

Supplementary information for

Atmospheric Oxidation of Folpet Initiated by OH Radicals, NO₃ Radicals, and O₃

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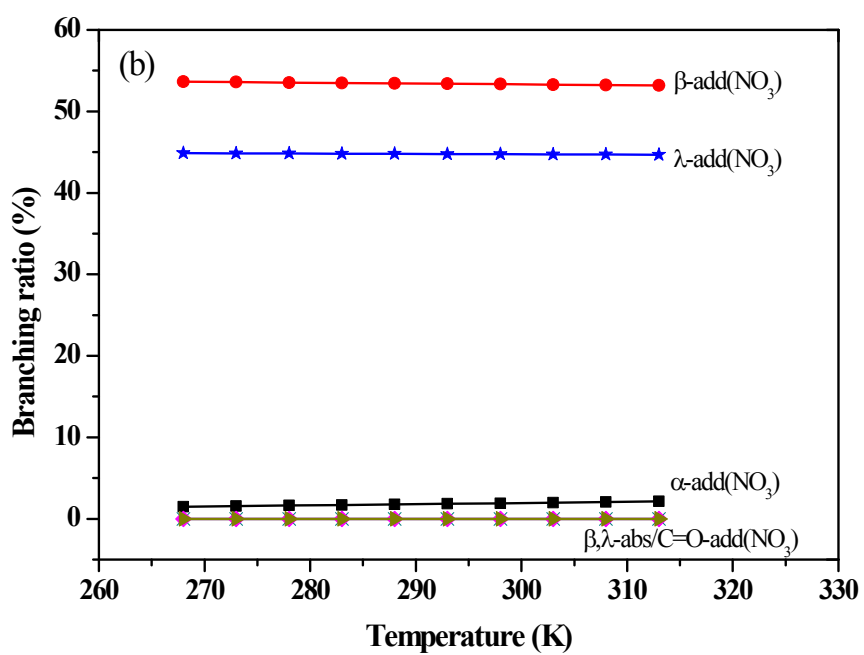


Fig. S1. The branching ratios of the reaction of Folpet with NO_3 radical at 268-313 K using the TST theory.

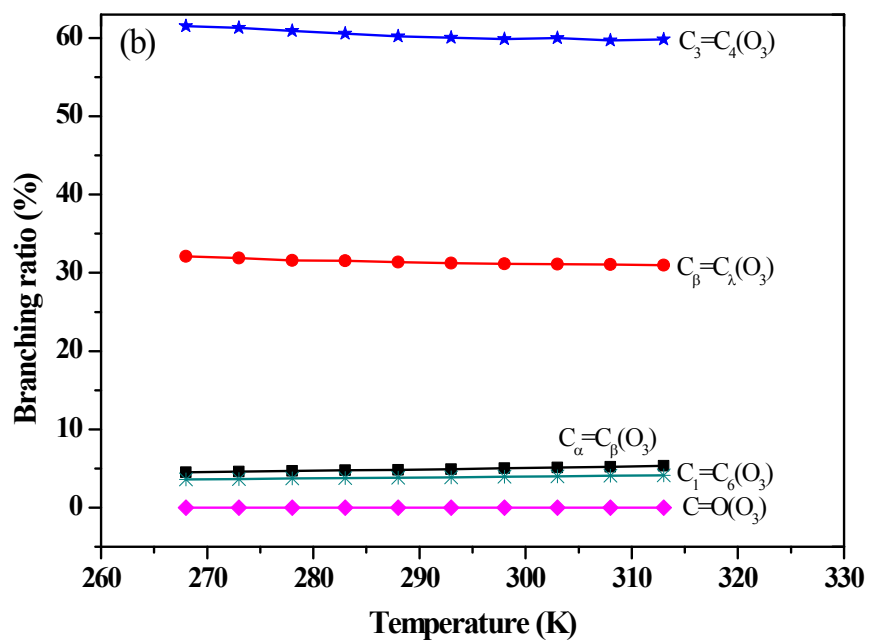


Fig. S2. The branching ratios of the reaction of Folpet with O_3 radical at 268-313 K using the TST theory.

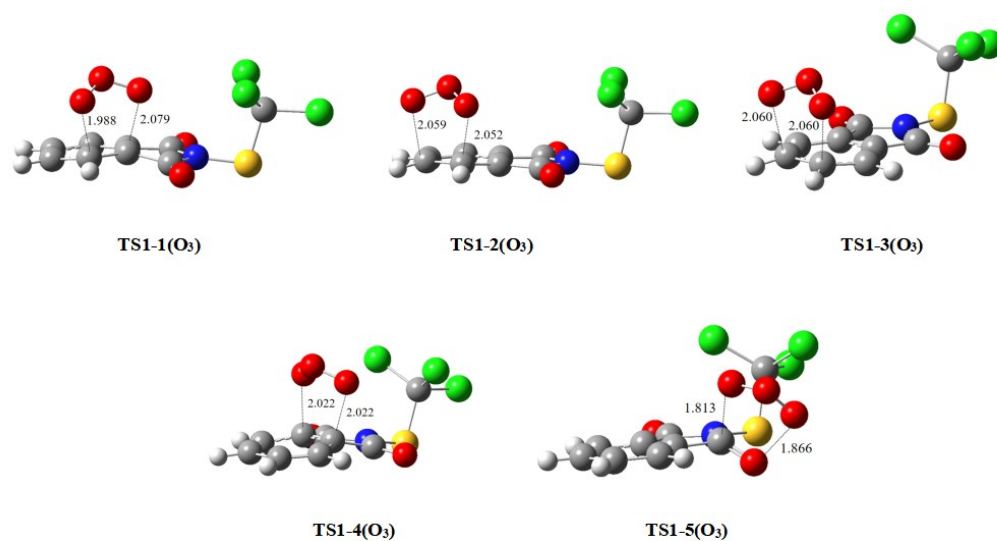


Fig. S3. The optimized transition state structures of Folpet with O₃

Table S1 The rate constants k (cm³ molecule⁻¹ s⁻¹) for each reaction site of Folpet with OH over the temperature range of 268-313 K

T(K)	$k_{\alpha\text{-add}}$	$k_{\beta\text{-add}}$	$k_{\lambda\text{-add}}$	$k_{\text{C=O-add}}$	$k_{\beta\text{-abs}}$	$k_{\lambda\text{-abs}}$	$k_{\text{total}}(\text{OH})$
268	6.79×10^{-16}	8.28×10^{-16}	5.49×10^{-15}	1.82×10^{-22}	1.13×10^{-14}	3.46×10^{-15}	2.18×10^{-14}
273	7.71×10^{-16}	9.52×10^{-16}	6.31×10^{-15}	2.66×10^{-22}	1.21×10^{-14}	3.90×10^{-15}	2.40×10^{-14}
278	8.71×10^{-16}	1.09×10^{-15}	6.83×10^{-15}	3.83×10^{-22}	1.29×10^{-14}	4.39×10^{-15}	2.61×10^{-14}
283	9.81×10^{-16}	1.25×10^{-15}	7.58×10^{-15}	5.46×10^{-22}	1.37×10^{-14}	4.92×10^{-15}	2.84×10^{-14}
288	1.10×10^{-15}	1.41×10^{-15}	8.39×10^{-15}	7.69×10^{-22}	1.47×10^{-14}	5.51×10^{-15}	3.11×10^{-14}
293	1.23×10^{-15}	1.60×10^{-15}	9.27×10^{-15}	1.07×10^{-21}	1.56×10^{-14}	6.16×10^{-15}	3.39×10^{-14}
298	1.38×10^{-15}	1.80×10^{-15}	1.02×10^{-14}	1.48×10^{-21}	1.66×10^{-14}	6.86×10^{-15}	3.68×10^{-14}
303	1.53×10^{-15}	2.03×10^{-15}	1.12×10^{-14}	2.01×10^{-21}	1.77×10^{-14}	7.63×10^{-15}	4.01×10^{-14}
308	1.70×10^{-15}	2.27×10^{-15}	1.23×10^{-14}	2.73×10^{-21}	1.88×10^{-14}	8.47×10^{-15}	4.35×10^{-14}

313 1.88×10^{-15} 2.54×10^{-15} 1.34×10^{-14} 3.66×10^{-21} 1.99×10^{-14} 9.39×10^{-15} 4.71×10^{-14}

Table S2 The rate constants k ($\text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$) for each reaction site of Folpet with O_3 over the temperature range of 268-313 K

T(K)	$k_{\text{C}\alpha=\text{C}\beta}$	$k_{\text{C}\beta=\text{C}\lambda}$	$k_{\text{C}3=\text{C}4}$	$k_{\text{C}1=\text{C}6}$	$k_{\text{C}=\text{O}}$	$k_{\text{total}}(\text{O}_3)$
268	9.61×10^{-25}	6.84×10^{-24}	1.31×10^{-23}	7.68×10^{-25}	4.10×10^{-36}	2.17×10^{-23}
273	1.43×10^{-24}	9.93×10^{-24}	1.91×10^{-23}	1.14×10^{-24}	9.59×10^{-36}	3.16×10^{-23}
278	2.10×10^{-24}	1.42×10^{-23}	2.74×10^{-23}	1.67×10^{-24}	2.18×10^{-35}	4.54×10^{-23}
283	3.05×10^{-24}	2.02×10^{-23}	3.88×10^{-23}	2.41×10^{-24}	4.81×10^{-35}	6.45×10^{-23}
288	4.36×10^{-24}	2.83×10^{-23}	5.43×10^{-23}	3.44×10^{-24}	1.03×10^{-34}	9.04×10^{-23}
293	6.18×10^{-24}	3.92×10^{-23}	7.53×10^{-23}	4.86×10^{-24}	2.17×10^{-34}	1.26×10^{-22}
298	8.66×10^{-24}	5.38×10^{-23}	1.03×10^{-22}	6.78×10^{-24}	4.43×10^{-34}	1.73×10^{-22}
303	1.20×10^{-23}	7.31×10^{-23}	1.41×10^{-22}	9.38×10^{-24}	8.87×10^{-34}	2.35×10^{-22}
308	1.65×10^{-23}	9.84×10^{-23}	1.89×10^{-22}	1.29×10^{-23}	1.74×10^{-33}	3.17×10^{-22}
313	2.25×10^{-23}	1.31×10^{-22}	2.53×10^{-22}	1.74×10^{-23}	3.33×10^{-33}	4.24×10^{-22}

Table S3 The rate constants k ($\text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$) for each reaction site of Folpet with NO_3 over the temperature range of 268-313 K

T(K)	$k_{\alpha\text{-add}}$	$k_{\beta\text{-add}}$	$k_{\lambda\text{-add}}$	$k_{\text{C}=\text{O}\text{-add}}$	$k_{\beta\text{-abs}}$	$k_{\lambda\text{-abs}}$	$k_{\text{total}}(\text{NO}_3)$
268	5.69×10^{-17}	2.04×10^{-15}	1.71×10^{-15}	1.27×10^{-29}	3.77×10^{-22}	1.01×10^{-20}	3.80×10^{-15}
273	6.34×10^{-17}	2.17×10^{-15}	1.82×10^{-15}	2.39×10^{-29}	5.12×10^{-22}	1.31×10^{-20}	4.05×10^{-15}
278	7.04×10^{-17}	2.31×10^{-15}	1.93×10^{-15}	4.42×10^{-29}	6.88×10^{-22}	1.68×10^{-20}	4.31×10^{-15}
283	7.79×10^{-17}	2.45×10^{-15}	2.05×10^{-15}	8.00×10^{-29}	9.16×10^{-22}	2.14×10^{-20}	4.57×10^{-15}
288	8.58×10^{-17}	2.59×10^{-15}	2.17×10^{-15}	1.42×10^{-28}	1.21×10^{-21}	2.72×10^{-20}	4.84×10^{-15}
293	9.43×10^{-17}	2.73×10^{-15}	2.29×10^{-15}	2.46×10^{-28}	1.59×10^{-21}	3.42×10^{-20}	5.12×10^{-15}

