

Supplementary Information for

**The Homogeneous Gas-phase Formation Mechanism of
PCPT/DT/DFs from Radical/Radical Cross-Condensation
of 2-CPR and 2-CTPR : A Theoretical Mechanistic and
Kinetic Study**

Ying Li^a, Yanan Han^a, Zhuochao Teng^a, Xianwei Zhao^a, Yanhui Sun^b, Fei Xu^{*a},
Qingzhu Zhang^a, Wenxing Wang^a

^aEnvironment Research Institute, Shandong University, Qingdao 266237, P. R. China

^bCollege of Environment and Safety Engineering, Qingdao University of Science &
Technology, Qingdao 266042, P. R. China

Keywords

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*Corresponding author. E-mail: xufei@sdu.edu.cn

Fax: 86-532-58631992

Contains two figures and five tables and ninety six pages:

Figure S1. PCTA/DT formation routes from self-coupling of 2-CTPR embedded with the potential barriers ΔE (in kcal/mol) and reaction heats ΔH (in kcal/mol). ΔH is calculated at 0 K.

Figure S2. Fitted plots of the CVT/SCT rate constants in the temperature range of 600–1200 K for the rate-determining steps in each PCPT/DT/DF formation routes from cross-condensation of 2-CPR and 2-CTPR.

Table S1. The comparison of calculated and experimental structural parameters of phenoxathiin. Distances are in angstrom.

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Table S3. CVT/SCT rate constants for the formation of PCPT/DT/DFs from cross-condensation of 2-CPR and 2-CTPR over the temperature range of 600–1200 K (units are s^{-1} and $\text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for unimolecular and bimolecular reactions, respectively).

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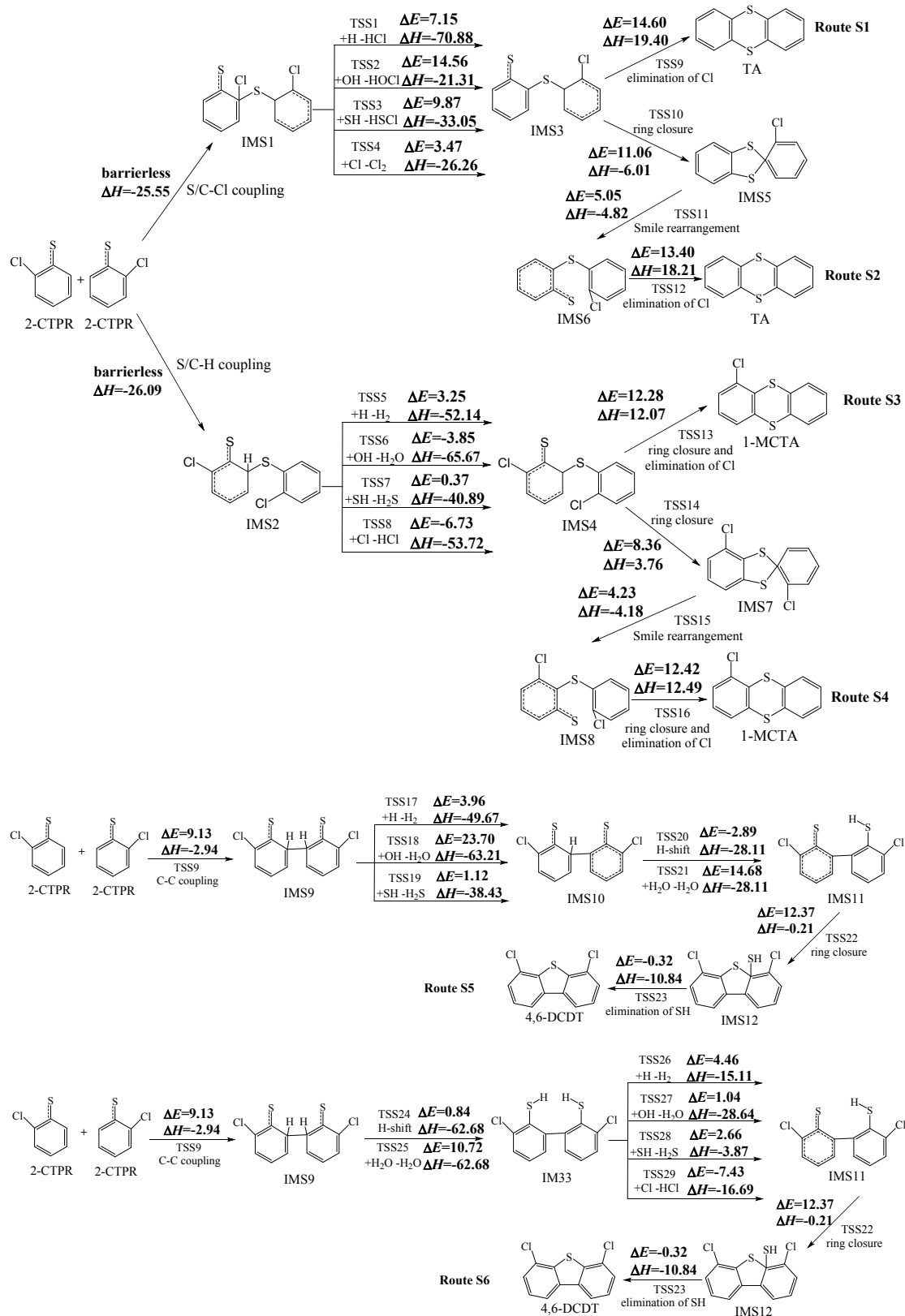


Figure S1.

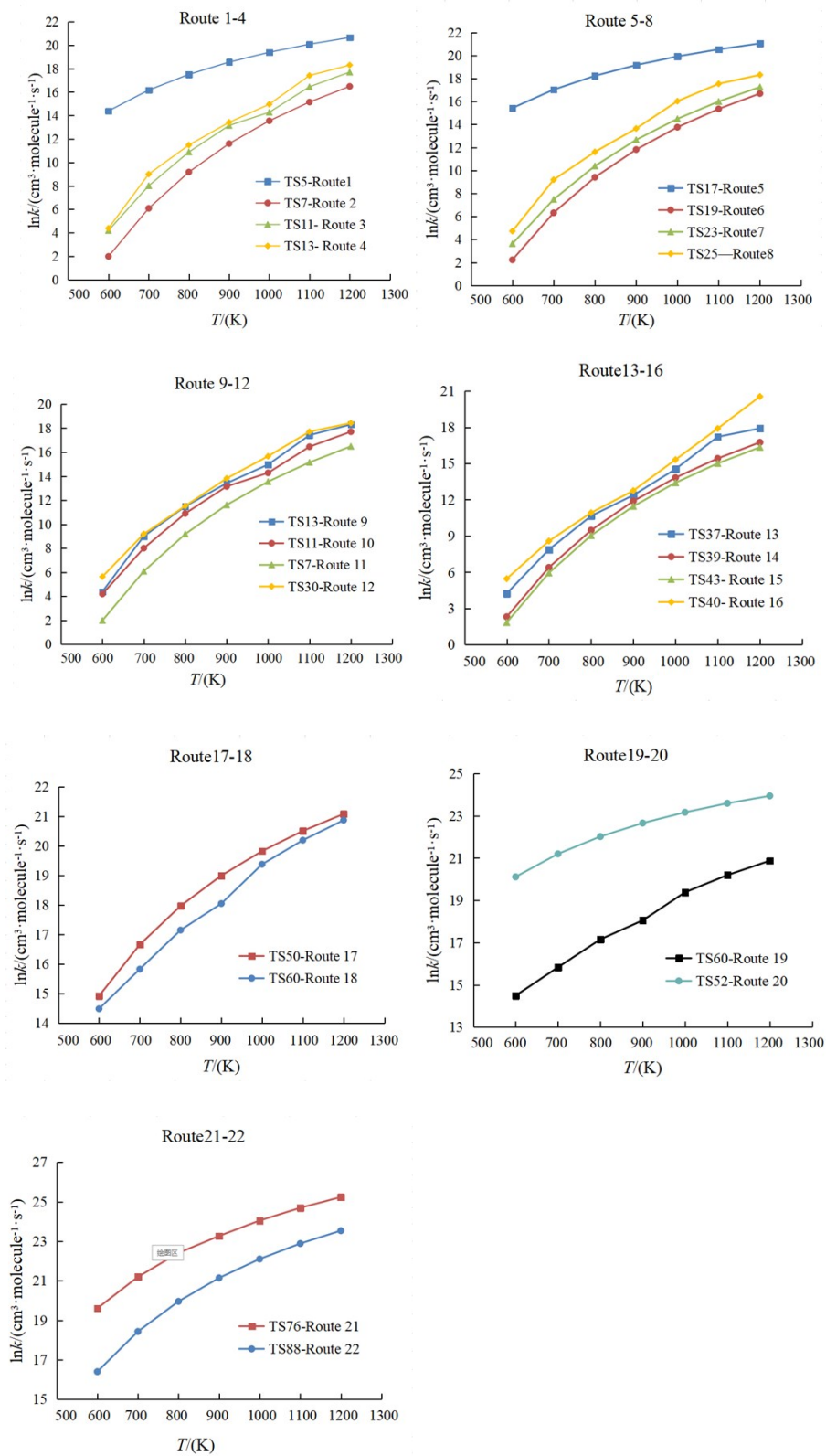


Figure S2.

Table S1. The comparison of calculated and experimental structural parameters of phenoxathiin. Distances are in angstrom.

Parameter	X-ray	MPWB1K	Discrepancy
C-O	1.387(3)	1.359	2.1%
C2-C3	1.384(4)	1.384	0.1%
C3-C4	1.381(4)	1.381	0%
C4-C5	1.388(5)	1.384	0.3%
C6-C7	1.396(4)	1.388	0.6%
C-S	1.762(3)	1.754	0.5%
C3-H	0.92(3)	1.078	16.8%
C4-H	0.93(4)	1.078	15.5%
O-C2-C3	117.2(3)	115.2	1.7%
C2-C3-C4	119.8(3)	120.5	0.6%
C3-C4-C5	120.3(3)	119.8	0.4%
C6-C7-S	119.5(3)	117.7	1.6%
C-S-C	97.7(1)	100.5	2.9%
C-O-C	117.4(2)	123.3	0.5%
C2-C3-H	116(2)	117.9	1.5%
C3-C4-H	118(2)	119.6	1.2%

Table S2. Imaginary frequencies (in cm^{-1}), zero point energies (ZPE, in a.u.) and total energies (in a.u.) for the transition states involved in the formation of PCPT/DF/DTs from cross-condensation of 2-CPR and 2-CTPR.

Transition States	Imaginary Frequencies	ZPE	Total Energies
TS1	-843i	0.17264	-1856.28898
TS2	-597i	0.18210	-1931.47943
TS3	-393i	0.17886	-2254.58840
TS4	-266i	0.17088	-2316.01258
TS5	-408i	0.16951	-1395.52143
TS6	-337i	0.16994	-1395.52980
TS7	-1047i	0.16259	-1395.48306
TS8	-388i	0.16908	-1395.52651
TS9	-636i	0.16781	-1395.50322
TS10	-540i	0.16843	-1395.50695
TS11	-1001i	0.16252	-1395.48646
TS12	-692i	0.16766	-1395.50538
TS13	-763i	0.16788	-1395.50077
TS14	-1571i	0.16964	-1856.27977
TS15	-420i	0.17615	-2254.59880
TS16	-252i	0.16995	-2316.02451
TS17	-408i	0.15985	-1855.21218
TS18	-336i	0.15996	-1855.22033
TS19	-1041i	0.15280	-1855.17340
TS20	-387i	0.15913	-1855.21775
TS21	-595i	0.15801	-1855.19525
TS22	-514i	0.15843	-1855.19767
TS23	-1000i	0.15272	-1855.17674
TS24	-629i	0.15784	-1855.19757
TS25	-693i	0.15803	-1855.19205
TS26	-991i	0.17218	-1856.31051
TS27	-530i	0.18192	-1931.52058
TS28	-432i	0.17875	-2254.60512
TS29	-286i	0.17058	-2316.02884
TS30	-635i	0.16781	-1395.50322
TS31	-388i	0.16909	-1395.52651
TS32	-395i	0.16901	-1395.52576
TS33	-1254i	0.17004	-1856.31850
TS34	-405i	0.17953	-1931.53349
TS35	-1009i	0.17424	-2254.62208
TS36	-169i	0.16952	-2316.04997
TS37	-754i	0.15800	-1855.19067
TS38	-538i	0.15876	-1855.19725

Table S2. *Cont.*

Transition States	Imaginary Frequencies	ZPE	Total Energies
TS39	-1118i	0.15278	-1855.17182
TS40	-660i	0.15798	-1855.19589
TS41	-389i	0.15941	-1855.21580
TS42	-329i	0.16011	-1855.21842
TS43	-1047i	0.15296	-1855.17122
TS44	-380i	0.15937	-1855.21537
TS45	-387i	0.15938	-1855.20732
TS46	-452i	0.17107	-1855.76596
TS47	-893i	0.17023	-1856.28053
TS48	-307i	0.18008	-1931.46762
TS49	-337i	0.17526	-2254.58558
TS50	-1380i	0.15519	-1855.18822
TS51	-1124i	0.18092	-1931.58144
TS52	-527i	0.15611	-1855.19295
TS53	-380i	0.15742	-1855.22769
TS54	-1185i	0.16967	-1856.27855
TS55	-571i	0.17941	-1931.51191
TS56	-1365i	0.17470	-2254.58134
TS57	-1534i	0.15570	-1855.16156
TS58	-1440i	0.18015	-1931.57558
TS59	-398i	0.15957	-1855.22554
TS60	-555i	0.15758	-1855.21168
TS61	-1513i	0.16596	-1855.77091
TS62	-737i	0.19285	-1932.16333
TS63	-1228i	0.19274	-1932.17595
TS64	-950i	0.17006	-1856.36690
TS65	-1016i	0.17469	-2254.67218
TS66	-924i	0.16849	-2316.09746
TS67	-2212i	0.16730	-1856.35490
TS68	-1769i	0.17707	-1931.59292
TS69	-2038i	0.17213	-2254.65566
TS70	-925i	0.16663	-2316.09065
TS71	-172i	0.17045	-1855.75589
TS72	-817i	0.17234	-1856.26943
TS73	-635i	0.18305	-1931.48411
TS74	-511i	0.17915	-2254.06268
TS75	-419i	0.17075	-2315.98745
TS76	-2211i	0.16359	-1395.50419
TS77	-972i	0.19074	-1471.89514

Table S2. Cont.

Transition States	Imaginary Frequencies	ZPE	Total Energies
TS78	-525i	0.16615	-1395.50497
TS79	-281i	0.16671	-1395.53582
TS80	-296i	0.17045	-1855.76103
TS81	-932i	0.17267	-1856.26815
TS82	-652i	0.18290	-1931.47759
TS83	-526i	0.17939	-2254.56271
TS84	-440i	0.17081	-2315.98340
TS85	-1897i	0.16487	-1395.48351
TS86	-1413i	0.18979	-1471.88517
TS87	-380i	0.16929	-1395.53466
TS88	-558i	0.16741	-1395.51991

Table S3. CVT/SCT rate constants for the formation of PCPT/DT/DFs from cross-condensation of 2-CPR and 2-CTPR over the temperature range of 600–1200 K (units are s^{-1} and $cm^3 \text{ molecule}^{-1} s^{-1}$ for unimolecular and bimolecular reactions, respectively).

T(K)	CVT/SCT Rate Constants			
	TS1	TS3	TS5	TS6
600	6.04×10^{-14}	7.71×10^{-14}	1.77×10^6	2.45×10^8
700	1.12×10^{-13}	1.76×10^{-13}	1.05×10^7	7.62×10^8
800	1.85×10^{-13}	3.43×10^{-13}	4.01×10^7	1.79×10^9
900	2.78×10^{-13}	5.96×10^{-13}	1.14×10^8	3.47×10^9
1000	3.94×10^{-13}	9.52×10^{-13}	2.64×10^8	5.91×10^9
1100	5.31×10^{-13}	8.07×10^{-13}	5.25×10^8	9.15×10^9
1200	6.90×10^{-13}	1.16×10^{-12}	9.31×10^8	1.24×10^{10}
	TS7	TS8	TS9	TS10
600	7.23×10^0	2.74×10^7	2.63×10^3	2.07×10^0
700	4.37×10^2	1.15×10^8	6.19×10^4	7.19×10^1
800	9.65×10^3	3.40×10^8	6.67×10^5	1.03×10^3
900	1.09×10^5	7.93×10^8	1.28×10^7	8.16×10^3
1000	7.62×10^5	1.57×10^8	5.54×10^7	4.28×10^4
1100	3.78×10^6	2.74×10^9	1.84×10^8	1.66×10^5
1200	1.44×10^7	4.36×10^9	4.99×10^8	1.72×10^6
	TS11	TS12	TS13	TS14
600	6.58×10^1	1.61×10^7	7.96×10^1	1.46×10^{-8}
700	2.99×10^3	1.21×10^8	8.07×10^3	1.99×10^{-8}
800	5.34×10^4	5.49×10^8	9.66×10^4	2.66×10^{-8}
900	5.10×10^5	1.79×10^9	6.68×10^5	3.45×10^{-8}
1000	1.58×10^6	4.62×10^9	3.14×10^6	4.33×10^{-8}
1100	1.39×10^7	1.00×10^{10}	3.64×10^7	5.29×10^{-8}
1200	4.86×10^7	1.92×10^{10}	8.86×10^7	6.32×10^{-8}
	TS17	TS18	TS19	TS20
600	5.00×10^6	8.92×10^8	9.23×10^0	3.76×10^8
700	2.48×10^7	2.40×10^9	5.52×10^2	1.27×10^9
800	8.24×10^7	5.04×10^9	1.21×10^4	3.20×10^9
900	2.10×10^8	9.01×10^9	1.35×10^5	6.59×10^9
1000	4.46×10^8	1.24×10^{10}	9.43×10^5	1.27×10^{10}
1100	8.25×10^8	1.82×10^{10}	4.65×10^6	1.89×10^{10}
1200	1.38×10^9	2.49×10^{10}	1.77×10^7	2.81×10^{10}

Table S3. Cont.

T(K)	CVT/SCT Rate Constants			
	TS21	TS22	TS23	TS24
600	2.32×10^4	2.43×10^3	3.76×10^1	4.98×10^7
700	4.64×10^5	3.41×10^4	1.77×10^3	3.64×10^8
800	4.39×10^6	2.47×10^5	3.24×10^4	1.62×10^9
900	2.55×10^7	1.15×10^6	3.15×10^5	5.20×10^9
1000	1.05×10^8	3.94×10^6	1.96×10^6	1.31×10^{10}
1100	3.36×10^8	1.08×10^7	8.83×10^6	2.80×10^{10}
1200	8.83×10^8	2.49×10^7	3.11×10^7	5.26×10^{10}
	TS25	TS26	TS27	TS28
600	1.12×10^2	6.85×10^{-14}	6.93×10^{-18}	3.08×10^{-16}
700	9.78×10^3	1.83×10^{-13}	5.12×10^{-17}	1.31×10^{-15}
800	1.10×10^5	3.94×10^{-13}	2.40×10^{-16}	4.03×10^{-15}
900	8.42×10^5	7.35×10^{-13}	8.22×10^{-16}	1.00×10^{-14}
1000	9.09×10^6	1.23×10^{-12}	2.26×10^{-15}	2.14×10^{-14}
1100	4.12×10^7	1.91×10^{-12}	5.30×10^{-15}	4.07×10^{-14}
1200	8.96×10^7	2.78×10^{-12}	1.10×10^{-14}	7.09×10^{-14}
	TS29	TS30	TS31	TS32
600	6.98×10^{-13}	2.77×10^2	2.19×10^9	3.20×10^{11}
700	1.43×10^{-12}	9.76×10^3	4.99×10^9	5.07×10^{11}
800	2.53×10^{-12}	1.00×10^5	9.09×10^9	7.16×10^{11}
900	4.01×10^{-12}	9.98×10^5	1.43×10^{10}	9.37×10^{11}
1000	5.90×10^{-12}	6.30×10^6	2.02×10^{10}	1.16×10^{12}
1100	8.14×10^{-12}	4.85×10^7	2.67×10^{10}	1.38×10^{12}
1200	1.10×10^{-11}	1.00×10^8	3.34×10^{10}	1.60×10^{12}
	TS33	TS34	TS37	TS38
600	1.10×10^{-12}	5.68×10^{-16}	6.90×10^1	8.89×10^0
700	1.35×10^{-12}	7.93×10^{-16}	2.62×10^3	3.34×10^2
800	1.87×10^{-12}	1.08×10^{-15}	4.23×10^4	7.59×10^3
900	2.49×10^{-12}	1.45×10^{-15}	2.36×10^5	6.83×10^4
1000	3.20×10^{-12}	1.91×10^{-15}	2.05×10^6	3.50×10^5
1100	4.01×10^{-12}	2.47×10^{-15}	2.97×10^7	1.40×10^6
1200	4.92×10^{-12}	3.14×10^{-15}	5.98×10^7	4.47×10^6

Table S3. Cont.

T(K)	CVT/SCT Rate Constants			
	TS39	TS40	TS41	TS42
600	1.00×10^1	2.34×10^2	6.20×10^{11}	4.06×10^8
700	5.96×10^2	5.30×10^3	9.31×10^{11}	1.21×10^9
800	1.30×10^4	5.52×10^4	1.26×10^{12}	2.77×10^9
900	1.45×10^5	3.43×10^5	1.60×10^{12}	4.61×10^9
1000	1.01×10^6	4.48×10^6	1.93×10^{12}	7.69×10^9
1100	4.96×10^6	5.90×10^7	2.25×10^{12}	1.17×10^{10}
1200	1.88×10^7	8.33×10^8	2.56×10^{12}	1.66×10^{10}
	TS43	TS44	TS45	TS47
600	6.26×10^0	4.21×10^{11}	5.46×10^5	1.88×10^{-14}
700	3.79×10^2	6.51×10^{11}	3.32×10^6	3.42×10^{-14}
800	8.39×10^3	9.03×10^{11}	1.29×10^7	5.54×10^{-14}
900	9.45×10^4	1.16×10^{12}	3.72×10^7	8.28×10^{-14}
1000	6.63×10^5	1.43×10^{12}	8.72×10^7	1.17×10^{-13}
1100	3.29×10^6	1.68×10^{12}	1.75×10^8	1.58×10^{-13}
1200	1.25×10^7	1.93×10^{12}	3.14×10^8	2.05×10^{-13}
	TS48	TS49	TS50	TS52
600	1.10×10^{-23}	3.90×10^{-18}	3.03×10^6	5.42×10^8
700	2.76×10^{-22}	5.85×10^{-18}	1.72×10^7	1.61×10^9
800	3.24×10^{-21}	8.39×10^{-18}	6.37×10^7	3.65×10^9
900	2.28×10^{-20}	1.16×10^{-17}	1.78×10^8	6.91×10^9
1000	1.11×10^{-19}	1.56×10^{-17}	4.08×10^8	1.15×10^{10}
1100	4.19×10^{-19}	2.05×10^{-17}	8.07×10^8	1.76×10^{10}
1200	1.29×10^{-18}	2.64×10^{-17}	1.43×10^9	2.50×10^{10}
	TS53	TS54	TS56	TS57
600	1.63×10^{12}	7.78×10^{-14}	2.33×10^{-15}	1.49×10^3
700	1.82×10^{12}	1.65×10^{-13}	5.01×10^{-15}	1.02×10^5
800	1.98×10^{12}	2.99×10^{-13}	9.41×10^{-15}	6.13×10^5
900	2.11×10^{12}	4.89×10^{-13}	1.60×10^{-14}	2.49×10^6
1000	2.22×10^{12}	7.42×10^{-13}	2.54×10^{-14}	7.67×10^6
1100	2.31×10^{12}	1.04×10^{-12}	3.81×10^{-14}	1.93×10^7
1200	2.39×10^{12}	1.38×10^{-12}	5.47×10^{-14}	4.16×10^7

Table S3. Cont.

