

Supporting Information for

Quantum Chemical and Kinetic Study on Dioxin Formation from the 2,4,6-TCP and 2,4-DCP Precursors

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Table S1. Imaginary frequencies (cm^{-1}), zero point energies (ZPE, a.u.), and total energies (a.u.) for the transition states involved in the formation of PCDDs from the 2,4,6-TCP precursor.

Transition States	Imaginary frequencies	ZPE	Total energies
TS1	895i	0.13612	-3372.01523
TS2	586i	0.13442	-3831.73535
TS3	370i	0.14588	-3447.22843
TS4	545i	0.13190	-2911.20945
TS5	871i	0.13139	-2911.21972
TS6	549i	0.13170	-2911.21893
TS7	448i	0.13201	-2911.20882

Table S2. Imaginary frequencies (cm^{-1}), zero point energies (ZPE, a.u.), and total energies (a.u.) for the transition states involved in the formation of PCDD/Fs from the 2,4-DCP precursor.

Transition States	Imaginary frequencies	ZPE	Total energies
TS8	847i	0.15578	-2452.64280
TS9	509i	0.15398	-2912.36391
TS10	308i	0.16487	-2527.85450
TS11	516i	0.15167	-1991.83425
TS12	447i	0.15211	-1991.83852
TS13	1000i	0.14592	-1991.81589
TS14	728i	0.15083	-1991.84174
TS15	461i	0.15127	-1991.84120
TS16	381i	0.15207	-1991.83915
TS17	1000i	0.14605	-1991.81593
TS18	524i	0.15108	-1991.84193
TS19	454i	0.15153	-1991.83453
TS20	1156i	0.15375	-2452.64667
TS21	331i	0.16354	-2527.87634
TS22	135i	0.15307	-2912.37678
TS23	497i	0.14166	-2451.52325
TS24	431i	0.14224	-2451.52734
TS25	1004i	0.13603	-2451.50313
TS26	717i	0.14116	-2451.53104
TS27	390i	0.14153	-2451.52995
TS28	347i	0.14234	-2451.52715
TS29	1000i	0.13604	-2451.50285
TS30	451i	0.14153	-2451.53060
TS31	418i	0.14181	-2451.52300
TS32	1250i	0.15289	-2452.63442
TS33	456i	0.16242	-2527.86664
TS34	2393i	0.13771	-2451.51812
TS35	563i	0.14190	-2451.53962
TS36	480i	0.14113	-2451.53869
TS37	1546i	0.14969	-2452.11007
TS38	2250i	0.15308	-2452.69998
TS39	912i	0.15537	-2452.62202
TS40	671i	0.16585	-2527.83185
TS41	446i	0.15312	-2912.33716
TS42	2201i	0.14767	-1991.83010
TS43	531i	0.15161	-1991.85235
TS44	493i	0.15096	-1991.85028

Table S3. Cartesian coordinates for the reactants and products.

2,4-DCP

C	-1.33005700	0.57842100	0.00000000
C	0.00000000	0.94538500	0.00000000
C	0.96551400	-0.04244300	0.00000000
C	0.62676000	-1.38925600	0.00000000
C	-0.71661200	-1.73108000	0.00000000
C	-1.69279900	-0.75705700	0.00000000
H	0.28848200	1.98313300	0.00000000
H	-0.97724300	-2.77706800	0.00000000
O	1.53600600	-2.37280600	0.00000000
H	2.42025100	-2.00268300	0.00000000
Cl	2.64134500	0.38518200	0.00000000
Cl	-2.54731800	1.80222900	0.00000000
H	-2.73482700	-1.03074100	0.00000000

2,4-DCPR

C	-1.31867700	0.47482900	0.00000000
C	0.00000000	0.92276000	0.00000000
C	1.01669400	0.00589100	0.00000000
C	0.75296300	-1.42167300	0.00000000
C	-0.63379000	-1.80808000	0.00000000
C	-1.63835000	-0.89031700	0.00000000
H	0.21255900	1.97897900	0.00000000
H	-0.83461400	-2.86749400	0.00000000
O	1.66235000	-2.25725400	0.00000000
Cl	2.63876500	0.51731200	0.00000000
Cl	-2.58444800	1.62608900	0.00000000
H	-2.67317200	-1.19172800	0.00000000

2,4,6-TCP

C	0.00671200	-1.60862800	0.00000000
C	-1.19760100	-0.93580200	0.00000000
C	-1.18297900	0.44412600	0.00000000
C	0.00000000	1.17382400	0.00000000
C	1.19414900	0.45982300	0.00000000
C	1.20457800	-0.92014300	0.00000000
H	-2.13309700	-1.46889000	0.00000000
O	0.04022000	2.50642700	0.00000000
H	-0.85146700	2.85922200	0.00000000

Cl	-2.67155400	1.32128800	0.00000000
Cl	0.01714100	-3.33279000	0.00000000
Cl	2.67621300	1.32487400	0.00000000
H	2.14305800	-1.44827200	0.00000000

2,4,6-TCPR

C	0.00007100	-1.56246500	0.00000000
C	-1.22198600	-0.88963000	0.00000000
C	-1.22643400	0.47585500	0.00000000
C	0.00000000	1.25585300	0.00000000
C	1.22637900	0.47597800	0.00000000
C	1.22205600	-0.88956000	0.00000000
H	-2.14565800	-1.44365300	0.00000000
O	0.00002100	2.48333000	0.00000000
Cl	-2.69238000	1.33681000	0.00000000
Cl	-0.00009900	-3.27236500	0.00000000
Cl	2.69243200	1.33698800	0.00000000
H	2.14577600	-1.44352100	0.00000000

1,3,6,8-TeCDD

C	1.19766400	0.62517300	0.00000000
C	0.01307000	1.34386700	0.00000000
C	0.06981900	2.72553200	0.00000000
C	1.28600600	3.38643700	0.00000000
C	2.44794500	2.64304600	0.00000000
C	2.41840900	1.26126700	0.00000000
O	1.19766400	-0.73385900	0.00000000
H	3.32101200	0.67411500	0.00000000
C	-0.01307000	-1.34386700	0.00000000
C	-0.06981900	-2.72553200	0.00000000
C	-1.28600600	-3.38643700	0.00000000
C	-2.44794500	-2.64304600	0.00000000
C	-2.41840900	-1.26126700	0.00000000
C	-1.19766400	-0.62517300	0.00000000
H	-3.32101200	-0.67411500	0.00000000
O	-1.19766400	0.73385900	0.00000000
Cl	3.96904800	3.45219700	0.00000000
Cl	-3.96904800	-3.45219700	0.00000000
Cl	1.39208400	-3.62250700	0.00000000
Cl	-1.39208400	3.62250700	0.00000000
H	-1.31374800	-4.46241800	0.00000000
H	1.31374800	4.46241800	0.00000000

1,3,7,9-TeCDD

C	-0.39320400	1.15205600	0.00000000
C	0.99272100	1.15919800	0.00000000
C	1.69994100	2.33990400	0.00000000
C	1.00255500	3.53319300	0.00000000
C	-0.37660000	3.55851400	0.00000000
C	-1.06776700	2.35918800	0.00000000
O	-1.10744200	-0.00000100	0.00000000
C	-0.39320800	-1.15205500	0.00000000
C	-1.06775800	-2.35919400	0.00000000
C	-0.37660000	-3.55852200	0.00000000
C	1.00255500	-3.53319300	0.00000000
C	1.69993800	-2.33990400	0.00000000
C	0.99271700	-1.15920300	0.00000000
H	2.77638200	-2.31275400	0.00000000
O	1.70267000	-0.00000300	0.00000000
Cl	1.87673500	-5.01790400	0.00000000
Cl	-2.78188700	-2.35999900	0.00000000
H	-0.91603700	-4.48994800	0.00000000
Cl	-2.78186700	2.35997400	0.00000000
Cl	1.87676900	5.01793700	0.00000000
H	-0.91603000	4.48994400	0.00000000
H	2.77638500	2.31276100	0.00000000

2,7-DCDD

C	-0.92897300	-0.97641400	0.00000000
C	0.42350900	-1.28000300	0.00000000
C	0.84184400	-2.59292500	0.00000000
C	-0.10326800	-3.60196800	0.00000000
C	-1.45391900	-3.31408300	0.00000000
C	-1.85957500	-1.99142300	0.00000000
O	-1.37585400	0.31039600	0.00000000
H	1.89695000	-2.80986700	0.00000000
H	-2.90570600	-1.73077800	0.00000000
C	-0.42350900	1.28000300	0.00000000
C	-0.84184400	2.59292500	0.00000000
C	0.10326800	3.60196800	0.00000000
C	1.45391800	3.31408300	0.00000000
C	1.85957500	1.99142300	0.00000000
C	0.92897300	0.97641400	0.00000000
H	-1.89695100	2.80986500	0.00000000
H	2.90570600	1.73077800	0.00000000

O	1.37585500	-0.31039700	0.00000000
Cl	0.42350900	-5.24521700	0.00000000
Cl	-0.42350900	5.24521800	0.00000000
H	2.17951500	4.10968600	0.00000000
H	-2.17951600	-4.10968600	0.00000000

2,8-DCDD

C	1.15638200	1.09215400	-0.00009700
C	1.15599900	-0.29394400	-0.00018300
C	2.34388700	-0.99192600	-0.00009800
C	3.53642200	-0.29248900	0.00006000
C	3.55289000	1.08859800	0.00014600
C	2.35213500	1.77578400	0.00007200
O	0.00001300	-1.01098600	-0.00036500
H	2.32221100	-2.06891500	-0.00016400
H	2.32845200	2.85365600	0.00013700
C	-1.15600500	-0.29393800	-0.00018600
C	-2.34388400	-0.99193200	-0.00010300
C	-3.53642500	-0.29249700	0.00005800
C	-3.55289200	1.08860900	0.00014500
C	-2.35214000	1.77579500	0.00006900
C	-1.15638100	1.09215800	-0.00009900
H	-2.32219900	-2.06892100	-0.00016900
H	-2.32845400	2.85366800	0.00013400
O	0.00000000	1.80977000	-0.00019700
Cl	5.02347700	-1.16881300	0.00015500
Cl	-5.02347900	-1.16881800	0.00015700
H	4.48915400	1.62086100	0.00027100
H	-4.48915900	1.62086900	0.00027200

1,3,7-TCDD

C	-1.33981000	0.84610600	0.00056600
C	-1.48314700	-0.52987500	0.00081900
C	-2.73667000	-1.10141400	0.00045800
C	-3.84905800	-0.27988400	-0.00014000
C	-3.72050100	1.09553500	-0.00024100
C	-2.45467900	1.65430600	0.00022700
O	-0.40472000	-1.36116300	0.00130000
H	-2.82851300	-2.17462500	0.00057500
H	-2.31615700	2.72345400	0.00020200
C	0.82040600	-0.77358000	0.00061900
C	1.92299400	-1.59851600	0.00020500

C	3.18275700	-1.02919400	-0.00020500
C	3.35121300	0.33946500	-0.00034700
C	2.22899600	1.14950600	-0.00001100
C	0.95680900	0.60627200	0.00051800
H	4.33362000	0.77915700	-0.00073300
O	-0.11185600	1.43716000	0.00087600
Cl	2.40880100	2.85553700	-0.00045100
Cl	-5.41962400	-0.99338200	-0.00090300
Cl	4.56844400	-2.05421800	-0.00053200
H	-4.59573200	1.72318400	-0.00062200
H	1.78397500	-2.66641700	0.00043100

1,3,8-TCDD

C	0.00000000	0.95482800	0.00000000
C	-0.18511000	2.32550400	0.00000000
C	0.89460500	3.19115500	0.00000000
C	2.16872300	2.66326300	0.00000000
C	2.38173900	1.29786800	0.00000000
C	1.29381300	0.45399700	0.00000000
O	-1.08641600	0.14581500	0.00000000
Cl	-1.78213700	2.95264600	0.00000000
H	0.73189900	4.25514100	0.00000000
C	-0.84358300	-1.19353500	0.00000000
C	-1.92828400	-2.04237300	0.00000000
C	-1.71151100	-3.40816100	0.00000000
C	-0.43179500	-3.92794900	0.00000000
C	0.64723900	-3.06235300	0.00000000
C	0.44462900	-1.70036600	0.00000000
H	-2.92280600	-1.62867600	0.00000000
H	1.65940600	-3.43363100	0.00000000
O	1.53439200	-0.88201900	0.00000000
Cl	3.52453000	3.72689900	0.00000000
Cl	-3.06776100	-4.47374600	0.00000000
H	3.37428200	0.88075000	0.00000000
H	-0.27812100	-4.99378600	0.00000000

2,4,8-TCDF

C	-1.03402300	2.63345000	0.00000000
C	-2.29467800	2.04457900	0.00000000
C	-2.41685100	0.66927600	0.00000000
C	-1.25960900	-0.08210600	0.00000000
C	0.00000000	0.50946600	0.00000000

C	0.12699100	1.88974200	0.00000000
H	-3.17883000	2.65955500	0.00000000
O	-1.19296800	-1.42958300	0.00000000
Cl	-3.95403400	-0.08783000	0.00000000
Cl	-0.93419400	4.35768000	0.00000000
H	2.95208000	0.14502000	0.00000000
C	2.30516100	-0.71686400	0.00000000
C	2.83297700	-1.99042500	0.00000000
C	0.92346500	-0.59626300	0.00000000
C	2.02615400	-3.12616600	0.00000000
C	0.12912500	-1.73764600	0.00000000
C	0.64943700	-3.01299500	0.00000000
H	0.01108800	-3.88079500	0.00000000
H	1.08936300	2.37393300	0.00000000
Cl	4.55010300	-2.19139400	0.00000000
H	2.48927400	-4.09911700	0.00000000

2,4,6,8-TeCDF

C	0.00000000	3.01254200	-1.22641500
C	0.00000000	3.36998400	0.11864200
C	0.00000000	2.39479700	1.09622300
C	0.00000000	1.07664800	0.68940700
C	0.00000000	0.72092000	-0.65504000
C	0.00000000	1.69733600	-1.63953800
H	0.00000000	4.40914100	0.40163700
O	0.00000000	0.00000000	1.50505700
Cl	0.00000000	2.79879700	2.76017700
Cl	0.00000000	4.26984500	-2.40920500
H	0.00000000	-4.40914100	0.40163700
C	0.00000000	-3.36998400	0.11864200
C	0.00000000	-3.01254200	-1.22641500
C	0.00000000	-2.39479700	1.09622300
C	0.00000000	-1.69733600	-1.63953800
Cl	0.00000000	-4.26984500	-2.40920500
C	0.00000000	-1.07664800	0.68940700
Cl	0.00000000	-2.79879700	2.76017700
C	0.00000000	-0.72092000	-0.65504000
H	0.00000000	1.45022900	-2.68806200
H	0.00000000	-1.45022900	-2.68806200

Table S4. Cartesian coordinates for the intermediates.