298	1.03×10^{-16}	2.88×10^{-15}	2.42×10^{-15}	4.19×10^{-28}	2.07×10^{-21}	4.28×10^{-20}	5.40×10^{-15}
303	1.13×10^{-16}	3.03×10^{-15}	2.54×10^{-15}	7.02×10^{-28}	2.67×10^{-21}	5.33×10^{-20}	5.68×10^{-15}
308	1.23×10^{-16}	3.18×10^{-15}	2.67×10^{-15}	1.16×10^{-27}	3.42×10^{-21}	6.60×10^{-20}	5.97×10^{-15}
313	1.33×10^{-16}	3.33×10^{-15}	2.80×10^{-15}	1.88×10^{-27}	4.36×10^{-21}	8.11×10^{-20}	6.27×10^{-15}

Table S4 The potential barriers E_b (kcal/mol) and reaction heats E_r (kcal/mol) at 298 K for the subsequent reactions of IM1-3(OH) and IM1-1'(OH)

Reaction	Potential barriers (E_b)	Reaction heat (E_r)
IM1-3(OH)→TS2-1→IM2-1	6.52	-10.70
IM1-3(OH)→TS2-2→IM2-2	4.12	-5.23
IM1-3(OH)→TS2-3→IM2-3	6.35	-10.54
IM2-2→TS3-1→IM3-1	38.46	13.59
IM2-2→TS3-2→IM3-2	37.49	12.85
IM2-2→TS3-3→IM3-3	38.57	23.73
IM2-2→TS3-4→IM3-4	38.65	38.65
IM2-2+NO→IM3-5	-	-21.38
IM3-2→TS4-1→IM4-1	28.82	-33.74
IM4-1+H ₂ O→TS5-1→P1+OH	10.80	9.35
IM3-5→TS4-2→IM4-2+NO ₂	51.35	14.96
IM4-2+H ₂ O→TS5-2→P2+OH	9.41	9.33
IM1-1'(OH)→IM2-O ₂	-	-44.59
IM1-1'(OH)→IM2-NO ₂	-	-70.94
IM1-1'(OH)→IM2-ONO	-	-76.80
IM1-1'(OH)→IM2-ON	-	-2.46
IM1-1'(OH)→IM2-NO	-	-51.62
IM2-ONO+H ₂ O→P3+HONO	10.08	-10.14

Table S5 Cartesian coordinates for all the optimized structures of reactants, transition states and products

Folpet

C 2.37127800 0.69503300 -0.13894100

C	2.37137100	-0.69505800	-0.13912300
C	3.49975000	-1.42364100	0.20141500
C	4.64290300	-0.69980300	0.55054600
C	4.64287400	0.69991900	0.55048900
C	3.49959800	1.42368500	0.20161100
C	1.02718900	1.18159400	-0.55943500
C	1.02719600	-1.18165900	-0.55937500
H	3.48570300	-2.50847700	0.19362700
H	5.54878600	-1.23035400	0.82533000
H	5.54878300	1.23053600	0.82506400
H	3.48549100	2.50851900	0.19382100
O	0.64273000	2.30582800	-0.72187400
O	0.64266200	-2.30590500	-0.72158100
N	0.24886200	-0.00004100	-0.75873300
S	-1.32390500	-0.00001600	-1.36269900
C	-2.27484100	-0.00007200	0.20706100
Cl	-1.94860100	1.44338500	1.18990300
Cl	-1.94772600	-1.44277700	1.19046300
Cl	-3.97163500	-0.00055300	-0.33691700
OH			
O	0.00000000	0.00000000	0.10841500
H	0.00000000	0.00000000	-0.86731800
IM1-1(OH)			
C	-2.15201600	-0.65364600	0.18508900
C	-2.22044500	0.83281500	0.09257900
C	-3.39543200	1.52213700	0.14587300
C	-4.60555000	0.79265000	0.13391200
C	-4.59998300	-0.61617200	-0.09363700

C	-3.43909300	-1.32383800	-0.16807100
C	-0.91127300	-0.98684100	-0.66017800
C	-0.90167100	1.35414800	-0.29679700
H	-3.39382500	2.60748300	0.10904500
H	-5.55161300	1.31771100	0.19886800
H	-5.55000300	-1.12151000	-0.23578200
H	-3.42367200	-2.39108400	-0.37005200
O	-0.60098300	-2.06268000	-1.09207200
O	-0.49694800	2.48368000	-0.34739700
N	-0.15503300	0.20084200	-0.73082300
S	1.39417400	0.30163400	-1.39906400
C	2.39208700	-0.01207000	0.11017500
Cl	2.12841700	-1.65049500	0.75341700
Cl	2.04900000	1.16311900	1.39357800
Cl	4.07227100	0.15490400	-0.45411300
O	-1.77272000	-0.98521200	1.53347600
H	-1.58167600	-1.93401100	1.57398200

IM1-2(OH)

C	-2.19245500	-0.31176900	-0.35692800
C	-2.08376600	1.04184500	-0.18075000
C	-3.14408600	1.82872900	0.27479200
C	-4.35729900	1.15096200	0.60725200
C	-4.50257000	-0.19447800	0.44990100
C	-3.44696700	-1.08684100	-0.14385400
C	-0.90525600	-0.86289600	-0.79092600
C	-0.68694500	1.45936600	-0.52376800
H	-3.02957300	2.89824900	0.40699500
H	-5.17827500	1.72678400	1.02219300

H	-5.42129100	-0.69028400	0.74849500
H	-3.81689000	-1.43829100	-1.12702400
O	-0.63109700	-2.00803100	-1.05820500
O	-0.21502100	2.56098100	-0.54806200
N	-0.00707900	0.24843400	-0.84622800
S	1.58748400	0.16022700	-1.37693000
C	2.44624500	-0.08586900	0.22879800
Cl	1.93191000	-1.58127900	1.03810700
Cl	2.18849600	1.27989200	1.33495100
Cl	4.16341600	-0.19207800	-0.22921800
O	-3.26460700	-2.20993500	0.70334200
H	-2.60474400	-2.78864600	0.29483500
IM1-3(OH)			
C	-2.06477700	-0.48466200	-0.48170000
C	-1.98636300	0.92174300	-0.30398900
C	-3.10519500	1.67533400	0.11209000
C	-4.28126800	1.01708500	0.31845700
C	-4.46100800	-0.46848200	0.11769200
C	-3.20301200	-1.18835800	-0.29127300
C	-0.71625600	-0.98535800	-0.88642600
C	-0.61335900	1.36566300	-0.57786700
H	-3.01017600	2.74444800	0.27269900
H	-5.16544200	1.54901700	0.65746300
H	-5.21600800	-0.61993200	-0.66974600
H	-3.24105800	-2.26699300	-0.41396600
O	-0.37872900	-2.10014100	-1.17317000
O	-0.15095500	2.47663500	-0.57324300
N	0.11952700	0.16687800	-0.88326400

S	1.73955500	0.15430200	-1.35068600
C	2.53542900	-0.09747400	0.28462500
Cl	2.06712500	-1.64494200	1.02483300
Cl	2.15368000	1.21294100	1.42223200
Cl	4.27545500	-0.09919200	-0.09130200
O	-5.05166800	-1.07355900	1.26379500
H	-4.44763900	-0.96965000	2.01069600
IM1-A(OH)			
C	-2.41843500	0.56255800	0.06372200
C	-2.34300000	-0.82188500	0.09000300
C	-3.43914100	-1.60902300	-0.22794800
C	-4.62634700	-0.95553100	-0.56418900
C	-4.70388000	0.44152100	-0.57157600
C	-3.59543200	1.22822400	-0.24726800
C	-1.06189400	1.15814200	0.42623800
C	-0.97112000	-1.24470000	0.48996900
H	-3.36138300	-2.69130100	-0.20951300
H	-5.50657300	-1.53693400	-0.81811800
H	-5.64353000	0.92232200	-0.82366600
H	-3.65767600	2.31218400	-0.22778000
O	-1.29498500	1.84012500	1.58471500
O	-0.55639400	-2.35904600	0.66968300
N	-0.23938500	-0.04879600	0.62793700
S	1.29612600	-0.00214800	1.29937100
C	2.40244000	-0.05523800	-0.18199000
Cl	2.62047700	1.52348700	-0.97002400
Cl	1.84279600	-1.23030400	-1.38239600
Cl	3.96798600	-0.56463900	0.51158400

O	-0.47251700	1.97018800	-0.53258200
H	-1.09253200	2.14986800	-1.24851200
IM1-1'(OH)			
C	-2.37835200	-0.75855700	-0.13317100
C	-2.40342200	0.63819000	-0.14277800
C	-3.53954200	1.35762800	0.19072100
C	-4.68439400	0.63826900	0.54904100
C	-4.68480500	-0.76573500	0.56726200
C	-3.52254500	-1.42469700	0.22083600
C	-1.02569900	-1.22868500	-0.55240300
C	-1.06398400	1.13842100	-0.56764900
H	-3.53091100	2.44219300	0.17091400
H	-5.59180900	1.17028600	0.81725900
H	-5.58118600	-1.31026600	0.84636600
O	-0.61897700	-2.34326300	-0.71182100
O	-0.69954400	2.26793000	-0.73829300
N	-0.27036200	-0.03117900	-0.75698700
S	1.30314100	-0.01004800	-1.36161400
C	2.25283300	0.01225400	0.20893500
Cl	1.94207800	-1.42677400	1.20203800
Cl	1.90841400	1.45933800	1.18054900
Cl	3.94914400	0.02843100	-0.33515500
IM1-2'(OH)			
C	2.40067000	0.73544100	-0.11194400
C	2.41945000	-0.65590400	-0.12717300
C	3.55097800	-1.38499200	0.21111100
C	4.69397300	-0.66114700	0.58010400
C	4.61741900	0.71880500	0.57851400

C	3.51806200	1.48366900	0.24564300
C	1.05114600	1.20943300	-0.53763700
C	1.08441800	-1.15286700	-0.56132400
H	3.54296100	-2.47015800	0.18794500
H	5.60972700	-1.17396500	0.85652400
H	3.50563600	2.56869000	0.25504900
O	0.65769300	2.33141000	-0.69072400
O	0.71463600	-2.27964900	-0.73788200
N	0.29130000	0.02089900	-0.75361500
S	-1.27925300	0.00529900	-1.36501900
C	-2.23571800	-0.01671400	0.20140800
Cl	-1.92651300	1.42194100	1.19641400
Cl	-1.89706900	-1.46419000	1.17408900
Cl	-3.92997100	-0.02975600	-0.34857800
TS1-1(OH)			
C	-2.20404700	-0.58725200	-0.21626200
C	-2.24460300	0.82359400	-0.13194700
C	-3.39471600	1.49563300	0.20393900
C	-4.55842700	0.73025900	0.39329500
C	-4.55943100	-0.65780900	0.19899900
C	-3.39731700	-1.33458800	-0.15214900
C	-0.89848000	-0.97795600	-0.84298400
C	-0.90180200	1.35760900	-0.47762200
H	-3.40237700	2.57697100	0.29217600
H	-5.48449600	1.22738200	0.66283000
H	-5.48851000	-1.20725200	0.30836400
H	-3.38386200	-2.40397200	-0.33877100
O	-0.55332000	-2.05505800	-1.24052100

