

Supplementary Materials for

Quantum chemical and kinetic study on radical/molecule formation mechanism of pre-intermediates for PCTA/PT/DT/DFs from 2-chlorothiophenol and 2-chlorophenol precursors

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Contains three figures and five tables

Figure S1. Pre-PCDD/DF formation pathways embedded with the potential barriers ΔE (in kcal/mol) and reaction heats ΔH (in kcal/mol) from the coupling reactions of CPR1 with 2-CP (a), CPR2 with 2-CP (b) and CPDR with 2-CP (c), PR2 with 2-CP (d) and PDR with 2-CP (e). ΔH is calculated at 0 K.

Figure S2. The optimized geometries for transition states for pre-PCTA formation routes from the S/C coupling of cross-condensation reactions of CTPR1 with 2-CTP. The red dotted line represents intramolecular hydrogen bonds (^aReference [24], previously calculated by Dar et al. at B3LYP/6-311+G(d,p) level of theory)

Figure S3. MPWB1K/6-31+G(d,p) optimized geometries for transition states of the coupling reactions of CTPR1 with 2-CTP, CTPR2 with 2-CTP, CTPDR with 2-CTP, CPR1 with 2-CP and PR2 with 2-CP. Distances are in Å.

Table S1. Imaginary frequencies (in cm^{-1}), zero point energies (ZPE, in a.u.) and total energies (without ZPE, in a.u.) for transition states involved in the formation of pre-PCTA/PT/DT/DF intermediates.

Table S2. TST rate constants for for pre-PCTA/PT/DT/DF formation routes from the cross-condensation reactions of 2-C(T)P with C(T)PR1, C(T)PR2 and (T)PR2, and C(T)PDR and (T)PDR over the temperature range of 600–1200 K (units are $\text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$).

Table S3. Activation enthalpies ($\Delta H^\ddagger$), activation Gibbs free energies ($\Delta G^\ddagger$), activation entropies ($\Delta S^\ddagger$), relative enthalpies ($\Delta_r H$), relative Gibbs free energies ($\Delta_r G$), relative entropies ($\Delta_r S$) calculated at 298.15 K and 1 atm. (unit is kcal/mol for $\Delta G^\ddagger$, $\Delta H^\ddagger$, $\Delta_r G$ and $\Delta_r H$, unit is $\text{cal mol}^{-1} \text{ K}^{-1}$ for $\Delta S^\ddagger$ and $\Delta_r S$)

Table S4. Cartesian coordinates for transition states involved in the formation routes of pre-intermediates for PCTA/PT/DT/DFs, x coordinate, y coordinate and z coordinate.

Table S5. Cartesian coordinates for reactions, intermediate and products involved in the formation routes of pre-intermediates for PCTA/PT/DT/DFs, x coordinate, y coordinate and z coordinate.

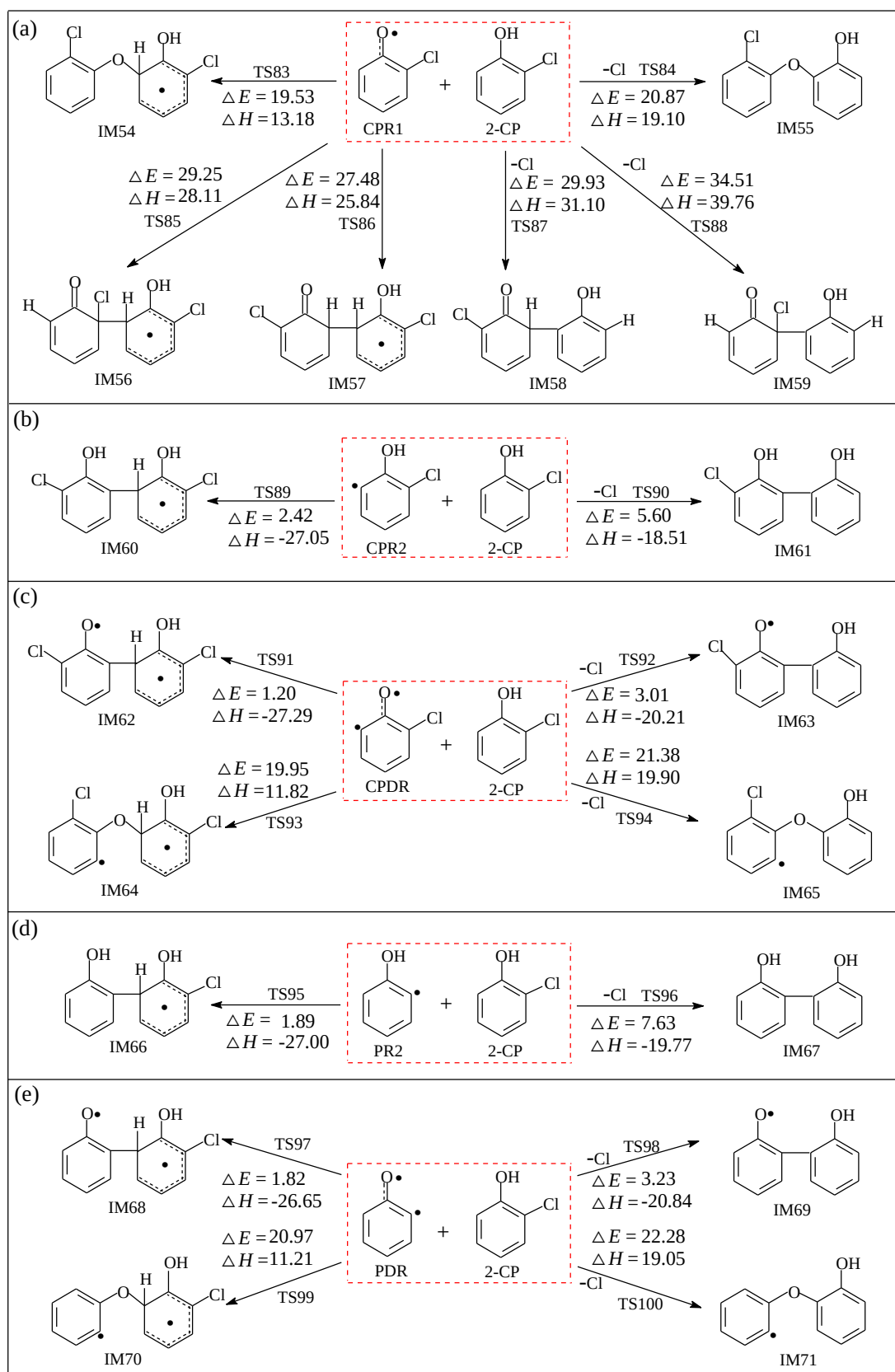


Figure S1. Pre-PCDD/DF formation pathways embedded with the potential barriers ΔE (in kcal/mol) and reaction heats ΔH (in kcal/mol) from the coupling reactions of CPR1 with 2-CP (a), CPR2 with 2-CP (b) and CPDR with 2-CP (c), PR2 with 2-CP (d) and PDR with 2-CP (e). ΔH is calculated at 0 K.

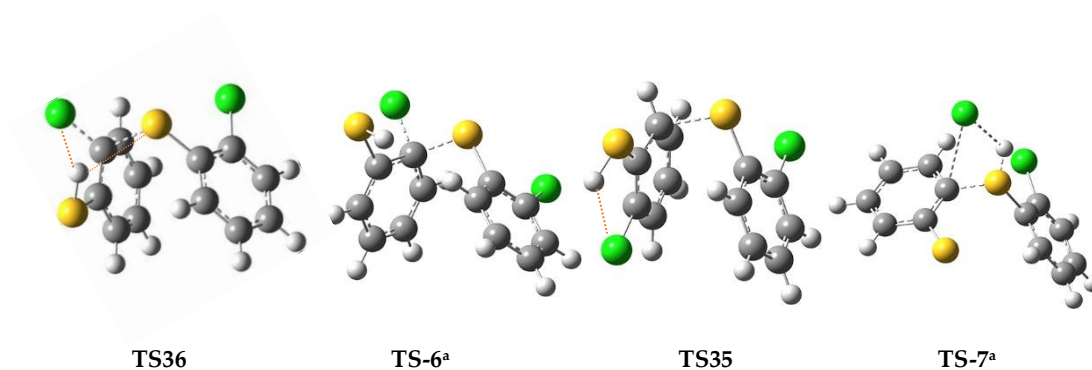


Figure S2. The optimized geometries for transition states for pre-PCTA formation routes from the S/C coupling of cross-condensation reactions of CTPR1 with 2-CTP. The red dotted line represents intramolecular hydrogen bonds (^aReference [24], previously calculated by Dar et al. at B3LYP/6-311+G(d,p) level of theory)

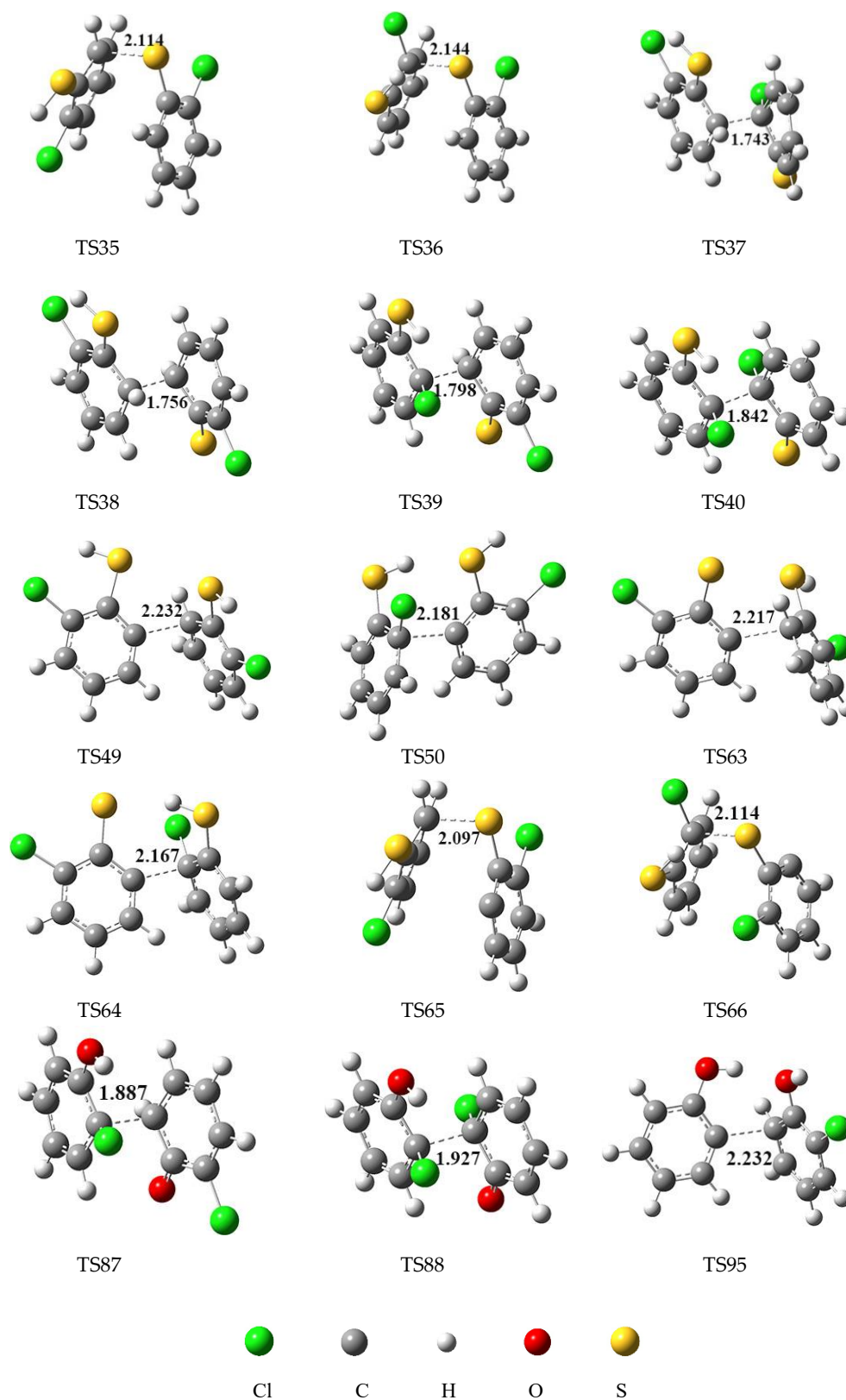


Figure S3. MPWB1K/6-31+G(d,p) optimized geometries for transition states of the coupling reactions of CTPR1 with 2-CTP, CTPR2 with 2-CTP, CTPDR with 2-CTP, CPR1 with 2-CP and PR2 with 2-CP. Distances are in Å.

Table S1. Imaginary frequencies (in cm^{-1}), zero point energies (ZPE, in a.u.) and total energies (without ZPE, in a.u.) for transition states involved in the formation of pre-PCTA/PT/DT/DF intermediates.

TS	Imaginary Frequencies	ZPE	Total Energies
TS1	-938i	0.09316	-1090.60937
TS2	-105i	0.10337	-1165.79578
TS3	-888i	0.09229	-1090.62576
TS4	-761i	0.10215	-1165.86250
TS5	-980i	0.09043	-1090.60320
TS6	-1722i	0.09812	-1165.84924
TS7	-853i	0.08834	-630.25694
TS8	-741i	0.09850	-705.49463
TS9	-936i	0.08393	-1089.96518
TS10	-142i	0.09384	-1165.16275
TS11	-1025i	0.08102	-1089.96954
TS12	-1767i	0.08845	-1165.21758
TS13	-886i	0.07910	-1089.93839
TS14	-791i	0.08886	-1165.17547
TS15	-910i	0.09904	-767.57783
TS16	-4i	0.10921	-842.76241
TS17	-2222i	0.09446	-767.57658
TS18	-2012i	0.10439	-842.82259
TS19	-896i	0.09627	-767.57039
TS20	-1767i	0.10362	-842.81822
TS21	-2182i	0.09065	-307.20602
TS22	-1428i	0.10143	-382.45499
TS23	-915i	0.08503	-766.92722
TS24	-125i	0.09485	-842.11252
TS25	-964i	0.08220	-766.92213
TS26	-1781i	0.09046	-842.17120
TS27	-2209i	0.08138	-766.88792
TS28	-1582i	0.09170	-842.13484
TS29	-625i	0.17903	-1856.55767
TS30	-636i	0.17850	-1856.55300
TS31	-564i	0.17813	-1856.53843
TS32	-584i	0.17867	-1856.54274
TS33	-647i	0.17836	-1856.53692
TS34	-601i	0.17825	-1856.52944
TS35	-337i	0.17673	-2179.62296
TS36	-399i	0.17624	-2179.61632
TS37	-275i	0.17571	-2179.56684
TS38	-384i	0.17615	-2179.57226
TS39	-547i	0.17585	-2179.56605
TS40	-545i	0.17559	-2179.55783

Table S1. *Cont.*

TS	Imaginary Frequencies	ZPE	Total Energies
TS41	-325i	0.18212	-1856.59007
TS42	-382i	0.18174	-1856.58447
TS43	-215i	0.18139	-1856.53709
TS44	-287i	0.18218	-1856.54196
TS45	-500i	0.18186	-1856.53736
TS46	-503i	0.18150	-1856.52936
TS47	-295i	0.17848	-1856.54362
TS48	-484i	0.17869	-1856.53370
TS49	-339i	0.17306	-2179.57473
TS50	-531i	0.17317	-2179.56316
TS51	-328i	0.17847	-1856.54353
TS52	-484i	0.17877	-1856.53534
TS53	-359i	0.18786	-1396.85838
TS54	-512i	0.18837	-1396.85110
TS55	-358i	0.18243	-1719.89213
TS56	-532i	0.18307	-1719.87982
TS57	-349i	0.18819	-1396.86203
TS58	-491i	0.18808	-1396.85247
TS59	-281i	0.16471	-1855.89841
TS60	-484i	0.16434	-1855.88904
TS61	-615i	0.16568	-1855.86993
TS62	-630i	0.16469	-1855.86513
TS63	-346i	0.16339	-2178.94438
TS64	-533i	0.16328	-2178.92911
TS65	-318i	0.16293	-2178.93558
TS66	-375i	0.16279	-2178.92802
TS67	-344i	0.16860	-1855.91178
TS68	-491i	0.16835	-1855.90371
TS69	-292i	0.16871	-1855.90348
TS70	-358i	0.16858	-1855.89774
TS71	-306i	0.17401	-1396.21549
TS72	-493i	0.17429	-1396.20684
TS73	-643i	0.17485	-1396.18659
TS74	-651i	0.17389	-1396.18234
TS75	-340i	0.17319	-1719.26436
TS76	-528i	0.17324	-1719.25053
TS77	-342i	0.17230	-1719.25362
TS78	-409i	0.17260	-1719.24825
TS79	-341i	0.17846	-1396.23194
TS80	-494i	0.17860	-1396.22480
TS81	-326i	0.17835	-1396.22144
TS82	-390i	0.17810	-1396.21651

Table S1. *Cont.*

TS	Imaginary Frequencies	ZPE	Total Energies
TS83	-611i	0.18411	-1533.52428
TS84	-613i	0.18378	-1533.52182
TS85	-537i	0.18347	-1533.50815
TS86	-573i	0.18434	-1533.51184
TS87	-623i	0.18375	-1533.50736
TS88	-588i	0.18372	-1533.50002
TS89	-286i	0.18377	-1533.51117
TS90	-442i	0.18394	-1533.50628
TS91	-287i	0.17014	-1532.86594
TS92	-435i	0.17047	-1532.86338
TS93	-604i	0.17119	-1532.83709
TS94	-606i	0.17053	-1532.83415
TS95	-358i	0.19363	-1073.82954
TS96	-458i	0.19292	-1073.81968
TS97	-293i	0.17960	-1073.18328
TS98	-442i	0.18006	-1073.18148
TS99	-629i	0.18032	-1073.15346
TS100	-632i	0.17994	-1073.15100

Table S2. TST rate constants for for pre-PCTA/PT/DT/DF formation routes from the cross-condensation reactions of 2-C(T)P with C(T)PR1, C(T)PR2 and (T)PR2, and C(T)PDR and (T)PDR over the temperature range of 600–1200 K (units are $\text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$).

T(K)	TST Rate Constants			
	TS29	TS30	TS31	TS32
600	1.91×10^{-23}	1.69×10^{-24}	6.42×10^{-28}	1.47×10^{-26}
700	2.40×10^{-22}	2.92×10^{-23}	3.31×10^{-26}	5.59×10^{-25}
800	1.68×10^{-21}	2.62×10^{-22}	6.72×10^{-25}	9.06×10^{-24}
900	7.99×10^{-21}	1.50×10^{-21}	7.30×10^{-24}	8.24×10^{-23}
1000	2.87×10^{-20}	6.29×10^{-21}	5.09×10^{-23}	4.98×10^{-22}
1100	8.42×10^{-20}	2.09×10^{-20}	2.57×10^{-22}	2.23×10^{-21}
1200	2.11×10^{-19}	5.82×10^{-20}	1.01×10^{-21}	7.97×10^{-21}
	TS33	TS34	TS35	TS36
600	2.79×10^{-28}	1.55×10^{-30}	6.32×10^{-17}	1.46×10^{-18}
700	1.62×10^{-26}	1.57×10^{-28}	9.39×10^{-17}	3.50×10^{-18}
800	3.59×10^{-25}	5.28×10^{-27}	1.34×10^{-16}	7.14×10^{-18}
900	4.18×10^{-24}	8.51×10^{-26}	1.84×10^{-16}	1.30×10^{-17}
1000	3.08×10^{-23}	8.51×10^{-26}	2.45×10^{-16}	1.30×10^{-17}
1100	1.62×10^{-22}	5.32×10^{-24}	3.20×10^{-16}	3.42×10^{-17}
1200	6.64×10^{-22}	2.60×10^{-23}	4.08×10^{-16}	5.10×10^{-17}
	TS37	TS38	TS39	TS40
600	8.21×10^{-30}	4.82×10^{-28}	7.43×10^{-30}	2.88×10^{-32}
700	7.80×10^{-28}	3.11×10^{-26}	7.53×10^{-28}	5.31×10^{-30}
800	2.52×10^{-26}	7.50×10^{-25}	2.55×10^{-26}	2.82×10^{-28}
900	3.93×10^{-25}	9.32×10^{-24}	4.13×10^{-25}	6.51×10^{-27}
1000	3.67×10^{-24}	7.24×10^{-23}	3.98×10^{-24}	8.32×10^{-26}
1100	2.35×10^{-23}	3.99×10^{-22}	2.62×10^{-23}	6.90×10^{-25}
1200	1.14×10^{-22}	1.70×10^{-21}	1.29×10^{-22}	4.12×10^{-24}
	TS41	TS42	TS43	TS44
600	1.20×10^{-16}	5.93×10^{-18}	6.96×10^{-29}	1.28×10^{-27}
700	2.04×10^{-16}	1.51×10^{-17}	6.02×10^{-27}	7.94×10^{-26}
800	3.20×10^{-16}	3.24×10^{-17}	1.81×10^{-25}	1.86×10^{-24}
900	4.76×10^{-16}	6.13×10^{-17}	2.68×10^{-24}	2.25×10^{-23}
1000	6.76×10^{-16}	1.06×10^{-16}	2.39×10^{-23}	1.72×10^{-22}
1100	9.28×10^{-16}	1.70×10^{-16}	1.48×10^{-22}	9.31×10^{-22}
1200	1.24×10^{-15}	2.59×10^{-16}	6.91×10^{-22}	3.90×10^{-21}
	TS45	TS46	TS47	TS48
600	5.33×10^{-29}	2.54×10^{-31}	9.20×10^{-17}	1.33×10^{-19}
700	4.58×10^{-27}	3.90×10^{-29}	1.68×10^{-16}	5.02×10^{-19}
800	1.37×10^{-25}	1.81×10^{-27}	2.79×10^{-16}	1.44×10^{-18}
900	2.02×10^{-24}	3.76×10^{-26}	4.31×10^{-16}	3.40×10^{-18}
1000	1.80×10^{-23}	4.41×10^{-25}	6.32×10^{-16}	7.01×10^{-18}
1100	1.11×10^{-22}	3.40×10^{-24}	8.89×10^{-16}	1.30×10^{-17}
1200	5.16×10^{-22}	1.92×10^{-23}	1.21×10^{-15}	2.23×10^{-17}

Table S2. *Cont.*

T(K)	TST Rate Constants			
	TS49	TS50	TS51	TS52
600	1.05×10^{-17}	4.78×10^{-21}	4.31×10^{-17}	1.15×10^{-19}
700	2.39×10^{-17}	2.51×10^{-20}	9.85×10^{-17}	4.77×10^{-19}
800	4.68×10^{-17}	9.18×10^{-20}	1.93×10^{-16}	1.46×10^{-18}
900	8.20×10^{-17}	2.63×10^{-19}	3.40×10^{-16}	3.64×10^{-18}
1000	1.33×10^{-16}	6.31×10^{-19}	5.54×10^{-16}	7.82×10^{-18}
1100	2.03×10^{-16}	1.33×10^{-18}	8.48×10^{-16}	1.50×10^{-17}
1200	2.96×10^{-16}	2.53×10^{-18}	1.24×10^{-15}	2.65×10^{-17}
	TS53	TS54	TS55	TS56
600	3.07×10^{-17}	7.81×10^{-20}	1.32×10^{-17}	2.18×10^{-21}
700	6.44×10^{-17}	2.85×10^{-19}	3.10×10^{-17}	1.28×10^{-20}
800	1.19×10^{-16}	7.93×10^{-19}	6.22×10^{-17}	5.11×10^{-20}
900	1.99×10^{-16}	1.84×10^{-18}	1.12×10^{-16}	1.56×10^{-19}
1000	3.11×10^{-16}	3.72×10^{-18}	1.84×10^{-16}	3.95×10^{-19}
1100	4.61×10^{-16}	6.81×10^{-18}	2.86×10^{-16}	8.69×10^{-19}
1200	6.56×10^{-16}	1.15×10^{-17}	4.21×10^{-16}	1.72×10^{-18}
	TS57	TS58	TS59	TS60
600	8.31×10^{-17}	1.28×10^{-19}	6.37×10^{-16}	1.63×10^{-18}
700	1.83×10^{-16}	5.61×10^{-19}	9.99×10^{-16}	4.94×10^{-18}
800	3.50×10^{-16}	1.79×10^{-18}	1.47×10^{-15}	1.20×10^{-17}
900	6.05×10^{-16}	4.62×10^{-18}	2.08×10^{-15}	2.50×10^{-17}
1000	9.70×10^{-16}	1.02×10^{-17}	2.84×10^{-15}	4.65×10^{-17}
1100	1.47×10^{-15}	2.00×10^{-17}	3.76×10^{-15}	7.96×10^{-17}
1200	2.12×10^{-15}	3.60×10^{-17}	4.86×10^{-15}	1.27×10^{-16}
	TS61	TS62	TS63	TS64
600	1.40×10^{-23}	3.10×10^{-24}	5.39×10^{-17}	5.15×10^{-21}
700	1.86×10^{-22}	5.71×10^{-23}	1.02×10^{-16}	2.95×10^{-20}
800	1.37×10^{-21}	5.37×10^{-22}	1.73×10^{-16}	1.15×10^{-19}
900	6.75×10^{-21}	3.21×10^{-21}	2.73×10^{-16}	3.49×10^{-19}
1000	2.50×10^{-20}	1.39×10^{-20}	4.07×10^{-16}	8.75×10^{-19}
1100	7.49×10^{-20}	4.74×10^{-20}	5.80×10^{-16}	1.91×10^{-18}
1200	1.91×10^{-19}	1.35×10^{-19}	7.97×10^{-16}	3.75×10^{-18}
	TS65	TS66	TS67	TS68
600	3.32×10^{-19}	1.72×10^{-21}	3.47×10^{-16}	8.04×10^{-19}
700	1.18×10^{-18}	1.12×10^{-20}	7.26×10^{-16}	2.96×10^{-18}
800	3.24×10^{-18}	4.84×10^{-20}	1.34×10^{-15}	8.31×10^{-18}
900	7.42×10^{-18}	1.58×10^{-19}	2.25×10^{-15}	1.94×10^{-17}
1000	1.49×10^{-17}	4.20×10^{-19}	3.52×10^{-15}	3.95×10^{-17}
1100	2.71×10^{-17}	9.65×10^{-19}	5.23×10^{-15}	7.29×10^{-17}
1200	4.57×10^{-17}	1.97×10^{-18}	7.44×10^{-15}	1.24×10^{-16}

Table S2. *Cont.*

T(K)	TST Rate Constants			
	TS69	TS70	TS71	TS72
600	4.30×10^{-19}	6.46×10^{-21}	3.78×10^{-16}	5.53×10^{-19}
700	1.66×10^{-18}	4.39×10^{-20}	6.42×10^{-16}	1.76×10^{-18}
800	4.86×10^{-18}	1.96×10^{-19}	1.01×10^{-15}	4.43×10^{-18}
900	1.17×10^{-17}	6.56×10^{-19}	1.49×10^{-15}	9.50×10^{-18}
1000	2.44×10^{-17}	1.78×10^{-18}	2.12×10^{-15}	1.81×10^{-17}
1100	4.59×10^{-17}	4.17×10^{-18}	2.89×10^{-15}	3.15×10^{-17}
1200	7.94×10^{-17}	8.65×10^{-18}	3.84×10^{-15}	5.11×10^{-17}
	TS73	TS74	TS75	TS76
600	1.70×10^{-23}	8.75×10^{-24}	6.55×10^{-17}	7.93×10^{-21}
700	2.55×10^{-22}	1.74×10^{-22}	1.25×10^{-16}	4.12×10^{-20}
800	2.04×10^{-21}	1.73×10^{-21}	2.14×10^{-16}	1.50×10^{-19}
900	1.08×10^{-20}	1.08×10^{-20}	3.40×10^{-16}	4.27×10^{-19}
1000	4.21×10^{-20}	4.86×10^{-20}	5.08×10^{-16}	1.02×10^{-18}
1100	1.32×10^{-19}	1.71×10^{-19}	7.26×10^{-16}	2.15×10^{-18}
1200	3.50×10^{-19}	4.98×10^{-19}	1.00×10^{-15}	4.08×10^{-18}
	TS77	TS78	TS79	TS80
600	9.16×10^{-19}	3.23×10^{-21}	2.26×10^{-16}	6.95×10^{-19}
700	3.76×10^{-18}	2.34×10^{-20}	4.71×10^{-16}	2.40×10^{-18}
800	1.15×10^{-17}	1.09×10^{-19}	8.63×10^{-16}	6.44×10^{-18}
900	2.85×10^{-17}	3.78×10^{-19}	1.44×10^{-15}	1.45×10^{-17}
1000	6.12×10^{-17}	1.06×10^{-18}	2.26×10^{-15}	2.86×10^{-17}
1100	1.18×10^{-16}	2.53×10^{-18}	3.34×10^{-15}	5.13×10^{-17}
1200	2.08×10^{-16}	5.36×10^{-18}	4.74×10^{-15}	8.55×10^{-17}
	TS81	TS82		
600	2.31×10^{-19}	8.96×10^{-21}		
700	1.04×10^{-18}	6.79×10^{-20}		
800	3.40×10^{-18}	3.29×10^{-19}		
900	8.91×10^{-18}	1.17×10^{-18}		
1000	2.00×10^{-17}	3.36×10^{-18}		
1100	3.97×10^{-17}	8.18×10^{-18}		
1200	7.21×10^{-17}	1.76×10^{-17}		

Table S3. Activation enthalpies ($\Delta H^\ddagger$), activation Gibbs free energies ($\Delta G^\ddagger$), activation entropies ($\Delta S^\ddagger$), relative enthalpies ($\Delta_r H$), relative Gibbs free energies ($\Delta_r G$), relative entropies ($\Delta_r S$) calculated at 298.15 K and 1 atm. (unit is kcal /mol for $\Delta G^\ddagger$, $\Delta H^\ddagger$, $\Delta_r G$ and $\Delta_r H$, unit is cal mol⁻¹ K⁻¹ for $\Delta S^\ddagger$ and $\Delta_r S$)