IM1

C	1.24366700	0.48806400	-0.54762800
C	1.42224500	-0.84764700	-0.87603600
C	2.64428200	-1.47045800	-0.72825500
C	3.71101600	-0.72812800	-0.26152800
C	3.57154400	0.60840800	0.05534200
C	2.33622800	1.20953200	-0.08978700
O	0.06891300	1.11955000	-0.80348200
Cl	0.07796700	-1.74419900	-1.46487000
H	2.75907900	-2.51101200	-0.97899000
C	-1.09588000	0.94686600	-0.07861300
C	-2.21364300	0.81638100	-1.04402000
C	-3.21320500	-0.02445700	-0.80731300
C	-3.25553700	-0.88241100	0.35897000
C	-2.24130500	-0.92041400	1.22778200
C	-1.02707300	-0.11696800	1.02413400
Cl	-1.42256700	2.45959100	0.87050600
H	-2.17140700	1.45041400	-1.91378900
O	-0.04079100	-0.22547900	1.69618000
Cl	5.24746800	-1.48397400	-0.07716600
Cl	-4.53955400	-0.15874200	-1.89428300
H	-4.12272700	-1.50593100	0.50548700
Cl	-2.24375200	-1.95267200	2.58499200
Cl	2.15141500	2.86591900	0.30035500
H	4.40942100	1.18064600	0.41533000

IM2

C	-1.19319900	-0.74745300	0.14702200
C	-2.11773200	-1.05903100	-0.83632100
C	-3.40648500	-0.56796800	-0.78101800
C	-3.76771600	0.24183500	0.27751600
C	-2.87018200	0.55774200	1.27782800
C	-1.58898500	0.04945500	1.20964300
O	0.03240100	-1.33786500	0.10687700
Cl	-1.63775800	-2.04936100	-2.15128200
H	-4.11078300	-0.81180300	-1.55786700
C	1.18046900	-0.65264300	0.00654500
C	2.31451600	-1.28495900	0.44590900
C	3.53392100	-0.63564900	0.32811800
C	3.65282300	0.64386700	-0.22598100

C	2.53103100	1.27178500	-0.67805000
C	1.22037900	0.65748800	-0.61363600
H	2.24394300	-2.26430300	0.88803300
O	0.20645500	1.19521300	-1.06330000
Cl	-5.37179600	0.86474000	0.35524000
Cl	4.94827300	-1.41566100	0.89346500
Cl	2.62081100	2.82592800	-1.36783700
H	4.61708700	1.11858800	-0.29255300
H	-3.15961300	1.18513200	2.10348000
Cl	-0.46744400	0.42534100	2.45657900

IM3

C	0.91969800	0.02205100	-0.14933300
C	1.72819700	-1.23412300	-0.10152900
C	3.07945600	-1.25641000	-0.10877400
C	3.79499800	-0.04999600	-0.16518600
C	3.13987300	1.19030600	-0.21435800
C	1.78895800	1.23565100	-0.20791000
O	0.05402200	-0.00475800	-1.28094200
Cl	0.81000800	-2.67032700	-0.03446300
H	3.60789100	-2.19456700	-0.07136600
C	-1.21968200	-0.00506300	-0.82338800
C	-2.37492900	-0.05327800	-1.55173200
C	-3.55404300	-0.03999400	-0.80922400
C	-3.56664800	0.01736800	0.56867400
C	-2.36457100	0.06574800	1.27253200
C	-1.20156100	0.05443600	0.55259700
H	-2.37857200	-0.09961600	-2.62653200
O	0.07358500	0.09489000	0.99521800
Cl	5.50209700	-0.09185700	-0.17355000
Cl	-5.05782600	-0.10025600	-1.65581600
H	3.71367900	2.10119200	-0.25609500
H	-4.49910600	0.02392200	1.10666500
Cl	0.94116600	2.71406600	-0.26419300
Cl	-2.34151700	0.13471800	2.98442900

IM4

C	-1.18778900	0.43198800	0.19413700
C	-2.10503700	1.06868200	-0.62453900
C	-3.39374800	0.58889200	-0.74893100
C	-3.75899900	-0.53680800	-0.03804100
C	-2.86635400	-1.18220900	0.79492000

C	-1.58502400	-0.68391000	0.91309000
O	0.23473900	-0.98459000	-1.57885300
Cl	-1.61814100	2.45403700	-1.50788700
H	-4.09540900	1.08785500	-1.39516800
C	1.25441700	-0.61947200	-0.97974400
C	2.54687100	-1.17185800	-1.27443100
C	3.64974400	-0.71304100	-0.63287400
C	3.56333100	0.30371600	0.33484600
C	2.33875600	0.85335100	0.65926500
C	1.18173700	0.40653200	0.04428800
H	2.59256300	-1.94287200	-2.02497800
O	0.03692800	1.00044000	0.37609600
Cl	-5.36316100	-1.14597500	-0.18803700
Cl	5.20604500	-1.35868200	-0.98622300
H	-3.16011700	-2.05621600	1.35068600
H	4.45288900	0.65350100	0.83129600
Cl	-0.46382100	-1.46648400	1.95214800
Cl	2.25139000	2.08509000	1.84813600

IM5

C	1.07180200	0.25126900	-0.63635200
C	1.64106200	-0.98223400	-0.36086900
C	2.99553500	-1.08956500	-0.11571300
C	3.77433400	0.05093600	-0.15556200
C	3.22292400	1.28490700	-0.44570300
C	1.86761800	1.37789000	-0.69357500
O	-0.25291000	0.30880500	-0.97867900
Cl	0.65163300	-2.38750900	-0.31683400
H	3.43199900	-2.04904700	0.10444000
H	1.41265300	2.32429200	-0.93273900
C	-1.23686500	0.69280000	-0.09580500
C	-2.52621100	0.39627500	-0.76953600
C	-3.50041200	-0.23554500	-0.12746700
C	-3.36406900	-0.69618500	1.24355300
C	-2.22598100	-0.53634300	1.92195100
C	-1.06884200	0.10982300	1.31681200
Cl	-1.20581200	2.49556500	0.16804000
H	-2.61711500	0.72416900	-1.79177400
H	-2.10137600	-0.88879100	2.93282000
O	-0.00994200	0.21646400	1.87859500
Cl	5.46719100	-0.07753900	0.15103300
Cl	-5.00497200	-0.56189400	-0.89704500
H	-4.21405600	-1.18453200	1.69397700

H	3.84866700	2.16098900	-0.48475700
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IM6

C	1.38185600	0.12845000	0.20190000
C	2.42207600	0.99831100	0.51508800
C	3.72930200	0.67115800	0.21684500
C	4.00030800	-0.53107700	-0.40816000
C	2.98197600	-1.40841700	-0.72188700
C	1.67641500	-1.07880600	-0.40631900
O	0.13308000	0.52465500	0.53505300
Cl	2.07785100	2.50329200	1.27041300
H	4.52313900	1.35633100	0.46255600
H	0.88700900	-1.78821500	-0.59203600
C	-0.95582700	0.10892000	-0.22967800
C	-1.85567900	1.26875400	-0.46667100
C	-3.16950800	1.08725500	-0.53654800
C	-3.78905100	-0.19884600	-0.28237100
C	-3.06756500	-1.25047100	0.12339800
C	-1.61988700	-1.12578500	0.36272100
H	-4.85865100	-0.28223100	-0.39202500
O	-0.97410500	-1.95756100	0.93949400
H	-0.61129600	-0.22760100	-1.22039200
Cl	-3.79036200	-2.74359800	0.52679700
Cl	5.63387500	-0.93506600	-0.79208600
Cl	-4.24084200	2.38201200	-0.91340300
H	3.20530200	-2.35224000	-1.19110000
H	-1.39266900	2.22765600	-0.63254900

IM7

C	-0.87109100	0.33338600	-0.30179200
C	-1.97141200	1.13153900	-0.03874400
C	-3.24248000	0.58853600	-0.05831200
C	-3.40153300	-0.75269400	-0.34441700
C	-2.31002100	-1.55522200	-0.62006800
C	-1.04626400	-1.00233100	-0.60632700
O	0.35555200	0.92800800	-0.34920600
Cl	-1.75725200	2.79592300	0.32052700
H	-4.09450700	1.21237900	0.15315600
H	-0.18434500	-1.61233600	-0.82830500
C	1.44700000	0.26645100	0.05955500
C	2.59214600	0.38847700	-0.68632400
C	3.75580700	-0.22946000	-0.24585400

C	3.79852300	-0.97282900	0.94428600
C	2.67343900	-1.08209600	1.70112500
C	1.43863800	-0.45260500	1.32081000
H	2.57587000	0.95395300	-1.60324900
H	2.66649900	-1.63233800	2.62850400
O	0.42423000	-0.49503700	2.02861800
Cl	-4.98891800	-1.42912000	-0.36320400
Cl	5.17839000	-0.09118200	-1.18803600
H	-2.44919200	-2.59853500	-0.84943600
H	4.72315500	-1.43936500	1.24254000

IM8

C	0.82476900	0.52996600	0.21122400
C	1.91181400	1.31546100	-0.01501300
C	3.19387400	0.75890500	-0.05125600
C	3.33839300	-0.63529200	0.11503800
C	2.29648800	-1.45966900	0.34676000
C	0.92752800	-0.92197800	0.49632900
O	-0.41136900	1.04561500	0.23652900
Cl	1.71227800	2.99966700	-0.28920800
H	4.05024300	1.38210400	-0.23878900
H	0.56403800	-1.09544100	1.52063900
C	-1.44970500	0.17340200	0.08953100
C	-2.72941100	0.67115900	0.22947800
C	-3.79638700	-0.17391200	0.00348100
C	-3.59984000	-1.49541500	-0.36007800
C	-2.31226500	-1.98199600	-0.47884100
C	-1.22975300	-1.15505300	-0.24933900
H	-2.87239900	1.70578800	0.49288300
H	-2.12746700	-3.00930600	-0.74884500
O	0.03295500	-1.63052500	-0.36324700
Cl	4.93647800	-1.28080000	0.00191800
Cl	-5.40312400	0.43424500	0.17204300
H	2.43033100	-2.52227700	0.46005300
H	-4.44619900	-2.13794900	-0.53688700

IM9

C	-0.76878200	-0.31740400	0.13271600
C	-1.62037200	0.89735200	-0.04196000
C	-2.96802500	0.84691400	-0.16992200
C	-3.62153300	-0.39221000	-0.13923400
C	-2.90257100	-1.59572600	0.02436000

C	-1.56211400	-1.57214300	0.15394400
O	0.19553000	-0.38329600	-0.92291100
Cl	-0.77701700	2.38061800	-0.07041000
H	-3.53628300	1.75406100	-0.29368500
H	-0.98895700	-2.47691800	0.28066800
C	1.42299100	-0.29877400	-0.35950700
C	2.63958900	-0.31966400	-0.98436400
C	3.75272200	-0.22500000	-0.15059500
C	3.64196400	-0.11745300	1.22035700
C	2.38631000	-0.09945100	1.82877800
C	1.29629300	-0.19178300	1.00868300
H	2.73567900	-0.40271600	-2.05314200
H	2.28209600	-0.01582900	2.89756400
O	-0.01754200	-0.20604300	1.34275500
Cl	-5.32202000	-0.44369100	-0.30209800
Cl	5.32334700	-0.24607200	-0.87425000
H	-3.44176400	-2.52910100	0.04410200
H	4.53323600	-0.04725300	1.82109500