O	-0.51291900	2.49236900	-0.47495300
N	-0.13680600	0.21939100	-0.88048200
S	1.45981800	0.30605500	-1.41641500
C	2.34033400	-0.01223000	0.16478400
Cl	2.04343900	-1.65228400	0.78051200
Cl	1.89918600	1.16031400	1.41970600
Cl	4.05813300	0.16684000	-0.27706500
O	-1.46274700	-0.96080100	1.56353700
H	-1.51027600	-1.93419000	1.58299100
TS1-2(OH)			
C	-2.20890700	-0.34728300	-0.50737700
C	-2.13272200	0.98635300	-0.14217200
C	-3.23065200	1.66858100	0.35842300
C	-4.43412900	0.95226500	0.48354500
C	-4.51992700	-0.38396100	0.12545900
C	-3.37894700	-1.10541300	-0.32652300
C	-0.87735100	-0.80349800	-0.98033900
C	-0.75133600	1.48010700	-0.40365800
H	-3.15704500	2.71510700	0.63497900
H	-5.31727500	1.45889800	0.85840900
H	-5.46156400	-0.91173100	0.23003100
H	-3.49189600	-2.07225100	-0.80395200
O	-0.55003400	-1.89364400	-1.36670000
O	-0.30190200	2.58437300	-0.28122800
N	-0.03007900	0.33605800	-0.87112800
S	1.58130700	0.37272400	-1.36487200
C	2.41071500	-0.07588900	0.21169400
Cl	1.96337500	-1.70459100	0.76567000

Cl	2.05136800	1.08256900	1.50887100
Cl	4.14162900	-0.02439800	-0.20095600
O	-2.83803500	-1.97556600	1.37378000
H	-2.06160700	-2.46576800	1.04430700
TS1-3(OH)			
C	-2.08999400	-0.46961400	-0.58535500
C	-2.04005800	0.89808100	-0.30906100
C	-3.16965400	1.61465400	0.06933500
C	-4.36298800	0.91049000	0.17548800
C	-4.41853000	-0.49493500	-0.04278800
C	-3.26269600	-1.18778900	-0.49466100
C	-0.73328300	-0.92976200	-0.99828700
C	-0.65084800	1.38589700	-0.52691300
H	-3.11282100	2.68114600	0.25947000
H	-5.27397500	1.42094200	0.46820800
H	-5.38733200	-0.96861200	-0.14100200
H	-3.29774200	-2.24815000	-0.71950900
O	-0.37771700	-2.01684400	-1.35698300
O	-0.21759300	2.50102300	-0.43828000
N	0.09774600	0.22763900	-0.89747700
S	1.72472900	0.26297300	-1.34120600
C	2.49885000	-0.09668100	0.28377900
Cl	2.03266100	-1.69424400	0.90685300
Cl	2.08881500	1.12958500	1.50342100
Cl	4.24307200	-0.05868400	-0.06641200
O	-4.45880500	-1.11848400	1.84890800
H	-3.59723000	-0.79714200	2.17042300

TS1-A(OH)

C	2.41972100	0.55740000	-0.22604900
C	2.40737400	-0.82014700	-0.05676100
C	3.55378900	-1.52105300	0.28616900
C	4.72726600	-0.78360300	0.45219100
C	4.73964800	0.60440200	0.27027100
C	3.57752800	1.30054700	-0.07186600
C	1.03595400	1.01236800	-0.57003600
C	1.04046100	-1.33568200	-0.34407300
H	3.52858200	-2.59858900	0.41109700
H	5.64805200	-1.29248500	0.71795100
H	5.67099800	1.14725700	0.39588000
H	3.57990400	2.37561400	-0.22137100
O	0.71700900	2.09050100	-1.11437600
O	0.63750400	-2.46543400	-0.33242200
N	0.27315000	-0.18607400	-0.69732600
S	-1.27233600	-0.28172400	-1.34491900
C	-2.37039400	-0.05612600	0.12542800
Cl	-2.71352100	1.65428800	0.47916100
Cl	-1.72181400	-0.84636200	1.56735600
Cl	-3.89605900	-0.83617100	-0.38396400
O	0.41297000	1.66511700	1.01757900
H	0.72355200	2.58835300	1.07513200
TS1-1'(OH)			
C	2.22460000	0.19663000	-0.14914300
C	2.06256800	-1.18639700	-0.14131900
C	3.09910800	-2.03511500	0.21063900
C	4.31877600	-1.44855800	0.56395800
C	4.49148800	-0.05699200	0.55988700

C	3.43044400	0.76430900	0.19673100
C	0.95358400	0.83654400	-0.58257400
C	0.66945200	-1.50423400	-0.56731400
H	2.96205300	-3.11129800	0.20987800
H	5.15473900	-2.07995600	0.84775000
H	5.44894100	0.37098700	0.83840800
H	3.54489700	2.02329300	0.17640000
O	0.71921800	2.00438000	-0.75843100
O	0.14720700	-2.56964000	-0.73091800
N	0.04155300	-0.23216600	-0.77480100
S	-1.52697100	-0.04422500	-1.36895900
C	-2.44766200	0.08910600	0.21543600
Cl	-1.95393400	1.51476400	1.15319300
Cl	-2.24465900	-1.35730400	1.22564000
Cl	-4.14217800	0.24912200	-0.30308000
O	3.33385200	3.20341700	0.03963400
H	2.40677200	3.18082100	-0.27335500
TS1-2'(OH)			
C	-2.00633700	-0.36257100	-0.42450400
C	-1.88270400	1.00960900	-0.23725700
C	-2.95358300	1.80065600	0.14956700
C	-4.18011900	1.15837200	0.35361500
C	-4.27634900	-0.21564400	0.15335800
C	-3.21327700	-1.02211500	-0.23446500
C	-0.68682300	-0.91843600	-0.84419100
C	-0.47753400	1.41337400	-0.52875900
H	-2.83669300	2.87077500	0.28738600
H	-5.05523100	1.72331800	0.65810800

H	-5.37852600	-0.73304800	0.30776200
H	-3.31138300	-2.09199500	-0.38704500
O	-0.39849500	-2.04442900	-1.13742100
O	0.01147700	2.50781500	-0.52445400
N	0.20228400	0.19812800	-0.84539700
S	1.81406400	0.12264200	-1.33592600
C	2.62196400	-0.16935600	0.28654700
Cl	2.11668000	-1.70826400	1.01837100
Cl	2.29384100	1.14278000	1.43861700
Cl	4.35569100	-0.21970300	-0.11333600
O	-6.41585500	-1.27002500	0.76982200
H	-6.13322500	-1.48024600	1.67727000

NO₃

O	0.00000000	1.09177500	-0.58348300
O	0.00000000	-1.09177500	-0.58348300
O	0.00000000	0.00000000	1.23901000
N	0.00000000	0.00000000	-0.08233600

IM1-1(NO₃)

C	1.95439500	0.07147500	-0.29946600
C	1.94568700	-1.30249100	0.28268900
C	3.08233000	-1.94344000	0.67075500
C	4.32867900	-1.33807200	0.38805600
C	4.39508500	-0.16251900	-0.41569200
C	3.27798700	0.49955700	-0.82889100
C	0.73654300	0.02028400	-1.24851500
C	0.57418500	-1.84105800	0.20880600

H	3.02237600	-2.92894100	1.12272600
H	5.24588500	-1.81937200	0.70679400
H	5.37020600	0.19275900	-0.73323600
H	3.31874800	1.36480200	-1.47921900
O	0.53731000	0.64456400	-2.24588600
O	0.10898100	-2.82711800	0.71061200
N	-0.11763400	-0.96615600	-0.68976800
S	-1.72495600	-1.17434500	-1.16560700
C	-2.50559000	-0.04515600	0.05668400
Cl	-1.88770300	1.61866500	-0.09715900
Cl	-2.24978900	-0.59414700	1.72457700
Cl	-4.23357800	-0.09376100	-0.35693600
O	1.54314800	0.87846200	0.88057100
N	1.33926200	2.24378000	0.67465000
O	1.48411200	2.66968200	-0.44174500
O	1.03433300	2.81723100	1.67816300
IM1-2(NO ₃)			
C	-1.72759800	0.63527800	-0.40359000
C	-1.28951900	1.90220400	-0.13617200
C	-2.12202700	2.90370200	0.37503400
C	-3.47338200	2.54240900	0.65778300
C	-3.95299600	1.28933500	0.42231300
C	-3.12893100	0.19117400	-0.18697800
C	-0.60518800	-0.19483200	-0.87538000
C	0.17342400	1.98142100	-0.45315700
H	-1.73924000	3.89772000	0.57421300
H	-4.13584400	3.28725900	1.08620300
H	-4.97898000	1.03455200	0.66815500

H	-3.58848500	-0.15693900	-1.12132400
O	-0.61264800	-1.34785800	-1.21578300
O	0.89661700	2.93613100	-0.40205100
N	0.53761300	0.66699000	-0.85191000
S	2.07733300	0.22270100	-1.37262400
C	2.79128100	-0.36877400	0.21459900
Cl	1.91734900	-1.77440100	0.85540100
Cl	2.80597300	0.90745000	1.45115000
Cl	4.45574500	-0.82271200	-0.22168800
O	-3.14408300	-0.92722500	0.73969900
N	-3.25701700	-2.20105300	0.15580600
O	-3.03172700	-3.07348100	0.93911800
O	-3.58234100	-2.26939200	-0.99872300
IM1-3(NO ₃)			
C	-1.30387500	0.21181700	-0.70352100
C	-1.00243400	1.50775200	-0.21593500
C	-2.00874900	2.36333300	0.27938300
C	-3.29450000	1.91656300	0.27198200
C	-3.69239700	0.57241900	-0.27235200
C	-2.55708600	-0.29185200	-0.74325500
C	-0.02789000	-0.43591600	-1.14182600
C	0.44763000	1.73615800	-0.31858600
H	-1.75001000	3.34555400	0.66083200
H	-4.10399200	2.52718600	0.65840400
H	-4.41985300	0.70416600	-1.08562800
H	-2.76960200	-1.28471800	-1.12747100
O	0.13489200	-1.50903100	-1.65041100
O	1.08486500	2.71997000	-0.04995200

N	0.98781900	0.51418100	-0.84221400
S	2.61521100	0.31224100	-1.24177800
C	3.23325000	-0.43999000	0.31500800
Cl	2.47217800	-2.01001400	0.64990300
Cl	2.98202600	0.62389000	1.71501800
Cl	4.97312900	-0.65535300	0.00696300
O	-4.40929700	-0.06304900	0.83117000
N	-5.26551400	-1.09109300	0.45476300
O	-5.83999700	-1.58252300	1.37994500
O	-5.33101600	-1.36364800	-0.71987200

IM1-A(NO₃)