Reactions	$\Delta H^\ddagger$	$\Delta G^\ddagger$	$\Delta S^\ddagger$	$\Delta_r H$	$\Delta_r G$	$\Delta_r S$
2-CTP + H $\rightarrow$ TPR2 + HCl via TS1	13.36	20.25	-23.11	-5.16	-8.06	9.72
2-CTP + OH $\rightarrow$ TPR2 + HClO via TS2	42.15	49.96	-26.17	44.17	42.28	6.35
2-CTP + H $\rightarrow$ CTPR1 + H ₂ via TS3	2.25	9.72	-25.07	-14.33	-14.64	1.04
2-CTP + OH $\rightarrow$ CTPR1 + H ₂ O via TS4	-0.74	7.97	-29.24	-28.15	-28.09	-0.20
2-CTP + H $\rightarrow$ CTPR2 + H ₂ via TS5	15.50	22.45	-23.29	10.50	9.65	2.87
2-CTP + OH $\rightarrow$ CTPR2 + H ₂ O via TS6	5.01	14.39	-31.45	-3.32	-3.81	1.63
TPR2 + H $\rightarrow$ TPDR + H ₂ via TS7	1.95	8.36	-21.49	-22.92	-23.67	2.53
TPR2 + OH $\rightarrow$ TPDR + H ₂ O via TS8	-1.53	6.01	-25.28	-36.75	-37.13	1.29
CTPR1 + H $\rightarrow$ TPDR + HCl via TS9	13.34	19.72	-21.39	-13.75	-17.09	11.21
CTPR1 + OH $\rightarrow$ TPDR + HClO via TS10	34.95	41.73	-22.74	35.58	33.24	7.83
CTPR1 + H $\rightarrow$ CTPDR + H ₂ via TS11	8.68	15.34	-22.35	3.12	1.78	4.49
CTPR1 + OH $\rightarrow$ CTPDR + H ₂ O via TS12	-3.20	5.83	-30.29	-10.71	-11.67	3.25
CTPR2 + H $\rightarrow$ CTPDR + H ₂ via TS13	2.31	9.35	-23.60	-21.71	-22.50	2.66
CTPR2 + OH $\rightarrow$ CTPDR + H ₂ O via TS14	-0.92	7.28	-27.48	-35.54	-35.96	1.42
2-CP + H $\rightarrow$ PR2 + HCl via TS15	13.73	20.12	-21.43	-2.79	-6.36	11.97
2-CP + OH $\rightarrow$ PR2 + HClO via TS16	43.65	50.84	-24.13	46.54	43.97	8.59
2-CP + H $\rightarrow$ CPR1 + H ₂ via TS17	11.49	18.10	-22.18	-12.89	-14.34	4.87
2-CP + OH $\rightarrow$ CPR1 + H ₂ O via TS18	2.45	11.40	-30.04	-26.71	-27.79	3.62
2-CP + H $\rightarrow$ CPR2 + H ₂ via TS19	16.72	23.07	-21.30	12.34	10.83	5.06
2-CP + OH $\rightarrow$ CPR2 + H ₂ O via TS20	4.91	13.59	-29.10	-1.49	-2.63	3.82
PR2 + H $\rightarrow$ PDR + H ₂ via TS21	9.86	16.61	-22.63	-15.81	-16.95	3.83
PR2 + OH $\rightarrow$ PDR + H ₂ O via TS22	-0.40	8.29	-29.14	-29.63	-30.41	2.59
CPR1 + H $\rightarrow$ PDR + HCl via TS23	13.56	20.07	-21.81	-5.72	-8.98	10.93
CPR1 + OH $\rightarrow$ PDR + HClO via TS24	42.89	49.65	-22.68	43.61	41.36	7.56
CPR1 + H $\rightarrow$ CPDR + H ₂ via TS25	15.00	21.50	-21.80	10.22	8.89	4.47
CPR1 + OH $\rightarrow$ CPDR + H ₂ O via TS26	2.80	12.15	-31.36	-3.61	-4.57	3.23
CPR2 + H $\rightarrow$ CPDR + H ₂ via TS27	10.60	17.44	-22.97	-15.00	-16.28	4.28
CPR2 + OH $\rightarrow$ CPDR + H ₂ O via TS28	1.34	10.25	-29.86	-28.83	-29.73	3.03
CPR1 + 2-CTP $\rightarrow$ IM1 via TS29	18.26	32.13	-46.49	11.21	24.53	-44.69
CPR1 + 2-CTP $\rightarrow$ IM2 + Cl via TS30	20.83	34.88	-47.10	18.15	22.39	-14.22
CPR1 + 2-CTP $\rightarrow$ IM3 via TS31	28.74	42.76	-47.04	28.74	42.76	-47.04
CPR1 + 2-CTP $\rightarrow$ IM4 + Cl via TS32	25.77	38.82	-43.79	25.77	38.82	-43.79
CPR1 + 2-CTP $\rightarrow$ IM5 via TS33	30.90	45.12	-47.68	32.17	37.50	-17.89
CPR1 + 2-CTP $\rightarrow$ IM6 + Cl TS34	35.39	50.46	-50.56	41.44	47.02	-18.73
CTPR1 + 2-CTP $\rightarrow$ IM7 via TS35	0.15	14.12	-46.83	-0.52	13.05	-45.49
CTPR1 + 2-CTP $\rightarrow$ IM8 via TS36	4.05	18.34	-47.93	11.01	15.85	-16.24
CTPR1 + 2-CTP $\rightarrow$ IM9 via TS37	34.67	49.08	-48.34	35.34	49.23	-46.59
CTPR1 + 2-CTP $\rightarrow$ IM10 via TS38	32.22	45.36	-44.07	32.22	45.36	-44.07
CTPR1 + 2-CTP $\rightarrow$ IM11 via TS39	35.34	49.50	-47.51	40.18	44.92	-15.89
CTPR1 + 2-CTP $\rightarrow$ IM12 + Cl TS40	40.18	55.25	-50.57	50.95	56.32	-18.01
CTPR1 + 2-CP $\rightarrow$ IM13 via TS41	0.70	13.32	-42.35	0.70	13.32	-42.35
CTPR1 + 2-CP $\rightarrow$ IM14 + Cl via TS42	4.50	17.75	-44.43	10.13	13.60	-11.67
CTPR1 + 2-CP $\rightarrow$ IM15 via TS43	34.56	47.41	-43.11	34.56	47.41	-43.11
CTPR1 + 2-CP $\rightarrow$ IM16 + Cl via TS44	32.02	44.54	-41.99	32.02	44.54	-41.99

Table S3. *Cont.*

Reactions	$\Delta H^\ddagger$	$\Delta G^\ddagger$	$\Delta S^\ddagger$	ΔH	ΔG	ΔS
CTPR1 + 2-CP $\rightarrow$ IM17 via TS45	33.98	47.64	-45.84	39.91	44.70	-16.07
CTPR1 + 2-CP $\rightarrow$ IM18 + Cl TS46	38.68	53.20	-48.71	47.19	52.09	-16.43
CPR2 + 2-CTP $\rightarrow$ IM19 via TS47	-27.85	-14.30	-45.43	-27.85	-14.30	-45.43
CPR2 + 2-CTP $\rightarrow$ IM20 + Cl via TS48	8.03	21.74	-46.00	-17.95	-12.81	-17.25
CTPR2 + 2-CTP $\rightarrow$ IM21 via TS49	3.76	16.99	-44.36	-25.11	-11.91	-44.29
CTPR2 + 2-CTP $\rightarrow$ IM22 + Cl via TS50	10.82	25.12	-47.94	-16.87	-11.62	-17.59
CTPR2 + 2-CP $\rightarrow$ IM23 via TS51	3.73	16.15	-41.66	-26.04	-11.48	-48.85
CTPR2 + 2-CP $\rightarrow$ IM24 + Cl TS52	8.80	22.21	-44.99	-16.30	-11.96	-14.55
PR2 + 2-CTP $\rightarrow$ IM25 via TS53	-25.80	-11.91	-46.58	-25.80	-11.91	-46.58
PR2 + 2-CTP $\rightarrow$ IM26 + Cl via TS54	7.80	21.94	-47.40	-19.69	-14.07	-18.85
TPR2 + 2-CTP $\rightarrow$ IM27 via TS55	3.99	16.98	-43.56	-25.43	-11.83	-45.62
TPR2 + 2-CTP $\rightarrow$ IM28 + Cl via TS56	11.79	26.06	-47.88	-17.46	-11.82	-18.92
TPR2 + 2-CP $\rightarrow$ IM29 via TS57	3.44	15.62	-40.85	-25.43	-11.98	-45.09
TPR2 + 2-CP $\rightarrow$ IM26 + Cl via TS58	9.22	22.37	-44.11	-17.33	-12.37	-16.61
CPDR + 2-CTP $\rightarrow$ IM30 via TS59	-27.58	-14.38	-44.25	-27.58	-14.38	-44.25
CPDR + 2-CTP $\rightarrow$ IM31 + Cl via TS60	6.12	19.31	-44.25	-17.54	-10.94	-22.16
CPDR + 2-CTP $\rightarrow$ IM32 via TS61	10.05	23.42	-44.87	10.05	23.42	-44.87
CPDR + 2-CTP $\rightarrow$ IM33 + Cl via TS62	21.30	34.77	-45.18	19.02	23.41	-14.75
CTPDR + 2-CTP $\rightarrow$ IM34 via TS63	2.16	15.22	-43.82	-25.03	-11.55	-45.23
CTPDR + 2-CTP $\rightarrow$ IM35 + Cl via TS64	11.48	25.42	-46.74	-9.03	-3.84	-17.40
CTPDR + 2-CTP $\rightarrow$ IM36 via TS65	7.36	20.87	-45.31	7.20	20.52	-44.69
CTPDR + 2-CTP $\rightarrow$ IM37 + Cl via TS66	11.88	26.09	-47.65	18.35	22.75	-14.76
CTPDR + 2-CP $\rightarrow$ IM38 via TS67	2.94	14.53	-38.88	-24.22	-11.31	-43.30
CTPDR + 2-CP $\rightarrow$ IM39 + Cl via TS68	7.70	20.54	-43.06	-8.37	-4.09	-14.35
CTPDR + 2-CP $\rightarrow$ IM40 via TS69	8.03	21.06	-43.67	8.02	20.63	-42.30
CTPDR + 2-CP $\rightarrow$ IM41 + Cl TS70	11.51	25.24	-46.07	17.62	20.77	-10.55
PDR + 2-CTP $\rightarrow$ IM42 via TS71	-27.61	-14.25	-44.82	-27.61	-14.25	-44.82
PDR + 2-CTP $\rightarrow$ IM43 + Cl via TS72	6.60	20.18	-45.56	-16.68	-11.20	-18.37
PDR + 2-CTP $\rightarrow$ IM44 via TS73	9.48	22.48	-43.60	9.48	22.48	-43.60
PDR + 2-CTP $\rightarrow$ IM45 + Cl TS74	21.92	34.47	-42.09	18.01	22.18	-13.98
TPDR + 2-CTP $\rightarrow$ IM46 via TS75	2.26	15.16	-43.26	-26.09	-13.01	-43.86
TPDR + 2-CTP $\rightarrow$ IM47 + Cl via TS76	10.72	24.77	-47.13	-15.02	-10.03	-16.74
TPDR + 2-CTP $\rightarrow$ IM48 via TS77	8.52	20.86	-41.38	7.93	20.57	-42.38
TPDR + 2-CTP $\rightarrow$ IM49 + Cl TS78	11.90	25.69	-46.27	19.92	23.85	-13.16
TPDR + 2-CP $\rightarrow$ IM50 via TS79	2.92	14.77	-39.75	-24.93	-12.71	-40.98
TPDR + 2-CP $\rightarrow$ IM51 + Cl via TS80	7.28	20.39	-43.99	-7.22	-2.86	-14.61
TPDR + 2-CP $\rightarrow$ IM52 via TS81	9.30	22.06	-42.80	9.01	21.26	-41.08
TPDR + 2-CP $\rightarrow$ IM53 + Cl TS82	12.30	25.19	-43.23	19.06	21.67	-8.76

Table S4. Cartesian coordinates for transition states involved in the formation routes of pre-intermediates for PCTA/PT/DT/DFs, x coordinate, y coordinate and z coordinate.

TS1			
0	2		
C	2.25897600	-1.14838400	0.00017200
C	0.93989600	-1.56578900	-0.00006100
C	-0.05451600	-0.61656600	-0.00046000
C	0.18476500	0.74289100	-0.00002200
C	1.52303200	1.13851600	0.00020800
C	2.54251900	0.20802200	0.00030800
H	3.05488100	-1.87624700	0.00030200
H	0.68442500	-2.61351800	-0.00010600
H	1.75510600	2.19328300	0.00037000
H	3.56633800	0.54781700	0.00055000
Cl	-1.84986500	-1.30490100	-0.00076700
H	-3.30857400	-1.87059100	0.01112500
S	-1.03610000	2.00350500	0.00002000
H	-2.09489600	1.19434700	-0.00039100
TS2			
0	2		
C	-2.18101900	-1.87355600	0.01179200
C	-0.79571100	-1.75420300	0.00122200
C	-0.29505100	-0.48522600	-0.00408500
C	-1.00786100	0.68273900	0.00340900
C	-2.39608000	0.52878900	0.01348000
C	-2.96589000	-0.73128300	0.01929200
H	-2.63512200	-2.85228100	0.01370300
H	-0.15157000	-2.61944200	-0.00493300
H	-3.02328500	1.40844800	0.01503600
H	-4.04093200	-0.82041700	0.02778300
Cl	2.15510500	-0.47863900	-0.07555500
O	3.87864200	-0.40404600	0.00103500
H	4.07080400	-0.56221500	0.92851400
S	-0.31199900	2.29471800	0.00810200
H	0.95584200	1.89609700	-0.10424200
TS3			
0	2		
C	-0.06851500	0.70050500	-0.02142300
C	-1.30695500	1.31615300	0.01874200
C	-2.45786700	0.55104300	0.04174600
C	-2.36904300	-0.82987800	0.03927900
C	-1.12947200	-1.43860400	0.02294200

C	0.04214000	-0.68894700	-0.01638700
H	-1.35747000	2.39295100	0.02187900
H	-3.41988300	1.03828300	0.06467200
H	-3.26228200	-1.43385800	0.06419500
H	-1.05043800	-2.51407300	0.04595500
H	2.22814800	-0.88929400	0.89238800
Cl	1.33852200	1.69602100	-0.06977800
H	2.71771400	-0.31937000	1.94132300
S	1.57047600	-1.54803900	-0.14709800
TS4			
0	2		
C	-0.47384100	0.73296400	-0.09650600
C	-1.76264800	1.10007100	0.24675100
C	-2.73941700	0.13517200	0.40632000
C	-2.42580200	-1.20184100	0.23267600
C	-1.13384100	-1.56640900	-0.08909300
C	-0.13783600	-0.60996900	-0.26481700
H	-1.99092200	2.14517000	0.37907000
H	-3.74273600	0.43238400	0.66783800
H	-3.18130400	-1.96090600	0.35970700
H	-0.87550500	-2.60748900	-0.20479900
H	2.20861700	-0.32317500	0.02581000
Cl	0.70180900	1.97158200	-0.30701400
O	2.73414800	-0.36003500	1.47825200
H	2.65580900	-1.26231300	1.81181900
S	1.44765100	-1.16251300	-0.76613700
TS5			
0	2		
C	0.08290900	-0.74144700	-0.00008300
C	0.02627900	0.65301100	0.00235500
C	-1.24408800	1.18851200	0.00104000
C	-2.41048100	0.47659700	-0.00211300
C	-2.31620100	-0.90954600	-0.00144500
C	-1.07163700	-1.50830600	0.00130900
H	-1.35526500	2.66277000	0.01997900
H	-3.36761000	0.97495900	-0.00238200
H	-3.20619600	-1.51924500	-0.00210800
H	-0.97942200	-2.58209300	0.00220400
Cl	1.60088600	-1.57198800	-0.00069800
H	-1.42170300	3.50141500	0.03414600
S	1.39878700	1.74551200	-0.01038500
H	2.33384800	0.80486000	0.11981700

TS6			
0	2		
C	-1.06879600	0.32112200	0.00389000
C	0.19905600	-0.26048500	-0.02598400
C	1.26862100	0.61380900	-0.04677000
C	1.15381900	1.98043500	-0.04184600
C	-0.12073100	2.52680600	-0.00633600
C	-1.22471100	1.69640700	0.02257900
H	2.43368300	0.15021200	-0.07486600
H	2.03209700	2.60563500	-0.05449400
H	-0.25476800	3.59698400	0.00318400
H	-2.22126800	2.10581600	0.05408100
Cl	-2.48614600	-0.66436000	0.03089800
O	3.50262900	-0.38980200	0.06302100
H	3.24853600	-1.15236300	0.59524700
S	0.52146300	-1.98676900	-0.09575800
H	-0.58177200	-2.37400400	0.54634600
TS7			
0	3		
C	-0.22041400	1.14017100	-0.13506900
C	-1.57840900	1.27313000	-0.09073000
C	-2.31486000	0.09718400	0.02789800
C	-1.66349300	-1.12341200	0.10758100
C	-0.27998600	-1.19532900	0.08391600
C	0.47941800	-0.03313900	-0.04836100
H	-2.06430700	2.23448000	-0.15417900
H	-3.39307600	0.14039800	0.05858100
H	-2.23728500	-2.03196000	0.20325400
H	0.22338700	-2.14665800	0.17180500
H	2.49245800	0.87364700	0.79368800
H	2.62997400	1.74327500	1.75916700
S	2.23845700	-0.11030100	-0.15648300
TS8			
0	3		
C	-0.45627200	0.92274900	-0.59939800
C	-1.74072000	1.34907000	-0.42239000
C	-2.62104300	0.44805500	0.17046900
C	-2.17318500	-0.80574700	0.55922700
C	-0.85285400	-1.17787700	0.37635700
C	0.04661700	-0.29711100	-0.22857300
H	-2.06581900	2.33033000	-0.73164500

H	-3.65105200	0.72991800	0.32762000
H	-2.85797800	-1.49901800	1.02192200
H	-0.50674400	-2.14826100	0.70067500
H	2.28542800	0.44616400	-0.36634700
O	2.97166100	1.16517800	0.83534200
H	2.54306800	0.87281700	1.64905000
S	1.70403500	-0.79301300	-0.52613500
TS9			
O	3		
C	2.27709000	-1.08683400	0.00000000
C	0.96725600	-1.53852600	0.00004200
C	-0.03959400	-0.60683100	0.00005300
C	0.17207200	0.75541500	0.00002600
C	1.49676300	1.19243600	-0.00001600
C	2.53125700	0.27550500	-0.00003700
H	3.09077800	-1.79474400	-0.00000300
H	0.73364900	-2.59150000	0.00009600
H	1.71029600	2.25048900	-0.00004600
H	3.54881600	0.63391800	-0.00007900
Cl	-1.85623600	-1.21951900	-0.00003700
H	-3.33147400	-1.73245700	0.00005500
S	-1.16407000	1.87619500	0.00001200
TS10			
O	3		
C	-2.19433700	-1.79485300	0.00496300
C	-0.80422000	-1.71784600	0.00704100
C	-0.26984800	-0.46439100	0.00385100
C	-0.96108800	0.73788200	0.00210900
C	-2.37076300	0.60553800	0.00058400
C	-2.96616600	-0.63506100	0.00182300
H	-2.67266700	-2.76265200	0.00707400
H	-0.18805200	-2.60310600	0.01127200
H	-2.96138900	1.50882700	-0.00176200
H	-4.04205000	-0.71097300	0.00090200
Cl	2.11171800	-0.55158800	-0.02576100
O	3.83528800	-0.40132000	0.03160500
H	3.97338500	0.54938200	0.03405300
S	-0.20576300	2.26365500	0.00070800
TS11			
O	3		
C	0.20580800	-0.71033500	-0.00001000

C	-0.01607900	0.69300300	0.00000700
C	-1.35897100	1.07300500	0.00003000
C	-2.43000900	0.22609600	0.00003400
C	-2.16031700	-1.13813800	0.00001400
C	-0.85036000	-1.59819900	-0.00000800
H	-1.66078700	2.50762000	0.00002600
H	-3.44273500	0.59834800	0.00005000
H	-2.97072600	-1.85122600	0.00001700
H	-0.64577800	-2.65622800	-0.00002300
Cl	1.80009400	-1.34096400	-0.00003100
H	-1.87665500	3.32283300	-0.00001500
S	1.22841600	1.85015300	0.00000500
TS12			
O	3		
C	1.07993900	0.28013900	0.00007800
C	-0.21385300	-0.30448000	0.00001300
C	-1.28266500	0.60124500	0.00008300
C	-1.15247500	1.96239500	0.00006900
C	0.13521600	2.48735100	-0.00005100
C	1.24112100	1.64978700	-0.00008000
H	-2.45482700	0.14979700	0.00002800
H	-2.01829200	2.60460500	0.00026400
H	0.28215800	3.55644800	0.00006200
H	2.23731500	2.06067900	-0.00014900
Cl	2.47890300	-0.70794400	-0.00002400
O	-3.50601700	-0.42239800	-0.00011700
H	-3.17541900	-1.32951000	-0.00005000
S	-0.48799100	-1.98040100	0.00003200
TS13			
O	3		
C	-0.11199600	0.66340500	-0.02744400
C	0.07856100	-0.72333400	-0.02542200
C	-1.07670900	-1.45893800	0.00955100
C	-2.35755700	-0.99106500	0.04238100
C	-2.50025100	0.39233900	0.05134000
C	-1.38377400	1.20985300	0.02299900
H	-3.21168000	-1.64901800	0.06535100
H	-3.48456500	0.83420500	0.07903700
H	-1.49070200	2.28207300	0.03099200
Cl	1.24265700	1.72784700	-0.07495700
H	2.26372300	-0.78431600	0.86922400
H	2.74163600	-0.17357700	1.90546300

S	1.63542400	-1.52727100	-0.13226400
TS14			
0	3		
C	-0.49458400	0.69624000	-0.10384000
C	-0.11841800	-0.64166900	-0.28204000
C	-1.12547600	-1.55409100	-0.10401000
C	-2.42456800	-1.30089400	0.22321300
C	-2.75403200	0.03855700	0.40216100
C	-1.79417000	1.02394900	0.24351900
H	-3.15496400	-2.08518200	0.34211600
H	-3.76355700	0.31586700	0.66466300
H	-2.04893000	2.06163000	0.38260200
Cl	0.65421200	1.96006800	-0.30281600
H	2.20763500	-0.31397500	0.01532000
O	2.70984400	-0.33032300	1.48305200
H	2.65973900	-1.23254400	1.82246200
S	1.47295100	-1.18730700	-0.76360800
TS15			
0	2		
C	-1.34374900	-1.34374900	0.00000200
C	-1.46885400	-1.46885400	-0.00001900
C	-0.32462600	-0.32462600	-0.00005000
C	0.94803300	0.94803300	-0.00000900
C	1.05621100	1.05621100	0.00002500
C	-0.07931900	-0.07931900	0.00002600
H	-2.22589900	-2.22589900	0.00000900
H	-2.43585700	-2.43585700	-0.00002100
H	2.04367400	2.04367400	0.00004900
H	0.02550700	0.02550700	0.00005000
O	2.06871800	2.06871800	-0.00001900
H	1.84201300	1.84201300	-0.00001300
Cl	-0.46709300	-0.46709300	-0.00000700
H	-0.58478400	-0.58478400	0.00035000
TS16			
0	2		
C	2.49412900	-1.38891500	0.01082000
C	1.10783900	-1.51220100	-0.00825600
C	0.39219700	-0.35280600	-0.01398300
C	0.89922700	0.92259500	-0.00031400
C	2.28702100	1.01842300	0.01950000
C	3.06498600	-0.12557400	0.02510500

H	3.11212200	-2.27306300	0.01417400
H	0.62745000	-2.47838400	-0.01984400
H	2.73074100	2.00243100	0.02967500
H	4.13917700	-0.02652300	0.04043400
Cl	-2.19659100	-0.32187100	-0.05642200
O	-3.88819300	-0.10601900	-0.01101800
H	-4.14029700	-0.42650600	0.85839900
O	0.15947600	2.04261400	-0.00448700
H	-0.76981100	1.81196400	-0.03686100
TS17			
0	2		
C	-0.35515700	-0.41173000	-0.03030600
C	0.53715100	-1.46238800	0.04320000
C	1.89750900	-1.20643900	0.06012900
C	2.36501200	0.09972200	0.02243500
C	1.47336200	1.14911100	-0.02389900
C	0.09890600	0.91310300	-0.07074300
H	0.16237800	-2.47247000	0.07801100
H	2.59112100	-2.03106100	0.10690200
H	3.42553300	0.29532500	0.03852800
H	1.80436200	2.17516400	-0.04533600
O	-0.73334600	1.93326600	-0.20587700
H	-1.46307700	2.01777800	0.67045700
Cl	-2.04575100	-0.70763800	-0.04094400
H	-1.97647200	2.09071300	1.48960600
TS18			
0	2		
C	-0.18576900	0.66208900	-0.07117600
C	-1.40346800	1.22484100	0.25390800
C	-2.53183500	0.42825600	0.34515000
C	-2.44054200	-0.93841400	0.11711700
C	-1.22476600	-1.50457700	-0.19141400
C	-0.07729100	-0.71650700	-0.29947100
H	-1.46049100	2.28725300	0.42738400
H	-3.47974500	0.87709600	0.59598600
H	-3.31958500	-1.55914100	0.18820400
H	-1.11957300	-2.56319100	-0.36697700
O	1.04818200	-1.29661700	-0.67218200
H	1.91761200	-0.95939200	-0.20344300
Cl	1.21356700	1.64611600	-0.19952400
O	2.81913100	-1.07796000	0.79345800
H	3.07465700	-2.00411800	0.85586600

TS19			
0	2		
C	0.46659700	-0.35701600	-0.00000500
C	-0.16358300	0.88474800	0.00000900
C	-1.54014700	0.86153400	0.00001500
C	-2.29419800	-0.27838200	0.00000700
C	-1.63738100	-1.50391900	-0.00000800
C	-0.25558800	-1.53696100	-0.00001300
H	-2.25713000	2.18252500	0.00002900
H	-3.37241800	-0.22681100	0.00001100
H	-2.19759000	-2.42547100	-0.00001400
H	0.27635900	-2.47445300	-0.00002400
Cl	2.20010000	-0.39175600	-0.00001200
O	0.49340900	2.05062100	0.00001800
H	1.43834900	1.88843300	0.00001200
H	-2.69074600	2.89062500	0.00002500
TS20			
0	2		
C	0.97884700	0.16587500	-0.00001700
C	-0.25989000	-0.46354200	0.00001100
C	-1.37618000	0.34537300	0.00002200
C	-1.31363600	1.71428900	0.00002600
C	-0.06335500	2.32143100	0.00001600
C	1.07990400	1.54468500	-0.00001300
H	-2.49431400	-0.26011700	-0.00004100
H	-2.21621800	2.30455000	0.00004000
H	0.01759500	3.39661300	0.00002400
H	2.05754100	1.99857300	-0.00002900
Cl	2.39929300	-0.82385000	-0.00002200
O	-0.41880900	-1.79633300	0.00005300
H	0.43730100	-2.22877600	0.00013300
O	-3.33984900	-1.08976700	-0.00009200
H	-2.79476700	-1.88527400	0.00029000
TS21			
0	3		
C	-0.14720600	-1.18824400	-0.08678900
C	1.21199000	-1.24292700	0.00536200
C	1.88960100	-0.02673600	0.06858300
C	1.18028400	1.16767700	0.05371200
C	-0.19925400	1.17052200	-0.01792500
C	-0.90750200	-0.03424200	-0.10173500

H	1.74643000	-2.18048300	0.01563500
H	2.96732400	-0.01739100	0.12775700
H	1.71210300	2.10484300	0.10356500
H	-0.76315100	2.09118200	-0.02087900
O	-2.23034300	-0.02782900	-0.24837800
H	-2.77239100	-0.33314200	0.68016000
H	-3.21504200	-0.51869200	1.55353500
TS22			
O	3		
C	-0.08039100	0.97507800	-0.34308100
C	-1.34674500	1.42259900	-0.11904800
C	-2.31271200	0.46699200	0.19319400
C	-1.95744000	-0.87449200	0.28318300
C	-0.65599100	-1.28076000	0.07546200
C	0.33043400	-0.34419200	-0.26186300
H	-1.59990900	2.46934400	-0.18932000
H	-3.33309700	0.77269400	0.36558200
H	-2.70826800	-1.60901700	0.52856500
H	-0.36479900	-2.31670900	0.15778600
O	1.55721300	-0.76008500	-0.51647000
H	2.27817700	-0.04807800	-0.33004900
O	3.18814500	0.58015300	0.48828500
H	3.90209700	-0.02012400	0.72582900
TS23			
O	3		
C	1.76062100	-1.38197300	-0.00004100
C	0.36690300	-1.44988100	-0.00029000
C	-0.34572000	-0.28735300	-0.00026600
C	0.26482100	1.01682500	-0.00010800
C	1.70848000	1.01849000	0.00022800
C	2.42054000	-0.14482400	0.00025500
H	2.33425000	-2.29600400	-0.00006000
H	-0.13955300	-2.40240400	-0.00050300
H	2.18655900	1.98557400	0.00041700
H	3.49909400	-0.12022800	0.00049500
O	-0.38560900	2.07001900	-0.00029000
Cl	-2.23877700	-0.35470900	0.00014000
H	-3.79014500	-0.32474600	0.00092000
TS24			
O	3		
C	2.27397100	-1.46945300	0.01618500

C	0.87458300	-1.45416200	0.01819400
C	0.27318000	-0.24076300	0.01008200
C	0.92116500	1.03452600	0.00551200
C	2.36732700	0.93879100	0.00391700
C	3.00216500	-0.26913900	0.00873800
H	2.79490000	-2.41463300	0.02472100
H	0.30549200	-2.37113200	0.02950400
H	2.90780500	1.87294900	-0.00389200
H	4.08029500	-0.30929200	0.00782500
O	0.33591200	2.12415400	0.00180400
Cl	2.13482100	-0.26442200	-0.08173000
O	3.84428700	-0.16204200	0.09542300
H	4.00387500	0.78157600	0.17766400
TS25			
O	3		
C	0.53705300	-0.30666400	-0.00000200
C	-0.18688200	0.95892800	-0.00000200
C	-1.61179800	0.81268600	0.00000200
C	-2.27511400	-0.37079300	0.00000300
C	-1.51769200	-1.54916800	0.00000200
C	-0.12192200	-1.50769600	0.00000000
H	-2.36849900	2.07841300	0.00001800
H	-3.35384400	-0.41167700	0.00000600
H	-2.01515200	-2.50687400	0.00000400
H	0.44588300	-2.42407100	-0.00000100
Cl	2.23947600	-0.24361200	-0.00000600
O	0.38773900	2.04968700	-0.00000400
H	-2.82326200	2.78435500	0.00008500
TS26			
O	3		
C	-1.01007700	0.11733300	-0.00001100
C	0.28824400	-0.53436200	-0.00019600
C	1.41220800	0.35716400	-0.00028000
C	1.31397700	1.71054400	-0.00009100
C	0.03202400	2.27939200	0.00002800
C	-1.11433400	1.48391700	0.00008000
H	2.52863900	-0.25123300	0.00034200
H	2.19133000	2.33788000	0.00005500
H	-0.07431600	3.35310700	0.00017300
H	-2.09025100	1.94170100	0.00020100
Cl	-2.39377900	-0.87202500	0.00006000
O	0.42019400	-1.76299200	-0.00009000

O	3.31689800	-1.13160900	0.00028400
H	2.70985400	-1.88414900	-0.00053000
TS27			
O	3		
C	-0.30474100	-0.39569500	-0.03375900
C	0.04986400	0.96555000	-0.08093800
C	1.40731600	1.21462600	-0.03261700
C	2.40145500	0.28554200	0.02221700
C	2.00361600	-1.04909800	0.06369500
C	0.65823500	-1.38349200	0.04383900
H	3.44441800	0.56045400	0.03645600
H	2.74575200	-1.83108800	0.11118700
H	0.34939100	-2.41519800	0.08175000
Cl	-1.97221300	-0.80364600	-0.03643900
O	-0.84238500	1.92971300	-0.21336600
H	-1.53207500	2.00600400	0.68024700
H	-2.03524800	2.07950900	1.52213800
TS28			
O	3		
C	-0.21610000	0.61807500	-0.07493700
C	-0.05245800	-0.75767900	-0.32291300
C	-1.20576000	-1.51096800	-0.21086100
C	-2.44825600	-1.05287700	0.09840400
C	-2.56466800	0.31480000	0.34193200
C	-1.45230900	1.13746200	0.25774200
H	-3.30283000	-1.70842200	0.15735300
H	-3.52403700	0.73819500	0.59585500
H	-1.53928600	2.19522700	0.44435300
Cl	1.15257000	1.64812000	-0.18525600
O	1.08525500	-1.30660200	-0.69422700
H	1.93766700	-0.94411800	-0.21961700
O	2.83380800	-1.04677600	0.79247900
H	3.11960200	-1.96478100	0.84919900
TS29			
O	2		
C	2.34790500	2.52960000	-0.15273200
C	1.10604000	2.52485600	-0.77018600
C	0.50779000	1.32891200	-1.10609400
C	1.13032400	0.10487200	-0.83554800
C	2.38808600	0.13833400	-0.21308100
C	2.99245800	1.33476000	0.11800600