IM10

C	-1.02291500	0.40221700	0.45795200
C	-2.11105900	1.07644400	-0.06764300
C	-3.31993400	0.42510100	-0.22535300
C	-3.42744200	-0.89927900	0.14960100
C	-2.34828100	-1.57811500	0.68609700
C	-1.14855500	-0.91726500	0.84651500
O	0.67651000	-0.48080900	-1.53678800
H	-4.16284400	0.95114300	-0.64077000
C	1.57778900	-0.23149400	-0.72615200
C	2.92337900	-0.70417400	-0.91193700
C	3.90607600	-0.35217700	-0.04451100
C	3.64011500	0.47923900	1.06009300
C	2.35890200	0.94076200	1.29237100
C	1.32852900	0.58335500	0.44905900
H	3.11098800	-1.32557900	-1.77191900
O	0.12258100	1.11117100	0.67883300
Cl	-4.93576400	-1.71297000	-0.04972800
H	-2.44952500	-2.60951400	0.98017300
H	2.14511300	1.57806200	2.13510500
Cl	-1.95750900	2.72074500	-0.53397700
H	-0.29625900	-1.42710500	1.26859700
H	4.44439500	0.74653100	1.72570500
Cl	5.52126100	-0.90801600	-0.27687200

IM11

C	-0.96296200	0.66642200	0.24853800
C	-2.18865400	1.17698300	-0.04672000
C	-3.30557100	0.34108300	-0.12777800
C	-3.13516700	-1.04692100	0.06541800
C	-1.94513900	-1.60633500	0.36568300
C	-0.74595500	-0.76593600	0.56863400
O	0.33367700	-1.26427900	-0.22527000
Cl	-2.36692700	2.85791000	-0.35525300
H	-4.27130500	0.74783400	-0.37033900
H	-0.40858600	-0.83579000	1.61380400
C	1.44409100	-0.50751200	-0.07221500
C	2.69194700	-1.07865700	-0.23367400
C	3.81581800	-0.29266000	-0.07474300
C	3.71661800	1.04879000	0.25456400
C	2.46643800	1.61391200	0.40949800
C	1.33624200	0.84174200	0.23691200
H	2.76501000	-2.12528100	-0.47772800
H	2.35099100	2.65919900	0.64662600
O	0.11821500	1.45307700	0.31407600
Cl	-4.53418800	-2.04471200	-0.10650300
Cl	5.37483500	-1.00579500	-0.27746000
H	-1.83725100	-2.66970300	0.49853600
H	4.60653400	1.64205000	0.38062200

IM12

C	1.15070500	-0.37302900	0.87067900
C	2.00431100	-1.45223300	0.95144700
C	3.27180700	-1.38263400	0.40892200
C	3.67670100	-0.21446600	-0.20879100
C	2.83969200	0.88248100	-0.27762300
C	1.57711200	0.80307300	0.27541900
O	-0.41768400	-0.92652300	-1.25072300
H	3.93830000	-2.22739900	0.45997400
C	-1.38352400	-0.60310000	-0.54531100
C	-2.70883400	-0.47990000	-1.08957100
C	-3.76107800	-0.17425400	-0.29137400
C	-3.58877000	0.03447600	1.09095400
C	-2.33513500	-0.05652800	1.65700000
C	-1.23514700	-0.34770700	0.87436100
H	-2.81961000	-0.65202900	-2.14725400
O	-0.06059500	-0.46028700	1.50431000

Cl	5.25537900	-0.11171600	-0.89678300
H	3.16324600	1.79398400	-0.75119800
Cl	0.53518300	2.16907400	0.21117100
H	1.65450700	-2.35132400	1.43193900
H	-2.19121500	0.10993500	2.71220400
Cl	-5.35061200	-0.03781800	-0.94564700
H	-4.44518200	0.27206700	1.70037800

IM13

C	-1.22780200	-0.66023400	-0.15847200
C	-2.32823500	-1.02701700	0.59722900
C	-3.56795100	-0.47858300	0.32813400
C	-3.69484400	0.43438800	-0.69957200
C	-2.60329800	0.79891900	-1.46645400
C	-1.37152800	0.23933800	-1.19617600
O	-0.04382000	-1.29053500	0.09612100
Cl	-2.15308500	-2.15693000	1.87679700
H	-4.42017500	-0.76202000	0.92243600
H	-0.51036200	0.50680500	-1.78908800
C	1.12212100	-0.64221500	-0.00337100
C	2.18910600	-1.31811000	-0.53193500
C	3.42970300	-0.69230300	-0.57333200
C	3.63093400	0.60611600	-0.09537500
C	2.57754500	1.28010000	0.45030000
C	1.25860600	0.68927200	0.56351100
H	4.60573900	1.06009100	-0.15469700
O	0.31578900	1.25315100	1.11823600
Cl	2.77166300	2.85700800	1.05930400
Cl	-5.24162400	1.12228400	-1.03193400
Cl	4.75974900	-1.53254800	-1.24544400
H	-2.71803900	1.50763800	-2.26963000
H	2.05698500	-2.31830500	-0.90907500

IM14

C	-1.12084500	0.80379400	0.23146800
C	-2.27197700	1.44629600	-0.10005000
C	-3.48856100	0.75743300	-0.11532800
C	-3.49831100	-0.62254900	0.18264100
C	-2.38734500	-1.30820400	0.52162000
C	-1.08670500	-0.61861100	0.65066800
O	0.05805500	1.44350300	0.23160400
Cl	-2.23570000	3.10721700	-0.53636700

H	-4.39642800	1.26624900	-0.38707300
H	-0.73481900	-0.66435600	1.69179700
C	1.18290400	0.67819900	0.16329600
C	2.39954700	1.32175400	0.25624700
C	3.55017200	0.57541200	0.10785200
C	3.50186200	-0.78614300	-0.12974100
C	2.27190400	-1.41037700	-0.20308000
C	1.09554500	-0.69121500	-0.05252600
H	4.40569600	-1.35887400	-0.24725900
O	-0.10107500	-1.30502700	-0.12673900
Cl	2.17974900	-3.10018900	-0.48251900
Cl	-5.01640800	-1.43924400	0.09121200
Cl	5.08213600	1.35885200	0.21416300
H	-2.41441800	-2.36383000	0.73358000
H	2.42876700	2.38547500	0.42132300

IM15

C	-1.01059600	-0.14004400	-0.35911700
C	-1.84190400	-0.26184700	0.87579700
C	-3.19630300	-0.26357600	0.85925800
C	-3.87578000	-0.15361500	-0.36103500
C	-3.17552100	-0.04182800	-1.58112200
C	-1.82876600	-0.03645200	-1.59241900
O	-0.12989400	-1.26479200	-0.46304100
Cl	-0.96978600	-0.39522800	2.33649200
H	-3.75015900	-0.34959800	1.77960300
H	-1.26962200	0.04858000	-2.51061200
C	1.13741600	-0.80933100	-0.34555100
C	2.29642300	-1.53433700	-0.35372600
C	3.47116800	-0.79528600	-0.22651100
C	3.47749300	0.57783400	-0.10129100
C	2.27270900	1.27902500	-0.09806300
C	1.11278700	0.56349800	-0.22018700
H	4.40612100	1.11392200	-0.00541400
O	-0.15996100	1.00832600	-0.25448800
Cl	2.24279000	2.98643600	0.05135300
Cl	-5.58390800	-0.15616300	-0.36932300
Cl	4.97712200	-1.64083300	-0.22730100
H	-3.73359600	0.03881100	-2.49995800
H	2.30562000	-2.60584000	-0.45035300

IM16

C	1.20261700	0.37898600	-0.15112900
C	2.27871900	0.82125100	0.59727900
C	3.51759600	0.22841600	0.44016100
C	3.66501100	-0.80024600	-0.46908700
C	2.59636200	-1.23946800	-1.22921100
C	1.36544800	-0.63718600	-1.07089300
O	-0.31170800	-1.27608900	1.44174400
H	4.35297500	0.56835500	1.02873900
C	-1.27719300	-0.82694400	0.81386600
C	-2.57070600	-1.45052500	0.85568900
C	-3.62318500	-0.88546200	0.21141300
C	-3.48261200	0.31079600	-0.51288400
C	-2.24958700	0.93360600	-0.59651200
C	-1.13968700	0.38349200	0.01856600
O	0.01340500	1.04396800	-0.02919000
Cl	5.21144800	-1.54043700	-0.66066700
H	2.72956100	-2.03713200	-1.94085600
Cl	2.07270300	2.09371800	1.72822100
H	0.51967100	-0.95690800	-1.66013100
H	-2.66348100	-2.35848100	1.42766800
H	-4.33374700	0.74332200	-1.01163200
Cl	-5.18112600	-1.61617100	0.26536800
Cl	-2.09804000	2.39215800	-1.48514400

IM17

C	1.14883300	0.48514900	0.17329100
C	2.31351900	1.09751000	-0.16948800
C	3.51282300	0.37911200	-0.18150800
C	3.49107300	-0.99707900	0.13249600
C	2.36568500	-1.65262500	0.48296900
C	1.08172600	-0.93161600	0.60501800
O	0.07920600	-1.60103400	-0.16676800
Cl	2.31482200	2.75346400	-0.62227600
H	4.43157300	0.86328200	-0.46159300
H	0.72837800	-0.95935700	1.64637300
C	-1.10970400	-0.96562600	-0.09226500
C	-2.27712000	-1.68839400	-0.23960600
C	-3.48475800	-1.02548700	-0.16225800
C	-3.55075600	0.33546800	0.07426400
C	-2.37557200	1.04735700	0.21452900
C	-1.15011700	0.40766100	0.12059100
H	-4.49834000	0.84135300	0.14349800
O	-0.01485000	1.15149500	0.17093600

Cl	-2.42128400	2.73982700	0.48416100
Cl	4.98970600	-1.84999900	0.04737100
Cl	-4.94896700	-1.91632100	-0.34521900
H	2.37065500	-2.70551100	0.70973100
H	-2.22361700	-2.75054600	-0.40817300

IM18

C	-1.32704300	0.59013100	-0.45181900
C	-2.20190400	0.69456900	-1.51162100
C	-3.51056900	0.27644900	-1.38085500
C	-3.93440300	-0.24124200	-0.17134000
C	-3.07314200	-0.33342700	0.90447400
C	-1.76730500	0.09472900	0.76480300
O	0.11428800	-1.64634400	-0.95710100
H	-4.19544600	0.34896400	-2.20911700
C	1.12153400	-1.00599300	-0.63038800
C	2.39823700	-1.63893900	-0.45002800
C	3.49336000	-0.89820800	-0.14921100
C	3.41472400	0.49837100	-0.00178600
C	2.20416100	1.14495400	-0.14977700
C	1.05122100	0.43143800	-0.43383800
O	-0.07274200	1.11904000	-0.61012200
Cl	-5.56540200	-0.77121100	0.00993800
H	-3.41094600	-0.72595500	1.84877000
Cl	-0.70090700	0.00688800	2.11062500
H	-1.83748800	1.09862000	-2.44190900
H	4.29878900	1.06715600	0.23285600
H	2.43958100	-2.70761600	-0.57700900
Cl	5.03147000	-1.64499300	0.05762700
Cl	2.12659900	2.84815600	0.03666300

IM19

C	2.05705000	-1.36554600	0.85901800
C	3.18733000	-0.55541200	0.46055200
C	3.07513500	0.37874100	-0.49304400
C	1.78273200	0.65528000	-1.13459500
C	0.68052900	-0.34889400	-0.88903100
C	0.87350600	-1.26986000	0.26070200
H	4.13010300	-0.70817600	0.96164500
H	0.68189900	-0.98302000	-1.78599500
O	1.60083900	1.61786200	-1.83858200
Cl	4.38821400	1.37660800	-0.93781100

Cl	2.33324300	-2.47478700	2.14964000
H	-4.13010300	0.70817600	0.96164600
C	-3.18733000	0.55541200	0.46055200
C	-2.05705000	1.36554600	0.85901800
C	-3.07513500	-0.37874200	-0.49304400
C	-0.87350600	1.26986000	0.26070100
Cl	-2.33324300	2.47478700	2.14964000
C	-1.78273200	-0.65528000	-1.13459400
Cl	-4.38821400	-1.37660900	-0.93781000
C	-0.68052900	0.34889400	-0.88903200
O	-1.60083900	-1.61786200	-1.83858200
H	-0.68189900	0.98302000	-1.78599600
H	0.05122500	-1.90594700	0.55030000
H	-0.05122600	1.90594800	0.55029900

IM20

C	-2.79892200	0.98123400	-0.81093900
C	-3.45815600	-0.00285800	0.01959000
C	-2.77718900	-1.01708200	0.56690600
C	-1.31831000	-1.13948900	0.39597100
C	-0.70470300	-0.27876400	-0.69869600
C	-1.51256200	0.88945200	-1.13513300
H	-4.51415700	0.10823800	0.20791100
H	-0.65190800	-0.97886400	-1.54630200
O	-0.64976200	-1.88955000	1.05446200
Cl	-3.52762100	-2.14945800	1.60176200
Cl	-3.77893600	2.28484700	-1.37193500
H	4.42732700	0.69544700	0.62322900
C	3.40734300	0.49865100	0.33814100
C	2.38731200	1.35732400	0.74100600
C	3.09260600	-0.59194100	-0.42475400
C	1.04850800	1.13365200	0.39984000
Cl	2.78443300	2.72501100	1.68804000
C	1.72828000	-0.87050900	-0.82766000
Cl	4.30542900	-1.66115200	-0.94849200
C	0.71335600	0.04838500	-0.35372200
O	1.44091400	-1.82382300	-1.55520700
H	-1.04522900	1.62544100	-1.77034000
H	0.29318300	1.82118700	0.74879400

