H	258.0882070000	190.2045150000	392.6931700000
H	255.7850820000	188.8567240000	393.3428620000
H	255.0794930000	188.2552730000	391.9040450000
H	258.3251140000	191.3970460000	390.4502870000
H	251.1072250000	184.6451670000	398.8047040000
H	252.0429650000	185.0705960000	396.4831890000
H	253.4066900000	184.0384650000	396.8412710000
H	254.1713490000	192.6894070000	399.7156110000
H	260.4578120000	186.6504370000	396.2726650000
H	258.5043690000	185.6776880000	400.4190710000
H	258.7202080000	187.3792770000	400.8362630000
H	260.0026460000	186.5153220000	399.9614690000
H	256.0457050000	193.3251940000	397.3322430000
H	254.2945420000	193.5514880000	397.4291860000
H	252.9638400000	191.4433310000	400.0587500000
H	257.0208620000	192.4846810000	390.9039070000
H	258.5428620000	192.5141070000	391.8249080000
H	260.6336130000	188.3183840000	396.8264790000
H	260.9590490000	186.9761880000	397.9445190000
H	251.3114010000	183.1147900000	397.9162140000
H	252.4801350000	183.6119170000	399.1662360000
Cl	253.9226840000	185.5782490000	394.1720250000
O	253.9873760000	187.3348900000	394.3384440000
H	252.6916320000	192.5950590000	398.7452000000
H	255.0545480000	193.1198930000	395.8947490000

### Int3Cl(O-O)

C	257.8289450000	191.8649240000	391.3050560000
C	257.1568911250	190.9221868625	392.3078329080
C	256.0190918898	190.1241187186	391.6616419748
O	255.8138103279	190.1565749955	390.4473425504
N	255.2635678601	189.3924436257	392.5165446813
C	251.8414800000	183.9707720000	398.3533320000
C	252.7136028817	184.7474714073	397.3553797324
C	253.5160121547	185.9105303065	397.9705656443
O	253.4207210807	186.2042586742	399.1584652663
O	254.2760258372	186.5008567058	397.0829324887
Mo	255.5013423275	188.1985971955	397.0335172250
C	253.4590040000	191.9940900000	399.2530890000
C	254.2866500008	191.0338361837	398.4195572951
S	254.2693187716	189.3551106576	398.8634615267
C	255.1115919568	191.4996925001	397.4306658756
S	256.3088370884	190.4602708630	396.7106508222

C	255.0789620000	192.9357490000	396.9759540000
C	260.3067490000	187.3169860000	397.1300150000
C	258.8196411350	187.3168796959	397.5320896318
S	257.7423795175	187.7337326355	396.2023850352
C	258.2475054807	187.0290835638	398.7511428116
S	256.5091462802	187.0577944937	398.9580615467
C	258.9150510000	186.6289720000	400.0610540000
O	244.8993191935	172.0038494226	382.9019983839
O	255.0497654911	188.1448296406	395.0840171437
H	256.7660055784	191.4677681693	393.1757768035
H	257.8825252105	190.2066383161	392.7172285333
H	255.4445627509	189.2553518528	393.5096749772
H	254.5568038666	188.7979222371	392.1104658243
H	258.1990486942	191.3031912981	390.4439289817
H	251.1258408651	184.6403181995	398.8396081118
H	252.1050431640	185.1757007470	396.5492745789
H	253.4309149538	184.0834920058	396.8574804475
H	254.0649827074	192.8351108095	399.6071480054
H	260.4677931752	186.6702647695	396.2610442680
H	258.4655208804	185.7095753223	400.4494405137
H	258.7761913259	187.4103124389	400.8156563773
H	259.9919495955	186.4592807517	399.9412300703
H	256.0318531031	193.4476232674	397.1703056419
H	254.2852405659	193.5089402517	397.4585897909
H	253.0451641000	191.4850833814	400.1278668620
H	257.1137489929	192.5998177055	390.9241993056
H	258.6648099077	192.3986391430	391.7702037452
H	260.6303247104	188.3281181051	396.8609712102
H	260.9400091812	186.9582564190	397.9484824039
H	251.2885492466	183.1684077545	397.8514277971
H	252.4571003898	183.5309176625	399.1440091916
Cl	245.7091056017	173.2521448342	383.7933338187
O	254.0014219490	188.7637304854	395.8063760511
H	252.6142612229	192.4028589187	398.6838631885
H	254.9106984826	192.9854788461	395.8938739994

## React<sub>N</sub>

C	257.8290000000	191.8650000000	391.3050000000
C	257.3240940242	190.8183259728	392.2991267695
C	256.4484969032	189.7598683302	391.6145713359
O	256.5010912040	189.5726448293	390.3939500304
N	255.6452881505	189.0683813849	392.4474488528
C	251.9230000000	184.0210000000	398.3810000000

C	252.5356262932	184.9153042026	397.3075797226
C	253.3951740917	186.0446635398	397.8999613110
O	253.4565746972	186.2188433681	399.1147937674
O	253.9896857126	186.7184561273	396.9594640196
Mo	255.5146660088	188.1491413613	397.0332036586
C	253.4590000000	191.9940000000	399.2530000000
C	254.1505026475	191.0314956682	398.2990386703
S	254.1129783722	189.3079850143	398.6568885900
C	254.8491012032	191.4793528913	397.2286926416
S	255.6802692918	190.3641437180	396.1558346697
C	255.0790000000	192.9360000000	396.9760000000
C	260.3070000000	187.3170000000	397.1300000000
C	258.8396729796	187.3726348188	397.5571311725
S	257.7928549586	187.9691216855	396.2619855274
C	258.2673140591	187.0633992991	398.7557364609
S	256.5055504120	187.1939743590	398.9522613730
C	258.9150000000	186.6290000000	400.0610000000
O	254.5371787823	186.3907204152	393.2176628041
O	255.1563198789	187.6394706669	394.8857875820
O	255.5514786547	185.4718571660	394.9245121651
H	256.7785117491	191.2736505642	393.1338311091
H	258.1686018533	190.2882994585	392.7598350454
H	255.6861192337	189.1515404991	393.4570056882
H	255.1735997075	188.2299370780	392.1301042206
H	258.3045466911	191.3713205415	390.4533651429
H	251.3194866237	184.6138537870	399.0754149731
H	251.7601274891	185.3802406676	396.6848914735
H	253.1711398794	184.3491454066	396.6170820209
H	254.1808751928	192.6402748724	399.7739316705
H	260.4251952114	186.6550210830	396.2639538683
H	258.5044273268	185.6711210281	400.4029595833
H	258.7188247813	187.3647841427	400.8507515751
H	260.0037519461	186.5140425371	399.9670650681
H	255.8948813494	193.3302157539	397.6028991859
H	254.1911799992	193.5459316177	397.1930895426
H	252.8950896827	191.4469041623	400.0148353162
H	256.9993098721	192.4611294338	390.9087462639
H	258.5462416360	192.5471240757	391.7762382817
H	260.6622524861	188.3108877285	396.8325733784
H	260.9570942329	186.9464696369	397.9336734419
H	251.2909548657	183.2362097694	397.9430595585
H	252.7075655408	183.5432863104	398.9764956793
H	252.7573501375	192.6553275284	398.7252840515
H	255.3603504231	193.1240990176	395.9340651461

N	255.0781090768	186.4578596088	394.3529977701
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## TS<sub>N</sub>

C	257.8290000000	191.8650000000	391.3050000000
C	257.1417340000	190.9701220000	392.3472950000
C	255.7861470000	190.4399320000	391.8586800000
O	255.2954130000	190.8230590000	390.7904750000
N	255.1876090000	189.5411740000	392.6703990000
C	251.9230000000	184.0210000000	398.3810000000
C	252.4693710000	184.9556560000	397.3090770000
C	253.3805740000	186.0382520000	397.9019260000
O	253.4515550000	186.2135150000	399.1133350000
O	254.0060190000	186.6886370000	396.9606760000
Mo	255.5015950000	188.1300320000	396.9272770000
C	253.4590000000	191.9940000000	399.2530000000
C	254.2010470000	191.0362000000	398.3258860000
S	254.0218380000	189.2999820000	398.5588680000
C	254.9944380000	191.4946700000	397.3342550000
S	255.9160650000	190.4383410000	396.2848550000
C	255.0790000000	192.9360000000	396.9760000000
C	260.3070000000	187.3170000000	397.1300000000
C	258.8384440000	187.3310720000	397.5401900000
S	257.8059890000	187.7959870000	396.1861450000
C	258.2620880000	187.0403780000	398.7433160000
S	256.5050750000	187.1586640000	398.9247800000
C	258.9150000000	186.6290000000	400.0610000000
O	253.0978600000	187.3246570000	393.8775520000
O	255.2554010000	187.8484730000	395.0677890000
O	254.4178570000	185.6203880000	394.1462670000
H	256.9731940000	191.5098830000	393.2882050000
H	257.7775480000	190.1186290000	392.6192900000
H	255.5251970000	189.2370250000	393.5824990000
H	254.2711890000	189.1961960000	392.4230700000
H	258.0382300000	191.3038210000	390.3888060000
H	251.4004820000	184.5923930000	399.1534140000
H	251.6587460000	185.4688070000	396.7755920000
H	253.0360660000	184.4184740000	396.5410820000
H	254.1389280000	192.7240620000	399.7106950000
H	260.4627850000	186.6484050000	396.2745900000
H	258.4984290000	185.6789540000	400.4161490000
H	258.7210560000	187.3785770000	400.8373650000
H	260.0028490000	186.5102460000	399.9661630000
H	256.1111490000	193.2430790000	396.7585980000

H	254.7006630000	193.5961380000	397.7638890000
H	252.9772320000	191.4404750000	400.0650000000
H	257.1759550000	192.6968640000	391.0269010000
H	258.7717500000	192.2645870000	391.6957000000
H	260.6330140000	188.3180570000	396.8235720000
H	260.9612630000	186.9805960000	397.9454930000
H	251.2332750000	183.2779140000	397.9586250000
H	252.7387980000	183.4887780000	398.8812220000
H	252.6740750000	192.5567830000	398.7278880000
H	254.4979120000	193.1534250000	396.0666690000
N	254.0587180000	186.7597930000	394.3908020000

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C	257.8290000000	191.8650000000	391.3050000000
C	257.0821594415	190.7888619063	392.1032947622
C	255.9663401274	190.1285796758	391.2663646871
O	255.8287701382	190.4324168861	390.0762410908
N	255.1980073657	189.2307648768	391.9140198930
C	251.9230000000	184.0210000000	398.3810000000
C	252.5744171994	184.9926181555	397.4020383909
C	253.5230192042	185.9852516306	398.0814704183
O	253.6540713021	186.0609194739	399.2931694396
O	254.1373118657	186.7150327841	397.1769567949
Mo	255.4951714933	188.1833070129	396.8531315147
C	253.4590000000	191.9940000000	399.2530000000
C	254.2271509615	191.0576700185	398.3455940690
S	253.8818271105	189.3277207739	398.4027194359
C	255.1356346936	191.5292095693	397.4716479224
S	256.3457054785	190.4929369486	396.7259590150
C	255.0790000000	192.9360000000	396.9760000000
C	260.3070000000	187.3170000000	397.1300000000
C	258.8236850960	187.3184196860	397.5274616240
S	257.7682991337	187.6195745249	396.1625158497
C	258.2521675312	187.0989418797	398.7678106328
S	256.5537010446	187.3392816468	399.0185560748
C	258.9150000000	186.6290000000	400.0610000000
O	253.1979340409	187.6601570479	390.6069873892
O	255.1810535725	188.1204029024	395.1621321928
O	251.8855518141	186.0051400336	390.9887972430
H	256.6505555709	191.2043115995	393.0234112115
H	257.7754181673	190.0044598850	392.4362139656
H	255.3528396389	189.0011353779	392.8879510722
H	254.4640175196	188.6992542801	391.4085984889

H	258.2358525891	191.4391987158	390.3836954704
H	251.3821669671	184.5654022706	399.1611013022
H	251.8240978235	185.5857954391	396.8652770922
H	253.1384147596	184.4687621959	396.6222124687
H	254.0257763176	192.9049518102	399.4605609501
H	260.4952834335	186.6217502432	396.3046636399
H	258.4404374386	185.7018861059	400.3978604695
H	258.7884767317	187.3726419501	400.8541309074
H	259.9891282717	186.4395717530	399.9384357423
H	256.0587412888	193.4363667456	396.9712317611
H	254.3876444541	193.5597430719	397.5471862737
H	253.2666381980	191.5003411263	400.2128059424
H	257.1465318424	192.6668775275	391.0073525944
H	258.6465104168	192.2976132250	391.8947718992
H	260.6076077296	188.3167694224	396.7983604365
H	260.9468831192	187.0294616956	397.9721863271
H	251.2223610983	183.3533694251	397.8658884429
H	252.6790514246	183.4091929768	398.8842314819
H	252.4776053207	192.2826897255	398.8476880648
H	254.7311560618	192.9325204529	395.9341329431
N	252.7279554703	186.8216476963	391.4406577693

## ReactCl,T

C	257.8290000000	191.8650000000	391.3050000000
C	257.0888058344	191.1516472923	392.4357793964
C	255.6851444323	190.7018243508	392.0052856045
O	255.3560055556	190.6860294335	390.8150093027
N	254.8743595919	190.3336266453	393.0194720954
C	251.9230000000	184.0210000000	398.3810000000
C	252.8307565564	184.7151639439	397.3678535984
C	253.6500142171	185.8463159510	397.9917889877
O	253.5638661414	186.1307143263	399.1807000563
O	254.4246669608	186.4286108140	397.1050585450
Mo	255.5141796668	188.1456593343	397.1475001992
C	253.4590000000	191.9940000000	399.2530000000
C	254.1327500007	191.0332101248	398.2980673487
S	253.7953379483	189.3114971344	398.5315320536
C	254.9600244512	191.4837781464	397.3293641189
S	256.0364678530	190.4189152315	396.4168104217
C	255.0790000000	192.9360000000	396.9760000000
C	260.3070000000	187.3170000000	397.1300000000
C	258.8245780849	187.3132937893	397.5320843249
S	257.7322693598	187.5646260731	396.1562351292

C	258.3033323120	187.2046995483	398.7950023189
S	256.6420970088	187.7067145067	399.1429967485
C	258.9150000000	186.6290000000	400.0610000000
O	252.7144522472	188.2404894564	393.2123694810
O	254.3669780378	188.2288585265	394.9965657180
O	253.5957953775	186.0867587059	394.0021773773
H	257.0168553868	191.7753305443	393.3348453802
H	257.6361033374	190.2532232979	392.7511203291
H	255.2260933776	190.2296145708	393.9676990584
H	254.0454286121	189.7845920016	392.8145301493
H	257.8310056014	191.2417108516	390.4069788187
H	251.2287322997	184.7401899459	398.8259696593
H	252.2624159278	185.1603922511	396.5443976537
H	253.5301576295	184.0115575655	396.8994889831
H	253.8170943201	193.0206289280	399.1478392032
H	260.5075351789	186.5981749293	396.3274155960
H	258.3905319471	185.7047551306	400.3328011212
H	258.8240822717	187.3173596170	400.9098425362
H	259.9785774828	186.3842878930	399.9347170160
H	255.9279567143	193.4311305825	397.4748414587
H	254.1752702114	193.5052565270	397.2138320705
H	253.6552464053	191.6799351308	400.2860695652
H	257.3292462443	192.8034184184	391.0402940191
H	258.8633071746	192.0927013577	391.5889124033
H	260.5715577311	188.3121857141	396.7551896769
H	260.9619359677	187.0832202396	397.9790375268
H	251.3409260678	183.2174194124	397.9108799414
H	252.5076445610	183.5945499010	399.2030325388
Cl	253.1717583541	187.4567743346	394.4203209090
O	252.0654100380	187.3856909553	395.4183539980
H	252.3650167469	191.9975723794	399.1346809469
H	255.2495736866	193.0452339698	395.8980508611

## TS1<sub>Cl,T</sub>

C	257.8287910000	191.8648120000	391.3051340000
C	256.8013750000	191.6980370000	392.4281110000
C	255.6490490000	190.7807410000	391.9884800000
O	255.2624580000	190.7782360000	390.8136990000
N	255.1084700000	190.0319390000	392.9643380000
C	251.9232450000	184.0211840000	398.3809670000
C	253.1588540000	184.4550210000	397.6019510000
C	253.7412300000	185.7745630000	398.1289820000
O	253.4798630000	186.1859630000	399.2564130000