H	2.82396000	3.46152000	0.10909000
H	0.60874100	3.45570800	-0.99414800
H	3.96683200	1.32357700	0.57952100
O	0.57850900	-1.03475300	-1.20220400
C	-0.62099400	-1.73586400	-0.07137900
C	-1.72253500	-0.81359200	-0.14211800
C	-1.82096100	0.15046600	0.83866300
C	-0.97811500	0.14478800	1.94526800
C	-0.04850000	-0.88419100	2.11592800
C	0.07831300	-1.85586800	1.16649500
H	-1.07579900	0.92650200	2.68035400
H	0.54963400	-0.91272500	3.01277300
H	0.77928200	-2.66485100	1.28142500
H	-0.44915700	1.30218400	-1.60515000
H	-0.70675500	-2.62358900	-0.67741200
Cl	3.21858100	-1.33960800	0.08777200
Cl	-3.01015900	1.40257600	0.74939000
S	-2.69994500	-0.92623100	-1.57253900
H	-3.62772300	-0.04351200	-1.19928300
TS30			
0	2		
C	-3.31340700	-1.66087800	-0.16737100
C	-2.17127400	-2.33134100	-0.57894700
C	-1.02244200	-1.62409400	-0.86215300
C	-0.98117800	-0.23044000	-0.74480200
C	-2.15203500	0.42499100	-0.33266600
C	-3.30479500	-0.28157200	-0.05153000
H	-4.21743200	-2.20706000	0.05215900
H	-2.18152200	-3.40508600	-0.68458900
H	-4.19164100	0.25359100	0.24770800
O	0.10607700	0.44495500	-1.06693400
C	1.33400800	-1.41884800	1.44874700
C	0.52703000	-0.83420800	2.41299400
C	0.20698500	0.52743600	2.33512500
C	0.66762600	1.27961400	1.29863300
H	1.59239600	-2.46381400	1.52793000
H	0.15946200	-1.43043200	3.23253400
H	-0.38104500	0.99007600	3.11178600
H	0.46176300	2.33328000	1.22342700
H	-0.12543200	-2.12069400	-1.19972200
Cl	-2.17074900	2.14345200	-0.23907100
C	1.35589200	0.66368000	0.20756600
Cl	2.35790700	1.74711000	-0.71231100

C	1.80723900	-0.69317000	0.37648600
S	2.78192600	-1.49933900	-0.81728500
H	2.62043100	-0.58665000	-1.77818900
TS31			
O	2		
C	-3.31884000	1.42951700	-0.54037300
C	-3.35834900	0.09905100	-0.74646300
C	-2.44878900	-0.79319600	-0.04665500
C	-1.25586200	-0.12497500	0.56778700
C	-1.42837700	1.26412900	0.95171900
C	-2.37576800	2.01891400	0.36613300
C	-0.11696500	-0.11217600	-0.91319200
C	1.14641000	0.50020100	-0.52027000
C	-0.03161200	-1.48552000	-1.35893200
C	2.21729300	-0.31586000	-0.22055900
C	1.05904300	-2.24761100	-1.07990600
C	2.17894400	-1.68375600	-0.46064100
O	-2.58815200	-1.99824000	-0.03272600
H	3.03501700	-2.28615100	-0.20634200
H	-0.73649500	1.68185000	1.66395900
H	-0.88838000	-1.92314100	-1.84235800
H	-4.04294100	2.06893000	-1.02337500
H	1.07212600	-3.29229000	-1.34660500
H	-2.45274200	3.06893400	0.59956700
H	-4.11731900	-0.36751600	-1.35427200
H	-0.73370900	0.53418300	-1.53262100
Cl	-0.47307900	-1.09794400	1.78388100
Cl	3.69804000	0.33601200	0.39483900
S	1.16818100	2.23726700	-0.47457400
H	2.45165900	2.36537100	-0.13310000
TS32			
O	2		
C	2.79065500	-1.60986800	0.09225700
C	2.93357100	-0.26892800	0.06507300
C	1.92363500	0.60927000	0.65287200
C	0.61895800	-0.03201700	0.94009800
C	0.61719200	-1.46074100	1.13931300
C	1.64077200	-2.21591200	0.68788200
C	-0.31949600	0.33201300	-0.64149200
C	-1.64125800	-0.25166100	-0.47907800
C	-0.27878400	1.76913500	-0.76042300
C	-2.65264700	0.54621800	0.01525800

C	-1.31628200	2.52788600	-0.30874200
C	-2.48973700	1.92068500	0.14627400
O	2.10022800	1.80004200	0.82515000
H	-3.30278300	2.50956700	0.53759600
H	0.32018200	-0.21334600	-1.32779700
H	-0.23784400	-1.92208700	1.60583700
H	0.62880600	2.23454300	-1.10439900
H	3.57624300	-2.23524600	-0.30288000
H	0.02092500	0.55523700	1.62551000
H	-1.24186900	3.60350100	-0.30668700
H	1.61663300	-3.28960500	0.78643900
Cl	4.34830400	0.47285100	-0.55659500
Cl	-4.20343200	-0.11396100	0.41142900
S	-1.78295100	-1.93008900	-0.89652400
H	-3.07718600	-2.05908800	-0.59836600
TS33			
O	2		
C	-2.42462300	-1.52082700	-0.44653600
C	-2.51202900	-0.18995900	-0.26692200
C	-1.41769100	0.70039100	-0.64835700
C	-0.13784200	0.04731100	-1.02747700
C	-0.17922500	-1.35924000	-1.34508900
C	-1.25334700	-2.10915900	-1.02160400
C	0.98068000	0.31536900	0.47424200
C	2.26300700	-0.21949400	0.03776000
C	0.93938600	1.74677800	0.66848700
C	3.13973900	0.62891500	-0.60929600
C	1.83985200	2.55295700	0.04586200
C	2.91724500	1.99593800	-0.65400300
H	3.62155800	2.63315400	-1.16428800
H	0.67216100	-1.80816500	-1.83014400
H	0.11126800	2.15620600	1.22029700
H	-3.26013400	-2.15043600	-0.18318300
H	0.43840700	0.67310300	-1.69952700
H	1.73028600	3.62342300	0.11189800
H	-1.26319400	-3.16704100	-1.23365500
Cl	-3.92771500	0.54532200	0.35550200
Cl	0.18713600	-0.56590600	1.78532600
H	4.03963900	0.21993300	-1.04354800
S	2.69189600	-1.89901600	0.14434800
H	1.65470400	-2.28020500	0.89211900
O	-1.51951100	1.91254000	-0.62700400

TS34			
0	2		
C	3.29293800	0.69103800	0.02001500
C	2.98964800	-0.53567300	0.47466400
C	1.75126000	-1.19466500	0.09929500
C	0.74753100	-0.36981900	-0.66054500
C	1.22400800	0.87673300	-1.22615100
C	2.40682500	1.40226800	-0.85735900
C	-0.57102400	0.03909100	0.69144100
C	-1.64636600	0.75562200	0.02124600
C	-0.93323400	-1.24222600	1.25231700
C	-2.80885600	0.08710700	-0.30629100
C	-2.09347500	-1.86265100	0.91526100
C	-3.03557700	-1.21393200	0.10639000
H	-3.95812100	-1.70514700	-0.15765100
H	0.60186900	1.36470000	-1.95790400
H	-0.22342700	-1.71842300	1.90587300
H	4.23643100	1.14543800	0.28289900
H	-2.29813600	-2.84807000	1.30212500
H	2.72629800	2.34585000	-1.27190500
Cl	0.34900400	1.02210800	1.85312700
H	-3.57216100	0.61349000	-0.85937200
Cl	-0.13822600	-1.33524900	-1.81684500
H	3.66511600	-1.11147800	1.08683500
O	1.51357800	-2.34866300	0.39685600
S	-1.52446700	2.41983000	-0.47025900
H	-0.42030100	2.71170800	0.21990900
TS35			
0	2		
C	1.82175900	2.67170900	-0.47131900
C	0.69541500	2.38015900	-1.22211900
C	0.36319900	1.06359600	-1.46808600
C	1.12847900	0.01097900	-0.96432500
C	2.26684800	0.33201000	-0.21928300
C	2.61235400	1.64982400	0.02148200
H	2.09545900	3.69653000	-0.27335400
H	0.07709800	3.17310500	-1.61233000
H	3.49829700	1.86533500	0.59656500
Cl	3.29229200	-0.89868200	0.41980500
C	-0.75609300	-1.81291800	0.34046300
C	-1.75734200	-0.78448000	0.16513100
C	-1.65134100	0.36314700	0.91961600
C	-0.71140800	0.48444400	1.94038700

C	0.13186300	-0.58691700	2.24319900
C	0.07663700	-1.73419100	1.50750500
H	-0.66035200	1.40530100	2.49705200
H	0.82231400	-0.50203300	3.06722100
H	0.72680000	-2.56586400	1.72488500
H	-0.51174700	0.81600400	-2.05047100
H	-1.06972100	-2.80692200	0.04665500
Cl	-2.70388400	1.70872600	0.64914700
S	0.61132300	-1.62780800	-1.26080500
S	-2.89698300	-1.06011200	-1.12161600
H	-3.73274000	-0.06965400	-0.80556300
TS36			
0	2		
C	3.29551800	1.71340100	0.02019700
C	2.20879100	2.34237500	-0.56367800
C	1.14263200	1.58728000	-1.00771500
C	1.13012100	0.19663800	-0.88365400
C	2.24489400	-0.41486100	-0.30024900
C	3.31622500	0.33657600	0.14802200
H	4.13715500	2.29063100	0.37064200
H	2.19254000	3.41535200	-0.67325400
H	4.16236900	-0.16417100	0.58993000
Cl	2.34385000	-2.12867100	-0.14117700
C	-1.49601300	-0.61230500	0.28399100
C	-1.69893300	0.79639600	0.52360200
C	-0.97471800	1.41563000	1.51874100
C	-0.14151800	0.69544300	2.36351100
C	-0.03694300	-0.69311800	2.22928500
C	-0.74194100	-1.34370600	1.26203900
H	-1.06095500	2.48537200	1.63415200
H	0.41654700	1.21109700	3.12828300
H	0.58626000	-1.25852100	2.90375100
H	-0.68802000	-2.41338000	1.14508200
Cl	-2.87042300	-1.50726900	-0.36483400
H	0.28423700	2.06105300	-1.46000900
S	-0.25054700	-0.69841100	-1.45901600
S	-2.73881600	1.76859900	-0.48269500
H	-2.73729300	0.94204300	-1.53356300
TS37			
0	2		
C	-2.85310800	2.01875400	-0.62619400
C	-3.10664200	0.70004300	-0.77545300

C	-2.38242600	-0.29391700	-0.03227000
C	-1.06835300	0.17529500	0.50650700
C	-1.05647000	1.59171600	0.90833500
C	-1.86679800	2.47456900	0.30730100
C	0.00382200	0.04228000	-0.86102300
C	1.37311200	0.44588500	-0.48056000
C	-0.08217700	-1.31831200	-1.39388100
C	2.31399600	-0.52730900	-0.22745100
C	0.88687200	-2.23496800	-1.16087600
C	2.07456800	-1.86758500	-0.51074200
H	2.83290300	-2.59795100	-0.28364500
H	-0.32533100	1.89629900	1.63767000
H	-0.97638300	-1.59658900	-1.92475000
H	-3.45399700	2.74296500	-1.15505800
H	0.76127800	-3.25293700	-1.49415400
H	-1.80070600	3.52454000	0.54475500
H	-3.92907500	0.35535200	-1.38160700
Cl	-0.40548600	-0.84224200	1.78008800
H	-0.46068400	0.77746100	-1.51780800
Cl	3.88318900	-0.12256500	0.38186800
S	-2.92612800	-1.82823500	0.09574300
S	1.66655100	2.15577400	-0.40742100
H	2.96589700	2.07323700	-0.11396800
TS38			
0	2		
C	-2.49882400	1.88354400	0.06489100
C	-2.74746200	0.55505400	-0.03082800
C	-1.85600300	-0.40981200	0.55688300
C	-0.49169100	0.09659600	0.83420600
C	-0.40536800	1.51143800	1.18356800
C	-1.35287500	2.36835600	0.76485800
C	0.40777000	-0.12366800	-0.65811500
C	1.78864200	0.33553700	-0.43522300
C	0.30774100	-1.53360900	-1.01838900
C	2.73361900	-0.58658400	-0.04347700
C	1.28602500	-2.41116200	-0.67774800
C	2.48040300	-1.95387000	-0.10469400
H	3.24325400	-2.64440200	0.21443300
H	-0.14178800	0.53478500	-1.32694800
H	0.46266700	1.86245800	1.71656400
H	-0.60359200	-1.88097700	-1.47445900
H	-3.21525400	2.58310200	-0.33622400
H	0.04064400	-0.56681000	1.50590400

Cl	4.32256700	-0.09472900	0.44046700
H	1.15593800	-3.46684400	-0.85488600
H	-1.26939300	3.42632700	0.95678300
Cl	-4.21106900	0.02477800	-0.76081200
S	-2.24813700	-1.97135400	0.85341900
S	2.06958900	2.03004900	-0.67612100
H	3.37696300	2.01147500	-0.40765600
TS39			
0	2		
C	-2.13669500	-1.79969900	-0.48782100
C	-2.35446300	-0.49581100	-0.20170600
C	-1.40584400	0.52108700	-0.57096400
C	-0.05456600	0.04444000	-0.94905300
C	0.03126900	-1.32970500	-1.42540400
C	-0.95001900	-2.21139400	-1.16507800
C	1.02808000	0.22606500	0.47520400
C	2.35324100	-0.21318400	0.01135900
C	0.97217600	1.63586300	0.84126300
C	3.19976000	0.72163500	-0.54586500
C	1.85337600	2.52660400	0.32100900
C	2.93766600	2.08021900	-0.44852400
H	3.61996800	2.78833200	-0.89042700
H	0.91040100	-1.63124800	-1.97043400
H	0.15228500	1.95618000	1.46074100
H	-2.89159200	-2.52870900	-0.23996500
H	0.44228500	0.76676300	-1.58841400
H	1.72685300	3.57879900	0.51966100
H	-0.86864400	-3.23674300	-1.49112400
Cl	-3.83705000	-0.03757600	0.53488200
Cl	0.32886200	-0.78512400	1.75870400
H	4.11416600	0.38748800	-1.01289000
S	-1.75563100	2.12358500	-0.59841600
S	2.86689400	-1.87112800	0.00160400
H	1.80937300	-2.37098500	0.64437400
TS40			
0	2		
C	2.77290800	1.78824100	-0.00816500
C	2.87192100	0.50030300	0.38253600
C	1.92078600	-0.49456200	-0.01482600
C	0.66499100	-0.00636700	-0.65864200
C	0.72376200	1.35201800	-1.19657900
C	1.69727800	2.21000700	-0.84913100

C	-0.63743000	-0.04242700	0.64334400
C	-1.89901800	0.41568200	0.04640200
C	-0.68848700	-1.39948100	1.16435600
C	-2.86856200	-0.50172100	-0.30126300
C	-1.67190500	-2.26662400	0.81869100
C	-2.75785900	-1.83791600	0.04037800
H	-3.53626100	-2.52927400	-0.23889700
H	-0.04837800	1.63838200	-1.88999400
H	0.10704900	-1.70469700	1.82122000
H	3.53542500	2.49760700	0.27400600
H	-1.63170800	-3.28245600	1.17846800
H	1.69512500	3.21311800	-1.24710000
Cl	-0.01721400	1.06834900	1.89881400
H	-3.75666300	-0.15105300	-0.80523800
Cl	0.04642100	-1.10924200	-1.88794700
H	3.71791600	0.15368000	0.95369500
S	2.23058300	-2.08659300	0.24162200
S	-2.23798000	2.08351300	-0.30603700
H	-1.23096100	2.60621800	0.39711400
TS41			
0	2		
C	1.56123300	2.78222300	-0.00651500
C	0.52610400	2.55426900	-0.89752700
C	0.28484500	1.27160600	-1.34546800
C	1.05389500	0.18820600	-0.91794000
C	2.10343600	0.44875400	-0.03206200
C	2.35437200	1.73266100	0.41880400
H	1.76310300	3.77967000	0.35213800
H	-0.08939800	3.37025600	-1.24208300
H	3.17235200	1.90066600	1.10056000
Cl	3.14293000	-0.81222000	0.51859600
C	-0.78443300	-1.94337700	-0.08712400
C	-1.85448700	-0.99097500	-0.22069000
C	-1.95486600	0.04211400	0.67806700
C	-1.13576000	0.11514300	1.80056700
C	-0.22363300	-0.91450900	2.04953400
C	-0.09617200	-1.95530900	1.17438900
H	-1.23541700	0.94961700	2.47437500
H	0.36866900	-0.88790400	2.95026500
H	0.59908800	-2.75626700	1.36414300
O	-2.64498600	-1.13577400	-1.28429800
H	-3.28894300	-0.42465300	-1.31118300
H	-0.51335500	1.07620400	-2.04560800

H	-0.99068900	-2.90179500	-0.54665100
Cl	-3.16060500	1.25529600	0.40019100
S	0.66673500	-1.40854600	-1.50782300
TS42			
0	2		
C	3.37928200	1.31311000	-0.08636100
C	2.42747600	2.00396600	-0.81693700
C	1.27358000	1.35923000	-1.21364600
C	1.03790300	0.02079100	-0.89566800
C	2.02024700	-0.65752300	-0.16718500
C	3.17914100	-0.01699000	0.23388000
H	4.28718900	1.80339700	0.22931300
H	2.58367400	3.03906100	-1.07713300
H	3.91913600	-0.56794500	0.79146200
Cl	1.84340300	-2.32414400	0.23656900
C	-1.70108000	-0.22588000	0.21791200
C	-1.74416200	1.21527100	0.21276200
C	-1.00272200	1.92640400	1.12356600
C	-0.30112500	1.26937900	2.12451700
C	-0.37196600	-0.12469700	2.24247200
C	-1.11297100	-0.85523000	1.36245100
H	-0.99278400	3.00153000	1.04283300
H	0.28119200	1.84127600	2.82875000
H	0.14027600	-0.62500300	3.04881000
H	-1.19752900	-1.92628700	1.44092400
Cl	-3.18510800	-0.98573600	-0.38500200
O	-2.40859600	1.86731700	-0.74088500
H	-2.87600800	1.24405700	-1.30208600
H	0.52006800	1.88253500	-1.78257700
S	-0.44306800	-0.73313700	-1.42477700
TS43			
0	2		
C	-2.88337100	1.90408100	-0.80619000
C	-3.06355100	0.56476300	-0.83227600
C	-2.27258000	-0.31724500	-0.02203600
C	-0.98596300	0.27365400	0.46060000
C	-1.04015500	1.72228100	0.71993700
C	-1.90712800	2.49853900	0.05667400
C	0.08576800	0.06289300	-0.88471800
C	1.40060700	0.60115900	-0.52956400
C	0.13157400	-1.34487000	-1.28405100
C	2.46058200	-0.22767800	-0.27267200

C	1.20887000	-2.13251700	-1.03211800
C	2.38347100	-1.59971100	-0.48208600
H	3.23371200	-2.22271700	-0.26152500
O	1.47089300	1.92785000	-0.42997000
H	2.35536400	2.18298500	-0.15265300
H	-0.30684300	2.13628200	1.38995700
H	-0.74474200	-1.76527700	-1.74654200
H	-3.53433800	2.54204000	-1.38472100
H	1.17510200	-3.18165900	-1.27972500
H	-1.89127600	3.56885900	0.18700300
H	-3.87490400	0.12223400	-1.38766900
Cl	-0.26553300	-0.58364600	1.82111700
H	-0.41135800	0.70626800	-1.61126800
Cl	3.94706400	0.48735700	0.25951400
S	-2.71641500	-1.86918700	0.23544800
TS44			
0	2		
C	-2.48773400	1.85797900	-0.21833800
C	-2.65906600	0.51670000	-0.12557700
C	-1.71924700	-0.30146300	0.59170600
C	-0.39101500	0.32283200	0.79753100
C	-0.38864000	1.77780300	0.94489400
C	-1.37970800	2.50689600	0.40643600
C	0.51634600	-0.03383000	-0.64352600
C	1.86327900	0.50090600	-0.45578500
C	0.49890100	-1.47361200	-0.88896600
C	2.90670800	-0.32502300	-0.12853700
C	1.56472100	-2.26525800	-0.59230800
C	2.77445800	-1.71046800	-0.15538200
H	3.61571500	-2.33118600	0.10369800
H	-0.03818200	0.54686300	-1.37874300
O	1.98016000	1.82430900	-0.55610600
H	2.89093500	2.08218600	-0.38842200
H	0.45671000	2.25176100	1.41461300
H	-0.41444200	-1.91243500	-1.25297800
H	-3.23994600	2.44958900	-0.71618900
H	0.16561400	-0.20836600	1.56026900
Cl	4.44334000	0.39530900	0.22771300
H	1.48954100	-3.33454100	-0.71005500
H	-1.36142500	3.58449600	0.44246500
Cl	-4.08406000	-0.19616900	-0.77273300
S	-2.00672400	-1.83431200	1.09041500

TS45				
0	2			
C	-2.22853700	-1.61416400	-0.44948800	
C	-2.25484700	-0.28677600	-0.18989600	
C	-1.16959900	0.57555500	-0.57566000	
C	0.09348400	-0.09892700	-0.95017600	
C	-0.01542600	-1.48472900	-1.39148900	
C	-1.11407800	-2.20897000	-1.11289000	
C	1.19315300	-0.04051800	0.46270100	
C	2.40681000	-0.71892500	0.00346000	
C	1.38715100	1.35628200	0.80736900	
C	3.44071800	0.00346200	-0.53061800	
C	2.44320100	2.04745300	0.30244300	
C	3.44794200	1.38929800	-0.42145200	
H	4.27162600	1.95045000	-0.83238400	
O	2.44715100	-2.04791800	-0.02238400	
H	1.69802400	-2.40367400	0.46554800	
H	0.81310500	-1.92165000	-1.92550900	
H	0.62772200	1.84055200	1.39648400	
H	-3.08119000	-2.22068000	-0.18923400	
H	0.68427400	0.52975400	-1.60765000	
H	2.51744900	3.10798200	0.48205300	
H	-1.18231100	-3.24286300	-1.41420200	
Cl	-3.65681400	0.39543800	0.53073700	
Cl	0.38772800	-0.96309200	1.75951400	
H	4.26394000	-0.53025900	-0.97766900	
S	-1.27470200	2.21310000	-0.61740300	
TS46				
0	2			
C	3.03476800	-1.17371400	0.12338000	
C	2.81443300	0.06551700	-0.36388100	
C	1.63636300	0.81669900	-0.04705100	
C	0.54403400	0.08701700	0.65852800	
C	0.92582900	-1.18018200	1.28554500	
C	2.08498700	-1.79251300	0.99427600	
C	-0.72874800	-0.28595300	-0.60072800	
C	-1.74124600	-1.11324400	0.05359400	
C	-1.23606300	0.95763600	-1.14702100	
C	-2.94843400	-0.58882100	0.43577700	
C	-2.44765000	1.44508000	-0.77329800	
C	-3.30193800	0.69513000	0.05014700	
H	-4.26066300	1.09464200	0.33866900	
O	-1.46182900	-2.38117900	0.34879900	

H	-0.66412400	-2.65441700	-0.11393800
H	0.23115700	-1.60508900	1.99144400
H	-0.60428200	1.49933500	-1.82894800
H	3.95489100	-1.68790400	-0.10717500
H	-2.76741200	2.40531100	-1.14550700
H	2.32508600	-2.73632600	1.45931200
Cl	0.15681200	-1.24612000	-1.83037700
H	-3.62579600	-1.21888800	0.98924700
Cl	-0.30894400	1.09176500	1.83232000
H	3.55517400	0.56754400	-0.96502900
S	1.51992700	2.40083400	-0.46607000
TS47			
0	2		
C	1.04840200	0.07208300	1.49330700
C	1.73069600	-0.61380600	0.46542300
C	2.75135800	0.05520500	-0.19358800
C	3.14783400	1.32713400	0.19355500
C	2.52934700	1.95436200	1.26423600
C	1.50247400	1.32032600	1.92873100
H	3.95163600	1.80740300	-0.34038100
H	2.86505000	2.93057300	1.57644900
H	1.01406200	1.79178200	2.76645500
C	-3.00188600	0.22836300	-0.34719100
C	-1.94417000	-0.06164600	0.50959100
C	-0.79230100	0.66372600	0.31937300
C	-0.63760100	1.62247300	-0.64017300
C	-1.71010500	1.89454600	-1.48353500
C	-2.89175200	1.19267400	-1.33293300
H	0.30022700	2.15070800	-0.74060500
H	-1.62555700	2.64430200	-2.25464000
H	-3.73608300	1.38253200	-1.97542000
O	-2.00751300	-0.99042400	1.47888700
H	-2.86157700	-1.42526200	1.45095100
H	0.36487900	-0.49102800	2.10962500
Cl	-4.48086100	-0.66077900	-0.15375200
Cl	3.59937300	-0.68082200	-1.50989500
S	1.14898300	-2.21985100	0.10556600
H	1.99527000	-2.47542300	-0.89136900
TS48			
0	2		
C	1.65128400	-0.13605200	0.65739900
C	1.96243100	-0.51512400	-0.67625800

C	2.66990200	0.37824000	-1.46744000
C	3.16857400	1.55935300	-0.95273500
C	2.97199900	1.87194700	0.39103400
C	2.25470200	1.02223100	1.19215900
H	2.84451100	0.12514200	-2.50189000
H	3.72959900	2.22458400	-1.58971000
H	3.40023900	2.76875100	0.81095700
H	2.11038200	1.22973300	2.24004200
C	-2.70451100	0.40578900	-0.10607500
C	-1.48213500	-0.21207100	0.14716100
C	-0.37948000	0.61198900	0.25526300
C	-0.45749800	1.97028800	0.10274100
C	-1.68758900	2.56219200	-0.15703900
C	-2.81698200	1.77396400	-0.25727400
H	0.43075400	2.57725700	0.18848100
H	-1.76372400	3.63163800	-0.27630700
H	-3.78493200	2.20519000	-0.45395700
Cl	-4.11638900	-0.59870700	-0.23300600
O	-1.37664700	-1.54660400	0.27697600
H	-2.24426300	-1.94288800	0.17141700
Cl	1.23190100	-1.35861400	1.82751000
S	1.49537000	-2.03911400	-1.38432000
H	0.49680600	-2.30275900	-0.53590600
TS49			
0	2		
C	1.08622000	-0.22440900	1.35926300
C	1.89063900	-0.64177100	0.27328000
C	2.92594000	0.18971400	-0.12591600
C	3.23019800	1.35086200	0.57087100
C	2.50008900	1.69628500	1.69867700
C	1.45356500	0.90033100	2.10797300
H	4.05041900	1.96249100	0.23191200
H	2.76605400	2.58171200	2.25409600
H	0.88055200	1.15338600	2.98561400
C	-2.95078300	0.52486300	-0.39443300
C	-1.89048100	-0.13723000	0.23070300
C	-0.68881100	0.53257000	0.23698300
C	-0.47028800	1.75704600	-0.33310900
C	-1.54143200	2.38614000	-0.95051200
C	-2.78122000	1.77291500	-0.96809100
H	0.50431200	2.22120200	-0.28749900
H	-1.41714200	3.35410800	-1.41153200
H	-3.62723400	2.25167800	-1.43344500

Cl	-4.52170600	-0.19614400	-0.45922400
H	0.39571500	-0.93393300	1.79210800
Cl	3.91303900	-0.20531200	-1.49055900
S	-1.99372900	-1.76218300	0.90528800
H	-3.24057800	-1.65744100	1.37065200
S	1.44276800	-2.15517900	-0.47247300
H	2.26879900	-2.07454900	-1.51477400
TS50			
0	2		
C	-1.71258600	-0.23498900	-0.62013600
C	-2.08463400	-0.32988900	0.75115500
C	-2.88159100	0.66732000	1.29208100
C	-3.41634600	1.67271800	0.50687200
C	-3.14126000	1.70941900	-0.85981200
C	-2.32569800	0.76111800	-1.41776100
H	-3.10176800	0.63442900	2.34808800
H	-4.05527600	2.41724600	0.95448000
H	-3.58315300	2.46915900	-1.48533600
H	-2.12358300	0.75257300	-2.47646300
Cl	-1.30471000	-1.68699100	-1.50388000
C	2.61497400	0.70924900	0.07283700
C	1.49396300	-0.09785700	-0.16363800
C	0.28457700	0.56985600	-0.27457400
C	0.15721600	1.92682200	-0.12599300
C	1.28203000	2.69279600	0.13168300
C	2.51389600	2.07929000	0.22575700
H	-0.81113200	2.39478000	-0.20153900
H	1.19944100	3.76146200	0.25568300
H	3.40749300	2.65034100	0.41681300
Cl	4.20308800	0.02599100	0.20092800
S	1.61950500	-1.85329000	-0.31408200
H	2.75685900	-1.95210200	0.37631400
S	-1.56847200	-1.62523600	1.79875100
H	-0.48507600	-1.98958800	1.09661900
TS51			
0	2		
C	1.23000100	-0.14101600	1.42886000
C	1.85129500	-0.76045200	0.32904400
C	2.90811500	-0.12203800	-0.29330100
C	3.41653900	1.07123300	0.19386500
C	2.86193000	1.63611600	1.33363300
C	1.79988000	1.02010800	1.96308400

H	4.24729900	1.53559900	-0.31197900
H	3.27901800	2.54746700	1.73174700
H	1.37370400	1.44648000	2.85713200
O	1.33676100	-1.91992000	-0.08790600
H	1.79412600	-2.21963400	-0.87593700
C	-2.81005800	0.43158500	-0.37829100
C	-1.73216600	-0.16743000	0.27946400
C	-0.57846800	0.58228400	0.33315600
C	-0.42110600	1.82363100	-0.21900800
C	-1.50958300	2.38943000	-0.86800700
C	-2.70288800	1.69471900	-0.93570600
H	0.52028700	2.34751800	-0.13697200
H	-1.43415600	3.36875500	-1.31546200
H	-3.56193900	2.12030800	-1.42811300
Cl	-4.32972600	-0.38664900	-0.51121400
H	0.54003100	-0.73149100	2.01181100
Cl	3.60874300	-0.86669500	-1.69051200
S	-1.75184400	-1.79366600	0.95753300
H	-3.04719300	-1.79915700	1.27907200
TS52			
0	2		
C	-1.82027600	-0.36983600	-0.45209100
C	-1.99941100	-0.56884200	0.94423000
C	-2.74849300	0.34265800	1.66561600
C	-3.41031600	1.37446500	1.02849900
C	-3.34442900	1.50281800	-0.35868500
C	-2.59584700	0.61838900	-1.09224900
H	-2.81416300	0.20406200	2.73273900
H	-4.00106100	2.06596900	1.60815500
H	-3.90296700	2.27704800	-0.86083200
H	-2.55931200	0.67387800	-2.16829300
Cl	-1.39385500	-1.75469100	-1.43513200
O	-1.43696200	-1.58147600	1.59498200
H	-0.75569500	-2.00687700	1.05964500
C	2.50562000	0.66764900	0.01445300
C	1.35768300	-0.12762300	-0.06160800
C	0.16922700	0.53032000	-0.31995400
C	0.08379700	1.88938000	-0.47976400
C	1.23596900	2.65398200	-0.38276500
C	2.44737700	2.04145200	-0.13372700
H	-0.86907100	2.35824200	-0.66850500
H	1.19059000	3.72576400	-0.50123200
H	3.35626400	2.61510200	-0.05646100