T(K)	CVT/SCT Rate Constants			
	TS59	TS60	TS61	TS64
600	9.63×10^7	1.96×10^6	5.62×10^7	1.89×10^{-13}
700	3.76×10^8	0.75×10^7	2.37×10^8	3.49×10^{-13}
800	1.05×10^9	2.81×10^7	7.03×10^8	5.78×10^{-13}
900	2.35×10^9	0.69×10^8	1.65×10^9	8.32×10^{-12}
1000	4.48×10^9	2.61×10^8	3.28×10^9	1.21×10^{-12}
1100	7.62×10^9	5.89×10^8	5.79×10^9	1.67×10^{-12}
1200	1.19×10^{10}	1.16×10^9	9.34×10^9	2.22×10^{-12}
	TS65	TS67	TS68	TS72
600	7.18×10^{-14}	5.48×10^{-16}	3.63×10^{-14}	2.65×10^{-16}
700	1.13×10^{-13}	2.37×10^{-15}	5.93×10^{-14}	3.34×10^{-16}
800	1.67×10^{-13}	7.47×10^{-15}	9.00×10^{-14}	3.97×10^{-16}
900	2.34×10^{-13}	1.89×10^{-14}	1.29×10^{-13}	4.56×10^{-16}
1000	3.18×10^{-13}	4.11×10^{-14}	1.78×10^{-13}	5.12×10^{-16}
1100	4.18×10^{-13}	7.93×10^{-14}	2.37×10^{-13}	5.66×10^{-16}
1200	5.37×10^{-13}	1.40×10^{-13}	3.09×10^{-13}	6.19×10^{-16}
	TS73	TS74	TS75	TS76
600	7.27×10^{-17}	2.31×10^{-15}	8.34×10^{-13}	3.26×10^8
700	2.60×10^{-16}	5.02×10^{-15}	1.27×10^{-12}	1.60×10^9
800	7.06×10^{-16}	9.38×10^{-15}	1.80×10^{-12}	5.38×10^9
900	5.98×10^{-16}	1.58×10^{-14}	2.41×10^{-12}	1.27×10^{10}
1000	1.14×10^{-15}	2.46×10^{-14}	3.10×10^{-12}	2.77×10^{10}
1100	1.96×10^{-15}	3.62×10^{-14}	3.86×10^{-12}	5.27×10^{10}
1200	3.15×10^{-15}	5.09×10^{-14}	4.69×10^{-12}	9.06×10^{10}
	TS78	TS79	TS81	TS82
600	3.44×10^9	6.58×10^{10}	1.63×10^{-13}	2.91×10^{-18}
700	8.12×10^9	8.65×10^{10}	3.31×10^{-13}	9.68×10^{-18}
800	1.47×10^{10}	1.06×10^{11}	5.79×10^{-13}	3.86×10^{-17}
900	2.44×10^{10}	1.24×10^{11}	9.15×10^{-13}	1.17×10^{-16}
1000	3.67×10^{10}	1.40×10^{11}	1.34×10^{-12}	2.92×10^{-16}
1100	5.12×10^{10}	1.54×10^{11}	1.86×10^{-12}	6.30×10^{-16}
1200	6.77×10^{10}	1.67×10^{11}	2.48×10^{-12}	1.22×10^{-15}

Table S3. Cont.

T(K)	CVT/SCT Rate Constants			
	TS83	TS84	TS85	TS87
600	2.16×10^{-16}	9.58×10^{-14}	1.67×10^8	2.35×10^7
700	7.17×10^{-16}	2.06×10^{-13}	6.75×10^9	1.05×10^8
800	1.84×10^{-15}	3.78×10^{-13}	1.94×10^9	3.24×10^8
900	3.96×10^{-15}	6.19×10^{-13}	4.45×10^9	7.82×10^8
1000	7.50×10^{-15}	9.35×10^{-13}	8.67×10^9	1.59×10^9
1100	1.29×10^{-14}	1.33×10^{-12}	1.50×10^{10}	2.85×10^9
1200	2.07×10^{-14}	1.81×10^{-12}	2.39×10^{10}	4.63×10^9
	TS88			
600	1.32×10^7			
700	1.01×10^8			
800	4.63×10^8			
900	1.52×10^9			
1000	3.96×10^9			
1100	8.65×10^9			
1200	1.66×10^{10}			

Table S4. Cartesian coordinates for the transition states involved in the formation of PCPT/DT/DFs from cross-condensation of 2-CPR and 2-CTPR.

TS1			
C	1.24766800	0.30313400	-0.62941800
C	1.94475800	-0.86570500	-0.36453500
C	3.25283300	-0.80627900	0.07763500
C	3.86329500	0.42330600	0.24184600
C	3.17212300	1.58855900	-0.04652000
C	1.86628700	1.52994300	-0.49237400
Cl	1.15861300	-2.38302900	-0.56381700
H	3.77961700	-1.72255200	0.28905600
H	1.30961900	2.42165900	-0.72592000
C	-1.17363000	0.34210900	-0.47369800
C	-2.25731800	0.01139800	-1.41515900
C	-3.31781100	-0.70788600	-1.04450200
C	-3.41349600	-1.22747800	0.29102900
C	-2.44349800	-1.01543600	1.20179500
C	-1.26913600	-0.24392500	0.91581700
Cl	-1.48828900	2.23830400	-0.15549900
H	-2.12682800	0.39164400	-2.41517700
H	-2.51560300	-1.41736200	2.19936300
H	-1.39064000	4.20804400	0.10189700
H	-4.28060200	-1.80953400	0.56308200
H	3.65229500	2.54707200	0.07071700
S	-0.14853300	0.03901500	2.06698200
H	-4.10218600	-0.92088400	-1.75305400
H	4.88388200	0.46741100	0.58773000
O	-0.00762400	0.21002000	-1.16656500
TS2			
C	1.41993800	-0.14168500	-0.17108300
C	1.54219300	-1.52039500	-0.19962300
C	2.79861400	-2.10330300	-0.18519700
C	3.93456400	-1.31897000	-0.13708000
C	3.81294500	0.05945100	-0.10438100
C	2.56472300	0.64728900	-0.12216300
H	2.87923000	-3.17857200	-0.20625000
C	-0.91658000	-0.18654200	-0.32530200
C	-1.17002600	-0.74673300	-1.62780200
C	-2.05257300	-1.76269800	-1.77812900
C	-2.68003400	-2.34498000	-0.64522500

C	-2.37384600	-1.93870700	0.61563600
C	-1.40989200	-0.91864700	0.85742800
Cl	-2.27826900	1.36716100	-0.39292300
H	-0.67561500	-0.27909700	-2.46428900
H	-2.81594000	-2.41187500	1.47730700
O	-3.12664000	3.24679800	-0.06679400
H	-2.38473600	3.64972700	0.39912200
H	-3.39317600	-3.14128400	-0.79095900
H	4.68449400	0.69273900	-0.06589800
H	4.91311200	-1.77113200	-0.12262200
H	-2.27609800	-2.13954300	-2.76347800
O	0.23640700	0.52487700	-0.18796600
S	-0.85353000	-0.57111600	2.36920100
Cl	2.41729600	2.35896400	-0.08762300
H	0.66345600	-2.14512200	-0.22525700

TS3

C	1.30697300	0.43460100	-0.54509900
C	2.52072000	-0.21503100	-0.39259400
C	3.62449700	0.48270300	0.05609600
C	3.51189900	1.83236300	0.33830200
C	2.30281400	2.48140200	0.15898100
C	1.19723700	1.78753700	-0.29713000
Cl	2.62673200	-1.90029800	-0.71986500
H	4.55988700	-0.03749400	0.18345100
H	0.25245400	2.28250000	-0.44868100
C	-0.81782600	-0.74563100	-0.49488800
C	-1.67505400	-1.39369700	-1.47405100
C	-2.55098100	-2.34518500	-1.11719100
C	-2.64478600	-2.76756200	0.24414200
C	-1.81817600	-2.26511100	1.18565700
C	-0.79400000	-1.30676300	0.88555600
Cl	-2.03846600	0.90840400	-0.03182600
H	-1.56844800	-1.04671400	-2.48855800
H	-1.86521800	-2.60207100	2.20827400
H	-2.96328200	3.35953000	-1.25581100
H	-3.37717100	-3.51131100	0.51625600
H	2.21526500	3.53616200	0.36552000
S	0.29615600	-0.87217500	2.02917400
S	-2.51756400	3.46851800	-0.00045900
H	-3.18793500	-2.79644400	-1.86096600
H	4.37458800	2.37516800	0.69081200
O	0.26524800	-0.26454700	-1.10970800

TS4

C	1.32884000	0.30573100	-0.59522700
C	2.47848700	-0.42650900	-0.35054600
C	3.61452800	0.21226200	0.10828300
C	3.59648600	1.58120600	0.30295200
C	2.45177200	2.30978400	0.02707600
C	1.31389900	1.67586100	-0.43467900
Cl	2.47059900	-2.13211000	-0.57968700
H	4.50011500	-0.36828700	0.30953800
H	0.41562200	2.23080600	-0.64945300
C	-0.86917100	-0.70576100	-0.50965200
C	-1.75932900	-1.38139500	-1.43531500
C	-2.67180300	-2.27408900	-1.00743800
C	-2.76291200	-2.60730700	0.37426300
C	-1.91707000	-2.06263800	1.28025400
C	-0.89420900	-1.13007800	0.92208700
Cl	-2.04356500	1.02516600	-0.33175800
H	-1.64466200	-1.11310500	-2.47247000
H	-1.97319800	-2.32668700	2.32359700
Cl	-2.12812300	3.50399500	0.01310100
H	-3.51089300	-3.31362800	0.69836500
H	2.43976900	3.37875400	0.16721000
S	0.13114100	-0.54623800	2.06104900
H	-3.33186500	-2.74722500	-1.71646900
H	4.48344500	2.07767800	0.66335600
O	0.24810200	-0.35134600	-1.14012000

TS5

C	-1.06794200	0.93521800	0.12707800
C	-1.28523400	-0.44902800	0.41683600
C	-2.60667300	-0.95192300	0.23371100
C	-3.58147300	-0.17334600	-0.31616600
C	-3.32966500	1.17178000	-0.61816100
C	-2.08171200	1.71486400	-0.38940900
Cl	-0.41136700	-1.13328700	1.76601000
H	-2.79487600	-1.97249300	0.52421500
H	-1.85702300	2.74209600	-0.62636000
C	1.29257100	0.82461400	0.06641100
C	2.44188600	1.39464800	0.58010600
C	3.66751600	0.80903200	0.33701500
C	3.73747100	-0.35833900	-0.40709300
C	2.58185600	-0.93297000	-0.89605100

C	1.33591900	-0.34709200	-0.68340900
H	2.34990900	2.29747900	1.16257500
H	2.62775400	-1.85516600	-1.45425200
H	4.68902500	-0.83064900	-0.59338400
H	-4.11267700	1.78734500	-1.03079000
S	-0.09966500	-1.09016000	-1.34194700
O	0.13233700	1.50536200	0.31364200
H	-4.56342900	-0.58737600	-0.48138500
H	4.56339300	1.25957100	0.73401900

TS6

C	-0.91815100	0.18044300	-0.36415400
C	-2.18073600	0.59035800	0.01879800
C	-3.24438800	-0.29285500	-0.02983600
C	-3.05418100	-1.60106700	-0.48913600
C	-1.81970300	-2.02231500	-0.89080900
C	-0.68422900	-1.16878400	-0.76584300
Cl	-2.41965500	2.20097900	0.56821500
H	-4.21813900	0.04486300	0.28440500
H	0.13919200	-1.32706600	-1.44943900
C	1.38615400	0.63147700	-0.21646100
C	2.34177100	1.52399600	-0.66678400
C	3.68169900	1.22224100	-0.53162300
C	4.06243700	0.01926400	0.04292500
C	3.10192200	-0.87490900	0.47188900
C	1.74435000	-0.58367500	0.36481400
H	2.01005700	2.45207600	-1.10450100
H	3.39201100	-1.82072000	0.90252400
H	5.10702900	-0.22895700	0.14553100
H	-1.67086700	-3.01760900	-1.27713200
S	0.53943500	-1.71072300	0.93903300
H	-3.90135300	-2.26560300	-0.54920600
H	4.42510800	1.92285200	-0.87744200
O	0.08980700	1.05625600	-0.30269900

TS7

C	-0.94056400	0.07110500	0.16590800
C	-2.20926100	0.57617500	-0.03902100
C	-3.25537700	-0.26853300	-0.37576400
C	-3.03073000	-1.62969500	-0.50541600
C	-1.76843400	-2.14818300	-0.32350700
C	-0.68951800	-1.29306100	-0.05983000
Cl	-2.49697100	2.25991000	0.15677400

H	-4.23761700	0.14956100	-0.52172500
H	-0.07696700	-1.06043600	-1.72138200
C	1.33594300	0.65946700	0.18114200
C	2.13061600	1.75030500	-0.10758400
C	3.46666400	1.55841500	-0.40614400
C	3.99687900	0.27909300	-0.43336600
C	3.18879800	-0.81041300	-0.16257200
C	1.85477100	-0.62533500	0.16361400
H	1.68717900	2.73266000	-0.08466200
H	3.58860300	-1.81204400	-0.19756000
H	5.03665100	0.12560100	-0.67478500
H	-1.58289700	-3.20597000	-0.42027400
S	0.81173600	-1.97027000	0.59110900
H	4.09164400	2.40979700	-0.62459900
H	-3.85293100	-2.28551300	-0.74271100
O	0.04104300	0.91702000	0.53500400

TS8

C	0.78430400	0.12970200	-0.35520700
C	0.90011300	1.48346800	-0.83128600
C	2.08764300	2.15271800	-0.75731100
C	3.23770900	1.49530100	-0.31754900
C	3.19620700	0.13950800	0.00493600
C	2.01952600	-0.55329200	-0.07265100
H	2.13856400	3.18770100	-1.05561100
C	-1.62963200	0.27126600	0.67774400
C	-2.91081900	0.58058500	1.10332500
C	-3.99487700	0.27629500	0.29346800
C	-3.80645700	-0.32245200	-0.94015300
C	-2.52717900	-0.62454900	-1.38425700
C	-1.46361900	-0.32532100	-0.56630100
H	-3.05945200	1.04677100	2.06437200
H	4.09382900	-0.38206600	0.29510800
H	-4.99143600	0.51409600	0.63099300
H	-2.35110300	-1.08820000	-2.34149700
H	-0.00335400	1.95605000	-1.18486300
Cl	1.95250100	-2.22144800	0.27680100
S	-0.14840800	0.50426300	1.55882200
H	4.17523500	2.02422700	-0.25729700
H	-4.65431000	-0.55143300	-1.56617600
O	-0.19043300	-0.65376400	-0.92004400

TS9

C	0.86624300	-0.08010700	-0.44005500
C	2.08787400	0.35047100	0.15985400
C	3.12057600	-0.53144300	0.36217600
C	3.02065800	-1.84279000	-0.08382600
C	1.87722900	-2.27602800	-0.75248500
C	0.84362400	-1.40693200	-0.96258800
H	4.01123800	-0.18948200	0.86350500
C	-1.43149000	-0.29572100	0.69933200
C	-2.49827900	-0.87064300	1.37829500
C	-3.78955300	-0.66630000	0.91744000
C	-4.02773200	0.06588700	-0.23217100
C	-2.96304400	0.61414100	-0.93643900
C	-1.68192100	0.44188100	-0.46063100
H	-2.30172100	-1.44719000	2.26771600
H	1.81343000	-3.28834300	-1.11832300
H	-5.03418300	0.19744600	-0.59616800
H	3.84275100	-2.52095800	0.08195200
H	-4.61559100	-1.10377500	1.45671900
S	-0.22735800	1.11853300	-1.17899100
O	-0.18519400	-0.40671100	1.12200800
H	-3.13463900	1.16635400	-1.84761600
H	-0.04630000	-1.71408100	-1.49017400
Cl	2.23760000	1.95545200	0.72804600

TS10

C	1.01737500	-0.09296800	-0.35156900
C	2.34646600	-0.22219700	0.02661900
C	3.17633800	0.87991400	0.08664400
C	2.69287700	2.14953100	-0.24296900
C	1.39876200	2.30366300	-0.65523300
C	0.52809900	1.19480100	-0.69186000
Cl	2.97292800	-1.77069000	0.44940900
H	4.19892100	0.74684900	0.40084500
H	-0.34631400	1.25319300	-1.32053400
C	-1.62312700	-0.62054900	-0.13757500
C	-2.75930500	-1.29169700	-0.55473500
C	-4.01705200	-0.76140700	-0.31532300
C	-4.13170200	0.46422500	0.31656500
C	-3.00080000	1.16966900	0.68644900
C	-1.72997500	0.63589900	0.48367600
H	-2.65875900	-2.24095400	-1.05928800
H	-3.07078600	2.13885900	1.15427800
H	-5.10602200	0.89117700	0.49811900

H	1.02060400	3.26842300	-0.95161500
H	3.35798300	2.99661600	-0.19104600
H	-4.89567300	-1.29976800	-0.63283000
O	-0.66193500	1.31796900	0.85540000
S	-0.07074900	-1.44060800	-0.26782600
TS11			
C	0.99283300	-0.05038700	0.16173800
C	2.33944000	-0.20434400	-0.11888500
C	3.16325000	0.88729900	-0.33927500
C	2.63784900	2.16804800	-0.26369100
C	1.30194700	2.35856100	0.00088000
C	0.45821200	1.25199700	0.12927400
Cl	3.02184300	-1.78717200	-0.14491100
H	4.20818800	0.72470700	-0.54451000
H	-0.06320400	1.14490400	-1.58197000
C	-1.59674400	-0.68813700	0.11818800
C	-2.66007400	-1.49469000	-0.25763600
C	-3.90990100	-0.94280400	-0.47367200
C	-4.09833600	0.42216100	-0.33575800
C	-3.03681000	1.23631600	0.01389500
C	-1.79752500	0.67580600	0.24635000
H	-2.50375900	-2.55621100	-0.37398200
H	-3.14868900	2.30357300	0.11775800
H	-5.07000500	0.85669000	-0.50964500
H	0.86482200	3.34012500	0.07920200
H	-4.73243100	-1.58028100	-0.75653000
H	3.28569000	3.01863400	-0.40213200
O	-0.78601100	1.50324800	0.63218600
S	-0.04304400	-1.41344800	0.50558500
TS12			
C	-1.09591600	-0.58672900	0.21900500
C	-1.50133500	0.78390800	0.28564400
C	-2.71440700	1.19513100	-0.22164000
C	-3.61475400	0.26060900	-0.69946000
C	-3.30143800	-1.10287200	-0.66657600
C	-2.09227600	-1.52055000	-0.19629700
Cl	-0.41976200	1.94362200	0.91909400
H	-2.95686700	2.24527500	-0.21791700
C	1.20674000	-0.23362400	-0.87899500
C	2.19172900	0.33302200	-1.68094200
C	3.48628400	0.43226500	-1.19961100

C	3.79988100	0.02405100	0.08594800
C	2.81005400	-0.49193900	0.91261200
C	1.52986300	-0.62194300	0.42409400
H	1.93259100	0.65292000	-2.67717300
H	-4.02200700	-1.82803100	-1.01031900
H	-1.83044500	-2.56567000	-0.17276200
H	3.03743500	-0.77395900	1.92908600
H	4.80625000	0.12798600	0.45926500
S	0.15021100	-1.22741300	1.32497400
H	-4.56794000	0.58786700	-1.08334900
H	4.25382700	0.84973100	-1.83281300
O	-0.01835100	-0.44088300	-1.31511300
TS13			
C	1.24825300	0.85286900	-0.06722000
C	1.33691300	-0.53538600	-0.34642500
C	2.47277000	-1.24277900	0.12585200
C	3.44141600	-0.59596400	0.82882400
C	3.35806500	0.78457800	1.07984800
C	2.26510100	1.48834100	0.64594500
Cl	0.63835500	-1.14265400	-1.82041700
H	2.54276200	-2.29373000	-0.09959300
H	2.15848100	2.53786100	0.87331600
C	-1.43878000	0.60785400	-0.12665100
C	-2.73769300	1.02508700	-0.41711500
C	-3.82484600	0.34645600	0.07545600
C	-3.62086500	-0.76078800	0.89967500
C	-2.35300500	-1.19112900	1.19058600
C	-1.22040100	-0.57190100	0.62330700
H	-2.87896400	1.91311400	-1.01550700
H	-2.17811200	-2.06120800	1.80257700
H	-4.46663400	-1.29186900	1.30875200
H	4.13805100	1.28248800	1.63261900
H	4.29797600	-1.15076700	1.17912200
H	-4.82247100	0.68461700	-0.15355300
O	-0.07018900	-1.14533100	0.79560000
S	-0.16519900	1.73273900	-0.50112200
TS14			
C	1.67023200	0.13821900	0.02583300
C	2.97487000	-0.29267600	-0.18833500
C	4.05221600	0.50143300	0.15420300
C	3.84065900	1.74058600	0.72924000

C	2.54818300	2.18209700	0.94233800
C	1.46953500	1.39412000	0.58235000
Cl	3.27367900	-1.83318600	-0.90334400
H	5.04960600	0.13535200	-0.02770600
H	0.46863700	1.77412600	0.69677400
C	-0.61072400	-0.67963000	0.40294200
C	-1.02965600	-2.03393600	0.76812000
C	-2.32328600	-2.35224900	0.86619400
C	-3.33821500	-1.39043000	0.54765800
C	-3.03045800	-0.16123900	0.08996500
C	-1.65255900	0.25275900	-0.14843300
H	-4.37557900	-1.66549000	0.65632300
H	-0.29227900	-0.18406100	1.44051800
Cl	-4.27878900	0.93132800	-0.33902500
H	2.36845000	3.15339100	1.37511200
H	-0.24829800	-2.73672700	1.00912400
H	0.06917000	0.28533200	2.45668900
H	-2.62598400	-3.33622100	1.18654600
H	4.68333700	2.35614000	1.00110800
O	0.63610100	-0.77849800	-0.37739400
S	-1.28273600	1.62396200	-0.89297000

TS15

C	-1.69391100	-0.05132100	-0.03194700
C	-3.02555400	0.30935700	-0.21919200
C	-4.02677100	-0.63613700	-0.12562300
C	-3.71359300	-1.95301100	0.16090800
C	-2.39272700	-2.31432000	0.34665400
C	-1.38437400	-1.37214700	0.24397800
Cl	-3.42415600	1.94775800	-0.56319500
H	-5.04861900	-0.32770300	-0.27640300
H	-0.35841900	-1.68103600	0.35626400
C	0.52806500	0.80949500	0.21209200
C	1.06329700	2.05738700	0.76038000
C	2.38816500	2.17905300	0.91773200
C	3.26118800	1.15315600	0.43452600
C	2.80849900	0.15317300	-0.35765300
C	1.41596500	0.08759700	-0.75046100
H	4.31646900	1.21113200	0.64936700
H	0.64206600	0.09807100	1.17144900
Cl	3.91831500	-0.96042700	-1.03674600
H	-0.24748900	-1.05665600	2.93545200
H	-2.13184400	-3.33917000	0.55826100

H	0.35060100	2.77667400	1.12986000
S	0.86035500	-0.68332400	-2.06659800
S	1.06127200	-0.87878300	2.72016300
H	-4.49915300	-2.68802500	0.23149500
H	2.81364300	3.03649000	1.41286300
O	-0.79418700	0.95570200	-0.12187800
TS16			
C	-1.57079300	0.08731800	0.14445700
C	-2.87194300	-0.18737500	0.58835200
C	-3.91187300	0.63375100	0.22951100
C	-3.68055000	1.74309600	-0.57921600
C	-2.40466400	2.02481100	-1.01561900
C	-1.34571500	1.21051600	-0.65309600
Cl	-3.15588800	-1.56726800	1.56887200
H	-4.90535200	0.40149600	0.57695200
H	-0.34723700	1.47543000	-0.94975200
C	0.63875800	-0.76419500	-0.02172600
C	1.15382900	-2.13481800	-0.14618900
C	2.46799600	-2.34050500	-0.28101600
C	3.37982200	-1.24291000	-0.16366800
C	2.97149800	-0.01432400	0.22281200
C	1.58913400	0.25309700	0.55616200
H	4.43073500	-1.40865700	-0.34075900
H	0.54618100	-0.45701200	-1.12926200
Cl	4.13204800	1.22493400	0.45955000
H	-2.21470600	2.88487300	-1.63643000
H	0.42061700	-2.91764400	-0.25337100
S	1.09478800	1.51477400	1.44874000
Cl	-0.22461400	-0.39668700	-2.93996800
H	-4.50579600	2.38036800	-0.85358200
H	2.85891700	-3.32408800	-0.48357500
O	-0.63365300	-0.78982300	0.51270600
TS17			
C	1.62528100	0.86828000	-0.31490100
C	1.63242900	-0.24002400	0.58725000
C	2.79393000	-1.06668700	0.58963900
C	3.78665500	-0.87713500	-0.32635000
C	3.73308500	0.19879100	-1.22261800
C	2.65851500	1.06505400	-1.20499700
Cl	0.87149900	-0.00818600	2.14240400
H	2.84238700	-1.85578500	1.32196700

H	2.58383600	1.89197400	-1.89222500
C	-0.69776700	1.30221700	-0.21034800
C	-1.62536600	2.30431800	-0.00293700
C	-2.96533400	1.98957500	0.07941800
C	-3.37638100	0.67421600	-0.03620100
C	-2.43351000	-0.31430000	-0.22807500
C	-1.06792200	-0.03824500	-0.32376100
H	-4.41812800	0.40650700	0.02426800
Cl	-2.97350000	-1.94597500	-0.37574000
H	4.53313300	0.35202900	-1.92866200
H	-1.27203200	3.31914100	0.08095600
S	0.08744700	-1.32023400	-0.56816900
H	4.63761400	-1.53959200	-0.33099200
H	-3.69335500	2.76989700	0.23266600
O	0.59246400	1.72549300	-0.34591000
TS18			
C	-1.44959900	0.19946400	0.36917900
C	-2.73005400	0.27963600	-0.14150400
C	-3.58448800	-0.80469700	-0.04588200
C	-3.16389200	-1.98001900	0.58699200
C	-1.90846300	-2.07373800	1.11455500
C	-0.97322800	-1.00939000	0.95448900
Cl	-3.24958000	1.72600600	-0.90914700
H	-4.57614400	-0.72623900	-0.46000500
H	-0.19823500	-0.90682800	1.70239400
C	0.71594500	1.12215200	0.30741600
C	1.40827200	2.24688600	0.71326200
C	2.78727900	2.24241500	0.69619500
C	3.47214600	1.11530700	0.27892000
C	2.76459000	-0.00427700	-0.11015400
C	1.36858600	-0.04093900	-0.11017800
H	4.54903100	1.09283900	0.25686800
Cl	3.64311000	-1.39371800	-0.62996100
H	-1.58790600	-2.96314900	1.63225500
H	0.84462100	3.11276900	1.02045300
S	0.48032500	-1.46263000	-0.58803000
H	3.33300800	3.11890300	1.00644400
H	-3.85426500	-2.80332900	0.67857700
O	-0.64098400	1.25892600	0.25707100
TS19			
C	1.44579300	0.02340400	0.15317000

