Electronic Supplementary Material (ESI) for RSC Advances.

Supplementary Information

Mechanistic Insight of TiCl4 Catalyzed [3+3] Cyclization of 1,3 – bis(silyl enol ethers) with 1,3-dielectrophiles

Riffat Un Nisa[a], Maria[a], Fatima Waseem[a],Tariq Mahmood[a], Ralf Ludwig[b,c], Khurshid Ayub*[a]

[a] *Department of Chemistry, COMSATS Institute for Information Technology, Campus Abbottabad, Abbottabad, Pakistan*

[b] *Leibniz-Institut für Katalyse e. V. an der Universität Rostock, Albert-Einstein-Str. 29a, 18059 Rostock, Germany*

[c] *Department of Physical Chemistry, University of Rostock, Dr.-Lorenz-Weg 1, 18059 Rostock, Germany*

Fax = +92-992-383441 khurshid@ciit.net.pk

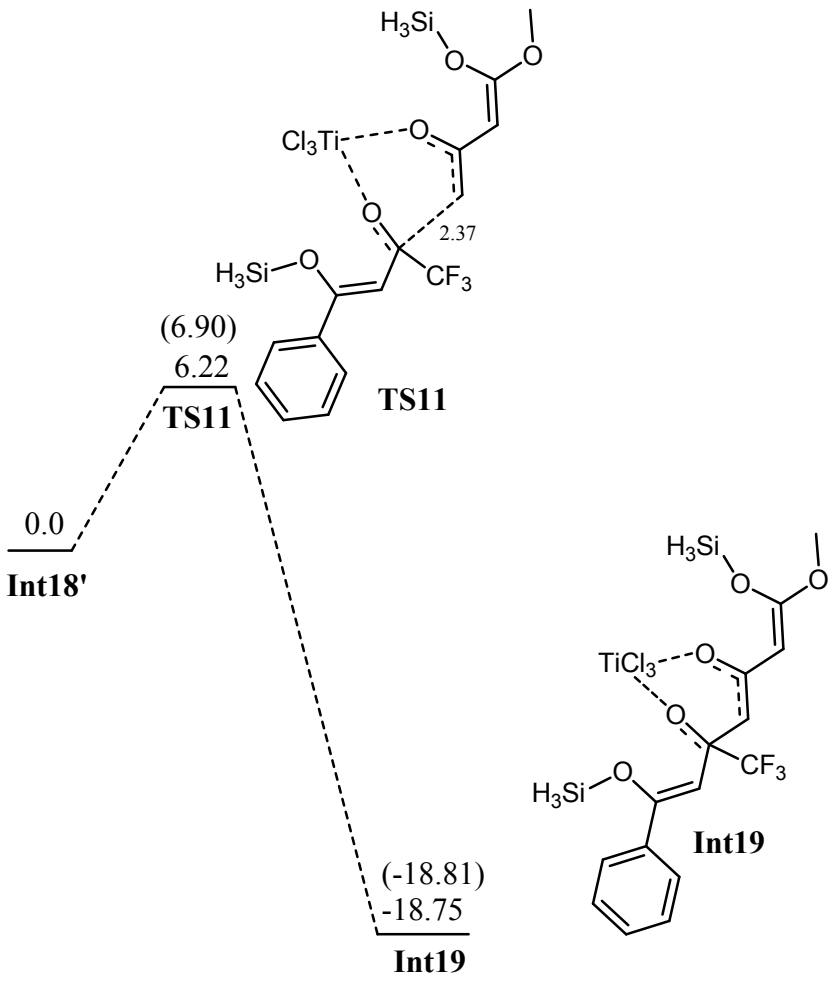

Figure SI1. Comparison of Potential energy diagram for 1,2 addition (**Int18' → Int19**) for SiH3 and $SiMe_3$ (values in parenthesis) substituted systems, All energies are relative to **Int18'** at 0 kcal mol^{-1}. All bond lengths are in Angstroms.

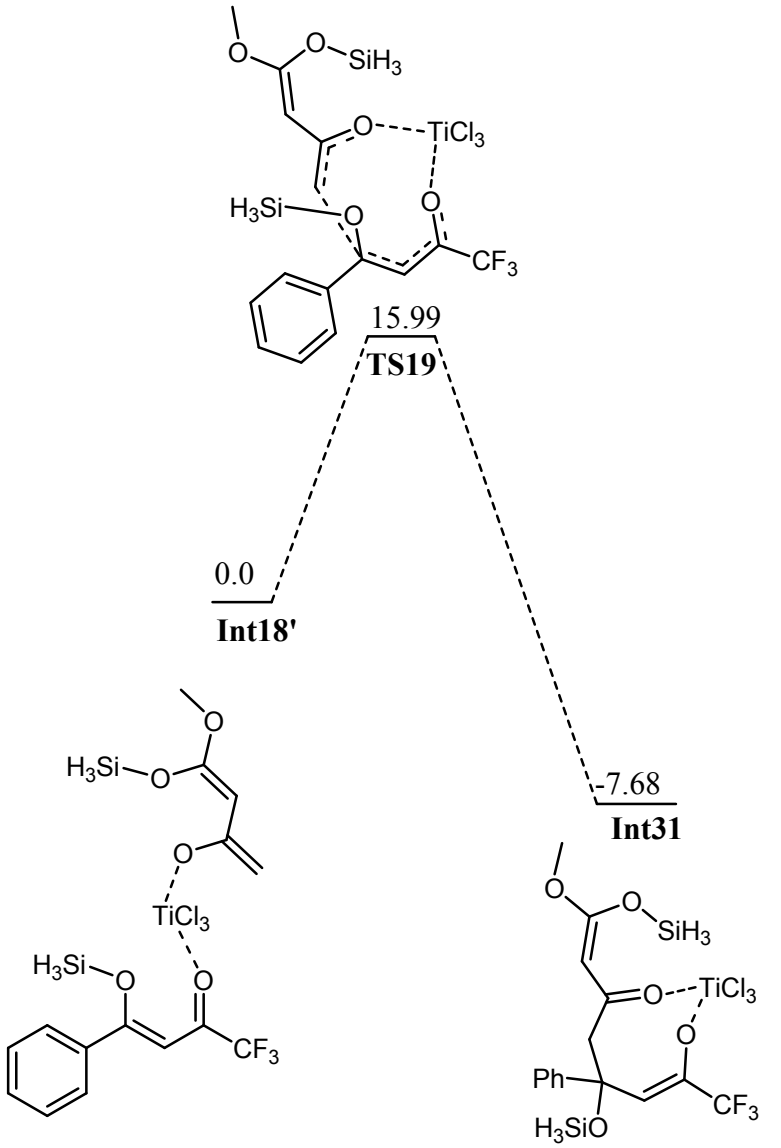

Figure SI2. Potential energy diagram for 1,4 addition on **Int18'** (**Int18'** → **Int31**). All energies are relative to **Int18'** at 0 kcal mol^{-1}.

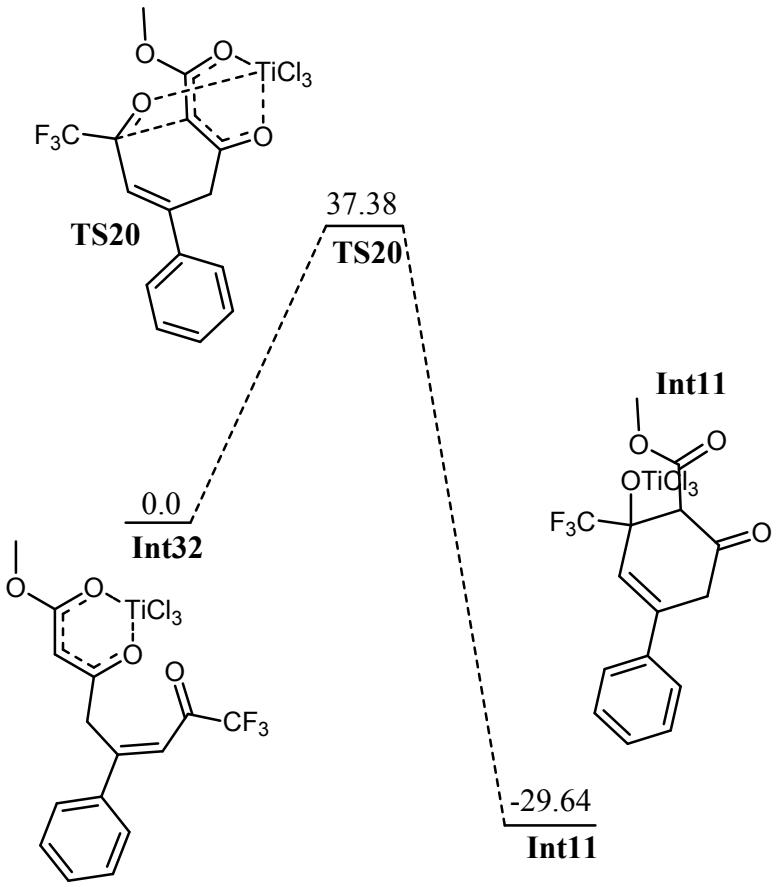

Figure SI2. Potential energy diagram for cyclization in **Int32** (**Int32 → Int11**), All energies are relative to **Int18'** at 0 kcal mol^{-1}.