Cl	4.05686600	-0.03862200	0.31524700
S	1.43348100	-1.88847300	0.11403400
H	2.35883900	-1.88837700	1.07670200
TS53			
O	2		
C	-0.37489400	-0.16555600	1.38449700
C	-1.28472200	0.41620600	0.47605200
C	-2.16561800	-0.40938500	-0.20227500
C	-2.21926100	-1.76904100	0.06248600
C	-1.41068700	-2.31057500	1.05354800
C	-0.51898700	-1.51592900	1.73525400
H	-2.91436900	-2.38429800	-0.48475700
H	-1.49570600	-3.35979000	1.28986600
H	0.11422300	-1.93008700	2.50321500
C	3.59558500	0.66814900	-0.39947400
C	2.34587000	0.83672000	0.18650800
C	1.47874000	-0.23376900	0.15119300
C	1.77297400	-1.42686600	-0.45405200
C	3.01728800	-1.57819000	-1.05346100
C	3.92301300	-0.52980700	-1.00905900
H	1.05663400	-2.23616000	-0.44729500
H	3.27680900	-2.50733400	-1.53709600
H	4.89648900	-0.64181900	-1.46121900
O	2.06172600	2.02006000	0.77188100
H	1.11254800	2.17840300	0.74048300
H	0.19489300	0.48623200	2.03090900
Cl	-3.23456300	0.23670500	-1.39253300
S	-1.23021400	2.16359000	0.29318000
H	-1.30992300	2.20671800	-1.03978000
H	4.28978900	1.49448200	-0.37449500
TS54			
O	2		
C	1.03466700	0.15549000	0.68683900
C	1.65420900	-0.16512600	-0.55257400
C	2.13377600	0.86188200	-1.34283100
C	2.13590000	2.17182700	-0.89150700
C	1.69786700	2.45730100	0.39783000
C	1.19912700	1.45987900	1.19718800
H	2.54818600	0.62089600	-2.30910100
H	2.53011200	2.95414000	-1.51994100
H	1.77000800	3.46186700	0.78509700
H	0.87263000	1.66025500	2.20458000

C	-3.20444200	-0.68682900	-0.37454800
C	-1.84489700	-0.87973800	-0.14542900
C	-1.06839400	0.24636700	0.06243600
C	-1.58241400	1.51753000	0.00772500
C	-2.93705100	1.69547400	-0.23717700
C	-3.74299300	0.58362000	-0.41656100
H	-0.94592100	2.37375100	0.16724500
H	-3.35202900	2.69074400	-0.27528300
H	-4.79982700	0.70504900	-0.59796800
O	-1.40457400	-2.14825800	-0.13774900
H	-0.44656600	-2.17300700	-0.20592400
Cl	0.84406600	-1.10332100	1.88602300
S	1.71205900	-1.80790800	-1.18240200
H	2.28175800	-2.36780800	-0.11007400
H	-3.81596300	-1.56288900	-0.52895300
TS55			
O	2		
C	-0.46798400	0.24618500	1.37004400
C	-1.32037300	0.62231700	0.30704600
C	-2.34809100	-0.23674700	-0.04662300
C	-2.60063800	-1.39529100	0.67350100
C	-1.83311700	-1.69450800	1.79032100
C	-0.79527700	-0.86770700	2.15688600
H	-3.41206500	-2.03623400	0.36995000
H	-2.06191900	-2.57301600	2.37305400
H	-0.19305500	-1.08997100	3.02322300
C	3.43842600	-0.36682600	-0.73385800
C	2.42100800	0.22948500	0.00807100
C	1.26348200	-0.49123100	0.18470700
C	1.05548200	-1.73856600	-0.34389000
C	2.08000600	-2.32098300	-1.07869200
C	3.26900700	-1.63496900	-1.26378000
H	0.12250300	-2.25912200	-0.18030400
H	1.94937200	-3.30621700	-1.50062300
H	4.06821900	-2.08256300	-1.83396600
H	0.22623500	0.97758300	1.75758000
Cl	-3.37967800	0.11725300	-1.38705000
S	2.69381100	1.83437000	0.71787400
H	1.65075200	2.43071800	0.12910900
H	4.35631900	0.17762900	-0.89835400
S	-0.99243900	2.15520800	-0.47511200
H	-1.44538000	1.82767200	-1.68640500

TS56			
0	2		
C	-1.19973000	-0.22299800	-0.64107000
C	-1.57058200	-0.33940300	0.72853200
C	-2.35452800	0.65769000	1.28776300
C	-2.87836900	1.68297900	0.52114000
C	-2.61084000	1.73623100	-0.84605300
C	-1.80876700	0.78717200	-1.42259900
H	-2.57154000	0.60969500	2.34378500
H	-3.50592300	2.42842900	0.98306000
H	-3.04802000	2.50963000	-1.45813900
H	-1.61386700	0.79137600	-2.48271500
C	3.12122300	0.69314200	0.25156400
C	2.00588200	-0.07957900	-0.07084600
C	0.80510000	0.57528000	-0.27778700
C	0.70001300	1.94130600	-0.16975700
C	1.81528200	2.69490900	0.16468400
C	3.02834500	2.06634900	0.37636900
H	-0.24787000	2.42951400	-0.33175000
H	1.73012500	3.76707000	0.25766300
H	3.90569000	2.64016500	0.63125200
Cl	-0.82071500	-1.67224300	-1.54907400
H	4.06784000	0.19474600	0.39799500
S	2.26647600	-1.83794300	-0.07369200
H	1.76564600	-2.09136400	-1.28280200
S	-1.07138400	-1.66270900	1.74907200
H	0.03043900	-1.99915300	1.05819600
TS57			
0	2		
C	0.55229200	-0.34050000	1.34015000
C	1.35445600	-0.76436400	0.26607000
C	2.40796000	0.02996900	-0.14331700
C	2.74154200	1.19127200	0.53631900
C	2.00865000	1.56012100	1.65513400
C	0.94586800	0.78592000	2.07214900
H	3.57565800	1.78120500	0.19310000
H	2.28697300	2.44642500	2.20282200
H	0.38015600	1.06231300	2.94735200
O	1.00997900	-1.90811800	-0.34216700
H	1.58465800	-2.06590400	-1.09398400
C	-3.41060400	0.23532900	-0.65363700
C	-2.32862100	-0.37146300	-0.01971400
C	-1.19330900	0.38377900	0.15356900

C	-1.06161900	1.67314300	-0.29095100
C	-2.14562700	2.26459600	-0.92712500
C	-3.31816600	1.54572300	-1.09215700
H	-0.14026800	2.21721700	-0.13647100
H	-2.07482400	3.28018000	-1.28652700
H	-4.16586100	2.00048700	-1.58100300
H	-0.13861500	-1.05065800	1.76780800
Cl	3.33197700	-0.47808800	-1.51757100
S	-2.48488700	-2.04192400	0.55038200
H	-1.27350600	-2.43840400	0.15065100
H	-4.31656600	-0.33078300	-0.81275400
TS58			
0	2		
C	-1.28822000	-0.34380200	-0.48716300
C	-1.51397200	-0.53172000	0.90309300
C	-2.26649400	0.39956800	1.59454200
C	-2.87892400	1.44724100	0.93339300
C	-2.75937100	1.57222100	-0.44972400
C	-2.01101800	0.66456500	-1.15542700
H	-2.37055900	0.26692700	2.65937900
H	-3.47194400	2.15469600	1.49106200
H	-3.27741700	2.36074500	-0.97265100
H	-1.93780100	0.71451500	-2.22994000
C	3.04149300	0.57560900	0.27785300
C	1.87864800	-0.16803500	0.09349700
C	0.72809900	0.49882300	-0.27860500
C	0.71087800	1.85768600	-0.47940900
C	1.87610900	2.58830500	-0.29302300
C	3.03985600	1.94615600	0.08998700
H	-0.20195800	2.35619400	-0.76708700
H	1.86867000	3.65737100	-0.44427400
H	3.94936400	2.50694800	0.23881900
Cl	-0.88611500	-1.74858500	-1.45533000
H	3.94716100	0.06304500	0.56548900
S	1.97967400	-1.91678800	0.42625900
H	1.76811200	-2.33899100	-0.82277500
O	-0.99553100	-1.55322200	1.57675300
H	-0.26270300	-1.96081900	1.09432300
TS59			
0	3		
C	-0.86826600	1.06624600	0.83721200
C	-1.93339000	0.15151000	0.71224100

C	-2.78950600	0.30080500	-0.36890200
C	-2.65918900	1.36177600	-1.25271500
C	-1.66196200	2.30569700	-1.06616300
C	-0.78236600	2.17294900	-0.01430600
H	-3.35331500	1.44546900	-2.07307100
H	-1.58559100	3.14228600	-1.74227000
H	0.00706200	2.88809000	0.15370700
C	1.75620500	-1.85093100	-1.36582000
C	0.62592500	-1.22676300	-0.82697100
C	0.81986600	-0.16315500	-0.00760300
C	2.09398900	0.37869000	0.35074300
C	3.22766000	-0.32768200	-0.23111900
C	3.04537100	-1.40011800	-1.06140300
H	1.64047000	-2.69567900	-2.02806600
H	-0.36770700	-1.58584800	-1.05496500
H	3.90440200	-1.89902700	-1.48000500
O	2.22984400	1.36054600	1.08958700
H	-0.27683100	1.06130800	1.74049100
Cl	4.79375300	0.22439100	0.16117500
Cl	-4.08254900	-0.81615800	-0.64848600
S	-2.00000100	-1.13246600	1.89636100
H	-3.14373000	-1.67562500	1.47881700
TS60			
O	3		
C	1.64612100	-0.06906300	0.65809800
C	1.96376900	-0.56430000	-0.63716700
C	2.64841600	0.27337700	-1.50704500
C	3.12093200	1.50741100	-1.10227000
C	2.93046000	1.93126600	0.21137900
C	2.23844500	1.13867000	1.08921600
H	2.82672100	-0.06786400	-2.51511400
H	3.66158800	2.12654400	-1.80052600
H	3.34695500	2.86783000	0.54831100
H	2.10038000	1.43077800	2.11778200
C	-2.76927700	0.32957400	-0.12709500
C	-1.46687100	-0.28736900	0.09858000
C	-0.37386200	0.63895600	0.22296800
C	-0.52120000	1.98391000	0.09920500
C	-1.79280100	2.51209800	-0.15054700
C	-2.91182900	1.68401200	-0.25259200
H	0.32807300	2.64419200	0.18902500
H	-1.91644000	3.57859300	-0.26326000
H	-3.88793000	2.10436400	-0.43273500

Cl	-4.11947300	-0.70595400	-0.24245800
O	-1.34950200	-1.51582300	0.15967400
Cl	1.22859700	-1.18231000	1.93134500
S	1.54531900	-2.16287200	-1.19116500
H	0.48266100	-2.32266000	-0.38970300

TS61

O 3

C	2.27785500	2.55187000	-0.26256900
C	1.00904200	2.50498500	-0.83507100
C	0.50205400	1.26726700	-1.09386400
C	1.10934100	0.04620100	-0.84612600
C	2.38298900	0.15213500	-0.24982100
C	2.95874300	1.37877300	0.02259200
H	2.73848000	3.50357600	-0.04576500
H	0.46393700	3.40701500	-1.06632400
H	3.94385600	1.40983600	0.45880300
O	0.58158900	-1.11457700	-1.15748900
C	-0.62866400	-1.74598300	-0.00756200
C	-1.71992800	-0.81521700	-0.12355300
C	-1.80568400	0.19619400	0.81032000
C	-0.95721700	0.23574100	1.91201700
C	-0.03524000	-0.79230800	2.12994900
C	0.07693500	-1.81228600	1.23108300
H	-1.04561500	1.05290300	2.60876600
H	0.56869500	-0.77878200	3.02326900
H	0.77865900	-2.61589300	1.37801000
H	-0.72480600	-2.66146500	-0.56962000
Cl	3.25080400	-1.29205700	0.10608900
Cl	-2.99001300	1.44764500	0.67142400
S	-2.70566700	-1.00345900	-1.53655700
H	-3.54005300	0.00553700	-1.28439800

TS62

O 3

C	3.22543600	1.74291800	-0.12728300
C	2.05525500	2.39520300	-0.50942300
C	0.98572200	1.60438000	-0.80035100
C	0.93440600	0.22003700	-0.76232800
C	2.14147000	-0.38966700	-0.36335200
C	3.26411800	0.35951600	-0.06108000
H	4.11021900	2.31403800	0.10942000
H	2.00800900	3.47121200	-0.57544800
H	4.17159900	-0.14894800	0.22086500

O	-0.12587300	-0.47725000	-1.10362700
C	-1.21079700	1.28175300	1.57723300
C	-0.47250600	0.54116000	2.48711000
C	-0.25592800	-0.82718900	2.27636900
C	-0.76288000	-1.43600100	1.16980500
H	-1.37324100	2.33475800	1.74870900
H	-0.06967400	1.02396100	3.36291900
H	0.29238400	-1.40620700	3.00232400
H	-0.62752000	-2.48797100	0.98492200
Cl	2.23162700	-2.10802400	-0.31125500
C	-1.40147200	-0.66674900	0.14771900
Cl	-2.49628000	-1.57290900	-0.85447000
C	-1.72559400	0.70554500	0.43526600
S	-2.57703100	1.70200200	-0.70505300
H	-2.43658700	0.87556200	-1.74460200

TS63

0 3

C	-1.10028100	-0.35357200	1.38280700
C	-1.83499200	-0.69275200	0.22182900
C	-2.87726300	0.14087300	-0.15499700
C	-3.25391700	1.22538700	0.62492800
C	-2.58830100	1.49283200	1.81291700
C	-1.53858600	0.69277800	2.20525900
H	-4.07779900	1.84009300	0.30073500
H	-2.90958800	2.31770200	2.42905600
H	-1.01838800	0.88156800	3.13082200
C	1.41887300	2.33280100	-0.92562100
C	0.40740100	1.73782100	-0.18269100
C	0.68473500	0.54574100	0.42368900
C	1.90767900	-0.12577500	0.36132300
C	2.91104600	0.52254500	-0.41214700
C	2.66399100	1.72442400	-1.03794000
H	1.24480600	3.27365700	-1.42610200
H	-0.56706900	2.19522600	-0.09003600
H	3.44729000	2.18682900	-1.61565800
Cl	4.46854200	-0.17944700	-0.58469200
H	-0.41178400	-1.08641200	1.77777900
Cl	-3.78302000	-0.15536200	-1.59871600
S	2.16125800	-1.60217000	1.16264600
S	-1.28710800	-2.10756700	-0.64090000
H	-2.15003900	-2.01973000	-1.65271200

TS64

0	3		
C	1.64815400	-0.10982200	0.66578700
C	2.17233400	-0.39871100	-0.62973600
C	2.98182000	0.54624700	-1.24221200
C	3.39769200	1.68552800	-0.57700300
C	2.99245900	1.91090700	0.73873200
C	2.15722600	1.02012500	1.35648700
H	3.31374000	0.36179800	-2.25241700
H	4.05148200	2.38481100	-1.07353200
H	3.35009800	2.77281700	1.28004800
H	1.85340700	1.15959000	2.38131400
Cl	1.20518400	-1.42449700	1.72741900
C	-2.70495200	0.61131300	-0.11312300
C	-1.51369500	-0.15850200	0.02473500
C	-0.31638500	0.57438900	0.05790800
C	-0.26208500	1.92629200	-0.14823700
C	-1.44291000	2.62674000	-0.35243300
C	-2.66440800	1.97332500	-0.31087400
H	0.68094100	2.44829200	-0.14284500
H	-1.41562600	3.69198000	-0.52610600
H	-3.58584000	2.51644900	-0.44025300
Cl	-4.24668100	-0.14579900	-0.07839700
S	-1.57653000	-1.85882300	0.03575000
S	1.83125700	-1.87272600	-1.48977900
H	0.71011700	-2.18292000	-0.81530800
TS65			
0	3		
C	1.80210500	2.67471600	-0.53653000
C	0.66844000	2.37165200	-1.28297300
C	0.41524400	1.04248800	-1.45752300
C	1.13535100	-0.01927000	-0.97087300
C	2.27371000	0.33567700	-0.23004000
C	2.60061100	1.66489700	-0.02313100
H	2.07140800	3.70525700	-0.35925400
H	0.03478700	3.14224200	-1.69219600
H	3.48344000	1.90442000	0.54657800
Cl	3.30246700	-0.87530800	0.43681600
C	-0.76073000	-1.80089200	0.33523200
C	-1.76164500	-0.77043200	0.14763900
C	-1.65645400	0.38243900	0.89496700
C	-0.71708600	0.51155500	1.91498700
C	0.12231300	-0.55990600	2.23224500
C	0.06535900	-1.71409000	1.50937700

H	-0.66681900	1.43679300	2.46447800
H	0.80835600	-0.46899500	3.05934200
H	0.71017400	-2.54669400	1.73916300
H	-1.08548900	-2.79767100	0.06156700
Cl	-2.71271200	1.72438700	0.61983700
S	0.60155800	-1.65378200	-1.25201200
S	-2.90244100	-1.06520500	-1.12938700
H	-3.69087900	-0.01889200	-0.88065900

TS66

0 3

C	3.82403400	-0.49711300	0.24905200
C	3.17183500	0.72566500	0.24849700
C	1.91626800	0.85538500	-0.32031600
C	1.27567400	-0.24665800	-0.91018400
C	1.99732600	-1.41370900	-0.87229800
C	3.23326300	-1.61497200	-0.32966100
H	4.80410300	-0.57448700	0.69571800
H	3.63746800	1.59214900	0.68864400
H	3.72877300	-2.57259400	-0.34746700
C	-1.53322800	-0.76918200	-0.05200500
C	-1.42076100	0.33366200	0.88259100
C	-0.56021200	0.20690800	1.95212200
C	0.04818200	-1.00436600	2.25169200
C	-0.22043400	-2.13856800	1.47297600
C	-1.02782500	-2.04508100	0.38207200
H	-0.37869800	1.07068500	2.57302500
H	0.71047400	-1.07318700	3.09966100
H	0.20483400	-3.09247200	1.74205500
H	-1.24957700	-2.89947900	-0.23596600
Cl	-3.05327000	-0.89312300	-0.93754300
S	-0.29274400	-0.21584400	-1.67234000
Cl	1.16516000	2.40133000	-0.30293800
S	-2.28602000	1.82737100	0.66113500
H	-2.32399900	1.77360600	-0.67542900

TS67

0 3

C	-1.14691200	-1.25124200	0.59797000
C	-1.93111400	-0.73755000	-0.45266600
C	-3.00395800	0.08302600	-0.15262200
C	-3.36793300	0.34824300	1.15830500
C	-2.64363400	-0.22216000	2.19580100
C	-1.56730100	-1.03838400	1.91831200

H	-4.21673600	0.98364100	1.35192700
H	-2.94148800	-0.03936800	3.21586000
H	-1.01229800	-1.49985700	2.71956200
O	-1.56248700	-1.03997900	-1.70007200
H	-2.14708500	-0.61192200	-2.32847600
C	1.28412400	2.34846000	0.51785200
C	0.27850300	1.40009100	0.65031300
C	0.60335900	0.09243900	0.42341300
C	1.87467000	-0.37161300	0.07642700
C	2.86962700	0.63787400	-0.05420400
C	2.57289300	1.96513200	0.16410700
H	1.07281300	3.39367400	0.68802700
H	-0.72767600	1.68280600	0.92504400
H	3.35208100	2.70212100	0.05942500
Cl	4.47941300	0.22509100	-0.48733600
H	-0.44789900	-2.03860400	0.36045700
Cl	-3.91762800	0.75241000	-1.46327600
S	2.19274300	-2.02475400	-0.15555500
TS68			
0	3		
C	1.76961900	-0.27635200	0.52190100
C	2.10762800	-0.71409700	-0.79066000
C	2.94296200	0.06666800	-1.56948800
C	3.53474800	1.20239400	-1.05149900
C	3.31212200	1.57054200	0.27565400
C	2.48026700	0.81767400	1.06278500
H	3.13140700	-0.25715200	-2.58037100
H	4.19445800	1.78868000	-1.67143800
H	3.81881900	2.42536300	0.69529400
H	2.32686600	1.05574900	2.10314800
Cl	1.25406400	-1.48121700	1.68168500
O	1.61996000	-1.83485700	-1.30377200
H	0.82954500	-2.11733000	-0.81662500
C	-2.58049600	0.58788800	-0.07214300
C	-1.37258800	-0.16554600	-0.07794500
C	-0.18950000	0.56960500	0.09830500
C	-0.16272400	1.93324700	0.20198700
C	-1.36144400	2.63344400	0.15454200
C	-2.56805600	1.96082900	0.03304100
H	0.77179500	2.45758800	0.32607600
H	-1.36087000	3.71089100	0.22584100
H	-3.50032400	2.50062300	0.01587800
Cl	-4.10277400	-0.19355700	-0.21961800

S	-1.38865800	-1.84576000	-0.34010400
TS69			
0	3		
C	1.51460300	2.79568800	-0.09612900
C	0.46078000	2.53737400	-0.96636600
C	0.30397000	1.23165400	-1.32926200
C	1.05091400	0.15247200	-0.92981700
C	2.10650600	0.46343400	-0.05885000
C	2.33236300	1.76825300	0.34630100
H	1.70646600	3.80604500	0.23300200
H	-0.18479400	3.32257600	-1.32627100
H	3.15337600	1.97485600	1.01307200
Cl	3.16284600	-0.76803500	0.52075300
C	-0.77848500	-1.93935200	-0.06479400
C	-1.85303400	-0.98922000	-0.21692800
C	-1.94936700	0.06534800	0.65631900
C	-1.12792400	0.16337700	1.77609600
C	-0.21974800	-0.86439500	2.05170700
C	-0.09387600	-1.92542000	1.20276700
H	-1.22582900	1.01382800	2.42988800
H	0.36921500	-0.81869600	2.95396200
H	0.59655600	-2.72529400	1.41375300
O	-2.64755500	-1.16778000	-1.27001400
H	-3.25999700	-0.43289700	-1.34727900
H	-0.99851100	-2.91151600	-0.48922500
Cl	-3.15430100	1.27268300	0.35425300
S	0.64990400	-1.45131000	-1.48888500
TS70			
0	3		
C	3.60015100	-0.84544800	0.03317800
C	3.09851000	0.42075900	0.28919400
C	1.85561000	0.79703100	-0.19048900
C	1.07831400	-0.09266800	-0.94983400
C	1.65427100	-1.32025600	-1.15992600
C	2.86813800	-1.75934900	-0.71678600
H	4.57286600	-1.11687700	0.41547200
H	3.67244600	1.12859700	0.86435700
H	3.24479300	-2.74671800	-0.93161000
C	-1.72050700	-0.42214300	-0.06599900
C	-1.40409300	0.42405300	1.06352400
C	-0.57346300	-0.04297600	2.05368700
C	-0.17242200	-1.37046800	2.06523200

C	-0.63571900	-2.26110700	1.08439700
C	-1.44507600	-1.82344700	0.08165600
H	-0.26940100	0.64546800	2.82558800
H	0.47496600	-1.72377600	2.85151300
H	-0.36750600	-3.30437400	1.13573800
H	-1.82156900	-2.48749700	-0.67868000
Cl	-3.28696700	-0.05098100	-0.81422400
O	-1.81793500	1.68616200	1.09847700
H	-2.35203500	1.88402800	0.32588500
S	-0.48956600	0.27311800	-1.62149100
Cl	1.28694900	2.38263200	0.15662200

TS71

0 3

C	0.41542100	-0.18143300	1.47682900
C	1.18396300	0.50419700	0.51002200
C	2.13614500	-0.22006900	-0.19271100
C	2.38918600	-1.55277600	0.09677000
C	1.69489100	-2.18847800	1.11453600
C	0.73292800	-1.49970400	1.82030800
H	3.14542800	-2.07450800	-0.46685900
H	1.92387400	-3.21419400	1.35688100
H	0.18802900	-1.97614400	2.61967700
C	-2.57007900	-1.28059700	-1.65010800
C	-1.46933100	-1.32306900	-0.79220000
C	-1.44679800	-0.47053800	0.26887500
C	-2.48596900	0.46548800	0.57082700
C	-3.59792600	0.47029400	-0.35122100
C	-3.62401000	-0.37872300	-1.41874800
H	-2.61223800	-1.94175700	-2.50276300
H	-0.65159400	-2.00811300	-0.97092300
H	-4.46138800	-0.36418700	-2.09928900
O	-2.44825200	1.22346100	1.55579100
H	-0.22656400	0.40216000	2.12093600
Cl	3.07763900	0.51587300	-1.44433500
S	0.78244600	2.18521300	0.26080800
H	1.68779900	2.41979700	-0.68901300
H	-4.39686000	1.16845600	-0.15327700

TS72

0 3

C	1.07057700	0.12313400	0.68521800
C	1.57972800	-0.22281300	-0.59787500
C	2.05250200	0.79838600	-1.40954200

C	2.14897200	2.10018200	-0.95482100
C	1.78425600	2.41010200	0.35360100
C	1.29077300	1.42946300	1.17439800
H	2.36847200	0.55286700	-2.41166300
H	2.53510500	2.86673000	-1.60788500
H	1.91275300	3.41181500	0.73342300
H	1.02680700	1.63697100	2.19895800
C	-3.22377600	-0.68548600	-0.38124900
C	-1.82538800	-0.90470600	-0.09098100
C	-1.04176400	0.27489900	0.15718300
C	-1.57264400	1.52862000	0.09662100
C	-2.92572300	1.68755200	-0.21279500
C	-3.74518100	0.57225500	-0.44259900
H	-0.95809400	2.39680000	0.28246800
H	-3.34479700	2.68079800	-0.27275100
H	-4.78982500	0.71756000	-0.67025400
O	-1.36616400	-2.06015600	-0.07736100
Cl	0.90531600	-1.10890400	1.90684000
S	1.65404000	-1.85750900	-1.20255900
H	0.59219600	-2.31327200	-0.51910600
H	-3.82229700	-1.56703300	-0.55259200
TS73			
0	3		
C	-3.15158600	-1.46372500	0.10564100
C	-2.07346300	-1.84193700	-0.69370200
C	-1.25119700	-0.85025000	-1.13919500
C	-1.39662800	0.50494200	-0.87854400
C	-2.48212300	0.84523300	-0.05482800
C	-3.34789900	-0.12475300	0.41470500
H	-3.83332800	-2.21380500	0.47729200
H	-1.90581000	-2.87774700	-0.94764600
H	-4.18603500	0.16385500	1.03021900
O	-0.59936900	1.42950200	-1.38121800
C	0.90876800	1.72115800	-0.46322000
C	1.47904400	0.41380700	-0.29164100
C	1.25212300	-0.23951100	0.90252600
C	0.61780400	0.39560500	1.96372800
C	0.24035500	1.73776300	1.85820200
C	0.44460500	2.41539600	0.69280400
H	0.44779000	-0.15458200	2.87434400
H	-0.19404900	2.23097600	2.71336100
H	0.16881000	3.45208700	0.58992900
H	1.31449000	2.31421400	-1.26734200

Cl	1.76556200	-1.87217700	1.13984400
S	2.22298600	-0.25502500	-1.70717600
H	2.58852000	-1.41540800	-1.16158900
H	-2.62657800	1.88944200	0.17979200
TS74			
0	3		
C	3.80105400	0.46360700	-0.09880500
C	2.88132100	1.51076000	-0.09737600
C	1.60867400	1.22164700	-0.49338800
C	1.15083100	-0.01929300	-0.91045100
C	2.10095900	-1.05292500	-0.88129000
C	3.40355600	-0.80765500	-0.49158700
H	4.82219900	0.64575700	0.20047600
H	3.17258800	2.50666600	0.20077600
H	4.12074000	-1.61391500	-0.49608000
O	-0.07624800	-0.23167800	-1.34996700
C	-0.56434800	0.50047800	1.90792400
C	-0.03515000	-0.69623900	2.36309200
C	-0.21450000	-1.87466000	1.62501700
C	-0.89793100	-1.84675900	0.44852800
H	-0.42089200	1.40366700	2.48072200
H	0.51243900	-0.71773400	3.29151800
H	0.16732100	-2.81028200	2.00209400
H	-1.07127900	-2.73746400	-0.13225800
C	-1.32687900	-0.60431200	-0.10954400
Cl	-2.64967600	-0.73693000	-1.23214500
C	-1.25526400	0.56991000	0.71570300
S	-1.84039800	2.11069800	0.16606200
H	-1.90073200	1.78176000	-1.12722600
H	1.78452400	-2.03575100	-1.19776100
TS75			
0	3		
C	0.42560300	0.55055200	1.23343000
C	1.34208200	0.69295800	0.16666600
C	2.38001800	-0.22178500	0.07371600
C	2.56907500	-1.20147100	1.03900500
C	1.71372100	-1.27830100	2.12817700
C	0.66732600	-0.39017200	2.24173400
H	3.39598500	-1.88468200	0.93365300
H	1.88560200	-2.02365300	2.88847600
H	0.00117600	-0.42912800	3.08885900
C	-1.99595700	-2.28835500	-1.06446200

C	-0.99543500	-1.62555900	-0.36434500
C	-1.28328000	-0.39585500	0.16204300
C	-2.52237500	0.23396400	0.04425200
C	-3.51867900	-0.46983800	-0.67421500
C	-3.25447300	-1.70527600	-1.21496400
H	-1.79911100	-3.25948300	-1.49400200
H	-0.01601100	-2.06530700	-0.23762000
H	-4.02473500	-2.22825200	-1.75999200
H	-0.27163400	1.35483400	1.41682400
Cl	3.51185100	-0.15985300	-1.23375200
S	-2.85088200	1.76810800	0.70922000
H	-4.48838800	-0.00905600	-0.78526600
S	1.00306100	1.98855000	-0.95396700
H	2.01502500	1.75053400	-1.78742600

TS76

0 3

C	1.14293100	-0.04463800	0.67732900
C	1.68651100	-0.33015000	-0.60852100
C	2.44134600	0.64779400	-1.23815600
C	2.78079400	1.82615100	-0.59774400
C	2.35658200	2.05455500	0.71033700
C	1.57782400	1.12502200	1.34676200
H	2.78914600	0.46132100	-2.24261500
H	3.39172600	2.55376700	-1.10796400
H	2.65638700	2.94947700	1.23297400
H	1.26114500	1.26762200	2.36726100
Cl	0.73349300	-1.35986000	1.75120100
C	-3.24553000	0.35305200	-0.20542100
C	-2.00005100	-0.29379000	-0.02398000
C	-0.86432200	0.52450100	0.05261500
C	-0.93433800	1.88120700	-0.13089600
C	-2.16612900	2.47955800	-0.36781600
C	-3.32580800	1.71290100	-0.38514500
H	-0.04183600	2.48563000	-0.08540100
H	-2.21992300	3.54682500	-0.52305600
H	-4.28435900	2.18108800	-0.54503400
S	-1.99485800	-2.00162500	-0.01364800
H	-4.13098600	-0.26368100	-0.22783900
S	1.43822000	-1.84146300	-1.43835200
H	0.31667400	-2.19200500	-0.78292500

TS77

0 3

C	3.00955800	1.59192000	-0.37361700
C	1.95667400	1.60114600	-1.28436000
C	1.24616700	0.44090600	-1.40214600
C	1.46291500	-0.72008300	-0.70052200
C	2.53047500	-0.69771100	0.20495900
C	3.29385000	0.44607800	0.35678500
H	3.61067500	2.47942300	-0.24220500
H	1.72230100	2.48139000	-1.86264000
H	4.11696200	0.44726800	1.05452100
C	-1.09830200	-1.63676300	0.42411800
C	-1.58279100	-0.32436300	0.05645800
C	-1.14783100	0.75907200	0.79076300
C	-0.38508200	0.60214200	1.94364600
C	-0.08266500	-0.67856100	2.41339100
C	-0.48384400	-1.77794400	1.71416300
H	-0.05940700	1.47892800	2.47802700
H	0.45026700	-0.78754400	3.34468100
H	-0.27277500	-2.77353100	2.06923600
H	-1.72707100	-2.45839200	0.10457100
Cl	-1.56197200	2.37436500	0.33037300
S	0.45869000	-2.12938100	-0.92149800
H	2.74516800	-1.58879900	0.77602900
S	-2.55440100	-0.26556900	-1.38211100
H	-2.81596300	1.04120000	-1.34263000
TS78			
0	3		
C	3.86321500	0.33938400	0.10568900
C	3.02385300	1.41936800	-0.13495100
C	1.77228500	1.23196700	-0.69135600
C	1.33162700	-0.05564700	-1.02428400
C	2.21101300	-1.07812000	-0.76435800
C	3.45644000	-0.95203800	-0.21555900
H	4.83983500	0.49980100	0.53803400
H	3.35147200	2.41672100	0.11437200
H	4.09829400	-1.80168200	-0.04084200
C	-1.40169300	-0.59165100	0.05682400
C	-1.16513500	0.61209100	0.81551400
C	-0.28398700	0.57193100	1.87500800
C	0.28398300	-0.62017100	2.29916900
C	-0.04462500	-1.82091500	1.65912700
C	-0.90822200	-1.82247800	0.60622800
H	-0.03603300	1.49361200	2.37893500
H	0.97139900	-0.61780900	3.12953800