C	2.79992800	0.21069400	-0.03915400
C	3.61726100	-0.86352000	-0.35575700
C	3.07485400	-2.13255400	-0.48158500
C	1.72394900	-2.33306100	-0.30974500
C	0.87971300	-1.24318100	-0.05888200
Cl	3.47496600	1.78060500	0.14515300
H	4.67245800	-0.69352800	-0.49199000
H	0.33698700	-0.87891900	-1.72465000
C	-0.63798600	1.12362300	0.16146000
C	-1.16065300	2.36670200	-0.12901200
C	-2.51239000	2.48946400	-0.38850700
C	-3.33482600	1.37868100	-0.36838500
C	-2.79128900	0.13881200	-0.08981400
C	-1.43811800	-0.01159200	0.18430100
H	-4.39048200	1.46085800	-0.56686900
Cl	-3.82305800	-1.24095900	-0.05203200
H	1.29163000	-3.31663800	-0.40175600
H	-0.49860800	3.21686300	-0.13426000
S	-0.73524300	-1.56280600	0.59008500
H	-2.93008000	3.45874300	-0.60867200
H	3.71882100	-2.96730600	-0.70699800
O	0.68541400	1.08324900	0.49278000

TS20

C	-1.43027600	-0.19801500	-0.62171100
C	-1.97855000	-0.45664900	0.68568600
C	-3.17277000	0.10329400	1.06296500
C	-3.93849800	0.79933800	0.13642100
C	-3.52611000	0.89089300	-1.19829900
C	-2.33509100	0.35466100	-1.58629500
Cl	-1.06660100	-1.38894900	1.78727600
H	-3.51725000	-0.02708300	2.07588900
C	1.17607800	0.24857000	-0.28879600
C	2.51292600	0.39910300	0.04074500
C	3.40836200	-0.64636300	-0.11199500
C	2.96283700	-1.86013000	-0.59966800
C	1.62985800	-2.04251900	-0.93517300
C	0.76656200	-0.98672200	-0.77432100
H	-4.16289000	1.36744700	-1.92628500
H	-1.99167700	0.38628600	-2.60731800
H	4.44217600	-0.49844200	0.15318300
H	1.25963200	-2.98241500	-1.31007500
Cl	3.06459500	1.92135800	0.63207500

S	-0.05749100	1.46005300	-0.18620900
H	-4.87836800	1.22972100	0.44279400
H	3.65899300	-2.67524100	-0.71563400
O	-0.53857900	-1.10560600	-1.13994200
TS21			
C	-1.23342600	-0.08460200	0.40566500
C	-1.34637600	0.84675700	1.47853800
C	-2.52597600	1.48113700	1.75147100
C	-3.67019500	1.15557700	1.02585500
C	-3.62343800	0.18631700	0.03273400
C	-2.44293400	-0.45355800	-0.25523000
H	-2.57332500	2.21656300	2.53852100
C	0.79235300	1.07413400	-0.70923000
C	1.64064700	2.07824000	-1.15744600
C	3.00844700	1.93604100	-0.98975800
C	3.54409800	0.83294200	-0.35264100
C	2.68875900	-0.15139500	0.11927800
C	1.32622200	-0.04115900	-0.05655300
H	-4.51172500	-0.07808800	-0.51728400
H	3.66836100	2.70980000	-1.34976600
H	-4.60610400	1.64709200	1.23986600
H	4.60601900	0.73026800	-0.20436000
O	-0.51021500	1.12313000	-0.90457700
S	0.13682500	-1.22674800	0.44231900
H	-0.45091300	1.06615900	2.03927600
H	1.21827200	2.93788600	-1.65088700
Cl	-2.41253300	-1.62710400	-1.49614900
Cl	3.32975800	-1.53462200	0.92603400
TS22			
C	-1.33248100	-0.08803900	0.29840700
C	-2.61891500	-0.45693800	-0.06950400
C	-3.67353800	0.42362300	0.06931400
C	-3.46541200	1.70282400	0.59259200
C	-2.21573000	2.08218700	0.99665100
C	-1.12281900	1.20726100	0.83455200
Cl	-2.91307900	-2.02248800	-0.72514900
H	-4.65771200	0.11171700	-0.24083800
H	-0.24012400	1.37319500	1.43141200
C	1.33106700	0.00776900	-0.09594300
C	2.63251500	-0.42035700	0.12224300
C	3.71930300	0.40862300	-0.10131300

C	3.49773100	1.70244000	-0.52895800
C	2.21125400	2.17283300	-0.71206000
C	1.11644600	1.33474400	-0.52023100
H	2.01947600	3.18639800	-1.02466100
H	4.33646500	2.35964800	-0.69711600
H	-2.04389000	3.04987400	1.43898200
H	-4.30352400	2.37322500	0.69560600
H	4.71477100	0.03424600	0.06832300
O	-0.09739200	1.80168900	-0.73525300
S	0.00975800	-1.14828000	0.00682900
Cl	2.93196200	-2.03581600	0.65377000

TS23

C	-1.33467400	0.02107000	0.18371400
C	-2.58998400	-0.49227000	-0.11865600
C	-3.67254500	0.33718800	-0.34422400
C	-3.50419200	1.70675000	-0.27644600
C	-2.26390100	2.24423600	0.01214800
C	-1.19810400	1.40123000	0.24606400
Cl	-2.82144300	-2.19927300	-0.18174200
H	-4.63223000	-0.09766600	-0.56859300
H	0.58637600	1.36852000	-1.61609100
C	1.13217700	1.40430100	0.09117300
C	2.22342900	2.26103900	-0.07641200
C	3.46745400	1.73362900	-0.33409300
C	3.65567900	0.36094500	-0.36370400
C	2.58806000	-0.48186500	-0.10319300
C	1.32560000	0.01352200	0.17349900
H	2.04589700	3.32280600	-0.03440800
H	-2.10206600	3.30812700	0.06817500
H	4.62469400	-0.06461300	-0.56438300
Cl	2.85797100	-2.18396900	-0.07457500
S	-0.00018700	-1.05660600	0.55193100
O	-0.00942300	1.97200800	0.58238900
H	4.30542900	2.39051000	-0.50313500
H	-4.34469900	2.35841200	-0.45341800

TS24

C	1.40185200	-0.47209100	-0.40491300
C	2.34660100	-0.77491600	-1.42951400
C	3.66275400	-0.44493600	-1.29853100
C	4.12519100	0.15298700	-0.12121100
C	3.26045600	0.38376200	0.93366900

C	1.93447100	0.02779200	0.82501700
H	4.35066400	-0.65145400	-2.10291800
C	-0.60569300	1.14233900	-0.67895100
C	-1.37418800	2.29984900	-0.62723800
C	-2.72792500	2.20243300	-0.35478400
C	-3.32233700	0.98263500	-0.08833200
C	-2.54087800	-0.16261200	-0.09831200
C	-1.19702600	-0.09059800	-0.38937300
H	-0.90519500	3.24740500	-0.83469500
H	3.61485300	0.81843900	1.85398500
H	-4.37148800	0.90880400	0.14416100
H	5.16512900	0.42145400	-0.02349500
H	-3.32914400	3.09797900	-0.33668700
S	-0.09282500	-1.44736600	-0.42052100
O	0.66287400	1.16266800	-1.02782400
H	1.96967400	-1.22979100	-2.33084200
Cl	0.89082800	0.26921900	2.15409500
Cl	-3.24917800	-1.69487600	0.25627300

TS25

C	-1.44350800	0.86376700	-0.21001900
C	-2.37063400	1.45544800	-1.06768500
C	-3.62660100	0.92391900	-1.21060200
C	-3.97822600	-0.23977800	-0.50517100
C	-3.10259100	-0.83122000	0.35197400
C	-1.80079100	-0.29696200	0.52246300
H	-4.33432000	1.38406000	-1.88099800
C	0.57460800	-1.21637500	-0.51884900
C	1.46843100	-2.23789800	-0.88941700
C	2.82373300	-2.06515400	-0.78439800
C	3.35946800	-0.85248100	-0.36396400
C	2.50150800	0.18202500	-0.08300000
C	1.11465200	0.04750700	-0.17916700
H	1.03885200	-3.17953600	-1.18904600
H	-3.37029500	-1.70526500	0.92169600
H	4.42282000	-0.70358600	-0.28275700
H	3.48514700	-2.88290300	-1.02472300
H	-4.96457000	-0.65967300	-0.62680600
H	-2.06847800	2.31993200	-1.63836200
Cl	-1.06270900	-0.59097100	2.06300700
Cl	3.16322400	1.71868600	0.35199100
O	-0.68738300	-1.52016400	-0.47793200
S	0.15380400	1.50127100	-0.11771900

TS26

C	1.32962800	0.28142400	-0.63444000
C	1.97834100	-0.86758400	-0.18735300
C	3.21714900	-0.78295800	0.42136800
C	3.81605500	0.45071700	0.59114600
C	3.18707700	1.60077800	0.14787800
C	1.95358100	1.51149400	-0.46571500
Cl	1.26739000	-2.42618300	-0.37293500
H	3.69960400	-1.68431500	0.76215000
H	1.45456300	2.39712200	-0.82427000
C	-1.42889700	0.54118600	-0.19456800
C	-2.74814100	0.41255400	-0.84481600
C	-3.58359300	-0.57554800	-0.52247400
C	-3.23547800	-1.55197300	0.48592600
C	-2.10159800	-1.46798300	1.19177800
C	-1.18645800	-0.34469700	1.01820200
Cl	-1.30957000	2.34425900	0.43350500
H	-2.98541900	1.13358800	-1.61158000
H	-1.84717400	-2.16910100	1.97026400
H	-1.13639200	3.99126600	1.15090200
H	-3.92588100	-2.36056100	0.67431200
H	3.65535500	2.56372800	0.27554200
H	-4.53373000	-0.66295100	-1.02549900
H	4.78124700	0.50871700	1.06973700
O	-0.27412500	-0.12658900	1.77594600
S	-0.21488200	0.21521600	-1.48252600

TS27

C	1.48226300	0.15848300	-0.61714100
C	2.42265300	-0.65959300	0.00088600
C	3.52112900	-0.10577500	0.63065600
C	3.68631100	1.26707200	0.64631400
C	2.76387500	2.08915700	0.02476100
C	1.67180300	1.53312600	-0.61478200
Cl	2.24512800	-2.37017000	0.01423300
H	4.23526100	-0.75484200	1.11045400
H	0.94854200	2.16090100	-1.10950400
C	-1.27397700	-0.40058100	-0.50492200
C	-2.48266700	-0.74573600	-1.21408000
C	-3.57083000	-1.19622800	-0.55717700
C	-3.56343300	-1.36129600	0.86795600
C	-2.45602000	-1.13112700	1.59066900

C	-1.19454900	-0.76831600	0.95341500
Cl	-1.71696100	1.68127000	-0.13495700
H	-2.49926100	-0.59808100	-2.28306000
H	-2.42177300	-1.26278600	2.66011500
O	-1.66457800	3.64253800	0.46579900
H	-1.32615900	3.49930800	1.35635900
H	-4.47157500	-1.67966700	1.35659200
H	2.89365100	3.15965200	0.02781600
H	4.54490300	1.69096800	1.14351200
H	-4.46920200	-1.42520400	-1.10796400
O	-0.14842800	-0.76185400	1.55840100
S	0.12821700	-0.51247200	-1.53343300
TS28			
C	1.51643500	0.07185900	-0.63928800
C	2.54086600	-0.60663200	0.01350900
C	3.56102500	0.09509700	0.62773300
C	3.56414500	1.47756600	0.59281400
C	2.55828500	2.16200900	-0.06511900
C	1.54531300	1.45862100	-0.68950600
Cl	2.56648700	-2.32461900	0.08836000
H	4.34136800	-0.44792200	1.13535500
H	0.76023800	1.98336900	-1.21009800
C	-1.16379900	-0.76839000	-0.50386900
C	-2.32294900	-1.28099400	-1.20696900
C	-3.35259900	-1.83016300	-0.53856100
C	-3.33873700	-1.94096100	0.89491300
C	-2.27021600	-1.56768300	1.61328800
C	-1.04902300	-1.09667900	0.96630900
Cl	-1.78903100	1.24161900	-0.18994200
H	-2.34678300	-1.17272600	-2.28043300
H	-2.22946200	-1.65865800	2.68667000
H	-0.99327600	3.41514100	1.41294200
H	-4.21127600	-2.33862300	1.39029400
H	2.56012800	3.23971100	-0.10233000
S	-1.61981300	3.68167700	0.26315200
H	-4.21376700	-2.18414900	-1.08272200
H	4.36196600	2.01737500	1.07886500
O	-0.00781600	-0.97800300	1.56560900
S	0.25007300	-0.78545100	-1.52677800
TS29			
C	1.57446400	0.23983500	-0.62660800

C	2.66186500	-0.30629200	0.04721700
C	3.58610200	0.52023700	0.65661100
C	3.42666100	1.89291300	0.59680800
C	2.35484600	2.44506900	-0.08034300
C	1.43818900	1.61816200	-0.70168300
Cl	2.87953300	-2.00859900	0.15134400
H	4.41935000	0.08173400	1.18084000
H	0.60197000	2.03545300	-1.23856300
C	-0.98037900	-0.91634700	-0.51984800
C	-2.05689400	-1.60124600	-1.19708300
C	-3.05441300	-2.17987100	-0.49912900
C	-3.08913400	-2.13675900	0.93602100
C	-2.08289900	-1.59809200	1.63969300
C	-0.87206000	-1.11820100	0.97468200
Cl	-1.92077000	1.02006400	-0.34593200
H	-2.05839800	-1.60002100	-2.27624400
H	-2.07446400	-1.56594600	2.71702400
Cl	-2.43183800	3.27098100	0.34491100
H	-3.94585000	-2.55061700	1.44495100
H	2.22907600	3.51455900	-0.13071900
H	-3.85840500	-2.66722300	-1.02749500
H	4.14957100	2.53032400	1.08154300
O	0.15491000	-0.91848500	1.57154300
S	0.43137900	-0.77427500	-1.51482600

TS30

C	0.86615500	0.07965100	-0.44020200
C	0.84256400	1.40624800	-0.96321800
C	1.87547800	2.27620500	-0.75330900
C	3.01909300	1.84408300	-0.08425300
C	3.12000900	0.53293100	0.36213500
C	2.08805900	-0.34985700	0.15985000
H	1.81097300	3.28832700	-1.11955100
C	-1.43150900	0.29568800	0.69945000
C	-2.49850600	0.86993800	1.37860700
C	-3.78967500	0.66573200	0.91733400
C	-4.02762000	-0.06606000	-0.23255900
C	-2.96273700	-0.61412000	-0.93667900
C	-1.68173000	-0.44181300	-0.46060600
H	-2.30225000	1.44607300	2.26836100
H	4.01087300	0.19183400	0.86369400
Cl	2.23929100	-1.95478100	0.72778800
H	-0.04764300	1.71261000	-1.49079100

H	-5.03397300	-0.19752300	-0.59685100
H	3.84051700	2.52302800	0.08167400
H	-4.61582900	1.10302800	1.45658500
S	-0.22702900	-1.11987700	-1.17778400
O	-0.18519700	0.40706400	1.12220300
H	-3.13407700	-1.16634900	-1.84788900
TS31			
C	-0.78420100	0.12968600	-0.35515100
C	-0.89961200	1.48347900	-0.83114700
C	-2.08697100	2.15302400	-0.75716200
C	-3.23720500	1.49583500	-0.31747600
C	-3.19608400	0.13998800	0.00480200
C	-2.01956100	-0.55308600	-0.07286500
H	-2.13770100	3.18799200	-1.05554300
C	1.46346700	-0.32519900	-0.56635500
C	2.52702500	-0.62448700	-1.38431000
C	3.80632700	-0.32247900	-0.94022400
C	3.99476200	0.27624100	0.29341900
C	2.91073600	0.58048600	1.10332800
C	1.62956200	0.27095400	0.67783400
H	2.35095800	-1.08802300	-2.34160800
H	-4.09386100	-0.38136700	0.29487900
H	3.05938400	1.04678600	2.06431600
Cl	-1.95301100	-2.22129500	0.27645900
H	0.00392400	1.95584600	-1.18484300
H	4.65418200	-0.55141500	-1.56625800
H	-4.17457100	2.02502900	-0.25709200
H	4.99131800	0.51417800	0.63085200
O	0.19041500	-0.65394500	-0.91980200
S	0.14842300	0.50361900	1.55911000
TS32			
C	-0.97871100	-0.29825600	0.54242200
C	-1.52957900	0.86621900	-0.10310800
C	-2.84516700	0.89200300	-0.49250400
C	-3.69702000	-0.14616300	-0.13721700
C	-3.23470500	-1.20176500	0.65768500
C	-1.92800600	-1.25095900	1.03933200
Cl	-0.48991700	2.17281600	-0.45953700
H	-3.21064400	1.73791100	-1.05160100
C	1.44733900	-0.68414300	-0.51785900
C	2.68671600	-0.71205700	-1.13699000

C	3.79451500	-0.19526400	-0.48339700
C	3.67069100	0.35603200	0.78042300
C	2.43372600	0.40130100	1.40481900
C	1.34615700	-0.11906900	0.74497500
H	2.78355900	-1.14067900	-2.12188200
H	-3.91994500	-1.96586400	0.98828400
H	-1.53809700	-2.03419300	1.66850300
H	2.30572700	0.83424200	2.38374000
H	4.53537000	0.75992800	1.28274600
H	-4.73091200	-0.11022600	-0.44106600
H	4.75700800	-0.22272200	-0.96963000
S	-0.03925900	-1.32263100	-1.15506500
O	0.12236700	-0.13518100	1.34532300
TS33			
C	1.73390600	0.24223800	-0.15125500
C	3.08071700	-0.10311500	-0.04915400
C	4.02031000	0.81413400	0.38451100
C	3.62967800	2.09436500	0.72845100
C	2.30043600	2.45871000	0.61683300
C	1.36514700	1.54621300	0.16574600
Cl	3.62683100	-1.68570600	-0.47185900
H	5.05258900	0.51140400	0.45383700
H	0.34228200	1.85002200	0.01390600
C	-0.88807800	-0.68149300	0.27523800
C	-1.43887800	-1.94887100	0.77671800
C	-2.75292400	-2.10550900	0.97107200
C	-3.68454300	-1.06107900	0.63805900
C	-3.28166500	0.08464800	0.06622500
C	-1.87593200	0.30905000	-0.29298600
H	-4.73470900	-1.21178800	0.83513500
H	-0.49575300	-0.11403300	1.24022800
Cl	-4.39127700	1.30494100	-0.38966800
H	1.98641300	3.46141800	0.86023000
H	-0.73516400	-2.72473200	1.03392300
H	-0.05677900	0.47124000	2.18911400
H	-3.13858900	-3.02373500	1.38449000
H	4.36666800	2.80348800	1.07094900
O	-1.52163300	1.25185700	-0.95733500
S	0.58329000	-0.96630500	-0.72212000
TS34			
C	1.73631700	0.19962700	-0.31084500

C	3.08352300	-0.13718700	-0.17714500
C	4.01782000	0.80536400	0.21257300
C	3.62495700	2.10353100	0.47651000
C	2.29655000	2.46105600	0.32589900
C	1.36633700	1.52227500	-0.08217500
Cl	3.63589600	-1.73958900	-0.49757700
H	5.04893600	0.50735900	0.31262500
H	0.34340500	1.81251900	-0.25899600
C	-0.88203700	-0.71096700	0.17421600
C	-1.44702400	-1.96468000	0.69875000
C	-2.76407000	-2.10841200	0.88313500
C	-3.68908800	-1.06943400	0.51473700
C	-3.27648800	0.05936400	-0.08112900
C	-1.86629900	0.26356200	-0.43894400
H	-4.74118400	-1.21103800	0.70774600
H	-0.53138300	-0.16243100	1.12974800
Cl	-4.37394000	1.27429000	-0.57517400
O	-0.15468200	0.52359600	2.43180200
H	0.65159500	1.01147900	2.21201200
H	1.98038300	3.47765700	0.50007800
H	-0.74988100	-2.73245700	0.99430400
H	4.35817300	2.83180100	0.78500600
H	-3.15723000	-3.01139700	1.32223900
O	-1.50872300	1.16902500	-1.14962100
S	0.59051200	-1.04368600	-0.80618300

TS35

C	1.79274200	0.07921600	-0.13693100
C	3.16959000	-0.11104800	-0.26081200
C	4.05224500	0.94508300	-0.16125500
C	3.57279400	2.22068900	0.07040800
C	2.21091300	2.42732200	0.18719900
C	1.32725200	1.37131500	0.07231500
Cl	3.80284800	-1.69313300	-0.54393200
H	5.10848600	0.75573400	-0.26348300
H	0.27214900	1.57260400	0.12080900
C	-0.84937300	-0.88276300	0.19701100
C	-1.59863100	-2.02072300	0.73033300
C	-2.94033200	-2.02079600	0.71221200
C	-3.67688300	-0.94741000	0.10532000
C	-3.05216400	0.03477800	-0.56692800
C	-1.59387200	0.00501400	-0.76636300
H	-4.75412500	-0.94561400	0.16634400

H	-0.77697700	-0.14163500	1.18788200
Cl	-3.91065600	1.27684300	-1.36325600
H	-2.27328500	0.45137900	2.61957700
H	1.82177700	3.41892800	0.35469000
H	-1.04271400	-2.80611200	1.21810000
S	-1.01603600	0.90860500	2.57253900
H	4.26267600	3.04558800	0.15052100
H	-3.49018800	-2.82894800	1.16734000
S	0.79802400	-1.36773600	-0.23153400
O	-1.03657000	0.66213000	-1.60633700

TS36

C	-1.68985500	-0.01964100	-0.28379800
C	-3.06180600	0.25877000	-0.41317800
C	-3.99125600	-0.74976600	-0.38229000
C	-3.57795100	-2.06984900	-0.23176300
C	-2.23713300	-2.36782100	-0.13037200
C	-1.29281800	-1.35700400	-0.17055000
Cl	-3.60270100	1.88421600	-0.59876200
H	-5.03713500	-0.50456600	-0.46950200
H	-0.24968200	-1.61130200	-0.18165900
C	0.92654500	0.72566900	0.35650000
C	1.62010900	1.76874700	1.13116400
C	2.95528800	1.81301800	1.17897000
C	3.76087500	0.90024500	0.41252600
C	3.21177100	0.01056600	-0.42866800
C	1.76137100	-0.03662300	-0.65274300
H	4.83487500	0.94428100	0.50555600
H	0.65108800	-0.06804900	1.15430700
Cl	4.16247300	-1.04050800	-1.38273600
H	-1.90625500	-3.38834600	-0.03012800
H	1.01536500	2.42651500	1.73547200
Cl	0.09437500	-1.25356800	2.55732500
H	-4.31597800	-2.85582800	-0.20876100
H	3.45359800	2.52930200	1.81211200
S	-0.62342000	1.34420200	-0.24888100
O	1.26219000	-0.65868600	-1.55489300

TS37

C	1.73990700	0.74805500	-0.35463600
C	1.58672300	-0.28708800	0.60336600
C	2.46440400	-1.39861000	0.54514800
C	3.43128600	-1.45712500	-0.40890900