IM21

C	2.76394000	-1.18449400	0.58425900
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C	3.55245000	-0.13639100	0.11209700
C	2.93693800	0.97458300	-0.39024700
C	1.49056200	1.09327500	-0.46065900
C	0.71886600	-0.03310300	0.04968200
C	1.36933800	-1.13340100	0.55526700
H	4.62692500	-0.20299600	0.15076100
H	-0.04217000	-2.01623500	-1.13958200
O	0.95261900	2.09288200	-0.93742800
Cl	3.85694500	2.28018400	-0.97215200
Cl	3.53075800	-2.56585400	1.23779000
H	-4.59989500	0.19819100	0.17414400
C	-3.52421100	0.16082400	0.13342800
C	-2.76094600	1.22892200	0.56775100
C	-2.89480200	-0.95820300	-0.36847800
C	-1.38709900	1.18095900	0.51325200
Cl	-3.54767800	2.63422000	1.18568700
C	-1.50732500	-1.03440900	-0.43089700
Cl	-3.83412300	-2.27852900	-0.93791800
C	-0.74599000	0.04085300	0.03711300
O	-0.97255100	-2.14682000	-0.95674700
H	0.80757900	-1.95443900	0.97445800
H	-0.80364000	2.02014600	0.85028300

IM22

C	-3.08112900	-1.21663300	-0.04038100
C	-3.39211600	0.12697700	-0.20161200
C	-2.39112400	1.08504700	-0.16012000
C	-1.09490300	0.66915600	0.04983200
C	-0.78815600	-0.68490700	0.20891900
C	-1.78538400	-1.64797600	0.15990400
H	-4.41338200	0.43146000	-0.35808200
H	0.49090100	0.62973900	2.40608300
O	-0.01815900	1.47391800	0.09542900
Cl	-2.75098900	2.74703200	-0.36868100
Cl	-4.36064400	-2.37417300	-0.09469800
H	4.24347800	0.23160100	-0.67783100
C	3.25082600	0.00494900	-0.32556600
C	2.87583800	-1.34795100	-0.13847700
C	2.36455400	0.99742500	-0.09609600
C	1.55590200	-1.72544800	0.10846500
Cl	4.06477800	-2.55771400	-0.37768800
C	1.06742900	0.68176600	0.56253400
Cl	2.73715600	2.63616300	-0.35932800

C	0.63854600	-0.73650700	0.31052100
O	1.25802200	0.93339700	1.91730500
H	-1.56700700	-2.69661500	0.27621100
H	1.27028200	-2.76233000	0.03090100

IM23

C	-2.80546400	1.05836900	0.78323400
C	-3.51748100	0.07224700	0.12684300
C	-2.83879800	-0.93862600	-0.52255600
C	-1.44753900	-0.97996900	-0.52691300
C	-0.73959500	0.01661400	0.14647400
C	-1.42600900	1.03563100	0.79714300
H	-4.59452700	0.08521400	0.11690300
H	-0.10760100	1.87508900	-1.12726200
O	-0.84473800	-1.97506300	-1.18476300
Cl	-3.71633400	-2.16170700	-1.34569800
Cl	-3.65269600	2.31863600	1.60051300
H	4.59452700	-0.08521400	0.11690300
C	3.51748100	-0.07224700	0.12684300
C	2.80546400	-1.05836900	0.78323300
C	2.83879800	0.93862600	-0.52255600
C	1.42600900	-1.03563100	0.79714300
Cl	3.65269600	-2.31863600	1.60051300
C	1.44753900	0.97996900	-0.52691300
Cl	3.71633400	2.16170700	-1.34569900
C	0.73959500	-0.01661400	0.14647400
O	0.84473800	1.97506300	-1.18476300
H	0.10760100	-1.87508900	-1.12726200
H	-0.87580700	1.79484500	1.33127000
H	0.87580700	-1.79484500	1.33127000

IM24

C	-1.48637700	1.45917900	-0.90390100
C	-2.35766500	0.92786500	0.12498400
C	-2.37387700	-0.38108200	0.40069700
C	-1.53228000	-1.32739600	-0.35855500
C	-0.40832500	-0.72559100	-1.17644100
C	-0.59529000	0.70772200	-1.54304200
H	-3.01484800	1.60646200	0.64506700
H	-0.30189300	-1.32920800	-2.07602200
O	-1.72014600	-2.51382400	-0.32788300
Cl	-3.43117200	-1.04813000	1.56377300

Cl	-1.68977100	3.12956700	-1.27623000
H	0.15589000	-0.23333900	1.52985600
C	0.98276400	-0.09894200	0.85021500
C	2.03112600	0.64330200	1.19055600
C	0.95160500	-0.83350000	-0.44465200
C	3.18399300	0.80762400	0.32504800
Cl	2.09389700	1.45015700	2.70957900
C	2.05777100	-0.43047300	-1.43236100
Cl	1.33557200	-2.55309000	-0.07247500
C	3.21405900	0.27847300	-0.90043400
O	1.94636500	-0.70549400	-2.60083400
H	4.05041000	0.41231400	-1.56693400
H	0.03434700	1.11933000	-2.31585400
H	4.01636800	1.38133200	0.70195900

IM25

C	2.19568700	1.35504600	0.47708600
C	2.96230600	0.35021300	-0.22525000
C	2.44586200	-0.85518800	-0.49362700
C	1.05645300	-1.19158200	-0.13269600
C	0.37486600	-0.23898000	0.83683100
C	0.97826400	1.11369600	0.95441500
H	3.96027500	0.59877400	-0.54971600
H	0.52042000	-0.74892700	1.80172200
O	0.49945800	-2.17310400	-0.54539400
Cl	3.31460300	-2.02862300	-1.38031000
Cl	2.95301900	2.89293800	0.67333500
H	-1.12198900	1.26352600	-0.90534300
C	-1.70252300	0.56750800	-0.31869700
C	-3.08188500	0.48516000	-0.52425300
C	-1.10288800	-0.23732600	0.60867100
C	-3.88400200	-0.40901300	0.19534100
Cl	-3.80868600	1.50222000	-1.69298400
C	-1.89619800	-1.15992500	1.39342500
C	-3.30784400	-1.21521600	1.13006900
O	-1.37277600	-1.85764900	2.27614400
H	-3.88859900	-1.91411100	1.71031900
H	0.42945600	1.87319500	1.48877200
H	-4.94351600	-0.44388600	-0.00035600

IM26

C	2.00847000	1.62418100	0.29071000
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C	3.03980200	0.75746300	-0.08049500
C	2.72990900	-0.54401900	-0.32996300
C	1.37450200	-1.05248200	-0.21229700
C	0.32815800	-0.10142000	0.12903800
C	0.68763200	1.20519700	0.38813100
H	4.05359700	1.11282000	-0.15627500
H	-0.06872000	-2.70874500	0.66953100
O	1.14708800	-2.25380600	-0.40738800
Cl	3.94161400	-1.65274900	-0.77275100
Cl	2.39363300	3.25287200	0.64095800
H	-1.60948700	1.39117900	-0.80959300
C	-1.99256100	0.50053800	-0.33805700
C	-3.35075800	0.32224900	-0.25726800
C	-1.09483800	-0.45995400	0.14686600
C	-3.87066600	-0.82440800	0.32332900
Cl	-4.41626000	1.52755800	-0.88817000
C	-1.62700900	-1.64557600	0.68392100
C	-3.00793400	-1.79041800	0.78259500
O	-0.89320700	-2.64252900	1.17802900
H	-3.37944300	-2.70071400	1.22438800
H	-0.06036300	1.91823400	0.69327000
H	-4.93762100	-0.96079000	0.39386200

IM27

C	2.57115700	1.39977800	0.02806300
C	3.11608900	0.14264900	-0.19665900
C	2.29899400	-0.97684100	-0.22515300
C	0.94703000	-0.81029700	-0.01926300
C	0.40511600	0.45980200	0.20568100
C	1.21767400	1.58428800	0.22530900
H	4.17663600	0.03134800	-0.34866100
H	-0.64632300	-1.14931400	2.30163400
O	0.02980000	-1.79073000	-0.04111800
Cl	2.95090900	-2.53557100	-0.51603400
Cl	3.62646600	2.76636800	0.05895500
H	-1.98709300	2.15087900	0.08430700
C	-2.08548700	1.07696600	0.10287900
C	-3.30999200	0.48564000	-0.19398600
C	-1.00799900	0.25414400	0.27979100
C	-3.42971200	-0.90955500	-0.45646300
Cl	-4.69045900	1.47587100	-0.41411500
C	-1.19179300	-1.22617500	0.44571200
C	-2.39689600	-1.74502200	-0.24370600

O	-1.33298900	-1.57829100	1.78738500
H	-2.45317800	-2.80166100	-0.44776200
H	0.81587200	2.57024100	0.39117500
H	-4.36304400	-1.27493600	-0.85378000

Table S5. Cartesian coordinates for the transition states.

TS1

C	1.27363646	0.34731550	-0.63684730
C	1.45221446	-0.98839550	-0.96525530
C	2.67425146	-1.61120650	-0.81747430
C	3.74098546	-0.86887650	-0.35074730
C	3.60151346	0.46765950	-0.03387730
C	2.36619746	1.06878350	-0.17900630
O	0.09888246	0.97880150	-0.89270130
Cl	0.10793646	-1.88494750	-1.55408930
H	2.78904846	-2.65176050	-1.06820930
C	-1.06591054	0.80611750	-0.16783230
C	-2.18367354	0.67563250	-1.13323930
C	-3.18323554	-0.16520550	-0.89653230
C	-3.22556754	-1.02315950	0.26975070
C	-2.21133554	-1.06116250	1.13856270
C	-0.99710354	-0.25771650	0.93491470
Cl	-1.41500853	2.42261664	0.84639702
H	-2.14143754	1.30966550	-2.00300830
O	-0.01082154	-0.36622750	1.60696070
Cl	5.27743746	-1.62472250	-0.16638530
Cl	-4.50958454	-0.29949050	-1.98350230
H	-4.09275754	-1.64667950	0.41626770
Cl	-2.21378254	-2.09342050	2.49577270
Cl	2.18138446	2.72517050	0.21113570
H	4.43939046	1.03989750	0.32611070
H	-1.73953976	3.95848916	1.82531228

TS2

C	1.37504800	0.12858800	-0.70533400
C	1.74116600	-1.20729500	-0.65214000
C	3.01995700	-1.58183900	-0.29801600
C	3.94604500	-0.59498600	-0.01853900
C	3.61394200	0.74298100	-0.08800900
C	2.32433200	1.09893100	-0.43441400
O	0.14464400	0.49738300	-1.16325200
Cl	0.56970800	-2.41095100	-1.01858700
H	3.28689700	-2.62354800	-0.24791500
C	-1.00440800	0.28785100	-0.50208900
C	-2.10836500	0.00351800	-1.36558900
C	-3.20519300	-0.60233200	-0.86440400

C	-3.29371700	-1.02548600	0.49993900
C	-2.25333200	-0.86308100	1.33496700
C	-0.97984800	-0.28407000	0.88495000
Cl	-1.63185800	2.22057700	0.16161400
H	-2.03423800	0.30806600	-2.39574700
O	0.00475000	-0.22568000	1.57708300
Cl	5.54902300	-1.04577700	0.41805100
Cl	-4.55869100	-0.90855100	-1.86695000
O	-1.56058700	4.07854400	0.99799000
H	-0.79711200	3.94961000	1.57239100
Cl	1.89192900	2.75241800	-0.52889800
Cl	-2.31161300	-1.37714700	2.95574400
H	4.34390200	1.50517300	0.12491700
H	-4.20814500	-1.47760800	0.84727200

TS3

C	1.45673500	-0.07474700	-0.73535500
C	1.91203600	-1.36249600	-0.50209300
C	3.20822200	-1.59312900	-0.09452600
C	4.05620000	-0.51160300	0.05501400
C	3.63171700	0.77759700	-0.19537800
C	2.32598200	0.99207900	-0.59635600
O	0.20708300	0.13486900	-1.25100000
Cl	0.82940100	-2.68171800	-0.70892100
H	3.54835000	-2.59636100	0.09686500
C	-0.93313600	-0.04342700	-0.58587300
C	-2.02018400	-0.44468100	-1.42257500
C	-3.10946900	-1.01959800	-0.86729700
C	-3.21437500	-1.28196400	0.53670500
C	-2.19381300	-0.99789700	1.36304200
C	-0.91912100	-0.45428700	0.86406700
Cl	-1.68755800	1.92137200	-0.14623500
H	-1.93939000	-0.25511600	-2.47947300
O	0.05516600	-0.31246500	1.55249000
Cl	5.67987100	-0.78253100	0.55676700
Cl	-4.43573600	-1.47121100	-1.84589600
Cl	-1.60509900	4.12750700	0.75201400
H	4.30242400	1.61202800	-0.08163100
H	-4.12651000	-1.70907900	0.91974800
Cl	-2.26868000	-1.31110000	3.03042800
Cl	1.77676400	2.57734000	-0.91955000