H	0.36786200	-2.75307700	2.01118200
H	-1.19089900	-2.73398000	0.10611200
Cl	-2.98297800	-0.74714300	-0.71019200
H	1.11338000	2.06898100	-0.87364600
S	-0.23937500	-0.33800500	-1.72700000
S	-1.85511200	2.14543900	0.35790700
H	-2.12542400	1.80758000	-0.90724600

TS79

O 3

C	-0.48943700	-1.18500700	0.69049200
C	-1.35724500	-0.79381900	-0.34609600
C	-2.43251000	0.02491500	-0.04997900
C	-2.71623700	0.40603800	1.25208100
C	-1.90682000	-0.04485100	2.28484600
C	-0.82672600	-0.85796400	2.01052200
H	-3.56901600	1.03666300	1.44379000
H	-2.14012900	0.22774100	3.30172700
H	-0.20459500	-1.22594500	2.81082700
O	-1.06431100	-1.20429200	-1.58320200
H	-1.70179300	-0.84915700	-2.20543000
C	1.85002500	2.46050000	0.11169400
C	0.87947000	1.51067400	0.40472200
C	1.20508500	0.18826100	0.26842700
C	2.45973500	-0.26651800	-0.13816300
C	3.42358900	0.72717700	-0.43367200
C	3.11860700	2.06189800	-0.30915900
H	1.62247200	3.51168500	0.20950200
H	-0.10747700	1.80470000	0.73403700
H	3.86606500	2.80584200	-0.53666500
H	0.22158900	-1.96896400	0.47744700
Cl	-3.45299200	0.54304100	-1.35115100
S	2.84874900	-1.92094400	-0.26992400
H	4.40302800	0.40736500	-0.75556000

TS80

O 3

C	1.24393400	-0.21357100	0.54889000
C	1.64620900	-0.63448000	-0.74956000
C	2.45592700	0.19256600	-1.50658200
C	2.95635100	1.36789700	-0.98000200
C	2.66557800	1.73024100	0.33488800
C	1.86079100	0.92794500	1.10261100
H	2.69661200	-0.12419900	-2.50861400

H	3.59684800	1.99169400	-1.58329800
H	3.09944600	2.62021600	0.76302800
H	1.65897200	1.16174200	2.13570000
Cl	0.75741900	-1.44397100	1.69494500
O	1.24467100	-1.78549800	-1.27300400
H	0.45056300	-2.11225100	-0.82062100
C	-3.13813200	0.32397800	-0.25882900
C	-1.87596600	-0.31168400	-0.19182700
C	-0.76062500	0.49908000	0.05773500
C	-0.86516800	1.85948300	0.18433800
C	-2.11473900	2.46016500	0.07975000
C	-3.25249200	1.68701700	-0.13026200
H	0.01203700	2.46092500	0.36764700
H	-2.20125700	3.53260900	0.17258800
H	-4.22165400	2.15599200	-0.19554400
S	-1.80301800	-1.99334400	-0.46738900
H	-4.00676800	-0.29355600	-0.42958200
TS81			
O	3		
C	2.88223600	1.76628800	0.02590600
C	1.90918800	1.82718100	-0.96774600
C	1.26053600	0.65942700	-1.25445900
C	1.47020600	-0.55729300	-0.65319000
C	2.45732900	-0.58435200	0.33873200
C	3.15344600	0.56526900	0.66672500
H	3.43214400	2.65729200	0.29060100
H	1.68780100	2.75023200	-1.48082600
H	3.91451100	0.52717100	1.43067900
C	-1.09048000	-1.76035100	0.17310300
C	-1.74044700	-0.54462400	-0.24013800
C	-1.54383900	0.60450600	0.48567700
C	-0.85555800	0.59381600	1.69472800
C	-0.39756300	-0.62197100	2.21180400
C	-0.56914300	-1.78204800	1.51189000
H	-0.71160100	1.51773400	2.22944100
H	0.07423500	-0.63612000	3.18148700
H	-0.23162100	-2.72544900	1.90948900
O	-2.44103000	-0.60617200	-1.37014200
H	-2.74042100	0.27134400	-1.61807600
H	-1.58056900	-2.65885500	-0.18007500
Cl	-2.21385000	2.08307500	-0.11854200
S	0.56502400	-1.98386800	-1.09892800
H	2.66335000	-1.51942900	0.83828500

TS82			
0	3		
C	-3.77879900	0.06757700	0.11698500
C	-3.05298400	-0.36544600	1.21878700
C	-1.78197700	-0.88780600	1.06647800
C	-1.20716400	-0.99189400	-0.20625900
C	-1.97706100	-0.54669000	-1.25232700
C	-3.23568800	-0.02122200	-1.16110900
H	-4.77215200	0.47051200	0.24840900
H	-3.48499400	-0.29448500	2.20493800
H	-3.78757600	0.30650300	-2.02854900
C	1.54677500	0.12762100	-0.27697700
C	1.23038000	0.64090700	1.03133100
C	0.37417400	1.70667500	1.16133600
C	-0.09824400	2.36901500	0.03797400
C	0.31850000	1.98092600	-1.24248600
C	1.17659100	0.93437900	-1.40069100
H	0.09205900	2.01437400	2.15537000
H	-0.77235600	3.20191800	0.15567400
H	-0.01804800	2.52881200	-2.10810500
H	1.52923100	0.62803400	-2.37158000
Cl	3.14837200	-0.62615600	-0.38617800
O	1.66856700	0.01789300	2.12491500
H	2.23584100	-0.71682700	1.87987800
H	-1.21305100	-1.22374400	1.92165700
S	0.38957300	-1.65611600	-0.44064000
TS83			
0	2		
C	2.01652000	2.59029800	0.30984400
C	0.84044600	2.61509700	-0.42471300
C	0.35539700	1.45302100	-0.98577100
C	1.02650800	0.23497000	-0.83302100
C	2.21601800	0.23883600	-0.08876900
C	2.70787000	1.40212700	0.47050700
H	2.40494700	3.49538700	0.74982600
H	0.30727300	3.54276400	-0.56323000
H	3.63300400	1.37066900	1.02344300
O	0.58055400	-0.86110600	-1.41638900
C	-0.66356700	-1.78448700	-0.52070300
C	-1.79007200	-0.90227600	-0.54946100
C	-2.05123400	-0.11369200	0.54637500
C	-1.32703100	-0.25239000	1.72296200

C	-0.35462100	-1.25254300	1.82135000
C	-0.08321200	-2.05972700	0.75270300
H	-1.54359400	0.39586900	2.55589000
H	0.16003000	-1.39566200	2.75793400
H	0.64998700	-2.84499900	0.82079500
H	-0.54702900	1.45182900	-1.57824500
H	-0.66519400	-2.56009600	-1.26869500
Cl	3.10955100	-1.22341400	0.08019400
Cl	-3.31960200	1.05925100	0.43248600
O	-2.45920900	-0.82740200	-1.69775500
H	-3.15744800	-0.17232300	-1.62796300
TS84			
0	2		
C	-3.37414000	-1.23646300	-0.21189400
C	-2.37501100	-1.98581600	-0.81456600
C	-1.15357000	-1.40861000	-1.08941800
C	-0.89578700	-0.07096400	-0.77492200
C	-1.92427800	0.66793800	-0.17209500
C	-3.15004000	0.09231700	0.10240300
H	-4.33366500	-1.67935400	0.00450600
H	-2.55309700	-3.01774100	-1.07438000
H	-3.92413000	0.69187200	0.55387900
O	0.26187500	0.48427500	-1.08895900
C	1.36415100	-1.93490600	0.98613000
C	0.72792500	-1.40997500	2.10038500
C	0.61098900	-0.02269900	2.27032500
C	1.10564900	0.83092200	1.33025700
H	1.49087800	-2.99790100	0.85884500
H	0.34001600	-2.07723300	2.85310300
H	0.15843100	0.37262400	3.16561000
H	1.06070700	1.89974300	1.44636200
H	-0.36508100	-1.96683400	-1.57079300
Cl	-1.67943100	2.33681200	0.17366700
C	1.59739600	0.31566600	0.09719900
Cl	2.71775400	1.32449200	-0.77855900
C	1.84738600	-1.09760500	0.01048400
O	2.42702600	-1.60970500	-1.07203500
H	2.67921900	-0.90272500	-1.67173500
TS85			
0	2		
C	3.32027500	-1.30609700	-0.74470000
C	3.29520800	0.04118900	-0.75229400

C	2.33175300	0.77635400	0.04829600
C	1.17585500	-0.03568400	0.54451100
C	1.40469200	-1.45859100	0.71363100
C	2.39571500	-2.07033900	0.04041900
C	0.05261300	0.11358200	-0.93819600
C	-1.15580200	-0.60747300	-0.60734200
C	-0.13279300	1.52141700	-1.20680900
C	-2.30475900	0.06893400	-0.28112200
C	-1.29150500	2.16140400	-0.88242900
C	-2.39071400	1.45058300	-0.39059200
O	2.39770600	1.97536100	0.22771200
H	-3.30716500	1.94968700	-0.12363300
H	0.71509600	-2.01310200	1.32740300
H	0.69797600	2.08111100	-1.60176500
H	4.08305600	-1.83001600	-1.30175300
H	-1.37498200	3.22687000	-1.02510600
H	2.51778800	-3.13950700	0.10815300
H	4.03793600	0.62771300	-1.26950100
H	0.69373800	-0.42939900	-1.62743600
Cl	0.32718500	0.71299600	1.87182000
Cl	-3.68585300	-0.85391400	0.21197700
O	-1.05669400	-1.93679400	-0.58444000
H	-1.89742800	-2.31797900	-0.31732500
TS86			
0	2		
C	-2.74934800	1.60603900	-0.18213400
C	-2.83548800	0.27191400	0.00018300
C	-1.78471300	-0.46404600	0.69711200
C	-0.51277600	0.27321700	0.87601400
C	-0.56698400	1.71513400	0.84682400
C	-1.62240800	2.34625400	0.29253900
C	0.42929700	-0.26704200	-0.64803400
C	1.71413700	0.38145200	-0.54539200
C	0.46618800	-1.70852500	-0.61358300
C	2.80046000	-0.31216800	-0.06931500
C	1.56815100	-2.37352700	-0.15812700
C	2.73991800	-1.68189700	0.15755300
O	-1.89926800	-1.62650300	1.03799500
H	3.61079700	-2.19656800	0.52817200
H	-0.22080000	0.18883500	-1.38740200
H	0.27742700	2.27722000	1.21059700
H	-0.43028000	-2.25166400	-0.85911400
H	-3.56475300	2.12837300	-0.65836300

H	0.10834000	-0.17983600	1.63782400
H	1.54592500	-3.44651100	-0.05519500
H	-1.64205700	3.42153100	0.21365300
Cl	-4.22518100	-0.61205700	-0.47810200
Cl	4.28587600	0.54829100	0.16833600
O	1.74568700	1.67667500	-0.85754800
H	2.63362600	2.02043700	-0.72956200

TS87

0	2		
C	2.43659000	1.36740400	-0.39330500
C	2.36332300	0.02819100	-0.27234300
C	1.16690000	-0.70788100	-0.67163600
C	-0.02172700	0.11092700	-1.01621600
C	0.18030800	1.51910900	-1.26178000
C	1.33873900	2.12024600	-0.91837400
C	-1.15417300	-0.09468700	0.47920300
C	-2.31404400	0.68787700	0.09912300
C	-1.36293900	-1.51475400	0.58938900
C	-3.35908100	0.08308500	-0.55278300
C	-2.42314600	-2.09193100	-0.04297000
C	-3.40178400	-1.30101500	-0.65761800
H	-4.23204700	-1.76853600	-1.16229900
H	-0.62053900	2.08855400	-1.70679800
H	-0.60553300	-2.10566000	1.07435700
H	3.34548000	1.87793000	-0.11560900
H	-0.67064600	-0.40891400	-1.71152600
H	-2.51732000	-3.16585800	-0.04801800
H	1.47235600	3.17910500	-1.07681700
Cl	3.68779900	-0.89650400	0.29706300
Cl	-0.25424900	0.62635700	1.82522200
H	-4.15665100	0.70150100	-0.93197400
O	1.11379200	-1.92406500	-0.68627000
O	-2.30407800	2.00999700	0.25081900
H	-1.55696200	2.26748800	0.79932500

TS88

0	2		
C	3.26949100	0.41223000	-0.14983100
C	2.82979500	-0.60422300	0.61172500
C	1.51001900	-1.17903000	0.42195500
C	0.61267900	-0.49189000	-0.56675100
C	1.21264000	0.51294400	-1.42188900
C	2.45397700	0.97743300	-1.18712900

C	-0.64993300	0.40130200	0.58268200
C	-1.49286100	1.16697500	-0.31259400
C	-1.30983200	-0.62545500	1.34315700
C	-2.75281100	0.72972300	-0.63569500
C	-2.56780000	-1.02910500	1.01454300
C	-3.29225200	-0.37117100	0.01035600
H	-4.28937400	-0.69830800	-0.23668000
H	0.62617100	0.87667600	-2.25083300
H	-0.75354400	-1.10693900	2.12890700
H	4.26634800	0.80121400	-0.00590100
H	-3.01705000	-1.84786500	1.55343400
H	2.86878000	1.74552800	-1.82141500
Cl	0.40604100	1.45659800	1.55661400
H	-3.31783000	1.29077300	-1.36247800
Cl	-0.37291200	-1.62472900	-1.46116100
H	3.44528700	-1.07183200	1.36352500
O	1.12345700	-2.15040500	1.04359700
O	-1.01681900	2.26955400	-0.89049500
H	-0.18377400	2.51738400	-0.47926200
TS89			
0	2		
C	1.00453100	-1.36311100	-0.29943800
C	1.93962700	-0.44010300	-0.79406500
C	2.94218200	0.01013600	0.04662500
C	3.08280800	-0.48318500	1.33371900
C	2.20944700	-1.45796400	1.79114900
C	1.19872100	-1.91537800	0.97117800
H	3.88066600	-0.11136700	1.95584700
H	2.33363300	-1.86093200	2.78340600
H	0.51816500	-2.67811800	1.31421000
C	-3.03537500	0.40699500	0.08122400
C	-1.96123400	-0.42654500	-0.21291600
C	-0.71276200	0.04620500	0.11342300
C	-0.48478100	1.25263400	0.71162100
C	-1.57528200	2.06830100	0.99824700
C	-2.85078900	1.64104400	0.67906500
H	0.52119500	1.56567100	0.95335000
H	-1.43239400	3.03001500	1.46596400
H	-3.71122000	2.25513900	0.88964700
Cl	-4.63425200	-0.14004500	-0.32065200
H	0.32666600	-1.82136600	-1.00202400
Cl	4.05187400	1.19521700	-0.56094800
O	1.78367500	-0.01090100	-2.05020900

H	2.45857000	0.63706000	-2.26042100
O	-2.09772900	-1.63713400	-0.78358500
H	-3.02497900	-1.80392000	-0.96142200

TS90

0	2		
C	-1.75574000	-0.38180800	-0.48480300
C	-1.88414900	-0.70426500	0.88996600
C	-2.60150700	0.14161900	1.71576100
C	-3.25283800	1.24433600	1.19769400
C	-3.21426300	1.51041100	-0.16950400
C	-2.51340800	0.68010500	-1.00837200
H	-2.64097900	-0.09565400	2.76666600
H	-3.81243200	1.88888100	1.85702500
H	-3.76078800	2.34641200	-0.57661900
H	-2.50150200	0.83807800	-2.07476800
C	2.58425900	0.38844000	0.06166800
C	1.35551800	-0.25802600	-0.01025200
C	0.25403000	0.51755000	-0.29780700
C	0.33100900	1.86948800	-0.49293500
C	1.56906900	2.49737000	-0.41333800
C	2.69865200	1.75170600	-0.13713900
H	-0.56164800	2.43845300	-0.70725100
H	1.65212100	3.56201800	-0.56692900
H	3.67006400	2.21377400	-0.07059400
Cl	3.99350100	-0.56239100	0.41788200
O	1.22892000	-1.58610700	0.19480900
H	2.08797500	-1.96429900	0.39425700
Cl	-1.30896000	-1.65890800	-1.58782400
O	-1.30256200	-1.77681000	1.42012900
H	-0.60465800	-2.10379600	0.84209800

TS91

0	3		
C	-0.97612800	1.20131900	0.68928500
C	-1.99993900	0.25604700	0.85454800
C	-2.92367700	0.08920400	-0.16198700
C	-2.90419100	0.88776700	-1.29368100
C	-1.94437700	1.88144400	-1.41432100
C	-1.00452500	2.05504500	-0.41972100
H	-3.64672100	0.73420600	-2.05985100
H	-1.94545600	2.52054500	-2.28265900
H	-0.24891600	2.82097600	-0.49307200
C	1.63114000	-2.14026000	-0.81336600

C	0.50254600	-1.41235900	-0.42183700
C	0.69162600	-0.17952000	0.11412900
C	1.96621500	0.44266700	0.30218900
C	3.09953700	-0.37362000	-0.11257600
C	2.91881500	-1.61799400	-0.65252500
H	1.51533600	-3.12142700	-1.24883200
H	-0.48852600	-1.82488800	-0.54696700
H	3.77769900	-2.19571900	-0.95378300
O	2.10330600	1.57751100	0.77320500
H	-0.35408700	1.43777300	1.53824800
Cl	4.66495400	0.27248100	0.09893100
Cl	-4.14140500	-1.13078800	0.02516600
O	-1.99303100	-0.48111500	1.97077300
H	-2.73411200	-1.08985400	1.96463500

TS92

0 3

C	1.74167900	-0.32318000	0.52175700
C	1.90382200	-0.80452200	-0.80450200
C	2.67658200	-0.07300300	-1.69014600
C	3.33604900	1.06861000	-1.27796600
C	3.25121200	1.49607700	0.04597800
C	2.50173200	0.78134000	0.94660400
H	2.74891500	-0.43109500	-2.70447500
H	3.93622500	1.61993200	-1.98460000
H	3.80211900	2.36315300	0.37472100
H	2.45903500	1.05908200	1.98769300
C	-2.65021600	0.33024000	-0.11272800
C	-1.34590000	-0.31413000	-0.07317300
C	-0.24357500	0.55907800	0.20700600
C	-0.37550500	1.89722300	0.39347800
C	-1.65213100	2.46597700	0.31760900
C	-2.78115200	1.67933200	0.07279700
H	0.48780000	2.51461300	0.59502900
H	-1.77518400	3.53008100	0.45225700
H	-3.75880400	2.13090700	0.02650400
Cl	-4.01136600	-0.65203900	-0.41053100
O	-1.22100200	-1.52922200	-0.28211900
Cl	1.22895500	-1.45087400	1.74989900
O	1.31134900	-1.91256300	-1.22782700
H	0.50253700	-2.08113000	-0.71709500

TS93

0 3

C	2.01327300	2.61197100	0.18895200
C	0.78903900	2.59745000	-0.47481900
C	0.36609900	1.39097200	-0.94577100
C	1.01566200	0.17235200	-0.83352900
C	2.23937200	0.24200300	-0.13719000
C	2.73174800	1.43810600	0.35115200
H	2.40942600	3.53955300	0.57317200
H	0.21468300	3.50036000	-0.61343000
H	3.68229200	1.44445000	0.85919900
O	0.56680200	-0.95032500	-1.34996600
C	-0.67018200	-1.80759100	-0.40100800
C	-1.80137800	-0.93591600	-0.51133800
C	-2.06954600	-0.05748500	0.51199700
C	-1.35071600	-0.09639800	1.70021900
C	-0.37697500	-1.08305400	1.88934400
C	-0.09650100	-1.97621400	0.89462700
H	-1.57540500	0.61760400	2.47525000
H	0.13073200	-1.14481900	2.83858000
H	0.64208900	-2.74804700	1.03076700
H	-0.66461900	-2.64293400	-1.08192900
Cl	3.15533500	-1.20136800	0.07091700
Cl	-3.34569900	1.09129200	0.29868500
O	-2.46797300	-0.97350500	-1.66037900
H	-3.13301100	-0.28142100	-1.67790000
TS94			
0	3		
C	-3.37833200	-1.26221900	-0.28923100
C	-2.35165600	-1.99890800	-0.87419500
C	-1.17384100	-1.34529000	-1.08051900
C	-0.88435300	-0.02865600	-0.76903100
C	-1.94994600	0.66579200	-0.16331600
C	-3.17426300	0.06313100	0.05985900
H	-4.33976000	-1.71960300	-0.11204100
H	-2.49199800	-3.03107900	-1.15559100
H	-3.96745800	0.63997400	0.50680700
O	0.26426900	0.55535600	-1.04223300
C	1.44213800	-2.05190500	0.70256800
C	0.76422000	-1.71090400	1.86264900
C	0.58191300	-0.36483700	2.21730900
C	1.04893700	0.62945100	1.41203300
H	1.62057200	-3.08093700	0.43594000
H	0.39311000	-2.49000800	2.50888000
H	0.09806300	-0.11588500	3.14825500

H	0.94383000	1.67041200	1.66511200
Cl	-1.72610200	2.31866600	0.26453700
C	1.58379400	0.30700600	0.13080600
Cl	2.66568700	1.47664400	-0.57735300
C	1.90805100	-1.06958400	-0.13771900
O	2.55050800	-1.40250800	-1.25094200
H	2.75249300	-0.61439400	-1.76136700

TS95

0 2

C	0.47121400	0.40890300	1.35976400
C	1.30740800	-0.44406400	0.62169900
C	2.25382300	0.08856100	-0.22850100
C	2.44750900	1.45765200	-0.31279000
C	1.68900100	2.30157400	0.48549400
C	0.73716400	1.78420000	1.33868400
H	3.19618600	1.84596700	-0.98352000
H	1.86399700	3.36506700	0.44762200
H	0.15940000	2.43688200	1.97344600
C	-3.43437200	-0.91540300	-0.30575200
C	-2.16380700	-0.93797100	0.25922700
C	-1.41169500	0.21536300	0.17642500
C	-1.84422100	1.35660300	-0.44465100
C	-3.11064500	1.36559000	-1.01513700
C	-3.89822800	0.22774600	-0.93177700
H	-1.21364000	2.23366500	-0.48019800
H	-3.47759100	2.25156800	-1.51000000
H	-4.88677800	0.22557000	-1.36475000
O	-1.74902500	-2.06952500	0.86303600
H	-0.79113600	-2.06800700	0.94256300
H	-0.10674500	-0.02265400	2.16286600
Cl	3.21214100	-0.99742400	-1.17640100
H	-4.03746100	-1.80899900	-0.24765000
O	1.09463700	-1.76799800	0.74875700
H	1.66356400	-2.25519000	0.14796900

TS96

0 2

C	-1.25017800	-0.33598100	-0.42182600
C	-1.36203800	-0.27410600	0.98996000
C	-1.90042000	0.86278900	1.56365400
C	-2.38038300	1.89485400	0.77979900
C	-2.34366700	1.80162700	-0.60907500
C	-1.82629000	0.67767800	-1.20468400

H	-1.92847600	0.91210700	2.64025100
H	-2.79826200	2.77019400	1.25136300
H	-2.75083600	2.59176300	-1.21987600
H	-1.82765300	0.55870800	-2.27607400
C	3.09609900	-0.24726400	0.39853600
C	1.80971400	-0.69045900	0.14416500
C	0.89847600	0.18680200	-0.39886900
C	1.21970200	1.48413700	-0.70331100
C	2.51388400	1.92562300	-0.45534400
C	3.44206700	1.06077000	0.10044400
H	0.47655300	2.15130900	-1.11560700
H	2.78976000	2.94279600	-0.68861600
H	4.44505400	1.40342800	0.30196100
Cl	-1.11496400	-1.91166500	-1.18401000
H	3.80825500	-0.93689800	0.82577100
O	-0.93069000	-1.24990300	1.78820600
H	-0.19275200	-1.73396700	1.39263800
O	1.47468400	-1.97951100	0.48594100
H	1.07900200	-2.40463900	-0.27751800
TS97			
0	3		
C	0.41569300	1.38725600	-0.34625300
C	1.30364900	0.39132900	-0.78625400
C	2.26289200	-0.08501200	0.09007400
C	2.41337300	0.45067300	1.35913600
C	1.59259600	1.49335800	1.76129000
C	0.62465300	1.97741500	0.90523200
H	3.17858800	0.05885100	2.00935900
H	1.72712600	1.93067700	2.73764600
H	-0.01175600	2.79454600	1.20531400
C	-2.42525700	-1.75196300	1.09115200
C	-1.26997100	-1.00825300	0.84625500
C	-1.36683300	0.09275900	0.05124200
C	-2.58544100	0.54780300	-0.54451900
C	-3.74937800	-0.26246000	-0.26453000
C	-3.65544600	-1.36938200	0.52737500
H	-2.37734900	-2.62878100	1.71954600
H	-0.32172300	-1.29724700	1.27930800
H	-4.53329500	-1.96387000	0.72888600
O	-2.65354400	1.56917800	-1.25077800
H	-0.23061900	1.85252400	-1.07570500
Cl	3.30763300	-1.35855400	-0.44911200
H	-4.68301800	0.04896800	-0.70764700

O	1.13822000	-0.08287300	-2.02460100
H	1.78168000	-0.77183400	-2.19996800
TS98			
O	3		
C	1.19820200	-0.24519200	0.53717500
C	1.53951000	-0.52486500	-0.81255000
C	2.21902000	0.43628400	-1.54066800
C	2.61910900	1.62085000	-0.95198600
C	2.36139500	1.86264600	0.39564700
C	1.70117800	0.91949900	1.14367200
H	2.42751300	0.22320300	-2.57680000
H	3.15079700	2.35307200	-1.53910300
H	2.71163400	2.76936700	0.86322900
H	1.53397000	1.05715200	2.20007100
C	-3.17159800	-0.35242100	-0.47923800
C	-1.78485900	-0.73080500	-0.35270600
C	-0.89282600	0.28384500	0.12986800
C	-1.30507800	1.54660700	0.42771100
C	-2.65253900	1.87473000	0.26253000
C	-3.57705900	0.91507100	-0.18387800
H	-0.60058800	2.28557600	0.78212800
H	-2.99006500	2.87662200	0.48197800
H	-4.61421900	1.19125100	-0.29398100
O	-1.40668300	-1.87660700	-0.66665800
Cl	0.82459100	-1.58591900	1.58959000
H	-3.85604400	-1.11143600	-0.82581600
O	1.19529800	-1.66121400	-1.40386300
H	0.38328800	-2.01911700	-1.00403200
TS99			
O	3		
C	3.07927500	1.48735900	0.27390800
C	2.02531500	1.86731100	-0.55510400
C	1.23211600	0.87313100	-1.04736100
C	1.37819200	-0.48400200	-0.80291700
C	2.43566100	-0.82418000	0.05575300
C	3.27558300	0.14537500	0.57036900
H	3.74200300	2.23757100	0.67816200
H	1.85508600	2.90514900	-0.79894000
H	4.09293800	-0.14577700	1.21206800
O	0.61681900	-1.41280400	-1.35490300
C	-0.91322700	-1.77321600	-0.51382300
C	-1.61538400	-0.52757500	-0.56765900

C	-1.57198800	0.31101200	0.52201300
C	-0.98379800	-0.08855800	1.71460800
C	-0.47746500	-1.38738400	1.83549300
C	-0.51152800	-2.24277400	0.77143900
H	-0.95130700	0.59946400	2.54305600
H	-0.08094800	-1.70902800	2.78535200
H	-0.13472300	-3.24917200	0.85358700
H	-1.19646100	-2.49315000	-1.26399800
Cl	-2.28996600	1.87919000	0.38340300
H	2.57965200	-1.87022700	0.28299500
O	-2.18784900	-0.21732500	-1.72687900
H	-2.52507800	0.68098700	-1.69619300
TS100			
0	3		
C	3.74127800	-0.02452800	-0.21682500
C	2.95388500	0.42994500	-1.27246900
C	1.65360100	0.01872700	-1.30074300
C	1.04521200	-0.81585700	-0.37722100
C	1.86424800	-1.23808800	0.68131500
C	3.19004000	-0.85479500	0.75017600
H	4.77932100	0.26594500	-0.15727700
H	3.36419200	1.07378300	-2.03579200
H	3.80377000	-1.20732100	1.56474000
O	-0.20502500	-1.23747400	-0.48449600
C	-0.72964100	2.06264400	-0.16692300
C	-0.22262500	2.11848500	1.12100400
C	-0.42558700	1.05790100	2.01774600
C	-1.10117000	-0.05700200	1.62238900
H	-0.60960900	2.88328200	-0.85535800
H	0.31444500	2.99628300	1.44239900
H	-0.07002500	1.13824000	3.03266200
H	-1.29336300	-0.87896400	2.29181900
C	-1.46951400	-0.21184900	0.25581200
Cl	-2.78627500	-1.30884700	-0.07365800
C	-1.40329900	0.94394000	-0.59610700
H	1.42782100	-1.88777000	1.42562600
O	-1.88025900	0.89551300	-1.83477200
H	-2.24618500	0.02546200	-2.01141800

Table S5. Cartesian coordinates for reactions, intermediate and products involved in the formation routes of pre-intermediates for PCTA/PT/DT/DFs, x coordinate, y coordinate and z coordinate.