O	254.5177940000	186.3296070000	397.2438850000
Mo	255.4857210000	188.1534090000	397.0603370000
C	253.4589480000	191.9939070000	399.2528160000
C	254.1407530000	191.0233980000	398.2907280000
S	253.8009290000	189.2952130000	398.4519140000
C	254.9657890000	191.4850830000	397.3182240000
S	256.0050010000	190.4421370000	396.3618820000
C	255.0791630000	192.9361500000	396.9761050000
C	260.3070640000	187.3171530000	397.1300590000
C	258.8289230000	187.3283130000	397.5363630000
S	257.7506430000	187.5715290000	396.1560460000
C	258.3035620000	187.2281300000	398.7996890000
S	256.6482500000	187.7553140000	399.1196620000
C	258.9147880000	186.6287950000	400.0609180000
O	252.9777980000	188.0121260000	393.2832600000
O	254.8900480000	187.8175130000	395.1310870000
O	253.3066080000	185.8041590000	394.3172670000
H	256.3599420000	192.6735430000	392.6758970000
H	257.2625360000	191.3256640000	393.3488270000
H	255.4478040000	190.0324160000	393.9212450000
H	254.3553950000	189.3819250000	392.7669650000
H	258.3543080000	190.9220120000	391.1174500000
H	251.1112720000	184.7427720000	398.2417710000
H	252.9504990000	184.5856020000	396.5363860000
H	253.9523340000	183.6973390000	397.6722730000
H	254.1654650000	192.7373350000	399.6394660000
H	260.5019110000	186.5918680000	396.3315750000
H	258.3764900000	185.7099520000	400.3224760000
H	258.8355010000	187.3085690000	400.9175740000
H	259.9740010000	186.3710360000	399.9262750000
H	256.0660090000	193.3506060000	397.2323030000
H	254.3226640000	193.5518220000	397.4721460000
H	253.0475950000	191.4486430000	400.1072980000
H	257.3165420000	192.1452670000	390.3809900000
H	258.5768630000	192.6268130000	391.5541270000
H	260.5791060000	188.3075480000	396.7479620000
H	260.9639900000	187.0849280000	397.9780780000
H	251.5629690000	183.0353990000	398.0573750000
H	252.1417930000	183.9883360000	399.4525120000
Cl	253.2454900000	187.2782930000	394.5833860000
O	252.1986730000	187.6072220000	395.5975070000
H	252.6255820000	192.5361660000	398.7826840000
H	254.9594610000	193.0767650000	395.8939840000

**Int1Cl,T**



C	257.8287910000	191.8648120000	391.3051340000
C	256.9401849415	191.1667186684	392.3432784973
C	255.8072160499	190.3492762158	391.6880740974
O	255.4763665421	190.5632470964	390.5177534214
N	255.2220414839	189.4393089498	392.4915256940
C	251.9232450000	184.0211840000	398.3809670000
C	252.8389298094	184.7117221413	397.3653477229
C	253.6023624008	185.9013732386	397.9466842930
O	253.3676582723	186.3508042010	399.0650290875
O	254.5021446838	186.3686556663	397.1092503319
Mo	255.4439087896	188.1786322345	396.8245570032
C	253.4589480000	191.9939070000	399.2528160000
C	254.2113310969	191.0232618070	398.3451969655
S	253.8814368403	189.3203418673	398.4963045932
C	255.1151193443	191.5084493836	397.4259711911
S	256.2601189596	190.5192309288	396.5988871519
C	255.0791630000	192.9361500000	396.9761050000
C	260.3070640000	187.3171530000	397.1300590000
C	258.8230000264	187.3432819185	397.5368885312
S	257.8104586645	187.6724325857	396.1398704798
C	258.2671879565	187.1930483315	398.7970547110
S	256.5897287984	187.5592072236	399.0966402787
C	258.9147880000	186.6287950000	400.0609180000
O	252.9190978271	187.5000825283	392.5583691661
O	255.0481664704	188.1688936763	395.1575129874
O	253.1142235645	185.0507952716	393.0639344452
H	256.4693378385	191.9104004543	393.0006970171
H	257.5310922204	190.5229115302	393.0056233386
H	255.5018817362	189.2884479402	393.4526478614
H	254.4264833912	188.8714698968	392.1964731830
H	258.3932942818	191.1311114666	390.7198413598
H	251.2147239690	184.7395274344	398.8033774429
H	252.2740220720	185.1008711414	396.5069891795
H	253.5697833027	184.0146581071	396.9392301795
H	254.1385746767	192.7392301663	399.6801110203
H	260.4753668443	186.6266512579	396.2966042803
H	258.4046159629	185.7018896103	400.3430052887
H	258.8171425804	187.3269906873	400.8992766452
H	259.9808348087	186.4015079020	399.9255389212
H	256.0812174182	193.3213918595	396.7548241024
H	254.6117917729	193.6116844621	397.6991387317
H	252.9865576076	191.4509988085	400.0759964441
H	257.2065884380	192.4255174765	390.6028794929

H	258.5415229408	192.5444228183	391.7866977583
H	260.6107385504	188.3169963447	396.8009971238
H	260.9532058523	187.0186452056	397.9642886402
H	251.3598802001	183.2078271032	397.9083394993
H	252.4982752141	183.6071863515	399.2172034383
Cl	253.0372245225	186.4548695450	393.7070606042
O	251.7438914539	186.5262535445	394.5502915595
H	252.6656517852	192.5277936991	398.7129679051
H	254.5027421574	193.0028075135	396.0438075237

## Int2b<sub>Cl,T</sub>

C	257.8290000000	191.8650000000	391.3050000000
C	257.1064960166	191.1637545875	392.4587122625
C	255.5870685128	191.0828391505	392.2334803817
O	255.0893106564	191.3464343707	391.1334200589
N	254.8781041507	190.7059143660	393.3170084748
C	251.9230000000	184.0210000000	398.3810000000
C	252.8368955646	184.6991391507	397.3632717964
C	253.6504949339	185.8466164664	397.9767866544
O	253.6004026711	186.0963192662	399.1775682270
O	254.3559759479	186.4681100489	397.0692897085
Mo	255.5293862370	188.1736375488	397.1221136569
C	253.4590000000	191.9940000000	399.2530000000
C	254.1926314407	191.0402574800	398.3394690925
S	253.8378156854	189.3196384989	398.5513774117
C	255.0574180203	191.5011710943	397.4088593644
S	256.2166720102	190.4545765473	396.5785224603
C	255.0790000000	192.9360000000	396.9760000000
C	260.3070000000	187.3170000000	397.1300000000
C	258.8225065953	187.2915438107	397.5227587362
S	257.7371730185	187.5358388635	396.1375569266
C	258.2915818044	187.1561894793	398.7803431985
S	256.6110798112	187.5648679729	399.1183307485
C	258.9150000000	186.6290000000	400.0610000000
O	252.3122600374	189.5239289147	394.4709195693
O	254.3973343075	188.3328500387	395.1380298105
O	252.3181872971	187.0268215409	394.5277047530
H	257.3050700833	191.6539956718	393.4192729694
H	257.4764244383	190.1368202004	392.5772814243
H	255.3221500549	190.3923522353	394.1767643764
H	253.9034538812	190.4380850070	393.2331251757
H	257.5761929610	191.3853614414	390.3557457465
H	251.2045336066	184.7384153665	398.7893114488

H	252.2785639270	185.1159174449	396.5170187127
H	253.5471246374	183.9858970709	396.9253392079
H	253.9858905092	192.9449186140	399.3739403386
H	260.5194267198	186.6079136686	396.3211292815
H	258.4060549983	185.7061451161	400.3644641904
H	258.8138132491	187.3434723349	400.8863515598
H	259.9832057880	186.3976228372	399.9434648176
H	256.0355904523	193.4369398582	397.1943640728
H	254.2774958840	193.5299226956	397.4226883310
H	253.3593156123	191.5448356875	400.2478725505
H	257.5158126586	192.9114814901	391.2264461456
H	258.9159498386	191.8371865076	391.4455528593
H	260.5659219689	188.3180621126	396.7670800300
H	260.9595097817	187.0800153702	397.9802476814
H	251.3661240503	183.1886834511	397.9303281439
H	252.5033764324	183.6399340845	399.2269755838
Cl	252.8005581642	188.2870257700	395.2412898094
H	252.4373223159	192.2128849620	398.9062280215
H	254.9482608027	192.9832279440	395.8864969795

## TS<sub>2Cl,T</sub>

C	257.8290000000	191.8650000000	391.3050000000
C	257.1245090000	191.1585690000	392.4656250000
C	255.6260490000	190.9580890000	392.1955840000
O	255.1252950000	191.2583880000	391.1064900000
N	254.9286670000	190.4467450000	393.2313060000
C	251.9230000000	184.0210000000	398.3810000000
C	253.0001340000	184.5315650000	397.4317130000
C	253.6534290000	185.8262660000	397.9450190000
O	253.4796290000	186.1919100000	399.1062450000
O	254.3608140000	186.4071350000	397.0249870000
Mo	255.5106820000	188.2080880000	397.0315430000
C	253.4590000000	191.9940000000	399.2530000000
C	254.1900990000	191.0420120000	398.3239420000
S	253.8261330000	189.3168100000	398.4629610000
C	255.0858140000	191.5102180000	397.4238560000
S	256.2782730000	190.4809230000	396.6332730000
C	255.0790000000	192.9360000000	396.9760000000
C	260.3070000000	187.3170000000	397.1300000000
C	258.8246550000	187.2884550000	397.5213280000
S	257.7559680000	187.5248440000	396.1194280000
C	258.2815880000	187.1309880000	398.7686810000
S	256.5728110000	187.4633370000	399.0733930000

C	258.9150000000	186.6290000000	400.0610000000
O	252.5412320000	188.7758970000	393.9946910000
O	254.8879300000	188.1502460000	395.1401900000
O	253.3426400000	186.3986020000	393.7751180000
H	257.2464600000	191.7069540000	393.4077780000
H	257.5685450000	190.1717070000	392.6492910000
H	255.3740480000	190.0870690000	394.0709070000
H	253.9844080000	190.1088540000	393.0867180000
H	257.6811550000	191.3092160000	390.3749750000
H	251.1037790000	184.7434730000	398.4600840000
H	252.6071500000	184.7183360000	396.4260960000
H	253.8000660000	183.7896750000	397.3052580000
H	254.0468790000	192.8924380000	399.4633680000
H	260.5158890000	186.6157500000	396.3131490000
H	258.4169470000	185.7052080000	400.3784500000
H	258.8029590000	187.3554950000	400.8745250000
H	259.9862570000	186.4125690000	399.9453100000
H	256.0527950000	193.4337860000	397.1027310000
H	254.3233420000	193.5420590000	397.4832070000
H	253.2654490000	191.4938100000	400.2084180000
H	257.4108180000	192.8642410000	391.1466710000
H	258.9040390000	191.9613160000	391.4970360000
H	260.5701940000	188.3202500000	396.7760320000
H	260.9615900000	187.0695440000	397.9760110000
H	251.5048250000	183.0617650000	398.0467740000
H	252.3343690000	183.9013510000	399.3869810000
Cl	253.1656860000	187.5766330000	394.7186550000
H	252.4800450000	192.3128390000	398.8622880000
H	254.8555340000	192.9714190000	395.9008180000

### **Int3<sub>Cl,T</sub>**

C	257.8290000000	191.8650000000	391.3050000000
C	257.0477684510	191.1003805458	392.3797019124
C	255.5640184536	190.9333688059	392.0028302977
O	255.1039229802	191.4850639394	390.9980376411
N	254.8405876737	190.1665830256	392.8431785775
C	251.9230000000	184.0210000000	398.3810000000
C	252.9628175047	184.5687301765	397.4037319765
C	253.6178546129	185.8745322081	397.8869785919
O	253.3461220311	186.3464314922	398.9903402900
O	254.4378333303	186.3608336128	397.0025304265
Mo	255.4641593829	188.2128940782	396.8255699792
C	253.4590000000	191.9940000000	399.2530000000

C	254.2283382241	191.0302181818	398.3521215642
S	253.9238313962	189.3161692859	398.5144990533
C	255.1251549193	191.5153006186	397.4356772117
S	256.3078606327	190.5283215215	396.6329760860
C	255.0790000000	192.9360000000	396.9760000000
C	260.3070000000	187.3170000000	397.1300000000
C	258.8212292985	187.3156236834	397.5318803256
S	257.7966612103	187.6570307682	396.1313285221
C	258.2570656478	187.1334246463	398.7767144846
S	256.5544660001	187.4307394452	399.0608086943
C	258.9150000000	186.6290000000	400.0610000000
O	252.0517942004	189.2284893770	392.9490560578
O	254.9038980826	188.2043099198	395.1957260637
O	251.2135085833	186.6798060664	393.0904915217
H	257.1018453386	191.6143519163	393.3486037475
H	257.4851813864	190.1089347181	392.5538444316
H	255.2391221439	189.7136813539	393.6572865490
H	253.8501898653	189.9744606569	392.6709877246
H	257.8110986017	191.3225739106	390.3546880016
H	251.1174617791	184.7465407041	398.5284632537
H	252.5206128577	184.7689740475	396.4207913705
H	253.7657184487	183.8410820379	397.2267359111
H	254.1127822396	192.7841620194	399.6371294080
H	260.4918678548	186.6314503377	396.2949174788
H	258.4319075294	185.6977884182	400.3756871084
H	258.7925687995	187.3534355489	400.8736284108
H	259.9886162412	186.4308540093	399.9370928491
H	256.0821489966	193.3609866395	396.8417755251
H	254.5221999425	193.5956047078	397.6482720033
H	253.0404164193	191.4540297858	400.1074158336
H	257.3683149843	192.8397333042	391.1216760629
H	258.8728466466	192.0123805547	391.6069695132
H	260.5999446421	188.3218484982	396.8052531643
H	260.9532933066	187.0237448731	397.9664356103
H	251.4854422074	183.0828768923	398.0156516587
H	252.3736202069	183.8427602278	399.3624483403
Cl	252.1850269823	187.8028468013	393.6731411980
H	252.6214526373	192.4707302537	398.7260820012
H	254.5890262068	192.9769603310	395.9938390232

## The Mo-perchlorate complex optimized using the bigger model

Mo	255.3426467622	188.1319885354	397.1631604495
P	253.3503101536	192.4813559380	404.4682840659
O	254.3281589871	193.4942089739	403.9404156111
O	253.7723604041	191.2232229871	405.1651000720
O	252.4016552480	191.9218685367	403.1280246228
O	252.9132761083	193.3203909207	401.0498530370
P	251.7562949441	192.8534081325	402.0171204109
O	250.9471261955	194.0098697143	402.5145578601
O	250.8242032011	191.8196665563	401.1857603191
O	252.1493765417	193.1651079425	405.3269893107
C	253.8004126477	192.3318995748	400.4266635397
C	253.4480223715	192.2695380757	398.9479426899
O	253.6653456093	193.6088872090	398.4722833127
C	254.1750777261	191.1894353916	398.1883014400
S	253.9910806666	189.5149385757	398.6967770535
C	254.8822861862	191.4826592560	397.0783074551
S	255.5859282330	190.2325254122	396.0993446541
C	255.2221385092	192.8989820317	396.7102486263
N	256.4459903480	193.2948210131	397.4306781652
C	256.6660989921	194.6841670127	397.5562271499
C	257.9465386364	195.1201437933	397.9840567728
O	258.9283387007	194.3837444790	398.2243935872
N	258.0585784303	196.5054500582	398.1183831360
C	257.0418690218	197.3643631617	397.8352391859
N	257.3342397021	198.7052912036	397.9283733457
N	255.8268627584	196.9647681518	397.5234794026
C	255.6542059759	195.6164378372	397.3747779754
N	254.4028288245	195.1994192118	396.9610807749
C	254.0619917117	193.8119114002	397.1026843576
P	262.3723918616	187.9623283630	394.5341209483
O	262.4866027982	189.5202211773	394.1603978828
O	261.0663556532	187.5660782360	393.6409251890
O	263.5597548934	187.1221345403	394.2782534441
O	261.8876569497	187.8028815721	396.0619236424
C	260.5575933160	188.1578643823	396.5148611786
C	260.0602279170	187.1754209567	397.5732096262
O	260.6743240583	187.5460127108	398.8234139883
C	258.5544198911	187.2430341803	397.7693543202
S	257.5362238620	187.6973458662	396.4246414541
C	257.9798318453	187.0646235500	398.9849218079