C	3.60147100	-0.41124600	-1.33425900
C	2.75496600	0.66562800	-1.30982200
Cl	0.96479600	0.09419900	2.17631900
H	2.34172200	-2.17943500	1.27675200
H	2.83663000	1.44975400	-2.04661000
C	-0.90945100	1.24516400	-0.11184500
C	-2.02807500	2.06775300	-0.00341200
C	-3.29374300	1.53423500	-0.02880900
C	-3.45644700	0.16193600	-0.18745600
C	-2.36098600	-0.65661400	-0.28717000
C	-1.04127100	-0.16249500	-0.17329000
H	-4.44023700	-0.27775800	-0.22067500
Cl	-2.57231500	-2.35602600	-0.45750200
H	4.37820500	-0.46973200	-2.07939500
H	-1.88882600	3.13533000	0.07680700
H	4.09048500	-2.31045400	-0.44289800
H	-4.15628000	2.17493800	0.05444700
O	-0.06545400	-1.00683800	-0.10249700
S	0.60981600	2.04284700	-0.41948600
TS38			
C	1.48045200	-0.15877900	0.37172600
C	2.76946600	0.07441300	-0.08196800
C	3.33267400	1.33366600	0.00129400
C	2.61323700	2.39731500	0.55417500
C	1.35403700	2.19086900	1.04355700
C	0.75191800	0.91919200	0.94003100
Cl	3.68057900	-1.20835800	-0.78335000
H	4.33058600	1.48496500	-0.37750600
H	-0.06032100	0.68444500	1.60952300
C	-0.99166600	-1.23947500	0.19749400
C	-1.90799000	-2.20399300	0.57153100
C	-3.26667800	-1.93807800	0.50412100
C	-3.70615600	-0.69437600	0.09623400
C	-2.78784100	0.28801000	-0.22823200
C	-1.41147600	0.04223600	-0.20541200
H	-4.75815800	-0.46351900	0.05050700
Cl	-3.33493800	1.84816500	-0.70145300
H	0.79829800	2.98933900	1.50720600
H	-1.55886600	-3.16858700	0.90670800
H	-3.97939600	-2.69752800	0.78223400
H	3.07185300	3.37144900	0.61026300
O	-0.55383500	0.98603700	-0.51487600

S	0.70818300	-1.68947400	0.10527500
TS39			
C	-1.40196900	-0.02961700	-0.24902900
C	-2.70644500	0.14700400	0.18106300
C	-3.19046700	1.39869400	0.52255300
C	-2.34508400	2.49721800	0.47843600
C	-1.04419600	2.36109500	0.05421600
C	-0.61096700	1.12044200	-0.42994700
Cl	-3.75926900	-1.21174700	0.29940300
H	-4.21252300	1.49628200	0.84865100
H	-1.08787300	1.37747600	-2.08457500
C	0.88900700	-1.31287500	-0.18871300
C	1.65733900	-2.36679400	0.27570200
C	2.97526800	-2.15252600	0.63304000
C	3.51984200	-0.88392000	0.55754300
C	2.74212200	0.17322700	0.12212900
C	1.42629200	-0.03763400	-0.26202000
H	4.54293300	-0.69909000	0.84096500
Cl	3.40730200	1.75592500	0.03494200
H	-0.35945900	3.19167200	0.01173600
H	1.21969500	-3.34996600	0.34829200
H	3.57971700	-2.97426200	0.98196100
H	-2.71037200	3.46211100	0.79161900
O	0.71947200	1.01088400	-0.74626000
S	-0.76305600	-1.58301300	-0.72639100
TS40			
C	-1.44685600	-0.47703700	-0.48060000
C	-1.77691100	-0.04211100	0.84197900
C	-2.82632800	0.82117100	1.06623500
C	-3.65311900	1.18751400	0.01988900
C	-3.43266800	0.68324400	-1.26715400
C	-2.37872200	-0.14595000	-1.50904700
Cl	-0.79522800	-0.52785900	2.15069100
H	-3.00364900	1.18513300	2.06498000
C	1.05185400	0.14398200	-0.46349600
C	2.22992600	0.82124500	-0.15447100
C	3.39412000	0.12106300	0.11089200
C	3.38871500	-1.26100700	0.11894700
C	2.21616500	-1.95926400	-0.13737000
C	1.07221400	-1.25422400	-0.43069700
H	-4.10086400	0.95018200	-2.07039000

H	-2.18488600	-0.53382200	-2.49557700
H	4.29597700	0.67195400	0.32364100
H	2.19757400	-3.03677100	-0.09210800
Cl	2.23048200	2.54081200	-0.16327800
H	-4.48061700	1.85382600	0.20497800
H	4.29470700	-1.79823500	0.34898900
O	-0.05598700	0.76181900	-0.79526700
S	-0.50000000	-1.96492400	-0.74994000
TS41			
C	1.05063900	0.03198400	0.27473800
C	1.18985700	-0.49192000	1.60783400
C	2.42318500	-0.74846800	2.13292100
C	3.57372100	-0.40229600	1.42230900
C	3.47641900	0.25037800	0.19453900
C	2.25063400	0.52825800	-0.34580500
H	2.50690300	-1.20370200	3.10673100
C	-1.10283700	-1.29455900	-0.44662800
C	-2.24160800	-2.07202800	-0.56725400
C	-3.48061900	-1.50965300	-0.30182200
C	-3.59223400	-0.18981100	0.09307600
C	-2.45173700	0.58706900	0.22573500
C	-1.22043900	0.03231300	-0.04864100
H	-2.16015900	-3.10262400	-0.87238500
H	4.36369500	0.56476600	-0.33058900
Cl	2.10521300	1.35887100	-1.82719600
H	0.28063500	-0.72636600	2.13982000
H	-4.55284000	0.24778900	0.30938900
Cl	-2.55936300	2.22894800	0.72341900
H	4.54827300	-0.60638400	1.83572600
H	-4.37062200	-2.11109900	-0.39790000
O	-0.08202100	0.76336400	0.00652400
S	0.53193400	-1.78061300	-0.78279900
TS42			
C	1.13079000	0.12552800	0.25739800
C	2.29854500	0.74656100	-0.13987100
C	3.52130100	0.15151900	0.11703800
C	3.58312400	-1.07190800	0.79383000
C	2.44195800	-1.69535700	1.20691800
C	1.16130800	-1.15542100	0.88414000
Cl	2.22367900	2.25176800	-0.96209800
H	4.42088400	0.64869500	-0.20642300

H	0.34330600	-1.37848900	1.55636800
C	-1.19374400	0.01027100	-0.04376100
C	-2.36416500	0.71058200	0.22127900
C	-3.59264000	0.09320900	0.10512600
C	-3.65248500	-1.23862000	-0.26528100
C	-2.49311600	-1.94775800	-0.50581200
C	-1.24814700	-1.33460800	-0.41149400
H	-2.53500600	-2.99198100	-0.77225400
H	-4.60940000	-1.72846100	-0.35005600
H	2.48274600	-2.62066500	1.75822500
S	0.21515800	-2.23061000	-0.73867500
H	4.54714700	-1.50346000	1.01118100
H	-4.48679300	0.65786500	0.31143300
O	-0.03760700	0.72156200	-0.00842600
Cl	-2.27432200	2.36410300	0.68331300

TS43

C	1.18484200	-0.02516700	0.19545100
C	2.24512600	0.82363100	-0.08509600
C	3.49221300	0.30336800	-0.37936900
C	3.67616700	-1.06610500	-0.41304500
C	2.61849300	-1.91838100	-0.15541500
C	1.37688200	-1.39855700	0.16627200
Cl	2.00354600	2.52290800	-0.05258500
H	4.30470600	0.97986200	-0.58756900
H	-0.59044700	-1.33352200	-1.72570900
C	-1.25278800	-1.41771000	-0.06923900
C	-2.50609500	-1.98014300	-0.34604800
C	-3.60074100	-1.16419900	-0.52402600
C	-3.48466500	0.20900300	-0.37829700
C	-2.26471100	0.76952000	-0.03121800
C	-1.16221600	-0.03706100	0.16773900
H	-2.58540700	-3.04998900	-0.45468500
H	2.74967600	-2.98803300	-0.19734400
H	-4.33420500	0.85629100	-0.52015800
Cl	-2.12605500	2.46660200	0.18526500
H	-4.55772900	-1.59508200	-0.77083800
H	4.64711000	-1.46942700	-0.65181400
O	-0.00036900	0.53586700	0.54885100
S	0.03230400	-2.44361900	0.58596800

TS44

C	1.21035400	-0.18176500	-0.51155900
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C	2.10738500	-0.26832800	-1.62585600
C	3.45627400	-0.26289900	-1.43887900
C	3.98754000	-0.29208300	-0.14357000
C	3.14865300	-0.38819700	0.95960000
C	1.78739800	-0.41038400	0.78923600
H	4.11694700	-0.26174200	-2.29096000
C	-0.92512000	1.39709500	-0.15209900
C	-2.01140500	2.17756700	0.20666400
C	-3.26318200	1.59418000	0.32430400
C	-3.44007500	0.24260100	0.09696200
C	-2.35251600	-0.54107300	-0.25165900
C	-1.10831000	0.03965300	-0.37288800
H	-1.87892000	3.23217000	0.38616600
H	3.55430000	-0.47393600	1.95453300
Cl	0.74268900	-0.60924600	2.12358900
H	1.65853000	-0.27257600	-2.60550800
H	-4.41013600	-0.21686200	0.19062200
Cl	-2.53861000	-2.22631400	-0.53708600
H	5.05568600	-0.28611600	0.00313800
H	-4.11016600	2.20213200	0.60016400
O	-0.03958400	-0.69384600	-0.76568100
S	0.70494400	1.94962700	-0.39780000

TS45

C	-1.22290700	0.86431000	-0.26492700
C	-2.16091700	1.64194700	-0.91115000
C	-3.50421600	1.35193500	-0.79427500
C	-3.92492300	0.25025000	-0.03704100
C	-3.01475300	-0.51043300	0.63357300
C	-1.61435700	-0.26387100	0.51758100
H	-4.22913300	1.96950500	-1.29965600
C	0.82751700	-1.19391600	-0.63033500
C	1.88879700	-2.08882200	-0.55074900
C	3.16426100	-1.64499700	-0.26287200
C	3.39988300	-0.30608400	-0.00553000
C	2.35075000	0.59055700	-0.05425600
C	1.07682000	0.15199400	-0.37422700
H	1.69611400	-3.13764700	-0.71117500
H	-3.32034700	-1.32443300	1.27048600
Cl	-0.70041800	-0.61019500	1.96822700
H	-1.80443900	2.45247600	-1.52577400
H	4.38636700	0.05196900	0.23892500
Cl	2.62257600	2.25771600	0.26444500

H	-4.97567300	0.02493400	0.05086600
H	3.97933600	-2.34934700	-0.21442500
S	-0.79480300	-1.73912900	-0.94793500
O	0.08902500	1.13419200	-0.52405700
TS46			
C	-2.58352700	2.24080000	-0.21590300
C	-3.21364700	1.00509600	0.10945700
C	-2.59189900	-0.17133300	-0.12896700
C	-1.28200600	-0.20873800	-0.74659600
C	-0.57629600	1.05252100	-0.83659900
C	-1.32324400	2.26986800	-0.69987500
H	-4.20764600	1.00634300	0.52827500
H	0.27968700	1.04248600	-1.49744500
Cl	-3.34684600	-1.66825100	0.20631400
H	0.64380800	3.05514800	1.25537300
C	1.16751200	2.19164600	0.87708500
C	2.41928300	2.29155700	0.38447500
C	0.49020700	0.92418100	0.85282700
C	3.09260000	1.14578900	-0.11937800
C	1.25602700	-0.27570200	0.60624100
C	2.53646100	-0.08689700	-0.01844500
H	-0.84765500	3.20600300	-0.94671700
H	4.07269000	1.24978500	-0.55639200
S	0.55747400	-1.74296200	0.86803300
H	2.93038900	3.24163700	0.37061500
H	-3.13917400	3.15514800	-0.07850700
O	-0.72921100	-1.26818100	-1.07136600
H	-0.35409600	0.79789400	1.51662400
Cl	3.41668700	-1.44906400	-0.57663000
TS47			
C	2.37129000	2.32245000	0.25075100
C	3.16613500	1.23055600	-0.22129500
C	2.69425900	-0.03613200	-0.25412300
C	1.34927100	-0.34757600	0.16561800
C	0.71005200	0.70556500	1.01842700
C	1.17679800	2.08578100	0.80318800
H	4.15371600	1.42629600	-0.60899000
H	1.15683100	0.44564800	2.05557700
Cl	3.66872100	-1.27665800	-0.93194600
H	-4.16581900	-1.32526000	0.53297400
C	-3.21418000	-0.83486300	0.67121400

C	-2.42925100	-1.15697500	1.83314300
C	-2.77779500	0.01329900	-0.27464600
C	-1.25056500	-0.56745500	2.04334900
C	-1.47659400	0.67525100	-0.16288500
Cl	-3.67438800	0.31436200	-1.70294800
C	-0.79223900	0.55629100	1.18527600
H	-1.13405400	1.46112200	1.70981700
H	-0.64198600	-0.82613500	2.89813400
H	0.56212000	2.89168100	1.17418000
S	0.58442900	-1.74312200	-0.18215900
H	1.63015400	0.10300300	3.26756500
O	-0.99155700	1.34855000	-1.03915300
H	-2.79314600	-1.91966100	2.50252700
H	2.74702100	3.32673200	0.14108700
TS48			
C	1.49583600	-1.17363900	2.15490300
C	2.78089700	-0.80719600	1.64477900
C	2.92908900	-0.16106400	0.46701100
C	1.79706600	0.22480700	-0.34269100
C	0.48421000	-0.37722000	0.07107300
C	0.39844200	-0.94653700	1.42601200
H	3.66163000	-1.03518000	2.22445000
H	0.47385400	-1.30113500	-0.60766700
Cl	4.50779100	0.28320300	-0.03869200
H	-4.11043700	2.02874300	0.95794600
C	-3.19009300	1.56596500	0.63545000
C	-1.94817300	2.27184500	0.82902200
C	-3.23515500	0.34298400	0.08395700
C	-0.79587700	1.75027300	0.40803400
C	-2.01148200	-0.35843400	-0.30520700
Cl	-4.70654000	-0.51375400	-0.09795000
C	-0.73883800	0.45469500	-0.31487700
H	-0.59962700	0.71873200	-1.37405100
O	0.37727700	-2.48943100	-1.61787600
H	-0.58655900	-2.57139800	-1.53692900
H	0.13430200	2.28476800	0.52777200
H	-0.57571600	-1.24831800	1.78059800
S	1.93129000	1.17798100	-1.66335800
H	-1.97647900	3.23405000	1.31468400
H	1.43456400	-1.64038300	3.12482200
O	-2.02389800	-1.52520400	-0.63459500

TS49

C	1.55450900	-0.25868100	2.52131600
C	2.80993700	-0.06686400	1.87703800
C	2.90015500	0.21602300	0.55469000
C	1.73340700	0.35381200	-0.27749000
C	0.45166800	-0.09897200	0.34880300
C	0.42058900	-0.24624300	1.80329000
H	3.71718400	-0.12588400	2.45732900
H	0.42861200	-1.21953900	-0.01444300
Cl	4.45274600	0.49218300	-0.12414800
H	-4.31262900	2.22665600	-0.11164000
C	-3.35597300	1.72705100	-0.09296600
C	-2.15125100	2.52254600	-0.09322500
C	-3.31932300	0.38796500	-0.03091700
C	-0.95041500	1.94594200	-0.14336700
C	-2.04123600	-0.32197800	0.11167500
Cl	-4.74195000	-0.55893900	0.06380300
C	-0.81520100	0.47093200	-0.27511600
H	-0.73114400	0.28830100	-1.35841100
H	-0.04692600	2.53588400	-0.16994600
H	-0.53327100	-0.43966200	2.26627600
S	1.80004300	0.84275700	-1.84067900
S	0.56385700	-2.78550000	-1.01573400
H	1.66652600	-2.24835700	-1.55627200
O	-1.97519300	-1.46978900	0.48330400
H	-2.24784100	3.59601200	-0.05948800
H	1.53390300	-0.42554300	3.58624200

TS50

C	2.80342600	1.92404300	0.99226500
C	3.54005600	0.89539600	0.35862900
C	2.92647800	-0.18347300	-0.18871100
C	1.50057400	-0.35540600	-0.12947400
C	0.74329800	0.73391000	0.49213400
C	1.45167700	1.85744400	1.01961100
H	4.61651600	0.95748600	0.31255400
H	0.25131200	-0.31563900	1.38690500
Cl	3.83343900	-1.42251000	-0.95759000
H	-4.29083100	1.20846800	-1.21321600
C	-3.27291400	1.13528300	-0.86715300
C	-2.37452300	2.17476300	-1.07422000
C	-2.85940100	-0.00240900	-0.21154700
C	-1.06384300	2.08365300	-0.64640000

C	-1.54600000	-0.10075000	0.25087700
Cl	-3.96816300	-1.28586400	0.06024700
C	-0.63345200	0.94407000	0.01542100
H	0.87215500	2.65826700	1.45534500
H	-0.36731800	2.88312300	-0.84388200
H	3.32837100	2.75846100	1.42776200
H	-2.70887500	3.06017900	-1.59191900
S	-0.89109000	-1.40827200	1.13184700
O	0.94426900	-1.40934900	-0.48210900
TS51			
C	2.12915900	-1.58591100	1.60226300
C	3.24728600	-1.03814000	0.92546600
C	3.12433200	0.05327200	0.12648800
C	1.85678300	0.75606400	-0.07190400
C	0.70607500	-0.00879800	0.42111400
C	0.90148700	-1.04748500	1.38460100
H	4.22772100	-1.46456700	1.07644300
H	0.98590000	-0.91085300	-0.75074500
Cl	4.51142200	0.75207400	-0.60782700
H	-4.11682300	2.30086300	0.20885100
C	-3.15099700	1.82355100	0.21172300
C	-1.98497100	2.56640000	0.37239500
C	-3.06545800	0.46843400	0.03665600
C	-0.75208800	1.95342500	0.38294600
C	-1.80991900	-0.20535500	0.00974500
C	-0.63294200	0.57460500	0.24726800
H	0.15193400	2.53030700	0.50195800
H	0.04054700	-1.42267700	1.91746700
O	1.01897500	-1.77941700	-1.51819200
H	1.65083900	-2.41120700	-1.15990000
H	0.09902200	-2.09651600	-1.30260000
S	-1.78771700	-1.86442100	-0.37223400
Cl	-4.53223700	-0.39664100	-0.19733600
H	-2.05352800	3.63396800	0.51102700
H	2.26963800	-2.38694100	2.30887300
O	1.76722500	1.79886900	-0.67686100
TS52			
C	3.17641700	1.82016100	0.42214300
C	3.55601300	0.53039100	0.03907400
C	2.62022600	-0.42621400	-0.27013900
C	1.25034300	-0.10526900	-0.23589600

C	0.88767500	1.20008900	0.19124200
C	1.84474300	2.15975600	0.49508500
H	4.60125500	0.26943900	-0.01489200
H	0.16421300	-0.27437400	2.15575100
Cl	3.09208600	-2.00514200	-0.75332600
H	-4.07829000	0.72962800	-1.32308000
C	-3.09984900	0.88925300	-0.89940700
C	-2.52107200	2.16365000	-0.92308700
C	-2.45521600	-0.16116900	-0.31132900
C	-1.24141400	2.35783400	-0.44248100
C	-1.18863400	0.02229600	0.31909100
Cl	-3.21750100	-1.69540000	-0.22133700
C	-0.54032700	1.29969000	0.10448500
H	1.54237200	3.14696800	0.81018600
H	-0.73783600	3.30025700	-0.59210800
S	-1.02596200	-0.81368500	1.86912900
H	-3.05690800	2.97669100	-1.38569700
H	3.93779800	2.54055000	0.67377000
O	0.30517700	-0.90797500	-0.57417700

TS53

C	3.19271600	1.88615700	-0.16325200
C	3.52545200	0.53440200	-0.16621800
C	2.54411300	-0.44068400	-0.15871800
C	1.23026000	-0.02479900	-0.14685100
C	0.88463600	1.32570500	-0.14039400
C	1.87547000	2.29769200	-0.15305600
H	4.55908400	0.22818300	-0.17339600
H	-2.03120500	0.82063300	2.16584600
Cl	2.93323400	-2.11064500	-0.16981500
H	-4.16977500	0.27973800	-0.92967300
C	-3.16131500	0.56114200	-0.67402200
C	-2.81159300	1.91794600	-0.58530800
C	-2.23017800	-0.41753600	-0.46424600
C	-1.50067200	2.31965300	-0.37257900
C	-0.93892600	-0.02795600	0.01750500
Cl	-2.59161300	-2.07413100	-0.62205100
C	-0.54671300	1.34789600	-0.16749300
H	1.62264500	3.34592500	-0.14849100
H	-1.22896400	3.36168200	-0.42744800
S	-1.16161400	-0.19512300	2.14145300
H	3.98539400	2.61696700	-0.16646900
H	-3.57601800	2.65943800	-0.75507500

O	0.15470000	-0.84088700	-0.16487700
TS54			
C	-2.50828400	-1.14926800	1.79725200
C	-3.24621700	-0.82697000	0.60874900
C	-2.74877600	-0.01591700	-0.34259100
C	-1.42335300	0.58635800	-0.20392400
C	-0.80071100	0.46849800	1.15895100
C	-1.31266800	-0.59355200	2.03174500
H	-4.21294600	-1.28154900	0.45460200
H	-1.22552500	1.45356300	1.66697400
Cl	-3.58904100	0.29235100	-1.80154100
H	4.08271300	1.51954400	-0.63270600
C	3.11629300	1.28528100	-0.21390400
C	2.28410000	2.35249100	0.25918500
C	2.70960900	-0.00179500	-0.20840400
C	1.11583500	2.07661400	0.83848200
C	1.39360500	-0.37698200	0.25311600
Cl	3.73075300	-1.20577600	-0.88615700
C	0.70202200	0.67168100	1.09862800
H	1.08639200	0.46044900	2.10955100
H	0.47312000	2.86347500	1.20312900
H	-0.74197400	-0.84871400	2.91255600
H	-1.62891300	2.48268300	2.14790900
H	2.61371400	3.36938900	0.12159500
H	-2.91930300	-1.88047800	2.47438000
S	0.70930300	-1.82331900	-0.03780100
O	-0.87174700	1.21304000	-1.07825200
TS55			
C	-1.44407700	-0.41136800	2.23018000
C	-2.78934000	-0.35977200	1.72110000
C	-3.04683000	-0.17147100	0.41658200
C	-1.95440400	-0.06382800	-0.55616300
C	-0.59180800	0.19853800	0.03213200
C	-0.39281200	-0.19135500	1.43097500
H	-3.61251500	-0.50218300	2.40421700
H	-0.65841700	1.36450200	0.07728200
Cl	-4.63813400	-0.18940900	-0.20710800
H	3.34958200	-2.61025200	0.18330900
C	2.59473100	-1.92139100	-0.16354100
C	1.42838500	-2.43859700	-0.81847900
C	2.80262600	-0.59735400	0.00742700

C	0.46521800	-1.60691200	-1.21852200
C	1.85904700	0.38504200	-0.46374700
Cl	4.25866700	-0.07594800	0.75598700
C	0.53511100	-0.14445300	-0.96096200
H	0.27860500	0.38269600	-1.87957400
O	-0.95020500	2.80033700	-0.11054900
H	-0.08447000	3.05507700	-0.46675400
H	-0.42358600	-1.96276800	-1.71593900
H	0.61452400	-0.21144500	1.81983900
H	1.35494300	-3.50171100	-0.98222000
H	-1.30234500	-0.63001400	3.27656100
O	-2.12066300	-0.14100700	-1.74952300
S	2.16915500	1.98687800	-0.44431200
TS56			
C	-1.29220600	-0.45922300	2.24637200
C	-2.64080900	-0.49546000	1.76884300
C	-2.92373800	-0.45712700	0.45151700
C	-1.85082800	-0.42259500	-0.54668100
C	-0.49944600	-0.06042500	-0.00969700
C	-0.25854400	-0.29396100	1.39890400
H	-3.44891400	-0.58313800	2.47860800
H	-0.65152500	1.19161700	-0.04640700
Cl	-4.52359300	-0.57690900	-0.13560900
H	3.53293800	-2.59518400	0.32559700
C	2.76284800	-1.95782900	-0.08065000
C	1.65918500	-2.55593700	-0.77990100
C	2.89029300	-0.62151700	0.05323700
C	0.66492900	-1.79676700	-1.24125400
C	1.92317700	0.29440000	-0.50926700
Cl	4.27264400	0.00991100	0.85390200
C	0.63604700	-0.32502200	-1.00729400
H	0.34628200	0.17787700	-1.92893800
H	-0.17816200	-2.21540800	-1.76779800
H	0.75407100	-0.23960500	1.76796500
S	-1.16479900	2.81380100	-0.19159600
H	-2.39078800	2.44637900	0.20619200
H	1.65909400	-3.62433500	-0.92613700
H	-1.11972800	-0.56130800	3.30573100
O	-2.03513500	-0.61414500	-1.72640200
S	2.14095600	1.90269900	-0.57586300

TS57

C	-2.65858400	2.12261200	-0.90178500
C	-3.40619200	1.04038600	-0.39779100
C	-2.81285700	-0.09712400	0.06834900
C	-1.40549100	-0.24452900	0.07875800
C	-0.61725500	0.89123400	-0.39905800
C	-1.30683500	2.04872300	-0.89319200
H	-4.48450800	1.08717700	-0.40152900
H	-0.21753300	0.14654000	-1.31740200
Cl	-3.80215400	-1.38511900	0.62995900
H	4.45819400	0.77438400	1.12109400
C	3.42500600	0.85706500	0.82314400
C	2.64915200	1.91594500	1.27099600
C	2.89007100	-0.11359800	-0.00224900
C	1.30979700	2.01305800	0.91337900
C	1.55767300	-0.01185000	-0.39703000
Cl	3.83895400	-1.43684100	-0.54191400
C	0.77610200	1.04449800	0.09478100
H	-0.70273800	2.86493500	-1.25973800
H	0.69970500	2.82432700	1.28042100
H	-3.17063600	2.98739000	-1.29107400
H	3.09244500	2.66277700	1.91051800
S	-0.62827200	-1.71625300	0.40858600
O	0.91853600	-0.83908800	-1.20328000