2-CTP				
0	1			
C	-2.40693700	0.60928100	-0.00002200	
C	-1.23620400	1.34006300	0.00002600	
C	-0.01153900	0.69432700	-0.00000900	
C	0.06931900	-0.69486100	0.00012200	
C	-1.12466300	-1.41295100	0.00012500	
C	-2.34636100	-0.77451000	-0.00002300	
H	-3.35675100	1.11961400	-0.00004500	
H	-1.25583700	2.41795400	0.00002200	
H	-1.08240200	-2.49162000	0.00031500	
H	-3.25261900	-1.35939700	-0.00002500	
Cl	1.41527100	1.67383000	-0.00006800	
S	1.55185800	-1.63175800	-0.00023100	
H	2.39658000	-0.60164200	0.00327600	
CTPR1				
0	2			
C	2.35886100	-0.70747300	0.00002100	
C	1.15370700	-1.38374900	0.00000500	
C	-0.02793300	-0.66935500	0.00001200	
C	-0.03619300	0.71959200	0.00006600	
C	1.18466500	1.38841100	0.00002900	
C	2.36906700	0.67780500	0.00001300	
H	3.28401200	-1.26119000	0.00000800	
H	1.11810600	-2.46130600	-0.00001600	
H	1.20074400	2.46724900	0.00001000	
H	3.30559400	1.21307700	-0.00000600	
Cl	-1.54089100	-1.50376300	-0.00000700	
S	-1.54539700	1.59092300	-0.00004700	
CTPR2				
0	2			
C	2.46039800	0.41505600	-0.00009800	
C	1.33466000	1.21607800	-0.00005600	
C	0.06539400	0.65776500	-0.00002000	
C	-0.11861400	-0.72779300	0.00017600	
C	1.04973100	-1.44753900	0.00025300	
C	2.32407400	-0.97057300	0.00001800	
H	3.44082500	0.86541700	-0.00023300	
H	1.42726600	2.28970800	-0.00006900	

H	3.18167700	-1.62460900	-0.00003200
Cl	-1.29132600	1.73109800	0.00001100
S	-1.64828400	-1.58266200	-0.00017600
H	-2.41854100	-0.49454600	0.00133700
CTPDR			
0	3		
C	-2.37787700	0.57323600	0.00006600
C	-1.19262100	1.30183500	0.00021100
C	0.02874200	0.66154600	0.00011800
C	0.10178100	-0.75781300	-0.00012900
C	-1.12948800	-1.39266200	-0.00025900
C	-2.36460000	-0.81913300	-0.00017700
H	-3.31925400	1.10203500	0.00014400
H	-1.22018000	2.37903700	0.00039800
H	-3.27675600	-1.39379600	-0.00029200
Cl	1.46181300	1.59998200	0.00030200
S	1.53560900	-1.66806400	-0.00027200
TPR2			
0	2		
C	2.27496600	-0.04520900	0.00002000
C	1.57576100	-1.24875500	0.00000600
C	0.21325100	-1.16671600	-0.00003300
C	-0.52874800	-0.01733700	-0.00012400
C	0.19289500	1.17611200	-0.00004000
C	1.57729700	1.15225300	0.00003600
H	3.35411500	-0.04889800	0.00006900
H	2.09103700	-2.19690400	0.00003800
H	-0.33370000	2.11948200	-0.00002600
H	2.11728500	2.08627100	0.00009200
S	-2.28813000	0.01535900	0.00003000
H	-2.45120200	-1.30778100	0.00016300
TPDR			
0	3		
C	2.21279700	-0.03271900	-0.00001200
C	1.53539500	-1.24938700	0.00001100
C	0.17256500	-1.18220300	-0.00000800
C	-0.59592800	-0.02904700	-0.00007500
C	0.13229500	1.18357600	0.00000100
C	1.50854000	1.17123700	0.00000300
H	3.29254300	-0.02345800	0.00000500
H	2.06749000	-2.18780000	0.00003300

H	-0.41955600	2.11133100	0.00003300
H	2.05109500	2.10357500	0.00002800
S	-2.29909700	-0.07327400	0.00002400
2-CP			
0	1		
C	-1.81954100	-1.26813400	-0.00008700
C	-0.45026800	-1.45388200	-0.00021700
C	0.38749800	-0.35566600	-0.00009700
C	-0.11792600	0.93874400	0.00016300
C	-1.49369500	1.11335100	0.00030000
C	-2.33476200	0.01917900	0.00017400
H	-2.47739100	-2.12216600	-0.00018100
H	-0.02189200	-2.44319600	-0.00041300
H	-1.87689400	2.12126600	0.00050200
H	-3.40232800	0.17426500	0.00028100
O	0.66604100	2.02579800	0.00028400
H	1.58739100	1.76066400	0.00029100
Cl	2.10793800	-0.56816300	-0.00024500
CPR1			
0	2		
C	1.70263800	-1.33082400	-0.00002200
C	0.31585600	-1.44405400	-0.00000800
C	-0.46131600	-0.31320000	-0.00002200
C	0.13568900	1.00842800	-0.00013600
C	1.57378900	1.06006200	-0.00000300
C	2.32696600	-0.07612200	0.00000800
H	2.30188400	-2.22785900	0.00000100
H	-0.15348600	-2.41463400	0.00002200
H	2.01535500	2.04395200	0.00004700
H	3.40405700	-0.01686400	0.00004900
O	-0.55080200	2.03838600	0.00004600
Cl	-2.16018400	-0.41867100	0.00003700
CPR2			
0	2		
C	-1.93114600	-1.11695700	-0.00009100
C	-0.57428700	-1.38058900	-0.00021900
C	0.33734100	-0.33886900	-0.00008300
C	-0.06937700	0.99461500	0.00018300
C	-1.42956900	1.17926200	0.00030000
C	-2.37771300	0.20319000	0.00017700
H	-2.63871200	-1.93101900	-0.00019800

H	-0.20752000	-2.39398800	-0.00042400
H	-3.43120100	0.43657600	0.00028300
O	0.77295700	2.03311700	0.00031800
H	1.67647900	1.71180500	0.00023300
Cl	2.04034200	-0.66660100	-0.00023800
CPDR			
0	3		
C	-1.82600500	-1.18598200	-0.00006700
C	-0.44095400	-1.37465300	-0.00020100
C	0.41088900	-0.30243300	-0.00008300
C	-0.08675100	1.07163800	0.00018600
C	-1.51357100	1.13863700	0.00030300
C	-2.38160700	0.10099900	0.00019200
H	-2.47511600	-2.04820300	-0.00016300
H	-0.03463200	-2.37302200	-0.00039800
H	-3.45104400	0.24403000	0.00029400
O	0.66181300	2.04952700	0.00030000
Cl	2.09966400	-0.52401500	-0.00024200
PR2			
0	2		
C	1.83148600	-0.00768400	0.00018100
C	1.16100800	-1.22746600	0.00030700
C	-0.20260800	-1.18500000	0.00016700
C	-0.97014400	-0.04829800	-0.00008800
C	-0.28339800	1.16028600	-0.00021200
C	1.10082700	1.17060700	-0.00007600
H	2.91008300	0.01439100	0.00028400
H	1.69937300	-2.16301300	0.00050800
H	-0.85387700	2.07681000	-0.00041500
H	1.61697200	2.11799600	-0.00017500
O	-2.31859900	-0.03595400	-0.00021500
H	-2.64678200	-0.93322900	-0.00015000
PDR			
0	3		
C	1.76165200	0.04596300	-0.00002100
C	1.15035800	-1.21191500	0.00001600
C	-0.20631600	-1.24273600	-0.00000400
C	-1.07646000	-0.10866500	-0.00017500
C	-0.37670300	1.15955000	-0.00001000
C	0.98647200	1.21820000	0.00000200
H	2.83885000	0.11475600	0.00000700

H	1.74200500	-2.11481200	0.00007000
H	-0.98995100	2.04789800	0.00006100
H	1.48422000	2.17546000	0.00005200
O	-2.31364300	-0.17321100	0.00012000
IM1			
0	2		
C	2.81525700	2.42741800	0.27927500
C	1.50886900	2.58067100	-0.15196400
C	0.77737400	1.48042000	-0.55941600
C	1.33939400	0.21407100	-0.52592100
C	2.65315600	0.07064200	-0.09457800
C	3.39043900	1.17043000	0.30328300
H	3.39179400	3.28379100	0.59156400
H	1.05891800	3.56050100	-0.18396900
H	4.40837100	1.03108900	0.62967700
O	0.66639700	-0.88151900	-0.96599500
C	-0.40822600	-1.36617500	-0.14627900
C	-1.66600200	-0.57928300	-0.38451200
C	-2.34984400	-0.03854800	0.66821800
C	-1.92574100	-0.19106400	1.99325300
C	-0.74806600	-0.91016200	2.27151400
C	-0.01632600	-1.46541200	1.28116800
H	-2.50205700	0.25788500	2.78414900
H	-0.43097000	-1.01134200	3.29791300
H	0.89090200	-2.01162300	1.48849200
H	-0.22939300	1.59149700	-0.92811700
H	-0.55757200	-2.36884200	-0.55479600
Cl	3.37169800	-1.49574300	-0.05990700
Cl	-3.79856000	0.87746700	0.41282300
S	-2.06497500	-0.44924600	-2.06890000
H	-3.28661500	0.05977200	-1.89838000
IM2			
0	1		
C	3.48996600	-1.43044700	0.88153600
C	2.27290500	-1.92945100	1.31231300
C	1.09450900	-1.29979200	0.95771800
C	1.12665400	-0.16697900	0.16135000
C	2.34876100	0.33499800	-0.26708600
C	3.52522700	-0.29426700	0.09429600
H	4.41065100	-1.91907600	1.15741600
H	2.23536800	-2.80971900	1.93455700
H	4.46159600	0.11376600	-0.25052900

O	0.01210200	0.52664500	-0.18089700
C	-1.18471100	-0.12130800	-0.32056300
C	-2.29993200	0.44851000	0.28103400
C	-3.53520900	-0.15987800	0.08867200
C	-3.65003100	-1.30424200	-0.67546800
C	-2.52914000	-1.85514400	-1.27534300
C	-1.29619700	-1.25649200	-1.10231200
H	-4.41106700	0.27590100	0.54468200
H	-4.61819600	-1.76057200	-0.80888100
H	-2.61376800	-2.74122500	-1.88417300
H	-0.41008300	-1.66067300	-1.56713800
H	0.14161000	-1.67615000	1.29482000
Cl	2.39387200	1.74964900	-1.24640500
S	-2.20233700	1.89132800	1.27524400
H	-0.92816800	2.16625300	0.99450600
IM3			
O	2		
C	-3.37968900	1.45057000	-0.46153500
C	-3.41414700	0.13940000	-0.73679500
C	-2.46161500	-0.77387300	-0.11263400
C	-1.18861300	-0.13398100	0.43357500
C	-1.38742200	1.26291100	0.89599600
C	-2.38777800	2.01140800	0.42855100
C	-0.15192900	-0.15166600	-0.81368600
C	1.15652200	0.48729500	-0.46463100
C	0.00575900	-1.54323800	-1.30784800
C	2.23196900	-0.30935300	-0.16838700
C	1.11481900	-2.26700800	-1.04222900
C	2.22001100	-1.68670800	-0.39440200
O	-2.62936400	-1.96789400	-0.09454000
H	3.08567200	-2.27203500	-0.13502700
H	-0.65568900	1.66215000	1.57887700
H	-0.82934200	-1.99557200	-1.81538100
H	-4.13563600	2.10580400	-0.86886200
H	1.16630900	-3.30214900	-1.34146900
H	-2.47878700	3.04332100	0.72862100
H	-4.19742700	-0.31009600	-1.32599000
H	-0.65982000	0.46610800	-1.55902600
Cl	-0.53334500	-1.11173600	1.75489900
S	1.18215000	2.22665300	-0.52186700
H	2.49668800	2.36640700	-0.33817200
Cl	3.72047500	0.37280800	0.40079300

IM4			
0	2		
C	2.84317400	-1.60798900	0.19549500
C	2.98301500	-0.27930400	0.07817700
C	1.93109200	0.62967200	0.55256700
C	0.57039000	0.01649100	0.76621200
C	0.58849000	-1.43473400	1.05533400
C	1.64697200	-2.19114800	0.75401000
C	-0.28932800	0.32564900	-0.56714200
C	-1.66072400	-0.26104900	-0.43847600
C	-0.32673000	1.79706100	-0.76949500
C	-2.66089900	0.52202300	0.07547700
C	-1.36507600	2.53007900	-0.30685000
C	-2.51044300	1.90434900	0.21937400
O	2.11853100	1.81240800	0.70936700
H	-3.31872600	2.48123100	0.63620800
H	0.24203000	-0.16934200	-1.38044900
H	-0.30046300	-1.87738900	1.47534300
H	0.54340600	2.27679700	-1.18407700
H	3.65530800	-2.25496600	-0.09928100
H	0.07255300	0.57842000	1.55384300
H	-1.33167200	3.60726100	-0.35411600
H	1.63251900	-3.25518800	0.92948500
Cl	4.42738300	0.43714400	-0.50221800
Cl	-4.21671000	-0.14395800	0.45413600
S	-1.81808500	-1.91021600	-0.95969700
H	-3.13488500	-2.01340100	-0.76743700
IM5			
0	1		
C	-2.88679100	1.15762600	0.52871300
C	-2.52852100	0.03725300	-0.11516300
C	-1.14484700	-0.44901700	-0.09514900
C	-0.16309500	0.30305700	0.78756700
C	-0.66851300	1.55968900	1.39528500
C	-1.94253000	1.93697300	1.29261900
C	1.17719900	0.46040800	0.11774000
C	2.14437300	-0.54478000	0.17353600
C	1.46358900	1.62878500	-0.57468000
C	3.37844500	-0.34359200	-0.42951800
C	2.69221800	1.82194000	-1.17924200
C	3.65694200	0.83465300	-1.09717800
O	-0.79547500	-1.42431800	-0.71693600
H	4.62083900	0.97285900	-1.56189900

H	0.03937400	2.14361100	1.96485800
H	0.70871900	2.39991800	-0.63148200
H	-3.91105600	1.49269200	0.46732300
H	-0.00587500	-0.39930900	1.62130900
H	2.89230500	2.73972000	-1.70994100
H	-2.29591000	2.83260600	1.77844600
H	4.11638000	-1.12861600	-0.38114400
Cl	-3.64542800	-0.86243200	-1.05205000
S	1.89170100	-2.05995400	1.05658000
H	0.83326400	-2.45630900	0.34041000

IM6

0 1

C	3.18634700	0.21264500	-1.35623500
C	3.02417700	0.95944900	-0.25836300
C	1.81517900	0.87371300	0.54490900
C	0.74184000	-0.16259100	0.14338300
C	1.05742100	-0.91807100	-1.10391700
C	2.17957500	-0.72629700	-1.79457400
C	-0.65093000	0.43083100	0.03809500
C	-1.81937600	-0.33662100	-0.11518000
C	-0.78066700	1.81700100	-0.01361600
C	-3.04185100	0.30277600	-0.28687000
C	-1.99820200	2.43926100	-0.21191100
C	-3.14023900	1.67763900	-0.34758700
O	1.65176900	1.55965900	1.52431000
H	-4.10343500	2.14306800	-0.48708100
H	0.31294200	-1.61956200	-1.44198600
H	0.08746100	2.43828200	0.10703100
H	4.09206400	0.30255900	-1.93775800
H	-2.04411700	3.51609100	-0.24803200
H	2.34974600	-1.28159400	-2.70352600
H	-3.92989900	-0.30476600	-0.36790300
H	3.76823000	1.65956500	0.08586700
Cl	0.88602900	-1.33627800	1.54025900
S	-1.95221700	-2.10061400	-0.21788400
H	-1.01381400	-2.42277800	0.67184100

IM7

0 2

C	1.97040400	2.67468900	-0.46605400
C	0.82832400	2.42136800	-1.20555700
C	0.43602300	1.11622600	-1.42684300
C	1.15941200	0.04409600	-0.91050000

C	2.31467800	0.32166000	-0.18016800
C	2.71754100	1.62756600	0.03982300
H	2.29119500	3.68936500	-0.28778800
H	0.24584600	3.23406800	-1.60972800
H	3.61609500	1.81259500	0.60575300
Cl	3.30074200	-0.94163900	0.45729200
C	-0.67064500	-1.75932800	0.21853500
C	-1.74617300	-0.75291800	0.08200200
C	-1.74318100	0.33691000	0.91280900
C	-0.86196500	0.44578300	1.99269500
C	0.01739800	-0.61084100	2.28153400
C	0.07342200	-1.70350400	1.48202300
H	-0.89412200	1.32781600	2.60954500
H	0.63948800	-0.55066400	3.16087500
H	0.74432500	-2.51945300	1.69690700
H	-0.44976600	0.89915600	-2.00458600
H	-1.04236600	-2.75960000	0.00245600
Cl	-2.87012700	1.63233900	0.68655500
S	0.58570300	-1.59044900	-1.21317800
S	-2.81628000	-1.01596200	-1.26484800
H	-3.75333600	-0.14286000	-0.89222700
IM8			
0	1		
C	-2.94764600	2.20157700	-0.49051200
C	-1.59054600	2.40484600	-0.66669300
C	-0.70638300	1.34732100	-0.57155000
C	-1.16143300	0.06450600	-0.29627700
C	-2.52934300	-0.12366100	-0.12325200
C	-3.41743900	0.93058000	-0.21883800
H	-3.64056800	3.02469300	-0.56300700
H	-1.21141200	3.39228000	-0.87825500
H	-4.46989600	0.74354800	-0.07877100
C	1.50253900	-0.62040200	-0.33552000
C	2.14005400	0.05628500	0.71172800
C	3.42707800	0.54479800	0.50624600
C	4.07398700	0.35926500	-0.69891300
C	3.45126400	-0.32576800	-1.72882200
C	2.17172100	-0.80978000	-1.53894600
H	3.92563400	1.06620400	1.30923100
H	5.07314200	0.74559200	-0.82888800
H	3.95399900	-0.47938700	-2.67034400
H	1.66458400	-1.34004800	-2.32985400
H	0.34949600	1.51565000	-0.71061100

Cl	-3.14435000	-1.70287700	0.21400400
S	-0.09946700	-1.34296100	-0.16439700
S	1.40911900	0.37756900	2.27138000
H	0.37143100	-0.45075300	2.10878900
IM9			
0	2		
C	-2.86520500	2.02620500	-0.60402100
C	-3.11490100	0.71152400	-0.77487100
C	-2.38375300	-0.29230000	-0.04765200
C	-1.05156000	0.16760200	0.47807000
C	-1.04569900	1.58636700	0.90131400
C	-1.86856600	2.47193900	0.32847800
C	-0.00621100	0.03253600	-0.83666600
C	1.37520100	0.44307400	-0.46735900
C	-0.07420300	-1.33482500	-1.38112000
C	2.31806800	-0.52448700	-0.21395900
C	0.90150200	-2.24206600	-1.14930400
C	2.08533400	-1.86925700	-0.49166400
H	2.84732700	-2.59495200	-0.26252700
H	-0.30455200	1.88306100	1.62395800
H	-0.96115800	-1.61685300	-1.92211200
H	-3.47294700	2.75754500	-1.11504300
H	0.78709600	-3.25875900	-1.49085300
H	-1.80667300	3.51816300	0.58291800
H	-3.94083200	0.37355600	-1.37997100
Cl	-0.41954300	-0.85084600	1.77477100
H	-0.44585900	0.75726300	-1.52370200
Cl	3.89075500	-0.11049200	0.38201600
S	-2.93764000	-1.81855100	0.08147400
S	1.66823500	2.15528700	-0.42216000
H	2.97743500	2.07809000	-0.17453300
IM10			
0	2		
C	-2.50713200	1.88058300	0.09869200
C	-2.75208900	0.55767100	-0.02886900
C	-1.85316400	-0.41775900	0.53981100
C	-0.46846200	0.08263100	0.78879600
C	-0.39128600	1.50268100	1.17324100
C	-1.35047900	2.35843300	0.79770600
C	0.38746200	-0.12182100	-0.62675100
C	1.78838700	0.33773400	-0.42144300
C	0.31167500	-1.54070300	-1.02172500

C	2.72911300	-0.58098100	-0.02545300
C	1.29116000	-2.41095200	-0.67844400
C	2.47711400	-1.95212900	-0.08106700
H	3.23831000	-2.64080400	0.24531800
H	-0.12831500	0.52550900	-1.33492900
H	0.48547700	1.84659900	1.69701900
H	-0.58488900	-1.88735400	-1.50696500
H	-3.23020400	2.58726100	-0.27774700
H	0.03630300	-0.57462300	1.48993400
Cl	4.32308600	-0.08919200	0.44547100
H	1.17584200	-3.46503500	-0.87563100
H	-1.27497000	3.41180600	1.01601900
Cl	-4.21824800	0.03583600	-0.75961000
S	-2.25342200	-1.96836100	0.84326200
S	2.07435600	2.02651300	-0.70044500
H	3.39145300	2.00093100	-0.48470200
IM11			
0	1		
C	-2.69968900	1.29088200	0.72247000
C	-2.42685700	0.17902100	0.00735900
C	-1.15007400	-0.48732700	0.08925000
C	-0.09210100	0.18075800	0.94186500
C	-0.51485200	1.37930000	1.70897100
C	-1.74069600	1.89409000	1.60528000
C	1.14297700	0.49924600	0.12127900
C	2.28252900	-0.30474300	0.15706600
C	1.13605600	1.62748400	-0.68683400
C	3.39409700	0.05539900	-0.59458000
C	2.24234700	1.97649800	-1.43779800
C	3.37984200	1.19117000	-1.38238400
H	4.25182500	1.45159600	-1.96203100
H	0.22730100	1.82356800	2.35519000
H	0.24598100	2.23994000	-0.72051800
H	-3.67842100	1.73609300	0.63124900
H	0.22218300	-0.56927300	1.67557000
H	2.21493000	2.85657300	-2.06122100
H	-2.03365800	2.76452200	2.17038600
H	4.26797600	-0.57611500	-0.56710300
Cl	-3.64539300	-0.46818200	-1.01684200
S	-0.82197700	-1.88464900	-0.68667000
S	2.39673700	-1.75826400	1.16423200
H	1.33592500	-2.37188200	0.61212500

IM12			
0	1		
C	-2.77946600	-0.37766000	1.85725700
C	-2.85875800	0.45747600	0.80339700
C	-1.85103100	0.50740000	-0.21145400
C	-0.62028000	-0.39125400	-0.03877800
C	-0.67838000	-1.30691900	1.13879900
C	-1.67319100	-1.27721100	2.02613700
C	0.68337700	0.39359700	0.07681900
C	1.96690500	-0.17928100	0.01341400
C	0.60107200	1.74854700	0.39188300
C	3.08353900	0.62817800	0.20220900
C	1.71774800	2.53094400	0.61376000
C	2.97246500	1.96953500	0.50672100
H	3.86095900	2.56350600	0.65324500
H	0.16064600	-1.97233300	1.26028800
H	-0.36390000	2.21428300	0.47945800
H	-3.57281800	-0.38550300	2.58949000
H	1.59593400	3.57401900	0.85880900
H	-1.65213200	-1.93316200	2.88196700
H	4.05941600	0.17825800	0.10430500
H	-3.70745500	1.10860500	0.66973700
Cl	-0.66857000	-1.44971600	-1.52519400
S	2.39878900	-1.88876100	-0.16289700
H	1.44651400	-2.25507000	-1.01971500
S	-2.01413100	1.47203900	-1.51399500
IM13			
0	2		
C	1.56991900	2.79887300	-0.00060700
C	0.52372600	2.56418000	-0.87601000
C	0.27942400	1.27755300	-1.31317100
C	1.05632100	0.20367400	-0.88559700
C	2.11426000	0.46611500	-0.01581200
C	2.36910700	1.75400100	0.42326700
H	1.77517500	3.79903700	0.34837800
H	-0.09725200	3.37704800	-1.21782900
H	3.19477200	1.92743900	1.09419500
Cl	3.16108200	-0.79047000	0.53073400
C	-0.67847000	-1.88376600	-0.19505000
C	-1.80353800	-0.94567300	-0.28749600
C	-1.98792600	0.00703300	0.67173000
C	-1.21981100	0.04238800	1.83938200
C	-0.27945400	-0.97627700	2.06177800

C	-0.06355700	-1.94661100	1.13606200
H	-1.38457900	0.82383800	2.56141200
H	0.26199300	-0.99333200	2.99474300
H	0.65482500	-2.73087200	1.31038600
O	-2.53748400	-1.04863700	-1.39697500
H	-3.22593600	-0.37949000	-1.39310700
H	-0.52856300	1.07408900	-2.00002000
H	-0.96008200	-2.85773400	-0.59114700
Cl	-3.23845800	1.18430100	0.42587600
S	0.66530700	-1.40718700	-1.47152900

IM14

0 1

C	-2.88400800	2.25645300	0.13944500
C	-1.52178800	2.49660000	0.10816900
C	-0.62884900	1.44816900	-0.01025100
C	-1.08118300	0.13841600	-0.09659800
C	-2.45361900	-0.08668500	-0.06389100
C	-3.34998800	0.95844500	0.05288200
H	-3.58354000	3.07205700	0.23083500
H	-1.14548300	3.50528800	0.17587000
H	-4.40614300	0.74314400	0.07441300
C	1.58686200	-0.51217700	-0.27520200
C	2.25986400	-0.30950100	0.93135900
C	3.53336300	0.24360600	0.92063000
C	4.12702500	0.58046600	-0.27789900
C	3.47100600	0.37040000	-1.48345000
C	2.20486800	-0.17819000	-1.47406800
H	4.03623700	0.39538600	1.86220400
H	5.11798300	1.00800600	-0.27248400
H	3.94374100	0.62915000	-2.41713700
H	1.67312000	-0.35367600	-2.39648100
O	1.71625900	-0.61919200	2.11345100
H	0.86571500	-1.04468400	1.96076400
H	0.43117300	1.64375800	-0.03784400
Cl	-3.06601700	-1.69923400	-0.16605700
S	-0.00761800	-1.26212000	-0.25572100

IM15

0 2

C	-2.89686000	1.89312200	-0.81884300
C	-3.06713400	0.55407500	-0.84869000
C	-2.27260900	-0.32275800	-0.03329400
C	-0.97716300	0.27260700	0.43984400

C	-1.04779900	1.72625000	0.70297900
C	-1.92383100	2.49467400	0.04670100
C	0.08142100	0.05774400	-0.86072200
C	1.40516900	0.59753700	-0.51173500
C	0.13783700	-1.35538300	-1.26657500
C	2.46875800	-0.22710900	-0.26853600
C	1.22175800	-2.13586500	-1.02768300
C	2.39815600	-1.60083300	-0.48144100
H	3.25325600	-2.21994800	-0.26966100
O	1.47222200	1.92531600	-0.41384700
H	2.35935900	2.18285200	-0.14746200
H	-0.31715000	2.14487800	1.37292800
H	-0.73691400	-1.77898200	-1.72903500
H	-3.55222500	2.52775700	-1.39615600
H	1.19281700	-3.18330800	-1.28347400
H	-1.92010300	3.56451400	0.18168100
H	-3.87500300	0.10623700	-1.40484900
Cl	-0.27806700	-0.56897800	1.82652600
H	-0.39147400	0.69255900	-1.61253800
Cl	3.95874000	0.49292700	0.24901000
S	-2.72050000	-1.86691200	0.24269900
IM16			
0	2		
C	-2.50487000	1.84998100	-0.22752900
C	-2.66509600	0.50925300	-0.13674200
C	-1.71948400	-0.29928800	0.58829900
C	-0.38328100	0.33108400	0.77596000
C	-0.40039000	1.79392200	0.92805700
C	-1.40037200	2.51152200	0.39815100
C	0.50693700	-0.02174700	-0.60983900
C	1.86906600	0.50410200	-0.43121800
C	0.49464400	-1.46848400	-0.87437800
C	2.91142800	-0.32651000	-0.12590600
C	1.56243500	-2.26146700	-0.59769600
C	2.77775600	-1.71419200	-0.16186200
H	3.62045900	-2.33821600	0.08338800
H	-0.01717900	0.55109500	-1.37524700
O	1.98987500	1.82844600	-0.52937900
H	2.90512800	2.08069000	-0.37828100
H	0.44115600	2.27575800	1.39649800
H	-0.41860700	-1.90337700	-1.24335700
H	-3.26234100	2.43567900	-0.72465300
H	0.15484600	-0.18164600	1.56557100

Cl	4.45700100	0.38589700	0.21158000
H	1.48685900	-3.32888600	-0.73243300
H	-1.39653700	3.58908500	0.43838300
Cl	-4.08303600	-0.21778800	-0.78339700
S	-2.00517700	-1.81966600	1.11089300

IM17

0 1

C	-2.38959500	1.55875700	0.21714900
C	-2.19603200	0.27252600	-0.14320400
C	-1.05643500	-0.47608200	0.32215400
C	0.02125500	0.30795200	1.03960100
C	-0.33683300	1.68858700	1.45101400
C	-1.47011100	2.27154900	1.05978600
C	1.30238000	0.32597100	0.21806900
C	2.25590100	-0.67539000	0.39783600
C	1.55441100	1.34266200	-0.69188800
C	3.45981500	-0.61090200	-0.28646300
C	2.74453100	1.39346300	-1.39292600
C	3.70362300	0.41829000	-1.17480800
H	4.64175400	0.45116000	-1.70712900
H	0.38488500	2.21326500	2.05882700
H	0.80908800	2.11041600	-0.84081500
H	-3.27822100	2.06326300	-0.12993300
H	0.25875300	-0.25277700	1.94716100
H	2.92385900	2.19120800	-2.09612300
H	-1.71366400	3.28018900	1.35301200
H	4.18336700	-1.39183600	-0.11491100
Cl	-3.36470600	-0.50365800	-1.13477900
O	2.06199100	-1.69891600	1.25708400
H	1.17109300	-2.05491600	1.11968400
S	-0.88964400	-2.08504700	0.09668000

IM18

0 1

C	-2.62972800	-0.14272300	1.87868300
C	-2.58101900	0.75276700	0.87307100
C	-1.59972700	0.68231400	-0.16590100
C	-0.54324300	-0.41507700	-0.06730500
C	-0.73144200	-1.37568200	1.05948300
C	-1.69118500	-1.22676100	1.97353700
C	0.86825600	0.12261200	0.05365500
C	1.98512500	-0.71526900	-0.07486100
C	1.08825400	1.44010600	0.44776500

C	3.25864800	-0.22286300	0.16025500
C	2.35696100	1.92516800	0.69441000
C	3.44773300	1.08765900	0.54622500
H	4.44666400	1.45280000	0.72799600
H	-0.00832300	-2.17319400	1.12812100
H	0.24871300	2.10062300	0.57765900
H	-3.39922700	-0.05488100	2.63081600
H	2.48669500	2.95121200	0.99877700
H	-1.76534700	-1.91816600	2.79780200
H	4.08739400	-0.90017300	0.02999400
H	-3.30473800	1.54818600	0.79801000
Cl	-0.75554300	-1.39648600	-1.60710800
O	1.90758200	-2.02502900	-0.38874400
H	1.12686900	-2.20114200	-0.92014300
S	-1.60668300	1.72885700	-1.41327100
IM19			
0	2		
C	-0.57980800	0.39757400	-1.03041100
C	-1.58014400	-0.47050800	-0.30888100
C	-2.78999700	0.03943700	0.06314900
C	-3.20142600	1.33639300	-0.27801900
C	-2.36026600	2.14451500	-1.06723100
C	-1.13800600	1.71452400	-1.45079900
H	-4.16940300	1.68266600	0.04127800
H	-2.70942600	3.11958000	-1.37112600
H	-0.49594200	2.33739900	-2.05461700
C	2.95749200	0.13992100	0.32787800
C	1.84389900	-0.05715400	-0.48025400
C	0.65927500	0.60171000	-0.17038700
C	0.61883500	1.42996200	0.93799100
C	1.73029900	1.61511600	1.73935300
C	2.91153400	0.96611700	1.43115900
H	-0.30890900	1.93336400	1.16919800
H	1.68117600	2.26152300	2.60071100
H	3.79502900	1.09226800	2.03567100
O	1.86803200	-0.86779800	-1.55087300
H	2.73168500	-1.27702600	-1.62879600
H	-0.25105400	-0.14252100	-1.92172300
Cl	4.42165000	-0.69160800	-0.08322000
Cl	-3.92658300	-0.91851500	0.95913900
S	-0.99994100	-2.08256300	-0.01826600
H	-2.06460700	-2.51743200	0.65672900

IM20				
0	1			
C	-1.27554200	0.51244000	-0.08486900	
C	-1.98624500	-0.61097200	0.34542300	
C	-3.33335000	-0.73376100	0.02337100	
C	-3.97699700	0.24011200	-0.71352400	
C	-3.28649800	1.36651500	-1.12576600	
C	-1.94867300	1.49225600	-0.80605000	
H	-3.88167700	-1.59788500	0.36715200	
H	-5.02223100	0.12168900	-0.95409800	
H	-3.78234700	2.13684500	-1.69502700	
H	-1.39352200	2.35861600	-1.13365900	
C	2.46739800	0.13780400	-0.11622700	
C	1.12445400	-0.09774600	-0.38621100	
C	0.15912500	0.71675500	0.21082700	
C	0.57479900	1.75027100	1.03696000	
C	1.91592000	1.97896200	1.29259500	
C	2.86993000	1.16483200	0.71350600	
H	-0.17853500	2.37596600	1.49068500	
H	2.21805500	2.78438100	1.94221500	
H	3.92165100	1.31625800	0.89519200	
Cl	3.64292300	-0.88878200	-0.86802800	
O	0.71200800	-1.07200200	-1.20306100	
H	1.46405200	-1.57442900	-1.52127000	
S	-1.29055200	-1.90361100	1.31461000	
H	-0.14830200	-1.28316000	1.61581000	
IM21				
0	2			
C	0.65097900	0.02057100	0.99442200	
C	1.72953800	-0.51276500	0.08695300	
C	2.93873400	0.11563300	0.01311300	
C	3.26633800	1.22115700	0.81126800	
C	2.33690100	1.69228700	1.75837600	
C	1.11480300	1.12848000	1.87917800	
H	4.23683200	1.67553200	0.70862100	
H	2.61615300	2.51462100	2.39909900	
H	0.40397100	1.49159700	2.60548100	
C	-2.84686900	0.41932500	-0.47761800	
C	-1.81477500	-0.08632800	0.31526400	
C	-0.54878100	0.48728600	0.17723500	
C	-0.34676200	1.52404200	-0.71838700	
C	-1.37869200	2.00764600	-1.49503400	
C	-2.63602300	1.44964400	-1.37272600	