S	256.2415428277	187.3091320215	399.1707729891
C	258.7541357045	186.6480256367	400.2140705226
N	258.3405142378	187.4030894184	401.3973371032
C	259.2071255402	187.3058582927	402.5025428477
C	258.7456110876	187.3507127337	403.8474003924
O	257.5540842654	187.3693643763	404.2713675332
N	259.7622468901	187.3933611485	404.8109556913
C	261.0907709687	187.3083994598	404.5199244236
N	261.9810053925	187.3882276583	405.5343749998
N	261.5247973905	187.1904580987	403.2757546900
C	260.5882965506	187.1997058552	402.2964014645
N	261.0730912209	187.0582871481	401.0256754348
C	260.2950467645	186.6700524946	399.8793722449
P	263.9359161216	190.4303773665	394.0207303057
O	263.5452257880	191.7868911089	393.5078785162
O	264.6395837716	190.2223417898	395.3379270271
O	264.6834759406	189.6053354063	392.8329547713
H	253.7111744344	191.3541225195	400.9108267390
H	254.8095675875	192.6991631364	400.5718471738
H	257.2684193714	192.8210013343	397.0536658420
H	259.0105687001	196.8796831057	398.1949222267
H	256.6777944657	199.2902556970	397.4313095743
H	258.3151830029	198.9384864842	397.8040157462
H	253.6455720835	195.8512315243	397.1599822385
H	260.5995870481	189.1519210283	396.9520941973
H	259.8659099077	188.1590319558	395.6743287953
H	260.3770094609	186.1591907376	397.2900031473
H	258.5101757362	185.5896592068	400.4104641349
H	258.0396260839	188.3705559712	401.2329099781
H	261.6319900931	187.1592617128	406.4542248135
H	262.9476255893	187.1097681586	405.3098903627
H	262.0779110853	187.0990197469	400.9077425418
H	260.5775945684	185.6473275969	399.5619340879
H	259.4762623599	187.5831711390	405.7708248421
H	260.5511716088	188.3373347221	393.3631477986
H	251.3161333501	191.1718185055	400.6515696301
H	264.7415522289	190.1787726623	392.0566070388
H	251.7824340150	193.9252412118	404.8480828699
H	252.3653929961	192.0534140144	398.8764160915
H	255.3568497494	192.9930395276	395.6219157346
H	253.2236580696	193.5791991997	396.4397013140
C	253.8140540000	181.3188680000	393.8543080000
C	252.5424124120	181.0576445410	393.0474978392
C	251.3389336117	181.8415405520	393.5500417123

C	251.4727354557	183.1357845726	394.0785876234
C	250.0429305121	181.3216401308	393.4398773021
C	250.3605026772	183.8830501013	394.4512374497
C	248.9166899800	182.0675238081	393.7927361367
C	249.0739260583	183.3645517087	394.2793059322
O	247.9474187118	184.0955003181	394.5679169690
H	252.3034710450	179.9851428704	393.0378049379
H	252.7384722369	181.3376314685	392.0035206443
H	249.9073178661	180.3159606347	393.0438822231
H	252.4503775729	183.5926086389	394.1927578039
H	247.9121376914	181.6726008793	393.6696315322
H	250.4944384563	184.8895174548	394.8329230433
H	248.1575587892	185.0334073910	394.4455600631
H	254.0007140496	182.3963583371	393.9175169236
H	254.7064280000	180.9465740000	393.3960950000
H	253.7446350000	180.9720910000	394.8641720000
C	250.7218750000	189.7719140000	397.2658080000
C	251.7060240000	190.2218780000	396.2069210000
O	251.8647674022	191.4565654704	396.0221619456
C	250.5460188405	188.2808886773	397.6451414216
C	249.4061914859	187.6567412058	396.8005847289
C	250.3113631321	188.1667288980	399.1609518446
C	248.9432257081	186.2623449126	397.2405294965
N	252.1860570000	189.2759060000	395.4019000000
C	253.0112190000	189.6169460000	394.2560170000
C	252.3723900000	189.5291300000	392.8819240000
O	251.1364736288	189.4602674440	392.7371449648
N	253.2205140000	189.6571500000	391.8670170000
C	252.7886420000	189.7523290000	390.4779890000
C	252.6395510000	188.3764130000	389.8628300000
O	253.3252895022	188.0314837546	388.8953326900
N	251.7414190000	187.5944470000	390.4436720000
C	251.5653020000	186.1915040000	390.0795090000
C	251.0844769709	185.3944637323	391.3114223821
C	249.8027465121	185.9103375739	391.8982627581
C	249.6985161854	186.7455341703	392.9781705530
C	248.4559674822	185.6481103571	391.4540849996
N	248.3572396375	186.9822480476	393.2795346224
C	247.5749203259	186.3564358871	392.3147960217
C	247.9150153684	184.8689850051	390.4198623882
C	246.1892774918	186.3237128998	392.1540782938
C	246.5353364434	184.8326046944	390.2545948636
C	245.6815445716	185.5573050421	391.1089056522
H	251.4759337792	187.7454399032	397.4444128643



H	249.4151038965	188.7281577556	399.4658204374
H	251.1838032688	188.5434875001	399.7048176848
H	250.1967679301	187.1286529109	399.4795880804
H	248.5370514659	188.3340553494	396.8308678527
H	249.7312741413	187.6283002434	395.7512074616
H	248.4315793728	186.2988868756	398.2075275591
H	248.2490726054	185.8190900116	396.5198815443
H	249.7806994337	185.5690652929	397.3457631116
H	251.0115930924	190.3326682146	398.1641257524
H	253.3354549581	190.6495932755	394.3930997585
H	253.9188480174	189.0240772534	394.2756317262
H	252.1221543900	188.2938305170	395.6431809930
H	251.8376716284	190.2983876909	390.4450411176
H	254.2394117205	189.5541720204	391.9926937122
H	251.8649469015	185.4417590176	392.0761495353
H	250.9741500026	184.3386739351	391.0327194795
H	250.4845647644	187.1919254754	393.5674400872
H	248.0528630088	187.7523945466	393.8560512462
H	248.5713670272	184.3052041033	389.7617154557
H	246.1040543346	184.2348532813	389.4549652785
H	245.5311319018	186.8716505627	392.8241032816
H	244.6061089670	185.5124567244	390.9540582380
H	252.5552566875	185.8203466156	389.7857053953
H	251.1773275943	187.9753479905	391.1990472680
H	253.5564373237	190.2844404743	389.9150804583
H	250.9372440000	186.0082860000	389.2328240000
H	249.7487980000	190.1330640000	397.0058230000
C	257.4170180000	180.5496190000	392.8123970000
C	257.7628094452	181.6672773861	391.7997673811
C	256.5074448815	182.1954233043	391.1407585830
C	255.7774013907	183.2297984612	391.7420016421
C	255.9907704689	181.5985199563	389.9838838551
C	254.5564574836	183.6458321301	391.2110266745
C	254.7731972564	182.0153677801	389.4445833459
C	254.0503173791	183.0394145325	390.0602365798
H	258.2675074382	182.4818451182	392.3304760957
H	258.4661751118	181.2919911677	391.0452003816
H	256.5484713584	180.7943473600	389.5057116424
H	256.1596191575	183.7138368584	392.6381762014
H	254.3894928103	181.5423665173	388.5428724882
H	254.0176868870	184.4552737654	391.6902725574
H	253.1013278270	183.3693268114	389.6436638737
H	258.2767548847	180.3597678855	393.4694967270
H	256.6113710000	180.8878910000	393.4299720000

H	257.1875720000	179.6226060000	392.3297990000
C	256.5883240000	185.6261280000	388.1369230000
C	256.7150441016	186.8781894657	389.0344266897
C	256.7739600512	186.4758381201	390.5141779354
C	257.9402440563	187.7231694488	388.6565171513
H	255.8170034929	187.4942084314	388.8906311104
H	257.9856753914	188.6324541365	389.2687876519
H	258.8724677524	187.1626615521	388.8156999398
H	257.9141542491	188.0316893748	387.6029009348
H	256.8331514121	187.3512742411	391.1641735067
H	257.6468047271	185.8352646996	390.7128992668
H	255.8836646678	185.9178838417	390.8080687929
H	255.6131032025	185.1558056310	388.3268276118
H	256.5961940000	185.9045290000	387.1038060000
H	257.3115520000	184.8931960000	388.4278720000
C	257.8298250000	191.8647110000	391.3055300000
C	258.2056898435	190.5219613039	391.9209715823
C	256.97444461522	189.7227254042	392.3232596777
O	255.9863920215	189.6614135549	391.5698072774
N	257.0856984730	189.0546302889	393.4824884345
H	258.8681614614	190.6495046394	392.7784785490
H	258.7394707232	189.9099984251	391.1799117355
H	257.6813349518	189.4525706484	394.2156853146
H	256.3069940743	188.4742503872	393.7804448445
H	257.1023133572	191.6838495238	390.5046649086
H	258.6811120000	192.3354150000	390.8598300000
H	257.3481020000	192.5081980000	392.0117640000
C	257.2030720000	182.8222950000	398.2411400000
C	256.2069930000	182.9722980000	399.3890710000
O	256.2821880969	183.9310983480	400.1593148203
C	257.0121449558	183.9124656563	397.1740408152
C	258.1361980062	183.9957519440	396.1546953470
C	259.4271600473	183.5033030620	396.3832371232
C	257.9149062484	184.7092552728	394.9656824963
C	260.4733067564	183.7475588333	395.4904614418
C	258.9480984739	184.9631823908	394.0672290620
C	260.2443023799	184.4995331501	394.3375495432
O	261.3007005584	184.7373536587	393.5057107770
N	255.2919070000	182.0103590000	399.5379370000
C	254.2768300000	182.0753700000	400.5798610000
C	253.0549250000	182.8554920000	400.1428150000
O	252.1626554079	183.0770732633	400.9620650072
N	253.0010500000	183.1645790000	398.8588310000
C	251.9221530000	184.0206930000	398.3808010000

C	252.4690510843	184.9551932170	397.3158661587
C	253.1652005595	186.1580308795	397.9195866794
O	252.9784236756	186.5514125698	399.0551766914
O	253.9105186918	186.7529389882	397.0110055056
H	256.9261884233	184.8805065278	397.6812452386
H	256.0562298927	183.7654921842	396.6524201720
H	256.9226559193	185.0983053039	394.7614081072
H	259.6488861907	182.9369240850	397.2842255002
H	258.7581240869	185.5441624835	393.1675112027
H	261.4810059975	183.3925908403	395.6875279591
H	261.1822776361	185.6094593536	393.0994105921
H	258.1835350660	182.9407539079	398.7142479583
H	254.6936692153	182.5880083668	401.4502536395
H	253.9685536092	181.0663945527	400.8692701899
H	255.2883860402	181.2282713403	398.8994160968
H	251.6701155053	185.3460001085	396.6789503753
H	253.1454769157	184.4511102409	396.6160199490
H	251.5605837337	184.5982494683	399.2355889690
H	253.8154388789	183.0472869385	398.2771758423
H	257.1736930000	181.8504670000	397.7943870000
H	251.0845350000	183.5184970000	397.9436560000
C	252.3745140000	194.4248920000	391.2271740000
C	251.5054576524	193.9016189296	392.3663140471
O	251.1949533191	194.9394889828	393.3314670345
C	252.1720238235	192.7081118011	393.0340499573
H	250.5218925224	193.6187942078	391.9701502368
H	251.5147935744	192.1480493673	393.6955505262
H	253.0341806859	193.0417781281	393.6284040979
H	252.5560118656	192.0160182993	392.2822842403
H	252.0005523615	195.0995934398	393.8446583110
H	252.2602702656	193.7357900801	390.3777436386
H	253.4131320000	194.3659120000	391.4775630000
H	252.0456620000	195.3824430000	390.8809740000
C	252.9229320000	197.6776770000	399.7280460000
C	251.9289630000	197.6087100000	398.5540210000
O	251.9969122022	196.6793022701	397.7246720956
C	252.8008925816	196.4051958950	400.5783523569
O	251.4358025034	196.3768834471	401.0032982454
C	253.7707965449	196.4222725131	401.7603637712
N	251.0510080000	198.6037450000	398.4339890000
C	250.2740630000	198.7447630000	397.1999590000
C	248.8842772386	198.0698632690	397.2984949971
C	248.3553800746	197.4133264003	396.0059014887
C	249.2768815575	196.3491408932	395.3546577164

N	249.9782129752	195.5463860278	396.3536604170
C	250.1969855416	194.2289682845	396.3440979174
N	249.7322246043	193.4380152880	395.3455393383
N	250.8528353434	193.6575244655	397.3628916649
H	253.0263706422	195.5408070455	399.9410620734
H	253.7056787769	195.4957655643	402.3390496479
H	253.5448616573	197.2639923201	402.4274439081
H	254.8061243976	196.5223108319	401.4118102022
H	251.2832863566	195.5463795596	401.4873044898
H	253.9186691456	197.7092455343	399.2640376454
H	248.9541417155	197.2974831101	398.0722144231
H	248.1400323485	198.7893298378	397.6602186742
H	247.3951400966	196.9453531522	396.2535390986
H	248.1440098232	198.1741104939	395.2427530260
H	250.0165579290	196.8159809595	394.6932479626
H	248.6733553148	195.6964939637	394.7201068480
H	250.6297899879	196.0633917770	396.9610560444
H	250.1156085929	192.4943112462	395.3869702925
H	249.8563183340	193.8715716718	394.4323559207
H	251.3137118229	194.2356423939	398.0574864242
H	251.2789445872	192.7431680042	397.1425294622
H	250.8704411129	198.2624109382	396.4196596952
H	251.0069655183	199.3081700417	399.1544609303
H	252.8224950000	198.5271910000	400.3708040000
H	250.2455750000	199.7824050000	396.9403670000
C	262.4397860000	198.8487360000	397.8030600000
C	261.3738350000	197.9836670000	397.1570730000
O	260.2203825551	197.9864287608	397.6259956583
N	261.7388800000	197.3096500000	396.0761030000
C	260.9409370000	196.2035970000	395.5761320000
C	261.7589980000	194.9406520000	395.8171980000
O	262.7446335192	194.7418188798	395.0956285957
C	260.5505033947	196.3398261664	394.0917305053
C	259.7468340232	195.1027098629	393.6584403627
C	259.7613511935	197.6341153925	393.8553936995
N	261.4030230000	194.1806740000	396.8512230000
C	262.2440980000	193.0757420000	397.2942690000
C	263.7130720000	193.5308170000	397.3752510000
O	263.9553574105	194.5963664466	397.9594471367
C	262.0623989095	191.8455108198	396.4121299705
C	260.6466636498	191.4701872538	396.2566215812
N	259.7759008811	191.2840382625	397.3085898823
C	259.9324084272	191.1774053383	395.1237955135
C	258.5965426080	190.8660375258	396.7754037699

N	258.6538123363	190.7922049039	395.4513359352
N	264.6520740000	192.7718210000	396.8362480000
C	266.0420760000	193.1748200000	397.0131920000
C	266.3610680000	194.3288050000	396.0731710000
O	267.3187262965	195.0748538669	396.3162340437
C	267.0286565507	191.9997130892	396.8647518721
O	267.0948696216	191.4469241431	395.5691167134
N	265.6370370000	194.4208050000	394.9661900000
C	265.9150260000	195.4717900000	393.9891710000
C	265.0112514548	195.2493560297	392.7560083816
O	265.1415108322	193.9468704180	392.2077275271
C	265.3587365507	196.2377538424	391.6456671746
H	263.0003318626	199.4225772693	397.0559898552
H	261.4823917904	196.3662103007	393.5119322918
H	258.8261961470	195.0041758318	394.2495383205
H	259.4585379675	195.1775007936	392.6042286812
H	260.3246303152	194.1820163893	393.7813885555
H	260.3329846791	198.5166814835	394.1643733300
H	258.8218551244	197.6284756803	394.4245637453
H	259.5092055095	197.7479551523	392.7950236008
H	260.0228034125	196.1876903549	396.1682686251
H	262.7286376815	197.2479105246	395.8565308562
H	262.6364588559	191.0060898396	396.8248354630
H	262.4532818778	192.0729477041	395.4195951794
H	260.3046159101	191.2162512836	394.1099144855
H	257.7499812967	190.5799229760	397.3714586346
H	261.9413864718	192.8506374844	398.3224693536
H	260.5494037791	194.3769792442	397.3758365393
H	266.7720487193	191.2438312211	397.6233520811
H	268.0203934414	192.4066975418	397.0970819156
H	266.3091397933	190.8791747029	395.4482394034
H	266.1541182638	193.5823053773	398.0228457377
H	264.4681174013	191.8763476298	396.3852393476
H	263.9734604211	195.4195631467	393.0840747707
H	265.3013228869	197.2744915185	391.9992157244
H	264.6717948952	196.1147857515	390.8022814561
H	266.3764516584	196.0483810020	391.2851719500
H	264.6205969444	193.3105726077	392.7310949267
H	266.9779338776	195.4484553327	393.7264095463
H	264.7782275118	193.8924243156	394.8843791019
H	259.9861439274	191.4208944874	398.3141653773
H	262.0015610000	199.5148990000	398.5165630000
H	263.1590353992	198.1978568205	398.3169184155
H	265.6769230000	196.4271170000	394.4081680000