TS4

C	-1.08245500	0.89689500	0.31977100
C	-1.24042400	-0.42442600	0.83427600
C	-2.48461900	-1.07625000	0.69428100
C	-3.49396500	-0.44323300	0.03427300
C	-3.35175700	0.86454200	-0.45021500
C	-2.14853300	1.52047900	-0.30673500
O	0.10690300	1.49886200	0.36058500
Cl	-0.27249500	-0.89753800	2.17822500
H	-2.61106600	-2.05755200	1.11757900
C	1.21634400	0.74086900	0.08773000
C	2.44818800	1.29076000	0.33810100
C	3.57100100	0.53821400	0.04220100
C	3.46388700	-0.74247200	-0.46134100
C	2.20760300	-1.28315100	-0.66711900
C	1.04703100	-0.54979200	-0.42402500
H	2.52302200	2.28224700	0.75133400
O	-0.15559100	-1.04282700	-0.63906600
Cl	-5.00777300	-1.22915300	-0.17663300
Cl	5.13313600	1.21227500	0.32201700
H	-4.17106700	1.34730000	-0.95561800
H	4.34238600	-1.32519200	-0.68042200
Cl	-1.94091400	3.09530700	-0.94640000
Cl	2.05230600	-2.88028500	-1.27439800

TS5

C	1.00913200	0.64197500	0.28476100
C	1.51258800	-0.30336400	1.22728900
C	2.79186700	-0.78859000	1.13338700
C	3.64325600	-0.24899800	0.18198000
C	3.23980400	0.78222200	-0.66724000
C	1.96139000	1.25046100	-0.58581000
O	0.15893500	-0.58902300	-0.93036800
Cl	0.44723200	-0.87882100	2.42416000
H	3.13364600	-1.55728800	1.80523400
C	-1.07690700	-0.37367300	-0.56857500
C	-2.19142000	-1.12915100	-0.90915500
C	-3.45505800	-0.72912800	-0.49976900
C	-3.59534400	0.39328900	0.29063300
C	-2.49945400	1.14716300	0.69730900
C	-1.27667700	0.73751600	0.24942600
O	-0.10654000	1.34886700	0.59694800
Cl	5.24541000	-0.83942200	0.06178500
H	3.93190300	1.20778300	-1.37380300

Cl	1.41711800	2.50489400	-1.59836900
H	-2.60534200	2.00101100	1.34410900
H	-4.31819400	-1.30021900	-0.79705800
Cl	-5.16954900	0.86475600	0.81503500
Cl	-1.99551800	-2.51660600	-1.89770200

TS6

C	1.05424400	0.43473100	0.13091600
C	1.56749300	-0.47495900	1.09832700
C	2.83456200	-0.98616200	0.98533500
C	3.65809700	-0.51202700	-0.02538500
C	3.24282400	0.47762500	-0.91442600
C	1.97530100	0.97562000	-0.80936800
O	0.17554300	-0.92171200	-1.01249100
Cl	0.53207800	-0.97193700	2.35310300
H	3.18899300	-1.72582700	1.68266200
C	-1.06035100	-0.64758500	-0.66824500
C	-2.17206300	-1.39941800	-1.01472500
C	-3.41744000	-0.94371700	-0.61215800
C	-3.58501700	0.19918900	0.14246200
C	-2.46038200	0.92781800	0.51091400
C	-1.22549900	0.50237800	0.10034200
H	-2.06254300	-2.29329700	-1.60365900
O	-0.06125600	1.14303800	0.41080700
Cl	5.24404500	-1.13906900	-0.16990000
Cl	-4.81443800	-1.85606000	-1.06143600
H	3.91436300	0.84919300	-1.66946200
H	-4.56312400	0.52152000	0.45438400
Cl	1.41760100	2.18745000	-1.86351400
Cl	-2.60649800	2.34178400	1.47148900

TS7

C	-1.11830000	0.61354100	0.22102800
C	-2.17613600	1.22264800	-0.44327800
C	-3.36639800	0.55587100	-0.60956200
C	-3.51045600	-0.74664800	-0.10802700
C	-2.51473100	-1.36150900	0.58738900
C	-1.28163700	-0.69701900	0.75284800
O	-0.14231300	-1.32673700	-0.70136900
Cl	-1.96235300	2.79137000	-1.09247300
H	-4.17622400	1.02305400	-1.14398900
C	1.05168900	-0.80144500	-0.49097000

C	2.20498400	-1.51847800	-0.78417900
C	3.43824900	-0.93500300	-0.56991700
C	3.56726000	0.33106900	-0.03433500
C	2.41820200	1.03614800	0.27732100
C	1.17699400	0.48682900	0.03812800
H	2.11589100	-2.51504200	-1.18126200
O	0.05789500	1.23169100	0.28711200
Cl	-5.01144400	-1.54785600	-0.34765500
Cl	4.86381600	-1.82921400	-0.95384300
H	-2.64604100	-2.33716500	1.02207500
H	4.53497900	0.76711800	0.14259800
Cl	-0.33387000	-1.15830900	2.11366300
Cl	2.53258300	2.60909000	0.95418700

TS8

C	1.11740100	0.14380800	-0.64225500
C	1.76611500	-1.03928200	-0.32630100
C	3.12138800	-1.04239600	-0.06665100
C	3.81947200	0.14842100	-0.13791200
C	3.18741800	1.32969300	-0.47472000
C	1.83029400	1.31983700	-0.73630000
O	-0.20799100	0.10290900	-1.00198900
Cl	0.87385700	-2.50370000	-0.23936800
H	3.62070900	-1.96115100	0.19051900
H	1.31516000	2.22377000	-1.01349800
C	-1.22753500	0.41214100	-0.17154100
C	-2.49386900	0.10766100	-0.84464100
C	-3.56493600	-0.23711700	-0.13128000
C	-3.52148700	-0.37456000	1.31066200
C	-2.37467300	-0.24367300	1.98266600
C	-1.11306000	-0.00226800	1.28747100
Cl	-1.29113100	2.35789200	0.07967200
H	-2.51167900	0.20875900	-1.91690800
H	-2.31311400	-0.37931300	3.05005100
O	-0.04047400	-0.09431300	1.82565000
Cl	5.51367300	0.14809900	0.18792100
Cl	-5.07334400	-0.54609300	-0.89374200
H	-1.10217900	4.30653100	0.23597400
H	3.75088000	2.24557600	-0.53956300
H	-4.44316300	-0.60190700	1.82274600

TS9

C	1.19026300	-0.09138300	-0.63331600
C	1.93773300	-1.21865100	-0.34027300
C	3.28536700	-1.10311900	-0.06789400
C	3.86986900	0.14920500	-0.10214800
C	3.13231700	1.27603600	-0.40990800
C	1.78374700	1.15029300	-0.68619400
O	-0.12676500	-0.25264100	-1.01289200
Cl	1.17720500	-2.75692900	-0.28773200
H	3.86576100	-1.97800100	0.17145400
H	1.18832100	2.01345400	-0.93084900
C	-1.16516800	-0.08194200	-0.20936500
C	-2.41181000	-0.40632000	-0.82981200
C	-3.50490900	-0.60619800	-0.06611700
C	-3.46129500	-0.53616600	1.36916000
C	-2.29997400	-0.33240900	2.00497700
C	-1.03893700	-0.23774600	1.27720100
Cl	-1.40791800	2.12117200	0.00746300
H	-2.44101300	-0.45772300	-1.90518900
H	-2.23002400	-0.30127100	3.07995400
O	0.03989200	-0.30204300	1.81933300
Cl	5.55371900	0.29631400	0.23976300
Cl	-5.01508500	-0.95437100	-0.79396000
O	-1.26931500	4.18916700	-0.14088900
H	-1.89444400	4.28762100	-0.86804000
H	3.60628500	2.24287200	-0.43829800
H	-4.38324900	-0.65757800	1.91461800

TS10

C	1.21496400	-0.30626900	-0.65894700
C	1.96750700	-1.40559000	-0.28549800
C	3.31216500	-1.26096100	-0.01562600
C	3.88694200	-0.00841200	-0.13193100
C	3.14234900	1.08944800	-0.51785300
C	1.79613100	0.93471300	-0.79249300
O	-0.10156400	-0.50102400	-1.03368600
Cl	1.21553800	-2.94070600	-0.12713200
H	3.89846600	-2.11237600	0.28585900
H	1.19824700	1.77514400	-1.10313700
C	-1.13907700	-0.32061600	-0.24006400
C	-2.38593300	-0.65083400	-0.85296000
C	-3.47976700	-0.84418500	-0.08226800
C	-3.43655800	-0.74816800	1.35180700
C	-2.27817900	-0.52179400	1.98515700

C	-1.01601500	-0.43214700	1.25697800
Cl	-1.46384600	1.86654000	-0.16471000
H	-2.41789100	-0.71534800	-1.92760200
H	-2.20993000	-0.46557200	3.05921100
O	0.05982000	-0.46252800	1.80044900
Cl	5.56692500	0.17501000	0.20685200
Cl	-4.98423900	-1.20850400	-0.80347400
Cl	-0.85742400	4.15968700	0.07461800
H	3.60824800	2.05630800	-0.60891300
H	-4.35857800	-0.86532100	1.89803800

TS11

C	-0.91852900	1.00996200	0.34553500
C	-1.27627000	-0.35666700	0.53117600
C	-2.61161000	-0.74571600	0.28599400
C	-3.50843200	0.17905700	-0.15718900
C	-3.15467300	1.52819100	-0.31074300
C	-1.86133700	1.93023800	-0.06440500
O	0.35311800	1.40089800	0.49468200
Cl	-0.39878800	-1.30264100	1.67452500
H	-2.89666800	-1.76866900	0.46224000
H	-1.55054700	2.95045400	-0.21829300
C	1.32980500	0.57872400	-0.00746600
C	2.63718000	0.86415700	0.30395400
C	3.63245700	0.06662500	-0.23151000
C	3.32210600	-1.01088800	-1.03887200
C	1.99753900	-1.30482400	-1.30707000
C	0.97291200	-0.50448600	-0.81551700
H	2.86658600	1.69683900	0.94762600
H	1.73259700	-2.15103600	-1.91989200
O	-0.29682500	-0.75685200	-1.09287600
Cl	-5.13068800	-0.29163000	-0.48825400
Cl	5.28344100	0.42400000	0.13103600
H	-3.89565100	2.23610500	-0.64323900
H	4.10907000	-1.62769200	-1.44042500

TS12

C	-0.82634800	0.49783100	-0.32846500
C	-1.91500200	1.27283200	0.04798000
C	-3.17157100	0.71204700	0.09096500
C	-3.34821400	-0.63638700	-0.24862100
C	-2.30167200	-1.41267700	-0.65077200

C	-1.00369100	-0.86435600	-0.66680800
O	0.39589600	1.02864700	-0.30313100
Cl	-1.68007800	2.91218300	0.48775700
H	-4.01433600	1.30739100	0.39994800
H	-0.25254700	-1.33480800	-1.28196900
C	1.44720100	0.18300500	-0.05687600
C	2.70928400	0.60359900	-0.40654400
C	3.79000300	-0.19028900	-0.06674900
C	3.60782700	-1.38769200	0.59797000
C	2.32841100	-1.81017200	0.91134300
C	1.22060700	-1.03101500	0.59921700
H	2.83809400	1.54180800	-0.92010700
H	2.16530900	-2.74903400	1.41533300
O	-0.01043300	-1.42109100	0.89700900
Cl	-4.94020300	-1.28794300	-0.18627500
Cl	5.38226500	0.32791300	-0.48971600
H	-2.45410700	-2.43493900	-0.95172000
H	4.45915500	-1.99780800	0.85163400

TS13

C	0.82863400	0.48584900	-0.14369400
C	1.93069500	1.30622300	-0.03656000
C	3.20350400	0.76932700	0.08226800
C	3.35797800	-0.60643500	0.08702900
C	2.27811800	-1.45334700	-0.01002800
C	0.99665700	-0.90505400	-0.03916200
O	-0.40225100	1.02366100	-0.24563600
Cl	1.71613500	3.00728600	-0.06785000
H	4.05560100	1.42223700	0.16092000
H	0.60349400	-0.88119300	1.71058200
C	-1.45408100	0.16264500	-0.14127000
C	-2.71460900	0.69868100	0.00388700
C	-3.79820400	-0.15740800	0.06680900
C	-3.63427800	-1.52787700	-0.00861900
C	-2.36029800	-2.05017200	-0.14351800
C	-1.27362200	-1.20766400	-0.21353200
H	-2.83425800	1.76766500	0.05847600
H	-2.19582300	-3.11403900	-0.20054100
O	-0.02865100	-1.73685800	-0.37952000
Cl	4.94520000	-1.26919800	0.19273000
H	2.39050700	-2.52367400	-0.02715400
Cl	-5.38163000	0.50459200	0.24188600
H	-4.49027800	-2.17959200	0.04230400