H	0.64495900	1.94676100	-0.79801400
H	-1.21115200	2.81295000	-2.19211000
H	-3.46288100	1.80537100	-1.96549700
Cl	-4.45215300	-0.22410800	-0.38151700
H	0.32800500	-0.80957100	1.62836100
Cl	4.17145200	-0.44832800	-1.06929600
S	-2.02081900	-1.39775300	1.46965500
H	-3.30621900	-1.62440300	1.20419400
S	1.22997400	-1.91836500	-0.80213300
H	2.38341800	-2.12541500	-1.43893700

IM22

0 1

C	-1.29556700	0.34615200	-0.43716700
C	-2.07727600	0.05777700	0.68389200
C	-3.41085900	-0.29833700	0.51424700
C	-3.96741800	-0.36740600	-0.74685300
C	-3.19990800	-0.08213200	-1.86327000
C	-1.87426800	0.26959900	-1.69882700
H	-4.01302700	-0.52408200	1.38138200
H	-5.00378100	-0.64760800	-0.85573200
H	-3.62736100	-0.13665800	-2.85190200
H	-1.25999200	0.48774600	-2.55958400
C	2.44828900	0.16750600	-0.13130900
C	1.12141100	-0.24559800	-0.23239800
C	0.12889900	0.74065300	-0.32040900
C	0.47758900	2.08114300	-0.31810700
C	1.80115400	2.46983300	-0.21942800
C	2.78668000	1.50858600	-0.12295200
H	-0.30698400	2.81873100	-0.38589700
H	2.06588800	3.51503400	-0.21429100
H	3.82546100	1.78482500	-0.04244900
Cl	3.73937400	-0.97878400	-0.01857100
S	0.58310100	-1.91382900	-0.26318400
H	1.78259000	-2.45239700	-0.04391000
S	-1.48635200	0.13292500	2.33795000
H	-0.21249600	0.40155400	2.04733100

IM23

0 2

C	0.74138100	-0.41791600	0.85515900
C	1.75579000	-0.58197200	-0.22540000
C	3.00152200	-0.04968400	-0.12866800
C	3.43896800	0.64212900	1.01306600

C	2.55691400	0.76861500	2.10144800
C	1.29880700	0.26758200	2.05877200
H	4.43636400	1.04536900	1.04358200
H	2.89921200	1.27535500	2.99082200
H	0.63332200	0.37421900	2.90120100
O	1.30615300	-1.27490800	-1.27219200
H	1.99039900	-1.33605900	-1.94304900
C	-2.77492200	0.51092600	-0.29775600
C	-1.72811700	-0.26757100	0.19952900
C	-0.47180700	0.33178000	0.31796400
C	-0.29300100	1.65336700	-0.05394700
C	-1.34065000	2.40589400	-0.54426400
C	-2.59025900	1.83008100	-0.66211300
H	0.69125600	2.08744800	0.05229000
H	-1.19103400	3.43431300	-0.83174000
H	-3.42936200	2.39214100	-1.03846600
Cl	-4.36901500	-0.14091500	-0.48199600
H	0.42038200	-1.42402600	1.14028500
Cl	4.09032400	-0.26644900	-1.46391700
S	-1.90574600	-1.95724800	0.65548100
H	-3.23784200	-1.96771800	0.65268100
IM24			
0	1		
C	-1.40660400	0.40721000	-0.12988200
C	-2.04590900	-0.25851100	0.91638900
C	-3.39140400	-0.57902000	0.82185400
C	-4.10436400	-0.23852000	-0.30944200
C	-3.48696200	0.42785300	-1.35674000
C	-2.14625900	0.74580100	-1.25664000
H	-3.85573900	-1.09349000	1.64794100
H	-5.15055700	-0.49556700	-0.37351500
H	-4.04266100	0.69347700	-2.24179100
H	-1.64707100	1.25945900	-2.06481700
O	-1.40955300	-0.59802100	2.05214400
H	-0.47411100	-0.40639600	1.97868600
C	2.35388200	0.20308500	-0.03836700
C	1.02339300	-0.19812600	-0.15089100
C	0.02383300	0.77873900	-0.02202100
C	0.37560600	2.10249500	0.19495700
C	1.70126300	2.48029100	0.29709500
C	2.69132100	1.52489100	0.18562700
H	-0.41198100	2.83365300	0.29116600
H	1.96519400	3.51140000	0.46932200

H	3.73246800	1.79183300	0.26676900
Cl	3.64917300	-0.93379400	-0.18750000
S	0.49400000	-1.83813100	-0.48522500
H	1.69417500	-2.40273500	-0.35145400
IM25			
0	2		
C	-0.00397400	0.48376400	0.87951800
C	1.07672400	-0.32779500	0.21535100
C	2.28886700	0.22191900	-0.07528000
C	2.59537700	1.56111700	0.21038900
C	1.60976500	2.38613700	0.78400000
C	0.38167000	1.90941200	1.08546200
H	3.57234900	1.94262200	-0.03201900
H	1.84649300	3.42101900	0.97888100
H	-0.37157600	2.55151900	1.51578500
C	-3.56005900	-0.55088900	-0.02298100
C	-2.32362700	-0.51523900	0.60378100
C	-1.33620100	0.36242300	0.16099100
C	-1.60414300	1.15610700	-0.94754200
C	-2.82786900	1.11330200	-1.58547400
C	-3.81256900	0.26156000	-1.10940400
H	-0.83375700	1.82924700	-1.29601700
H	-3.01492300	1.74294700	-2.44091600
H	-4.77687300	0.22212200	-1.59220200
O	-2.15362400	-1.32870200	1.67637000
H	-1.27393500	-1.70829000	1.66733800
H	-0.15478500	0.04923700	1.87794800
Cl	3.53317100	-0.72631000	-0.81828200
S	0.60921500	-1.98034000	-0.10802700
H	1.82405000	-2.52450900	0.00097900
H	-4.30315600	-1.23450600	0.35562600
IM26			
0	1		
C	-0.65923700	-0.51889200	-0.00309900
C	-1.49590900	0.56884300	-0.28136200
C	-2.87660400	0.41954700	-0.18546000
C	-3.43221700	-0.79178200	0.17117100
C	-2.61589100	-1.88124600	0.42735400
C	-1.24595000	-1.73494500	0.33941500
H	-3.51592500	1.25988500	-0.41029600
H	-4.50501400	-0.88633200	0.23789400
H	-3.04254600	-2.83375200	0.69926200

H	-0.59617600	-2.57137700	0.54909400
C	2.92224900	0.37327400	0.78419000
C	1.53738400	0.32690400	0.84379100
C	0.81586100	-0.43246300	-0.07997500
C	1.51972200	-1.15336600	-1.03914600
C	2.89923600	-1.11441900	-1.10114800
C	3.59641100	-0.34284600	-0.18411500
H	0.95949300	-1.74316400	-1.74950000
H	3.42447200	-1.67555400	-1.85744000
H	4.67413300	-0.29996300	-0.22052700
O	0.93970900	1.02878100	1.82276300
H	-0.01308100	0.94857900	1.75773500
S	-0.90616800	2.15626400	-0.76612800
H	0.35793500	1.78923700	-0.99256500
H	3.44740600	0.97030300	1.51259900
IM27			
O	2		
C	0.10119100	0.24626400	0.91723100
C	1.18888200	-0.38777500	0.09048400
C	2.43873400	0.15663200	0.04742200
C	2.78130900	1.31911600	0.75375100
C	1.80091300	1.97213800	1.52401300
C	0.53961100	1.49366800	1.60628800
H	3.78534500	1.70119600	0.68497200
H	2.07004100	2.87349100	2.05333800
H	-0.20804000	2.00394200	2.19400300
C	-3.41815100	0.04681900	-0.57032500
C	-2.31121600	-0.26037000	0.21346100
C	-1.14562200	0.49514600	0.08595200
C	-1.11224600	1.52153700	-0.84914100
C	-2.21217900	1.82206900	-1.62764900
C	-3.37461700	1.08509000	-1.48083000
H	-0.20045000	2.09276700	-0.95294900
H	-2.16287100	2.62660500	-2.34486600
H	-4.24322100	1.30781500	-2.08092300
H	-0.18340700	-0.47891600	1.68853800
Cl	3.69494000	-0.57648100	-0.89642200
S	-2.49749200	-1.56819600	1.40351400
H	-1.54153600	-2.37180800	0.92312500
H	-4.31208300	-0.54722800	-0.46343900
S	0.66333400	-1.81413300	-0.76425000
H	1.86912600	-2.35243400	-0.95478500

IM28			
0	1		
C	-0.73644800	0.56631600	-0.07626400
C	-1.56571700	-0.34605200	0.58410700
C	-2.94427400	-0.27272600	0.40882700
C	-3.50263300	0.69532500	-0.40153800
C	-2.69153400	1.61391600	-1.04609000
C	-1.32258300	1.54139700	-0.87712900
H	-3.58084900	-0.97697200	0.92303700
H	-4.57424700	0.73468200	-0.52175700
H	-3.12005900	2.37703600	-1.67633200
H	-0.67614000	2.24582100	-1.37870800
C	2.94214800	-0.27831300	-0.40821300
C	1.56306100	-0.35260900	-0.57926000
C	0.73668500	0.56386100	0.07950700
C	1.32578300	1.53961200	0.87770300
C	2.69548000	1.61380700	1.04070200
C	3.50394600	0.69429600	0.39427000
H	0.68104100	2.24551700	1.37954800
H	3.12620900	2.37875700	1.66719300
H	4.57602200	0.73353200	0.51046700
S	-0.97003100	-1.61462300	1.64662700
H	0.31325700	-1.24780500	1.63019900
H	3.57661100	-0.98871100	-0.91658700
S	0.96919500	-1.61116600	-1.65324400
H	-0.33195500	-1.36220900	-1.49092100
IM29			
0	2		
C	0.15941200	0.08381100	0.95115200
C	1.18343500	-0.52123700	0.05009400
C	2.42384300	0.00975000	-0.09660600
C	2.84915400	1.13944700	0.62116900
C	1.95416100	1.73083500	1.53059100
C	0.69786800	1.25435800	1.70405100
H	3.84377500	1.52326700	0.47388700
H	2.28466100	2.58459300	2.10247100
H	0.02446100	1.72355900	2.40461800
O	0.75576800	-1.61826000	-0.58731400
H	1.44524200	-1.94517600	-1.17072100
C	-3.32735200	-0.04208900	-0.60738500
C	-2.19610200	-0.42569700	0.10246400
C	-1.09770600	0.43180600	0.17000900
C	-1.15312000	1.64078800	-0.50974900

C	-2.27789800	2.01778700	-1.21929200
C	-3.37482800	1.17572700	-1.25898300
H	-0.29555900	2.29668600	-0.46420700
H	-2.29721500	2.96532600	-1.73510500
H	-4.26151800	1.45737200	-1.80557800
H	-0.13421000	-0.69124300	1.66959800
Cl	3.52219300	-0.76450300	-1.19795600
S	-2.26549800	-1.98249900	0.95046800
H	-1.16271000	-2.50641100	0.40979400
H	-4.16758800	-0.71707200	-0.65356800

IM30

0 3

C	0.57382200	0.42531500	-1.02824100
C	1.58263300	-0.46172700	-0.34391600
C	2.78051700	0.05117800	0.06352800
C	3.17320600	1.36753200	-0.21752400
C	2.32983500	2.19288100	-0.98700800
C	1.11830700	1.76186500	-1.40184500
H	4.13271500	1.71511500	0.12507700
H	2.67161400	3.18086300	-1.25534700
H	0.47895400	2.39421900	-1.99847100
C	-1.73986400	1.42201300	1.82385400
C	-0.60743000	1.30489000	1.01708900
C	-0.64918000	0.58337800	-0.14478200
C	-1.87537000	-0.06723000	-0.55729700
C	-3.02347500	0.09083300	0.31497300
C	-2.94557800	0.81657800	1.47216200
H	-1.68668900	1.99220700	2.73819100
H	0.31571300	1.78440300	1.31002200
H	-3.81378000	0.91634000	2.10323000
O	-1.94014600	-0.72446500	-1.60311600
H	0.21654200	-0.08710000	-1.92585700
Cl	-4.47907900	-0.66124700	-0.15075100
Cl	3.92214900	-0.92902300	0.92639000
S	1.01899200	-2.09118200	-0.13078400
H	2.06550100	-2.53185000	0.56878600

IM31

0 2

C	-2.52091100	0.14659200	-0.11616400
C	-2.88135300	1.22473600	0.64555100
C	-1.89016200	2.05469500	1.16235900
C	-0.53718300	1.80398300	0.92453900

C	-0.13321400	0.72396100	0.18245900
C	-1.13029700	-0.15423500	-0.40346500
H	-3.92295200	1.42383200	0.83859900
H	5.08195500	0.13835700	-0.79132000
C	4.02609600	0.24713300	-0.59779600
C	3.36201600	1.40231600	-0.96419300
C	3.33027900	-0.77933400	0.01658100
C	2.00857800	1.52093500	-0.70860300
C	1.97123100	-0.67111600	0.27233800
C	1.29553700	0.49868900	-0.09073500
H	1.48163200	2.41659700	-1.00214800
H	3.89070200	2.20799400	-1.44927100
O	-0.81738000	-1.10220500	-1.13202600
H	-2.17584400	2.90333300	1.76404900
H	0.20818600	2.45831300	1.35003100
Cl	-3.70083000	-0.88863300	-0.77700800
H	3.83970500	-1.68463200	0.30657000
S	1.20611400	-1.98061400	1.19196400
H	0.34823200	-2.35970300	0.24019200
IM32			
0	3		
C	2.46691400	2.29583600	-1.10854200
C	1.14409800	2.37827000	-0.68918400
C	0.63198200	1.29509000	-0.03650500
C	1.29983300	0.13049900	0.24756300
C	2.62577200	0.07971900	-0.18774500
C	3.19735700	1.14797200	-0.85473400
H	2.92450700	3.12199900	-1.63002700
H	0.55022400	3.26015400	-0.87341500
H	4.22356000	1.06756200	-1.17405100
O	0.80059000	-0.93907600	0.89260300
C	-0.56729000	-0.90307400	1.31357400
C	-1.49143100	-0.81707800	0.13142000
C	-2.38635200	0.21156200	0.04008100
C	-2.50848000	1.18725400	1.03605000
C	-1.70833200	1.11591800	2.19517500
C	-0.79495200	0.13478300	2.35069300
H	-3.22629300	1.97970700	0.90821400
H	-1.83656100	1.86370400	2.96252700
H	-0.17058200	0.07573300	3.22844200
Cl	3.55490600	-1.33880000	0.11662100
S	-1.21613500	-2.07059500	-1.03102200
H	-2.22832300	-1.75113200	-1.83982500

Cl	-3.43504100	0.36097600	-1.32920900
H	-0.67552200	-1.89309900	1.76057000
IM33			
O	2		
C	3.34473000	-1.63138400	0.89188000
C	2.08193100	-2.18290300	1.08437400
C	1.01972700	-1.46216900	0.62565300
C	1.08437900	-0.25402000	-0.01845600
C	2.36100300	0.27441100	-0.19889800
C	3.47530600	-0.40977700	0.25500700
H	4.22264700	-2.15241600	1.24037500
H	1.95249400	-3.13212800	1.58064000
H	4.44791100	0.02841000	0.10163500
O	0.01917200	0.44882800	-0.45425500
C	-1.21892200	-0.14069200	-0.40002900
C	-2.23195500	0.54540000	0.25699500
C	-3.50196400	-0.01912700	0.27364200
C	-3.74723100	-1.22980400	-0.34462400
C	-2.72848400	-1.89269200	-1.00856100
C	-1.46255400	-1.33928100	-1.04333200
H	-4.30167600	0.50217400	0.77727600
H	-4.74023000	-1.65000000	-0.31571200
H	-2.91802100	-2.82991700	-1.50699700
H	-0.65577200	-1.82507300	-1.56969700
Cl	2.53836700	1.79422500	-0.98884200
S	-1.96444400	2.07127200	1.08087200
H	-0.73767100	2.27837100	0.60097700
IM34			
O	3		
C	-0.65242900	0.09546300	1.01973300
C	-1.71595000	-0.51105600	0.14362300
C	-2.91870600	0.11565000	-0.01296700
C	-3.25662500	1.28453000	0.68416800
C	-2.34830300	1.82223500	1.61630300
C	-1.13114600	1.26713000	1.80768100
H	-4.22173200	1.73321700	0.52249000
H	-2.64224900	2.68781400	2.19013700
H	-0.44002600	1.67917100	2.52696200
C	1.40625000	1.89262000	-1.58273300
C	0.36065100	1.47510900	-0.77962400
C	0.54954500	0.49850300	0.17747800
C	1.82717100	-0.09465000	0.35648300

C	2.87595500	0.36711800	-0.48263800
C	2.66818100	1.33927200	-1.43412900
H	1.24413300	2.65410300	-2.32977500
H	-0.62273000	1.90832400	-0.89485100
H	3.48937500	1.66008300	-2.05355200
Cl	4.45961500	-0.27915300	-0.34143000
H	-0.30120100	-0.67566800	1.70949800
Cl	-4.13052800	-0.53439000	-1.07010900
S	2.09577500	-1.31237300	1.51246700
S	-1.20544500	-1.99338700	-0.60499200
H	-2.33288500	-2.23619400	-1.27458900
IM35			
0	2		
C	-2.45626800	0.23738700	-0.04364900
C	-2.78283500	1.40833300	0.61058200
C	-1.78035300	2.27994900	0.99240500
C	-0.45153500	1.97955000	0.72954700
C	-0.10701600	0.80933300	0.08101500
C	-1.11524700	-0.09922400	-0.33876600
H	-3.81749300	1.62989700	0.81465000
H	5.08045300	-0.03682900	-0.87906100
C	4.03219400	0.13012400	-0.68555500
C	3.33429300	1.09079500	-1.39560300
C	3.39256000	-0.60762400	0.29131800
C	1.99309500	1.29097000	-1.12768100
C	2.04306200	-0.41578500	0.55611700
C	1.32555000	0.53436400	-0.17343100
H	1.43629900	2.03359400	-1.67948300
H	3.82775400	1.68083900	-2.15167500
H	-2.03635300	3.19551900	1.50250600
H	0.32981600	2.65564000	1.03995900
Cl	-3.74278500	-0.80099200	-0.50198800
H	3.94547700	-1.33460000	0.86649100
S	-0.70257900	-1.52334700	-1.17815800
S	1.32920000	-1.43710400	1.80170900
H	0.27044800	-0.66901400	2.06577900
IM36			
0	3		
C	1.91233100	2.68414100	-0.53752800
C	0.76385400	2.40692800	-1.27087900
C	0.46420500	1.08405400	-1.41911700
C	1.15567100	0.01111100	-0.92230500

C	2.30927800	0.33606800	-0.19777500
C	2.67994600	1.65807700	-0.01247600
H	2.21730500	3.70797300	-0.38049100
H	0.15590100	3.19123600	-1.69257200
H	3.57467100	1.87699700	0.54670500
Cl	3.31335900	-0.89591700	0.46810000
C	-0.68219300	-1.76170200	0.22541100
C	-1.74610400	-0.74593800	0.07399500
C	-1.73172800	0.35349500	0.89382100
C	-0.84460600	0.46866700	1.96708600
C	0.02538900	-0.59222200	2.26813200
C	0.06533200	-1.69775900	1.48552000
H	-0.86757000	1.35828500	2.57344900
H	0.65164000	-0.52545900	3.14405000
H	0.72904800	-2.51724800	1.70944200
H	-1.06054400	-2.76134600	0.01767800
Cl	-2.85318400	1.65305500	0.66312500
S	0.58555000	-1.62487500	-1.20759300
S	-2.82205500	-1.02522700	-1.25996200
H	-3.66759700	-0.02968500	-0.99153100

IM37

0 2

C	-2.77969400	2.26039700	-0.60573800
C	-1.40286100	2.39052700	-0.75862400
C	-0.66578100	1.25597500	-0.59223000
C	-1.13475600	0.00698700	-0.28810200
C	-2.51928500	-0.08201000	-0.14072000
C	-3.33043300	1.02864100	-0.29888100
H	-3.42154500	3.11963200	-0.72480500
H	-0.94794300	3.33960500	-0.99451700
H	-4.39547500	0.91735400	-0.17764400
C	1.48755200	-0.66679700	-0.30124100
C	2.10588100	0.08564600	0.70358500
C	3.37874500	0.59519500	0.46665700
C	4.02934700	0.35704500	-0.72706500
C	3.42508500	-0.40426000	-1.71327300
C	2.15930100	-0.91004500	-1.49282900
H	3.86439500	1.17514100	1.23667000
H	5.01781000	0.76132800	-0.88186100
H	3.93105900	-0.60000800	-2.64520300
H	1.66591800	-1.49891300	-2.25019000
Cl	-3.23507400	-1.60529700	0.24524400
S	-0.10412400	-1.40853900	-0.08917100

S	1.37907900	0.46898200	2.25222800
H	0.36417300	-0.39498100	2.15025400
IM38			
O	3		
C	-0.77069800	0.18862500	1.01493900
C	-1.66065800	-0.56914900	0.08620500
C	-2.93340900	-0.17269600	-0.17396000
C	-3.51376600	0.95036800	0.43685500
C	-2.74590300	1.68403400	1.35921100
C	-1.46514900	1.34666000	1.64687500
H	-4.52815700	1.22263900	0.20203100
H	-3.19651000	2.53289200	1.85073700
H	-0.89347400	1.92052800	2.35997700
O	-1.07742800	-1.64063700	-0.45323000
H	-1.69200500	-2.08480700	-1.04236500
C	1.53517800	2.11853000	-1.27447800
C	0.43114100	1.71806000	-0.54084500
C	0.48743500	0.60414600	0.27100800
C	1.68205400	-0.15816700	0.36089100
C	2.78903700	0.28307800	-0.40719700
C	2.71788100	1.40187200	-1.20720100
H	1.47769000	2.99255600	-1.90461200
H	-0.49218400	2.27530100	-0.59675900
H	3.58314800	1.70570500	-1.77295700
Cl	4.28063900	-0.56609000	-0.36454900
H	-0.44486400	-0.51814800	1.78608900
Cl	-3.87268000	-1.11481200	-1.29061300
S	1.78447600	-1.54490000	1.34047700
IM39			
O	2		
C	-2.37685300	0.21814700	-0.01596800
C	-2.67851600	1.52530800	0.29842000
C	-1.65408100	2.44001900	0.47021700
C	-0.33140800	2.04662500	0.34588400
C	-0.00392500	0.73772200	0.04037400
C	-1.03749300	-0.22138300	-0.16933400
H	-3.70907700	1.82175400	0.40386300
H	0.44926300	-0.88609900	1.78809900
H	5.19399700	-0.40201800	-0.37639000
C	4.14179500	-0.17585100	-0.29735800
C	3.54916100	0.70193700	-1.19109000
C	3.39466200	-0.76579300	0.70164200

C	2.20102300	0.97650300	-1.07079300
C	2.04084500	-0.49245200	0.81360400
C	1.42512900	0.38059400	-0.08316000
O	1.38519600	-1.07660000	1.83438300
H	1.72199800	1.65307200	-1.76314500
H	4.12899000	1.16433900	-1.97374800
H	-1.89115400	3.46396600	0.71418200
H	0.46414900	2.75869100	0.49977900
Cl	-3.68491300	-0.86995600	-0.23016800
H	3.83904600	-1.44433500	1.41211100
S	-0.66608100	-1.80972400	-0.65760000

IM40

0 3

C	1.61533800	2.79096700	-0.09681500
C	0.54673900	2.55781000	-0.95550300
C	0.34509000	1.25367300	-1.30229600
C	1.06236900	0.15908000	-0.89782500
C	2.13590300	0.44242600	-0.04368700
C	2.40473900	1.74379500	0.34844000
H	1.84120700	3.79800800	0.22068000
H	-0.07507500	3.35980700	-1.31990500
H	3.23833000	1.93087200	1.00517500
Cl	3.16782900	-0.81282400	0.52848000
C	-0.72077500	-1.87874200	-0.13843300
C	-1.84300700	-0.94400800	-0.26163500
C	-1.99299900	0.06770500	0.64318900
C	-1.19983500	0.15635800	1.79079000
C	-0.27470800	-0.86529000	2.05805300
C	-0.08999300	-1.88885400	1.18360600
H	-1.34069400	0.97925400	2.47075500
H	0.27783000	-0.84108800	2.98433700
H	0.61371100	-2.67802700	1.39201700
O	-2.60962400	-1.11902400	-1.33667500
H	-3.25903000	-0.41433700	-1.39334300
H	-0.99925600	-2.86574200	-0.50128400
Cl	-3.24073200	1.23914800	0.36306900
S	0.61788500	-1.44584800	-1.45554200

IM41

0 2

C	-2.69217100	2.35164500	0.15250900
C	-1.31008700	2.50735100	0.11530400
C	-0.57620800	1.36515200	-0.00994500

C	-1.05572700	0.08680000	-0.10033900
C	-2.44503800	-0.02878100	-0.05930200
C	-3.25228600	1.08901400	0.06557300
H	-3.33180600	3.21523300	0.25009100
H	-0.84925500	3.48020600	0.18308600
H	-4.32176000	0.95899800	0.09314600
C	1.56514500	-0.54822700	-0.28190700
C	2.22712800	-0.33238100	0.92756800
C	3.48455700	0.25557700	0.92197200
C	4.07123700	0.61475400	-0.27334800
C	3.42411400	0.39302000	-1.48129400
C	2.17398000	-0.19085300	-1.47778100
H	3.98056500	0.41723000	1.86553800
H	5.04978900	1.06994500	-0.26329900
H	3.89081400	0.67101400	-2.41247900
H	1.64939100	-0.37596500	-2.40232500
O	1.69232700	-0.66635400	2.10772400
H	0.85044500	-1.10686500	1.95387000
Cl	-3.16832400	-1.59263700	-0.16415700
S	-0.01769600	-1.33140900	-0.27080100

IM42

0	3		
C	-0.03190800	0.34913500	-1.07217700
C	1.05624600	-0.42185900	-0.36656500
C	2.15574400	0.23152400	0.11181500
C	2.38812700	1.59299800	-0.12709700
C	1.48930600	2.31799800	-0.93355700
C	0.36479800	1.74531700	-1.41616300
H	3.27517300	2.05386000	0.27260400
H	1.71822300	3.34481700	-1.17519600
H	-0.31744400	2.30212000	-2.03995000
C	-2.51072700	1.07740000	1.72098200
C	-1.36517700	1.10459900	0.92878400
C	-1.28224200	0.35040100	-0.21430900
C	-2.39898300	-0.48074900	-0.60452500
C	-3.56319800	-0.48127000	0.23916200
C	-3.60912700	0.28101200	1.36944100
H	-2.55192000	1.67719400	2.61707000
H	-0.52681300	1.72384600	1.21553400
H	-4.48686300	0.27440200	1.99696800
O	-2.35633600	-1.17287100	-1.63895400
H	-0.30439400	-0.19215000	-1.98235000
Cl	3.37158400	-0.61335700	1.01654700

S	0.69919300	-2.11436400	-0.20892500
H	1.76893200	-2.43471200	0.52096200
H	-4.38537100	-1.10856000	-0.06724900
IM43			
O	2		
C	-2.98826100	0.46425100	0.68690500
C	-3.62892600	-0.37533800	-0.17538500
C	-2.88139800	-1.25349000	-0.96911600
C	-1.48980900	-1.27859800	-0.89343900
C	-0.80163800	-0.43457700	-0.05250700
C	-1.55451300	0.46869900	0.79601900
H	-4.70529900	-0.36949000	-0.24896500
H	4.50635500	-0.92689800	0.24759400
C	3.43433300	-0.81893800	0.18988400
C	2.60653800	-1.89359800	0.45373900
C	2.88339800	0.40538300	-0.14494100
C	1.23537700	-1.73288700	0.37713300
C	1.50884800	0.57629000	-0.22086700
C	0.66526500	-0.50876200	0.04174900
H	0.58285100	-2.56597100	0.59243000
H	3.02201500	-2.85278900	0.72069200
O	-0.98817100	1.21658500	1.61386900
H	-3.38600600	-1.91757600	-1.65375600
H	-0.93526300	-1.95834100	-1.52284100
H	3.52095300	1.25029800	-0.35209900
S	0.91635900	2.14274800	-0.80296300
H	0.22407200	2.46194300	0.29362000
H	-3.52133700	1.15157000	1.32473200
IM44			
O	3		
C	-3.44141600	-0.94861700	-1.35111400
C	-2.15100500	-1.42656000	-1.15361900
C	-1.34425100	-0.73626900	-0.29384400
C	-1.70884400	0.39607200	0.39171000
C	-3.00365600	0.86147900	0.18185100
C	-3.85374300	0.19244600	-0.67908400
H	-4.11156000	-1.46369700	-2.02187900
H	-1.80021400	-2.31159300	-1.66300200
H	-4.85372300	0.56948100	-0.82739800
O	-0.93170800	1.09865700	1.24859700
C	0.37961900	0.61376200	1.53597400
C	1.25118400	0.63439000	0.31053200

C	1.87599900	-0.50806400	-0.10277900
C	1.75844400	-1.71767100	0.59256000
C	0.99148400	-1.78033400	1.77329000
C	0.33980800	-0.69440500	2.23815900
H	2.26729800	-2.58913500	0.21682300
H	0.93035600	-2.71842100	2.30306200
H	-0.26039000	-0.73513500	3.13362000
S	1.27947200	2.18586000	-0.46026900
H	2.18229700	1.88078100	-1.39347700
Cl	2.86116600	-0.52018600	-1.52729100
H	0.74576400	1.37979400	2.22346200
H	-3.31927700	1.75069000	0.70644200

IM45

0 2

C	4.00189700	-0.42091400	0.58918400
C	2.89051900	-1.02208700	1.17341200
C	1.66123700	-0.65572300	0.70765700
C	1.44256700	0.24620000	-0.30240800
C	2.55846200	0.83412100	-0.88250200
C	3.82399100	0.50036200	-0.43051300
H	4.99325900	-0.67378100	0.93170300
H	2.99969000	-1.74257300	1.96989600
H	4.68335400	0.96502100	-0.88804700
O	0.21562100	0.62491600	-0.74344400
C	-0.86633300	-0.15303000	-0.42733100
C	-1.98971200	0.47967400	0.09137900
C	-3.11443300	-0.29051800	0.36185300
C	-3.11577100	-1.65087700	0.12334500
C	-1.99179100	-2.26550600	-0.40295300
C	-0.86877900	-1.51171900	-0.68524500
H	-3.99352600	0.18791200	0.76599100
H	-3.99907500	-2.22910400	0.34449800
H	-1.98981000	-3.32526100	-0.60253500
H	0.01251500	-1.96575400	-1.11064000
S	-2.03869100	2.20218300	0.42299000
H	-0.81818400	2.46593600	-0.04298400
H	2.41473500	1.54344700	-1.68345000