C	-2.34112200	-0.07468700	0.25152300
C	-2.16321700	-1.41122000	-0.08901300
C	-3.21024400	-2.19463400	-0.54839500
C	-4.46831500	-1.59904500	-0.63871200
C	-4.65369100	-0.26522400	-0.26444400
C	-3.59413300	0.52156200	0.19502700
C	-0.98750200	0.49242400	0.69326900
C	-0.76001600	-1.82632300	0.15505500
H	-3.03846800	-3.23301400	-0.81315400
H	-5.31600100	-2.17840500	-0.98960200
H	-5.64464200	0.17249800	-0.32750500
H	-3.74886800	1.55035300	0.49115400
O	-1.10658700	1.01176900	1.92411000
O	-0.25134100	-2.90524500	0.02861400
N	-0.10475900	-0.66019700	0.62639700
S	1.43080500	-0.68896400	1.30917800
C	2.53969600	-0.24651100	-0.10974900

Cl	2.73844300	1.50741000	-0.31882200
Cl	1.98370400	-0.96372900	-1.62601900
Cl	4.10991800	-0.94217200	0.37706200
O	-0.36486100	1.40284900	-0.25293500
N	-0.87539200	2.69598100	-0.33517500
O	-0.16467400	3.42805500	-0.95571700
O	-1.93724800	2.91979700	0.18575000

IM1-1'(NO₃)

C	-2.37835200	-0.75855700	-0.13317100
C	-2.40342200	0.63819000	-0.14277800
C	-3.53954200	1.35762800	0.19072100
C	-4.68439400	0.63826900	0.54904100
C	-4.68480500	-0.76573500	0.56726200
C	-3.52254500	-1.42469700	0.22083600
C	-1.02569900	-1.22868500	-0.55240300
C	-1.06398400	1.13842100	-0.56764900
H	-3.53091100	2.44219300	0.17091400
H	-5.59180900	1.17028600	0.81725900
H	-5.58118600	-1.31026600	0.84636600
O	-0.61897700	-2.34326300	-0.71182100
O	-0.69954400	2.26793000	-0.73829300
N	-0.27036200	-0.03117900	-0.75698700
S	1.30314100	-0.01004800	-1.36161400
C	2.25283300	0.01225400	0.20893500
Cl	1.94207800	-1.42677400	1.20203800
Cl	1.90841400	1.45933800	1.18054900
Cl	3.94914400	0.02843100	-0.33515500

IM1-2'(NO₃)

C	2.40067000	0.73544100	-0.11194400
C	2.41945000	-0.65590400	-0.12717300
C	3.55097800	-1.38499200	0.21111100
C	4.69397300	-0.66114700	0.58010400
C	4.61741900	0.71880500	0.57851400
C	3.51806200	1.48366900	0.24564300
C	1.05114600	1.20943300	-0.53763700
C	1.08441800	-1.15286700	-0.56132400
H	3.54296100	-2.47015800	0.18794500
H	5.60972700	-1.17396500	0.85652400
H	3.50563600	2.56869000	0.25504900
O	0.65769300	2.33141000	-0.69072400
O	0.71463600	-2.27964900	-0.73788200
N	0.29130000	0.02089900	-0.75361500
S	-1.27925300	0.00529900	-1.36501900
C	-2.23571800	-0.01671400	0.20140800
Cl	-1.92651300	1.42194100	1.19641400
Cl	-1.89706900	-1.46419000	1.17408900
Cl	-3.92997100	-0.02975600	-0.34857800
TS1-1(NO ₃)			
C	-2.01244300	-0.13812700	0.56800600
C	-1.98359700	-1.35196700	-0.18115300
C	-3.10576700	-1.85899000	-0.77849400
C	-4.31996600	-1.17483500	-0.55921800
C	-4.39201600	-0.05216600	0.28654400
C	-3.26209400	0.45908400	0.89818600
C	-0.72597200	-0.07975400	1.35725700
C	-0.59655400	-1.89149800	-0.16016400

H	-3.06223600	-2.76639100	-1.37160700
H	-5.22808900	-1.54289200	-1.02532900
H	-5.35637200	0.41036700	0.46710900
H	-3.28695500	1.31876300	1.55738500
O	-0.45628600	0.60058900	2.30074700
O	-0.15162000	-2.84208400	-0.73971800
N	0.11182800	-1.05950400	0.75271200
S	1.74962000	-1.24957200	1.12226100
C	2.45279600	-0.04564100	-0.07899400
Cl	1.91558300	1.61412000	0.25948500
Cl	2.03085200	-0.45313900	-1.75093100
Cl	4.20943900	-0.18412900	0.17381900
O	-1.36280700	0.94834700	-0.88792600
N	-1.22181800	2.26847200	-0.65522300
O	-1.50129200	2.70146000	0.44042200
O	-0.81131100	2.88011300	-1.61081600
TS1-2(NO ₃)			
C	-1.53714800	0.75915800	-0.74429000
C	-1.20824200	1.80571000	0.08276200
C	-2.18257300	2.56022300	0.74264100
C	-3.52460300	2.21675600	0.53438600
C	-3.87247100	1.14646500	-0.28096300
C	-2.87583500	0.33235700	-0.90074600
C	-0.29442100	0.16984500	-1.31633900
C	0.27804600	1.96602100	0.09774000
H	-1.89626700	3.38685300	1.38477500
H	-4.30589600	2.79296800	1.01784000
H	-4.91331500	0.87554400	-0.42120500

H	-3.14308700	-0.38120000	-1.67249400
O	-0.18037300	-0.71817800	-2.11218100
O	0.93560800	2.79525300	0.65963600
N	0.77053600	0.91778900	-0.73007000
S	2.40014900	0.70471000	-1.11669800
C	2.87266300	-0.50255800	0.18604000
Cl	4.59804800	-0.79950000	-0.13221200
Cl	1.95233300	-2.01421600	0.05463800
Cl	2.65296300	0.16154300	1.81802500
O	-2.80827100	-1.10665000	0.50891200
N	-3.86403100	-1.92779600	0.44914100
O	-3.82526500	-2.82344300	1.25760100
O	-4.73153500	-1.71152900	-0.37275500
TS1-3(NO ₃)			
C	-1.36642000	0.63306300	-0.88409400
C	-1.10172300	1.66433600	0.01755600
C	-2.11492100	2.38690300	0.64972500
C	-3.41780900	2.02422600	0.36506400
C	-3.70670500	0.92038300	-0.49722900
C	-2.65188900	0.24947900	-1.18721600
C	-0.07304400	0.10259600	-1.40688300
C	0.37693800	1.84741900	0.12027700
H	-1.87468200	3.20229400	1.32354900
H	-4.24771900	2.54657100	0.82833900
H	-4.72460100	0.77462900	-0.84010300
H	-2.86937500	-0.55491500	-1.88193300
O	0.11633800	-0.74568100	-2.23030100
O	0.98520300	2.66561200	0.75095900

N	0.93635500	0.84683700	-0.72354200
S	2.58874900	0.69251400	-1.04061600
C	3.03738700	-0.54119900	0.24499600
Cl	2.13265200	-2.05694900	0.05456100
Cl	2.76757700	0.08223100	1.88587600
Cl	4.77256000	-0.81662200	-0.03215100
O	-3.95709500	-0.46313400	0.96061600
N	-4.59431100	-1.55561800	0.51971000
O	-4.77549100	-2.38683500	1.37606700
O	-4.92223000	-1.61468600	-0.64824200

TS1-A(NO₃)

C	2.29901400	-0.18990600	-0.48929600
C	2.15233500	-1.41364300	0.15603900
C	3.23361300	-2.07972900	0.70908200
C	4.48597800	-1.47335600	0.58670100
C	4.63481100	-0.25292000	-0.08024100
C	3.53820200	0.41417400	-0.63396900
C	0.95154300	0.25025400	-0.96489900
C	0.73428400	-1.85101100	0.06888000
H	3.10099600	-3.03609300	1.20396300
H	5.36079000	-1.96050700	1.00487400
H	5.62300500	0.18592800	-0.17088800
H	3.64371300	1.36230600	-1.14756200
O	0.72597900	1.07148200	-1.91019900
O	0.21619900	-2.85295900	0.47045500
N	0.07014700	-0.81795100	-0.66994500
S	-1.49995300	-0.98093500	-1.25507800
C	-2.53400300	-0.18410200	0.05962900

Cl	-2.70568800	1.57029700	-0.17327000
Cl	-1.91455000	-0.51183300	1.68235500
Cl	-4.13272700	-0.94503900	-0.16821900
O	0.33889000	1.43219700	0.24641900
N	1.02265700	2.58509000	0.52283800
O	0.54913200	3.16696300	1.46259900
O	1.97565700	2.87313800	-0.14998100
TS1-1'(NO ₃)			
C	-1.38843000	0.73977000	-0.25877800
C	-0.80358900	2.00102400	-0.15196100
C	-1.53047900	3.11876400	0.22405700
C	-2.88830300	2.94784300	0.50408600
C	-3.50283600	1.68907600	0.40591300
C	-2.72778700	0.60866700	0.02097500
C	-0.35740600	-0.24681600	-0.69631600
C	0.64010100	1.88695900	-0.51681100
H	-1.05215500	4.09001000	0.29668600
H	-3.49015700	3.79977100	0.80355400
H	-4.55708900	1.56163300	0.62472900
H	-3.24902600	-0.55404200	-0.09272300
O	-0.48818700	-1.41094600	-0.94133600
O	1.46504600	2.75259700	-0.59322800
N	0.85197200	0.50283700	-0.78657700
S	2.30842200	-0.13488200	-1.35439600
C	3.07652400	-0.63164600	0.23867300
Cl	2.10054300	-1.83976200	1.09957000
Cl	3.34142800	0.75912700	1.31224200
Cl	4.63397000	-1.33488500	-0.25518400

O	-3.69626400	-1.69453700	-0.25252500
N	-5.00661900	-1.68655300	0.10607900
O	-5.53148700	-2.75781000	-0.02111300
O	-5.48680400	-0.64821100	0.49818600
TS1-2'(NO ₃)			
C	-1.14810900	0.24147300	-0.50484200
C	-0.78358100	1.55222400	-0.22053000
C	-1.69880300	2.49849600	0.21365800
C	-3.02641900	2.08002900	0.36779100
C	-3.33836400	0.76016300	0.07437500
C	-2.45598200	-0.21037600	-0.36766900
C	0.05939100	-0.51403500	-0.95571900
C	0.67929400	1.71284100	-0.46972900
H	-1.39596100	3.51846600	0.42727400
H	-3.79165600	2.76928900	0.70975800
H	-4.54509700	0.44542000	0.22934200
H	-2.75225300	-1.23061600	-0.58663600
O	0.14344800	-1.64776400	-1.33153100
O	1.35419400	2.69954700	-0.38434500
N	1.13408500	0.42072600	-0.86616600
S	2.72544100	0.07347600	-1.30894900
C	3.38975600	-0.48085900	0.31113900
Cl	2.54171800	-1.91677200	0.92253500
Cl	3.30802600	0.79821000	1.54175900
Cl	5.08680000	-0.87503100	-0.05115000
O	-5.76714300	0.26311700	0.47122700
N	-6.03989400	-1.05053700	0.24912400
O	-7.19372000	-1.32314400	0.43512700