TS14

C	0.88395700	-0.36017100	-0.67416000
C	1.43591900	0.85361100	-0.16579400
C	2.75904700	0.92107100	0.19920100
C	3.58277700	-0.16200300	-0.05653800
C	3.10444800	-1.31051100	-0.70039000
C	1.78949900	-1.38925200	-1.03991600
O	0.19695500	-1.00474900	1.01292900
Cl	0.40493000	2.19046300	0.05484400
H	3.15141900	1.81544400	0.65285300
C	-1.07034000	-0.72561900	0.81009200
C	-2.08076600	-0.75147700	1.75861100
C	-3.38693500	-0.49189100	1.36745500
C	-3.67045600	-0.16859300	0.05539100
C	-2.66937600	-0.09144400	-0.90693100
C	-1.39711100	-0.37737800	-0.49856400
H	-1.84715400	-1.00794400	2.77865900
O	-0.31019900	-0.32733100	-1.32684400
Cl	5.23642800	-0.07839300	0.38506200
H	3.78539300	-2.11308800	-0.93041600
H	1.38276000	-2.24960400	-1.54483000
H	-4.18553500	-0.53479900	2.08970900
H	-2.88153700	0.19064200	-1.92433700
Cl	-5.29920200	0.17486700	-0.41055700

TS15

C	0.87330500	0.42070200	0.54686600
C	1.15961900	-0.83139500	1.15120600
C	2.33695100	-1.47443000	0.90242000
C	3.29708000	-0.84679000	0.10866100
C	3.09527200	0.42635500	-0.41439700
C	1.91600400	1.07657200	-0.16408700
O	-0.17643300	-0.36130200	-0.93999300
H	2.53669500	-2.44884500	1.31573800
C	-1.35388500	-0.17110100	-0.38842000
C	-2.54856200	-0.71559500	-0.83099400
C	-3.70924400	-0.40434900	-0.13663800
C	-3.71314600	0.40802400	0.97878100
C	-2.51144300	0.94839800	1.42747100
C	-1.37088000	0.65658900	0.73438700
H	-2.56867300	-1.35229200	-1.69874100
O	-0.13543000	1.17804800	1.02846600

Cl	4.77473100	-1.64945600	-0.21554100
H	3.86219600	0.90190300	-1.00220600
H	-2.47419200	1.58736200	2.29483500
Cl	1.63649400	2.64342700	-0.76384200
H	0.39285500	-1.27544500	1.76627100
Cl	-5.20215400	-1.08335000	-0.68949800
H	-4.63461000	0.61491600	1.49576700

TS16

C	-0.96715700	0.62326600	0.40463100
C	-2.14968000	1.16065000	-0.09266600
C	-3.25822400	0.35969100	-0.23084700
C	-3.19418700	-0.99349900	0.13372800
C	-2.05756800	-1.53922500	0.65206500
C	-0.90376200	-0.74039400	0.77128500
O	0.34153400	-1.11051600	-0.68324300
Cl	-2.20295900	2.80893700	-0.55744400
H	-4.16996800	0.76883700	-0.63265800
C	1.42785600	-0.46730400	-0.29050400
C	2.69369200	-1.00440500	-0.49933900
C	3.81168200	-0.31022600	-0.07732100
C	3.71324800	0.90234400	0.57878100
C	2.45640500	1.43920800	0.79676900
C	1.33858700	0.77011600	0.35729600
H	2.78128300	-1.95667200	-0.99470100
O	0.11822800	1.38848700	0.47282400
Cl	-4.61204600	-1.95077800	-0.05174100
H	-2.03151600	-2.56785600	0.96854300
H	-0.13126400	-1.04274100	1.46104300
H	2.33523500	2.38860200	1.29326000
H	4.59890200	1.41737100	0.90977100
Cl	5.37229200	-1.00125500	-0.35229600

TS17

C	-0.95609400	0.62738100	-0.10975900
C	-2.22340100	1.15881300	-0.00483900
C	-3.33383600	0.33281600	0.07708900
C	-3.15819200	-1.03997200	0.04629900
C	-1.90660000	-1.60364700	-0.04977300
C	-0.79231400	-0.76610100	-0.03997500
O	0.40651300	-1.32217000	-0.37962900
Cl	-2.42209700	2.86220400	0.00462700

H	-4.31796100	0.76195500	0.15390700
H	-0.43916900	-0.70001000	1.71686100
C	1.48714700	-0.51684600	-0.18748700
C	2.73652700	-1.09292500	-0.12341400
C	3.84054700	-0.27572000	0.03619600
C	3.70611300	1.09571800	0.14434900
C	2.44399400	1.65885100	0.08627100
C	1.33880100	0.85472600	-0.08210600
H	2.83241400	-2.16270300	-0.20326300
H	2.30301300	2.72474800	0.16391200
O	0.11154500	1.44437500	-0.17826200
Cl	-4.54249900	-2.06462000	0.10502800
Cl	5.40957800	-0.98864900	0.10785400
H	-1.76018000	-2.66920100	-0.09448900
H	4.57656000	1.71711200	0.27142800

TS18

C	-0.97243100	0.25356600	0.86440100
C	-1.50670400	0.87329600	-0.30307800
C	-2.73583000	0.49922800	-0.78900500
C	-3.50065800	-0.39968100	-0.06289100
C	-3.06346200	-0.91461900	1.16320500
C	-1.83775500	-0.55950900	1.63665600
O	0.05419200	-1.10887100	-0.12036500
Cl	-0.55893600	2.02485400	-1.12234600
H	-3.10609400	0.91806000	-1.70942100
C	1.24649200	-0.59663500	0.08508100
C	2.41954900	-1.03007400	-0.51350300
C	3.60715300	-0.40986100	-0.15568600
C	3.65549500	0.63405800	0.74607700
C	2.47372800	1.08732500	1.32336200
C	1.30600200	0.46416900	0.98558800
H	2.40148500	-1.84340700	-1.21840100
O	0.08388700	0.81388500	1.50187200
Cl	-5.03812100	-0.86032000	-0.66133000
H	-3.70481500	-1.57617300	1.72132400
H	-1.46422700	-0.92407200	2.57915000
H	2.47041600	1.90988000	2.01980600
H	4.59700200	1.09554900	0.99069300
Cl	5.07659400	-0.96615400	-0.88199700

TS19

C	-1.09206800	1.19749500	-0.00960600
C	-2.10016800	1.69040300	-0.81690800
C	-3.26754900	0.98190700	-0.97131300
C	-3.43051000	-0.24833400	-0.31398600
C	-2.47492900	-0.74025900	0.52264100
C	-1.26243900	-0.03524200	0.68240600
O	-0.01821100	-0.83135900	-0.59151700
H	-4.05294600	1.34780600	-1.61163100
C	1.14645800	-0.23629500	-0.39385500
C	2.33660200	-0.94421400	-0.52565600
C	3.54293300	-0.29775800	-0.33838300
C	3.60659100	1.03656800	0.01552400
C	2.42515500	1.74057400	0.17244700
C	1.22213200	1.11423400	-0.04358100
H	2.29600200	-1.98929500	-0.78208900
O	0.06893500	1.85571300	0.05269100
Cl	-4.89915500	-1.11599800	-0.53936300
H	-2.62280600	-1.65320900	1.07349600
H	2.43001100	2.78198700	0.45161600
Cl	-0.40369900	-0.29845100	2.15274700
H	-1.92880300	2.61385900	-1.34503700
Cl	5.00880300	-1.19538000	-0.52641100
H	4.55838800	1.51662600	0.16734200

TS20

C	-1.35520500	-0.28548200	0.09588500
C	-2.43690800	-1.09422100	0.43594700
C	-3.73051000	-0.68136100	0.19432000
C	-3.94992700	0.54727500	-0.39961000
C	-2.89076300	1.36258300	-0.74045900
C	-1.59667200	0.94752800	-0.48433900
O	-0.13067600	-0.79234600	0.36667900
Cl	-2.16211100	-2.62924500	1.15817800
H	-4.55543100	-1.31921000	0.46373800
H	-0.78154000	1.61525900	-0.70120500
C	1.01488300	-0.26461400	-0.18764300
C	2.01890600	-1.31959900	-0.39308200
C	3.30644000	-0.98359100	-0.47769000
C	3.76272800	0.36749900	-0.24317900
C	2.91944800	1.31599400	0.18850300
C	1.51074300	0.99550200	0.47596300
H	4.80888000	0.58923800	-0.38165800
O	0.79075400	1.69795600	1.13397200

H	0.77086200	0.11615700	-1.28256600
Cl	3.44935200	2.88745700	0.58942000
Cl	-5.56772800	1.06200900	-0.70608800
Cl	4.51664800	-2.14873200	-0.84787200
H	0.42821200	0.39167000	-2.44281900
H	1.66489700	-2.32457300	-0.55272100
H	-3.07022000	2.32618000	-1.18751600

TS21

C	-1.37024500	0.27119700	-0.26442400
C	-2.44823000	1.10973000	-0.54456400
C	-3.74151100	0.70559000	-0.28804100
C	-3.96680100	-0.54337800	0.26144700
C	-2.91320600	-1.38951200	0.53997700
C	-1.61802400	-0.98439500	0.26696800
O	-0.14582200	0.76486300	-0.54082500
Cl	-2.16646900	2.66840300	-1.20783800
H	-4.56269600	1.36669200	-0.50864000
H	-0.80639700	-1.67330100	0.42891800
C	0.99137400	0.25348700	0.05681700
C	1.97200300	1.32622200	0.28464100
C	3.26739400	1.02071100	0.36494100
C	3.76237300	-0.31348200	0.10711500
C	2.94622300	-1.27897800	-0.33506200
C	1.52732700	-0.99473000	-0.61077900
H	4.81453800	-0.50688200	0.24179600
O	0.82680100	-1.70664600	-1.27815300
H	0.73974300	-0.11543300	1.12354400
Cl	3.51568600	-2.83116200	-0.75335700
Cl	-5.58395500	-1.04368300	0.58880700
Cl	4.44458100	2.20881900	0.76152700
O	0.31307800	-0.40230800	2.58000000
H	-0.65401700	-0.40146500	2.56207500
H	1.59499400	2.31838400	0.46873100
H	-3.09801000	-2.37043500	0.94582900

TS22

C	-1.34010400	0.33187000	-0.32897500
C	-2.42454400	1.15639800	-0.66745400
C	-3.71207600	0.73007400	-0.46123600
C	-3.93403800	-0.52754800	0.08896100
C	-2.88192900	-1.35508300	0.42259000

C	-1.58694700	-0.93146100	0.20629100
O	-0.13093400	0.85383100	-0.54444000
Cl	-2.13424800	2.71025100	-1.32681600
H	-4.53952200	1.36970400	-0.71795800
H	-0.77366800	-1.60151400	0.41543300
C	1.01599100	0.29396800	-0.02289100
C	2.03489500	1.32958400	0.19203700
C	3.32225000	0.97929000	0.22301200
C	3.76120300	-0.36278700	-0.08501900
C	2.89944300	-1.28683900	-0.53017200
C	1.48394300	-0.94999000	-0.75276700
H	4.80883400	-0.59753100	0.01462800
O	0.74037400	-1.61273900	-1.42238500
H	0.77148200	-0.09175800	1.03836500
Cl	3.39811800	-2.84687200	-1.00101600
Cl	-5.54985200	-1.04984300	0.33917600
Cl	4.54848300	2.11420400	0.61692700
Cl	-0.00370400	-0.30706200	2.78443700
H	1.69724600	2.32627200	0.42248100
H	-3.06797600	-2.33029800	0.83934300

TS23

C	-1.17229200	-1.30322200	-0.21747900
C	-1.45660900	-0.22532400	0.67131100
C	-2.75612300	0.32854700	0.66908400
C	-3.68803600	-0.15478300	-0.19901900
C	-3.40717700	-1.23644600	-1.04899000
C	-2.14995900	-1.79673900	-1.05583600
O	0.06943800	-1.79707500	-0.30377000
Cl	-0.57155000	-0.10237500	2.14452100
H	-2.98646000	1.11787100	1.36378400
H	-1.89336000	-2.59458700	-1.73307100
C	1.11226500	-0.90960300	-0.27099900
C	2.38168300	-1.41488500	-0.13794800
C	3.44309500	-0.52806100	-0.14088600
C	3.23875700	0.83248700	-0.24634100
C	1.94564100	1.31420100	-0.34205900
C	0.84452200	0.45959900	-0.37938700
H	4.06852300	1.51856800	-0.23970500
O	-0.38978100	0.90640900	-0.48777200
Cl	1.66998400	3.00489800	-0.45289100
Cl	-5.26676600	0.52733900	-0.22794500
Cl	5.05086900	-1.13754100	-0.00013800