C	259.4897310000	190.5143660000	408.0813510000
C	258.6587620000	191.0442650000	406.9172830000
O	258.5406951912	190.3903731806	405.8721881059
C	260.4829444746	189.4262441614	407.6504961945
O	259.8945277970	188.1155302521	407.5878560373
N	258.0657450000	192.2112760000	407.1151720000
C	257.1357700000	192.7791890000	406.1320980000
C	257.8807970000	193.5141070000	405.0200630000
O	259.1076137822	193.6938400042	405.1076119211
C	256.2723573404	193.7279421140	406.9864120040
C	257.3013601733	194.2893686485	407.9830107692
C	258.2007263094	193.0766364452	408.3012140050
N	257.1568240000	193.9310180000	403.9930070000
C	257.7578510000	194.5809260000	402.8279760000
C	257.0864514262	194.0991343951	401.5356667670
C	257.2154710173	192.6125856994	401.3017532254
N	256.9960690920	192.0851816216	400.0389223615
C	257.4874911919	191.5128367127	402.0939272419
C	257.1375950805	190.7354266754	400.1184358296
N	257.4384892039	190.3528697212	401.3453211062
H	261.3386889588	189.4099114447	408.3411863144
H	260.8602876874	189.6172642742	406.6445271373
H	259.5750700633	187.8726591827	408.4654424876
H	260.0615641785	191.3314720364	408.5378019429
H	255.4951918045	193.1483222503	407.4978324501
H	255.7781523566	194.4890929616	406.3782294466
H	256.8519673491	194.7153341714	408.8851913050
H	257.8998368891	195.0672548873	407.4970102920
H	257.8601888174	192.5466883574	409.2016010715
H	259.2441245586	193.3749235244	408.4523087253
H	256.5357473298	191.9764471069	405.6930680131
H	256.0253481582	194.3927886218	401.5495983483
H	257.5431892544	194.6327614934	400.6919278116
H	257.7369429693	191.4778512749	403.1444390302
H	256.9752936313	190.0722607608	399.2824145746
H	258.8076397441	194.2901377569	402.8129003199
H	256.1508132540	193.7317852682	403.9608780580
H	256.7685315813	192.5947839282	399.1729502880
H	257.7515080000	195.6461040000	402.9292550000
H	258.8823310000	190.1066000000	408.8621790000
C	262.5168400000	191.6281260000	404.4244280000
C	261.4201509413	190.7936664071	403.7028710366
C	261.0506163995	191.3313418244	402.3506719621
N	260.6905767010	192.6547063414	402.1579937114

C	260.9522253494	190.7605177361	401.1028001488
C	260.3709366695	192.8233330016	400.8410541042
N	260.5297145845	191.6957477065	400.1720614814
H	260.5199433286	190.7311266527	404.3315841667
H	261.7793597466	189.7702613271	403.5585723281
H	261.1105332082	189.7265071999	400.8279388157
H	260.0367504874	193.7568467788	400.4089178205
H	262.8558902266	191.0799442721	405.3136033504
H	260.5566231764	193.3161603087	402.9128573992
H	262.1234480000	192.5625320000	404.7665220000
H	263.3515270000	191.7182260000	403.7610420000
C	247.8968980000	194.0107940000	404.4931570000
C	248.2018860000	195.4878030000	404.7371180000
O	247.4392671576	196.1674477404	405.4302715158
C	246.8110551461	193.8121132878	403.4317410939
O	247.2376320367	194.2721112368	402.1553715058
N	249.3138700000	195.9618030000	404.1770870000
C	249.8018600000	197.3148150000	404.4650490000
H	245.9229902815	194.3985705716	403.6917163639
H	246.5210276049	192.7479458378	403.4017740874
H	248.1122140685	193.8939690096	401.9829295084
H	248.8024453066	193.4946303106	404.1336649049
H	249.0916164567	197.7709458974	405.1562330287
H	249.8643105596	195.3649926049	403.5703763621
H	250.7882180108	197.2675537056	404.9429456145
H	249.8830000000	197.9214530000	403.5873780000
H	247.6468730000	193.5209220000	405.4109870000
C	248.0799800000	189.8886070000	402.3844170000
C	249.0950770000	189.0787130000	403.1734010000
O	248.7625889751	188.1261682305	403.8784487311
N	250.3660440000	189.4517880000	403.0173110000
C	251.5131280000	188.7688930000	403.5982810000
C	251.3882420000	188.5089510000	405.0893020000
O	251.8643037023	187.5043697476	405.6380918017
N	250.8692160000	189.5059460000	405.7982900000
C	250.6663130000	189.3999970000	407.2253080000
H	248.3899608104	190.9347020409	402.2625751537
H	248.0291863568	189.4693477240	401.3704928772
H	252.3947158694	189.3978306554	403.4464156978
H	251.6978245727	187.8146242489	403.1063338955
H	250.5513975920	190.2825941632	402.4785549947
H	251.6174581966	189.3224183734	407.7650115262
H	250.1701882348	190.3105881769	407.5737624834
H	250.5301263594	190.3224713740	405.3113969549

H	247.0858900000	189.8760150000	402.7800520000
H	250.0645750000	188.5600940000	407.5034690000
C	252.9378530000	183.9059790000	405.2635470000
C	253.9995486879	185.0058777937	405.0994378062
C	253.9636636549	185.6823421686	403.7660610408
N	254.9277711036	186.5883250207	403.3478686273
C	252.9665426879	185.7687627319	402.8234734830
C	254.4650692333	187.1672249756	402.1978653228
N	253.2777698556	186.7068779158	401.8637080519
H	253.8373117343	185.7769420835	405.8579292750
H	255.0007480883	184.5828731592	405.2855331570
H	252.0414030358	185.2111560812	402.7827749084
H	255.0507649587	187.8852705960	401.6416300869
H	253.0331810313	183.1995697108	404.4257883859
H	255.8784082783	186.7203955439	403.6923363936
H	253.0726070000	183.3277390000	406.1537030000
H	251.9386620000	184.2827480000	405.1959970000
C	256.1358660000	184.2685110000	410.0932670000
C	254.8571621363	185.0209344471	409.6706484347
C	254.9167586773	185.6305892722	408.2492866664
C	255.8167733025	186.8742988567	408.0875492678
N	255.9056880651	187.4162640498	406.7206628175
C	255.2494547991	188.5118284002	406.2802128126
N	254.0996253527	188.9042700038	406.9003944060
N	255.7413625249	189.2221731201	405.2777015871
H	254.6221921378	185.8060283182	410.4043567219
H	254.0071888679	184.3270223313	409.6900374884
H	253.9007533841	185.9050393479	407.9453755561
H	255.2473804431	184.8593426378	407.5445166791
H	255.4554269073	187.6766145486	408.7413898923
H	256.8441219367	186.6382739817	408.3945767310
H	256.6795243124	187.1326308932	406.1167788140
H	253.3909255651	188.1689414305	406.9349532219
H	253.7150520494	189.7560275553	406.4854808294
H	255.1538702510	189.9494746820	404.8688770800
H	256.6272164213	188.9489709998	404.8495835612
H	256.9582533735	184.9972048431	410.1881854735
H	256.0755190000	183.8111360000	411.0587020000
H	256.4554930000	183.6147070000	409.3088700000
C	258.2849300000	182.3635890000	407.6132630000
C	259.1217889788	183.2904727140	406.6981256099
C	259.3499163488	182.7090374103	405.2893218563
C	259.9006494372	183.7988565329	404.3720755068
O	260.9337191655	184.3997072311	404.6570853267



N	259.1654314017	184.0705193153	403.2578217655
H	258.5750341339	184.2387420271	406.5853832593
H	260.0917932905	183.5514803439	407.1351085784
H	260.0777707695	181.8891565204	405.3292531365
H	258.4130010232	182.2944385914	404.8938944727
H	258.2387247861	183.6976841745	403.1121667317
H	259.3928387018	184.9117962962	402.7411125713
H	258.8566984944	181.4959574940	407.9618037769
H	257.9773220000	182.9532090000	408.4514900000
H	257.4950910000	182.0183080000	406.9793570000
C	266.7507380000	184.8294110000	405.9897060000
C	266.9140867077	184.5525328686	404.4814378303
C	266.4498880323	185.7240498689	403.5859981532
C	265.0000585622	186.1274944022	403.8338663203
O	264.6656712991	186.6214137807	404.9231448925
N	264.1211458518	185.9029493167	402.8381772729
H	266.3732299625	183.6400123655	404.1970953249
H	267.9714340987	184.3679103022	404.2497155186
H	267.0576085331	186.6091559996	403.8099017675
H	266.6134007850	185.4761397027	402.5302620223
H	263.1594947319	186.2499074775	402.9565109474
H	264.4319316469	185.5769867301	401.9356858638
H	265.7109394100	184.6899706764	406.2974305537
H	267.3703190000	184.1798560000	406.5720270000
H	266.9701810000	185.8609910000	406.1702230000
C	265.3832440000	185.7487040000	399.2267180000
C	264.4405810393	186.2102651526	398.0950545712
C	264.8540629925	187.5966941375	397.5507517650
C	264.6471831620	188.7528249946	398.5274105469
O	265.5545383027	189.4911761985	398.8981491893
N	263.3650798650	188.8968124490	398.9999506133
H	263.3955538533	186.2332512117	398.4322444985
H	264.4750662948	185.4943976546	397.2648627044
H	265.9167019813	187.6014949583	397.2882571856
H	264.3026404208	187.8170565862	396.6353619670
H	263.1688273041	189.7316094717	399.5363524471
H	262.5746489109	188.4126910658	398.5920669183
H	265.3435984682	186.4734504075	400.0543466807
H	266.3826300000	185.7928110000	398.8470050000
H	265.1504780000	184.7840630000	399.6269520000
C	264.6901830000	186.5738150000	390.9080180000
C	266.0211440000	186.4578400000	391.6570910000
O	266.9669562207	185.8591136006	391.1234004800
N	266.1040810000	187.0408770000	392.8470770000

C	267.3460400000	187.0189030000	393.6281430000
H	264.0513272713	187.3744428292	391.2915925595
H	264.1458197043	185.6266789106	390.9894760682
H	268.1859580965	186.8795538599	392.9460723429
H	265.2703857139	187.4197715910	393.2819259980
H	267.4444875410	187.9553812594	394.1846273143
H	264.9293500000	186.7388150000	389.8782240000
H	267.2858450000	186.1920680000	394.3046200000
O	254.3385773890	186.5680584150	392.6936827910
O	255.0452693805	187.4047971085	394.8535690196
O	254.5314812646	184.9822792638	394.5604283216
Cl	254.1352403319	186.3589946354	394.1509619445
O	252.6895256899	186.6053122664	394.4866284359

## The TS for the O-Cl cleavage of perchlorate optimized using the bigger model

Mo	255.3478180000	188.1085230000	397.0566890000
P	253.2903890000	192.3660170000	404.4419010000
O	254.2120130000	193.4495160000	403.9666630000
O	253.7618410000	191.1078910000	405.1049060000
O	252.4052990000	191.8092890000	403.0571620000
O	252.9087250000	193.2694720000	401.0167550000
P	251.7555330000	192.7723780000	401.9755810000
O	250.9408050000	193.9062540000	402.5102170000
O	250.8269950000	191.7645780000	401.1088980000
O	252.0319190000	192.9516950000	405.2959060000
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C	253.4511690000	192.2332390000	398.9066420000
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C	256.9771360000	197.3724670000	397.8026780000
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N	257.4105140000	190.3498360000	401.3484090000
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H	260.8875630000	189.6428700000	406.6606860000
H	259.5236020000	187.8636300000	408.3887470000
H	260.0629450000	191.3296590000	408.5365390000
H	255.5040250000	193.1553700000	407.5021780000
H	255.7834900000	194.4922770000	406.3787920000
H	256.8647450000	194.7265430000	408.8746350000
H	257.9134580000	195.0604650000	407.4843410000
H	257.8485960000	192.5506770000	409.1979580000

H	259.2417770000	193.3679460000	408.4571180000
H	256.5339730000	191.9769970000	405.6954620000
H	256.0427410000	194.3921740000	401.5289570000
H	257.5696570000	194.6352430000	400.6924290000
H	257.7282120000	191.4831510000	403.1395030000
H	256.9415030000	190.0646480000	399.2868660000
H	258.8080580000	194.2912520000	402.8244220000
H	256.1544980000	193.7235090000	403.9590580000
H	256.7805630000	192.5910080000	399.1620040000
H	257.7515080000	195.6461040000	402.9292550000
H	258.8823310000	190.1066000000	408.8621790000
C	262.5168400000	191.6281260000	404.4244280000
C	261.4129990000	190.8045410000	403.7057490000
C	261.0431300000	191.3210220000	402.3463060000
N	260.7274850000	192.6487300000	402.1107340000
C	260.9073870000	190.7117540000	401.1184780000
C	260.4000640000	192.7855730000	400.7921730000
N	260.5096440000	191.6305380000	400.1608650000
H	260.5152380000	190.7568250000	404.3368860000
H	261.7604840000	189.7774350000	403.5718590000
H	261.0304550000	189.6669280000	400.8734000000
H	260.0896060000	193.7151400000	400.3354030000
H	262.8513780000	191.0759470000	405.3108240000
H	260.6310110000	193.3428820000	402.8390990000
H	262.1234480000	192.5625320000	404.7665220000
H	263.3515270000	191.7182260000	403.7610420000
C	247.8968980000	194.0107940000	404.4931570000
C	248.2018860000	195.4878030000	404.7371180000
O	247.4392020000	196.1679310000	405.4283440000
C	246.8102050000	193.8237450000	403.4316120000
O	247.2304760000	194.3093830000	402.1627230000
N	249.3138700000	195.9618030000	404.1770870000
C	249.8018600000	197.3148150000	404.4650490000
H	245.9206600000	194.4011000000	403.7031090000
H	246.5249650000	192.7599380000	403.3836040000
H	248.0985800000	193.9256350000	401.9715370000
H	248.7995410000	193.4960330000	404.1281320000
H	249.0911220000	197.7703550000	405.1551580000
H	249.8684100000	195.3635560000	403.5768610000
H	250.7882450000	197.2666380000	404.9413240000
H	249.8830000000	197.9214530000	403.5873780000
H	247.6468730000	193.5209220000	405.4109870000
C	248.0799800000	189.8886070000	402.3844170000
C	249.0950770000	189.0787130000	403.1734010000

O	248.7586140000	188.1330730000	403.8845680000
N	250.3660440000	189.4517880000	403.0173110000
C	251.5131280000	188.7688930000	403.5982810000
C	251.3882420000	188.5089510000	405.0893020000
O	251.8545890000	187.4985500000	405.6337840000
N	250.8692160000	189.5059460000	405.7982900000
C	250.6663130000	189.3999970000	407.2253080000
H	248.3922330000	190.9324820000	402.2587640000
H	248.0257450000	189.4648590000	401.3732800000
H	252.3950310000	189.3930570000	403.4441300000
H	251.6924910000	187.8122520000	403.1094240000
H	250.5540920000	190.2555830000	402.4426620000
H	251.6192730000	189.3197430000	407.7614190000
H	250.1722150000	190.3112810000	407.5712370000
H	250.5591400000	190.3360940000	405.3162370000
H	247.0858900000	189.8760150000	402.7800520000
H	250.0645750000	188.5600940000	407.5034690000
C	252.9378530000	183.9059790000	405.2635470000
C	254.0004680000	184.9975270000	405.0807530000
C	253.9420330000	185.6533960000	403.7399920000
N	254.8752550000	186.5805870000	403.2935630000
C	252.9299640000	185.6949850000	402.8102360000
C	254.3819860000	187.1214520000	402.1364620000
N	253.2021770000	186.6224870000	401.8292280000
H	253.8511620000	185.7758900000	405.8328480000
H	255.0013660000	184.5741670000	405.2604930000
H	252.0215120000	185.1112740000	402.7924250000
H	254.9393420000	187.8418780000	401.5556740000
H	253.0276420000	183.1952180000	404.4299590000
H	255.8266830000	186.7345120000	403.6221240000
H	253.0726070000	183.3277390000	406.1537030000
H	251.9386620000	184.2827480000	405.1959970000
C	256.1358660000	184.2685110000	410.0932670000
C	254.8627970000	185.0196980000	409.6631750000
C	254.9282180000	185.6057730000	408.2345290000
C	255.8630290000	186.8183250000	408.0516760000
N	255.9537760000	187.3529380000	406.6829880000
C	255.2934850000	188.4481740000	406.2471110000
N	254.1406720000	188.8281600000	406.8689610000
N	255.7846180000	189.1750520000	405.2580480000
H	254.6336210000	185.8168040000	410.3840310000
H	254.0095680000	184.3313990000	409.6926650000
H	253.9186560000	185.9030490000	407.9337460000
H	255.2305770000	184.8156990000	407.5391810000