Table 1. Total electronic, zero-point corrected and Gibbs free energies of the optimized geometries

Structure	Total Energy	Zero point corrected energy	Gibbs Free energy
5	-828.2496239	-828.056858	-828.098358
TS1	-828.2451912	-828.052219	-828.091633
5'	-828.2506638	-828.057436	-828.099187
9	-1125.9582569	-1125.788366	-1125.833270
TS2	-1125.9518805	-1125.781886	-1125.825073
9'	-1125.9597783	-1125.789795	-1125.835269
11	-3518.729896	-3518.530783	-3518.587340
11'	-3518.7389014	-3518.539342	-3518.596538
12	3816.4460613	-3816.269505	-3816.328462
12'	-3816.4465525	-3816.270121	-3816.329787
Int5	-4818.865185	-4818.527619	-4818.606352
TS3	4818.8337685	-4818.496755	-4818.575059
Int6'	4067.3309294	-4067.021884	-4067.097096
TS4	-4067.3226478	-4067.013451	-4067.083649
Int7	4067.3603386	-4067.048583	-4067.120271
Int8	4067.3322631	-4067.022413	-4067.099301
Int9	4161.0133637	-4160.730803	-4160.797089
TS5	4160.9482175	4160.667270	-4160.730272
Int10	3409.5188122	-3409.264326	-3409.324514
Int10'	-3409.4615101	-3409.20889	-3409.269272
TS6	-3409.4048537	-3409.153431	-3409.212319
Int11	3409.5193462	-3409.264762	-3409.324535
TS7	-4067.3150455	-4067.006409	-4067.074759
Int12	-4067.3645644	-4067.052991	-4067.122094
TS8	-4067.368496	-4067.055904	-4067.121019
Int13	-4067.3852568	-4067.074457	-4067.145110
Int14	4161.0206308	-4160.739589	-4160.811331
Int15	-3409.4754867	-3409.222685	-3409.283969
TS9	-3409.4236397	-3409.172093	-3409.231363
Int16	-3409.4784102	-3409.224999	-3409.285027
Int17	4818.875717	-4818.540054	-4818.628437
Ts10	-4818.8322317	-4818.495130	-4818.572310
Int18	-4818.8640183	-4818.526476	-4818.604288
Int18'	4067.3386567	-4067.029944	-4067.103933
TS11	4067.3290769	-4067.020027	-4067.090122
Int19	4067.3719669	-4067.059823	-4067.129887
Int20			
TS12	3409.4236398	-3409.172093	-3409.239361

Int21	3409.5098945	-3409.255829	-3409.319405
Int22	4521.1596446	-4520.798943	-4520.875120
TS13	-4521.1292691	-4520.769081	-4520.845161
Int23	3769.6365254	-3769.304614	-3769.378818
Int23'	3769.6351131	-3769.303068	-3769.375638
TS14	-3769.617516	-3769.285174	3769.353607
Int24	3769.6576863	-3769.322240	-3769.389072
TS15	3769.6271358	-3769.293876	-3769.364114
Int25	3769.6640305	3769.330576	-3769.405402
Int26	-3863.3056605	-3863.001258	-3863.069575
Int27	-3863.294042	-3862.99142	-3863.062801
TS16	3111.7126711	-3111.438196	-3111.494015
Int28	3111.7700052	-3111.493247	-3111.548951
Int27'	3111.7981838	-3111.520346	-3111.576058
TS17	3769.6027339	-3769.270751	-3769.337149
Int29	-3769.6414997	-3769.306776	-3769.373618
Int29'	3769.6458181	-3769.309384	-3769.370686
TS18	-3769.6334288	-3769.299038	-3769.360513
Int30	-3769.6623314	-3769.328939	-3769.396800
TS19	-4067.3128718	-4067.004459	-4067.074332
Int31	-4067.354105	-4067.042194	-4067.112140
Int32	-3409.4707696	-3409.217524	-3409.278859
TS20	-3409.4095081	-3409.157949	-3409.324535
Int6'-SiMe3	-4303.3153672	-4302.8336	-4302.922500
TS4-SiMe3	-4303.3078864	-4302.825873	-4302.909038
Int7-SiMe3	-4303.3454393	-4302.860993	-4302.943589
TS7-SiMe3	-4303.3000695	-4302.818464	-4302.900473
Int12-SiMe3	-4303.3479989	-4302.863274	-4302.945167
Int18'-SiMe3	-4303.3227679	-4302.840770	-4302.927630
TS11-SiMe3	-4303.3121996	-4302.829966	-4302.912201
Int19-SiMe3	-4303.3561825	-4302.870757	-4302.953343

Cartesian Coordinates of the optimized geometries

5

C	-2.35190000	1.11630000	-0.04080000
C	-0.92610000	1.15030000	-0.18970000
H	-0.45540000	2.09580000	-0.42600000
C	-0.13860000	0.04360000	0.02090000

C	-3.12400000	2.41280000	-0.15960000
H	-4.18850000	2.22330000	-0.01110000
H	-2.77430000	3.14000000	0.58310000
O	-0.61000000	-1.17540000	0.24880000
O	-2.97840000	0.06270000	0.20050000
Si	-2.12750000	-1.98470000	-0.00330000
H	-1.47290000	-3.33220000	-0.12300000
H	-3.01130000	-2.15560000	1.17120000
H	-2.76290000	-1.81680000	-1.33410000
H	-2.96690000	2.85990000	-1.14890000
C	1.34360000	0.10250000	0.01550000
C	2.03980000	1.31060000	0.19550000
C	2.07920000	-1.08050000	-0.16950000
C	3.43150000	1.33590000	0.17240000
H	1.49540000	2.23020000	0.38340000
C	3.47150000	-1.05120000	-0.19620000
H	1.54550000	-2.01550000	-0.29570000
C	4.15230000	0.15600000	-0.02800000
H	3.95490000	2.27630000	0.32100000
H	4.02570000	-1.97330000	-0.34780000
H	5.23860000	0.17760000	-0.04520000

TS1

C	0.09090000	0.01780000	-0.00810000

C	0.89310000	1.14360000	0.23270000
H	0.45010000	2.09420000	0.49340000
C	2.26420000	1.07940000	-0.01450000
O	2.88280000	-0.01550000	-0.30360000
O	0.60570000	-1.13670000	-0.27700000
C	-1.39120000	0.07500000	-0.00750000
C	-2.09690000	1.29060000	-0.01160000
C	-2.11380000	-1.13070000	-0.00680000
C	-3.48920000	1.29850000	-0.00510000
H	-1.56360000	2.23480000	-0.04240000
C	-3.50560000	-1.11950000	0.00330000
H	-1.56530000	-2.06590000	-0.00980000
C	-4.19710000	0.09420000	0.00570000
H	-4.02260000	2.24480000	-0.01420000
H	-4.05220000	-2.05830000	0.01000000
H	-5.28370000	0.10260000	0.01220000
Si	2.34170000	-1.76580000	0.14020000
H	3.74320000	-2.09440000	-0.28540000
H	2.31320000	-1.63570000	1.62350000
H	1.71650000	-3.08340000	-0.22220000
C	3.12590000	2.31260000	-0.00060000
H	3.90540000	2.20460000	0.76230000
H	3.63540000	2.40760000	-0.96610000
H	2.55020000	3.22000000	0.19630000

5’

C	-0.00890000	-0.04920000	0.01890000
C	-0.80480000	1.14560000	-0.08250000
H	-0.32780000	2.10840000	-0.20200000
C	-2.17160000	1.12860000	-0.02570000
O	-2.94290000	0.05780000	0.09510000
O	-0.54530000	-1.17600000	0.11930000
C	1.48450000	0.01970000	0.00760000
C	2.19960000	1.22480000	0.09850000
C	2.19840000	-1.18650000	-0.08820000
C	3.59340000	1.22250000	0.08850000
H	1.67790000	2.17090000	0.19570000
C	3.58960000	-1.18740000	-0.10390000
H	1.63740000	-2.11250000	-0.15050000
C	4.29150000	0.01800000	-0.01620000
H	4.13430000	2.16160000	0.16510000
H	4.12900000	-2.12720000	-0.18380000
H	5.37810000	0.01840000	-0.02680000
C	-2.98090000	2.39410000	-0.08530000
H	-3.67070000	2.35310000	-0.93630000
H	-3.59520000	2.47920000	0.81870000
H	-2.34890000	3.28050000	-0.17510000
Si	-2.75710000	-1.66290000	0.00150000
H	-2.34930000	-2.36920000	1.23700000
H	-4.23480000	-1.91200000	-0.06110000