H	-4.17527700	-1.60403700	-1.70904200
H	2.53160600	-2.47657200	-0.03863800

TS24

C	-1.12697700	-0.80301100	-0.30625700
C	-2.26541300	-1.37420000	0.24477300
C	-3.46038200	-0.69181700	0.20105200
C	-3.52454200	0.57336200	-0.40085300
C	-2.42804400	1.14495500	-0.97547000
C	-1.19012600	0.47523400	-0.91095900
O	0.04157900	-1.43683900	-0.19578500
Cl	-2.16621500	-2.90512000	1.00691600
H	-4.34147400	-1.12417400	0.64486500
H	-0.42402600	0.73847600	-1.62349300
C	1.17748200	-0.67346200	-0.14354500
C	2.37563400	-1.28243800	-0.43026700
C	3.53845700	-0.54728100	-0.28257700
C	3.50296500	0.76966300	0.12713200
C	2.28028600	1.36618300	0.37877700
C	1.08246100	0.66275000	0.26135000
H	4.41050000	1.33901100	0.23544100
O	-0.08836700	1.22171200	0.49620200
Cl	2.21574300	3.00927700	0.87237000
Cl	-5.04311500	1.38061500	-0.43390100
Cl	5.05593100	-1.29290700	-0.62309200
H	2.39314400	-2.31172000	-0.74663300
H	-2.49448200	2.09809300	-1.47141200

TS25

C	-1.12993800	0.73411100	-0.15405000
C	-2.31607400	1.42735500	-0.05787900
C	-3.51934700	0.75155400	0.07708700
C	-3.51876100	-0.63278600	0.10916900
C	-2.35044700	-1.35481200	0.02484800
C	-1.14173500	-0.66364700	-0.01911700
O	0.03499000	1.40140700	-0.27727400
Cl	-2.29837800	3.14059200	-0.12472800
H	-4.43999600	1.30490100	0.14667600
H	-0.74551200	-0.56520200	1.72719300
C	1.17662500	0.67181900	-0.14134000
C	2.36270200	1.35531700	0.00173900
C	3.53444400	0.62893500	0.09912100

C	3.53280900	-0.75108300	0.06094900
C	2.32687000	-1.41615200	-0.07344200
C	1.14201200	-0.71271300	-0.18177500
H	4.44990800	-1.30919300	0.13887000
O	-0.02653400	-1.37880400	-0.34877400
Cl	2.29190800	-3.12961400	-0.11972000
Cl	-5.01990500	-1.46817100	0.23410900
Cl	5.02959700	1.46664900	0.27297400
H	2.35709800	2.43166300	0.02945100
H	-2.33889100	-2.43113700	0.02955000

TS26

C	-1.12030200	-0.73410300	-0.62536900
C	-1.66874100	-0.72994200	0.69174300
C	-2.96803000	-0.33649900	0.90482400
C	-3.77626800	-0.06727400	-0.18679500
C	-3.30755300	-0.20840300	-1.49998500
C	-2.01540800	-0.57388900	-1.71329200
O	-0.29265800	1.02057200	-0.51283800
H	-3.35571400	-0.26523000	1.90694200
C	0.94299200	0.62048300	-0.36322700
C	2.03529000	1.39923900	-0.00558700
C	3.30393000	0.83955500	0.05843300
C	3.47201700	-0.50607400	-0.19190500
C	2.39837100	-1.33028200	-0.50909900
C	1.17085800	-0.73677300	-0.58723300
O	0.02625300	-1.42559900	-0.86985200
Cl	-5.40054400	0.40839700	0.07170900
H	-3.97914100	-0.03814800	-2.32493300
H	4.14757100	1.46008800	0.30908500
H	2.52232400	-2.38693300	-0.67297100
Cl	5.05114600	-1.19509000	-0.08721800
Cl	1.80891300	3.07348800	0.29695600
Cl	-0.65891100	-1.14803400	1.99584600
H	-1.61701000	-0.70472400	-2.70564200

TS27

C	-1.08137000	0.42272100	-0.18438000
C	-1.40723700	-0.36510000	-1.31862500
C	-2.64230100	-0.92987300	-1.44189100
C	-3.61217500	-0.65643300	-0.47640300
C	-3.36033000	0.19496600	0.59439700

C	-2.12194800	0.76702500	0.72059800
O	-0.19552200	-1.07312600	0.79830800
H	-2.88054000	-1.57017000	-2.27460700
C	1.02921100	-0.75256500	0.45632800
C	2.15237200	-1.54006800	0.65279100
C	3.37906700	-1.04530700	0.23523200
C	3.52410600	0.18386800	-0.37381700
C	2.39162200	0.96549700	-0.56762100
C	1.17486900	0.49768600	-0.14812000
O	0.01384800	1.21210100	-0.21140800
Cl	-5.16328400	-1.36493300	-0.62177900
H	-4.13344900	0.41252000	1.31174700
Cl	-1.77504300	1.83212200	1.99885600
H	-0.63125100	-0.53807900	-2.04761300
H	2.06691200	-2.50305800	1.12537900
H	4.48782800	0.53504600	-0.69863600
Cl	4.78285900	-2.02460400	0.47216900
Cl	2.50773700	2.50432300	-1.31997600

TS28

C	-1.15092700	0.48355100	0.21691800
C	-2.29356700	1.04043500	-0.34866800
C	-3.47510200	0.33934200	-0.32056400
C	-3.52558000	-0.92842500	0.28024600
C	-2.42771300	-1.48467900	0.86601400
C	-1.20172400	-0.79428400	0.81834300
O	-0.05473900	-1.52067500	-0.58833500
H	-4.35843800	0.75739700	-0.77347300
C	1.10297700	-0.93840700	-0.34115400
C	2.29947100	-1.62772400	-0.50161100
C	3.49387900	-0.98959700	-0.22907200
C	3.54404800	0.31182900	0.22930100
C	2.35318300	0.99738000	0.39204000
C	1.14826200	0.39164800	0.09736400
O	0.00456800	1.13674200	0.12667100
Cl	-5.03216400	-1.75793200	0.29498000
H	-2.48633600	-2.43920500	1.36020100
Cl	-2.20712500	2.57524900	-1.10174900
H	-0.43305800	-1.04806100	1.53173400
H	2.27402200	-2.64955600	-0.83952900
H	4.48109700	0.78989200	0.45538300
Cl	2.37057800	2.62210500	0.94593300
Cl	4.96993700	-1.85974000	-0.43304200

TS29

C	1.14622600	0.41496100	-0.14731700
C	2.34813600	1.07884600	-0.03621900
C	3.53564900	0.37140200	0.07529700
C	3.50310100	-1.01291300	0.06840600
C	2.31847300	-1.70515400	-0.03336400
C	1.12550700	-0.98591900	-0.05436400
O	-0.00653500	-1.66546500	-0.40250200
Cl	2.36782800	2.79203400	-0.05487500
H	4.46892200	0.90142600	0.15746800
H	0.73510200	-0.93092200	1.69571000
C	-1.16642900	-0.98210600	-0.21437000
C	-2.34186400	-1.69270300	-0.13529800
C	-3.52579400	-0.99625200	0.01990400
C	-3.54465600	0.38109500	0.10846300
C	-2.35003800	1.07546000	0.03423100
C	-1.15395500	0.40126900	-0.13103800
H	-4.47028500	0.91619700	0.23308100
O	-0.00318400	1.11227800	-0.24599600
Cl	-2.34373200	2.78614900	0.13293600
Cl	4.98502300	-1.88587900	0.16507900
Cl	-5.00833500	-1.86884500	0.11185200
H	2.28389100	-2.78064200	-0.05997400
H	-2.31936000	-2.76727900	-0.19915000

TS30

C	1.17176900	0.52979000	-0.49140600
C	1.72138900	0.29610200	0.80223000
C	3.00715100	-0.16780300	0.93598000
C	3.79788200	-0.29468200	-0.19525000
C	3.32740300	0.05831500	-1.46534100
C	2.04734100	0.50157900	-1.60270200
O	0.30579700	-1.25200700	-0.63730300
H	3.39985100	-0.40570700	1.91001900
C	-0.92741100	-0.84780100	-0.44116800
C	-2.02365400	-1.67653800	-0.26000700
C	-3.26816600	-1.08758600	-0.09512700
C	-3.45169100	0.27926100	-0.08060800
C	-2.34247800	1.10045000	-0.24291900
C	-1.10951800	0.53359800	-0.42393200
O	0.03273600	1.25298500	-0.62190800
Cl	5.40472700	-0.86101300	-0.02882600

H	3.98474900	-0.01354000	-2.31570100
Cl	0.73708300	0.53682400	2.16804200
H	1.64505200	0.79570800	-2.55783200
H	-4.42793800	0.70909000	0.06066800
H	-1.90449500	-2.74602300	-0.26680100
Cl	-4.64243000	-2.11400900	0.11612500
Cl	-2.50559100	2.80905300	-0.21976300

TS31

C	-1.24011000	0.97226200	-0.19181300
C	-2.20914000	1.47502000	-1.04027500
C	-3.45195700	0.89219600	-1.08291500
C	-3.73106800	-0.22039000	-0.27135900
C	-2.81147100	-0.71161900	0.60485800
C	-1.52544700	-0.13169000	0.65911200
O	-0.38994800	-1.21594100	-0.51156300
H	-4.21145600	1.26443600	-1.75026700
C	0.83375200	-0.73356700	-0.39500200
C	1.93773700	-1.57701700	-0.43896700
C	3.20650700	-1.04286900	-0.32880900
C	3.41996100	0.30787900	-0.14013400
C	2.31975600	1.14421400	-0.07782700
C	1.04517000	0.63831000	-0.21881800
O	-0.01378100	1.50012200	-0.23274600
Cl	-5.29452100	-0.93126700	-0.35946800
H	-3.04488600	-1.52468500	1.27056200
Cl	-0.66621800	-0.29480000	2.14236800
H	-1.94992900	2.30058200	-1.68240000
Cl	4.56766500	-2.10304400	-0.39889800
Cl	2.53882400	2.83122300	0.16029200
H	4.41348900	0.70893600	-0.04110300
H	1.78273200	-2.63499400	-0.56361700

TS32

C	2.14010200	-1.38063000	0.82890700
C	3.24375600	-0.53838700	0.44338200
C	3.07599000	0.47328100	-0.42241500
C	1.75299700	0.78517500	-0.97283300
C	0.69905100	-0.26072900	-0.77016400
C	0.92255300	-1.24267400	0.29600500
H	4.21158000	-0.72302500	0.88176400
H	0.81296300	-0.87914200	-1.77314900

O	1.51908800	1.79793300	-1.59042500
Cl	4.35571800	1.52278200	-0.84199100
Cl	2.46845400	-2.58208900	2.01826900
H	-4.21963600	0.68203600	0.86237700
C	-3.25492900	0.52970000	0.40475200
C	-2.17908700	1.43237000	0.74882300
C	-3.06589600	-0.48751700	-0.44611400
C	-0.97558400	1.34426000	0.19059600
Cl	-2.54867000	2.64737900	1.91485100
C	-1.73882400	-0.76380600	-1.01248400
Cl	-4.31179800	-1.59338200	-0.82322600
C	-0.70326500	0.32668800	-0.85994900
O	-1.48106500	-1.79353800	-1.58534300
H	-0.73801500	0.87551800	-1.81143700
H	0.82507700	-1.35653800	-2.87742300
H	-0.19663400	2.05227200	0.42449400
H	0.11632800	-1.90241400	0.57413500

TS33

C	2.02899500	-0.93124100	1.36245700
C	3.16643600	-0.26265100	0.78050800
C	3.04824600	0.45279700	-0.34731900
C	1.74205400	0.62066700	-0.99944300
C	0.66810900	-0.33426700	-0.55582000
C	0.83240900	-0.94555000	0.76932500
H	4.11738900	-0.33028400	1.28433100
H	0.87974000	-1.19876800	-1.30377200
O	1.53701700	1.44250700	-1.85861000
Cl	4.36224400	1.30997800	-1.01622800
Cl	2.29010500	-1.71747700	2.87072400
H	-4.22408200	0.91443500	0.77827700
C	-3.26859400	0.67531800	0.33868200
C	-2.21880200	1.66652100	0.39189900
C	-3.07203600	-0.52173600	-0.23080900
C	-1.02501000	1.45875000	-0.15514400
Cl	-2.60535100	3.14367300	1.19071400
C	-1.76779300	-0.89419400	-0.78476100
Cl	-4.29509600	-1.71337800	-0.26817900
C	-0.72477100	0.19642100	-0.88242100
O	-1.53710700	-2.02051400	-1.16324500
H	-0.69708800	0.46291500	-1.94718700
O	0.98210600	-2.23198100	-2.35344200
H	0.08962200	-2.58517900	-2.20913300

H	-0.26319300	2.22194200	-0.14216100
H	0.00369900	-1.47769200	1.20956700

TS34

C	-2.88775500	1.12156300	-0.64144900
C	-3.49289100	0.03926700	0.06091500
C	-2.74073200	-0.91374800	0.64757800
C	-1.27736800	-0.86329900	0.64512100
C	-0.71430300	0.15698200	-0.26689100
C	-1.54900600	1.20399600	-0.77797400
H	-4.56828700	-0.00537300	0.12706500
H	-0.37082700	-0.80328300	-1.20348500
O	-0.58160600	-1.61470300	1.29954200
Cl	-3.46206900	-2.18750700	1.53180900
Cl	-3.92848600	2.31207400	-1.32982900
H	4.57906900	0.10650500	0.17364500
C	3.50797100	0.15536700	0.06891200
C	2.80357900	1.22470700	0.64102300
C	2.83792000	-0.81709900	-0.61812300
C	1.41619100	1.34082400	0.56715200
Cl	3.69213400	2.40282600	1.50217500
C	1.43009900	-0.69695100	-0.76735500
Cl	3.64763100	-2.12239400	-1.34654700
C	0.72673100	0.36351900	-0.09381000
O	0.71293400	-1.41648300	-1.51404100
H	0.91206400	2.15164200	1.06657400
H	-1.10181200	2.02426100	-1.31773300