H	255.5344730000	187.6316290000	408.7082340000
H	256.8848830000	186.5507170000	408.3460360000
H	256.7368800000	187.0812360000	406.0877900000
H	253.4334080000	188.0923630000	406.8979510000
H	253.7479830000	189.6755370000	406.4538900000
H	255.1887640000	189.8940170000	404.8475600000
H	256.6712060000	188.9097580000	404.8260030000
H	256.9583690000	184.9953450000	410.1883750000
H	256.0755190000	183.8111360000	411.0587020000
H	256.4554930000	183.6147070000	409.3088700000
C	258.2849300000	182.3635890000	407.6132630000
C	259.1092420000	183.2957540000	406.6922790000
C	259.2723700000	182.7455670000	405.2642050000
C	259.8239020000	183.8300640000	404.3431540000
O	260.8486530000	184.4405300000	404.6362040000
N	259.1105850000	184.0761880000	403.2093590000
H	258.5773790000	184.2553530000	406.6208690000
H	260.0973530000	183.5290770000	407.1002810000
H	259.9747230000	181.9032480000	405.2605120000
H	258.3115080000	182.3655610000	404.8947700000
H	258.1857640000	183.7027800000	403.0571740000
H	259.3460890000	184.9081180000	402.6827430000
H	258.8614100000	181.4988260000	407.9573980000
H	257.9773220000	182.9532090000	408.4514900000
H	257.4950910000	182.0183080000	406.9793570000
C	266.7507380000	184.8294110000	405.9897060000
C	266.9164000000	184.5275970000	404.4879500000
C	266.4671900000	185.6759990000	403.5590560000
C	265.0260240000	186.1079570000	403.7924280000
O	264.7069350000	186.6488510000	404.8631050000
N	264.1392650000	185.8544980000	402.8111190000
H	266.3714680000	183.6120630000	404.2246640000
H	267.9725030000	184.3290190000	404.2655720000
H	267.0858160000	186.5584370000	403.7579390000
H	266.6294260000	185.3939390000	402.5126090000
H	263.1863660000	186.2297170000	402.9090000000
H	264.4459330000	185.4980640000	401.9197250000
H	265.7109440000	184.6914060000	406.2968720000
H	267.3703190000	184.1798560000	406.5720270000
H	266.9701810000	185.8609910000	406.1702230000
C	265.3832440000	185.7487040000	399.2267180000
C	264.4312750000	186.2206410000	398.1124760000
C	264.8181610000	187.6245780000	397.6021050000
C	264.6154920000	188.7445680000	398.6168640000

O	265.5210490000	189.4834500000	398.9884010000
N	263.3434590000	188.8520870000	399.1314070000
H	263.3893130000	186.2201020000	398.4562730000
H	264.4697620000	185.5263160000	397.2655310000
H	265.8756910000	187.6513560000	397.3251770000
H	264.2505120000	187.8656660000	396.7022320000
H	263.1520590000	189.6841410000	399.6737050000
H	262.5470570000	188.4137190000	398.6838320000
H	265.3490530000	186.4660410000	400.0597340000
H	266.3826300000	185.7928110000	398.8470050000
H	265.1504780000	184.7840630000	399.6269520000
C	264.6901830000	186.5738150000	390.9080180000
C	266.0211440000	186.4578400000	391.6570910000
O	266.9671610000	185.8614880000	391.1225250000
N	266.1040810000	187.0408770000	392.8470770000
C	267.3460400000	187.0189030000	393.6281430000
H	264.0515220000	187.3727040000	391.2942440000
H	264.1469150000	185.6266930000	390.9901040000
H	268.1853960000	186.8791370000	392.9467790000
H	265.2697980000	187.4174730000	393.2821760000
H	267.4425180000	187.9549060000	394.1844390000
H	264.9293500000	186.7388150000	389.8782240000
H	267.2858450000	186.1920680000	394.3046200000
O	254.4633600000	186.5556430000	392.8152820000
O	255.1333920000	187.5253410000	394.9868180000
O	254.5425800000	184.9648010000	394.6867230000
Cl	254.1544360000	186.3404800000	394.2535210000
O	252.6820470000	186.5828370000	394.4844660000

**The intermediate resulted from the O-Cl cleavage of perchlorate optimized using the bigger model**

Mo	255.3953993946	188.1251972035	397.0189293661
P	253.3283951885	192.5575711950	404.5838763763
O	254.3322596766	193.4660670190	403.9334784952
O	253.7100876996	191.3266114629	405.3482778084
O	252.2929827371	191.9670135727	403.3119440172
O	252.8078539705	193.2526993333	401.1465994079
P	251.6910285861	192.9360598990	402.2128950147
O	251.0536279220	194.1758677152	402.7569021902
O	250.6010526516	192.0029889378	401.4519030099
O	252.2202483732	193.3733358679	405.4428501990

C	253.6665999505	192.1968676425	400.5837660475
C	253.4339972079	192.2328878761	399.0793365575
O	253.7452588112	193.5811909414	398.7052795024
C	254.1673441192	191.1730215932	398.2918887393
S	253.8276742706	189.4898909800	398.6411616647
C	254.9450628030	191.5285800371	397.2464334920
S	255.5882813276	190.3749409946	396.1440721535
C	255.2712638874	192.9523203779	396.8975211063
N	256.5246529329	193.3373024728	397.5610209351
C	256.7373336064	194.7207952060	397.7374574615
C	258.0170208175	195.1437078419	398.1734718193
O	259.0030620952	194.4006050545	398.3738689710
N	258.1233794865	196.5214362922	398.3760043440
C	257.1056568977	197.3869502529	398.1140622256
N	257.4025483037	198.7243480189	398.2279090671
N	255.8878791480	196.9924910932	397.8041414817
C	255.7120714848	195.6486387668	397.6213196584
N	254.4551204581	195.2337002667	397.2416044881
C	254.1181517250	193.8470539985	397.3398711384
P	262.2149750911	187.8803057182	394.7169320954
O	262.3571856184	189.4274006866	394.3088655452
O	260.7810381136	187.5332295253	394.0311633312
O	263.3167839002	186.9787177404	394.3269983312
O	261.9457773918	187.7721653278	396.3068362101
C	260.7496401403	188.2314379312	396.9659190711
C	260.1173341547	187.1198521837	397.8192434599
O	260.7172107102	187.1778845978	399.1262777881
C	258.6097987025	187.2869985356	397.9463299867
S	257.6917224871	187.5309711619	396.5046748218
C	257.9499550735	187.1603085844	399.1302165540
S	256.2575330052	187.5087514470	399.2493327101
C	258.6299965096	186.7166971415	400.3941327025
N	258.6411832790	187.7621449853	401.4126421467
C	259.2593597360	187.3822207666	402.5948544708
C	258.7305000789	187.5631043353	403.9007675969
O	257.5785220557	187.9562203789	404.2210347392
N	259.6223487253	187.2474182615	404.9357762750
C	260.7890222991	186.5726827210	404.7473672568
N	261.5290281996	186.2195925332	405.8390375630
N	261.1815102746	186.2168526998	403.5403160267
C	260.4239755054	186.6265038520	402.4887224245
N	260.8889686856	186.2431017366	401.2461742358
C	260.0803390808	186.2917892036	400.0578489314
P	263.7982348253	190.3178199224	394.0545312210

O	263.3847435061	191.6562629105	393.5142454526
O	264.5857018116	190.1517394068	395.3297761063
O	264.4712471241	189.4453706928	392.8526858578
H	253.4219370186	191.2159236926	401.0027948234
H	254.6871765293	192.4587964058	400.8491398406
H	257.3340323000	192.8759190915	397.1434652248
H	259.0756069914	196.8903613072	398.4365313153
H	256.7273173583	199.3184699570	397.7678665744
H	258.3772826401	198.9552594379	398.0539650312
H	253.6896118713	195.8899994194	397.3837421427
H	261.0259155873	189.0594767824	397.6177535615
H	260.0236537106	188.5889120168	396.2381598027
H	260.3437336274	186.1505753124	397.3471697107
H	258.1081088481	185.8111485061	400.7545598018
H	257.8570045420	188.4138347533	401.4840580246
H	261.3442442277	186.7462204868	406.6829795937
H	262.5053520862	185.9891076592	405.6150565687
H	261.6269970904	185.5530959831	401.2637727143
H	260.0426680882	185.2918782848	399.5952745198
H	259.3245560774	187.4843756642	405.8785531975
H	260.1799692041	188.2891997065	393.9462583045
H	250.9068852117	191.6654496833	400.5948956584
H	264.4748952914	189.9865145617	392.0516724144
H	251.8525425467	194.0996810609	404.9122218875
H	252.3505231011	192.0553562901	398.9235282831
H	255.3538737441	193.0592448763	395.8050080411
H	253.2703086117	193.6350258297	396.6823942168
C	253.8150000000	181.3190000000	393.8550000000
C	252.5791329879	180.9303775592	393.0281292638
C	251.2872952951	181.5945617396	393.4748554355
C	251.2856346426	182.9297125089	393.9025982562
C	250.0526270178	180.9377892222	393.4017125992
C	250.1043556722	183.5909703667	394.2154518563
C	248.8534874508	181.5941710925	393.6965878110
C	248.8779209709	182.9342541005	394.0834393710
O	247.6827205084	183.5738137995	394.3212997482
H	252.4525091818	179.8381105718	393.0273370802
H	252.7766756759	181.2143822368	391.9847133767
H	250.0197739855	179.8966027149	393.0811264440
H	252.2098030831	183.4899681877	393.9807434374
H	247.8945791238	181.0912907024	393.6039406387
H	250.1505688142	184.6343004104	394.5126522383
H	247.8256789552	184.5208058800	394.1784797533
H	253.9351088524	182.4041028117	393.8918031331



H	254.7073923500	180.9467449100	393.3967838500
H	253.7456652600	180.9723263200	394.8649059600
C	250.7220000000	189.7720000000	397.2660000000
C	251.7060000000	190.2220000000	396.2070000000
O	251.9298692665	191.4585575831	396.0719980614
C	250.4922929230	188.2628497232	397.5373738907
C	249.3743189659	187.7555861118	396.5900282679
C	250.1591673746	188.0585858190	399.0222088160
C	248.9621103780	186.2891371583	396.7518628097
N	252.1860000000	189.2760000000	395.4020000000
C	253.0110000000	189.6170000000	394.2560000000
C	252.3720000000	189.5290000000	392.8820000000
O	251.1358986317	189.4610284565	392.7432904716
N	253.2200000000	189.6570000000	391.8670000000
C	252.7880000000	189.7520000000	390.4780000000
C	252.6390000000	188.3760000000	389.8630000000
O	253.3131431110	188.0421800094	388.8822793095
N	251.7410000000	187.5940000000	390.4440000000
C	251.5650000000	186.1910000000	390.0800000000
C	251.0693729136	185.3618587544	391.2763216756
C	249.6674306350	185.6868660114	391.6875204349
C	249.2901330827	186.5274704038	392.6993465079
C	248.4549355195	185.1513192813	391.1194380679
N	247.8988739351	186.5081783420	392.8381627552
C	247.3631803514	185.7021632829	391.8411402835
C	248.1981841531	184.2397733408	390.0825335827
C	246.0380846973	185.3845136994	391.5367954352
C	246.8810345620	183.9180982959	389.7729346071
C	245.8122708959	184.4915059670	390.4920723288
H	251.4140827055	187.7135532101	397.3395097050
H	249.2519236949	188.6174824722	399.2990414418
H	250.9949702696	188.3871860052	399.6472569084
H	249.9970259256	187.0052025166	399.2618720562
H	248.4847420399	188.3874426852	396.7494196721
H	249.6914697267	187.9290618919	395.5529646277
H	248.5485477737	186.0872804771	397.7457796811
H	248.1946140689	186.0149905034	396.0181307904
H	249.8041375068	185.6115599206	396.5961579679
H	251.0250868360	190.2793354106	398.1887373919
H	253.3580246690	190.6403578176	394.3996861951
H	253.9023469397	188.9882316449	394.2651854334
H	251.9287593547	188.2904864214	395.4846725901
H	251.8353172120	190.2950672945	390.4478043373
H	254.2306528575	189.5169857689	391.9984371477

H	251.7463303131	185.5218063654	392.1162025194
H	251.1327947759	184.2990756007	391.0088947890
H	249.9206615016	187.1045917546	393.3624646365
H	247.3789816961	187.2041057319	393.3501797466
H	249.0254994364	183.7941793568	389.5360698204
H	246.6686285706	183.2143611765	388.9719235372
H	245.2121044692	185.8108202096	392.1016559956
H	244.7897074334	184.2254525828	390.2338951361
H	252.5584663987	185.8265023109	389.7894292043
H	251.2259868963	187.9528685780	391.2431718797
H	253.5534569774	190.2860021043	389.9132478569
H	250.9368908000	186.0076258400	389.2333874900
H	249.7488626700	190.1330501900	397.0061029300
C	257.4180000000	180.5500000000	392.8130000000
C	257.7583052900	181.6745165622	391.8048797718
C	256.5036105820	182.2232539600	391.1577874638
C	255.7377740871	183.1874086074	391.8283142620
C	256.0329190718	181.7326879349	389.9341743887
C	254.5292720255	183.6442411755	391.3034987284
C	254.8266867439	182.1880058540	389.3984252012
C	254.0709737293	183.1420107075	390.0834788994
H	258.2701923416	182.4824466399	392.3413460514
H	258.4557733922	181.3054017283	391.0416692424
H	256.6175203336	180.9859446847	389.3980909188
H	256.0837007626	183.5824427126	392.7798767330
H	254.4786668138	181.8003072942	388.4428748780
H	253.9650646976	184.3931993629	391.8501642608
H	253.1323686574	183.4993090087	389.6666199919
H	258.2791107944	180.3609039524	393.4689259071
H	256.6123453200	180.8882626800	393.4305750100
H	257.1886380500	179.6229026800	392.3305234100
C	256.5880000000	185.6260000000	388.1370000000
C	256.6573261440	186.8748696699	389.0403755852
C	256.5328259409	186.4802819021	390.5178497770
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H	262.6198608181	188.0849063117	399.0542047625
H	265.3565431340	186.4689490284	400.0599560148
H	266.3824140000	185.7920594000	398.8473548600
H	265.1501260700	184.7833374000	399.6271197500
C	264.6900000000	186.5740000000	390.9080000000
C	266.0210000000	186.4580000000	391.6570000000
O	266.9664674224	185.8537615159	391.1301520182
N	266.1040000000	187.0410000000	392.8470000000
C	267.3460000000	187.0190000000	393.6280000000
H	264.0463961084	187.3694450346	391.2931955511
H	264.1486993680	185.6252281309	390.9885477351
H	268.1849256659	186.8783305300	392.9449559921
H	265.2779639031	187.4562107623	393.2604835234
H	267.4464641743	187.9556170042	394.1839949377
H	264.9291132400	186.7390321500	389.8781994100
H	267.2858396200	186.1921445100	394.3044545300
O	253.6859776606	186.7137963228	392.8177258468
O	255.4053079575	187.7946728443	395.3061663046
O	253.7971263724	184.7664762346	394.3670338486
Cl	253.4814677554	186.2662810913	394.2639941995
O	251.9629807066	186.4825426672	394.6039937543

## The Mo-chlorate complex optimized using the bigger model

Mo	255.3278338966	188.1350285191	397.0515443574
P	253.3435476764	192.4662396389	404.4910672627
O	254.3292105721	193.4727806103	403.9690632636
O	253.7514648850	191.1981066740	405.1774979393
O	252.3900101184	191.9276448191	403.1427369946
O	252.9066774559	193.3102628800	401.0537383504
P	251.7598967747	192.8950721181	402.0548015183
O	251.0190063651	194.0802725304	402.5890798649
O	250.7500510943	191.9193878546	401.2423852763
O	252.1486716527	193.1530915491	405.3543475252
C	253.7714845979	192.2962047454	400.4341047243
C	253.4394310697	192.2609127443	398.9488464617
O	253.6696357876	193.6054043472	398.4951374357
C	254.1689582899	191.1868093788	398.1788402027
S	253.9349092942	189.5066466661	398.6316938382
C	254.9003439722	191.4984609361	397.0879431871
S	255.5987258138	190.2706227707	396.0780070576
C	255.2389272313	192.9175868028	396.7368320881
N	256.4558516761	193.3153606261	397.4653728101
C	256.6730837665	194.7048319660	397.5784191771
C	257.9548560095	195.1437070969	397.9959458736
O	258.9375207118	194.4083411845	398.2359285094
N	258.0649126302	196.5286126724	398.1202267621
C	257.0445958689	197.3840817975	397.8418992551
N	257.3346896404	198.7257284495	397.9330341699
N	255.8282152422	196.9821568084	397.5379766393
C	255.6574782622	195.6326325745	397.3971756109
N	254.4048558847	195.2099832441	396.9941971871
C	254.0717014547	193.8208976839	397.1284495326
P	262.3967838756	187.9520246137	394.5372920400
O	262.4936002939	189.5126596881	394.1696002172
O	261.1106267919	187.5400425198	393.6228212011
O	263.5984990371	187.1275115352	394.2972376240
O	261.8923187962	187.7859709746	396.0566857884
C	260.5576531493	188.1539200185	396.4879768898
C	260.0424232731	187.1811170689	397.5443659328
O	260.6473517028	187.5460228836	398.7981484105
C	258.5365716147	187.2581076025	397.7279665706
S	257.5458888671	187.6897123644	396.3670593236
C	257.9426518646	187.0556245947	398.9326637407
S	256.1929459186	187.2456562705	399.0735942693
C	258.7112799417	186.6372153067	400.1668918155