TS58

C	-1.78933100	-2.01567900	-1.45913500
C	-2.97925600	-1.39504400	-1.01645500
C	-2.95813500	-0.24512200	-0.29126400
C	-1.73952200	0.42689800	0.08340400
C	-0.52865000	-0.28609800	-0.30053700
C	-0.60122100	-1.45364800	-1.14004100
H	-3.93428100	-1.83245600	-1.26261800
H	-0.54965800	-0.99785100	0.89122800
H	4.33688800	1.97264900	-0.70597300
C	3.36374800	1.52521500	-0.58423200
C	2.20324800	2.24283000	-0.90975500
C	3.25409400	0.25310700	-0.11792300
C	0.94484700	1.69015600	-0.76510300
C	1.96137300	-0.36506800	0.07404200
C	0.78364600	0.39518400	-0.31208500
H	0.07083300	2.26474900	-1.02166400
H	0.32584800	-1.89733600	-1.47003300
O	-0.29645300	-1.66993400	1.90228200

H	-0.82886500	-2.46623200	1.92951300
H	0.62124800	-1.88549400	1.60552400
Cl	4.63599300	-0.66355700	0.29249500
O	1.88002400	-1.50220400	0.58421300
S	-1.72440700	1.80922200	1.00652000
H	-1.84046500	-2.90945900	-2.05932200
H	2.30135100	3.24348400	-1.30026300
Cl	-4.46364000	0.44597600	0.16820100

TS59

C	3.04931400	1.91737900	0.69290900
C	3.53708500	0.67515000	0.33064200
C	2.66783000	-0.32396200	-0.07716400
C	1.30390600	-0.09441100	-0.12435900
C	0.82700700	1.16918200	0.25044700
C	1.68763600	2.17138300	0.64912200
H	4.59498700	0.46901800	0.35848400
H	-1.27596500	-1.27772900	1.85437600
Cl	3.29697800	-1.85844600	-0.54862000
H	-4.24547600	0.60715100	-1.15512600
C	-3.23892700	0.78276300	-0.81130900
C	-2.56197500	1.95162600	-1.16109100
C	-2.63911000	-0.13401900	0.00442900
C	-1.25342200	2.16393100	-0.73828400
C	-1.30023100	0.04961100	0.48511200
Cl	-3.46564300	-1.55045100	0.51366400
C	-0.61757000	1.24834500	0.06084300
H	1.29650600	3.13501900	0.93726400
H	-0.70281100	3.02246300	-1.09038600
H	-3.04864500	2.67315000	-1.79709500
H	3.73497400	2.68559300	1.01292900
S	0.10297100	-1.24084400	-0.67245300
O	-0.98788300	-0.37147100	1.73316000

TS60

C	3.05150300	2.07160500	-0.03414200
C	3.54902500	0.77348700	-0.06037400
C	2.68228000	-0.29977500	-0.07990600
C	1.31464600	-0.08221500	-0.07320300
C	0.81671800	1.22544200	-0.04532800
C	1.69322000	2.30396700	-0.02944900
H	4.61152300	0.59165700	-0.06494100
H	-1.78915300	0.66976300	2.17000600

Cl	3.29039400	-1.91043500	-0.12043000
H	-4.41015900	0.61367800	-0.52010400
C	-3.35637300	0.78124700	-0.36916500
C	-2.83772300	2.07997100	-0.36042400
C	-2.52157100	-0.29146900	-0.20302200
C	-1.48144600	2.31067400	-0.22451100
C	-1.14727500	-0.08037000	0.07824700
Cl	-3.11987500	-1.89309900	-0.23889500
C	-0.61972300	1.23883300	-0.07186100
H	1.31298500	3.31334900	-0.00705200
H	-1.09468000	3.31603100	-0.27985800
H	3.74215500	2.89943800	-0.01604800
H	-3.51192400	2.91108400	-0.49378700
O	-1.25154100	-0.11013700	1.99098900
S	0.08706600	-1.31013800	-0.11054900

TS61

C	-1.32111600	1.11508700	1.72010300
C	-2.65419600	1.12365900	1.91145400
C	-3.52244500	0.44695500	1.00183300
C	-3.07573000	-0.18206000	-0.11424200
C	-1.68245700	-0.14257100	-0.40861800
C	-0.75942000	0.32905400	0.63492300
H	-4.58515600	0.45830400	1.19199200
C	0.54586100	0.63460200	-0.05808800
C	1.62836000	-0.28801000	0.23966900
C	0.82441900	1.95424800	-0.53886500
C	2.90571500	0.10929500	-0.25679600
C	2.07516500	2.28869800	-0.93468600
H	0.00594700	2.65183700	-0.63930700
C	3.11300800	1.34018200	-0.80321900
H	4.10912300	1.59498700	-1.13072400
H	0.04957800	0.03150100	-1.12403500
H	-0.64951800	1.60094300	2.41085800
Cl	-4.14137400	-0.90114800	-1.24519000
Cl	4.24219200	-0.95783600	-0.08852900
H	-0.44744200	-0.68334200	1.12243900
S	1.33356500	-1.71164000	1.05585200
O	-1.14940800	-0.49149700	-1.47688800
H	-3.09105200	1.63323100	2.75472300
H	2.28985700	3.25866400	-1.35206100

TS62

C	1.60673000	-0.59842100	2.21974300
C	2.88747800	-0.38572100	1.66862900
C	3.05053100	0.06522900	0.39464400
C	1.93128100	0.40208600	-0.46112500
C	0.64981600	0.00999000	0.09181700
C	0.50650300	-0.36331300	1.44895700
H	3.76582500	-0.57282900	2.26775800
H	0.95234400	-1.37769700	-0.49414500
Cl	4.62316600	0.36458100	-0.23361900
H	-3.59297000	2.44421300	0.67618300
C	-2.75455400	1.90458600	0.26192800
C	-1.58628600	2.62257700	-0.11109400
C	-2.87860200	0.55799500	0.10617800
C	-0.54601900	1.95108700	-0.62449700
C	-1.82593800	-0.23290600	-0.43372400
C	-0.54449100	0.47791900	-0.75456200
H	0.36601100	2.43394200	-0.94146800
H	-0.48436000	-0.52466700	1.85049400
O	0.86372700	-2.36983800	-1.00819800
H	1.20553300	-3.06094500	-0.43512500
H	-0.15277000	-2.41147900	-1.04175500
H	-0.26289600	0.25303800	-1.78969100
Cl	-4.36234300	-0.18424100	0.56215500
S	-2.02225100	-1.85891900	-0.69050800
O	2.03595400	0.90381000	-1.58329300
H	-1.56040000	3.69155900	0.02310000
H	1.50956900	-0.93664200	3.23822300

TS63

C	-1.49146500	-1.58711500	-1.89588100
C	-2.75758700	-1.19047500	-1.42029800
C	-2.89357900	-0.26845400	-0.42552300
C	-1.77049000	0.37784400	0.19455400
C	-0.49310400	-0.17867600	-0.20005500
C	-0.38350900	-1.05326900	-1.32155600
H	-3.64969100	-1.61014600	-1.85855600
H	-0.62923000	-1.15925600	0.78539500
Cl	-4.48212500	0.18280000	0.05157000
H	4.21111100	1.70318400	-1.23347000
C	3.26000900	1.38211200	-0.83558100
C	2.09265600	2.17310100	-1.10019100
C	3.21711500	0.24794100	-0.10827500
C	0.90949400	1.80707800	-0.59997000

C	1.96699600	-0.25288300	0.42392100
C	0.74448700	0.59647200	0.23481800
H	0.01565600	2.39363600	-0.75159000
H	0.60116000	-1.34131800	-1.66243800
O	-0.41727900	-1.94770100	1.70706500
H	-0.72761000	-2.82919200	1.49668000
H	0.57809100	-1.89688300	1.61410600
H	0.48237200	0.98467200	1.23900000
Cl	4.62488000	-0.68912800	0.17744700
O	1.92603000	-1.32279100	1.02773000
S	-1.91027300	1.58970100	1.33289700
H	-1.41778000	-2.29468800	-2.70537800
H	2.19729700	3.06420900	-1.69752900
TS64			
C	-2.43056200	2.22714000	-1.02129700
C	-3.30894500	1.19560100	-0.75586200
C	-2.84297500	0.03111200	-0.17488200
C	-1.50053300	-0.12423300	0.18023500
C	-0.61515600	0.92846000	-0.10684700
C	-1.09274400	2.08531000	-0.70926100
H	-4.35487400	1.27765800	-1.00248400
H	0.28237000	-0.71994700	-1.57086300
Cl	-3.98455400	-1.22852000	0.11418700
H	4.57732600	0.66812900	1.08717600
C	3.52643900	0.73347600	0.85580300
C	2.71536900	1.66530000	1.47743300
C	2.99588500	-0.12766500	-0.08362100
C	1.37253600	1.71949000	1.15971100
C	1.64554200	-0.07793400	-0.41092100
Cl	4.00973600	-1.27035500	-0.87506500
C	0.82297900	0.84701400	0.23119600
H	-1.92705100	-1.71835200	1.87592600
H	-2.77492900	-1.71929400	2.81624600
H	0.72438700	2.43198700	1.64674000
H	-0.39348400	2.87753800	-0.92763000
S	-0.88501000	-1.58212400	0.95081800
O	1.19128300	-0.92425700	-1.34773300
H	-2.79008800	3.13404600	-1.48091400
H	3.13113900	2.33870800	2.20937400
TS65			
C	-1.81884100	2.98510600	0.24065200

C	-2.77687400	2.14034000	-0.28285000
C	-2.45509500	0.82108600	-0.53928700
C	-1.18307600	0.31189300	-0.26065800
C	-0.21588900	1.18659000	0.26165100
C	-0.54723400	2.51131800	0.50302300
H	-3.77177000	2.49274700	-0.49984800
H	2.13087200	-0.31248400	-2.22400100
Cl	-3.68584000	-0.18881300	-1.19231600
H	4.75878400	-0.37826000	1.42797600
C	3.75286700	-0.05862600	1.20910000
C	2.94252100	0.48446500	2.18714000
C	3.26435800	-0.19252500	-0.07469100
C	1.65525700	0.87976000	1.86856500
C	1.97447900	0.19989400	-0.40528800
Cl	4.26093800	-0.85511600	-1.32602000
C	1.15215600	0.73476200	0.58511700
H	-1.89833300	-1.94198500	0.23429500
H	1.01115400	1.29323700	2.62961800
H	0.21012000	3.17346600	0.89323300
S	-0.78488700	-1.36346200	-0.54705000
H	-1.75495200	-2.75271900	2.26162700
S	-2.84340100	-2.46574800	1.54032400
O	1.48420500	0.10073200	-1.64853500
H	-2.06410400	4.01716300	0.43619700
H	3.31273900	0.59273700	3.19366400

TS66

C	-1.85180400	2.86097300	0.76805600
C	-2.81290500	2.12532500	0.10240200
C	-2.50197200	0.86967300	-0.38130700
C	-1.22540400	0.32023400	-0.18983600
C	-0.24898800	1.08764500	0.47794600
C	-0.57753900	2.34975600	0.94360100
H	-3.80488800	2.51700200	-0.05128500
H	0.81211000	1.13311800	-1.65868000
Cl	-3.72135000	0.00260300	-1.21945200
H	4.66718500	-0.79869600	1.30647600
C	3.67153300	-0.41408400	1.15543900
C	2.82229300	-0.19621100	2.22503400
C	3.25353800	-0.13283100	-0.12995400
C	1.55113000	0.29360900	1.99897000
C	1.97713200	0.36282000	-0.36657000
Cl	4.31818300	-0.38225500	-1.45690800

C	1.11471900	0.56344700	0.70987000
H	-2.02139900	-1.92869600	-0.38131300
H	0.87024100	0.44906000	2.82154700
H	0.17859600	2.92846200	1.45033200
S	-0.80286100	-1.27520000	-0.73105900
Cl	-2.53451400	-2.73146300	1.09071400
O	1.62506800	0.62810300	-1.63582100
H	-2.09709100	3.84209000	1.14292800
H	3.15064200	-0.41714500	3.22756900
TS67			
C	-2.66526400	1.72494500	-1.46186500
C	-3.51814800	0.81431400	-0.86409300
C	-3.00334200	-0.11301100	0.01802900
C	-1.63693600	-0.13708600	0.32831700
C	-0.78271600	0.80550100	-0.26825300
C	-1.31123600	1.71725200	-1.16682100
H	-4.57398500	0.81327200	-1.08050900
H	-0.12599900	-1.35952700	-1.22441400
Cl	-4.03830100	-1.23831600	0.79509600
H	4.35611800	1.26267000	1.10306000
C	3.31774600	1.17145300	0.82896600
C	2.40809000	2.16584500	1.12425000
C	2.89436000	0.03854900	0.16278300
C	1.08688200	2.00653200	0.75405700
C	1.56675200	-0.14689800	-0.21838600
Cl	4.06362900	-1.17397800	-0.21629500
C	0.64931100	0.86462500	0.09616600
H	-1.51614100	-0.96881300	2.20646600
H	-1.81358500	-0.78027300	3.10539300
H	0.36373700	2.77319300	0.98694500
H	-0.64911700	2.42682300	-1.63837700
O	-1.13030700	-1.05800600	1.13002000
S	1.17944400	-1.60418400	-1.11358000
H	2.72713300	3.05625900	1.64170500
H	-3.06036500	2.44424800	-2.16167800
TS68			
C	2.44403500	-2.37048700	-0.93330200
C	3.33871600	-1.32815100	-0.76954600
C	2.89136100	-0.11748700	-0.28372000
C	1.54377400	0.06886400	0.05655000
C	0.64214300	-0.99755600	-0.10967500

C	1.10735800	-2.20178500	-0.60692000
H	4.38055900	-1.44398200	-1.02009400
H	-0.03930100	0.54745800	-1.86128600
Cl	3.98701400	1.18534900	-0.07510300
H	-4.41068600	-0.64052800	1.57638100
C	-3.39017800	-0.71557900	1.23763200
C	-2.48385200	-1.54274000	1.86915200
C	-2.98736100	0.02612200	0.14494000
C	-1.18488700	-1.60723200	1.40243500
C	-1.68363200	-0.02235000	-0.34420600
Cl	-4.15073800	1.03181100	-0.63992600
C	-0.76783300	-0.85413000	0.31340900
H	1.66225700	1.74451400	1.17591600
H	-0.46348800	-2.24140400	1.89453400
H	0.40936500	-3.01399400	-0.73860600
H	1.14537200	2.20719100	2.90323100
O	1.96769700	2.00195700	2.44539300
O	1.07470300	1.22612400	0.47541900
S	-1.31629800	0.92157200	-1.77529000
H	2.79116900	-3.31625200	-1.31791800
H	-2.78821400	-2.12946300	2.72098500

TS69

C	1.54282000	-2.61244000	1.34285500
C	2.71947000	-2.21147200	0.72503300
C	2.72545500	-1.06172000	-0.02769200
C	1.55285700	-0.28335100	-0.18130100
C	0.36895200	-0.69099300	0.48337200
C	0.38328700	-1.86070600	1.21941200
H	3.62400900	-2.78847500	0.82606100
H	-1.01443200	-2.16197400	-0.94167900
Cl	4.15514100	-0.53141000	-0.79789800
H	-3.93683200	2.44786000	0.59151000
C	-3.05833800	1.82490100	0.54728200
C	-1.83275500	2.28258400	0.99134800
C	-3.16199600	0.55130500	0.02595200
C	-0.73232200	1.45369500	0.92556100
C	-2.06262900	-0.30060400	-0.06122800
Cl	-4.70350400	0.01452800	-0.53457900
C	-0.83412300	0.16102900	0.42654100
H	2.27728000	1.62650700	-0.72037100
H	0.22812600	1.79815700	1.27883700
H	-0.52172200	-2.17681900	1.71529500

H	1.81192600	3.67004500	-0.39568500
S	2.88040000	2.94109400	-0.06017500
O	1.53321300	0.75299100	-0.95785200
S	-2.30987700	-1.87433400	-0.80670700
H	-1.74068000	3.27928900	1.39198000
H	1.53634700	-3.51306200	1.93628500
TS70			
C	2.11804500	-2.79599000	0.68691500
C	3.07164900	-1.96486200	0.12378300
C	2.72071100	-0.68930800	-0.25825000
C	1.39944200	-0.22150100	-0.06464900
C	0.42944200	-1.08680900	0.50277100
C	0.80851500	-2.35867700	0.86877800
H	4.08351400	-2.30282400	-0.02774500
H	-0.33575700	-1.14384800	-1.79492600
Cl	3.86512000	0.34691300	-0.97519800
H	-4.43066600	0.78327200	1.63935700
C	-3.45138200	0.39352800	1.41417200
C	-2.55568700	0.08660000	2.41831800
C	-3.09420900	0.19447300	0.09517800
C	-1.30742100	-0.40384800	2.08871200
C	-1.84213800	-0.29865700	-0.26253600
Cl	-4.24162400	0.56440300	-1.13752500
C	-0.93502600	-0.58630300	0.76422900
H	1.68259100	1.74023000	-0.28260100
H	-0.59042800	-0.62665100	2.86367800
H	0.07289500	-3.01845700	1.30118700
Cl	2.25915200	3.07285400	0.72734700
H	2.39438100	-3.79597700	0.98146100
H	-2.82662600	0.23893900	3.45043600
S	-1.52262100	-0.55943600	-1.96749200
O	1.01692200	0.96669000	-0.42051400
TS71			
C	-1.06505900	2.11317900	-0.97422900
C	-2.20328600	1.53608000	-0.33694500
C	-2.34974500	0.19848600	-0.26284800
C	-1.35328000	-0.69712900	-0.85768200
C	-0.11957400	-0.04793300	-1.32244400
C	-0.08091400	1.33350600	-1.51433500
H	-2.96561300	2.18160700	0.07063800
H	0.58934500	-0.70697900	-1.80167400

Cl	-3.72619900	-0.52369200	0.44509200
H	-0.55628600	0.03255500	2.05609900
C	0.26479500	0.45117900	1.49721200
C	0.54134000	1.78046100	1.52623300
C	1.02060800	-0.40916900	0.66986500
C	1.68409300	2.28485800	0.84438700
C	2.26619600	0.05539300	0.04477900
Cl	0.79898100	-2.08229600	0.88771200
C	2.50676100	1.46340400	0.15383000
H	3.39595400	1.83837500	-0.32663800
H	0.75981200	1.78101600	-2.01813100
H	1.90934700	3.33879700	0.90690200
S	3.32244900	-0.93717200	-0.73434700
H	-0.05914600	2.44272300	2.12959000
H	-1.02301700	3.18681300	-1.07210900
O	-1.51481200	-1.89653000	-0.95746600

TS72

C	-1.27627100	2.34252000	-0.63781700
C	-2.44289900	1.69623000	-0.07793900
C	-2.56917300	0.36319900	-0.07547400
C	-1.53833800	-0.49486100	-0.68950300
C	-0.18964400	0.14835400	-0.96257400
C	-0.23378500	1.63624100	-1.07274800
H	-3.23956000	2.30574900	0.32060300
H	0.18787800	-0.28955200	-1.88539600
Cl	-3.96616800	-0.42016100	0.52829500
H	-0.60884900	0.06593500	1.73986700
C	0.43272300	0.19308100	1.48938500
C	1.31063500	0.60809500	2.40720000
C	0.84932000	-0.18998600	0.12407400
C	2.70086600	0.73964800	2.07689900
C	2.26189000	0.19549000	-0.25204400
Cl	1.00597800	-2.08158700	0.22629400
C	3.14950500	0.53034800	0.82342700
H	4.18906000	0.66194400	0.57122700
H	0.80166600	-4.05885200	0.06787000
H	0.63116300	2.12218300	-1.49655700
H	3.39661700	1.02731400	2.85036400
S	2.78441800	0.18628900	-1.80139000
H	-1.27722600	3.41891300	-0.70816000
H	0.97981200	0.84016800	3.40706500
O	-1.75212500	-1.64435800	-0.97374600

TS73

C	1.42937800	-2.54662200	-0.67806900
C	2.57066200	-1.85867400	-0.11968900
C	2.62505100	-0.52113900	-0.05302900
C	1.53426300	0.30987900	-0.58310700
C	0.23010100	-0.39786600	-0.91374000
C	0.34645000	-1.87759700	-1.06976200
H	3.41203400	-2.43839300	0.22818800
H	-0.14668300	0.04232300	-1.83668000
Cl	3.99800100	0.30193100	0.55254600
H	0.56315500	-0.34608600	1.79230800
C	-0.47520300	-0.45292300	1.51790400
C	-1.39652800	-0.78378400	2.44563100
C	-0.84687000	-0.16789800	0.14799300
C	-2.76890800	-0.90842200	2.09168400
C	-2.23825500	-0.48294800	-0.24156200
Cl	-1.08913600	1.88530800	0.17204600
C	-3.16849700	-0.75399100	0.80718200
H	-4.20114300	-0.87613200	0.52385400
O	-0.33860500	3.75347100	-0.17964100
H	0.50312700	3.43680300	-0.53626500
H	-0.51002000	-2.38923600	-1.48117800
H	-3.49316000	-1.14507900	2.85541200
S	-2.72879700	-0.51471800	-1.82306500
H	-1.09280700	-0.95529600	3.46621100
H	1.47968100	-3.61947200	-0.77546300
O	1.66935600	1.49589200	-0.75711100

TS74

C	1.68050100	-2.52062100	-0.96321600
C	2.76636100	-1.81286200	-0.32355100
C	2.71081600	-0.49246000	-0.10200700
C	1.55465600	0.30232900	-0.54617500
C	0.30581500	-0.46656100	-0.94264700
C	0.54260600	-1.90241300	-1.27583600
H	3.65433500	-2.35893700	-0.04364100
H	-0.12773200	0.04946700	-1.79877100
Cl	4.01495700	0.36672000	0.59861700
H	0.69211900	-0.70769900	1.75292600
C	-0.33099700	-0.90278700	1.47098900
C	-1.18495100	-1.47218900	2.34294700
C	-0.76463300	-0.46368000	0.15318500

C	-2.54181300	-1.71014300	1.97836800
C	-2.12432500	-0.89875300	-0.27579100
Cl	-1.15646500	1.48657500	0.52571300
C	-2.98755900	-1.42640700	0.73281500
H	-4.00473700	-1.63374200	0.44295300
H	0.34354300	3.59192400	-0.37920600
H	-0.27049700	-2.43120300	-1.74845800
H	-3.21525800	-2.13865600	2.70435300
S	-0.93171100	3.87864900	-0.09322300
H	-0.84202600	-1.75047600	3.32687600
H	1.81823600	-3.56621000	-1.18887800
O	1.59738600	1.50470800	-0.60828600
S	-2.64205700	-0.75357900	-1.83239900
TS75			
C	2.21415400	-2.16098800	-0.91432200
C	3.14112800	-1.25054300	-0.27798800
C	2.84421700	0.04420200	-0.10900300
C	1.57125600	0.60236800	-0.60332600
C	0.48503500	-0.39580700	-0.97335700
C	0.98824800	-1.77366100	-1.26251400
H	4.10424000	-1.62027600	0.03899100
H	-0.03452700	0.00644200	-1.84144300
Cl	3.94911400	1.14994300	0.58541400
H	0.89840700	-0.30277000	1.73376300
C	-0.04781500	-0.75303800	1.47839400
C	-0.76043100	-1.42341300	2.41510900
C	-0.55311400	-0.55406900	0.13632800
C	-2.01430200	-2.00089500	2.09315500
C	-1.79081500	-1.30215000	-0.22588500
Cl	-1.36717900	1.28494600	0.45859800
C	-2.50805400	-1.93455500	0.82897300
H	-3.44996000	-2.39196800	0.57370900
Cl	-2.36981300	3.38981700	-0.18028500
H	0.30167900	-2.45666300	-1.73783100
H	-2.57528600	-2.50990700	2.86127300
H	2.54727500	-3.16773700	-1.11170800
H	-0.37038000	-1.51876200	3.41594700
S	-2.34877100	-1.37003700	-1.77605000
O	1.39197000	1.78468700	-0.71408200
TS76			
C	1.88488100	-1.81930000	-1.38767500

C	2.86459800	-1.02219100	-0.72248500
C	2.50334500	-0.05705400	0.14680800
C	1.09270800	0.18945700	0.47911300
C	0.09914300	-0.48217500	-0.42239200
C	0.56209200	-1.58692100	-1.21676500
H	3.91187000	-1.21050300	-0.90047800
H	-0.06145900	0.49733400	-1.26088400
Cl	3.66285300	0.86271200	0.99855600
H	-1.28702400	-2.26894800	1.20694900
C	-1.87345400	-1.42537400	0.87524900
C	-3.18077500	-1.26974300	1.30153700
C	-1.30771700	-0.47258600	0.04927000
C	-3.91499200	-0.16065400	0.90386500
C	-2.06218900	0.62066200	-0.38346100
C	-3.36348900	0.79426300	0.07145900
H	-3.93780900	1.65410300	-0.23475500
H	-0.17496900	-2.18590600	-1.72927700
H	-4.92989300	-0.03834900	1.24966800
S	-1.26566200	1.65188400	-1.53432500
H	-3.62232800	-1.99992500	1.96123400
H	2.21999600	-2.61538500	-2.03349000
O	0.75485000	0.90262800	1.39345700