H	-2.26910000	-2.20800000	-1.28790000

9

C	-1.82580000	0.02180000	-0.01940000
C	-0.48900000	-0.44200000	0.18210000
H	-0.34540000	-1.47620000	0.45990000
C	0.61620000	0.34710000	-0.04310000
C	-2.94500000	-1.04460000	0.05060000
O	0.56420000	1.64860000	-0.30750000
O	-2.16570000	1.17340000	-0.30490000
Si	-0.48240000	2.95590000	0.07880000
H	0.57290000	3.99000000	0.29590000
H	-1.29350000	3.43410000	-1.05580000
H	-1.17140000	2.80080000	1.37850000
C	1.99490000	-0.19130000	-0.02580000
C	2.25510000	-1.56670000	-0.16460000
C	3.07870000	0.69090000	0.12760000
C	3.56130000	-2.04550000	-0.13240000
H	1.43860000	-2.26260000	-0.32670000
C	4.38400000	0.20760000	0.16310000
H	2.88440000	1.75290000	0.22370000
C	4.62980000	-1.16090000	0.03560000
H	3.74660000	-3.10950000	-0.24860000
H	5.21090000	0.90060000	0.29020000
H	5.64890000	-1.53690000	0.05990000
F	-2.66300000	-2.00240000	0.96330000

F	-4.11990000	-0.49590000	0.37120000
F	-3.07120000	-1.65180000	-1.14820000

TS2

C	0.09090000	0.01780000	-0.00810000
C	0.89310000	1.14360000	0.23270000
H	0.45010000	2.09420000	0.49340000
C	2.26420000	1.07940000	-0.01450000
O	2.88280000	-0.01550000	-0.30360000
O	0.60570000	-1.13670000	-0.27700000
C	-1.39120000	0.07500000	-0.00750000
C	-2.09690000	1.29060000	-0.01160000
C	-2.11380000	-1.13070000	-0.00680000
C	-3.48920000	1.29850000	-0.00510000
H	-1.56360000	2.23480000	-0.04240000
C	-3.50560000	-1.11950000	0.00330000
H	-1.56530000	-2.06590000	-0.00980000
C	-4.19710000	0.09420000	0.00570000
H	-4.02260000	2.24480000	-0.01420000
H	-4.05220000	-2.05830000	0.01000000
H	-5.28370000	0.10260000	0.01220000
Si	2.34170000	-1.76580000	0.14020000
H	3.74320000	-2.09440000	-0.28540000
H	2.31320000	-1.63570000	1.62350000
H	1.71650000	-3.08340000	-0.22220000

C	3.12590000	2.31260000	-0.00060000
H	3.90540000	2.20460000	0.76230000
H	3.63540000	2.40760000	-0.96610000
H	2.55020000	3.22000000	0.19630000

9’

C	-0.55380000	4.84030000	-0.53990000
C	0.12710000	3.62900000	-0.61030000
C	-0.37920000	2.49170000	0.04700000
C	-1.57250000	2.59820000	0.78380000
C	-2.23300000	3.81910000	0.87470000
C	-1.72940000	4.93940000	0.20930000
H	-0.16860000	5.70680000	-1.06900000
H	1.02780000	3.56160000	-1.21220000
H	-1.95770000	1.72840000	1.30300000
H	-3.14460000	3.89480000	1.45970000
H	-2.25310000	5.88920000	0.27210000
C	0.31780000	1.18590000	-0.00610000
C	1.76630000	1.18450000	-0.12170000
H	2.25570000	2.13570000	-0.27050000
O	-0.32280000	0.11370000	0.09400000
C	2.57860000	0.10630000	0.03080000
O	2.16700000	-1.10790000	0.32660000
Si	2.80670000	-2.69420000	0.32950000
H	4.12810000	-2.69670000	0.99690000

H	1.82290000	-3.46490000	1.10890000
H	2.91960000	-3.16580000	-1.06680000
Ti	-1.93630000	-1.20630000	-0.08420000
Cl	-2.83910000	0.29390000	-1.47080000
Cl	-3.71580000	-2.55070000	-0.09960000
Cl	-1.93680000	-1.02840000	2.16520000
Cl	-0.56840000	-2.63440000	-1.11560000
C	4.09250000	0.28930000	-0.06100000
F	4.66550000	0.07220000	1.13730000
F	4.60680000	-0.61230000	-0.92840000
F	4.44500000	1.51260000	-0.47950000

11

C	0.10040000	-1.54020000	0.02490000
C	1.52950000	-1.40260000	-0.00870000
H	2.09710000	-2.32440000	0.01190000
C	2.24660000	-0.23310000	-0.10050000
C	-0.48140000	-2.92570000	0.12940000
H	-1.08440000	-3.12660000	-0.76350000
H	0.28510000	-3.69610000	0.23160000
O	1.63920000	0.94310000	-0.26970000
O	-0.67180000	-0.54870000	-0.03440000
Si	1.58390000	2.32060000	0.72370000
H	2.94610000	2.59020000	1.25080000
H	1.13800000	3.41040000	-0.16360000

H	0.65520000	2.07920000	1.84810000
H	-1.16110000	-2.96420000	0.98790000
C	3.72590000	-0.22560000	-0.10850000
C	4.46730000	-1.17180000	0.62090000
C	4.41020000	0.73960000	-0.86870000
C	5.85900000	-1.15330000	0.58630000
H	3.95280000	-1.89870000	1.24180000
C	5.80180000	0.74620000	-0.91020000
H	3.84390000	1.46150000	-1.44830000
C	6.52920000	-0.19800000	-0.18190000
H	6.42150000	-1.87980000	1.16550000
H	6.31900000	1.48690000	-1.51310000
H	7.61510000	-0.18730000	-0.20960000
Ti	-2.66830000	0.05390000	-0.05820000
Cl	-4.85570000	0.50770000	-0.03190000
Cl	-2.80580000	-1.17910000	-1.93630000
Cl	-1.97390000	2.14860000	-0.32790000
Cl	-2.68060000	-0.74730000	2.05170000

11’

C	-3.53360000	3.14820000	-0.54580000
C	-2.16460000	2.89840000	-0.52280000
C	-1.66280000	1.76310000	0.13830000
C	-2.55790000	0.89260000	0.78480000
C	-3.92370000	1.15940000	0.77740000

C	-4.41450000	2.28310000	0.10840000
H	-3.91460000	4.01410000	-1.07940000
H	-1.49120000	3.56000000	-1.05840000
H	-2.17720000	0.03180000	1.32490000
H	-4.60430000	0.48820000	1.29230000
H	-5.48220000	2.48350000	0.09390000
C	-0.21310000	1.45820000	0.15260000
C	0.73280000	2.53880000	0.11720000
H	0.33040000	3.54250000	0.14700000
O	0.17220000	0.25800000	0.22770000
C	2.09910000	2.42980000	0.08980000
O	2.69260000	1.24250000	0.08050000
Si	4.32880000	0.77520000	0.06390000
H	5.02440000	1.39410000	1.22010000
H	4.30310000	-0.69180000	0.16180000
H	4.95410000	1.23920000	-1.19950000
Ti	-0.13180000	-1.69840000	-0.07660000
Cl	-0.68830000	-0.97210000	-2.17490000
Cl	-1.64270000	-3.33760000	-0.16010000
Cl	-0.16120000	-1.69470000	2.22440000
Cl	1.82970000	-2.62750000	-0.46650000
C	2.97940000	3.64830000	0.07200000
H	3.63780000	3.65750000	0.94970000
H	3.62000000	3.64250000	-0.81920000
H	2.39290000	4.56860000	0.07020000

12’

C	-0.55380000	4.84030000	-0.53990000
C	0.12710000	3.62900000	-0.61030000
C	-0.37920000	2.49170000	0.04700000
C	-1.57250000	2.59820000	0.78380000
C	-2.23300000	3.81910000	0.87470000
C	-1.72940000	4.93940000	0.20930000
H	-0.16860000	5.70680000	-1.06900000
H	1.02780000	3.56160000	-1.21220000
H	-1.95770000	1.72840000	1.30300000
H	-3.14460000	3.89480000	1.45970000
H	-2.25310000	5.88920000	0.27210000
C	0.31780000	1.18590000	-0.00610000
C	1.76630000	1.18450000	-0.12170000
H	2.25570000	2.13570000	-0.27050000
O	-0.32280000	0.11370000	0.09400000
C	2.57860000	0.10630000	0.03080000
O	2.16700000	-1.10790000	0.32660000
Si	2.80670000	-2.69420000	0.32950000
H	4.12810000	-2.69670000	0.99700000
H	1.82290000	-3.46490000	1.10890000
H	2.91960000	-3.16580000	-1.06680000
Ti	-1.93630000	-1.20630000	-0.08420000