N	258.2961142330	187.3928891697	401.3492441974
C	259.1660081086	187.3114831002	402.4557466075
C	258.7087137488	187.3787900471	403.8004962924
O	257.5177755389	187.4025962233	404.2275217013
N	259.7258577769	187.4398714843	404.7633497317
C	261.0530766681	187.3353147904	404.4761603797
N	261.9435298785	187.4181397638	405.4918204038
N	261.4854674030	187.1972251131	403.2341901172
C	260.5480436116	187.1961574519	402.2548017170
N	261.0342385321	187.0265456957	400.9900908910
C	260.2545500822	186.6601462038	399.8397178275
P	263.9360938079	190.4301765276	394.0134845133
O	263.5341039353	191.7842915375	393.5029729277
O	264.6552301016	190.2271394250	395.3228191148
O	264.6723676267	189.6066800457	392.8170008327
H	253.6357716825	191.3161272397	400.9023975748
H	254.7903902189	192.6261506908	400.6029483859
H	257.2811700657	192.8398634412	397.0964880898
H	259.0174128725	196.9040701187	398.1888670224
H	256.6740183961	199.3102568369	397.4412841287
H	258.3143359322	198.9610663154	397.8043642520
H	253.6443303913	195.8592690420	397.1881304645
H	260.5999668683	189.1509225784	396.9177151675
H	259.8784969391	188.1517596028	395.6374592674
H	260.3516478447	186.1612570238	397.2652649121
H	258.4677669807	185.5787547163	400.3631337694
H	257.9832867206	188.3557838403	401.1838732243
H	261.5896090820	187.1935674081	406.4112932115
H	262.9055605229	187.1198347293	405.2746014285
H	262.0388435446	187.0675827200	400.8716345930
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H	259.4398118207	187.6425062330	405.7203831587
H	260.6029023110	188.3082322468	393.3243722455
H	251.1922204315	191.3105351987	400.6265498384
H	264.7185296253	190.1810995260	392.0406653862
H	251.7858083115	193.9163062079	404.8765059348
H	252.3554495789	192.0499976452	398.8624833011
H	255.3785241817	193.0208374128	395.6497697834
H	253.2377007109	193.5853876516	396.4602408685
C	253.8150000000	181.3190000000	393.8550000000
C	252.5635933948	180.9619200096	393.0411455483
C	251.2924136426	181.5392567415	393.6346272352
C	251.1883209024	182.9124939455	393.9071696204
C	250.1850407162	180.7357139369	393.9278908511

C	250.0170084678	183.4616336784	394.4232713056
C	248.9991086997	181.2743865084	394.4310701798
C	248.9051576147	182.6457230784	394.6590548898
O	247.7139761836	183.1529328453	395.1236257006
H	252.4651771627	179.8712066598	392.9573858822
H	252.6993286298	181.3411976425	392.0189715138
H	250.2424658789	179.6641162861	393.7420414949
H	252.0351784267	183.5657553153	393.7114693535
H	248.1320356955	180.6507692574	394.6307564533
H	249.9486125264	184.5284168740	394.6156763396
H	247.5568126365	184.0015698219	394.6837448426
H	253.9448728155	182.4055731306	393.9064819374
H	254.7073920000	180.9467450000	393.3967840000
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C	250.7220000000	189.7720000000	397.2660000000
C	251.7060000000	190.2220000000	396.2070000000
O	251.8460855099	191.4536789285	396.0043258419
C	250.5334320536	188.2793908903	397.6265878490
C	249.4880064492	187.6392645514	396.6773338319
C	250.1692513383	188.1582049743	399.1147987371
C	248.9594543960	186.2568851019	397.0843719751
N	252.1860000000	189.2760000000	395.4020000000
C	253.0110000000	189.6170000000	394.2560000000
C	252.3720000000	189.5290000000	392.8820000000
O	251.1337542020	189.4649005166	392.7382464083
N	253.2200000000	189.6570000000	391.8670000000
C	252.7880000000	189.7520000000	390.4780000000
C	252.6390000000	188.3760000000	389.8630000000
O	253.3225173485	188.0320722934	388.8944469139
N	251.7410000000	187.5940000000	390.4440000000
C	251.5650000000	186.1910000000	390.0800000000
C	251.1683527749	185.3603629361	391.3215764107
C	249.8981715310	185.7546619615	392.0276564188
C	249.7700239885	186.7604511115	392.9567451116
C	248.6086729847	185.1154488867	391.9520748070
N	248.4734935754	186.7988334616	393.4434091607
C	247.7372952018	185.7923747880	392.8572446605
C	248.1222455641	183.9996933329	391.2543545765
C	246.4115833211	185.3905234103	393.0596750058
C	246.8105381674	183.5902444251	391.4600565801
C	245.9633524384	184.2790698333	392.3501786687
H	251.4867731752	187.7642036450	397.5118892238
H	249.2508463242	188.7174084921	399.3488036300
H	250.9919492328	188.5329550742	399.7330114857

H	250.0234420331	187.1176926872	399.4140004712
H	248.6271841710	188.3238387199	396.5926444905
H	249.9308716450	187.5850903348	395.6746290845
H	248.3104395051	186.3176487404	397.9642409383
H	248.3772036029	185.7991285902	396.2764391776
H	249.7661780909	185.5621722741	397.3290826731
H	251.0143234639	190.3194898419	398.1709467884
H	253.3475240312	190.6455658069	394.3923828407
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H	254.2416448566	189.5553629758	391.9915333739
H	252.0005305671	185.4471207208	392.0273258201
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H	245.7621750816	185.9185544606	393.7538640261
H	244.9455511258	183.9282892177	392.4996059276
H	252.5550950117	185.8433079035	389.7580291914
H	251.1664289548	187.9879656016	391.1820958367
H	253.5574980297	190.2825925813	389.9161495367
H	250.9368910000	186.0076260000	389.2333870000
H	249.7488630000	190.1330500000	397.0061030000
C	257.4180000000	180.5500000000	392.8130000000
C	257.7617099699	181.6817782123	391.8153783433
C	256.4984823997	182.2301500237	391.1886449033
C	255.7844411609	183.2513711603	391.8303856779
C	255.9581349463	181.6637950605	390.0274019811
C	254.5570163168	183.6875829210	391.3330618694
C	254.7321366524	182.0988747848	389.5229344883
C	254.0255200748	183.1100417834	390.1782215609
H	258.2770473671	182.4837809580	392.3574424802
H	258.4523419864	181.3176725272	391.0437581367
H	256.5042078784	180.8713543828	389.5171046717
H	256.1800196076	183.7091837853	392.7342950673
H	254.3298818525	181.6513144488	388.6161361725
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C	256.6669305720	186.8821193891	389.0303769045
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C	257.9614868232	187.6710864175	388.7873805979
H	255.8178550296	187.5297602479	388.7726076227
H	257.9651785643	188.5954568919	389.3779787793
H	258.8445353126	187.0831482997	389.0754471834
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H	256.5749369367	187.3929668725	391.1493219912
H	257.3081581425	185.8064101174	390.8216038253
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C	257.8290000000	191.8650000000	391.3050000000
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C	256.9458612704	189.7398021317	392.3193107753
O	255.9563188705	189.7100097931	391.5631000593
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H	257.1015509819	191.6865717487	390.5035767777
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C	257.2040000000	182.8230000000	398.2410000000
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O	256.2894022204	183.9253973917	400.1668080560
C	257.0281171353	183.9067693354	397.1660052247
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C	259.4557697147	183.4835163559	396.4142698018
C	257.9710998308	184.6949142450	394.9724658993
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C	259.0189162666	184.9384057892	394.0882221177
C	260.3083883809	184.4685289591	394.3777504250
O	261.3782957814	184.7011576513	393.5611979946
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C	254.2780000000	182.0760000000	400.5800000000
C	253.0560000000	182.8560000000	400.1430000000
O	252.1616594241	183.0761867666	400.9602125268
N	253.0020000000	183.1650000000	398.8590000000
C	251.9230000000	184.0210000000	398.3810000000
C	252.4608408591	184.9475077614	397.2970995874
C	253.1020814240	186.1974454613	397.8744650658

O	253.0034946798	186.5281102049	399.0388032435
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H	256.9334149976	184.8780271809	397.6640126312
H	256.0831131169	183.7562245004	396.6264354706
H	256.9840076711	185.0895910650	394.7535671180
H	259.6617772286	182.9164637532	397.3185650623
H	258.8451576473	185.5194124664	393.1850963792
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H	258.1824608964	182.9380570219	398.7191849287
H	254.6954276770	182.5891091691	401.4498111236
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H	251.6579483162	185.2727737636	396.6241293353
H	253.1819971612	184.4465131409	396.6379996293
H	251.5669161766	184.6062640798	399.2327200633
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H	257.1746610000	181.8511420000	397.7943120000
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C	252.1747265032	192.7119677940	393.0373262289
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H	253.0364822573	193.0493955658	393.6300902835
H	252.5603561249	192.0184068667	392.2877112361
H	251.9920132761	195.1045920329	393.8426232474
H	252.2600649967	193.7359943940	390.3774444215
H	253.4126370000	194.3660190000	391.4773090000
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C	252.9230000000	197.6780000000	399.7280000000
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O	251.9939806400	196.6780766898	397.7257462416
C	252.7978124272	196.4111379927	400.5852917934
O	251.4363686610	196.4001273061	401.0212653392
C	253.7793308675	196.4274906690	401.7581231569
N	251.0510000000	198.6040000000	398.4340000000
C	250.2740000000	198.7450000000	397.2000000000
C	248.8837399353	198.0714680801	397.2995373960
C	248.3531104956	197.4169079235	396.0068774590
C	249.2734445502	196.3534285638	395.3531548515
N	249.9771969060	195.5500149904	396.3499725523
C	250.1926908497	194.2326587709	396.3404122320



N	249.7217242943	193.4423074671	395.3441184905
N	250.8511581061	193.6603590613	397.3577820532
H	253.0106807400	195.5400999472	399.9523679481
H	253.7086983383	195.5074003366	402.3464869195
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H	254.8119436070	196.5119289768	401.3981332561
H	251.2899706129	195.5877057869	401.5371434059
H	253.9189292041	197.7074243258	399.2644069111
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H	250.0120489214	196.8207978504	394.6909860729
H	248.6690081943	195.7011152815	394.7192064794
H	250.6293330587	196.0663230372	396.9578803255
H	250.1008106541	192.4970428287	395.3848905886
H	249.8446826783	193.8744259511	394.4300303959
H	251.3175856632	194.2383699999	398.0490267717
H	251.2756533791	192.7469907469	397.1354323427
H	250.8698610931	198.2624035381	396.4194807432
H	251.0083161381	199.3091697095	399.1538536497
H	252.8225450000	198.5275040000	400.3707690000
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C	260.9410000000	196.2040000000	395.5760000000
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C	260.5508472772	196.3401328073	394.0915610289
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C	259.7622252976	197.6346716266	393.8545704616
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C	262.2440000000	193.0760000000	397.2940000000
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C	262.0631811009	191.8450145689	396.4126294127
C	260.6476975597	191.4693155748	396.2571806298
N	259.7792230229	191.2719701002	397.3090131856
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N	258.6536675954	190.7992626653	395.4483268309
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C	265.9150000000	195.4720000000	393.9890000000
C	265.0111104634	195.2493043497	392.7559420109
O	265.1412790817	193.9465960864	392.2080644030
C	265.3583903986	196.2374486995	391.6452159283
H	263.0009388160	199.4227517276	397.0561355757
H	261.4829075001	196.3659782396	393.5120046665
H	258.8264825960	195.0046397351	394.2499188654
H	259.4584505434	195.1778238655	392.6044406573
H	260.3246007679	194.1824075924	393.7815274991
H	260.3345485325	198.5173078670	394.1621684849
H	258.8231840377	197.6300125917	394.4245306841
H	259.5092838975	197.7475136597	392.7942796074
H	260.0228051371	196.1879205529	396.1681086510
H	262.7288420674	197.2481352307	395.8568128144
H	262.6379701815	191.0065147081	396.8263695037
H	262.4538406351	192.0717911327	395.4197934771
H	260.3016227859	191.2358095672	394.1084179527
H	257.7552978743	190.5647858197	397.3701252414
H	261.9410461536	192.8512263666	398.3222618032
H	260.5498973449	194.3781256675	397.3759594277
H	266.7655197880	191.2391582875	397.6147992974
H	268.0190946762	192.4040873407	397.1052315149
H	266.3178673318	190.8910575295	395.4329810810
H	266.1541299362	193.5816537228	398.0229527164
H	264.4687793179	191.8758640037	396.3862472666
H	263.9733584494	195.4196390091	393.0840135067
H	265.2998490091	197.2743089976	391.9983298233
H	264.6720243266	196.1134594677	390.8015227077
H	266.3765287610	196.0489156345	391.2854140180
H	264.6192837782	193.3108349331	392.7310770981
H	266.9778965839	195.4485606819	393.7262839606
H	264.7768609135	193.8945867455	394.8855615751
H	259.9902778795	191.3975947262	398.3160329384
H	262.0018150000	199.5151590000	398.5165310000
H	263.1589992723	198.1979183243	398.3169720835
H	265.6768690000	196.4273180000	394.4079990000
C	259.4900000000	190.5140000000	408.0810000000
C	258.6590000000	191.0440000000	406.9170000000

O	258.5400436772	190.3892314467	405.8726575877
C	260.4812549566	189.4252635252	407.6491976064
O	259.8843101669	188.1203624347	407.5601549382
N	258.0660000000	192.2110000000	407.1150000000
C	257.1360000000	192.7790000000	406.1320000000
C	257.8810000000	193.5140000000	405.0200000000
O	259.1074852770	193.6947720115	405.1086287647
C	256.2739006863	193.7286325734	406.9867085720
C	257.3044399429	194.2903699664	407.9816469149
C	258.2030269682	193.0772023564	408.3000572919
N	257.1570000000	193.9310000000	403.9930000000
C	257.7580000000	194.5810000000	402.8280000000
C	257.0920859252	194.0970895825	401.5322626598
C	257.2062384245	192.6080633302	401.2982769777
N	256.9678748228	192.0864301346	400.0362920306
C	257.4681545785	191.5024480147	402.0860503337
C	257.0885908734	190.7338120324	400.1114839682
N	257.3941826153	190.3447685870	401.3356574886
H	261.3270474013	189.3935829914	408.3516974172
H	260.8744026714	189.6272027411	406.6513170266
H	259.5499085824	187.8682093715	408.4295665918
H	260.0631625881	191.3300413002	408.5377340711
H	255.4973695912	193.1497319570	407.4999445229
H	255.7789446054	194.4895328124	406.3789179351
H	256.8563589322	194.7176749007	408.8838581430
H	257.9030271983	195.0670787287	407.4940794652
H	257.8629344744	192.5483016944	409.2013018179
H	259.2468565255	193.3747505269	408.4498730259
H	256.5355289617	191.9765056546	405.6931547568
H	256.0332802901	194.3997044577	401.5343383734
H	257.5603621251	194.6241088308	400.6906950255
H	257.7237252678	191.4622186845	403.1351107095
H	256.9085116478	190.0743364565	399.2751860355
H	258.8084016492	194.2908998548	402.8159767056
H	256.1517910358	193.7292216011	403.9617496879
H	256.7402468546	192.6047773126	399.1733916021
H	257.7516640000	195.6461680000	402.9293770000
H	258.8826200000	190.1061770000	408.8618140000
C	262.5170000000	191.6280000000	404.4240000000
C	261.4195273910	190.7912610889	403.7061034990
C	261.0470455038	191.3209405411	402.3514220802
N	260.6955862942	192.6451199179	402.1482918334
C	260.9385035276	190.7400034507	401.1089016096
C	260.3728925993	192.8051221128	400.8309961917