TS77

C	1.59660800	-1.58146400	1.56572500
C	2.72498200	-0.94975200	0.98857700
C	2.58972500	0.14111600	0.19402400
C	1.30126400	0.76765900	-0.09113700
C	0.15788800	-0.04101600	0.34136700
C	0.35721200	-1.11056000	1.27259600
H	3.71642500	-1.32143600	1.19984100
H	0.46124500	-0.92531800	-0.85386000
H	-4.83058600	1.93327200	0.19434300
C	-3.83228100	1.52555400	0.17588000
C	-2.72138400	2.36397300	0.28349700
C	-3.63927100	0.17989900	0.03822300
C	-1.44165000	1.85054800	0.28308700
C	-2.33633900	-0.37130000	-0.02176700
C	-1.20536400	0.48180700	0.17602300
H	-0.59538900	2.50767600	0.38040700
H	-0.51507300	-1.56575700	1.71792000
O	0.50005400	-1.76343900	-1.62475200
H	1.21536000	-2.35104200	-1.36282600

H	-0.37776500	-2.16863500	-1.37764900
S	-2.25282800	-2.01979200	-0.45305000
O	1.20907600	1.80849200	-0.73017200
H	1.73256400	-2.40010400	2.25318900
H	-2.86160300	3.42828200	0.39454200
H	-4.47441500	-0.49406300	-0.06852500
Cl	3.97606600	0.92791800	-0.44857400
TS78			
C	2.19148200	2.27082300	0.57845800
C	2.92319000	1.16029100	0.14549800
C	2.29510200	0.00224100	-0.23995300
C	0.89162200	-0.06514300	-0.22994200
C	0.16811900	1.05967100	0.23978900
C	0.81805800	2.22696600	0.62196500
H	4.00045300	1.20216200	0.11368700
H	-2.05344200	-1.32639700	2.27855200
Cl	3.19314900	-1.35786000	-0.78105900
H	-2.00375600	2.71862600	-0.27272200
C	-2.21265700	1.65972100	-0.28372900
C	-3.39617200	1.18465000	-0.80238800
C	-1.22492200	0.76885600	0.11819100
C	-3.59309100	-0.19758800	-0.95937800
C	-1.49392200	-0.64439000	0.13250400
C	-2.66578000	-1.10042900	-0.51969400
H	-2.84577000	-2.16151800	-0.57576200
H	0.24988700	3.07408700	0.97482100
H	-4.51008200	-0.55434000	-1.40279100
S	-0.97509800	-1.63735200	1.54928900
H	-4.15187900	1.87425500	-1.14361000
H	2.71900900	3.15756000	0.89095600
O	0.21343100	-1.08215300	-0.64770900
TS79			
C	2.37423600	2.24172600	0.29732000
C	3.02232000	1.03692600	0.04969100
C	2.30187900	-0.12295300	-0.18465700
C	0.92665800	-0.04884300	-0.15754000
C	0.26559800	1.15704500	0.09378100
C	0.99462800	2.31816100	0.31473200
H	4.09926700	0.99008300	0.03726600
H	-1.46593900	0.00383300	2.29242800
Cl	3.08870600	-1.61335600	-0.51047900

H	-2.22886100	2.68013600	-0.16229600
C	-2.25589100	1.60536900	-0.25768700
C	-3.39935300	0.97163700	-0.73257700
C	-1.12820900	0.85511400	-0.03206700
C	-3.37253700	-0.39813300	-1.09458000
C	-1.19859300	-0.62519700	-0.04315600
C	-2.29483600	-1.17913200	-0.84721000
H	-2.25201100	-2.21915600	-1.12900600
H	0.49509800	3.25543200	0.50290200
H	-4.22824200	-0.81921800	-1.59885500
S	-1.48429400	-1.21379600	1.74789500
H	2.96489800	3.12562800	0.47755400
H	-4.28799500	1.55030600	-0.92739900
O	0.09113800	-1.07369500	-0.40213300
TS80			
C	0.23764500	-2.23075900	-1.10934900
C	1.41006700	-2.02938300	-0.33164400
C	1.91203600	-0.78726900	-0.12629400
C	1.27722400	0.37059300	-0.69550800
C	-0.04694900	0.14101300	-1.24454400
C	-0.44985300	-1.16927000	-1.59910700
H	1.93511600	-2.88154700	0.07024100
H	-0.49682600	0.98976100	-1.74139700
Cl	3.37110100	-0.60459200	0.75897400
H	0.02832300	-0.33445600	2.06573100
C	-0.82182700	-0.47532500	1.41751000
C	-1.50639300	-1.63799700	1.38356500
C	-1.18580300	0.58554500	0.53852300
C	-2.69760000	-1.76345600	0.59138200
C	-2.46897100	0.52140800	-0.23038500
Cl	-0.68615300	2.15348700	0.96178600
C	-3.16413200	-0.75291100	-0.16258900
H	-4.07767000	-0.82755300	-0.73062000
H	-1.32827300	-1.30476400	-2.20810900
H	-3.24191700	-2.69555400	0.63000200
H	-1.20708000	-2.45823900	2.01659000
H	-0.07063600	-3.23987800	-1.33353100
O	-2.87022400	1.46801500	-0.88268300
S	1.92524900	1.87773400	-0.72185700
TS81			
C	-0.80427800	-2.25593500	1.26081100

C	-1.89869000	-1.95284600	0.37597500
C	-2.17500300	-0.68939300	-0.00022000
C	-1.40009600	0.42958000	0.50280700
C	-0.04607900	0.07866600	1.06660400
C	0.05985600	-1.30528100	1.61675200
H	-2.54064300	-2.75176700	0.03891800
H	0.21697600	0.80442900	1.83221500
Cl	-3.53626700	-0.38475800	-1.00293800
H	-0.12704500	-0.54083000	-1.67798700
C	0.86224900	-0.55891300	-1.24797400
C	1.87285500	-1.16813300	-1.87429700
C	1.07443000	0.18288000	0.00684100
C	3.21183300	-1.15318300	-1.33148500
C	2.43429200	-0.01376800	0.66501800
Cl	1.23507200	1.99705400	-0.55500500
C	3.49375900	-0.58395800	-0.15181900
H	4.48317600	-0.58642200	0.27602400
H	1.12881900	3.86058600	-0.81522800
H	0.89170200	-1.50902300	2.27213500
H	3.99964100	-1.62300400	-1.90141100
H	-0.70505800	-3.26428200	1.63042700
H	1.70019100	-1.67128600	-2.81255000
O	2.59791900	0.30293100	1.82128900
S	-1.92634700	1.96192800	0.48363000

TS82

C	1.32029100	-2.44597000	-1.11615900
C	2.32200900	-1.90728100	-0.23556300
C	2.37133900	-0.59503500	0.06864500
C	1.42772400	0.34342300	-0.50475100
C	0.17080100	-0.26667800	-1.07454400
C	0.31642900	-1.67925600	-1.54287500
H	3.08322700	-2.56268300	0.15820000
H	-0.18445300	0.35609700	-1.89181900
Cl	3.64260000	-0.00740200	1.06247100
H	0.24200000	-0.61404000	1.71224000
C	-0.73587900	-0.76722800	1.28353100
C	-1.73630400	-1.30091200	2.02486700
C	-0.97377500	-0.31857400	-0.05955000
C	-3.05161600	-1.47746000	1.48590900
C	-2.28781300	-0.69440100	-0.68534300
Cl	-1.46426500	1.66636400	0.36047000
C	-3.33223600	-1.16692300	0.20739100

H	-4.30823400	-1.31160800	-0.22672700
O	-1.62701000	3.57683700	-0.02384400
H	-0.78812700	3.69447800	-0.48621000
H	-0.45827000	-2.05521800	-2.19197100
H	-3.82379700	-1.87385900	2.12747100
H	-1.54575800	-1.59286700	3.04549400
H	1.40291700	-3.47655100	-1.42284200
O	-2.44410100	-0.60371700	-1.88693500
S	1.69074200	1.94416900	-0.55230800

TS83

C	2.08810100	-2.12310600	-1.19089900
C	2.91259500	-1.35672200	-0.29467200
C	2.60075500	-0.09196400	0.05091300
C	1.43144000	0.56766100	-0.49715700
C	0.38179100	-0.34865800	-1.07676300
C	0.90678100	-1.65105300	-1.59121900
H	3.82853400	-1.78895600	0.07722100
H	-0.15080500	0.17384500	-1.86776300
Cl	3.66796800	0.79376800	1.06386800
H	0.61713500	-0.77431900	1.69049800
C	-0.28626000	-1.18180000	1.26522400
C	-1.06894500	-2.01433000	1.98519900
C	-0.68112700	-0.75402300	-0.05403000
C	-2.29595600	-2.53336700	1.45310900
C	-1.84530100	-1.47050500	-0.68514200
Cl	-1.70970800	0.98231100	0.43636700
C	-2.68968700	-2.25748000	0.19772400
H	-3.59433700	-2.65744100	-0.23084900
H	-1.57212400	3.53335100	-0.49912100
H	0.25982800	-2.20711700	-2.25049000
H	-2.90509100	-3.16432800	2.08251500
S	-2.73597600	3.09690800	-0.00605700
H	-0.77583800	-2.29105700	2.98558200
H	2.44858300	-3.08085200	-1.53127900
O	-2.04617500	-1.38177800	-1.87925700
S	1.24835000	2.17870800	-0.51269100

TS84

C	2.22337600	-2.08438900	-1.09695800
C	2.98855300	-1.26481900	-0.19274100
C	2.62609800	0.00088800	0.09188600
C	1.46521600	0.60740200	-0.53538900

C	0.45863700	-0.36600100	-1.10128200
C	1.04272800	-1.66808800	-1.55617600
H	3.89905100	-1.65749100	0.23222800
H	-0.07636600	0.10977400	-1.91923600
Cl	3.61595100	0.95621300	1.11921300
H	0.62871100	-0.60180200	1.69514800
C	-0.24750500	-1.06647800	1.27201400
C	-1.04298600	-1.85840500	2.04133800
C	-0.59694200	-0.77512300	-0.08298500
C	-2.23286700	-2.45444100	1.52206600
C	-1.73521400	-1.55510900	-0.68316300
Cl	-1.73461000	0.96293100	0.35069400
C	-2.58910000	-2.29321600	0.23322700
H	-3.47159700	-2.74534400	-0.18950200
Cl	-3.00447600	2.85545300	-0.02830100
H	0.44204400	-2.26501000	-2.22332800
H	-2.84753600	-3.04525500	2.18360300
H	2.63011700	-3.03722600	-1.39691100
H	-0.77643600	-2.03456000	3.07146700
O	-1.90845500	-1.56079400	-1.88409700
S	1.23581100	2.20386200	-0.64743800

TS85

C	1.82462100	2.43381400	-0.14876500
C	2.75208000	1.36631500	-0.09682600
C	2.35941500	0.06261500	-0.03332600
C	0.98071800	-0.27983400	-0.03820200
C	0.04915600	0.81533800	0.07505800
C	0.49808200	2.16707800	-0.10072300
H	3.80900000	1.58315700	-0.12594900
H	-0.23460200	0.73365300	1.31334900
Cl	3.53409600	-1.19004800	-0.04312500
H	-1.49179600	0.60152900	-2.35891100
C	-2.00645900	0.34430800	-1.44653000
C	-3.32208200	-0.07017500	-1.47006900
C	-1.34656000	0.38717000	-0.23338600
C	-3.98914800	-0.44062900	-0.28332000
C	-2.03978100	0.09233400	0.99613600
C	-3.38036100	-0.37330100	0.93455400
H	-3.88981000	-0.62694100	1.84949800
H	-0.23554500	2.95873600	-0.12751900
H	-5.01388300	-0.77363600	-0.34709700
H	-3.85044200	-0.12579000	-2.40874700

H	2.18946700	3.44514600	-0.22166900
O	-1.38836200	0.31069500	2.05219200
S	0.34167500	-1.81754900	-0.13656100
TS86			
C	1.39865100	2.00096600	-1.41254500
C	2.52601700	1.23877900	-1.03069200
C	2.40217700	0.07753500	-0.33438900
C	1.12969900	-0.46578900	0.06812100
C	-0.00530300	0.39009900	-0.24852900
C	0.16689300	1.56523700	-1.06203300
H	3.51482500	1.57500200	-1.30144400
H	0.13581400	1.05759700	0.95010700
H	-5.08581800	-1.35243700	-0.54542800
C	-4.07150400	-0.99869400	-0.44418100
C	-3.00325400	-1.81292400	-0.87137000
C	-3.81973400	0.22411900	0.08614000
C	-1.69428100	-1.39262300	-0.75331200
C	-2.47259800	0.69091300	0.24108400
C	-1.38348200	-0.14772300	-0.23073500
H	-0.89281200	-2.03085300	-1.08628500
H	-0.71733300	2.11739500	-1.34287300
O	-0.02419800	1.73054400	1.99007800
H	0.55767400	2.49153900	1.99478500
H	-0.94082700	2.00582200	1.72142500
O	-2.26381900	1.79464500	0.80486800
S	0.98584500	-1.86623900	0.95049400
H	1.52913800	2.90111800	-1.99082700
H	-3.21196400	-2.77418700	-1.31441100
Cl	3.83556500	-0.79013100	0.05119300
H	-4.60236200	0.88017400	0.43183600
TS87			
C	2.13709200	2.35305200	0.31028500
C	2.89289600	1.21581900	0.08274500
C	2.27364800	-0.00635900	-0.12023000
C	0.89073500	-0.10845800	-0.09797200
C	0.14028400	1.05574300	0.13620500
C	0.75411000	2.27744100	0.33542100
H	3.96970500	1.26613300	0.06009700
H	-0.35794000	-0.41712600	2.11130400
Cl	3.22978200	-1.40630500	-0.42609100
H	-1.87367400	2.27855100	-1.29386600

C	-2.17529800	1.37622600	-0.78336700
C	-3.42262100	0.81163700	-1.03922800
C	-1.28560700	0.76155500	0.06013600
C	-3.77173400	-0.41463400	-0.45933300
C	-1.63707800	-0.49833200	0.69515500
C	-2.92451300	-1.05264400	0.39781700
H	-3.20521200	-1.95853300	0.91021600
H	0.15618100	3.15694200	0.51888700
H	-4.73879900	-0.84471300	-0.66895100
H	-4.10891900	1.30630200	-1.70758800
H	2.63284800	3.29662900	0.47319700
O	-1.25667400	-0.72646600	1.97864100
S	-0.03491000	-1.56197200	-0.38091700
TS88			
C	2.08579100	2.43456100	0.12094000
C	2.90052900	1.31066600	0.04108700
C	2.33703000	0.05571100	-0.06711000
C	0.96027800	-0.08229500	-0.09498000
C	0.14049500	1.04957600	-0.01252000
C	0.71298400	2.31218600	0.09188500
H	3.97399400	1.40641900	0.06358700
H	-2.30787700	-0.36298300	2.07599100
Cl	3.33514200	-1.34394200	-0.17536300
H	-2.24911200	2.58528000	-0.20371300
C	-2.36177200	1.51204100	-0.21244600
C	-3.60922400	0.94666100	-0.40158300
C	-1.25027200	0.69423200	-0.08600300
C	-3.76665200	-0.44420800	-0.48772400
C	-1.42916300	-0.72173200	-0.02442700
C	-2.69300700	-1.28033000	-0.34509000
H	-2.80229100	-2.35097400	-0.40348700
H	0.08596400	3.18787300	0.15678200
H	-4.74408100	-0.85853900	-0.67808800
H	2.53984400	3.40870300	0.20841500
H	-4.47130600	1.58495800	-0.51544300
O	-1.53861100	-0.90847200	1.87751500
S	0.08901400	-1.57552300	-0.24219800

Table S5. Cartesian coordinates for the reactants, intermediates and products involved in the formation of PCPT/DT/DFs from cross-condensation of 2-CPR and 2-CTPR.

IM1			
C	-1.19329400	-0.29057800	-0.65423400
C	-1.81026500	0.91900600	-0.36487400
C	-3.12727000	0.94584300	0.05452000
C	-3.83037600	-0.23783500	0.17739900
C	-3.22243100	-1.44349500	-0.13132900
C	-1.90838000	-1.47047500	-0.55470400
Cl	-0.92724600	2.38616300	-0.53043900
H	-3.58874000	1.89359800	0.27932800
H	-1.41826000	-2.39524400	-0.80796600
C	1.20839200	-0.57670900	-0.41729700
C	2.33852800	-0.26964200	-1.33886300
C	3.27790600	0.61951900	-1.03473400
C	3.23520100	1.34073000	0.21408100
C	2.27384700	1.12016000	1.12673100
C	1.25251600	0.12815600	0.93874900
Cl	1.31361200	-2.36239500	-0.10752400
H	2.31743700	-0.79947700	-2.27737000
H	2.25090100	1.65875200	2.06020500
H	3.99848300	2.07750400	0.41298100
H	-3.77430100	-2.36638800	-0.04890000
S	0.17938300	-0.22333800	2.10463400
H	-4.85760900	-0.21436000	0.50525700
H	4.07571300	0.82387700	-1.73099100
O	0.07397000	-0.27712300	-1.16424600
IM2			
C	1.64263700	0.13215700	0.16191000
C	2.93216300	-0.26873900	-0.17638900
C	4.02086000	0.51039900	0.16041000
C	3.83993100	1.69832400	0.84623000
C	2.56179300	2.10315800	1.18140500
C	1.46758900	1.32995100	0.83500300
Cl	3.16916700	-1.75645900	-1.01047300
H	5.00703800	0.17211600	-0.11387300
H	0.47211100	1.68182300	1.05519100
C	-0.58828600	-0.63412100	0.45622700
C	-1.02239200	-2.01556000	0.79831000
C	-2.31351800	-2.28405900	0.97959800

C	-3.30353800	-1.26828400	0.72736700
C	-2.98765000	-0.08688600	0.16122300
C	-1.62674700	0.21418100	-0.24815100
H	-4.33884300	-1.47987800	0.94470100
H	-0.46086000	-0.13427000	1.43138800
Cl	-4.23766000	1.02207100	-0.23168800
H	2.40452600	3.03460300	1.70199200
H	-0.23928000	-2.73768800	0.96633800
S	-1.22247600	1.36498000	-1.30962500
H	4.69395200	2.30149900	1.10932800
H	-2.64281000	-3.25769300	1.30488900
O	0.63639000	-0.68984000	-0.20350900

IM3

C	0.97492200	0.05540900	-0.41629300
C	2.25290100	-0.39438400	-0.11232600
C	3.31907000	0.48305000	-0.12891900
C	3.12003000	1.81382600	-0.45082300
C	1.84826400	2.25957300	-0.76158900
C	0.77791100	1.38416200	-0.74970800
Cl	2.50100500	-2.04803400	0.28858800
H	4.30131900	0.11210700	0.11545400
H	-0.21529600	1.72710500	-0.99403100
C	-1.31621300	-0.47642000	-0.40120900
C	-2.09007400	-0.77249800	-1.50279100
C	-3.43923300	-0.45742700	-1.50567000
C	-4.01975400	0.16277100	-0.40600300
C	-3.24924700	0.45302500	0.69607500
C	-1.87945900	0.13223200	0.74330300
H	-1.62195500	-1.25258500	-2.34708500
H	-3.68100500	0.92274700	1.56562800
H	1.68172400	3.29390200	-1.01834100
H	-5.06946500	0.40979600	-0.41282600
S	-0.96690800	0.43066700	2.14935400
H	3.95646200	2.49407800	-0.45850300
H	-4.03771000	-0.69415200	-2.37173200
O	-0.01941900	-0.86837600	-0.42481200

IM4

C	0.92786500	0.17905000	0.17905000
C	2.18717100	0.60881200	0.60881200
C	3.27125000	-0.27329000	-0.27329000
C	3.06154900	-1.61924100	-1.61924100

C	1.82928700	-2.08985400	-2.08985400
C	0.63417900	-1.22671900	-1.22671900
Cl	2.44820400	2.25636600	2.25636600
H	4.25289100	0.09106400	0.09106400
H	0.05099100	-1.28435800	-1.28435800
C	-1.38665500	0.64666300	0.64666300
C	-2.33362300	1.59801000	1.59801000
C	-3.67588200	1.30990200	1.30990200
C	-4.07670300	0.06512500	0.06512500
C	-3.12916800	-0.88715300	-0.88715300
C	-1.77181400	-0.60979700	-0.60979700
H	-1.99025200	2.55896400	2.55896400
H	-3.43114300	-1.86618300	-1.86618300
H	-5.12488000	-0.16753700	-0.16753700
H	1.67953100	-3.11933200	-3.11933200
S	-0.56673400	-1.81087500	-1.81087500
O	-0.08934900	1.05270400	1.05270400
H	3.91031900	-2.28438100	-2.28438100
H	-4.40912800	2.05685300	2.05685300

IM5

C	0.90691000	-0.44813400	0.23947800
C	1.59048200	0.83667700	-0.06932200
C	2.94247300	0.94631500	-0.16742400
C	3.76552200	-0.14778500	0.11938300
C	3.19581500	-1.35876800	0.56143800
C	1.85544900	-1.50100000	0.66577100
Cl	0.57523400	2.18047200	-0.36990600
H	3.37297800	1.89277300	-0.45317100
H	1.40106800	-2.41140900	1.02234900
C	-1.34971500	-0.18438400	0.74287400
C	-2.40982100	0.22118100	1.51857500
C	-3.67124200	0.25374300	0.93867800
C	-3.85224600	-0.10871000	-0.38433500
C	-2.77243400	-0.51584500	-1.15666100
C	-1.51960500	-0.55540200	-0.58035200
H	-2.24766300	0.50680400	2.54512100
H	-2.90986400	-0.79692300	-2.18866300
H	3.83989600	-2.17820400	0.84011900
S	-0.00624500	-1.05932900	-1.28912000
H	-4.83624000	-0.07305600	-0.82430400
H	4.83528800	-0.04753500	0.03678800
H	-4.51545800	0.57186400	1.52997000

O	-0.08857500	-0.27629900	1.22968600
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IM6

C	1.06767700	0.04033000	-0.38659100
C	2.36389000	-0.21427300	0.04199800
C	3.31040800	0.79497100	0.08084000
C	2.96868400	2.07470900	-0.30710100
C	1.68212500	2.33979000	-0.74707200
C	0.74618800	1.32814800	-0.79647800
Cl	2.83339300	-1.80188500	0.52954100
H	4.30676900	0.56497700	0.42191800
H	-0.25151700	1.53323100	-1.15258200
C	-1.62527200	-0.52069300	-0.23220400
C	-2.68270200	-0.87884500	-1.04507400
C	-3.96145900	-0.39051400	-0.81093200
C	-4.21226300	0.49107500	0.25157300
C	-3.19765400	0.86126200	1.08061600
C	-1.85924600	0.35311500	0.91138500
H	-2.50498900	-1.53515100	-1.88316900
H	-3.34900000	1.53174400	1.91191200
H	1.40786600	3.33475900	-1.06053300
H	-5.21028900	0.87066000	0.40653400
H	3.70715100	2.85979000	-0.26956900
H	-4.76588600	-0.68026600	-1.46884800
O	-0.96517000	0.63708700	1.71658200
S	-0.08679300	-1.28867600	-0.49289300

IM7

C	-1.00997600	-0.09619500	0.16226600
C	-2.35892400	-0.22064000	-0.02186600
C	-3.20922800	0.88484100	-0.02161100
C	-2.66333400	2.17619000	0.14242100
C	-1.34106400	2.36462600	0.33626400
C	-0.39006000	1.23269900	0.43483700
Cl	-3.04014600	-1.78768700	-0.28098100
H	-4.26486200	0.74178200	-0.17720800
H	0.05059500	1.20516400	1.44212500
C	1.61482100	-0.65410100	0.10212000
C	2.74867300	-1.42569200	0.32921300
C	4.00823200	-0.88474100	0.16911200
C	4.14657100	0.44017000	-0.21698600
C	3.02683800	1.22196200	-0.42038600
C	1.76274000	0.68191600	-0.25694200

H	2.63420000	-2.45960100	0.61886700
H	3.10372600	2.25960100	-0.70403800
H	5.12796700	0.86875700	-0.34611900
H	-0.91942600	3.35136500	0.44429400
O	0.69172600	1.48172100	-0.46230600
S	0.05320100	-1.45546400	0.14505100
H	-3.32545000	3.02719600	0.10120200
H	4.87898600	-1.49614300	0.34452800