Cl	-2.83910000	0.29390000	-1.47080000
Cl	-3.71580000	-2.55070000	-0.09960000
Cl	-1.93680000	-1.02840000	2.16520000
Cl	-0.56830000	-2.63440000	-1.11560000
C	4.09250000	0.28930000	-0.06100000
F	4.66550000	0.07220000	1.13730000
F	4.44500000	1.51260000	-0.47950000
F	4.60680000	-0.61230000	-0.92840000

12

C	-0.77470000	0.45850000	0.03040000
C	0.30600000	-0.51700000	-0.07010000
H	0.08780000	-1.56400000	-0.21600000
C	1.61160000	-0.17500000	0.04240000
O	2.16640000	1.01130000	0.22300000
O	-0.52110000	1.66830000	0.14340000
C	-2.19890000	0.00880000	0.00810000
C	-2.58390000	-1.34180000	0.00090000
C	-3.19530000	1.00020000	0.00440000
C	-3.93350000	-1.69040000	-0.01190000
H	-1.84090000	-2.13180000	0.01650000
C	-4.54120000	0.65090000	-0.01210000
H	-2.88590000	2.03960000	0.01450000
C	-4.91370000	-0.69660000	-0.02040000

H	-4.21910000	-2.73850000	-0.01370000
H	-5.30180000	1.42650000	-0.01780000
H	-5.96510000	-0.97100000	-0.03220000
C	2.69620000	-1.24660000	-0.00430000
Si	1.74880000	2.64750000	-0.09950000
H	1.12330000	3.36030000	1.03130000
H	3.13750000	3.17830000	-0.20460000
H	1.12720000	2.84700000	-1.42660000
F	3.38820000	-1.26610000	1.14890000
F	3.56300000	-0.99350000	-1.00190000
F	2.18820000	-2.47970000	-0.20190000

Int5

C	3.35320000	0.68160000	0.48730000
C	2.08820000	0.27870000	0.71150000
H	1.92330000	-0.46470000	1.48280000
C	0.90710000	0.59460000	-0.10400000
Cl	-0.31520000	-2.10500000	1.97690000
Cl	1.95920000	-2.87790000	-0.43690000
C	-2.92950000	-0.43770000	-0.42000000
C	-2.82950000	0.38310000	0.77900000
H	-2.36520000	-0.10290000	1.62590000
C	-3.24690000	1.66050000	0.92510000
O	-3.81470000	2.37690000	-0.05970000
Si	-4.43640000	3.94480000	0.12800000

Cl	-0.53080000	-2.10080000	-2.56830000
H	-4.94150000	4.25600000	-1.22860000
H	-5.55050000	3.97470000	1.10590000
H	-3.38570000	4.91850000	0.50920000
O	-3.16270000	2.39780000	2.06010000
C	-3.37200000	-0.14340000	-1.65040000
H	-3.72280000	0.85210000	-1.88580000
H	-3.36850000	-0.89680000	-2.42830000
C	-2.63070000	1.79250000	3.23890000
H	-3.22660000	0.92010000	3.52810000
H	-1.58940000	1.49000000	3.08360000
H	-2.68580000	2.55720000	4.01410000
O	3.72170000	1.52870000	-0.48150000
Si	5.06110000	1.61540000	-1.52520000
H	4.70280000	2.73230000	-2.42480000
H	6.29800000	1.93390000	-0.77680000
H	5.19890000	0.34500000	-2.27180000
C	0.60850000	1.94980000	-0.59850000
C	1.18240000	3.09260000	-0.01310000
C	-0.31430000	2.09500000	-1.65150000
C	0.84380000	4.35900000	-0.47830000
H	1.87420000	2.98620000	0.81520000
C	-0.63400000	3.36380000	-2.12410000
H	-0.76340000	1.20820000	-2.08530000
C	-0.05780000	4.49550000	-1.53830000

H	1.28020000	5.23970000	-0.01640000
H	-1.33280000	3.47200000	-2.94840000
H	-0.31270000	5.48560000	-1.90670000
C	4.48630000	0.19580000	1.37700000
F	4.08290000	-0.65890000	2.32050000
F	5.07900000	1.24810000	1.98050000
F	5.43330000	-0.41720000	0.62610000
O	0.09060000	-0.31980000	-0.35440000
Cl	-0.97540000	-4.53190000	-0.28950000
Si	-3.75970000	-2.86380000	0.27410000
O	-2.50220000	-1.77270000	-0.16510000
Ti	-0.22160000	-2.41800000	-0.32950000
H	-4.92010000	-2.01920000	0.64650000
H	-4.10870000	-3.71580000	-0.88420000
H	-3.32910000	-3.66470000	1.43580000

TS3

C	-3.64870000	0.36610000	-0.46520000
C	-2.35570000	0.09920000	-0.73840000
H	-2.14480000	-0.71740000	-1.41870000
C	-1.18140000	0.65830000	-0.06460000
Cl	0.75210000	-1.65340000	-2.04670000
Cl	-1.39280000	-3.24580000	-0.10540000
C	2.90820000	-0.30940000	0.71830000
C	3.26350000	0.32740000	-0.54370000

H	3.17300000	-0.30310000	-1.41620000
C	3.65140000	1.60870000	-0.72590000
O	3.77230000	2.50310000	0.27300000
Si	4.24950000	4.11580000	0.05380000
Cl	0.08590000	-1.86700000	2.48960000
H	4.19250000	4.65670000	1.43210000
H	5.63190000	4.21690000	-0.47140000
H	3.30640000	4.86170000	-0.81380000
O	3.96930000	2.18260000	-1.91280000
C	3.00300000	0.15180000	1.97710000
H	3.39830000	1.13910000	2.17480000
H	2.69620000	-0.46900000	2.80920000
C	3.89000000	1.39520000	-3.10270000
H	4.58350000	0.54880000	-3.05090000
H	2.87010000	1.02700000	-3.25570000
H	4.17570000	2.06220000	-3.91650000
O	-4.06650000	1.28350000	0.41130000
Si	-5.38080000	1.38950000	1.48900000
H	-5.12600000	2.66920000	2.18310000
H	-6.66450000	1.44440000	0.75500000
H	-5.34550000	0.24860000	2.43030000
C	-1.01700000	2.07860000	0.26960000
C	-1.78120000	3.07630000	-0.36300000
C	-0.02540000	2.44360000	1.20140000
C	-1.56510000	4.41590000	-0.05870000

H	-2.52210000	2.80160000	-1.10520000
C	0.17150000	3.78430000	1.51370000
H	0.57460000	1.66930000	1.66830000
C	-0.59600000	4.77030000	0.88480000
H	-2.14780000	5.18460000	-0.55740000
H	0.92390000	4.06220000	2.24570000
H	-0.43560000	5.81740000	1.12690000
C	-4.75660000	-0.38470000	-1.18980000
F	-4.29750000	-1.30690000	-2.03760000
F	-5.52420000	0.48600000	-1.87830000
F	-5.55980000	-0.99760000	-0.28680000
O	-0.23680000	-0.12330000	0.20780000
Cl	1.71610000	-4.14720000	0.27660000
Si	3.78400000	-3.04920000	0.46390000
H	4.50290000	-2.28020000	1.51620000
H	4.29940000	-4.42780000	0.73410000
H	4.21600000	-2.73300000	-0.91680000
O	2.44110000	-1.62920000	0.53600000
Ti	0.48160000	-2.02710000	0.23350000

Int6

C	3.81890000	-0.33990000	-0.30660000
C	2.82200000	-0.28400000	0.59450000
H	2.65430000	-1.15350000	1.21950000
C	1.79280000	0.76460000	0.70250000

Cl	0.40770000	-1.86150000	2.75190000
Cl	-1.89150000	-3.26860000	0.75380000
C	-3.21800000	0.41840000	0.82660000
C	-4.09630000	-0.28600000	-0.10090000
H	-3.75680000	-1.26850000	-0.39780000
C	-5.26880000	0.16410000	-0.59800000
O	-5.79670000	1.36140000	-0.29110000
Si	-7.23670000	1.97430000	-0.94770000
Cl	0.09300000	-1.55340000	-1.28920000
H	-7.34570000	3.30280000	-0.30290000
H	-7.14280000	2.13240000	-2.41920000
H	-8.40640000	1.13850000	-0.58690000
O	-6.07180000	-0.50240000	-1.46210000
C	-3.39820000	1.56310000	1.51050000
H	-4.32060000	2.11900000	1.42310000
H	-2.61710000	1.93250000	2.16440000
C	-5.66790000	-1.79290000	-1.92480000
H	-4.71260000	-1.73010000	-2.45710000
H	-5.57870000	-2.49330000	-1.08770000
H	-6.45440000	-2.12100000	-2.60470000
O	4.10270000	0.63110000	-1.18540000
Si	4.60970000	0.63810000	-2.80660000
H	4.57890000	2.07490000	-3.15380000
H	5.98630000	0.10850000	-2.93610000
H	3.66100000	-0.13500000	-3.63890000