O	-5.13250100	-1.76902700	-0.09442200
HNO ₃			
H	-1.72929100	0.14367000	0.00004300
O	-1.08920300	-0.58920100	-0.00000700
N	0.13783300	0.03737300	0.00000200
O	1.07060800	-0.70749500	0.00000200
O	0.11415300	1.24603500	-0.00000300
O ₃			
O	0.00000000	0.00000000	0.42403200
O	0.00000000	1.06278900	-0.21201600
O	0.00000000	-1.06278900	-0.21201600
IM1-1(O ₃)			
C	-1.91822300	-0.21535600	-0.07248700
C	-1.82930100	1.25539300	0.13761300
C	-2.91026200	2.03618000	0.24309300
C	-4.24577700	1.44057000	0.14449000
C	-4.41891800	0.16996900	-0.24835600
C	-3.27883200	-0.77644600	-0.52143100
C	-0.69676000	-0.50807900	-0.95704100
C	-0.43144500	1.68524800	-0.09809400
H	-2.79669900	3.11301300	0.33588000
H	-5.10711600	2.06887900	0.34453900
H	-5.41639200	-0.24499000	-0.35881100
H	-3.24715100	-1.12848200	-1.55932100
O	-0.51443600	-1.44955700	-1.67151400
O	0.08486100	2.74979100	0.09536400

N	0.20267100	0.56151000	-0.72114900
S	1.78466500	0.60399700	-1.32242500
C	2.65336100	-0.12447000	0.12243200
Cl	2.10142500	-1.77883500	0.45747900
Cl	2.44137600	0.85703200	1.58635300
Cl	4.36176100	-0.12863400	-0.37673600
O	-1.70144900	-0.88919000	1.17441600
O	-2.18360100	-2.18002100	0.86551700
O	-3.47620000	-1.89646800	0.36154200
IM1-2(O ₃)			
C	-1.72214700	-0.01563500	-0.63396000
C	-1.56595300	1.25017100	-0.22594400
C	-2.64503800	2.09697200	0.25127600
C	-3.88660600	1.59522200	0.27453200
C	-4.21732500	0.19165800	-0.16404100
C	-3.02866500	-0.72612100	-0.61809700
C	-0.41849600	-0.56314600	-1.09813800
C	-0.12426000	1.63828800	-0.36939400
H	-2.41948500	3.10848800	0.57126300
H	-4.72273600	2.19028900	0.62971800
H	-4.99591400	0.19883400	-0.93564700
H	-3.24855200	-1.20785000	-1.57640800
O	-0.18383300	-1.62450400	-1.60244400
O	0.37977000	2.70228500	-0.14327600
N	0.53004700	0.47805800	-0.85684300
S	2.15705100	0.41010700	-1.28947900
C	2.87266900	-0.23094000	0.27696700
Cl	2.25708100	-1.84767300	0.67625900

Cl	2.55459200	0.85638200	1.64539600
Cl	4.61823300	-0.29922700	-0.06172500
O	-2.98296700	-1.71411800	0.41157500
O	-4.34701400	-1.83487400	0.75689700
O	-4.70719700	-0.48852600	0.99757600
IM1-3(O ₃)			
C	-1.59718300	-0.72929600	-0.71956000
C	-1.59715500	0.72979700	-0.71938400
C	-2.69067200	1.46347400	-0.52553500
C	-4.02137100	0.78670400	-0.31899300
C	-4.02149000	-0.78627900	-0.31966800
C	-2.69076100	-1.46300500	-0.52626600
C	-0.19715000	-1.19240800	-0.93257300
C	-0.19710300	1.19290900	-0.93234800
H	-2.65680400	2.54868000	-0.49029500
H	-4.75863000	1.17592000	-1.02670500
H	-4.75857100	-1.17481000	-1.02794000
H	-2.65695500	-2.54822400	-0.49146400
O	0.22252200	-2.30960300	-1.04668100
O	0.22256600	2.31011200	-1.04635400
N	0.58623900	0.00024500	-0.99908800
S	2.24573300	0.00018100	-1.33132600
C	2.90724600	-0.00010600	0.38153200
Cl	2.41132900	-1.44377600	1.28831500
Cl	2.41229000	1.44392800	1.28832000
Cl	4.67071300	-0.00075900	0.13760100
O	-4.54846900	-1.09259400	0.97481400
O	-4.09549400	-0.00075900	1.75055100

O	-4.54790500	1.09202000	0.97591900
IM1-4(O ₃)			
C	2.34704800	0.20184600	0.06813200
C	2.26051900	-1.15817800	-0.18233700
C	3.33630000	-2.00742300	0.03467300
C	4.51275700	-1.43513100	0.51864400
C	4.59644100	-0.06039200	0.77115800
C	3.50698500	0.78497200	0.55071100
C	1.04046400	0.86335800	-0.28063600
C	0.89730700	-1.47836100	-0.68236600
H	3.25110100	-3.07057900	-0.16464300
H	5.37824800	-2.06235700	0.70591500
H	5.52546100	0.35394700	1.14916400
H	3.56137700	1.85040500	0.74923600
O	1.10357700	1.79919200	-1.36401300
O	0.44186900	-2.53120500	-1.03200600
N	0.19579900	-0.23779800	-0.68029600
S	-1.36061800	-0.07485900	-1.28877200
C	-2.40738000	-0.31354300	0.21795800
Cl	-2.57957200	1.16561300	1.19387900
Cl	-1.79866400	-1.61782100	1.24901500
Cl	-4.00180300	-0.73796200	-0.45901000
O	0.57928500	1.62746600	0.81803600
O	-0.02319700	2.75432300	0.19394900
O	0.97360700	3.05533800	-0.72582800
IM1-5(O ₃)			
C	2.34704800	0.20184600	0.06813200
C	2.26051900	-1.15817800	-0.18233700

C	3.33630000	-2.00742300	0.03467300
C	4.51275700	-1.43513100	0.51864400
C	4.59644100	-0.06039200	0.77115800
C	3.50698500	0.78497200	0.55071100
C	1.04046400	0.86335800	-0.28063600
C	0.89730700	-1.47836100	-0.68236600
H	3.25110100	-3.07057900	-0.16464300
H	5.37824800	-2.06235700	0.70591500
H	5.52546100	0.35394700	1.14916400
H	3.56137700	1.85040500	0.74923600
O	1.10357700	1.79919200	-1.36401300
O	0.44186900	-2.53120500	-1.03200600
N	0.19579900	-0.23779800	-0.68029600
S	-1.36061800	-0.07485900	-1.28877200
C	-2.40738000	-0.31354300	0.21795800
Cl	-2.57957200	1.16561300	1.19387900
Cl	-1.79866400	-1.61782100	1.24901500
Cl	-4.00180300	-0.73796200	-0.45901000
O	0.57928500	1.62746600	0.81803600
O	-0.02319700	2.75432300	0.19394900
O	0.97360700	3.05533800	-0.72582800
TS1-1(O ₃)			
C	-1.94324500	-0.08733400	-0.60253500
C	-1.87983400	1.20380600	-0.02628900
C	-2.99311700	1.83028900	0.45131500
C	-4.25822700	1.19830000	0.24491000
C	-4.36522600	0.01138900	-0.43289100
C	-3.20022200	-0.72639200	-0.82651300

C	-0.63577600	-0.36810500	-1.27615300
C	-0.47571400	1.68387000	-0.10234600
H	-2.92250000	2.80665600	0.92031100
H	-5.15680200	1.70184500	0.58572600
H	-5.34088600	-0.41659200	-0.63519600
H	-3.26289800	-1.52638900	-1.55635900
O	-0.35494300	-1.25959900	-2.02390500
O	0.00359300	2.70353300	0.30764000
N	0.22648000	0.67334800	-0.83454100
S	1.85762800	0.78916700	-1.25612800
C	2.59608700	-0.13311100	0.15164500
Cl	2.05139600	-1.82188500	0.19421200
Cl	2.22191900	0.62774800	1.71157500
Cl	4.34585800	-0.05873700	-0.16977000
O	-1.29283900	-1.20693900	1.02403400
O	-3.17702700	-2.06964500	0.63834700
O	-2.45611200	-1.45273200	1.50715800
TS1-2(O ₃)			
C	-1.78122900	0.09420700	-0.89871600
C	-1.68647200	1.24377400	-0.16449800
C	-2.81904700	1.90111000	0.36797600
C	-4.04586600	1.33037400	0.14539600
C	-4.16482900	0.05119300	-0.48569400
C	-3.00514200	-0.59870500	-1.03691900
C	-0.43363700	-0.30226900	-1.38625400
C	-0.25855700	1.68030600	-0.13072000
H	-2.70604900	2.84227400	0.89530600
H	-4.95068700	1.81823000	0.49100900

H	-5.14368900	-0.28843300	-0.80258500
H	-3.11050800	-1.39634100	-1.76269600
O	-0.12454800	-1.22101300	-2.09166800
O	0.21485000	2.66456700	0.36399300
N	0.45593500	0.67663100	-0.84706600
S	2.10727600	0.74180500	-1.17355800
C	2.74621400	-0.22141200	0.25458600
Cl	2.12859700	-1.88617500	0.26161400
Cl	2.34155000	0.54249700	1.80723500
Cl	4.50890900	-0.21808700	0.00660800
O	-2.67752100	-2.01332000	0.41327500
O	-4.38219300	-1.07406800	1.22428400
O	-3.14928700	-1.36897700	1.41657100
TS1-3(O ₃)			
C	1.64730300	0.71012000	-0.85275600
C	1.64736900	-0.70918500	-0.85336700
C	2.79425800	-1.43872100	-0.77516000
C	4.00525800	-0.72029100	-0.53752800
C	4.00519800	0.72105600	-0.53666200
C	2.79411800	1.43968100	-0.77377500
C	0.24761700	1.18642600	-1.03465200
C	0.24770100	-1.18545100	-1.03559700
H	2.78792200	-2.52126300	-0.83976800
H	4.95584000	-1.22930900	-0.64373900
H	4.95573400	1.23032800	-0.64203100
H	2.78771400	2.52228400	-0.83731300
O	-0.16381800	2.30756000	-1.14184800
O	-0.16365300	-2.30653700	-1.14360200

N	-0.54713000	0.00047200	-1.08122900
S	-2.21444300	0.00052100	-1.34586800
C	-2.80345700	-0.00022200	0.39365100
Cl	-2.26682600	1.44360000	1.27833100
Cl	-2.26656300	-1.44458300	1.27727600
Cl	-4.57596400	-0.00032400	0.23142100
O	4.10951300	1.05326500	1.49355000
O	3.49747200	-0.00119100	1.88950800
O	4.11056100	-1.05459000	1.49250800
TS1-4(O ₃)			
C	2.04134200	0.71639500	-0.33916100
C	2.04137200	-0.71641700	-0.33907300
C	3.26325300	-1.43683200	-0.38560500
C	4.42265200	-0.71725700	-0.28811100
C	4.42262300	0.71731500	-0.28818300
C	3.26319400	1.43684300	-0.38576300
C	0.70645700	1.18079100	-0.84292900
C	0.70652000	-1.18087100	-0.84284200
H	3.24528000	-2.51849600	-0.45811600
H	5.37642600	-1.23437000	-0.26092700
H	5.37637500	1.23447100	-0.26106800
H	3.24520700	2.51850000	-0.45837900
O	0.34779700	2.30059600	-1.06511700
O	0.34791500	-2.30070500	-1.06497400
N	-0.06432400	-0.00006500	-1.02082200
S	-1.67412800	-0.00019900	-1.53570000
C	-2.51699400	0.00000100	0.09673600
Cl	-2.12166400	1.44330800	1.04976100