IM8

C	-1.32359000	0.24017200	-0.64552700
C	-1.62113500	-0.83011000	0.19131700
C	-2.77390700	-0.82848400	0.95612000
C	-3.65563700	0.23172500	0.87056200
C	-3.38353600	1.29331400	0.02504500
C	-2.22137500	1.29583300	-0.72016400
Cl	-0.57033000	-2.19330000	0.30896800
H	-2.97467800	-1.66515900	1.60541400
C	1.46408700	1.02053400	0.59592500
C	2.64911300	0.93908000	1.41161300
C	3.72966200	0.20817000	1.02461100
C	3.69457400	-0.50704600	-0.18296400
C	2.56160300	-0.50045900	-0.98347800
C	1.44391200	0.22419400	-0.62034000
H	2.63558400	1.50684500	2.32858200
H	-4.06521700	2.12633300	-0.04163600
H	-1.97972200	2.13270100	-1.35569800
H	2.53998900	-1.08802900	-1.88859400
H	4.55055300	-1.09039500	-0.48475500
S	0.08506500	0.25997300	-1.70995600
H	-4.55470200	0.22497000	1.46669900
H	4.61511100	0.17287500	1.64022700
O	0.52312700	1.76060900	0.91253400

IM9

C	-1.52398300	0.27371300	0.36298000
C	-2.76082600	0.12504800	-0.24908500
C	-3.72478600	-0.67928600	0.32648800
C	-3.46313100	-1.33797800	1.51478500
C	-2.23279900	-1.18343100	2.12704200
C	-1.26545600	-0.37607600	1.55658500
Cl	-3.08093300	0.93854000	-1.72886500
H	-4.67647300	-0.78536000	-0.16872400

H	-0.30464400	-0.25056600	2.03103500
C	0.68069300	1.03359000	0.08477400
C	1.24065700	2.11029100	0.73283500
C	2.59533700	2.10314800	1.02067900
C	3.38819700	1.02344700	0.66860600
C	2.82578200	-0.05074100	0.01255200
C	1.45035100	-0.08625500	-0.32198500
H	4.44090000	1.01325500	0.89704800
Cl	3.85136200	-1.35677200	-0.41263000
H	-2.01896100	-1.68951300	3.05522000
H	0.60757000	2.93969300	1.00221600
S	0.73996000	-1.35738800	-1.19194500
H	3.03954400	2.94421600	1.52942100
H	-4.21950600	-1.96713800	1.95571600
O	-0.63316300	1.11134200	-0.23036400
IM10			
C	-1.45173600	0.16833700	0.28310300
C	-2.74732000	0.28005100	-0.12362700
C	-3.60906800	-0.82093200	-0.07689100
C	-3.13343300	-2.05253400	0.40876900
C	-1.85409500	-2.20682600	0.82716800
C	-0.88053900	-1.10014400	0.76060300
Cl	-3.33140500	1.78796200	-0.71344000
H	-4.62550600	-0.70860100	-0.41296900
H	-0.37695000	-0.95060700	1.71925300
C	0.70588800	1.13582000	0.27626400
C	1.38190900	2.30387500	0.58169500
C	2.75884700	2.32929900	0.53251900
C	3.46690900	1.19302700	0.18038200
C	2.77949100	0.03120700	-0.10359000
C	1.38782000	-0.03373700	-0.05706400
H	4.54291600	1.19764900	0.12953100
Cl	3.67098900	-1.37744800	-0.54424700
H	-1.50234800	-3.15043300	1.21301900
H	0.80389400	3.17799900	0.83365600
S	0.51738400	-1.51298700	-0.39357600
H	3.28787500	3.23992700	0.76336700
H	-3.81454600	-2.88777100	0.46080700
O	-0.64930800	1.24327800	0.25440300
IM11			
C	1.30863700	-0.03449700	-0.51980700

C	2.03567000	0.35221200	0.71919300
C	3.34684600	0.05669200	0.92577100
C	4.10373800	-0.55319000	-0.07988100
C	3.51917900	-0.82274700	-1.33390900
C	2.21719300	-0.54682800	-1.56953200
Cl	1.11398400	1.14910500	1.91975200
H	3.80023800	0.31504700	1.86938400
H	1.75725200	-0.72634300	-2.52806800
C	-1.22707700	-0.20369400	-0.26096400
C	-2.56899600	-0.34516500	0.01840800
C	-3.43819800	0.71607600	-0.18678500
C	-2.94718500	1.91238400	-0.67429900
C	-1.59874800	2.07471200	-0.96330600
C	-0.76116000	1.00681900	-0.74990200
H	-1.20481400	3.00372000	-1.34048900
H	4.12520500	-1.23762000	-2.12413100
H	-4.48471100	0.59369600	0.03801100
Cl	-3.15407200	-1.85270000	0.61269200
S	0.04734800	-1.37750000	-0.11956800
H	5.14205100	-0.78078400	0.09701600
H	-3.62500000	2.73649600	-0.83000700
O	0.55928800	1.05253100	-1.03376400

IM12

C	-1.34696500	-0.22153800	0.49114300
C	-1.28293500	0.65237600	1.56804200
C	-2.37964800	1.40792200	1.92965100
C	-3.56704700	1.27429500	1.22983500
C	-3.65248600	0.38803800	0.17407400
C	-2.54594600	-0.35660400	-0.19548200
H	-2.31030100	2.08987300	2.76235600
C	1.00628300	1.21919200	-0.87032800
C	2.08592400	2.15784000	-1.03628000
C	3.35094700	1.85417500	-0.64276300
C	3.62434800	0.61573400	-0.04569000
C	2.60922700	-0.30239300	0.17775900
C	1.29382100	-0.03164700	-0.16683900
H	-4.57035400	0.27237000	-0.37896900
H	4.15768200	2.55449400	-0.79094500
H	-4.43218500	1.85583000	1.50718500
H	4.62701300	0.36451500	0.25976200
O	-0.11309300	1.45422500	-1.33376200
S	0.05821600	-1.21704000	0.09251100

H	-0.35796300	0.73554000	2.11795000
H	1.83608700	3.09063900	-1.51553700
Cl	-2.68870200	-1.43574000	-1.52934900
Cl	3.03282800	-1.80360000	0.91460600
IM13			
C	-1.33405400	-0.05739200	0.14273000
C	-2.61528200	-0.48630400	-0.06244600
C	-3.70590200	0.37808300	0.03012700
C	-3.48536400	1.74227800	0.31601300
C	-2.24408200	2.22734400	0.53053900
C	-1.04690700	1.35407800	0.52407900
Cl	-2.90892200	-2.14240300	-0.45679600
H	-4.69828700	-0.00082900	-0.14478700
H	-0.58148600	1.35530700	1.51993300
C	1.33144200	0.02382000	-0.01590900
C	2.63872100	-0.44884700	0.07757900
C	3.72662400	0.37960000	-0.10036100
C	3.51645100	1.71790200	-0.38118700
C	2.23370900	2.22028500	-0.46047900
C	1.14849800	1.38300600	-0.27242500
H	2.04216600	3.26154400	-0.66308100
H	4.36050500	2.37299300	-0.52650000
H	-2.07176000	3.27257000	0.73267300
O	-0.08479900	1.92468700	-0.36413300
S	0.01390600	-1.13175300	0.05238100
H	4.72074100	-0.02799800	-0.02373700
H	-4.33420300	2.40729800	0.35366600
Cl	2.91098700	-2.12427000	0.38957600
IM14			
C	-1.57846600	-0.60616200	0.36116000
C	-2.53158700	-0.80820800	1.34820300
C	-3.83364600	-0.38010400	1.17357900
C	-4.19361000	0.26761900	0.00579500
C	-3.25592700	0.47224500	-0.98918000
C	-1.95968400	0.02475800	-0.81839300
H	-4.55949300	-0.54181300	1.95462800
C	0.81181700	1.34963700	0.76399200
C	1.82448800	2.35157300	0.55648600
C	3.07833600	2.01672500	0.15324300
C	3.40382600	0.67409800	-0.08408100
C	2.44951200	-0.32034900	0.06160600

C	1.14733800	-0.03364700	0.43804300
H	1.53438300	3.36872300	0.76488100
H	-3.52202600	0.97182800	-1.90651300
Cl	-0.82890600	0.28550700	-2.09339300
H	-2.23406800	-1.29168000	2.26518800
H	4.39807800	0.39743200	-0.39504000
Cl	2.93078800	-1.94801200	-0.25000800
S	0.01133700	-1.33215500	0.60163000
H	-5.20459800	0.61545800	-0.13686600
H	3.83522500	2.77309000	0.01840600
O	-0.29190900	1.65436700	1.22804100
IM15			
C	-1.27956900	-0.29355900	-0.64090100
C	-1.90922000	0.86895300	-0.19705600
C	-3.16960900	0.81544600	0.36952400
C	-3.81390700	-0.39987100	0.49969600
C	-3.20949500	-1.56256400	0.05536700
C	-1.95407900	-1.50349800	-0.51570000
Cl	-1.15447200	2.41091700	-0.34540600
H	-3.63409300	1.72713400	0.70774700
H	-1.47502500	-2.39813600	-0.87874400
C	1.45063000	-0.71915700	-0.05845500
C	2.79023700	-0.62567800	-0.69545900
C	3.55029400	0.45792700	-0.54667700
C	3.12860700	1.56186500	0.28851300
C	2.00664300	1.50691000	1.01491600
C	1.19094200	0.29596700	1.04893900
Cl	1.18363900	-2.36332400	0.55444500
H	3.08556600	-1.45314300	-1.32102400
H	1.70310700	2.30018100	1.67867800
H	3.75522700	2.44001800	0.33226400
H	-3.71406300	-2.51106800	0.14789300
H	-4.79577200	-0.43312600	0.94564500
H	4.50125900	0.52101600	-1.05178000
O	0.32746400	0.11457700	1.86943600
S	0.29808800	-0.27093900	-1.42537900
IM16			
C	-1.87358400	-0.56219400	-0.34652600
C	-2.70740300	0.55126500	-0.26704200
C	-3.98580300	0.44243300	0.25695900
C	-4.44365500	-0.77861800	0.71180500

C	-3.63069400	-1.89730000	0.63993200
C	-2.36190500	-1.78448600	0.10738500
Cl	-2.18765900	2.10258600	-0.80889300
H	-4.61100300	1.31922300	0.30395400
H	-1.72367700	-2.65124200	0.02388400
C	0.72843600	-0.46174900	0.51108700
C	0.57105600	0.85863700	1.15984100
C	1.58846600	1.71496500	1.25376700
C	2.89802400	1.37501300	0.75144500
C	3.16609900	0.17773300	0.20996600
C	2.14110600	-0.86722000	0.13016500
H	3.68817800	2.10691300	0.82230200
H	0.33382600	-1.26463700	1.13075600
Cl	4.72930700	-0.23368900	-0.35401300
H	-3.98672700	-2.85521700	0.98457600
H	-0.41301500	1.11804600	1.52014200
H	-5.44039200	-0.85404800	1.11781900
H	1.45080100	2.68775300	1.69817500
O	2.37741500	-1.99463100	-0.22149000
S	-0.25413700	-0.50199200	-1.04831300

IM17

C	-0.90696400	-0.44814200	0.23950700
C	-1.59045800	0.83668500	-0.06935100
C	-2.94244900	0.94637200	-0.16747900
C	-3.76555200	-0.14767500	0.11934200
C	-3.19591600	-1.35868100	0.56144700
C	-1.85555900	-1.50096500	0.66580200
Cl	-0.57516000	2.18043500	-0.36994900
H	-3.37290100	1.89284300	-0.45326300
H	-1.40121300	-2.41137900	1.02240900
C	1.51960000	-0.55544000	-0.58031200
C	2.77241400	-0.51590000	-1.15665400
C	3.85224600	-0.10872200	-0.38437800
C	3.67127200	0.25378800	0.93862500
C	2.40986800	0.22123400	1.51855500
C	1.34973500	-0.18436800	0.74290100
H	2.90980600	-0.79700600	-2.18865400
H	2.24773900	0.50689500	2.54509500
H	-3.84004000	-2.17807900	0.84013900
H	4.51550500	0.57193300	1.52988300
H	-4.83531000	-0.04737300	0.03671000
H	4.83623000	-0.07307200	-0.82436500

O	0.08859400	-0.27631900	1.22976200
S	0.00623400	-1.05942100	-1.28905900
IM18			
C	-1.19350500	0.00389500	-0.77646000
C	-1.55175600	-0.83440800	0.26927700
C	-2.82742500	-0.76518000	0.80229000
C	-3.75827300	0.10613500	0.27125800
C	-3.41341700	0.90872400	-0.80389600
C	-2.13713800	0.85442800	-1.32307700
Cl	-0.43278000	-1.97529200	0.91621800
H	-3.08084100	-1.41344200	1.62563600
C	1.50256200	0.84849200	0.32921700
C	2.81156500	0.78737900	0.85720600
C	3.78470300	-0.00479400	0.30530700
C	3.47785900	-0.78210700	-0.80937200
C	2.20362300	-0.77654300	-1.33666700
C	1.21330700	0.00545600	-0.76879800
H	3.02433900	1.41515500	1.70798300
H	-4.13628300	1.58413300	-1.23333900
H	-1.83404800	1.48087500	-2.14625100
H	1.94259600	-1.38854200	-2.18477600
H	4.23505100	-1.40453100	-1.26060900
H	-4.75055100	0.14769600	0.69118500
H	4.77806300	-0.01836000	0.72431900
O	0.01826700	-0.04935800	-1.39860400
S	0.39751000	1.96643700	0.97445400
IM19			
C	1.56030500	-0.18899200	0.44609800
C	2.76101100	0.06317700	-0.20508300
C	3.51007800	1.18529700	0.10332500
C	3.06425700	2.06923700	1.06575600
C	1.87512200	1.82190800	1.73162600
C	1.13908200	0.69511600	1.43095800
Cl	3.35403000	-1.02049600	-1.40856300
H	4.43537300	1.35675600	-0.42233600
H	0.22090500	0.49259200	1.96086300
C	-1.00176000	-1.13102600	0.27836600
C	-1.87554300	-1.92118600	0.98879000
C	-3.22480700	-1.58993300	1.07538100
C	-3.73197800	-0.44322200	0.46223200
C	-2.89544400	0.36168100	-0.25829000

C	-1.48494600	0.04988000	-0.43190000
H	-4.77519900	-0.18800400	0.55440500
Cl	-3.47887400	1.76796500	-1.02278100
H	1.52438100	2.50211800	2.49160300
H	-1.50407700	-2.79606200	1.49905100
H	-3.88946400	-2.21862200	1.64673300
H	3.64866300	2.94589200	1.29611900
O	-0.75805300	0.73248000	-1.14893400
S	0.64712100	-1.65581800	0.08589600
IM20			
C	1.45942600	-0.11657400	0.19338600
C	2.78506700	0.09180100	-0.06214400
C	3.35837500	1.36203400	0.00643900
C	2.54395000	2.47249900	0.31525000
C	1.22735600	2.33160500	0.57890900
C	0.56966800	1.00460000	0.60775600
Cl	3.78919400	-1.24419200	-0.50000700
H	4.40663500	1.48260600	-0.20749200
H	0.19704000	0.79691400	1.62070700
C	-0.96812700	-1.26603000	0.16400400
C	-1.87422400	-2.30200400	0.35111900
C	-3.23005600	-2.06243600	0.26766900
C	-3.69610500	-0.78603700	0.00397300
C	-2.79739400	0.24922200	-0.15671800
C	-1.42747300	0.02639000	-0.07323600
H	-4.75186100	-0.58111000	-0.06402200
Cl	-3.36600300	1.84416800	-0.45820000
H	0.59754800	3.17965100	0.79565600
H	-1.50679200	-3.29803400	0.54571800
H	-3.92937900	-2.87087700	0.40780900
H	2.99036300	3.45463900	0.32863900
O	-0.58585900	1.06292200	-0.23265200
S	0.73664400	-1.68107300	0.09658000
IM21			
C	1.18911900	0.06514400	-0.47983300
C	1.85483400	-0.22542800	0.81727100
C	3.19104500	-0.45686400	0.92145600
C	3.99108600	-0.52855400	-0.22344400
C	3.40361200	-0.40803500	-1.49894800
C	2.07989100	-0.17089900	-1.63673100
Cl	0.86081600	-0.18756200	2.20887200

H	3.62297000	-0.60290100	1.89861100
H	1.60682000	-0.09954700	-2.60292700
C	-1.12613800	-0.02728800	-0.35006200
C	-2.34661500	-0.64904300	-0.20420100
C	-3.46981300	0.12085800	0.06149400
C	-3.35864900	1.49309100	0.17829100
C	-2.13016500	2.12266300	0.03007000
C	-1.02098200	1.34960100	-0.23929500
H	-2.04421500	3.19311000	0.12297100
H	4.01520000	-0.52805500	-2.37948700
H	-4.42190900	-0.36995200	0.17974900
Cl	-2.45898600	-2.35740800	-0.35099900
H	5.04801700	-0.71439600	-0.12602700
H	-4.23743300	2.08071200	0.39058900
O	0.00572000	-0.69990000	-0.63472200
S	0.62439600	1.86207900	-0.51537300

IM22

C	1.12669600	0.17028500	0.24829000
C	0.97825300	-0.12033300	1.59187800
C	2.09517000	-0.34174400	2.37700000
C	3.36143800	-0.26649800	1.82602500
C	3.50840500	0.03287200	0.48326900
C	2.39630800	0.25141100	-0.30581500
H	1.96909800	-0.56951400	3.42368700
C	-1.51645900	-1.34412800	-0.27405400
C	-2.84655000	-1.69536500	0.01103900
C	-3.78995200	-0.73565300	0.29956200
C	-3.43061700	0.60300300	0.32284200
C	-2.12130000	0.97721900	0.06021000
C	-1.16343800	0.02377100	-0.23657700
H	-3.10727300	-2.74099000	-0.01799400
H	4.48576500	0.09600100	0.03284700
Cl	2.57706600	0.61477700	-1.97542100
H	-0.01219000	-0.17197800	2.01684500
H	-4.15641000	1.36796100	0.54712600
Cl	-1.68410100	2.63709000	0.10377800
H	4.23452000	-0.43858900	2.43471400
H	-4.80959700	-1.01861400	0.50612500
O	0.07431800	0.43444700	-0.57177100
S	-0.37291100	-2.53816400	-0.68582800

IM23

C	-1.14925900	0.10543600	-0.19029700
C	-2.28356100	0.79574500	0.11775500
C	-3.54263200	0.21335300	-0.05760500
C	-3.63688400	-1.09566500	-0.56432500
C	-2.53522000	-1.81619200	-0.88448100
C	-1.17558400	-1.27919900	-0.68719200
Cl	-2.16964700	2.39547300	0.73869300
H	-4.42309400	0.77750600	0.19799300
H	-0.57290200	-1.36816600	-1.59492200
C	1.26296100	-1.36743200	0.31607200
C	2.50373600	-1.98139700	0.42274100
C	3.66392300	-1.25455800	0.24975200
C	3.60026500	0.09296200	-0.06023600
C	2.37265100	0.70922400	-0.18223200
C	1.19732600	-0.00908200	0.01603600
H	2.54469300	-3.03724700	0.63994100
H	-2.61783900	-2.81260700	-1.28856000
H	4.49522500	0.67331300	-0.21282700
Cl	2.28517400	2.38280900	-0.56089200
H	4.62258600	-1.73946600	0.34062800
H	-4.61540500	-1.52500000	-0.71409900
O	0.04523000	0.69781500	-0.03105000
S	-0.21408700	-2.27880100	0.55510500
IM24			
C	-1.34821300	-0.32373500	0.57716400
C	-2.32579300	-0.09504800	1.52787400
C	-3.65229400	-0.02361600	1.15931800
C	-4.01165100	-0.18009600	-0.16999000
C	-3.04031500	-0.43397600	-1.11778800
C	-1.70966300	-0.52701900	-0.74603200
H	-4.40490200	0.16385600	1.90862500
C	1.04923300	1.48823100	0.08741500
C	2.24631900	1.97852600	-0.47140000
C	3.35818200	1.18476300	-0.59792800
C	3.30846300	-0.13843100	-0.17850900
C	2.14108900	-0.65850900	0.34556400
C	1.00159000	0.12660600	0.46572900
H	2.26280200	3.01280900	-0.77487500
H	-3.30082100	-0.58157500	-2.15342400
Cl	-0.52895400	-0.92167400	-1.93770600
H	-2.01277300	0.04321900	2.54989800
H	4.16984500	-0.78061100	-0.26730400

Cl	2.08820500	-2.30765600	0.82335100
H	-5.04543700	-0.11550600	-0.46958500
H	4.26951400	1.58143200	-1.01534000
O	-0.06862200	-0.45735500	1.03207300
S	-0.24988700	2.55297700	0.35130900

IM25

C	1.61366900	0.07346300	2.23452300
C	2.93756500	0.02690200	1.65890200
C	3.13629500	-0.10921700	0.33903300
C	2.00256600	-0.15649100	-0.59119800
C	0.65136200	-0.41888500	0.03130800
C	0.53181000	-0.09943000	1.47484700
H	3.79259200	0.13007900	2.30970000
H	0.53644500	-1.51230300	-0.04705400
Cl	4.70333500	-0.08880600	-0.35030000
H	-3.45003300	2.41841100	0.32055600
C	-2.64146900	1.78567100	-0.01168900
C	-1.41921800	2.39502600	-0.45431300
C	-2.82683300	0.44790400	-0.00911400
C	-0.40336300	1.63182500	-0.85896200
C	-1.80026000	-0.46610000	-0.44585100
Cl	-4.33765900	-0.17863800	0.51817500
C	-0.48028100	0.15116300	-0.84665100
H	-0.24982400	-0.19960000	-1.85470800
H	-0.45922100	-0.08353800	1.90567200
H	0.52068400	2.06379900	-1.21388600
S	-1.99522900	-2.08421500	-0.49711900
O	2.12892900	-0.02653100	-1.78501600
H	1.52453900	0.24735500	3.29498600
H	-1.35050200	3.47106600	-0.46012300

IM26

C	0.46271900	1.52554700	0.71081500
C	1.61481600	2.25616100	0.95580000
C	2.86029100	1.73613500	0.65102000
C	2.95077100	0.47809600	0.09831700
C	1.79583000	-0.30090700	-0.17190200
C	0.53232200	0.26796900	0.15313300
H	3.75811800	2.30133300	0.83860300
C	-0.72539100	-0.53507800	-0.05400000
C	-1.90122300	0.30115000	-0.51182200
C	-0.98097100	-1.44669200	1.09629000

C	-3.22052800	-0.10354100	-0.01551700
C	-2.21283900	-1.67378200	1.55062900
H	-0.12539100	-1.95416500	1.51584100
C	-3.35230000	-1.00987300	0.96475200
H	-4.33892700	-1.24193800	1.33580600
H	-0.54039100	-1.20138000	-0.90806300
H	-0.49790300	1.95730900	0.93943100
Cl	4.51595700	-0.12134200	-0.26402800
Cl	-4.57454200	0.71237600	-0.67529800
S	1.91725800	-1.84626500	-0.86590400
H	-2.38526000	-2.36547400	2.35988700
H	1.54162500	3.24302300	1.38560100
O	-1.75412700	1.22285600	-1.27614800
IM27			
C	2.73369600	1.65896700	1.44523100
C	3.54506700	0.73813100	0.80933400
C	3.00315900	-0.14112800	-0.10530500
C	1.64280300	-0.10576400	-0.39253300
C	0.80643700	0.81261300	0.25210800
C	1.38092800	1.68889400	1.16120700
H	4.60322000	0.68923600	1.01100000
H	0.14786400	-1.22632700	1.36264400
Cl	3.98234600	-1.29171700	-0.93061200
H	-4.34557200	1.23668600	-1.08119500
C	-3.30611500	1.15941900	-0.80688300
C	-2.41637200	2.17992100	-1.07681400
C	-2.86181900	0.01963900	-0.16736200
C	-1.09020000	2.03694800	-0.71921500
C	-1.53152000	-0.14195400	0.21541900
Cl	-4.00143200	-1.22934300	0.17722000
C	-0.63114300	0.88829500	-0.08844200
H	0.73487300	2.39817500	1.65595400
H	-0.37976400	2.81766500	-0.94362800
S	-1.10096200	-1.60541100	1.08210700
H	3.15575500	2.34540400	2.16075800
H	-2.75468600	3.07542200	-1.57274800
O	1.14108000	-0.94444300	-1.28241400
IM28			
C	3.20399600	1.86459200	-0.16973500
C	3.52184400	0.51143100	-0.20225700
C	2.52876600	-0.45489800	-0.16851000