C	2.10890000	2.20630000	0.68220000
C	3.40470000	2.68230000	0.94460000
C	1.06560000	3.12290000	0.45420000
C	3.65320000	4.05170000	0.97120000
H	4.20690000	1.98160000	1.14780000
C	1.32270000	4.48900000	0.46620000
H	0.06610000	2.74540000	0.26600000
C	2.61570000	4.95480000	0.72610000
H	4.65370000	4.41530000	1.18610000
H	0.51740000	5.19290000	0.27790000
H	2.81340000	6.02320000	0.74190000
C	4.73890000	-1.54790000	-0.36780000
F	4.41610000	-2.49730000	0.51580000
F	6.01420000	-1.17000000	-0.14050000
F	4.70200000	-2.09560000	-1.60730000
O	0.60450000	0.41930000	0.85810000
O	-2.01620000	-0.23240000	0.99780000
Ti	-0.69640000	-1.35310000	0.83210000

Int6’

C	1.48170000	1.10220000	-0.69300000
O	1.31750000	0.37200000	0.31020000
Ti	1.44160000	-1.48620000	1.20350000
Cl	0.17010000	-1.82830000	3.02000000

Cl	3.15790000	-0.37920000	2.31730000
O	0.18380000	-1.85520000	-0.00580000
C	-0.89110000	-1.68580000	-0.82360000
C	-2.14950000	-1.80860000	-0.08880000
H	-2.03510000	-2.02380000	0.96490000
C	-3.39940000	-1.68850000	-0.58380000
O	-3.67160000	-1.41250000	-1.87250000
Si	-5.23560000	-1.30820000	-2.52000000
Cl	2.69210000	-3.30000000	0.78460000
H	-4.97480000	-1.01480000	-3.94810000
H	-5.97480000	-2.58680000	-2.39180000
H	-6.00940000	-0.19690000	-1.91470000
O	-4.55020000	-1.81820000	0.12340000
C	-0.67770000	-1.45760000	-2.13690000
H	-1.50480000	-1.33440000	-2.82150000
H	0.33400000	-1.43370000	-2.52380000
C	-4.47250000	-2.13870000	1.51310000
H	-3.94050000	-1.35420000	2.06230000
H	-5.50450000	-2.20310000	1.85910000
H	-3.96600000	-3.09860000	1.66050000
C	2.41590000	0.70740000	-1.77340000
C	2.22340000	1.13360000	-3.10060000
C	3.51070000	-0.11940000	-1.46610000
C	3.09920000	0.72390000	-4.10110000
H	1.36660000	1.74840000	-3.35860000

C	4.39500000	-0.50870000	-2.46860000
H	3.68890000	-0.41960000	-0.43870000
C	4.18860000	-0.09370000	-3.78600000
H	2.93150000	1.03870000	-5.12690000
H	5.24450000	-1.13670000	-2.21850000
H	4.87520000	-0.40630000	-4.56780000
C	0.83140000	2.39980000	-0.78840000
C	-0.06980000	2.95700000	0.06100000
H	1.13940000	3.04150000	-1.60510000
C	-0.67060000	2.26540000	1.29480000
F	-1.65450000	3.04660000	1.81460000
F	0.24120000	2.08570000	2.25250000
F	-1.23180000	1.09280000	0.98120000
O	-0.47970000	4.19810000	-0.19080000
Si	-1.36800000	5.42900000	0.58260000
H	-2.81600000	5.12880000	0.56230000
H	-0.86450000	5.65780000	1.95430000
H	-1.08100000	6.59820000	-0.27630000

TS4

C	0.61290000	1.20620000	0.08380000
O	1.21450000	0.10940000	0.41680000

Ti	2.24560000	-1.41430000	-0.18640000
Cl	1.59690000	-3.51480000	0.24980000
Cl	3.45310000	-1.15300000	1.74200000
O	1.04520000	-1.21940000	-1.64880000
C	-0.06060000	-0.54970000	-1.89250000
C	-1.27230000	-1.30850000	-1.72120000
H	-1.11610000	-2.32920000	-1.40030000
C	-2.55450000	-0.87520000	-1.88330000
O	-2.88070000	0.34760000	-2.30390000
Si	-4.48340000	0.91550000	-2.47610000
Cl	4.02650000	-1.37460000	-1.53540000
H	-4.27200000	2.31730000	-2.89830000
H	-5.19800000	0.15680000	-3.52790000
H	-5.21460000	0.86340000	-1.19040000
O	-3.65180000	-1.61340000	-1.64460000
C	0.07160000	0.82030000	-2.11030000
H	-0.79270000	1.42690000	-2.34320000
H	1.03980000	1.17510000	-2.43900000
C	-3.51390000	-2.91480000	-1.05210000
H	-2.96550000	-2.84100000	-0.10870000
H	-4.53190000	-3.26160000	-0.87690000
H	-2.99920000	-3.59530000	-1.73720000
C	1.46510000	2.41680000	-0.16980000
C	0.94140000	3.61840000	-0.67960000
C	2.82920000	2.35690000	0.15430000

C	1.76350000	4.72480000	-0.86750000
H	-0.10510000	3.68960000	-0.96040000
C	3.64830000	3.47060000	-0.03150000
H	3.24160000	1.44850000	0.57860000
C	3.12170000	4.65570000	-0.54380000
H	1.34440000	5.64230000	-1.27130000
H	4.70010000	3.40700000	0.23170000
H	3.76170000	5.52130000	-0.69040000
C	-0.75790000	1.44470000	0.56260000
C	-1.52820000	0.73080000	1.40760000
H	-1.24090000	2.33000000	0.16640000
C	-1.11060000	-0.51160000	2.19150000
F	-2.04380000	-0.78460000	3.14080000
F	0.05650000	-0.35560000	2.82020000
F	-1.03100000	-1.60800000	1.40700000
O	-2.82220000	1.11070000	1.57220000
Si	-3.75000000	1.40350000	2.95580000
H	-4.58110000	0.22910000	3.30510000
H	-2.88110000	1.80560000	4.08750000
H	-4.63700000	2.52480000	2.56400000

Int7

C	0.17500000	0.33120000	-0.73630000
O	1.09260000	-0.71360000	-0.44340000

Ti	1.16640000	-2.37380000	0.17180000
Cl	1.47910000	-2.62370000	2.37950000
Cl	3.27090000	-2.83440000	-0.48720000
O	-0.87680000	-1.94990000	0.74580000
C	-1.68190000	-1.13080000	0.23920000
C	-2.98790000	-1.06060000	0.83240000
H	-3.11620000	-1.74200000	1.66320000
C	-4.05840000	-0.28250000	0.47930000
O	-4.05780000	0.59730000	-0.51520000
Si	-5.41090000	1.53580000	-1.00300000
Cl	0.16960000	-3.96570000	-1.09070000
H	-4.86020000	2.30240000	-2.13900000
H	-6.51570000	0.65250000	-1.43670000
H	-5.83280000	2.43660000	0.09260000
O	-5.24780000	-0.30930000	1.09420000
C	-1.22900000	-0.31250000	-0.95210000
H	-1.95030000	0.45910000	-1.21260000
H	-1.14830000	-0.99820000	-1.80500000
C	-5.47940000	-1.19790000	2.20030000
H	-4.80170000	-0.96280000	3.02580000
H	-6.51180000	-1.01890000	2.49830000
H	-5.35130000	-2.23780000	1.88660000
C	0.58190000	1.00940000	-2.05600000
C	0.01780000	2.24090000	-2.41210000
C	1.46000000	0.37980000	-2.94360000

C	0.32470000	2.83350000	-3.63690000
H	-0.65390000	2.74900000	-1.72460000
C	1.76960000	0.97720000	-4.16690000
H	1.91730000	-0.56360000	-2.66790000
C	1.20250000	2.20200000	-4.51980000
H	-0.11730000	3.79180000	-3.89670000
H	2.46180000	0.48130000	-4.84190000
H	1.44690000	2.66460000	-5.47210000
C	0.08930000	1.29860000	0.44000000
C	1.06270000	1.87600000	1.15750000
H	-0.91310000	1.52740000	0.79400000
C	2.55820000	1.73770000	0.94540000
F	3.14320000	2.96080000	1.10600000
F	2.89450000	1.29930000	-0.26810000
F	3.10300000	0.92310000	1.86690000
O	0.72370000	2.60420000	2.25270000
Si	1.40070000	3.90400000	3.08420000
H	2.66310000	3.54560000	3.77010000
H	1.60090000	5.07180000	2.19050000
H	0.36130000	4.22250000	4.09120000