IM46

0 3

C	0.06000300	-0.05248300	0.99142200
C	1.18186700	0.49166000	0.14686200
C	2.36681800	-0.17982100	0.06125000

C	2.63319600	-1.34009000	0.80304200
C	1.66563800	-1.82185900	1.70567200
C	0.46219600	-1.21916600	1.82798000
H	3.58810900	-1.82557700	0.69695500
H	1.90178300	-2.68191500	2.31355300
H	-0.27495400	-1.58829900	2.52452900
C	-1.99581200	-1.84177700	-1.63489600
C	-0.96218500	-1.45597200	-0.79919500
C	-1.12136300	-0.42619300	0.11045500
C	-2.36611000	0.24206300	0.18606500
C	-3.40541900	-0.17087000	-0.67385100
C	-3.22558000	-1.19539300	-1.57065000
H	-1.84381500	-2.64698500	-2.33726800
H	-0.00568600	-1.95758600	-0.85044700
H	-4.03212100	-1.49467900	-2.22143500
H	-0.28950200	0.75144700	1.64538600
Cl	3.64700100	0.39638100	-0.95832700
S	-2.65870300	1.53459300	1.26152200
H	-4.34904600	0.34694700	-0.60852400
S	0.76008000	1.96738700	-0.66794000
H	1.92468000	2.14588800	-1.29344200
IM47			
0	2		
C	2.93881200	-0.29464000	0.44145000
C	3.51498900	0.63984000	-0.38979800
C	2.70851400	1.54352800	-1.06597000
C	1.33082000	1.50101900	-0.91113600
C	0.73046600	0.56836300	-0.08296600
C	1.54611800	-0.34899200	0.62334500
H	4.58648700	0.66832300	-0.51197600
H	-4.58340500	0.70963100	0.42540000
C	-3.50940700	0.68147700	0.32435800
C	-2.72683500	1.66576200	0.90039000
C	-2.92086200	-0.34413500	-0.39105300
C	-1.35293800	1.60609700	0.75926000
C	-1.54112900	-0.40488400	-0.53434700
C	-0.74347600	0.57537000	0.05785300
H	-0.72818900	2.36217300	1.21076300
H	-3.18001400	2.47094900	1.45669100
H	3.14997700	2.28010300	-1.71959200
H	0.70622300	2.19836200	-1.44833600
H	-3.54122900	-1.10107700	-0.84683700
S	0.88761400	-1.48951200	1.71409900

H	3.54631100	-1.00284700	0.98223800
S	-0.75796700	-1.67288300	-1.47344600
H	-1.88094900	-2.32012900	-1.78710600
IM48			
O	3		
C	3.02646800	1.64625600	-0.37485800
C	1.98109700	1.63808100	-1.29374700
C	1.26565500	0.47836600	-1.38829400
C	1.47842300	-0.66292700	-0.65968400
C	2.53468100	-0.62726500	0.25238400
C	3.30019700	0.51888200	0.38547800
H	3.62982500	2.53453900	-0.26008800
H	1.75573500	2.50473200	-1.89550900
H	4.11679900	0.53383500	1.09049500
C	-0.93899100	-1.67321200	0.34278800
C	-1.52739100	-0.35804700	0.00511000
C	-1.21568000	0.72510500	0.78637300
C	-0.50481700	0.59929100	1.98175600
C	-0.14280800	-0.67675300	2.44602600
C	-0.40435100	-1.78059100	1.70617800
H	-0.27784200	1.48326700	2.55315300
H	0.32796800	-0.76916300	3.41248500
H	-0.14222900	-2.76613500	2.05661600
H	-1.62601600	-2.48287100	0.10319100
Cl	-1.72967100	2.31863900	0.34540400
S	0.47624300	-2.09333500	-0.87275100
H	2.74150900	-1.50526800	0.84613200
S	-2.43485500	-0.33319700	-1.47488800
H	-2.89844300	0.91160100	-1.35316700
IM49			
O	2		
C	3.66005200	0.18625600	1.33896300
C	2.35465400	0.24589500	1.81578900
C	1.36050700	-0.06864700	0.93404000
C	1.53309400	-0.43191400	-0.37307200
C	2.84923300	-0.48236300	-0.83264000
C	3.89463000	-0.17722700	0.02151900
H	4.48409800	0.42406100	1.99413600
H	2.14202200	0.52901400	2.83526500
H	4.90678400	-0.22323300	-0.34928200
C	-1.19916900	-0.57124500	-0.44798400
C	-1.67552300	0.70609600	-0.13168800

C	-2.82001300	0.81586800	0.65264900
C	-3.48535900	-0.30637700	1.10176900
C	-3.02511000	-1.57013900	0.77274700
C	-1.88615100	-1.69229900	0.00189500
H	-3.19471400	1.79740900	0.90036400
H	-4.37268300	-0.19060900	1.70485200
H	-3.54341500	-2.45140800	1.11565200
H	-1.50382700	-2.66699200	-0.25782800
S	0.21326300	-0.83235200	-1.47597100
H	3.04886000	-0.76191900	-1.85736200
S	-0.91663800	2.20528800	-0.63008000
H	-0.07820800	1.65327200	-1.51291100
IM50			
0	3		
C	-0.14415700	-0.10033600	0.94704800
C	-1.17837200	-0.56384100	-0.02369100
C	-2.41942800	-0.01469900	-0.07007000
C	-2.82927500	1.00036400	0.80958300
C	-1.91818000	1.45473300	1.78024100
C	-0.66219800	0.95290800	1.86736400
H	-3.82498600	1.40222800	0.73647200
H	-2.23594000	2.21825200	2.47399000
H	0.02165100	1.31177700	2.62110600
O	-0.75521200	-1.54513200	-0.82220100
C	2.13946800	2.03610200	-1.18811400
C	1.05457200	1.57709400	-0.45944100
C	1.09064200	0.35845000	0.19244100
C	2.26166000	-0.43203500	0.11164400
C	3.35056200	0.05279000	-0.64128300
C	3.29443900	1.26882900	-1.27910300
H	2.08348800	2.99169600	-1.68672100
H	0.15666000	2.17461600	-0.39029900
H	4.14017400	1.62269200	-1.84764500
H	0.16346300	-0.97896100	1.52368900
Cl	-3.53924200	-0.61773500	-1.25385000
S	2.41805700	-1.94120900	0.89429800
H	4.23476100	-0.56165300	-0.70144100
H	-1.45777200	-1.80089200	-1.42455700
IM51			
0	2		
C	2.89621300	0.44054500	-0.17693500
C	3.44812700	-0.76103200	0.19976000

C	2.61567400	-1.83885600	0.47296600
C	1.23962300	-1.69997900	0.38436600
C	0.65586200	-0.49713400	0.01595900
C	1.50133700	0.60232700	-0.29129500
H	4.51894400	-0.86599700	0.27661600
H	-0.01298700	1.16929300	1.64453200
H	-4.67342300	-0.31669900	-0.22598000
C	-3.59571900	-0.35111100	-0.18171900
C	-2.89089700	-1.19749000	-1.02319400
C	-2.92781200	0.45063400	0.72086600
C	-1.51215700	-1.22454900	-0.94954800
C	-1.54389800	0.42397700	0.78646600
C	-0.81642900	-0.41239800	-0.06088300
O	-0.96571400	1.20219700	1.72125900
H	-0.94722000	-1.87232400	-1.60373500
H	-3.40850700	-1.82554400	-1.73051400
H	3.03811800	-2.78771400	0.76604900
H	0.59737300	-2.53582400	0.61651100
H	-3.45828000	1.10718800	1.39180000
S	0.88316300	2.08828700	-0.86727800
H	3.52155200	1.28786100	-0.40976000

IM52

0 3

C	2.86574100	1.81492400	0.02374800
C	1.91001600	1.85140200	-0.98739900
C	1.26989600	0.67518500	-1.25876700
C	1.47375300	-0.52289700	-0.62541200
C	2.44236500	-0.52945800	0.38019300
C	3.12937300	0.63034200	0.69548400
H	3.40732900	2.71375300	0.27891600
H	1.69379900	2.76227500	-1.52376200
H	3.87640600	0.61169200	1.47373500
C	-0.95262500	-1.77005900	0.07564100
C	-1.67133800	-0.54556200	-0.29483800
C	-1.56819800	0.57125600	0.48310500
C	-0.92979800	0.55004800	1.72630600
C	-0.44525400	-0.67200900	2.22029500
C	-0.51556100	-1.80606200	1.47541000
H	-0.85670600	1.45704700	2.30173800
H	-0.03262600	-0.70490600	3.21671400
H	-0.15533700	-2.74754000	1.85826900
O	-2.32524900	-0.60316800	-1.45349600
H	-2.67999900	0.26203700	-1.67073100

H	-1.51671500	-2.64965300	-0.22794000
Cl	-2.29621500	2.03857600	-0.08618800
S	0.57562600	-1.97285900	-1.06258600
H	2.64127800	-1.45208200	0.90499500
IM53			
O	2		
C	-3.61025700	1.32963900	0.27141900
C	-2.30145700	1.78241800	0.40337300
C	-1.30857300	0.87710100	0.15922100
C	-1.48625200	-0.42943400	-0.20385900
C	-2.80511800	-0.86303900	-0.33392000
C	-3.84925700	0.01386900	-0.09503100
H	-4.43381300	2.00303300	0.45337000
H	-2.08570100	2.80106700	0.68720000
H	-4.86422100	-0.33644500	-0.20069600
C	1.24318000	-0.49653400	-0.36065500
C	1.83877300	-0.32328800	0.88953100
C	2.95886200	0.48842100	1.00620800
C	3.47648200	1.11156300	-0.10989700
C	2.89502900	0.93770000	-1.35841300
C	1.78159900	0.13110700	-1.47609100
H	3.40466200	0.61283100	1.98000900
H	4.34830100	1.73923200	-0.00560000
H	3.30702500	1.42424900	-2.22780100
H	1.31058900	-0.02229100	-2.43460900
O	1.36649900	-0.91035500	1.99514900
H	0.62016600	-1.46781600	1.75155400
S	-0.15805800	-1.55901600	-0.50570600
H	-3.00814200	-1.88390100	-0.62464000
IM54			
O	2		
C	2.42023900	2.43723000	0.65557300
C	1.19494300	2.61588000	0.03654900
C	0.58610700	1.55782100	-0.61238800
C	1.18427300	0.30753800	-0.63627600
C	2.42165100	0.14305700	-0.02403300
C	3.03831200	1.20129900	0.61797200
H	2.90288200	3.26000500	1.15902000
H	0.71646100	3.58261600	0.04674100
H	3.99920500	1.04716100	1.08180300
O	0.62138000	-0.72812300	-1.30889100
C	-0.49070900	-1.39119100	-0.68007600

C	-1.71716000	-0.54587600	-0.72219300
C	-2.37378500	-0.17762200	0.41207500
C	-1.96575100	-0.60111100	1.68105600
C	-0.85095700	-1.45384300	1.78515200
C	-0.15981000	-1.85457800	0.69196900
H	-2.50707900	-0.27434500	2.55226500
H	-0.55062700	-1.79639000	2.76338400
H	0.69511400	-2.50543900	0.78077700
H	-0.34948700	1.68819800	-1.13237900
H	-0.64348500	-2.23838700	-1.35075500
Cl	3.21254800	-1.38726400	-0.08596400
Cl	-3.76970900	0.84205000	0.25507800
O	-2.07549900	-0.18014200	-1.95259200
H	-2.88240200	0.33970200	-1.91620700

IM55

0 1

C	-3.25778000	1.71848200	0.42772600
C	-2.01395800	2.23906000	0.73860300
C	-0.87711600	1.46357100	0.60370500
C	-0.97893900	0.15942600	0.14950600
C	-2.22863100	-0.36407900	-0.15703500
C	-3.36258100	0.41319000	-0.01689300
H	-4.14555400	2.32148100	0.53123900
H	-1.92223900	3.25333200	1.09389500
H	-4.32097800	-0.01482800	-0.26265800
O	0.08899000	-0.67133700	0.03061600
C	1.34596500	-0.15376400	-0.16326300
C	2.33583000	-0.67821600	0.65627500
C	3.64394200	-0.25944300	0.48534600
C	3.94663000	0.66741500	-0.49516000
C	2.95362400	1.17836700	-1.31637100
C	1.64510000	0.75888300	-1.15336900
H	4.40560700	-0.67152300	1.12770800
H	4.96843000	0.98953200	-0.62094100
H	3.19536300	1.89407800	-2.08558500
H	0.85198100	1.13529900	-1.78100100
H	0.09531300	1.86074500	0.84747100
Cl	-2.36109100	-1.98931900	-0.70734500
O	2.03565900	-1.58109100	1.60416300
H	1.10091200	-1.78762800	1.54207800

IM56

0 2

C	3.37425700	-1.27971600	-0.80262200
C	3.32417400	0.05998700	-0.82625500
C	2.34740400	0.77633400	-0.01342700
C	1.13147800	-0.03542000	0.42133500
C	1.42736300	-1.47834500	0.61503800
C	2.45322800	-2.05976100	-0.00822700
C	0.07071400	0.14351900	-0.78784600
C	-1.18950300	-0.58415500	-0.50163000
C	-0.16825000	1.58005400	-1.07844000
C	-2.35657500	0.07463500	-0.25929900
C	-1.35650400	2.18469800	-0.83657300
C	-2.47153400	1.46179000	-0.38274700
O	2.44818000	1.95241000	0.23490000
H	-3.41027900	1.94332300	-0.16945200
H	0.74310700	-2.04363400	1.22400800
H	0.66324900	2.16068000	-1.44020200
H	4.15155700	-1.79702000	-1.34593700
H	-1.45735200	3.24456200	-1.01072300
H	2.61840800	-3.12075100	0.09120900
H	4.05959800	0.65990100	-1.33808700
H	0.57202500	-0.35444200	-1.62428200
Cl	0.43323300	0.64886500	1.89687700
Cl	-3.75631400	-0.86895500	0.14417500
O	-1.07743700	-1.91579000	-0.48952000
H	-1.93138700	-2.30577800	-0.28330900
IM57			
O	2		
C	-2.81256700	1.60153400	-0.14896600
C	-2.88726800	0.26756600	-0.02626200
C	-1.81250300	-0.48312000	0.63321700
C	-0.48978800	0.22925100	0.75739200
C	-0.58714200	1.70607400	0.79055700
C	-1.66809400	2.33871200	0.32812500
C	0.40342400	-0.24655800	-0.50373200
C	1.73907900	0.39674700	-0.44961100
C	0.50641800	-1.72843700	-0.52715800
C	2.84136500	-0.29480500	-0.04643200
C	1.63406200	-2.37651800	-0.14317200
C	2.81293800	-1.67790000	0.16480800
O	-1.94734300	-1.62489700	1.00408200
H	3.70371400	-2.18734500	0.49024300
H	-0.12200800	0.13446200	-1.38184100
H	0.26185300	2.26404800	1.14906100

H	-0.37884300	-2.28848700	-0.77573400
H	-3.64418200	2.14079900	-0.57646300
H	0.01569500	-0.16841000	1.63392600
H	1.63838600	-3.45413700	-0.09212100
H	-1.71289100	3.41603700	0.31079100
Cl	-4.28065900	-0.61300900	-0.49771600
Cl	4.34183200	0.56634600	0.10247200
O	1.75541800	1.68940900	-0.78881500
H	2.65418500	2.02493600	-0.73343800

IM58

0	1		
C	-2.59795100	1.33805100	0.03454200
C	-2.32768200	0.03839600	-0.16014500
C	-1.07108500	-0.54364500	0.30414600
C	-0.04383700	0.38555100	0.91780200
C	-0.47566700	1.79336300	1.09591900
C	-1.66904800	2.22722600	0.69227900
C	1.28710900	0.27340500	0.19818800
C	2.09576500	-0.84126400	0.42642600
C	1.74460200	1.27508200	-0.64566200
C	3.36245700	-0.90129100	-0.13227800
C	2.99863500	1.20314000	-1.22486300
C	3.81214800	0.11662700	-0.95062800
O	-0.84184400	-1.73321000	0.22413600
H	4.79718900	0.05373400	-1.38698200
H	0.22615400	2.45998700	1.57476300
H	1.11134800	2.12854000	-0.83921500
H	-3.54367400	1.73184600	-0.30567700
H	0.12330000	-0.03083600	1.91960700
H	3.33804400	1.99234500	-1.87678800
H	-1.96765100	3.25224600	0.84415900
H	3.97043500	-1.76668500	0.07774900
Cl	-3.43213400	-1.01470300	-0.93563400
O	1.69547500	-1.85487300	1.21925300
H	0.76942500	-2.05441400	1.01671500

IM59

0	1		
C	2.98440600	-0.62010000	1.31855800
C	2.72912500	-1.22860000	0.15366400
C	1.55992900	-0.88408500	-0.63772300
C	0.63934700	0.23565000	-0.12267100
C	1.04624600	0.82769400	1.18546200

C	2.12175400	0.41153000	1.85022400
C	-0.80810800	-0.17775500	-0.04813300
C	-1.80611700	0.76844900	0.21770600
C	-1.18016400	-1.51682700	-0.12544200
C	-3.11628400	0.36874600	0.41716200
C	-2.48742500	-1.91448400	0.07640700
C	-3.45679900	-0.96686900	0.35438100
O	1.30656600	-1.43088200	-1.68315700
H	-4.48173000	-1.26513500	0.51201800
H	0.40028700	1.59126300	1.59015200
H	-0.43790500	-2.26272300	-0.35132400
H	3.86002900	-0.89750600	1.88678200
H	-2.74316900	-2.95985200	0.01192600
H	2.36279100	0.84476300	2.80807300
H	-3.85126300	1.13259300	0.61426000
H	3.36849200	-1.99356700	-0.25651100
Cl	0.88326300	1.55009900	-1.38664200
O	-1.56001900	2.09247400	0.32711300
H	-0.82083600	2.34565000	-0.23167100
IM60			
0	2		
C	-0.62811100	0.44736500	-0.89563500
C	-1.66973200	-0.51769800	-0.43715800
C	-2.89436600	-0.10789900	-0.01698900
C	-3.28579600	1.24116300	-0.03110000
C	-2.37876500	2.19749000	-0.52188500
C	-1.14190600	1.84928500	-0.95195800
H	-4.26695200	1.51660300	0.31498100
H	-2.68495300	3.23187600	-0.55947400
H	-0.45837400	2.59614700	-1.32494800
C	2.92637100	-0.06537400	0.34063200
C	1.83077100	-0.00587400	-0.51392600
C	0.59463500	0.36249500	0.00320900
C	0.48901800	0.66738500	1.34899900
C	1.58363800	0.60327300	2.19133400
C	2.81461500	0.23190200	1.68262400
H	-0.47852000	0.96035300	1.73205900
H	1.48375100	0.84092500	3.23808300
H	3.68736100	0.17267400	2.31248200
O	1.92837500	-0.28485600	-1.82365100
H	2.82603800	-0.54991100	-2.03141000
H	-0.30914900	0.13045700	-1.89179800
Cl	4.45731000	-0.53103800	-0.32690900

Cl	-4.01838000	-1.31377300	0.53341300
O	-1.26976400	-1.79003800	-0.46929000
H	-1.97212100	-2.35926300	-0.14590100
IM61			
0	1		
C	-1.37951900	0.28371500	-0.05912800
C	-1.96784300	-0.85745900	0.49581400
C	-3.33849900	-1.05094500	0.39441600
C	-4.13298600	-0.14014100	-0.26958700
C	-3.56355600	0.98162500	-0.85096300
C	-2.20316300	1.18120300	-0.73746000
H	-3.75477400	-1.93546300	0.84967500
H	-5.19601400	-0.31133900	-0.34263100
H	-4.17172000	1.69111900	-1.38933400
H	-1.74930700	2.05009600	-1.19115300
C	2.40021000	0.12145900	-0.04665000
C	1.07561800	-0.27013200	-0.17963700
C	0.04776600	0.62718000	0.10192300
C	0.40528900	1.90852900	0.50887700
C	1.72611300	2.29541500	0.63416900
C	2.73767200	1.39628300	0.35463100
H	-0.38335100	2.60561400	0.74609300
H	1.97036500	3.29399800	0.95881800
H	3.77624900	1.66822800	0.44830600
Cl	3.63461400	-1.03688700	-0.41609500
O	0.74537200	-1.51708600	-0.58282200
H	1.54007800	-2.01462000	-0.78986500
O	-1.27547700	-1.77725700	1.19814600
H	-0.42173200	-1.92619600	0.78268400
IM62			
0	3		
C	-0.59027900	0.69042700	0.53181100
C	-1.82911400	-0.12579800	0.64320400
C	-2.94120100	0.15326400	-0.08470000
C	-3.01667800	1.25029000	-0.95789300
C	-1.90679300	2.10918600	-1.05302200
C	-0.76884000	1.88426500	-0.35510700
H	-3.91905200	1.42632000	-1.51733800
H	-1.97550700	2.97561300	-1.69298000
H	0.07145400	2.55729700	-0.41527100
C	1.61807200	-1.97126300	-1.08272200
C	0.48007400	-1.29034400	-0.64248200

C	0.59371500	-0.12452700	0.06081800
C	1.90328600	0.42352000	0.35225400
C	3.05042600	-0.32174000	-0.12836400
C	2.89971600	-1.48923100	-0.82612000
H	1.50553900	-2.89107400	-1.63516700
H	-0.49741000	-1.69396400	-0.85766500
H	3.76837000	-2.02543000	-1.17221600
O	2.02878800	1.48211200	0.97929000
H	-0.32295900	1.04196400	1.53531500
Cl	4.59735700	0.30620900	0.20985900
Cl	-4.32666800	-0.87556300	0.11359100
O	-1.73105000	-1.13657800	1.51402300
H	-2.56833800	-1.60427700	1.56410900
IM63			
0	2		
C	-2.47286300	0.11615700	-0.05326800
C	-2.75834200	1.40405300	0.28324000
C	-1.70385800	2.27967700	0.55852800
C	-0.38289300	1.87072100	0.47251700
C	-0.03280700	0.57747000	0.11951100
C	-1.10744700	-0.37337400	-0.12518400
H	-3.78234000	1.73397800	0.34612900
H	5.23458700	-0.20099500	-0.27986100
C	4.16483600	-0.07028900	-0.22326000
C	3.57614500	1.10373300	-0.67757600
C	3.38129100	-1.08216400	0.27889500
C	2.21319100	1.24572900	-0.58010000
C	1.99596600	-0.95964500	0.34775100
C	1.38350200	0.24509700	-0.05046200
H	1.75046000	2.14873300	-0.94799200
H	4.17441900	1.89089200	-1.10744400
O	-0.89588900	-1.56489600	-0.39613600
H	-1.92644900	3.29415400	0.85021600
H	0.39786200	2.57476500	0.71101800
Cl	-3.71825900	-1.00052900	-0.38079300
H	3.80998400	-2.01019900	0.62148700
O	1.34056400	-2.00059400	0.86021100
H	0.45414200	-2.04140700	0.46378200
IM64			
0	3		
C	2.33115500	2.51847800	-0.05680300
C	0.98596000	2.37304300	0.26182600

C	0.50026600	1.10014600	0.33775500
C	1.21357600	-0.05401200	0.12945300
C	2.56247900	0.12778900	-0.18611100
C	3.10891200	1.39498500	-0.27730100
H	2.76940200	3.50140400	-0.13226100
H	0.35492200	3.23018200	0.43952000
H	4.15388300	1.48967900	-0.52363600
O	0.74103600	-1.30949100	0.19396000
C	-0.62076100	-1.51676700	0.58678900
C	-1.56815600	-0.92603100	-0.40203700
C	-2.45547300	0.04113600	-0.04312600
C	-2.56019400	0.50125700	1.27518900
C	-1.76394400	-0.09254900	2.27532300
C	-0.86772900	-1.06133100	1.97939900
H	-3.26259500	1.28283400	1.50992900
H	-1.88300300	0.23800800	3.29559500
H	-0.25547300	-1.51153400	2.74475000
Cl	3.55241600	-1.25513900	-0.46102000
Cl	-3.48299500	0.70827600	-1.26887800
H	-0.69895300	-2.60237600	0.51622500
O	-1.43152600	-1.41570800	-1.63048300
H	-2.03095700	-0.96680200	-2.23180000
IM65			
0	2		
C	-3.14222400	1.82338100	0.55400900
C	-1.85333600	2.32772400	0.69687400
C	-0.82512300	1.47432100	0.42653700
C	-0.94757600	0.17329900	0.01362500
C	-2.24872900	-0.30525100	-0.12358800
C	-3.33072900	0.51435100	0.14726000
H	-3.99530800	2.45018700	0.76149700
H	-1.67889500	3.34388400	1.01480300
H	-4.32414800	0.11250300	0.03326500
O	0.08428400	-0.65979300	-0.23881700
C	1.35990300	-0.14250100	-0.24910000
C	2.27703200	-0.81873600	0.54356600
C	3.59473500	-0.39699700	0.55508900
C	3.97824200	0.68048600	-0.22255700
C	3.05886100	1.34018500	-1.02211300
C	1.73993200	0.92002000	-1.04163800
H	4.29992800	-0.92456900	1.17704200
H	5.00753000	1.00309400	-0.20706800
H	3.36541400	2.17199800	-1.63555300

H	1.00788800	1.40411100	-1.66887500
Cl	-2.49908000	-1.93203200	-0.62913000
O	1.89882200	-1.86701500	1.29233200
H	0.97116900	-2.04389100	1.12420100
IM66			
0	2		
C	0.04794800	0.32929200	0.98269800
C	1.10369400	-0.48093700	0.31077100
C	2.25753500	0.05688200	-0.15320800
C	2.57332700	1.41346600	0.02916300
C	1.66963500	2.22070000	0.74441400
C	0.49446200	1.73406500	1.21088900
H	3.49856800	1.80440900	-0.35733800
H	1.92819000	3.25294500	0.92530900
H	-0.18610200	2.37021000	1.75551000
C	-3.39466700	-0.80918400	-0.19143500
C	-2.15503600	-0.80268700	0.42793800
C	-1.27325600	0.25879600	0.22687300
C	-1.64396900	1.26993600	-0.64808800
C	-2.87179900	1.25956700	-1.28314700
C	-3.75370000	0.21997500	-1.03977100
H	-0.95668500	2.08588700	-0.81587000
H	-3.14051600	2.05983200	-1.95443000
H	-4.72035800	0.20233700	-1.51930800
O	-1.86611300	-1.83325000	1.25685700
H	-0.94004300	-2.06495400	1.16903600
H	-0.13828400	-0.13882800	1.95929600
Cl	3.38433700	-0.98576000	-0.96396100
H	-4.05539100	-1.63957500	0.00104700
O	0.78795300	-1.78309200	0.21481700
H	1.47712900	-2.26282900	-0.25188200
IM67			
0	1		
C	-0.73859400	0.32969600	-0.03057300
C	-1.47231300	-0.68656800	0.58652100
C	-2.85866600	-0.68707500	0.53342600
C	-3.52224600	0.33095100	-0.12009700
C	-2.81380500	1.35940800	-0.72384800
C	-1.43395800	1.34894700	-0.67520000
H	-3.39219600	-1.48627300	1.02277400
H	-4.60083600	0.32398700	-0.15397300
H	-3.33260200	2.15633500	-1.23231600

H	-0.86558600	2.13468200	-1.15032800
C	2.85865000	-0.68706700	-0.53348000
C	1.47226800	-0.68661700	-0.58643400
C	0.73857300	0.32966200	0.03066200
C	1.43397500	1.34892100	0.67525300
C	2.81380900	1.35940500	0.72378900
C	3.52225100	0.33096500	0.11996100
H	0.86563200	2.13465900	1.15041200
H	3.33265200	2.15634800	1.23218800
H	4.60084200	0.32408700	0.15378000
O	0.87789500	-1.69502600	-1.25301700
H	-0.06669500	-1.54077900	-1.31313400
H	3.39207900	-1.48630900	-1.02287600
O	-0.87784400	-1.69500400	1.25298500
H	0.06663400	-1.54027300	1.31384100

IM68

0 3

C	-0.01124800	0.81182200	0.56044400
C	-1.11944100	-0.18340400	0.61790900
C	-2.28254800	-0.00504100	-0.05968500
C	-2.54005000	1.14121100	-0.82920200
C	-1.55958000	2.14856600	-0.88130300
C	-0.37824000	2.02693300	-0.22899200
H	-3.47794600	1.23741300	-1.34821200
H	-1.76423700	3.04347600	-1.44906200
H	0.35895000	2.81351700	-0.27008800
C	2.42560400	-1.04777900	-1.69304800
C	1.25621000	-0.47557400	-1.19830500
C	1.24555400	0.17287100	0.01123000
C	2.46834000	0.27734800	0.77470600
C	3.65375900	-0.32895200	0.23165900
C	3.62384400	-0.97354900	-0.96964700
H	2.40771400	-1.55383200	-2.64598600
H	0.34135200	-0.54165900	-1.77076900
H	4.51798800	-1.42589600	-1.36981200
O	2.49961200	0.87791600	1.86543000
H	0.23730000	1.10057800	1.58687800
Cl	-3.50115200	-1.23765800	0.06351900
H	4.55459100	-0.24705900	0.81913900
O	-0.84435600	-1.24370100	1.38096300
H	-1.59139200	-1.84677400	1.38235800

IM69

0	2		
C	3.00294900	0.67586300	-0.31044200
C	3.56333800	-0.50008000	0.06882200
C	2.72959100	-1.56172100	0.46232500
C	1.35447700	-1.43207100	0.43920300
C	0.72002200	-0.25894300	0.03984300
C	1.57665600	0.86332400	-0.31279700
H	4.63519500	-0.62080400	0.08377200
H	-4.60880800	-0.61099000	-0.04692000
C	-3.53384600	-0.51529500	-0.05630900
C	-2.73674500	-1.58757200	-0.44169600
C	-2.95398100	0.68112100	0.29036600
C	-1.37183800	-1.43977400	-0.43004000
C	-1.57075500	0.85096900	0.26849100
C	-0.73960800	-0.24190900	-0.05593600
H	-0.75289700	-2.26435300	-0.74855100
H	-3.17901500	-2.52002300	-0.75371800
O	1.12145000	1.98298800	-0.62489600
H	3.16695500	-2.49012200	0.79548400
H	0.74937900	-2.26193200	0.76759300
H	-3.54844800	1.53477700	0.57370000
H	3.59070200	1.53155000	-0.60227600
O	-1.12515600	2.05259500	0.62152500
H	-0.26497600	2.21376800	0.18691200
IM70			
0	3		
C	-3.29582200	-1.57822100	0.44798400
C	-1.99933600	-1.50913000	0.94502700
C	-1.22107000	-0.46084900	0.54221300
C	-1.62037400	0.53557000	-0.31398300
C	-2.92082800	0.44976000	-0.80415100
C	-3.74208200	-0.59558100	-0.42298000
H	-3.94492300	-2.38940800	0.73945000
H	-1.62263300	-2.25866000	1.62483400
H	-4.74661300	-0.64172200	-0.81418700
O	-0.87041400	1.58351400	-0.72175100
C	0.47212000	1.69274800	-0.24591300
C	1.31025900	0.55273000	-0.71874700
C	1.94210500	-0.27636600	0.15553700
C	1.87081200	-0.08918100	1.54131100
C	1.16975900	1.02361500	2.04771900
C	0.53006800	1.88778700	1.22685000
H	2.36695400	-0.78400900	2.19728000

H	1.15222100	1.18185100	3.11507000
H	-0.01096900	2.73505200	1.61773900
Cl	2.85833200	-1.60178200	-0.48447700
H	0.81391300	2.59075600	-0.76346100
H	-3.26324400	1.21622300	-1.48303800
O	1.34930500	0.43243100	-2.04290100
H	1.85884300	-0.34464800	-2.28556700
IM71			
0	2		
C	3.81279700	-0.64565800	0.47893500
C	2.66207700	-1.22649600	1.00476700
C	1.46309800	-0.68844400	0.63679600
C	1.31038900	0.36835500	-0.22365800
C	2.46380300	0.93479000	-0.74830700
C	3.70164700	0.42787100	-0.39032100
H	4.78291900	-1.03309300	0.74878400
H	2.71959100	-2.06380300	1.68371100
H	4.59138300	0.87665900	-0.80341800
O	0.11292300	0.91176800	-0.56686200
C	-1.02864200	0.17932000	-0.34572100
C	-2.06520600	0.86907100	0.26867500
C	-3.27219100	0.22717800	0.47855500
C	-3.43125700	-1.08640900	0.07507300
C	-2.39465300	-1.76612300	-0.54356000
C	-1.18653100	-1.12597100	-0.76185200
H	-4.06937000	0.77084700	0.95976500
H	-4.37497200	-1.58089300	0.24433000
H	-2.52477500	-2.78765500	-0.86277200
H	-0.36807000	-1.62922100	-1.25251700
H	2.37099300	1.76335300	-1.43398400
O	-1.90346900	2.14549900	0.65661200
H	-1.01530900	2.42076100	0.42181100