C	1.21909200	-0.03336600	-0.09735100
C	0.89003400	1.32415700	-0.06319600
C	1.88986000	2.28627400	-0.10531600
H	4.55078200	0.19372500	-0.25319200
H	-0.12581500	0.33291000	2.41570300
Cl	2.90503500	-2.12799600	-0.22310800
H	-4.08651400	0.30942300	-1.13944000
C	-3.11204300	0.58470100	-0.76888200
C	-2.76321000	1.95023400	-0.66863700
C	-2.22861200	-0.39216300	-0.44746600
C	-1.45748500	2.33497700	-0.38271300
C	-0.96602600	-0.02734400	0.22323100
Cl	-2.58952400	-2.05163700	-0.61229200
C	-0.54031600	1.36735500	-0.06815100
H	1.64579500	3.33655000	-0.08380500
H	-1.15433200	3.36403600	-0.49727700
S	-1.30957700	-0.18252100	2.06588600
H	4.00223800	2.58890600	-0.19513600
H	-3.50091700	2.69401900	-0.92215000
O	0.14286400	-0.84264600	-0.08289800
IM29			
C	-0.51151100	-1.00926900	0.98061700
C	-1.63110600	-1.61691700	1.55839400
C	-2.92576900	-1.26217600	1.18979600
C	-3.11214800	-0.29029400	0.24387300
C	-1.98839300	0.38034700	-0.37954400
C	-0.66182100	-0.03998900	0.02975200
H	-3.77746000	-1.74545800	1.64006000
C	0.48698900	0.69380400	-0.62491100
C	1.75257000	-0.13152700	-0.62929500
C	0.55996200	2.03082700	0.03235300
C	2.81649400	0.33183500	0.22694200
C	1.62508800	2.40055600	0.74444500
H	-0.30367800	2.66765000	-0.08270400
C	2.75292600	1.51986100	0.86509900
H	3.59180800	1.82591900	1.47097400
H	0.18624400	0.84744300	-1.66243600
H	0.47432200	-1.32924100	1.28015800
Cl	-4.67512900	0.17448700	-0.24320200
Cl	4.22741400	-0.63328600	0.40636000
H	1.66379400	3.36023100	1.23464000
H	-1.48935500	-2.38405700	2.30343100

O	-2.14431900	1.27136100	-1.22169000
S	1.84002200	-1.47851000	-1.53808900
IM30			
C	-2.50653400	2.10130500	-1.11953000
C	-3.35595000	1.05606500	-0.80317300
C	-2.86126300	-0.04870200	-0.14015600
C	-1.52232200	-0.12790700	0.22664900
C	-0.66727000	0.92975000	-0.10007900
C	-1.16830800	2.03302700	-0.77330000
H	-4.40123200	1.08948800	-1.06539300
H	0.24344600	-0.56204800	-1.65883700
Cl	-3.91270400	-1.35079700	0.27545200
H	0.60897600	2.18084100	1.91366700
C	1.27325800	1.54042100	1.35433500
C	2.60215100	1.42747600	1.70808500
C	0.75884900	0.82184600	0.28266500
C	3.43396800	0.58957900	0.98456100
C	1.60111700	-0.01656200	-0.45460900
C	2.93944900	-0.12426400	-0.08702300
H	-0.49480600	2.83796700	-1.02481500
H	4.47504900	0.48352900	1.24374500
H	2.99370600	1.98220600	2.54524800
H	-2.89021700	2.96409200	-1.63984500
O	1.18155900	-0.70469300	-1.52207400
S	-0.89229700	-1.49454000	1.10146900
Cl	3.97896900	-1.15026700	-0.99493600
IM31			
C	3.10185400	2.01780100	0.09570300
C	3.56265400	0.71678700	-0.03859400
C	2.66218300	-0.33301900	-0.10811800
C	1.30442500	-0.08882500	-0.03858000
C	0.84194400	1.22923000	0.08826100
C	1.74671800	2.28096900	0.15511100
H	4.61897100	0.50779400	-0.08808100
H	-0.49689500	-0.13290600	2.23960700
Cl	3.23344700	-1.94787500	-0.29157200
H	-4.31166400	0.65904700	-0.86680000
C	-3.29322400	0.81999800	-0.55159900
C	-2.74338900	2.11943400	-0.58362900
C	-2.54902600	-0.23443900	-0.15029400
C	-1.39196200	2.32775800	-0.31595100

C	-1.19197700	-0.04574200	0.42853200
Cl	-3.18629700	-1.82158200	-0.11241000
C	-0.59467500	1.28185100	0.05567800
H	1.38958300	3.29374200	0.26116100
H	-0.95706700	3.30055600	-0.49049400
H	3.81250800	2.82667600	0.15504200
H	-3.36510200	2.94315500	-0.89456600
S	0.04052100	-1.29339800	-0.13973200
O	-1.35917200	-0.14672000	1.82105300
IM32			
C	-1.34654900	1.66683000	1.20346300
C	-2.69395100	1.63376400	1.50521900
C	-3.51690400	0.73171700	0.85527700
C	-2.99308900	-0.12654500	-0.09068000
C	-1.63743600	-0.09845600	-0.40383100
C	-0.80330100	0.80451400	0.25998700
H	-4.57168000	0.68453400	1.07311400
C	0.63261600	0.88552200	-0.09234800
C	1.54050100	-0.13680600	0.22415200
C	1.08926400	2.02553700	-0.74324400
C	2.87240300	0.02410300	-0.15760400
C	2.41579200	2.16944300	-1.09839900
H	0.37559100	2.80042800	-0.97691800
C	3.31128000	1.15775100	-0.81108700
H	4.35100100	1.23779100	-1.08369300
H	-0.15037200	-1.20851000	1.35753200
H	-0.69011300	2.36050100	1.70615200
Cl	-4.01858300	-1.23833200	-0.90910400
Cl	4.01495200	-1.21613900	0.20425400
H	-0.24186100	-0.83693600	-1.45553300
S	1.10111200	-1.59682200	1.09506300
O	-1.18738500	-0.94362900	-1.33787500
H	-3.10488600	2.30255300	2.24402500
H	2.75159500	3.05956700	-1.60565500
IM33			
C	-1.10104900	1.84189100	-1.50235000
C	-2.32227700	1.50522400	-0.80413300
C	-2.51613200	0.28777500	-0.28197200
C	-1.50461700	-0.77318600	-0.43804600
C	-0.12079600	-0.33443600	-0.87865700
C	-0.07946600	0.98926300	-1.56186800

H	-3.10424600	2.24542500	-0.72916000
H	0.27411700	-1.11420100	-1.53108000
Cl	-3.97555500	-0.14983700	0.49783000
H	-0.59784200	0.39069500	1.80109600
C	0.37235700	0.62595400	1.39022000
C	1.08152800	1.65755400	1.84361700
C	0.87401200	-0.28721200	0.32293600
C	2.39613700	1.92381400	1.32280700
C	2.27092600	0.03923400	-0.21021900
Cl	0.99159700	-1.90226900	1.09731700
C	2.95784200	1.15382300	0.37182700
H	3.95039600	1.35646600	0.00327200
H	0.82759000	1.24699700	-2.08689800
H	2.95014300	2.76051800	1.72121300
S	2.93467600	-0.83899200	-1.41088400
O	-1.75276900	-1.93114800	-0.22552700
H	-1.04178300	2.80482500	-1.98469900
H	0.68545500	2.28996000	2.62216200

IM34

C	1.96363500	1.97066200	1.21606700
C	2.89868900	1.13652300	0.49879600
C	2.51579100	0.01058800	-0.11962300
C	1.10948900	-0.41675000	-0.13790100
C	0.15882100	0.35401400	0.76861300
C	0.67958200	1.62882200	1.32081100
H	3.93385700	1.43786400	0.44737600
H	0.04533200	-0.34174900	1.61617600
Cl	3.61903900	-0.94690700	-1.01400200
H	-0.80674100	2.37601500	-0.71096700
C	-1.52774300	1.57810200	-0.60843900
C	-2.76288200	1.68284200	-1.23028200
C	-1.19753300	0.46311700	0.13849500
C	-3.69101400	0.65748300	-1.11803000
C	-2.13450900	-0.58876400	0.25929300
C	-3.37603700	-0.46653000	-0.38934700
H	-4.07762900	-1.28034400	-0.29869900
H	-0.01729300	2.25201600	1.86191400
H	-4.65047700	0.73611800	-1.60465500
S	-1.80569000	-1.98835000	1.17893800
O	0.72324700	-1.34634300	-0.79840500
H	2.33334100	2.87731600	1.66835100
H	-2.99673500	2.56387400	-1.80794500

IM35

C	1.95275500	1.93735300	1.30791600
C	2.89186800	1.12372600	0.70194500
C	2.48311600	0.11163200	-0.14164900
C	1.13020100	-0.09641800	-0.38510200
C	0.16663100	0.71145400	0.22974800
C	0.60737200	1.72648800	1.06570800
H	3.94759200	1.26304600	0.87177100
H	-0.15871100	-1.30495900	1.62297900
Cl	3.62279100	-0.91201100	-0.92874400
H	-1.38721600	2.38901100	-1.07204300
C	-1.94078700	1.51244800	-0.77022600
C	-3.27523800	1.38788900	-1.10155400
C	-1.26832000	0.51584500	-0.07023800
C	-3.96190400	0.24600500	-0.72540800
C	-1.97581100	-0.62196200	0.32836000
C	-3.31960600	-0.74376800	-0.00959900
H	-3.86593800	-1.61923800	0.30718000
H	-0.13665800	2.35130300	1.53628900
H	-5.00427000	0.12818000	-0.97802300
S	-1.27930800	-1.93698500	1.26772000
H	-3.77150800	2.16992900	-1.65402000
H	2.27041600	2.72875500	1.96685100
O	0.75576500	-1.05928000	-1.20940600

IM36

C	2.38704500	2.23685800	0.30640700
C	3.03058100	1.03074600	0.05347500
C	2.30548400	-0.12627900	-0.18276600
C	0.93018300	-0.04703200	-0.15465600
C	0.27327300	1.16142600	0.09915700
C	1.00763800	2.31831200	0.32640700
H	4.10732300	0.98001800	0.03898500
H	-0.51813500	-0.58743400	2.24524900
Cl	3.08658800	-1.61900200	-0.51236600
H	-2.21174900	2.69717000	-0.12476600
C	-2.24498200	1.62399400	-0.23339200
C	-3.39689300	1.00071400	-0.69438000
C	-1.12006800	0.86342300	-0.02561700
C	-3.37707400	-0.36659400	-1.08088800
C	-1.20358100	-0.61863200	-0.04385400
C	-2.29866700	-1.15355700	-0.86738800

H	-2.25335700	-2.18575200	-1.17490500
H	2.98112200	3.11806600	0.48859700
H	-4.23721100	-0.77194300	-1.59121100
S	-1.56603800	-1.22047800	1.70372700
H	0.51151700	3.25631900	0.51939800
H	-4.28821900	1.58194800	-0.86744100
O	0.09196200	-1.07224700	-0.38729200
IM37			
C	-0.60634500	-2.10160100	1.42481000
C	-1.73803300	-1.93463800	0.55028200
C	-2.10291600	-0.72256900	0.09088900
C	-1.38469900	0.47558400	0.48297700
C	0.00202600	0.24800400	1.02502200
C	0.20560300	-1.07576200	1.68057700
H	-2.33631900	-2.79469600	0.29287700
H	0.25172000	1.05092100	1.71534200
Cl	-3.50662000	-0.57763500	-0.88896000
H	-0.12746100	-0.49248400	-1.72191000
C	0.84253200	-0.55143200	-1.25275400
C	1.79117200	-1.35439600	-1.72834700
C	1.08497900	0.35788000	-0.09968800
C	3.11551900	-1.38351000	-1.14435200
C	2.45748300	0.19923700	0.57495300
Cl	1.13087300	2.01607000	-0.78697800
C	3.44743100	-0.63646500	-0.08395100
H	4.43042400	-0.65528900	0.35820500
H	1.05656000	-1.17849800	2.33559500
H	3.85517300	-2.02992700	-1.59347600
H	-0.43945500	-3.06867500	1.87231500
H	1.59016400	-1.98079900	-2.58307000
O	2.66627500	0.75383600	1.62722300
S	-1.99448900	1.97146100	0.35467300
IM38			
C	1.04335600	2.40469400	-0.71129200
C	2.13306800	1.48817500	-0.89649400
C	2.18682300	0.29084300	-0.27501400
C	1.15110300	-0.14586400	0.62857600
C	-0.08865400	0.71468300	0.68347600
C	0.00011500	2.05917500	0.04435700
H	2.95164800	1.77333300	-1.53922700
H	-0.35275300	0.85846200	1.73219700

Cl	3.55418700	-0.71885700	-0.53374000
H	-0.22037400	-1.26364900	-1.26547700
C	-1.18744800	-0.92727200	-0.92421300
C	-2.33800200	-1.49362400	-1.47469500
C	-1.27957600	0.02668300	0.05542100
C	-3.61327800	-1.10794900	-1.04485600
C	-2.58547500	0.46055200	0.50931300
C	-3.74371100	-0.15586100	-0.07657800
H	-4.70480200	0.17101100	0.28768200
H	-0.83693100	2.72062500	0.20695400
H	-4.48621100	-1.56745900	-1.48151800
H	1.09201600	3.36947800	-1.19047500
H	-2.23853500	-2.24690100	-2.24074500
S	1.24063200	-1.50078800	1.52552500
O	-2.69315900	1.34160700	1.38097200

IM39

C	1.76931100	2.45802800	0.25570900
C	2.73686600	1.47453700	0.15415200
C	2.35763600	0.16239800	-0.04450600
C	1.01576900	-0.19156800	-0.15384500
C	0.04112700	0.80784400	-0.04126500
C	0.42996700	2.12228000	0.16328800
H	3.78526500	1.71547200	0.22505500
H	-0.45487800	-0.25148900	2.01957900
Cl	3.56029900	-1.06517700	-0.18839200
H	-1.63860500	1.21060100	-2.10169700
C	-2.12888800	0.71108100	-1.27967800
C	-3.45946400	0.35746000	-1.37177600
C	-1.38459200	0.42328900	-0.14071400
C	-4.06364300	-0.29497900	-0.30608900
C	-2.01228100	-0.22244100	0.92916600
C	-3.34942300	-0.58293600	0.83740300
H	-3.80625900	-1.07888600	1.67881200
H	-0.33251700	2.88088300	0.25188600
H	-5.10295900	-0.57929100	-0.36644300
H	-4.02010900	0.58150400	-2.26500000
H	2.06362700	3.48354000	0.41136200
O	-1.38025100	-0.49010800	2.08392900
S	0.51931600	-1.83021400	-0.45833700

IM40

C	2.12042400	2.41063700	0.16372600
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C	2.90796600	1.27979700	0.00780600
C	2.31413600	0.03279600	-0.10069500
C	0.93982400	-0.08850200	-0.04779400
C	0.14512400	1.05830000	0.10366800
C	0.74306400	2.30773800	0.20792400
H	3.98256600	1.35587700	-0.02968200
H	-0.80859000	-0.59957800	2.20008400
Cl	3.28815300	-1.37204700	-0.31440800
H	-2.13626100	2.59743800	-0.46379300
C	-2.29939800	1.53984800	-0.31628100
C	-3.54136500	0.98588800	-0.61087300
C	-1.25501500	0.73326300	0.05219100
C	-3.72191300	-0.42103800	-0.60600100
C	-1.49275800	-0.71118900	0.38320500
C	-2.74373600	-1.25594400	-0.20094600
H	-2.88425900	-2.32497200	-0.17458100
H	0.13220900	3.18879300	0.33085300
H	-4.66243700	-0.82716100	-0.94542400
H	-4.35346400	1.62452900	-0.91922500
H	2.59350700	3.37560800	0.25258400
O	-1.61687500	-0.89220300	1.77505000
S	0.02968800	-1.57235400	-0.20761600
CPR1			
C	0.31581100	-1.44385300	-0.00022000
C	-0.46099100	-0.31302000	-0.00006600
C	0.13573600	1.00832200	0.00005100
C	1.57368600	1.05986000	0.00031800
C	2.32680200	-0.07616800	0.00019600
C	1.70247200	-1.33072000	-0.00011300
H	-0.15374000	-2.41425700	-0.00041200
H	2.01521000	2.04373500	0.00056400
H	3.40381400	-0.01685000	0.00035400
H	2.30158700	-2.22777500	-0.00028700
O	-0.55072600	2.03815600	0.00001500
Cl	-2.16012700	-0.41862500	-0.00007800
CTPR1			
C	-2.35878900	-0.70642400	-0.00000100
C	-2.36847400	0.67862900	-0.00000100
C	-1.18392900	1.38882000	0.00000300
C	0.03673700	0.71954300	0.00000000
C	0.02777900	-0.66939800	-0.00000300

C	-1.15408800	-1.38314100	0.00000000
H	-3.28420500	-1.25985100	0.00000000
H	-3.30517300	1.21371600	0.00000000
H	-1.19990300	2.46761600	0.00001100
H	-1.12004600	-2.46083900	0.00000100
Cl	1.53972200	-1.50435400	0.00000100
S	1.54616500	1.59032500	-0.00000100

4-MCDF

C	2.02352900	2.25082800	0.00021200
C	2.75050300	1.06341900	0.00029900
C	2.10580400	-0.15809900	0.00004000
C	0.72608800	-0.15483600	-0.00027000
C	-0.01294400	1.02591700	-0.00039600
C	0.64226700	2.24832000	-0.00017600
H	3.82830000	1.08287700	0.00055100
Cl	2.97667000	-1.63814900	0.00006600
H	-2.69512900	2.30804000	-0.00027100
C	-2.62539800	1.23131700	-0.00005100
C	-3.76480800	0.45066900	0.00033100
C	-1.39025800	0.59708000	-0.00023900
C	-3.68265200	-0.94129400	0.00029500
C	-1.34048400	-0.79328800	-0.00010100
C	-2.46256200	-1.59209100	-0.00006200
H	-2.38416600	-2.66669900	-0.00005700
H	0.08935300	3.17426900	-0.00038800
H	-4.59057600	-1.52395600	0.00036000
H	2.55892700	3.18693600	0.00050300
H	-4.73447600	0.92305500	0.00057500
O	-0.06126600	-1.25045500	-0.00021200

4-MCDT

C	1.88927000	2.43016100	0.00009800
C	2.74090200	1.33007900	0.00013900
C	2.21507800	0.05665400	0.00001900
C	0.84080600	-0.12222300	-0.00007700
C	-0.01623400	0.98322200	-0.00010000
C	0.52068400	2.26600400	-0.00005100
H	3.81074600	1.46132900	0.00023100
Cl	3.25257600	-1.31956300	0.00001000
H	-2.46698500	2.43497300	-0.00021400
C	-2.54808100	1.35856300	-0.00012100
C	-3.78739600	0.75615400	0.00006100

C	-1.40052200	0.57156400	-0.00012400
C	-3.89908700	-0.63245900	0.00016200
C	-1.52912000	-0.81971600	-0.00007000
C	-2.77441500	-1.43102400	0.00008200
H	-2.86170500	-2.50626400	0.00010600
H	-0.13084000	3.12617300	-0.00018000
H	-4.87550400	-1.09137800	0.00036000
H	2.31255800	3.42211900	0.00022100
H	-4.67907800	1.36312400	0.00011800
S	0.00535600	-1.64121100	-0.00005800

4-MCPT

C	0.00000000	0.99549700	0.00000000
C	-0.15071900	2.37817700	0.00000000
C	0.92947400	3.23936000	0.00000000
C	2.20522100	2.71023400	0.00000000
C	2.38668900	1.34208800	0.00000000
C	1.29594400	0.49398900	0.00000000
H	0.75993000	4.30303000	0.00000000
C	-0.68984100	-1.60748900	0.00000000
C	-1.53254400	-2.71065300	0.00000000
C	-1.02455400	-3.99567700	0.00000000
C	0.34590400	-4.19028800	0.00000000
C	1.19261800	-3.09976600	0.00000000
C	0.67828300	-1.81615200	0.00000000
H	-2.60067600	-2.55163700	0.00000000
H	2.26472300	-3.21556900	0.00000000
H	3.36966500	0.89998800	0.00000000
H	0.75746500	-5.18703200	0.00000000
S	-1.43233800	-0.01479300	0.00000000
O	1.60738200	-0.82488300	0.00000000
H	-1.69888300	-4.83703000	0.00000000
H	3.06061900	3.36646000	0.00000000
Cl	-1.74549100	3.03656700	0.00000000

1-MCPT

C	1.35670000	0.66549100	0.00000000
C	2.28132200	1.69840100	0.00000000
C	1.86948800	3.01584400	0.00000000
C	0.52086100	3.31486100	0.00000000
C	-0.40265200	2.28770200	0.00000000
C	0.00000000	0.95693500	0.00000000
H	2.59841400	3.80998000	0.00000000

C	0.48846300	-1.89277200	0.00000000
C	0.57942500	-3.27739700	0.00000000
C	-0.55565100	-4.06425800	0.00000000
C	-1.80366700	-3.46464900	0.00000000
C	-1.90433300	-2.08743300	0.00000000
C	-0.76476700	-1.30421700	0.00000000
H	1.55678600	-3.73646300	0.00000000
H	-2.86014100	-1.58828100	0.00000000
H	-2.69916000	-4.06543800	0.00000000
S	1.98127700	-0.97326500	0.00000000
O	-0.98858000	0.03822800	0.00000000
H	-0.46246900	-5.13846900	0.00000000
H	0.17138200	4.33401700	0.00000000
H	3.33366900	1.45836700	0.00000000
Cl	-2.08361200	2.65303800	0.00000000

4,6-DCDF

C	3.02554300	1.88244600	0.00035400
C	3.36981700	0.53320400	0.00036400
C	2.39520000	-0.44621000	0.00002500
C	1.07818600	-0.03577500	-0.00028800
C	0.72079000	1.30934000	-0.00036600
C	1.70536500	2.28651900	-0.00000800
H	4.40570000	0.23492900	0.00059900
Cl	2.79247700	-2.11526400	-0.00005000
H	-4.40573700	0.23485900	0.00039900
C	-3.36985500	0.53313600	0.00021300
C	-3.02563000	1.88238200	0.00013900
C	-2.39519800	-0.44627100	0.00007600
C	-1.70544200	2.28648600	-0.00013400
C	-1.07819400	-0.03577700	-0.00014800
Cl	-2.79238100	-2.11532000	0.00013800
C	-0.72083000	1.30934100	-0.00033800
H	1.44794100	3.33377900	-0.00017300
H	-1.44811700	3.33377000	-0.00024800
H	3.81276900	2.61937500	0.00067900
H	-3.81286100	2.61931200	0.00029900
O	0.00002000	-0.85112800	-0.00030000

4,6-DCDT

C	2.95289000	2.07628400	0.00081800
C	3.46066300	0.78088400	0.00062600
C	2.60007200	-0.29500000	0.00008700

C	1.22992300	-0.08172400	-0.00036800
C	0.72141700	1.22066800	-0.00061400
C	1.59387300	2.30254000	0.00031500
H	4.52425600	0.60604800	0.00068600
Cl	3.21267200	-1.90521000	-0.00019600
H	-4.52433500	0.60562800	0.00066900
C	-3.46077900	0.78058200	0.00026200
C	-2.95327100	2.07603600	-0.00027700
C	-2.59992700	-0.29522000	0.00028500
C	-1.59436700	2.30245700	-0.00041500
C	-1.22996200	-0.08169500	-0.00076900
Cl	-3.21225200	-1.90549100	0.00058900
C	-0.72171000	1.22064000	-0.00051500
H	1.20999000	3.31076500	0.00061600
H	-1.21062900	3.31072400	-0.00025100
H	3.63863200	2.90857800	0.00150300
H	-3.63917400	2.90822000	-0.00078500
S	0.00007400	-1.30667300	-0.00035900

1,9-DCPT

C	1.33950100	-0.04268800	0.00000000
C	2.63279600	0.46802900	0.00000000
C	3.74743800	-0.34757700	0.00000000
C	3.57292300	-1.71699500	0.00000000
C	2.30048700	-2.25395600	0.00000000
C	1.19639200	-1.42343000	0.00000000
H	4.72902800	0.09569700	0.00000000
C	-1.33941100	-0.04282200	0.00000000
C	-2.63271600	0.46784300	0.00000000
C	-3.74735600	-0.34774600	0.00000000
C	-3.57288500	-1.71718000	0.00000000
C	-2.30046700	-2.25414300	0.00000000
C	-1.19645300	-1.42358600	0.00000000
H	-4.43112100	-2.36965100	0.00000000
S	0.00000000	1.08868400	0.00000000
O	-0.00045300	-2.06309700	0.00000000
H	-4.72894200	0.09554600	0.00000000
H	4.43115400	-2.36948100	0.00000000
H	2.13406000	-3.31883700	0.00000000
H	-2.13403800	-3.31902800	0.00000000
Cl	2.85505400	2.17882100	0.00000000
Cl	-2.85493600	2.17865600	0.00000000

PT			
C	-1.34847700	0.63249200	0.00000000
C	-2.62960400	1.16647000	0.00000000
C	-3.74315400	0.34946900	0.00000000
C	-3.58057400	-1.02498000	0.00000000
C	-2.30965900	-1.56651000	0.00000000
C	-1.19622100	-0.74508000	0.00000000
H	-4.72895000	0.78629100	0.00000000
C	1.34880300	0.63134000	0.00000000
C	2.63035600	1.16429100	0.00000000
C	3.74327600	0.34643500	0.00000000
C	3.57972100	-1.02789900	0.00000000
C	2.30840600	-1.56846000	0.00000000
C	1.19569300	-0.74615000	0.00000000
H	2.74800200	2.23773100	0.00000000
H	2.14827600	-2.63493200	0.00000000
H	-2.15034600	-2.63310300	0.00000000
H	4.43737000	-1.68175800	0.00000000
S	0.00062400	1.75267200	0.00000000
O	0.00000000	-1.39122700	0.00000000
H	4.72939800	0.78253300	0.00000000
H	-2.74642900	2.24000700	0.00000000
H	-4.43870500	-1.67822100	0.00000000