Int8

C	-1.44700000	-2.42850000	-0.30810000
C	-1.36390000	-1.82610000	0.91600000
H	-2.11230000	-2.13880000	1.63150000

C	-0.46460000	-0.79030000	1.30980000
O	-1.18470000	0.68340000	-0.78920000
Ti	-1.07700000	2.29020000	-1.03220000
O	1.55500000	-2.15280000	2.54180000
C	1.93190000	-1.49450000	1.57610000
C	3.34250000	-1.43030000	1.22190000
H	3.97550000	-1.98700000	1.90080000
C	3.92250000	-0.77190000	0.17800000
O	3.23840000	-0.10880000	-0.74800000
Si	3.89560000	0.92840000	-1.94590000
H	2.69940000	1.42620000	-2.64580000
H	4.66570000	2.01700000	-1.30330000
H	4.75910000	0.14820000	-2.86460000
O	5.24630000	-0.71310000	-0.05920000
C	0.90890000	-0.70060000	0.72390000
C	6.15980000	-1.32770000	0.85520000
H	6.00410000	-2.41080000	0.88570000
H	7.15340000	-1.10510000	0.46670000
H	6.04360000	-0.90430000	1.85790000
O	-0.69570000	-2.17250000	-1.35140000
Si	-1.00590000	-1.48840000	-2.91080000
H	0.91670000	-1.10980000	-0.28430000
H	1.22250000	0.34190000	0.63260000
Cl	-2.89010000	3.28730000	-0.09730000
Cl	0.84760000	2.99650000	0.00580000

Cl	-0.94580000	2.64800000	-3.27120000
H	0.17190000	-0.64960000	-3.18500000
H	-2.29810000	-0.78700000	-2.91210000
H	-1.03260000	-2.64550000	-3.83980000
C	-0.84120000	0.08090000	2.39590000
C	0.13300000	0.84540000	3.08630000
C	-2.20210000	0.23400000	2.76910000
C	-0.23530000	1.69420000	4.11920000
H	1.17900000	0.75620000	2.82430000
C	-2.56590000	1.10180000	3.78560000
H	-2.97600000	-0.28660000	2.21700000
C	-1.58280000	1.82790000	4.46830000
H	0.52370000	2.26380000	4.64580000
H	-3.61340000	1.22960000	4.03890000
H	-1.86990000	2.50870000	5.26470000
C	-2.49120000	-3.52070000	-0.55120000
F	-3.29820000	-3.71570000	0.50260000
F	-3.25790000	-3.19330000	-1.61280000
F	-1.87450000	-4.68020000	-0.83340000

Int9

C	1.18340000	2.39280000	0.15820000
C	0.07130000	1.34420000	0.02050000
C	-1.26280000	2.01310000	0.19070000

C	2.60540000	1.86410000	0.14610000
O	-1.76890000	2.04300000	1.36530000
O	0.92180000	3.57820000	0.19670000
C	2.75090000	0.35720000	0.09020000
C	1.72180000	-0.45650000	0.37480000
C	0.34840000	0.02240000	0.80720000
O	-0.62320000	-0.91870000	0.50060000
C	-3.09240000	2.62410000	1.59330000
Cl	-2.82730000	-2.79620000	1.37850000
H	0.09720000	0.99490000	-1.02350000
H	-3.24070000	2.52760000	2.66600000
H	-3.08430000	3.66800000	1.27880000
H	-3.82030000	2.03510000	1.03370000
H	3.10390000	2.26550000	1.03940000
H	3.10800000	2.34740000	-0.70050000
H	1.82390000	-1.53530000	0.32680000
Cl	-1.25060000	-0.41890000	-2.41430000
Cl	-1.51930000	-3.54580000	-1.53350000
Cl	-3.85650000	-0.33330000	-0.48810000
Ti	-1.97600000	-1.66460000	-0.40310000
O	-1.87700000	2.59540000	-0.75780000
C	4.09400000	-0.19330000	-0.23130000
C	4.89780000	0.36650000	-1.23860000
C	4.58670000	-1.30370000	0.47600000
C	6.14380000	-0.17960000	-1.54250000

H	4.54140000	1.21610000	-1.81450000
C	5.83400000	-1.84640000	0.17430000
H	3.99420000	-1.72450000	1.28300000
C	6.61670000	-1.28750000	-0.83740000
H	6.74360000	0.25950000	-2.33490000
H	6.19780000	-2.70160000	0.73690000
H	7.59010000	-1.70910000	-1.07180000
C	0.36370000	0.17140000	2.36540000
F	1.06440000	-0.82950000	2.92210000
F	-0.85200000	0.16220000	2.91820000
F	0.97420000	1.33980000	2.70420000
Si	-1.64990000	2.90630000	-2.47730000
H	-2.75250000	2.21890000	-3.15720000
H	-1.81530000	4.37630000	-2.48660000
H	-0.28300000	2.52910000	-2.87040000

Int10

C	1.07940000	2.28720000	-0.69340000
C	-0.07150000	1.26610000	-0.63090000
C	-1.51510000	1.74320000	-0.61590000
C	2.45360000	1.64440000	-0.83620000
O	-1.71930000	3.03420000	-0.68170000
O	0.93720000	3.48630000	-0.69590000

C	2.61510000	0.27480000	-0.20560000
C	1.57820000	-0.35840000	0.36820000
C	0.18730000	0.21430000	0.49570000
O	-0.74720000	-0.82970000	0.40590000
C	-3.10140000	3.47850000	-0.68750000
Cl	-2.20830000	-3.48220000	0.08940000
H	0.01090000	0.66550000	-1.54980000
H	-3.04070000	4.56410000	-0.73610000
H	-3.61850000	3.07140000	-1.55840000
H	-3.59860000	3.14950000	0.22650000
H	3.19100000	2.35130000	-0.44020000
H	2.65190000	1.58380000	-1.91780000
H	1.68760000	-1.34880000	0.79720000
Cl	-2.47660000	-1.32500000	-2.49070000
Cl	-4.17060000	-0.88470000	0.96640000
Ti	-2.34600000	-1.28370000	-0.25250000
O	-2.44540000	0.93210000	-0.58520000
C	3.97200000	-0.33020000	-0.22900000
C	4.86090000	-0.08510000	-1.28990000
C	4.40510000	-1.16130000	0.82010000
C	6.12500000	-0.67270000	-1.31540000
H	4.56320000	0.55410000	-2.11550000
C	5.66860000	-1.74590000	0.79560000
H	3.75550000	-1.32690000	1.67410000
C	6.53350000	-1.50690000	-0.27440000

H	6.79040000	-0.47730000	-2.15170000
H	5.98260000	-2.37960000	1.62030000
H	7.52080000	-1.95990000	-0.29160000
C	0.01870000	0.84350000	1.90600000
F	0.25390000	-0.06310000	2.86240000
F	-1.22630000	1.33200000	2.09070000
F	0.88360000	1.86710000	2.06930000

TS5

C	-1.63070000	1.02710000	2.09070000
C	-0.64880000	0.05160000	1.64580000
C	0.69250000	0.04480000	1.92030000
C	-2.80550000	1.34320000	1.08480000
O	1.24150000	0.86850000	2.79560000
O	-1.59160000	1.68820000	3.11280000
C	-2.95530000	0.48880000	-0.14730000
C	-1.93830000	0.32320000	-1.05360000
C	-0.62980000	0.94470000	-1.00550000
O	0.40580000	0.28710000	-1.21300000
C	2.61320000	0.68480000	3.20100000
Cl	2.92610000	1.74470000	-0.20280000
H	-0.95260000	-0.67940000	0.91520000
H	2.78170000	1.45980000	3.94790000
H	2.74560000	-0.30330000	3.64930000
H	3.29550000	0.81370000	2.36110000

H	-2.60880000	2.37950000	0.79070000
H	-3.73150000	1.37770000	1.66130000
H	-1.97690000	-0.51880000	-1.74000000
C	-0.47180000	2.49480000	-0.90790000
Cl	1.34340000	-2.64380000	-0.74750000
Cl	2.71220000	-0.41040000	-2.94130000
Si	1.34670000	-2.76700000	1.61040000
H	0.59680000	-2.31740000	2.81620000
H	0.69020000	-4.08570000	1.37400000
H	2.78190000	-2.97260000	1.87510000
Cl	4.32390000	-1.23080000	-0.11760000
Ti	2.38500000	-0.34770000	-0.75540000
O	1.50120000	-0.79820000	1.23480000
C	-4.18220000	-0.31830000	-0.30590000
C	-4.87870000	-0.81830000	0.81140000
C	-4.68160000	-0.60950000	-1.59080000
C	-6.02140000	-1.59720000	0.64670000
H	-4.50870000	-0.62760000	1.81390000
C	-5.83320000	-1.37340000	-1.75180000
H	-4.17990000	-0.20200000	-2.46350000
C	-6.50480000	-1.87440000	-0.63340000
H	-6.53470000	-1.98810000	1.52040000
H	-6.21160000	-1.57270000	-2.75020000
H	-7.40240000	-2.47300000	-0.75950000
F	0.41880000	2.88750000	-1.82380000

F	-0.05860000	2.89120000	0.30410000
F	-1.63820000	3.11560000	-1.17480000

Int10’