N	260.5205853904	191.6705124308	400.1714469954
H	260.5205148546	190.7306496238	404.3366433022
H	261.7790296144	189.7677349121	403.5655047057
H	261.0886501472	189.7029302378	400.8411465843
H	260.0449062796	193.7377517380	400.3922088245
H	262.8571594626	191.0808959365	405.3134352034
H	260.5726374638	193.3154392428	402.8968267239
H	262.1236480000	192.5623940000	404.7661720000
H	263.3516530000	191.7181200000	403.7605750000
C	247.8970000000	194.0110000000	404.4930000000
C	248.2020000000	195.4880000000	404.7370000000
O	247.4356305146	196.1675465888	405.4263702565
C	246.7935033607	193.8165447900	403.4481702848
O	247.1966848642	194.2729142428	402.1630017715
N	249.3140000000	195.9620000000	404.1770000000
C	249.8020000000	197.3150000000	404.4650000000
H	245.9140494777	194.4083511379	403.7244346764
H	246.4968958120	192.7540295118	403.4246059553
H	248.0534571680	193.8691730634	401.9634260836
H	248.7974205724	193.4925164159	404.1245116857
H	249.0923258967	197.7718077535	405.1563875480
H	249.8752459633	195.3596520079	403.5858354191
H	250.7886165797	197.2671855464	404.9422670409
H	249.8831630000	197.9216560000	403.5873430000
H	247.6469520000	193.5211100000	405.4108150000
C	248.0800000000	189.8890000000	402.3840000000
C	249.0950000000	189.0790000000	403.1730000000
O	248.7615071676	188.1245080397	403.8747114099
N	250.3660000000	189.4520000000	403.0170000000
C	251.5130000000	188.7690000000	403.5980000000
C	251.3880000000	188.5090000000	405.0890000000
O	251.8603146857	187.5023320440	405.6367980724
N	250.8690000000	189.5060000000	405.7980000000
C	250.6660000000	189.4000000000	407.2250000000
H	248.3907836075	190.9347843343	402.2619320434
H	248.0297666682	189.4686746962	401.3704261054
H	252.3942764236	189.3981981616	403.4462918147
H	251.6971049937	187.8148426415	403.1052706190
H	250.5522244809	190.2909872431	402.4906347684
H	251.6166897720	189.3225926796	407.7656487399
H	250.1695077113	190.3104679794	407.5733560965
H	250.5426030167	190.3290153064	405.3135065566
H	247.0858870000	189.8764540000	402.7795790000
H	250.0641850000	188.5601270000	407.5030850000

C	252.9370000000	183.9060000000	405.2630000000
C	253.9953393915	185.0087713497	405.0933771874
C	253.9451163300	185.6811539080	403.7580656003
N	254.8949190468	186.5963920363	403.3270364579
C	252.9414955796	185.7469360384	402.8209183914
C	254.4184786724	187.1585257900	402.1740507276
N	253.2347633189	186.6801851424	401.8513921200
H	253.8351360927	185.7801730474	405.8519549993
H	254.9992499631	184.5894931350	405.2734953399
H	252.0241040503	185.1762434582	402.7895429628
H	254.9929263984	187.8756593102	401.6041643398
H	253.0318651310	183.1989691833	404.4256911562
H	255.8468763997	186.7416259419	403.6635405042
H	253.0716360000	183.3276930000	406.1531320000
H	251.9378550000	184.2828830000	405.1954110000
C	256.1350000000	184.2680000000	410.0930000000
C	254.8553806033	185.0187203736	409.6702820098
C	254.9121653038	185.6245965094	408.2473938196
C	255.8268217625	186.8564973777	408.0781008501
N	255.9042987246	187.4047594035	406.7131835319
C	255.2437036863	188.5027190167	406.2842492684
N	254.0967267902	188.8882884156	406.9146635569
N	255.7290327041	189.2213052226	405.2853160842
H	254.6216330954	185.8060271938	410.4020179474
H	254.0054771042	184.3247639495	409.6929910682
H	253.8972402028	185.9110016703	407.9507294731
H	255.2281527555	184.8482572978	407.5415647099
H	255.4862851969	187.6600017494	408.7418298118
H	256.8549426130	186.6040879895	408.3687164818
H	256.6726672505	187.1253918342	406.1010023229
H	253.3904284308	188.1508993493	406.9478890328
H	253.7061992708	189.7388351398	406.5029995073
H	255.1351289671	189.9468937590	404.8824542720
H	256.6079781486	188.9443939717	404.8433410681
H	256.9567099738	184.9973173875	410.1879359463
H	256.0745740000	183.8105880000	411.0584130000
H	256.4546020000	183.6142020000	409.3085880000
C	258.2840000000	182.3630000000	407.6130000000
C	259.1096293005	183.2921987907	406.6870560592
C	259.2682166878	182.7344988326	405.2590449042
C	259.8065810452	183.8256062530	404.3353402587
O	260.8323489033	184.4400927356	404.6184289591
N	259.0746392345	184.0778082666	403.2148784587
H	258.5808572065	184.2542318481	406.6128407580

H	260.1009027512	183.5243377136	407.0906275627
H	259.9755884814	181.8954008012	405.2540513095
H	258.3066143782	182.3490906233	404.8942221392
H	258.1532235466	183.6939261443	403.0641065184
H	259.3001988323	184.9138807516	402.6888923521
H	258.8592512696	181.4965761055	407.9580470764
H	257.9764080000	182.9526100000	408.4512410000
H	257.4941570000	182.0178150000	406.9790470000
C	266.7500000000	184.8280000000	405.9900000000
C	266.9001875939	184.5479974432	404.4817004945
C	266.4174775764	185.7113903933	403.5857507581
C	264.9645794501	186.1065344424	403.8346952915
O	264.6231634275	186.5853577585	404.9284147153
N	264.0917555582	185.8975186927	402.8299803704
H	266.3637684371	183.6299097564	404.2068881230
H	267.9564518199	184.3705984585	404.2393833242
H	267.0183670876	186.6030707162	403.8027126243
H	266.5793156615	185.4612021407	402.5302704752
H	263.1309758081	186.2495461706	402.9410626553
H	264.4089794759	185.5841268102	401.9252196840
H	265.7114548768	184.6909610663	406.3035068529
H	267.3694890000	184.1783430000	406.5723060000
H	266.9695250000	185.8595460000	406.1706120000
C	265.3830000000	185.7480000000	399.2270000000
C	264.4432234788	186.2104994924	398.0930859064
C	264.8541069539	187.6007320199	397.5558814541
C	264.6230370190	188.7576434566	398.5261880931
O	265.5167189575	189.5105769344	398.9010784052
N	263.3347395642	188.8863325209	398.9856785060
H	263.3964413576	186.2272269043	398.4247728153
H	264.4848677360	185.4981162160	397.2602560740
H	265.9203955044	187.6138911876	397.3087559397
H	264.3153968390	187.8159412485	396.6318279161
H	263.1220572000	189.7207664897	399.5164072680
H	262.5546802817	188.3947791027	398.5670682980
H	265.3426477412	186.4730018130	400.0544393488
H	266.3824140000	185.7920590000	398.8473550000
H	265.1501260000	184.7833370000	399.6271200000
C	264.6900000000	186.5740000000	390.9080000000
C	266.0210000000	186.4580000000	391.6570000000
O	266.9661311045	185.8584337608	391.1227612069
N	266.1040000000	187.0410000000	392.8470000000
C	267.3460000000	187.0190000000	393.6280000000
H	264.0510522500	187.3746603424	391.2913326616

H	264.1458942140	185.6266796446	390.9893510852
H	268.1859766895	186.8796061215	392.9459567354
H	265.2703876944	187.4185107360	393.2832713776
H	267.4446587913	187.9554945615	394.1844293371
H	264.9291130000	186.7390320000	389.8781990000
H	267.2858400000	186.1921450000	394.3044550000
O	253.9780346699	186.6675604659	392.9438138891
O	255.1533876990	187.4622201972	394.9670406283
O	254.6826034628	184.9449291301	394.6331302771
Cl	254.0610250083	186.3164659590	394.4230783310

## The TS for the O-Cl cleavage of chlorate optimized using the bigger model

Mo	255.2937440000	188.1294480000	397.0070700000
P	253.3062710000	192.3555910000	404.4788230000
O	254.2422140000	193.4300780000	404.0120700000
O	253.7587060000	191.0867450000	405.1340410000
O	252.4231590000	191.8184010000	403.0809650000
O	252.9036120000	193.2826530000	401.0329040000
P	251.7761110000	192.8254520000	402.0390870000
O	251.0494600000	193.9850400000	402.6409590000
O	250.7548580000	191.8851220000	401.1997000000
O	252.0525960000	192.9487190000	405.3316610000
C	253.7835340000	192.2952800000	400.3967120000
C	253.4381120000	192.2518310000	398.9170090000
O	253.6464330000	193.5952430000	398.4565010000
C	254.1702530000	191.1788510000	398.1457210000
S	253.9331530000	189.5026180000	398.6107610000
C	254.8960580000	191.4906180000	397.0523520000
S	255.5900200000	190.2636450000	396.0346400000
C	255.2161360000	192.9141740000	396.7016630000
N	256.4292890000	193.3194790000	397.4300680000
C	256.6367430000	194.7088320000	397.5395000000
C	257.9112870000	195.1555560000	397.9686790000
O	258.8917280000	194.4229750000	398.2217040000
N	258.0160630000	196.5411240000	398.0864460000
C	256.9845810000	197.3882590000	397.8294610000
N	257.2573190000	198.7305200000	397.9564350000
N	255.7729810000	196.9788140000	397.5175790000
C	255.6150760000	195.6285370000	397.3602850000
N	254.3676030000	195.1993900000	396.9506780000

C	254.0422040000	193.8093450000	397.0914450000
P	262.3620040000	187.9930540000	394.5170060000
O	262.4724890000	189.5535410000	394.1518100000
O	261.0805020000	187.5805610000	393.5957780000
O	263.5542410000	187.1547470000	394.2843650000
O	261.8535240000	187.8341440000	396.0348750000
C	260.5105780000	188.1765540000	396.4541110000
C	260.0050390000	187.1961790000	397.5040080000
O	260.6155880000	187.5569090000	398.7539170000
C	258.5011360000	187.2677260000	397.6956420000
S	257.5110410000	187.6703870000	396.3286830000
C	257.9174750000	187.0719200000	398.9056030000
S	256.1691660000	187.2553190000	399.0524840000
C	258.7007720000	186.6426670000	400.1326070000
N	258.3075440000	187.3863470000	401.3289640000
C	259.1975750000	187.3073630000	402.4167280000
C	258.7618700000	187.3840200000	403.7679860000
O	257.5807250000	187.4200370000	404.2119300000
N	259.7910900000	187.4482920000	404.7115700000
C	261.1123820000	187.3376830000	404.4091630000
N	262.0090610000	187.4323930000	405.4195530000
N	261.5316420000	187.1927720000	403.1617910000
C	260.5759430000	187.1860700000	402.1959290000
N	261.0411320000	187.0059950000	400.9263740000
C	260.2371550000	186.6581660000	399.7885120000
P	263.9321590000	190.4456420000	393.9981260000
O	263.5364440000	191.8099130000	393.5110950000
O	264.6621410000	190.2102230000	395.2958490000
O	264.6576130000	189.6306200000	392.7882440000
H	253.6798990000	191.3127840000	400.8649910000
H	254.7950290000	192.6496650000	400.5535650000
H	257.2550690000	192.8505800000	397.0565160000
H	258.9656220000	196.9225230000	398.1615270000
H	256.5936600000	199.3207720000	397.4770540000
H	258.2327260000	198.9857270000	397.8426870000
H	253.6059030000	195.8437330000	397.1513110000
H	260.5292290000	189.1728300000	396.8828780000
H	259.8387060000	188.1630960000	395.5996870000
H	260.3170090000	186.1787390000	397.2162350000
H	258.4518270000	185.5852840000	400.3211770000
H	257.9680270000	188.3405540000	401.1832100000
H	261.6771230000	187.2093740000	406.3472480000
H	262.9739570000	187.1483300000	405.2025050000
H	262.0403190000	187.0729030000	400.7782150000



H	260.5019050000	185.6415250000	399.4410100000
H	259.5125970000	187.6496940000	405.6707200000
H	260.5431350000	188.3403320000	393.3288110000
H	251.1913610000	191.2516690000	400.6048770000
H	264.6678240000	190.1977880000	392.0052710000
H	251.6835900000	193.7228630000	404.8751200000
H	252.3567250000	192.0293480000	398.8450240000
H	255.3550830000	193.0192820000	395.6154040000
H	253.2084790000	193.5658340000	396.4250460000
C	253.8150000000	181.3190000000	393.8550000000
C	252.5509510000	180.9780500000	393.0556580000
C	251.2937540000	181.5629680000	393.6681230000
C	251.1910170000	182.9390950000	393.9237400000
C	250.1932620000	180.7589190000	393.9910800000
C	250.0286100000	183.4918570000	394.4558490000
C	249.0166450000	181.3008020000	394.5111730000
C	248.9241780000	182.6761440000	394.7259380000
O	247.7427730000	183.1886210000	395.2079520000
H	252.4399730000	179.8899460000	392.9670440000
H	252.6763320000	181.3610780000	392.0345070000
H	250.2499140000	179.6867650000	393.8143890000
H	252.0299710000	183.5915950000	393.7004510000
H	248.1543400000	180.6791220000	394.7309310000
H	249.9629210000	184.5604840000	394.6322380000
H	247.5805780000	184.0269340000	394.7533650000
H	253.9491600000	182.4024890000	393.9072610000
H	254.7073920000	180.9467450000	393.3967840000
H	253.7456650000	180.9723260000	394.8649060000
C	250.7220000000	189.7720000000	397.2660000000
C	251.7060000000	190.2220000000	396.2070000000
O	251.8433070000	191.4527730000	396.0035430000
C	250.5315130000	188.2866230000	397.6393930000
C	249.4874210000	187.6385240000	396.6981810000
C	250.1705410000	188.1805550000	399.1285230000
C	248.9772620000	186.2533310000	397.1091310000
N	252.1860000000	189.2760000000	395.4020000000
C	253.0110000000	189.6170000000	394.2560000000
C	252.3720000000	189.5290000000	392.8820000000
O	251.1354750000	189.4611570000	392.7335590000
N	253.2200000000	189.6570000000	391.8670000000
C	252.7880000000	189.7520000000	390.4780000000
C	252.6390000000	188.3760000000	389.8630000000
O	253.3248730000	188.0306510000	388.8962370000
N	251.7410000000	187.5940000000	390.4440000000

C	251.5650000000	186.1910000000	390.0800000000
C	251.1707360000	185.3711240000	391.3253670000
C	249.8954980000	185.7557310000	392.0253600000
C	249.7438060000	186.7675240000	392.9450680000
C	248.6229050000	185.0809780000	391.9570650000
N	248.4506050000	186.7675540000	393.4416870000
C	247.7379640000	185.7424050000	392.8599240000
C	248.1595900000	183.9486930000	391.2694500000
C	246.4220390000	185.3110020000	393.0713100000
C	246.8571930000	183.5103810000	391.4818990000
C	245.9957010000	184.1854230000	392.3701880000
H	251.4832830000	187.7691030000	397.5298410000
H	249.2532250000	188.7414380000	399.3580860000
H	250.9960190000	188.5616090000	399.7376820000
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H	248.6211310000	188.3149140000	396.6169550000
H	249.9243800000	187.5876360000	395.6932040000
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H	249.7992410000	185.5802270000	397.3555650000
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N	264.1106900000	185.8293020000	402.8049290000
H	266.3643890000	183.6031160000	404.2339110000
H	267.9609550000	184.3307410000	404.2592980000
H	267.0510490000	186.5531370000	403.7481660000
H	266.6039100000	185.3772180000	402.5108530000
H	263.1537420000	186.1984270000	402.8989170000
H	264.4226660000	185.4797340000	401.9127070000
H	265.7112000000	184.6911190000	406.3028320000
H	267.3694890000	184.1783430000	406.5723060000
H	266.9695250000	185.8595460000	406.1706120000
C	265.3830000000	185.7480000000	399.2270000000
C	264.4295640000	186.2151670000	398.1123850000
C	264.8063150000	187.6221720000	397.6038480000
C	264.5707590000	188.7452830000	398.6072900000
O	265.4582270000	189.5054820000	398.9802360000
N	263.2929750000	188.8309530000	399.1126430000
H	263.3871170000	186.2058340000	398.4543260000

H	264.4749420000	185.5220950000	397.2647670000
H	265.8678580000	187.6625270000	397.3441920000
H	264.2523520000	187.8505560000	396.6921920000
H	263.0862730000	189.6687420000	399.6407410000
H	262.5059030000	188.3970010000	398.6438880000
H	265.3502320000	186.4639810000	400.0604840000
H	266.3824140000	185.7920590000	398.8473550000
H	265.1501260000	184.7833370000	399.6271200000
C	264.6900000000	186.5740000000	390.9080000000
C	266.0210000000	186.4580000000	391.6570000000
O	266.9664090000	185.8613630000	391.1221500000
N	266.1040000000	187.0410000000	392.8470000000
C	267.3460000000	187.0190000000	393.6280000000
H	264.0513870000	187.3733240000	391.2937570000
H	264.1470450000	185.6268150000	390.9897140000
H	268.1854470000	186.8786640000	392.9466540000
H	265.2721690000	187.4188260000	393.2858590000
H	267.4423330000	187.9543030000	394.1844880000
H	264.9291130000	186.7390320000	389.8781990000
H	267.2858400000	186.1921450000	394.3044550000
O	253.9936460000	186.6059390000	392.9321250000
O	255.1186120000	187.5206390000	394.9883180000
O	254.6572100000	184.9321170000	394.6923290000
Cl	254.0127500000	186.2827650000	394.4184390000