Cl	-2.12147600	-1.44294800	1.05021000
Cl	-4.24605600	-0.00016200	-0.33609800
O	1.44552400	1.05517400	1.56360300
O	1.93921000	0.00000700	2.11043200
O	1.44541200	-1.05502600	1.56345400
TS1-5(O ₃)			
C	2.41890600	0.29637700	-0.19806800
C	2.34980700	-1.08455700	-0.08810900
C	3.45469300	-1.83778600	0.28513800
C	4.63846600	-1.14966800	0.54889400
C	4.70394600	0.24449700	0.42943300
C	3.58875200	0.99387800	0.04958000
C	1.07539500	0.80885900	-0.62812600
C	0.98617200	-1.54640000	-0.46129500
H	3.38578500	-2.91801400	0.36134200
H	5.52569400	-1.69995800	0.84423700
H	5.64164800	0.75109500	0.63402200
H	3.63173000	2.07346900	-0.05076000
O	0.96148300	1.81398300	-1.39862200
O	0.55355600	-2.66337500	-0.52734200
N	0.25893100	-0.35889900	-0.77164200
S	-1.30571300	-0.37046800	-1.37060700
C	-2.35219300	-0.33187400	0.16135000
Cl	-2.72147900	1.31937500	0.73240100
Cl	-1.63453100	-1.25231200	1.48773200
Cl	-3.88198100	-1.08203500	-0.36988100
O	0.45614500	1.45762900	0.94709800
O	-0.31567300	2.79876500	-0.46075600

O 0.31401800 2.73396700 0.62653500

IM2-1

C	1.63354900	0.76619200	-0.57875500
C	1.59173500	-0.67816900	-0.77708700
C	2.64178500	-1.48435200	-0.61347000
C	3.94799700	-0.87514900	-0.16720800
C	4.06945300	0.65006400	-0.41508600
C	2.77169700	1.41719600	-0.33850000
C	0.25172400	1.29481300	-0.70812200
C	0.18361900	-1.05923300	-1.09447900
H	2.55589500	-2.56338300	-0.70065000
H	4.80830400	-1.37476300	-0.61815500
H	4.40312600	0.74120100	-1.46023000
H	2.81539900	2.49113800	-0.17618800
O	-0.14527600	2.42369300	-0.63461700
O	-0.25910100	-2.13371400	-1.39002200
N	-0.56378000	0.14920400	-0.98200400
S	-2.21504100	0.25155900	-1.33694800
C	-2.91681900	-0.00949100	0.33834600
Cl	-2.42671000	1.26113600	1.47792900
Cl	-2.46370000	-1.58799300	1.01582100
Cl	-4.67389700	0.05836000	0.05971000
O	5.09828900	1.21602800	0.35269300
H	4.85276300	1.17237800	1.28716500
O	4.13145300	-1.18706000	1.24864900
O	3.36168600	-0.45678700	2.00461900

IM2-2

C	1.84744200	0.77083900	-0.34091500
C	1.76568000	-0.71143100	-0.23711500
C	2.98892800	-1.44057300	-0.66613000
C	4.15603100	-0.79488300	-0.63685000
C	4.30686900	0.66908600	-0.27444900
C	3.00237500	1.43081800	-0.34120600
C	0.48787200	1.30610700	-0.60764800
C	0.42284200	-1.04817500	-0.89466000
H	2.89707600	-2.49830400	-0.89303800
H	5.08257300	-1.32467400	-0.84244500
H	5.00471700	1.13106900	-0.98174800
H	3.02881900	2.51557200	-0.41106800
O	0.10733500	2.44073600	-0.64976500
O	0.05902600	-2.11762900	-1.28752000
N	-0.31554700	0.15670100	-0.90671100
S	-1.92803200	0.25601800	-1.42145400
C	-2.75849300	0.03422800	0.20188000
Cl	-2.33882400	1.32605800	1.34477600
Cl	-2.35997000	-1.53199600	0.93807100
Cl	-4.48939900	0.10515500	-0.20399900
O	4.92037900	0.81825000	0.99417300
H	4.33677900	0.39884200	1.64444600
O	2.39372900	-0.68644400	2.00247700
O	1.46820400	-1.07972400	1.19266500
IM2-3			
C	-1.74014100	-0.11301500	-0.62974900
C	-1.61854400	1.15207800	-0.19811600
C	-2.70655500	1.93361300	0.35912000

C	-3.92838200	1.38388800	0.31737600
C	-4.21673900	0.08140300	-0.39976800
C	-3.01438100	-0.88276600	-0.53221400
C	-0.42482600	-0.62317600	-1.09335600
C	-0.18988400	1.58525200	-0.36213800
H	-2.50266800	2.90211000	0.80130800
H	-4.79901500	1.88797200	0.72866400
H	-4.47110000	0.35996600	-1.43369800
H	-3.16136100	-1.56870100	-1.36904600
O	-0.15935000	-1.68506600	-1.58316700
O	0.28573300	2.66164800	-0.13480200
N	0.49342900	0.44833700	-0.86690000
S	2.11394800	0.43407000	-1.32804800
C	2.88069600	-0.17378800	0.22771200
Cl	2.31995100	-1.80404500	0.65181600
Cl	2.56197300	0.91448400	1.59503500
Cl	4.62048900	-0.19631200	-0.14763900
O	-5.35324300	-0.57385000	0.09933900
H	-5.17763300	-0.85923200	1.00655000
O	-2.93758300	-1.79684400	0.60188500
O	-2.95479300	-1.15672400	1.73718100
TS2-1			
C	1.73979200	0.78117300	-0.59711900
C	1.68228200	-0.63766300	-0.88030300
C	2.77505500	-1.44782200	-0.81854500
C	3.93683200	-0.86761900	-0.25719800
C	4.16781800	0.62777700	-0.29880600
C	2.88021200	1.41799600	-0.30496300

C	0.36091300	1.33476400	-0.71117900
C	0.27928800	-0.99285300	-1.21016100
H	2.69376400	-2.51641600	-0.98825900
H	4.83654900	-1.46182100	-0.12637800
H	4.68850400	0.84507200	-1.24820800
H	2.92275300	2.48686800	-0.11424400
O	-0.01636100	2.46569000	-0.58421800
O	-0.17338800	-2.04774900	-1.56081300
N	-0.46407100	0.21567300	-1.03664400
S	-2.11779200	0.34158300	-1.36279900
C	-2.79664900	0.00429700	0.30919800
Cl	-2.29683400	1.22772300	1.49598600
Cl	-2.32741600	-1.59886500	0.91128200
Cl	-4.55808300	0.07641300	0.05796400
O	5.06793900	1.05372100	0.69927700
H	4.68509700	0.85944400	1.56492000
O	3.37436900	-0.95821200	1.68294800
O	2.15405200	-0.95071000	1.84767800

TS2-2

C	-1.85176500	-0.69303600	-0.60907700
C	-1.76780900	0.74240200	-0.55081300
C	-2.96191800	1.53718600	-0.58166200
C	-4.13285600	0.90722900	-0.35668400
C	-4.28206200	-0.58825100	-0.19977200
C	-2.99802800	-1.35348400	-0.39202900
C	-0.48762500	-1.23178000	-0.87065100
C	-0.40000900	1.13688100	-0.99477300
H	-2.88500700	2.61483700	-0.68315100

H	-5.05810900	1.47184600	-0.27601700
H	-4.99823800	-0.93889300	-0.95724200
H	-3.03624700	-2.43959600	-0.36755400
O	-0.12313500	-2.36995500	-0.95591900
O	0.02111200	2.23382100	-1.23485000
N	0.33933300	-0.07926600	-1.04940800
S	1.98140400	-0.16067300	-1.44189300
C	2.70234200	-0.05577500	0.24483600
Cl	2.17190800	-1.39944300	1.27723800
Cl	2.29854200	1.47486400	1.04972600
Cl	4.45446000	-0.15468500	-0.04920700
O	-4.89240400	-0.91462000	1.03683700
H	-4.29812600	-0.61309600	1.73912000
O	-2.23571600	0.39923000	2.03760000
O	-1.32575000	0.89774700	1.37919000
TS2-3			
C	-1.81039600	-0.10299000	-0.87771200
C	-1.71160600	1.13163900	-0.29533600
C	-2.82658200	1.79889300	0.32477500
C	-4.01996300	1.17339300	0.30642300
C	-4.24174800	-0.16403400	-0.36941500
C	-2.95399700	-0.88659500	-0.67984700
C	-0.46180300	-0.54927600	-1.32317500
C	-0.30087300	1.60212400	-0.39026300
H	-2.67835100	2.76308900	0.79901900
H	-4.90358400	1.62233200	0.75150200
H	-4.73811600	0.03509200	-1.33545900
H	-3.02551100	-1.89231700	-1.08348600

O	-0.14819300	-1.57287400	-1.86319300
O	0.16019900	2.65781000	-0.05476500
N	0.41548300	0.52269500	-0.98478000
S	2.06309700	0.54786300	-1.33557300
C	2.73084500	-0.16923400	0.21964700
Cl	2.11967600	-1.80857800	0.52125400
Cl	2.36495900	0.84408500	1.63139300
Cl	4.48793900	-0.20806900	-0.06742100
O	-5.15645500	-0.97571400	0.33334100
H	-4.76049100	-1.22591500	1.17847900
O	-2.51278000	-1.46695200	1.20087500
O	-1.68888300	-0.74188400	1.76038700
TS2-ONO			
C	-1.66106300	0.74918800	0.00678800
C	-1.10753400	2.02443100	-0.17910900
C	-1.79999100	3.18919400	0.05926800
C	-3.12609200	3.04327800	0.51052800
C	-3.69735800	1.79657100	0.69704800
C	-2.98785400	0.58223100	0.45880800
C	-0.65862000	-0.25729200	-0.37371300
C	0.28475900	1.87920200	-0.68090000
H	-1.34169300	4.15910800	-0.09654000
H	-3.71891900	3.92925100	0.71800000
H	-4.71976300	1.70231700	1.04897800
O	-0.72917800	-1.46771100	-0.42820000
O	1.07786500	2.71913000	-1.00426900
N	0.51339600	0.46777000	-0.73258400
S	1.90469700	-0.24211300	-1.35822100

C	2.88978300	-0.43798900	0.17951400
Cl	2.06618500	-1.46442800	1.37633700
Cl	3.26820000	1.12273400	0.93580100
Cl	4.38501000	-1.22938300	-0.37769300
O	-3.57448300	-0.56324600	0.65697700
N	-3.77802700	-2.22555700	-0.86443100
O	-4.82534400	-2.56077000	-0.74988800
O	-2.82314600	-2.83787900	0.65292500
H	-2.99211500	-1.83626400	0.93293000
H	-1.90184800	-2.79688600	0.33195800

IM3-1

C	-1.77333500	-0.56861900	-0.52588500
C	-1.76100200	0.83019100	-0.03527400
C	-2.96366500	1.57516500	-0.54842100
C	-4.09722600	0.87855800	-0.68596600
C	-4.22229500	-0.59907600	-0.35071100
C	-2.89708500	-1.13716700	0.24155500
C	-0.45206100	-0.97960400	-0.97457100
C	-0.36624500	1.33883600	-0.40476500
H	-2.88737200	2.63950600	-0.74723500
H	-5.01752800	1.36297700	-1.00256200
H	-4.47453600	-1.17105200	-1.25075500
H	-2.90951300	-2.21693600	0.39906400
O	-0.06150500	-2.04454800	-1.37446000
O	0.03286400	2.46498100	-0.35176100
N	0.35415500	0.21099600	-0.86808800
S	1.96329700	0.28862600	-1.38822600