C	0.46850000	-1.30910000	1.08670000
C	-0.94180000	-1.76680000	0.97070000
C	-1.33140000	-2.61080000	-0.18900000
C	1.34550000	-1.29990000	-0.20070000
O	-1.45150000	-3.79650000	-0.32800000
O	-1.68130000	-1.70060000	-1.19970000
O	0.95590000	-0.96860000	2.14820000
C	2.34290000	-0.17230000	-0.19830000
C	1.93150000	1.13810000	-0.28580000
H	2.67120000	1.92750000	-0.33980000
C	0.56700000	1.55450000	-0.31030000
O	-0.42110000	0.80370000	-0.24690000
Ti	-2.27270000	-0.07220000	0.31760000
C	-2.29980000	-2.23430000	-2.39720000
Cl	-3.14820000	1.00270000	-1.48630000
Cl	-2.23800000	1.20310000	2.12280000
H	-1.62100000	-2.95580000	-2.85430000
H	-3.24120000	-2.71880000	-2.13140000
H	-2.47180000	-1.37840000	-3.04600000
H	0.70420000	-1.23610000	-1.08310000

H	1.85460000	-2.26840000	-0.21770000
Cl	-4.07070000	-1.29390000	0.84240000
H	-1.27950000	-2.18740000	1.91800000
C	0.30230000	3.06820000	-0.48800000
F	-0.93330000	3.39610000	-0.12410000
F	1.17830000	3.79230000	0.23720000
F	0.47700000	3.38650000	-1.78650000
C	3.77760000	-0.47330000	-0.09570000
C	4.32070000	-1.63680000	-0.67780000
C	4.64910000	0.40590000	0.58140000
C	5.68620000	-1.89610000	-0.60860000
H	3.68050000	-2.32280000	-1.22310000
C	6.00890000	0.12990000	0.67080000
H	4.24580000	1.27950000	1.08300000
C	6.53360000	-1.01730000	0.06940000
H	6.08870000	-2.78710000	-1.08150000
H	6.65980000	0.80570000	1.21750000
H	7.59690000	-1.22910000	0.13590000

TS6

C	0.54710000	0.65800000	-1.73330000
C	-0.88730000	0.58350000	-1.35950000
C	-1.71340000	1.81550000	-1.26170000
C	1.54780000	1.47290000	-0.84130000

O	-2.91860000	1.85340000	-1.40450000
O	-0.98250000	2.94630000	-1.03290000
O	1.02200000	0.01480000	-2.65330000
C	2.04600000	0.50050000	0.18700000
C	1.16260000	-0.05090000	1.08080000
H	1.42850000	-0.96770000	1.60360000
C	-0.19970000	0.33030000	1.30410000
O	-1.09000000	-0.56280000	1.55280000
Ti	-1.71180000	-1.52630000	-0.01870000
C	-1.74970000	4.15670000	-0.92660000
Cl	-3.70480000	-1.17470000	-0.83350000
Cl	-2.20190000	-3.21620000	1.36240000
H	-2.31330000	4.33570000	-1.84510000
H	-2.44530000	4.09500000	-0.08630000
H	-1.01920000	4.94990000	-0.76260000
H	1.03560000	2.32770000	-0.40720000
H	2.34850000	1.80970000	-1.49820000
Cl	-0.37970000	-2.63930000	-1.37650000
H	-1.38080000	-0.08010000	-2.07300000
C	-0.59970000	1.70830000	1.89060000
F	-1.85150000	2.04770000	1.57290000
F	-0.53750000	1.54120000	3.22770000
F	0.22750000	2.71160000	1.57280000
C	3.41810000	-0.02540000	0.08500000
C	4.46880000	0.83140000	-0.29880000

C	3.72710000	-1.36610000	0.39360000
C	5.78240000	0.37340000	-0.33920000
H	4.26190000	1.87110000	-0.53110000
C	5.03790000	-1.82630000	0.32870000
H	2.93210000	-2.06550000	0.63170000
C	6.07140000	-0.95700000	-0.02960000
H	6.58070000	1.05520000	-0.61770000
H	5.25190000	-2.86840000	0.54680000
H	7.09480000	-1.31790000	-0.07750000

Int11

C	1.08860000	2.17250000	-0.97890000
C	-0.06060000	1.18180000	-0.73280000
C	-1.49280000	1.69040000	-0.74370000
C	2.49710000	1.65700000	-0.68800000
O	-2.43470000	0.89230000	-0.71700000
O	-1.67220000	2.98630000	-0.76680000
O	0.92380000	3.26650000	-1.46580000
C	2.61440000	0.26510000	-0.10510000
C	1.55440000	-0.33620000	0.45980000
H	1.63580000	-1.30110000	0.94850000
C	0.17420000	0.27140000	0.51290000
O	-0.78210000	-0.75660000	0.53650000
Ti	-2.33980000	-1.29260000	-0.16170000
C	-3.04500000	3.45680000	-0.73590000

Cl	-4.22530000	-0.78880000	0.91670000
Cl	-2.20790000	-3.44300000	0.41130000
H	-3.58520000	3.08090000	-1.60660000
H	-3.53120000	3.11480000	0.17940000
H	-2.96500000	4.54200000	-0.76090000
H	2.95590000	2.39590000	-0.01690000
H	3.05880000	1.73160000	-1.62760000
Cl	-2.35230000	-1.56430000	-2.38510000
H	-0.00820000	0.47160000	-1.57230000
C	0.00580000	1.07010000	1.83320000
F	-1.25110000	1.54220000	1.97610000
F	0.28480000	0.31040000	2.89700000
F	0.83900000	2.13680000	1.83980000
C	3.94630000	-0.38900000	-0.15270000
C	5.12680000	0.37380000	-0.12600000
C	4.06110000	-1.78850000	-0.23510000
C	6.37760000	-0.24200000	-0.15520000
H	5.07460000	1.45650000	-0.06180000
C	5.31040000	-2.40240000	-0.26820000
H	3.16430000	-2.39720000	-0.30210000
C	6.47470000	-1.63180000	-0.22530000
H	7.27640000	0.36750000	-0.12270000
H	5.37450000	-3.48450000	-0.33980000
H	7.44910000	-2.11130000	-0.25460000

TS7

C	0.05510000	0.39540000	1.17380000
O	1.08510000	-0.22500000	0.73940000
Ti	2.51170000	-0.67960000	-0.60470000
Cl	4.05550000	-1.32840000	-2.12070000
Cl	3.36930000	-1.98630000	1.02850000
O	1.14500000	-1.07050000	-1.78280000
C	-0.12940000	-0.64780000	-1.86400000
C	-0.28320000	0.77610000	-1.99040000
H	0.63870000	1.34040000	-2.02260000
C	-1.45090000	1.48460000	-2.03870000
O	-2.65840000	0.92470000	-2.04300000
Si	-4.13980000	1.77150000	-2.01170000
Cl	3.10940000	1.50660000	-0.67090000
H	-5.13720000	0.68130000	-2.01300000
H	-4.24620000	2.57650000	-0.77130000
H	-4.29250000	2.62440000	-3.21180000
O	-1.53580000	2.82350000	-2.09920000
C	-1.14210000	-1.58130000	-1.74920000
H	-2.15810000	-1.31430000	-1.99730000
H	-0.86990000	-2.62830000	-1.77190000
C	-0.33620000	3.61730000	-2.08370000
H	0.27740000	3.39700000	-2.96210000
H	-0.67740000	4.65160000	-2.11490000

H	0.23320000	3.43050000	-1.16910000
C	0.28740000	1.67030000	1.90780000
C	-0.68020000	2.68780000	1.99510000
C	1.52910000	1.85730000	2.53920000
C	-0.41130000	3.85860000	2.69930000
H	-1.63410000	2.58430000	1.48720000
C	1.78690000	3.02200000	3.25760000
H	2.27810000	1.07700000	2.46890000
C	0.82000000	4.02600000	3.33860000
H	-1.16250000	4.64200000	2.74810000
H	2.74690000	3.14740000	3.74960000
H	1.02530000	4.93750000	3.89310000
C	-1.26020000	-0.09970000	1.03530000
C	-1.70920000	-1.34100000	0.56430000
H	-2.06670000	0.56900000	1.31140000
C	-1.05590000	-2.68890000	0.89910000
F	-1.64750000	-3.69700000	0.22690000
F	-1.28210000	-2.92620000	2.22240000
F	0.25380000	-2.76040000	0.69090000
O	-3.05520000	-1.46120000	0.44130000
Si	-4.24460000	-2.12140000	1.44830000
H	-4.15120000	-1.49570000	2.79120000
H	-5.50810000	-1.74150000	0.77860000
H	-4.13810000	-3.59290000	1.55810000