TS35

C	3.07197200	1.12613300	0.23617100
C	3.40348500	-0.14026000	-0.25425900
C	2.43029700	-1.08089900	-0.47967400
C	1.07380900	-0.76988800	-0.24842400
C	0.78466200	0.51472900	0.28971700
C	1.77050500	1.46784500	0.50970500
H	4.43438200	-0.38149400	-0.45595900
H	0.02984300	-1.18267800	1.97866800
O	0.08704900	-1.54836700	-0.49904300
Cl	2.83250500	-2.62875300	-1.09601100
Cl	4.33950300	2.26198400	0.51742300
H	-4.36580600	0.01896400	-0.46572900
C	-3.33084100	0.16640600	-0.20513200

C	-2.76037200	1.44509000	-0.31196800
C	-2.59458800	-0.87902600	0.26259200
C	-1.42237300	1.66729900	-0.04211000
Cl	-3.73948000	2.73037100	-0.88298500
C	-1.24143600	-0.67296800	0.67842700
Cl	-3.28566600	-2.42230200	0.47945700
C	-0.64214200	0.61780000	0.38834900
O	-0.88782700	-1.36310300	1.75689300
H	1.52782200	2.44049900	0.90670600
H	-0.97454100	2.62081500	-0.27088800

TS36

C	-3.08652500	-1.23575600	-0.04259200
C	-3.42321400	0.11291200	-0.11133800
C	-2.43591900	1.07944100	-0.12944600
C	-1.12444700	0.65832100	-0.07436100
C	-0.78983500	-0.69114200	-0.00371200
C	-1.77774600	-1.66391800	0.00991400
H	-4.45805000	0.40912100	-0.15054800
H	1.63574600	0.14537800	2.34074500
O	-0.04060800	1.46196100	-0.10391900
Cl	-2.82042900	2.74422900	-0.22221300
Cl	-4.36038800	-2.39998600	-0.02157300
H	4.34348100	0.30033700	-0.32434300
C	3.30469700	0.04048300	-0.21009100
C	2.92612600	-1.30409800	-0.14468100
C	2.35436000	1.02968000	-0.14900800
C	1.60532800	-1.70565800	-0.04678900
Cl	4.16097900	-2.50018400	-0.22277500
C	1.02011400	0.64899200	0.08124600
Cl	2.75916600	2.67715000	-0.26824000
C	0.64486200	-0.71650400	0.01271500
O	1.01543200	0.81728300	2.03698000
H	-1.54408500	-2.71404400	0.06455600
H	1.34894500	-2.75182300	-0.05443200

TS37

C	-2.79753100	0.98246800	-0.91757900
C	-3.48429600	0.06136600	-0.05897800
C	-2.84064000	-0.88190700	0.66899700
C	-1.41973600	-0.92273000	0.59666100
C	-0.72085300	-0.17193100	-0.46814500

C	-1.47153400	0.91478100	-1.10147900
H	-4.55651100	0.14923500	0.02718500
H	-0.60622500	-0.96595900	-1.26176900
O	-0.67304000	-1.54718100	1.37270200
Cl	-3.65642500	-1.90837400	1.76168900
Cl	-3.76182700	2.17123900	-1.70719200
H	4.50678000	0.48822700	0.35059800
C	3.44748600	0.33963900	0.21244900
C	2.54039100	1.24221900	0.82491500
C	3.00967100	-0.68956600	-0.55119100
C	1.20686000	1.08010000	0.68462600
Cl	3.19010000	2.54404800	1.75847200
C	1.59947000	-0.89772800	-0.81575500
Cl	4.11934800	-1.73344600	-1.33639300
C	0.71532900	-0.05426200	-0.03120500
O	1.15791100	-1.73564300	-1.60145500
H	0.35867000	-1.02713200	0.97288100
H	0.51897600	1.76914500	1.15120100
H	-0.95869600	1.58543700	-1.77177100

TS38

C	-2.73474300	1.34053100	-0.55484500
C	-3.53358300	0.30326600	-0.10431300
C	-2.92152900	-0.83324700	0.37313800
C	-1.52609100	-0.95113100	0.39423000
C	-0.72930100	0.11506100	-0.04841700
C	-1.35521900	1.25661600	-0.52816200
H	-4.60733700	0.37948600	-0.12804800
H	0.22937300	-2.35766000	-0.49545300
O	-0.97053400	-2.08672500	0.80284800
Cl	-3.87016700	-2.13016500	0.96167100
Cl	-3.48157700	2.76268200	-1.16654300
H	4.60203800	0.35911900	0.04448100
C	3.52720000	0.29035600	0.04443400
C	2.74991500	1.31303600	0.55186600
C	2.90767500	-0.83641600	-0.45350000
C	1.37703000	1.21895800	0.54007800
Cl	3.50939600	2.71736300	1.20702300
C	1.51908000	-0.97197700	-0.45978300
Cl	3.87035400	-2.11203300	-1.08195300
C	0.74440500	0.08924600	0.02617200
O	1.00664500	-2.08247400	-0.99639500
H	-0.69787000	-2.10193900	1.89703400

H	-0.45967900	-2.07454100	2.86136200
H	0.78286800	2.02383500	0.94220000
H	-0.76339600	2.07609100	-0.90194500

TS39

C	-1.73317900	1.46678000	-0.71462200
C	-2.49519600	0.74606800	0.28423000
C	-2.35290400	-0.57576200	0.43443500
C	-1.44419700	-1.34685400	-0.43722500
C	-0.43446400	-0.54827100	-1.23783500
C	-0.79310400	0.88466100	-1.45317000
H	-3.20235800	1.29340100	0.88699100
H	-0.30926500	-1.04649400	-2.19738600
O	-1.49399100	-2.54517900	-0.50760900
Cl	-3.27972600	-1.46362400	1.56036000
Cl	-2.13094400	3.13202600	-0.91236400
H	0.18059200	-0.22450500	1.46196400
C	1.00349200	-0.02362000	0.79423100
C	2.08602600	0.62816900	1.22315800
C	0.95077500	-0.55522700	-0.57614900
C	3.22591400	0.88527400	0.36836800
Cl	2.19224500	1.19830700	2.84157000
C	1.99886900	-0.00060400	-1.52855500
Cl	1.55399400	-2.36028900	-0.44373600
C	3.20267500	0.56194200	-0.92833200
O	1.82224600	-0.04166000	-2.72268800
H	4.02385800	0.77727100	-1.59229000
H	1.84168400	-4.24389400	-0.47618500
H	-0.24269800	1.43486400	-2.19910100
H	4.08923500	1.35959900	0.80805700

TS40

C	2.21428900	-1.22832000	-0.73244500
C	2.75508800	-0.40328200	0.32757800
C	2.28385700	0.82903400	0.55509700
C	1.22061900	1.40002200	-0.29023900
C	0.45473200	0.42583600	-1.16310600
C	1.16402000	-0.85467800	-1.45750300
H	3.57027800	-0.79291200	0.91660200
H	0.22310400	0.93837800	-2.09534200
O	0.97028800	2.57805300	-0.28678600
Cl	2.94625000	1.84341100	1.75798800

Cl	3.02153000	-2.72397300	-1.01529000
H	-0.16616200	-0.20557800	1.49008100
C	-0.92805900	-0.49002600	0.78148100
C	-1.95837700	-1.27425300	1.17022300
C	-0.88609200	0.03097500	-0.55485800
C	-3.00774500	-1.66385400	0.27028300
Cl	-2.05325000	-1.84390700	2.78372500
C	-1.82171300	-0.58013000	-1.55509500
Cl	-1.89341200	1.84535300	-0.32524100
C	-2.96036800	-1.31402700	-1.02409100
O	-1.61326400	-0.46524400	-2.74545300
H	-3.71448000	-1.61899800	-1.73112300
O	-2.02178200	3.77688800	-0.57640700
H	-1.07693400	3.96976500	-0.51134400
H	-3.82299900	-2.25215500	0.66028500
H	0.76473600	-1.47489600	-2.24402500

TS41

C	-2.69267700	0.34141400	-0.97313600
C	-3.00506000	-0.47011400	0.18489500
C	-2.15714100	-1.41328900	0.61100100
C	-0.88952700	-1.67787300	-0.09963100
C	-0.43414800	-0.61566300	-1.08484000
C	-1.52088600	0.27652400	-1.59769900
H	-3.95089000	-0.31926900	0.68049000
H	0.05047700	-1.12152300	-1.91758700
O	-0.24053700	-2.66710900	0.10093700
Cl	-2.52111300	-2.42670700	1.93524800
Cl	-3.94508500	1.39069500	-1.51956900
H	-0.16848300	0.23572000	1.56762700
C	0.41599100	0.80263800	0.86057800
C	1.04233500	1.94232200	1.25766800
C	0.59874900	0.31304100	-0.46767700
C	1.85937500	2.71809900	0.37183000
Cl	0.87770300	2.49179900	2.86641400
C	1.25176000	1.23393300	-1.46060000
Cl	2.32263100	-0.85465700	-0.12001800
C	1.98565100	2.37018600	-0.91872700
O	1.15390000	1.02607100	-2.64916300
H	2.57327100	2.94539600	-1.61544300
Cl	4.11325800	-2.24855000	-0.61717400
H	2.36109200	3.58616800	0.76860800
H	-1.30460200	0.88063800	-2.46313900

TS42

C	2.34240400	1.42191800	0.18951700
C	3.07450200	0.27659600	-0.24030300
C	2.45981300	-0.90888400	-0.42805600
C	1.01523900	-1.07501200	-0.25809800
C	0.35081300	0.08122000	0.38203400
C	1.02515100	1.34471500	0.46193300
H	4.13274100	0.37106900	-0.42490100
H	0.24273500	-0.58478200	1.58507300
O	0.41776300	-2.08540100	-0.57363900
Cl	3.32631900	-2.27254000	-0.99114300
Cl	3.20567000	2.90513700	0.36801100
H	-1.68411200	1.35037800	-1.24672500
C	-2.00649100	0.65939000	-0.48495800
C	-3.35517700	0.34166300	-0.35201100
C	-1.11243200	0.02112700	0.33230600
C	-3.82164300	-0.60451100	0.58264700
Cl	-4.49320300	1.08587200	-1.38734200
C	-1.58569500	-0.87573900	1.35540600
C	-2.95439000	-1.23214500	1.42470400
O	-0.70066500	-1.22709600	2.18682200
H	-3.28362400	-1.94955700	2.15757200
H	0.48106800	2.21560600	0.79313000
H	-4.87751300	-0.81874800	0.61772800

TS43

C	2.48345000	1.40773700	0.12223900
C	3.05820200	0.19813000	-0.27955000
C	2.29322300	-0.93436100	-0.39853900
C	0.90620000	-0.88769500	-0.14409300
C	0.36948500	0.35311100	0.30303900
C	1.14514800	1.50124200	0.41168800
H	4.11282200	0.15477900	-0.49743400
H	-0.00607100	-1.33952600	2.14303800
O	0.09605400	-1.86720200	-0.29831700
Cl	2.99346600	-2.41418600	-0.90933900
Cl	3.49815800	2.79566900	0.27176300
H	-1.80826400	2.01609900	-0.30892400
C	-2.04011900	1.00527300	-0.01332500
C	-3.30566400	0.49491600	-0.22358600
C	-1.04288900	0.16995000	0.44875200
C	-3.59014600	-0.87297900	-0.02198500

Cl	-4.54606900	1.51106500	-0.83109500
C	-1.36911400	-1.19229600	0.83761000
C	-2.64905700	-1.70930900	0.48359800
O	-0.87088000	-1.71596800	1.95717400
H	-2.86275100	-2.74007500	0.71155800
H	0.71627000	2.43496000	0.73882400
H	-4.58014800	-1.23651900	-0.24557500

TS44

C	2.57726100	1.40762200	0.01078200
C	3.14338200	0.14192800	-0.10756500
C	2.33773300	-0.97840100	-0.17969400
C	0.97231900	-0.79513600	-0.12809700
C	0.40878000	0.47319400	-0.00688200
C	1.21369600	1.60012300	0.06084100
H	4.21421500	0.03087700	-0.14205700
H	-1.87282600	-0.92295700	2.24767500
O	0.04578800	-1.77058400	-0.20990900
Cl	3.00785600	-2.54696100	-0.33173400
Cl	3.62990300	2.77351500	0.09856400
H	-2.05661500	2.13017100	-0.01602500
C	-2.12666500	1.05549100	-0.05167200
C	-3.35636200	0.43609900	-0.18698000
C	-1.00721100	0.24778600	-0.01297500
C	-3.49079500	-0.95422700	-0.30809200
Cl	-4.77840700	1.40601200	-0.24502400
C	-1.14878000	-1.16364600	-0.00476900
C	-2.38952800	-1.76959700	-0.26218700
O	-1.11602300	-1.42657800	1.92913200
H	-2.46243800	-2.83966600	-0.35583000
H	0.80106400	2.59087500	0.15436300
H	-4.47349000	-1.37303600	-0.44885700