C	2.81622600	-0.10464000	0.19079000
Cl	2.41609300	-1.73094700	0.77975300
Cl	2.43183100	1.07310200	1.46213300
Cl	4.54067300	-0.01241800	-0.24044600
O	-5.27295300	-0.81870200	0.55738800
H	-5.03114300	-0.39523900	1.39432200
O	-2.72970200	-0.51491800	1.54062800
O	-1.82842700	0.62298200	1.38200400

IM3-2

C	1.77467500	0.77313200	-0.43846800
C	1.75355700	-0.73008800	-0.34483100
C	2.97518100	-1.27617800	-0.99544100
C	3.97630100	-0.79969700	0.00167200
C	4.22286200	0.72398900	-0.12681900
C	2.91234400	1.46054600	-0.34054100
C	0.40421300	1.26011900	-0.72334000
C	0.35344500	-1.12333100	-0.81456800
H	3.02311500	-2.17616900	-1.59258100
H	4.91807800	-1.35053700	0.04138300
H	4.88806100	0.91356400	-0.97778700
H	2.93388600	2.54628600	-0.39744900
O	-0.00140000	2.38120000	-0.84221800
O	-0.04081900	-2.22235500	-1.07108000
N	-0.39016800	0.07823500	-0.89534200
S	-2.01568200	0.12120200	-1.37706200
C	-2.81870000	0.04333500	0.27256900
Cl	-2.41623100	1.45030400	1.27742600
Cl	-2.38315500	-1.43353200	1.15499700

Cl	-4.55610700	0.04302200	-0.11721500
O	4.89243500	1.20738000	1.01108900
H	4.38245600	0.93263300	1.78785600
O	3.32044200	-1.00887100	1.27872200
O	1.89891600	-1.15236800	1.01586700
IM3-3			
C	1.76213500	0.94966800	-0.26229900
C	1.79728600	-0.53450800	-0.21173500
C	3.09395200	-1.23518500	-0.62154100
C	4.23864000	-0.29927400	-0.71732200
C	4.20114300	0.99724700	0.04887700
C	2.86508600	1.69182600	-0.15664000
C	0.38209900	1.39686200	-0.57766100
C	0.45682400	-0.96544200	-0.81273200
H	3.02540100	-1.96519300	-1.43060700
H	5.18146900	-0.65136900	-1.11857900
H	5.00472300	1.65021000	-0.29797200
H	2.81607800	2.77652800	-0.21106200
O	-0.06056200	2.50772000	-0.65097100
O	0.14295300	-2.06341200	-1.16894600
N	-0.35059600	0.19705200	-0.85315200
S	-1.95951300	0.19223000	-1.38874100
C	-2.80068900	-0.01954300	0.22999600
Cl	-2.47988300	1.33983900	1.32609300
Cl	-2.32127200	-1.52914700	1.03187200
Cl	-4.52628800	-0.06745100	-0.20341000
O	4.45780600	0.80711700	1.43665500
H	3.82097800	0.16576600	1.78849000

O	3.06564400	-1.91996000	0.67811900
O	1.96233400	-1.07596300	1.12021300
IM3-4			
C	-1.88197200	-0.64751900	-0.04255400
C	-1.77922600	0.85761800	0.13292200
C	-2.97764600	1.67299000	-0.19328500
C	-4.14276900	1.07652900	-0.46287700
C	-4.36156200	-0.42485100	-0.47909400
C	-3.08771200	-1.19080000	-0.66912200
C	-0.54933900	-1.09148700	-0.64258900
C	-0.45352000	1.27551600	-0.49324300
H	-2.87310000	2.75354400	-0.16287600
H	-5.02818800	1.68135700	-0.64050900
H	-5.06262600	-0.67388500	-1.28025500
H	-3.08729400	-2.19728400	-1.07059800
O	-0.22937200	-2.20308300	-0.94823400
O	-0.05897800	2.38732500	-0.69175100
N	0.24179100	0.07556200	-0.79314600
S	1.81238400	0.04902500	-1.44164000
C	2.76461400	-0.05927600	0.12528400
Cl	2.36836500	-1.52597900	1.04117700
Cl	2.49620300	1.35509400	1.16301300
Cl	4.45657000	-0.10888100	-0.42639600
O	-5.02321600	-0.83799600	0.71652100
H	-4.41769100	-0.70622900	1.46098200
O	-1.84713800	-0.77628000	1.41911900
O	-1.57458900	0.65164000	1.55889100

IM3-5

C	1.99916000	-0.85456500	-0.40124300
C	1.92804500	0.17674400	0.68276400
C	3.10516600	0.14956300	1.61235200
C	4.26852300	-0.30555800	1.14748400
C	4.45196700	-0.85066300	-0.25721100
C	3.15101800	-1.33449200	-0.86054900
C	0.63856700	-1.38939700	-0.65540500
C	0.54772100	-0.06735600	1.31875500
H	2.98176800	0.59089600	2.59630800
H	5.16499900	-0.25241100	1.75931500
H	5.14889000	-1.69362200	-0.22163200
H	3.17373800	-2.09363900	-1.63856400
O	0.25494600	-2.13535200	-1.51020200
O	0.14303200	0.38393900	2.35155200
N	-0.16264300	-0.91184200	0.43608000
S	-1.70601700	-1.53577700	0.76030800
C	-2.75426500	-0.23659300	-0.00162000
Cl	-2.31285300	0.06557300	-1.69128900
Cl	-2.67994300	1.29571200	0.89701000
Cl	-4.39566400	-0.91768800	0.10656100
O	5.09083700	0.10761900	-1.08946800
H	4.53298200	0.89755900	-1.12560700
O	1.98231400	1.51563300	0.13881800
O	0.98799600	1.64411800	-0.85695400
N	0.08671500	2.67476200	-0.38961300
O	-0.65740200	2.92353800	-1.24384100
TS3-1			
C	-1.80162200	-0.59248500	-0.61471300

C	-1.74269800	0.81513800	-0.11629400
C	-2.97071300	1.59545200	-0.46101700
C	-4.13071000	0.93354100	-0.50104100
C	-4.25981400	-0.56095700	-0.29083400
C	-2.90985100	-1.24155900	-0.11387500
C	-0.45247800	-1.03177400	-0.99279500
C	-0.37067300	1.31218100	-0.56242500
H	-2.88819800	2.66921100	-0.59709300
H	-5.06790500	1.45874500	-0.66696600
H	-4.71289400	-1.00449100	-1.18881400
H	-2.91841300	-2.31840200	0.04298400
O	-0.06419600	-2.11916900	-1.32127700
O	0.02319600	2.44097000	-0.59523200
N	0.35578300	0.15385800	-0.93581300
S	1.98118000	0.18554700	-1.41392100
C	2.77561500	-0.09084000	0.21968600
Cl	2.32251100	-1.65519000	0.92534500
Cl	2.37666400	1.19482700	1.37653400
Cl	4.51477000	-0.06498700	-0.15998000
O	-5.14456600	-0.86704800	0.75701600
H	-4.77589000	-0.48540300	1.56666300
O	-2.60139700	-0.32844100	1.61499300
O	-1.62371800	0.59035600	1.32002600
TS3-2			
C	1.79283200	0.75926700	-0.42894300
C	1.74381400	-0.73114500	-0.30536000
C	2.97729300	-1.38581300	-0.85646600
C	4.07864500	-0.79885000	-0.26454700

C	4.24179500	0.71342200	-0.17338500
C	2.92969800	1.44508200	-0.33403600
C	0.42570700	1.26394900	-0.70949700
C	0.36159700	-1.10845300	-0.83364600
H	2.93794100	-2.39975400	-1.23823400
H	5.00593400	-1.35805700	-0.15889800
H	4.89826200	1.01076300	-1.00345700
H	2.94827700	2.53116200	-0.38562000
O	0.03571400	2.39183400	-0.81403700
O	-0.02316700	-2.20234500	-1.12806800
N	-0.37894800	0.09440600	-0.90404300
S	-2.00230300	0.15543700	-1.38986700
C	-2.80585500	0.04558600	0.25802800
Cl	-2.39263600	1.42631000	1.29378200
Cl	-2.37713500	-1.45416900	1.10499600
Cl	-4.54338900	0.06410100	-0.12943000
O	4.92321700	1.10340400	0.99186000
H	4.37965600	0.82850500	1.74482900
O	3.07390400	-0.84141100	1.48898300
O	1.78657800	-1.15083300	1.07572900
TS3-3			
C	1.77015100	0.95558800	-0.28354000
C	1.79357600	-0.53551700	-0.25966500
C	3.07690100	-1.15498000	-0.79030600
C	4.20991600	-0.38214100	-0.68775800
C	4.20334100	0.94296400	0.04567400
C	2.88300800	1.67164000	-0.14063400
C	0.38891100	1.41662100	-0.56945800

C	0.45589200	-0.93876400	-0.88731800
H	3.02687200	-2.04297800	-1.41053300
H	5.16575700	-0.77025700	-1.02390700
H	5.01373500	1.56724500	-0.33918200
H	2.86261700	2.75827500	-0.14410000
O	-0.05198300	2.53001300	-0.60186600
O	0.13785900	-2.02033000	-1.28762600
N	-0.34833100	0.22751200	-0.87828800
S	-1.96594400	0.24767800	-1.38783200
C	-2.77855700	-0.02306900	0.23620000
Cl	-2.40344000	1.27375300	1.38963700
Cl	-2.31607300	-1.57915500	0.95527200
Cl	-4.51360600	-0.01463200	-0.16038100
O	4.49787400	0.76720200	1.42355000
H	3.89031700	0.10363200	1.78691500
O	2.90459000	-1.95796600	0.91659200
O	1.87144800	-0.99952300	1.09534900

TS3-4

C	-1.86007500	-0.65200200	-0.33443600
C	-1.83514800	0.82566200	-0.00554200
C	-3.04685600	1.58790600	-0.42651800
C	-4.20057000	0.92298000	-0.52901800
C	-4.32706000	-0.56476500	-0.24576000
C	-3.04614000	-1.30345200	-0.54781700
C	-0.52243600	-1.05196200	-0.87057400
C	-0.48035400	1.30189100	-0.53764100
H	-2.96220800	2.66072000	-0.56922100
H	-5.12046100	1.45064500	-0.76448900

H	-5.13578800	-0.98288900	-0.85019300
H	-3.06264900	-2.34811300	-0.84221500
O	-0.16567200	-2.13262300	-1.24166600
O	-0.09626400	2.43145500	-0.62723900
N	0.25204900	0.14018100	-0.89344200
S	1.85887100	0.18652000	-1.43923000
C	2.71160600	-0.06108000	0.16950300
Cl	2.33002200	-1.63799800	0.88719300
Cl	2.30458700	1.21321700	1.33521500
Cl	4.43675900	0.01937800	-0.26372400
O	-4.72078800	-0.79549900	1.10061200
H	-4.00847400	-0.49451100	1.68611900
O	-1.45784600	-0.65676700	1.50099600
O	-1.78289900	0.72960300	1.42866800
IM4-1			
C	1.77180600	0.81449500	-0.14844600
C	1.65501800	-0.67922500	0.08073500
C	2.90636900	-1.46606300	-0.24699500
C	4.17840800	-0.73873600	-0.43834700
C	4.26433800	0.77843500	-0.31686600
C	2.91712300	1.46956500	-0.30507700
C	0.40783600	1.34196200	-0.42641300
C	0.38554200	-0.99662900	-0.75667200
H	2.76173500	-2.44998200	-0.68866600
H	4.97208900	-1.21265500	-1.01222900
H	4.80993700	1.15738500	-1.18773100
H	2.89861700	2.54269500	-0.48443500
O	0.02085400	2.47419300	-0.45648900