**The intermediate resulted from the O-Cl cleavage of chlorate  
optimized using the bigger model**

Mo	255.3273912696	188.1493704448	396.9647251504
P	253.3459730212	192.5020703414	404.5027221867
O	254.3309246364	193.4811700622	403.9307945094
O	253.7531354235	191.2394139468	405.1989257614
O	252.3427353291	191.9552817512	403.1914610027
O	252.8633523285	193.3163736043	401.0915573115
P	251.7158062154	192.9183062002	402.0983907706
O	250.9878445442	194.1139526332	402.6243728996
O	250.6956665832	191.9485996132	401.2924489951
O	252.1939309702	193.2319919999	405.3860092501
C	253.7199449280	192.2920518181	400.4844467433
C	253.4165384882	192.2868164737	398.9924297390
O	253.6832832908	193.6329404241	398.5703600651
C	254.1490492769	191.2141468038	398.2226787329

S	253.8229837330	189.5406004942	398.6191192476
C	254.9259034593	191.5454285890	397.1691755096
S	255.5929743775	190.3843300724	396.0854630125
C	255.2608016870	192.9639307371	396.8167598558
N	256.4868302781	193.3516333826	397.5249234236
C	256.7043037516	194.7387758359	397.6551495297
C	257.9850350733	195.1692087716	398.0770951536
O	258.9663374778	194.4263748313	398.2986198302
N	258.0956965722	196.5508122675	398.2295833579
C	257.0801098231	197.4118552885	397.9488483245
N	257.3758121863	198.7513507950	398.0403776062
N	255.8628697594	197.0151697940	397.6398882580
C	255.6878065190	195.6679151625	397.4889745726
N	254.4347476537	195.2503141150	397.0895720564
C	254.0947487990	193.8646112742	397.2101931921
P	262.3706501875	187.9483707978	394.5168341054
O	262.4790047093	189.5124975139	394.1653087196
O	261.0498468528	187.5771222344	393.6353979972
O	263.5615079093	187.1173614115	394.2493235647
O	261.8952934087	187.7612356252	396.0452099907
C	260.5852329628	188.1564246109	396.5150768962
C	260.0664394370	187.1734307936	397.5629258845
O	260.6651945131	187.5285241624	398.8199490630
C	258.5590069840	187.2583908880	397.7393882194
S	257.5753743308	187.5333767757	396.3497475418
C	257.9613396791	187.0913684631	398.9525087650
S	256.2524908415	187.3908628855	399.1257799251
C	258.7178641723	186.6507612051	400.1859379883
N	258.3056675684	187.4050140139	401.3686881797
C	259.1677941662	187.3021987976	402.4800557848
C	258.7045923295	187.3640697412	403.8234710683
O	257.5133171744	187.3974861808	404.2464725987
N	259.7186618127	187.4064413889	404.7898498769
C	261.0468437819	187.3051451695	404.5044146280
N	261.9342649001	187.3786870873	405.5208986177
N	261.4828484487	187.1765706206	403.2619903487
C	260.5489383442	187.1809033944	402.2816339757
N	261.0379678177	187.0137684981	401.0161381742
C	260.2617338545	186.6477129858	399.8640677406
P	263.9290960476	190.4245199602	394.0303049797
O	263.5372091448	191.7830295011	393.5242586824
O	264.6299452800	190.2101717634	395.3481348875
O	264.6754967713	189.6043655754	392.8391474695
H	253.5511195334	191.3081329558	400.9344746596

H	254.7430225474	192.5948020032	400.6804719856
H	257.3081390228	192.8756145674	397.1479213313
H	259.0493416695	196.9220704679	398.2899924501
H	256.7115429768	199.3375688365	397.5552508505
H	258.3546698679	198.9814046741	397.8944400200
H	253.6727461864	195.9052329339	397.2550232668
H	260.6675437509	189.1396862441	396.9709960432
H	259.8891204356	188.2006006465	395.6794063848
H	260.3698520382	186.1547493717	397.2744341505
H	258.4458276930	185.5962881555	400.3653848113
H	258.0092493662	188.3744846407	401.2088561475
H	261.5782205086	187.1657896110	406.4421064887
H	262.8983019891	187.0862694336	405.3036818916
H	262.0430705017	187.0459494349	400.9018039700
H	260.5284587586	185.6237643812	399.5384190277
H	259.4311094960	187.6070690529	405.7468606651
H	260.6157358285	188.3643998168	393.2769173575
H	251.1255121967	191.3556727585	400.6531777360
H	264.7450044099	190.1843317789	392.0686354929
H	251.8409262974	194.0004330016	404.9093185016
H	252.3329695014	192.0895302930	398.8799049862
H	255.3839504147	193.0631210911	395.7271173200
H	253.2657751193	193.6346759097	396.5339121835
C	253.8150000000	181.3190000000	393.8550000000
C	252.5638720701	180.9617139077	393.0410709039
C	251.2928701996	181.5507229717	393.6249962770
C	251.2139039128	182.9204571643	393.9276522603
C	250.1622661257	180.7643909400	393.8715898643
C	250.0392708663	183.4815677727	394.4229486319
C	248.9749633065	181.3173394144	394.3571267093
C	248.9040242183	182.6853606320	394.6102830723
O	247.7096218995	183.2116155920	395.0533004462
H	252.4574592622	179.8710295738	392.9593259747
H	252.7037932855	181.3375440209	392.0178596599
H	250.2021816333	179.6960491081	393.6622874492
H	252.0832568659	183.5567054107	393.7814475016
H	248.0897802243	180.7084112194	394.5204563635
H	249.9895073901	184.5455416338	394.6361997615
H	247.5616518350	184.0483086597	394.5879450036
H	253.9428532183	182.4057378035	393.9089519727
H	254.7073920000	180.9467450000	393.3967840000
H	253.7456650000	180.9723260000	394.8649060000
C	250.7220000000	189.7720000000	397.2660000000
C	251.7060000000	190.2220000000	396.2070000000

O	251.8665345477	191.4546521394	396.0177645737
C	250.5357542974	188.2739811753	397.6160691758
C	249.4912939491	187.6380739919	396.6608154954
C	250.1658845456	188.1411016866	399.1020294685
C	248.9559757605	186.2556836504	397.0591609120
N	252.1860000000	189.2760000000	395.4020000000
C	253.0110000000	189.6170000000	394.2560000000
C	252.3720000000	189.5290000000	392.8820000000
O	251.1328415466	189.4859549923	392.7417293868
N	253.2200000000	189.6570000000	391.8670000000
C	252.7880000000	189.7520000000	390.4780000000
C	252.6390000000	188.3760000000	389.8630000000
O	253.3168685885	188.0387405289	388.8869188460
N	251.7410000000	187.5940000000	390.4440000000
C	251.5650000000	186.1910000000	390.0800000000
C	251.1417284756	185.3539726404	391.3097424794
C	249.8721816842	185.7677408362	392.0057500129
C	249.7551226740	186.7776561873	392.9311386373
C	248.5705965530	185.1537993451	391.9224837858
N	248.4542723464	186.8441868708	393.4074092139
C	247.7039260618	185.8503912608	392.8178260212
C	248.0664779881	184.0466283861	391.2238677901
C	246.3685901781	185.4754928607	393.0083634894
C	246.7457334793	183.6626216391	391.4190460018
C	245.9042095065	184.3704291066	392.2992838712
H	251.4915341969	187.7600306554	397.4962039860
H	249.2389701573	188.6872766814	399.3320879859
H	250.9768553460	188.5256667915	399.7297580418
H	250.0274233227	187.0975027394	399.3946696999
H	248.6331956171	188.3259145967	396.5786842065
H	249.9327193304	187.5862188681	395.6575535452
H	248.3119885570	186.3130271119	397.9430763455
H	248.3669466667	185.8096604023	396.2500947579
H	249.7583892007	185.5514834310	397.2909920131
H	251.0128232732	190.3149199371	398.1730365931
H	253.3661278913	190.6375243229	394.3969156607
H	253.8878245133	188.9684073611	394.2603415487
H	252.1802404036	188.3144600541	395.7180244608
H	251.8375510183	190.2989284179	390.4448489098
H	254.2333828559	189.5159542629	391.9922027564
H	251.9675742139	185.4214305377	392.0223280934
H	251.0620227999	184.3040019999	391.0025867118
H	250.4909973524	187.4862619048	393.2793861176
H	248.1273770071	187.5081296092	394.0905258942

H	248.7139768335	183.4835181671	390.5583484069
H	246.3565164023	182.7920310591	390.8972438492
H	245.7242199656	186.0171883010	393.6969261117
H	244.8787168393	184.0394240880	392.4416847215
H	252.5560636358	185.8366550664	389.7698354648
H	251.1953126691	187.9741102866	391.2093118465
H	253.5564711559	190.2834939920	389.9152765898
H	250.9368910000	186.0076260000	389.2333870000
H	249.7488630000	190.1330500000	397.0061030000
C	257.4180000000	180.5500000000	392.8130000000
C	257.7539374745	181.6820163373	391.8126552678
C	256.4905495135	182.2292477928	391.1826376068
C	255.7687524732	183.2453791011	391.8236273593
C	255.9615699217	181.6698417370	390.0125688765
C	254.5496378732	183.6912751863	391.3143672753
C	254.7417182181	182.1104680572	389.4978402537
C	254.0319180523	183.1223326401	390.1493949602
H	258.2670418344	182.4862961645	392.3533878467
H	258.4460925231	181.3197192022	391.0411617056
H	256.5112108380	180.8785574969	389.5038272458
H	256.1428840362	183.6915460152	392.7412732336
H	254.3467707463	181.6665666150	388.5858047688
H	254.0263264562	184.4877718183	391.8330664416
H	253.0830402765	183.4703994274	389.7478651689
H	258.2789607383	180.3592391997	393.4687119089
H	256.6123450000	180.8882630000	393.4305750000
H	257.1886380000	179.6229030000	392.3305230000
C	256.5880000000	185.6260000000	388.1370000000
C	256.6761829415	186.8799446224	389.0333854327
C	256.5677814728	186.4999591913	390.5156731983
C	257.9622375066	187.6752300616	388.7644082291
H	255.8189119483	187.5248538250	388.7965418117
H	257.9757315929	188.5992786026	389.3558706622
H	258.8538215675	187.0901715446	389.0320894272
H	258.0552333640	187.9546977548	387.7061506037
H	256.6581394835	187.3778841864	391.1580125889
H	257.3504610777	185.7798570794	390.7966535151
H	255.6026860802	186.0414295647	390.7406024036
H	255.6156118036	185.1441018016	388.3148558532
H	256.5957310000	185.9043160000	387.1038590000
H	257.3113660000	184.8932020000	388.4279430000
C	257.8290000000	191.8650000000	391.3050000000
C	258.1993542650	190.5259999275	391.9308770576
C	256.9548578185	189.7399649336	392.3196082453

O	255.9748523176	189.7018126201	391.5565673762
N	257.0430182706	189.0621717302	393.4739529629
H	258.8518931990	190.6571577066	392.7961656732
H	258.7388227530	189.9072971486	391.1997191376
H	257.6618005419	189.4166731681	394.2077179264
H	256.2584373164	188.4861329904	393.7708507857
H	257.1018913443	191.6808625886	390.5051658791
H	258.6802010000	192.3357680000	390.8592030000
H	257.3472600000	192.5084820000	392.0112270000
C	257.2040000000	182.8230000000	398.2410000000
C	256.2080000000	182.9730000000	399.3890000000
O	256.2815390090	183.9339700334	400.1581120872
C	256.9858270833	183.8994151308	397.1654345768
C	258.0917872555	183.9798924753	396.1278088340
C	259.3997001290	183.5367417429	396.3616305793
C	257.8303396320	184.6435966549	394.9175191345
C	260.4305435492	183.7882607653	395.4537343322
C	258.8526507076	184.9095168491	394.0080509811
C	260.1664688836	184.5022474796	394.2847895994
O	261.2125140289	184.7539993111	393.4409517668
N	255.2930000000	182.0110000000	399.5380000000
C	254.2780000000	182.0760000000	400.5800000000
C	253.0560000000	182.8560000000	400.1430000000
O	252.1684938211	183.0865698710	400.9651373238
N	253.0020000000	183.1650000000	398.8590000000
C	251.9230000000	184.0210000000	398.3810000000
C	252.4774342191	184.9847411576	397.3451683735
C	253.1740945732	186.1679554980	397.9955486438
O	253.1552026914	186.4218955974	399.1800021275
O	253.7431543707	186.9180389358	397.0625427751
H	256.9026017454	184.8709754054	397.6665735166
H	256.0241420391	183.7424568920	396.6576712408
H	256.8153630216	184.9787586292	394.7063677914
H	259.6452874724	183.0037487210	397.2769352370
H	258.6375726251	185.4530132117	393.0904002703
H	261.4507491518	183.4698921904	395.6497286334
H	261.0795636704	185.6247317330	393.0374730356
H	258.1865180956	182.9523324468	398.7060755466
H	254.6940178904	182.5904243111	401.4496874891
H	253.9709827561	181.0669383344	400.8704935877
H	255.2932680752	181.2266066392	398.9021636244
H	251.6831505211	185.3787727220	396.7014283726
H	253.1738024435	184.5003606953	396.6479001230
H	251.5550004673	184.5771483886	399.2479317939



H	253.8037017445	183.0197594471	398.2660327620
H	257.1746610000	181.8511420000	397.7943120000
H	251.0853860000	183.5187120000	397.9439530000
C	252.3740000000	194.4250000000	391.2270000000
C	251.4955866777	193.8964736925	392.3562881291
O	251.1711154948	194.9327200708	393.3200768018
C	252.1557871697	192.7024935199	393.0295533444
H	250.5169223157	193.6133700998	391.9486386893
H	251.4882003921	192.1331159649	393.6728322448
H	253.0036051180	193.0373408417	393.6434788689
H	252.5594111824	192.0164742864	392.2823543546
H	251.9722604111	195.0957532192	393.8389892912
H	252.2641750554	193.7387169149	390.3745964791
H	253.4126370000	194.3660190000	391.4773090000
H	252.0451240000	195.3825470000	390.8808150000
C	252.9230000000	197.6780000000	399.7280000000
C	251.9290000000	197.6090000000	398.5540000000
O	251.9968458324	196.6791431393	397.7241513971
C	252.7876494171	196.4157657501	400.5909944168
O	251.4249329841	196.4171768621	401.0240271612
C	253.7662297409	196.4313478328	401.7659443066
N	251.0510000000	198.6040000000	398.4340000000
C	250.2740000000	198.7450000000	397.2000000000
C	248.8862484297	198.0660931648	397.2970115063
C	248.3569377620	197.4146849951	396.0020325604
C	249.2794483778	196.3566537584	395.3427056904
N	249.9842010046	195.5469038080	396.3341720192
C	250.1911013989	194.2279421288	396.3240208128
N	249.7109164689	193.4396668190	395.3312786653
N	250.8521358621	193.6525539412	397.3386698231
H	252.9951712692	195.5397559039	399.9639738663
H	253.6921276776	195.5124379362	402.3553996974
H	253.5576374575	197.2837284752	402.4251343982
H	254.7998667209	196.5123158853	401.4079007821
H	251.2713324517	195.6114218310	401.5475922534
H	253.9207524391	197.7041622267	399.2685000859
H	248.9598233168	197.2899694739	398.0666903171
H	248.1405331283	198.7813682710	397.6637696381
H	247.3985028771	196.9426697596	396.2487913781
H	248.1420056112	198.1786230850	395.2430945820
H	250.0185478667	196.8292680767	394.6848418850
H	248.6773462852	195.7082026166	394.7028556248
H	250.6369837862	196.0598572738	396.9435481875
H	250.0790527337	192.4906404538	395.3712661652

H	249.8315489706	193.8685472546	394.4151482731
H	251.3110595455	194.2313951091	398.0338636322
H	251.2765708468	192.7371819161	397.1131780993
H	250.8717360359	198.2642303224	396.4197089066
H	251.0031464743	199.3050789640	399.1575345262
H	252.8225450000	198.5275040000	400.3707690000
H	250.2454670000	199.7826420000	396.9404150000
C	262.4400000000	198.8490000000	397.8030000000
C	261.3740000000	197.9840000000	397.1570000000
O	260.2183477020	197.9918090944	397.6199981183
N	261.7390000000	197.3100000000	396.0760000000
C	260.9410000000	196.2040000000	395.5760000000
C	261.7590000000	194.9410000000	395.8170000000
O	262.7421308455	194.7393334116	395.0931707660
C	260.5568384793	196.3410382934	394.0896929010
C	259.7633498551	195.1005775060	393.6467674626
C	259.7624823553	197.6317366687	393.8517653784
N	261.4030000000	194.1810000000	396.8510000000
C	262.2440000000	193.0760000000	397.2940000000
C	263.7130000000	193.5310000000	397.3750000000
O	263.9541675188	194.5960824205	397.9602980664
C	262.0522372641	191.8430617485	396.4201908800
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