O	0.09620200	-2.05031200	-1.24033500
N	-0.36669800	0.19512100	-0.78979000
S	-1.95029500	0.28976000	-1.38496500
C	-2.85883300	-0.00075400	0.18544200
Cl	-2.48909900	1.23541600	1.40172300
Cl	-2.49722500	-1.60147000	0.86551800
Cl	-4.56830100	0.09297400	-0.29969400
O	5.03732900	1.14314800	0.80539200
H	4.70030400	0.64740100	1.56627300
O	3.87475300	-1.39513100	0.78331500
O	1.25735000	-0.81974800	1.39340300

IM4-2

C	-1.98411800	-0.67844400	-0.24996600
C	-1.87218900	0.79146000	0.10080300
C	-3.11170900	1.57702200	-0.21860800
C	-4.28450100	0.94721700	-0.29094500
C	-4.44664900	-0.54972800	-0.12699300
C	-3.15328800	-1.30296800	-0.34979700
C	-0.63565100	-1.17918700	-0.62527600
C	-0.55967100	1.18755200	-0.60680300
H	-3.01831300	2.65611100	-0.29690600
H	-5.20497900	1.50859900	-0.42750900
H	-5.17750400	-0.90998000	-0.85809900
H	-3.19321700	-2.35382200	-0.62734500
O	-0.27975600	-2.30540700	-0.82661900
O	-0.20187600	2.29050000	-0.89907300
N	0.16675100	-0.01253600	-0.80183700
S	1.75216200	-0.05949700	-1.39637700

C	2.66563800	-0.05420800	0.19576600
Cl	2.28819800	-1.47624500	1.18803300
Cl	2.33705200	1.40951600	1.14557000
Cl	4.37312700	-0.09069700	-0.31014700
O	-5.01683900	-0.87287800	1.13324600
H	-4.44735600	-0.51290400	1.82725500
O	-1.60653700	0.74974100	1.46365300
TS4-1			
C	1.74484600	0.78983300	-0.37045800
C	1.70332800	-0.70924300	-0.26693200
C	2.92015400	-1.31838200	-0.88934800
C	4.05455500	-0.78495300	-0.06242900
C	4.21475700	0.75370300	-0.18891100
C	2.88684200	1.47316300	-0.31420800
C	0.37959100	1.29519700	-0.64624600
C	0.32041000	-1.08077400	-0.84652100
H	2.91584100	-2.30382700	-1.33941300
H	5.00603900	-1.28442100	-0.29735300
H	4.79702800	0.97101900	-1.09321300
H	2.90306200	2.55899000	-0.37891300
O	-0.02373800	2.42031100	-0.72443500
O	-0.05328500	-2.16309200	-1.18513500
N	-0.41696400	0.12366100	-0.88390600
S	-2.03964000	0.19122300	-1.37435100
C	-2.84278800	0.02880100	0.26949200
Cl	-2.44595800	1.38642600	1.34146000
Cl	-2.39413500	-1.48798000	1.07735100
Cl	-4.58014000	0.03587300	-0.11675600

O	4.96763000	1.24976700	0.88881100
H	4.57242900	0.90188300	1.70239300
O	3.75760300	-1.13790200	1.26404400
O	1.75333800	-1.16112600	1.04945000
TS4-2			
C	2.02637800	-1.11640700	-0.14902900
C	1.97229900	0.22767000	0.52931500
C	3.18768100	0.46238000	1.40725600
C	4.34652400	-0.05434900	0.99167600
C	4.44321200	-0.85234000	-0.30112300
C	3.17705100	-1.65347600	-0.54341100
C	0.68004300	-1.72935100	-0.14124100
C	0.60374100	0.20930500	1.24056700
H	3.08040300	1.14389400	2.24532000
H	5.27210400	0.15046800	1.52252500
H	5.30500700	-1.52219800	-0.26298300
H	3.22379200	-2.62302000	-1.03237000
O	0.28670400	-2.73790400	-0.65699200
O	0.17610500	1.01262600	2.02323200
N	-0.11870700	-0.88461600	0.70477700
S	-1.69548900	-1.29793100	1.16211900
C	-2.66362800	-0.34403100	-0.06968000
Cl	-2.09289600	-0.61673500	-1.72637700
Cl	-2.65214700	1.41268000	0.25889000
Cl	-4.32101400	-0.95920600	0.13098100
O	4.69332500	0.01982800	-1.39625800
H	3.96330900	0.66024300	-1.42247100
O	2.00456100	1.28345800	-0.35893600

O	0.13144000	1.79537600	-1.11372000
N	0.12112300	2.83252700	-0.58337000
O	-0.57345200	3.77676200	-0.44221900
TS5-1			
C	-1.56827700	-1.20426400	-0.18328800
C	-1.63623200	0.29878100	-0.30281200
C	-2.91481100	0.75794500	-1.00187200
C	-4.11451600	-0.05117800	-0.72293300
C	-3.99078300	-1.25585900	0.23097600
C	-2.64450200	-1.94797000	0.05583100
C	-0.16859700	-1.64270100	-0.41160900
C	-0.33221900	0.63541900	-1.04489600
H	-2.79277700	1.31539300	-1.92805900
H	-4.91574500	-0.08902000	-1.45718200
H	-4.79203900	-1.96185700	0.00252600
H	-2.56717200	-3.02624100	0.16865800
O	0.31154000	-2.73517200	-0.29762000
O	-0.06882300	1.64689700	-1.62747200
N	0.52118500	-0.48265100	-0.87920800
S	2.14621200	-0.49941200	-1.35912200
C	2.90707400	0.06859500	0.21326400
Cl	2.55716400	-1.03623000	1.55804900
Cl	2.36233000	1.70079700	0.65630500
Cl	4.65049600	0.07524400	-0.14309900
O	-4.17809100	-0.88420000	1.57597200
H	-3.55961500	-0.16365700	1.77638600
O	-3.92820500	1.22729600	-0.13145000
O	-1.54985700	0.76359300	1.02249700

H	-1.50910300	1.88903100	1.08834600
O	-1.94286100	2.98022400	0.85276800
H	-2.91352000	2.88699300	0.88487400
TS5-2			
C	-1.86311500	-0.97679600	-0.10857000
C	-1.81051700	0.52396800	-0.18702600
C	-3.07075100	1.13004000	-0.73146900
C	-4.21737900	0.45843000	-0.62635600
C	-4.32584400	-0.93787300	-0.04837400
C	-2.99936400	-1.66370900	-0.03709500
C	-0.50516000	-1.52123000	-0.35653000
C	-0.49924000	0.76450600	-0.95813200
H	-3.02330600	2.15342500	-1.09275200
H	-5.15697400	0.92520700	-0.91010600
H	-5.02662300	-1.52054200	-0.65521300
H	-2.98920200	-2.75054800	-0.00318100
O	-0.09602600	-2.64169900	-0.25383700
O	-0.14154900	1.79947300	-1.45845800
N	0.25494400	-0.41483300	-0.86484600
S	1.86451100	-0.54445200	-1.38395300
C	2.71381200	-0.09517200	0.18135400
Cl	2.34651200	-1.23509000	1.49025700
Cl	2.29586500	1.54568000	0.72413300
Cl	4.43873400	-0.17933200	-0.24793900
O	-4.91165100	-0.91327700	1.24592900
H	-4.35519900	-0.36839100	1.81969700
O	-1.54532300	0.97446300	1.13054400
H	-1.44497800	2.09182200	1.17876100

O	-1.28572400	3.22695300	0.79178400
H	-0.69187400	3.19240700	0.01578800
P1			
C	1.75283300	0.85018400	-0.19097400
C	1.66812700	-0.63340800	0.00844200
C	2.91397800	-1.38283700	-0.42325600
C	4.17988400	-0.62983400	-0.53075900
C	4.23771700	0.86626700	-0.20846800
C	2.88301300	1.54312200	-0.28230400
C	0.38762000	1.35807300	-0.49134900
C	0.39103600	-0.99088200	-0.76945800
H	2.76045300	-2.29629100	-0.99607800
H	4.96227200	-1.01087200	-1.18373500
H	4.89125100	1.34458400	-0.94414600
H	2.85297900	2.62029800	-0.42888900
O	-0.01933000	2.48330100	-0.54278200
O	0.07001300	-2.07440500	-1.17253500
N	-0.37484600	0.19239200	-0.83292200
S	-1.96970400	0.25462900	-1.39833600
C	-2.85085600	-0.00016800	0.19269400
Cl	-2.45893500	1.25704900	1.37994700
Cl	-2.48723400	-1.59045200	0.90275600
Cl	-4.56936900	0.08624400	-0.26245600
O	4.84857900	1.08570700	1.04404700
H	4.42299000	0.49456200	1.68326100
O	3.90641100	-1.45933100	0.58740400
O	1.36173900	-0.84297700	1.37782500
H	1.29397800	-1.79284900	1.55014300

P2

C	-1.97375600	-0.70172500	-0.19394200
C	-1.86732800	0.76963400	0.06084700
C	-3.09893300	1.52593900	-0.34114100
C	-4.27083000	0.89186300	-0.39531100
C	-4.43149300	-0.59495600	-0.15022200
C	-3.12987100	-1.35079400	-0.28792400
C	-0.62981500	-1.22662600	-0.54622500
C	-0.55710900	1.13880900	-0.64937400
H	-3.00950100	2.60007800	-0.48546200
H	-5.18999700	1.44249700	-0.57757900
H	-5.14072000	-0.99773200	-0.88062600
H	-3.15622900	-2.41904100	-0.48843200
O	-0.25657100	-2.35745400	-0.67792700
O	-0.17887300	2.24134600	-0.93395400
N	0.16617500	-0.06352500	-0.80981700
S	1.74907000	-0.13247200	-1.40670400
C	2.67262200	-0.05785000	0.17755000
Cl	2.30398700	-1.43244000	1.23573600
Cl	2.35063900	1.44884500	1.06772400
Cl	4.37775700	-0.11097000	-0.33377800
O	-5.04167100	-0.84252600	1.10995800
H	-4.46149500	-0.49105100	1.79941800
O	-1.60336500	0.93483800	1.45865300
H	-1.37798600	1.86167200	1.62468700

P3

C	-2.21459200	-0.33198200	-0.16795100
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C	-2.11282100	1.05586300	-0.13234500
C	-3.17986100	1.85347900	0.22733400
C	-4.37343900	1.18866700	0.55889800
C	-4.48776200	-0.19831200	0.52513300
C	-3.39249400	-0.99450000	0.15165200
C	-0.93841900	-0.92053000	-0.59535300
C	-0.72749700	1.42495000	-0.54924400
H	-3.09796400	2.93405200	0.25119300
H	-5.24086800	1.77242900	0.84993600
H	-5.42056100	-0.68867500	0.78242000
O	-0.68412300	-2.08915900	-0.77286600
O	-0.23633400	2.50726600	-0.69748900
N	-0.05475800	0.17458000	-0.77486700
S	1.51688200	0.04189000	-1.36906600
C	2.44542400	-0.07479100	0.21167700
Cl	1.99236500	-1.51805500	1.14444400
Cl	2.20999200	1.36031200	1.23055900
Cl	4.14313500	-0.18928900	-0.31117300
O	-3.51017600	-2.33104000	0.11431800
H	-2.66693500	-2.72416600	-0.17003400