Int12

C	1.69280000	-0.89990000	0.52390000
O	1.96500000	0.21660000	-0.16790000
Ti	1.32310000	1.86390000	-0.63050000
Cl	-0.21630000	3.20860000	-1.68380000
Cl	2.92190000	2.22000000	-2.15900000
O	-0.40230000	1.10330000	0.25010000
C	-1.49090000	0.48810000	0.29710000
C	-2.55290000	1.11600000	1.02890000
H	-2.28180000	2.07630000	1.44620000
C	-3.84040000	0.67810000	1.19920000
O	-4.30120000	-0.46880000	0.72000000
Si	-5.91730000	-1.03180000	0.87620000
Cl	1.98340000	3.11850000	1.07890000
H	-5.86820000	-2.32050000	0.15740000
H	-6.25200000	-1.22760000	2.30430000
H	-6.84920000	-0.08570000	0.22440000
O	-4.78930000	1.34910000	1.86000000
C	-1.67280000	-0.85410000	-0.38510000
C	-4.50360000	2.63600000	2.43690000
H	-4.19860000	3.34130000	1.65900000
H	-5.43910000	2.95750000	2.89280000
H	-3.72350000	2.54660000	3.19820000
C	2.65270000	-1.17400000	1.62930000

C	2.29810000	-1.94330000	2.74940000
C	3.95200000	-0.64730000	1.55570000
C	3.22570000	-2.19880000	3.75670000
H	1.28530000	-2.32280000	2.84840000
C	4.87830000	-0.90600000	2.56470000
H	4.22920000	-0.04040000	0.70070000
C	4.52110000	-1.68430000	3.66650000
H	2.93230000	-2.79070000	4.61960000
H	5.88140000	-0.49540000	2.48870000
H	5.24270000	-1.88130000	4.45470000
C	0.66540000	-1.72560000	0.22640000
C	0.06980000	-1.13520000	-2.22990000
F	-0.83600000	-1.44730000	-3.17440000
F	1.24180000	-1.68740000	-2.58130000
F	0.21160000	0.21870000	-2.30060000
O	-0.91850000	-2.95620000	-1.05990000
Si	-0.14220000	-4.34310000	-1.60400000
H	1.13700000	-4.58240000	-0.88810000
H	-1.10640000	-5.42630000	-1.29560000
H	0.11190000	-4.31010000	-3.06530000
C	-0.40910000	-1.63890000	-0.83800000
H	-2.35460000	-0.73380000	-1.23730000
H	-2.19560000	-1.52140000	0.30370000
H	0.55770000	-2.61600000	0.83440000

TS8

C	-1.56690000	0.49520000	-0.98780000
C	-2.85150000	1.06370000	-0.98830000
C	-4.03630000	0.41260000	-0.65610000
C	-0.40310000	1.39680000	-1.35760000
O	-4.25830000	-0.87020000	-0.57270000
O	-5.07890000	1.19130000	-0.39960000
O	-1.33920000	-0.73060000	-0.72550000
C	0.37280000	2.00310000	-0.12580000
C	1.84600000	1.69260000	-0.21730000
C	2.30010000	0.42320000	-0.31280000
O	1.41480000	-0.59670000	-0.24160000
Ti	0.16270000	-1.72670000	0.38540000
C	-6.35190000	0.58430000	-0.09860000
Cl	1.57720000	-2.64810000	1.91180000
H	-2.93140000	2.13540000	-1.11480000
H	-6.28110000	-0.02130000	0.80730000
H	-7.02870000	1.42400000	0.05440000
H	-6.69170000	-0.03380000	-0.93310000
H	-0.77130000	2.20580000	-1.99170000
H	0.28670000	0.80420000	-1.95750000
O	-0.22620000	1.50320000	1.06750000
Si	0.13570000	1.89440000	2.67440000
H	-0.40060000	0.77130000	3.46670000
H	1.59940000	2.03510000	2.87420000

H	-0.54070000	3.15460000	3.07420000
H	2.55280000	2.51210000	-0.22180000
Cl	-1.49100000	-1.70210000	1.96490000
Cl	0.04880000	-3.45980000	-1.01940000
Si	-3.63050000	-2.26910000	-1.37110000
H	-4.89500000	-2.95690000	-1.73760000
H	-2.93140000	-1.85890000	-2.60430000
H	-2.87350000	-3.08150000	-0.41620000
C	0.17810000	3.53270000	-0.17200000
F	0.82000000	4.14280000	0.84980000
F	-1.12390000	3.87180000	-0.09100000
F	0.66720000	4.05260000	-1.31790000
C	3.71280000	0.04710000	-0.55880000
C	4.60690000	0.96470000	-1.13920000
C	4.17830000	-1.23610000	-0.23230000
C	5.93560000	0.61540000	-1.36220000
H	4.25660000	1.94650000	-1.44260000
C	5.50940000	-1.58250000	-0.46110000
H	3.50190000	-1.95370000	0.21550000
C	6.39310000	-0.66020000	-1.02190000
H	6.61130000	1.33540000	-1.81590000
H	5.85410000	-2.57810000	-0.19610000
H	7.42920000	-0.93400000	-1.20130000

Int12

C	-1.54243700	0.81129400	-0.83188100
C	-2.78553100	1.48082700	-0.94547300
C	-4.03048100	0.93315900	-0.67507900
C	-0.30532400	1.58703800	-1.31248900
O	-4.33264000	-0.33475100	-0.55379000
O	-5.04007300	1.78721200	-0.53326500
O	-1.40614700	-0.36087600	-0.39928100
C	0.56003100	2.17150300	-0.22252200
C	1.77578800	1.73586600	0.13975200
C	2.40217000	0.50946900	-0.40740500
O	1.70926600	-0.49080300	-0.65704100
Ti	0.11902400	-1.72192200	0.39196400
C	-6.37353100	1.26826900	-0.36308900
Cl	-0.12850000	-2.64115100	-1.74497700
H	-2.77728800	2.54126600	-1.16246500
H	-6.44388200	0.68482800	0.55741300
H	-7.00918400	2.15120300	-0.30434700
H	-6.66106200	0.64855000	-1.21620100
H	-0.63747700	2.40500600	-1.95821400
H	0.27813100	0.88757000	-1.91335700
H	2.34137300	2.29626300	0.87599400
Cl	1.89471100	-3.00665700	0.99143000
Si	-3.83725500	-1.70332600	-1.49820300
H	-5.14060300	-2.19845100	-2.01442300
H	-3.02296400	-1.19825700	-2.61885500

H	-3.22070900	-2.68862600	-0.60855200
C	-0.01701600	3.37749000	0.48687100
F	0.88685800	4.03819800	1.23201700
F	-1.02222800	2.99578500	1.30909800
F	-0.54300900	4.26351000	-0.39203000
C	3.85613700	0.47542800	-0.64907400
C	4.64191700	1.64248700	-0.62557300
C	4.46140400	-0.76683500	-0.91965700
C	6.01022900	1.56746700	-0.86745600
H	4.18373100	2.60856200	-0.43663000
C	5.83079900	-0.83541000	-1.15020500
H	3.84410800	-1.65869500	-0.92820900
C	6.60495100	0.32903300	-1.12573700
H	6.61305300	2.47070800	-0.85499900
H	6.29720500	-1.79595600	-1.34760400
H	7.67465000	0.27182200	-1.30820000
Cl	-1.44789700	-2.95705300	1.45572500
O	0.28624000	-0.47813400	1.69030900
Si	-0.03116900	-0.01647300	3.25424800
H	0.33122200	-1.09050200	4.21324500
H	0.78300800	1.19309200	3.56366700
H	-1.46763100	0.33260600	3.41375500

Int14

C	2.12960000	-0.36860000	0.13080000

C	3.42670000	0.26060000	0.11640000
C	3.76180000	1.36010000	0.86840000
C	1.96380000	-1.60920000	-0.78660000
O	2.92090000	1.88820000	1.73850000
O	1.17070000	-0.02250000	0.81750000
C	0.68940000	-1.55410000	-1.58420000
C	-0.55490000	-1.38720000	-1.10830000
C	-0.96960000	-1.26920000	0.30950000
O	-1.78040000	-0.37320000	0.62370000
C	3.26850000	3.10650000	2.42010000
Cl	-3.17090000	1.72810000	2.12850000
H	4.18190000	-0.14370000	-0.54690000
H	2.39910000	3.33210000	3.03650000
H	4.15370000	2.96410000	3.04490000
H	3.44450000	3.91410000	1.70510000
H	1.95050000	-2.47110000	-0.10850000
H	2.82250000	-1.73310000	-1.44890000
H	-1.36950000	-1.23500000	-1.81100000
C	-0.63810000	-2.29730000	1.32190000
C	-0.24590000	-3.59220000	0.94720000
C	-0.80280000	-1.98720000	2.68260000
C	-0.00790000	-4.56020000	1.92170000
H	-0.15620000	-3.84660000	-0.10450000
C	-0.55250000	-2.95310000	3.65070000
H	-1.11390000	-0.98550000	2.95830000

C	-0.15510000	-4.24020000	3.27270000
H	0.28260000	-5.56420000	1.62620000
H	-0.66990000	-2.70670000	4.70200000
H	0.03270000	-4.99470000	4.03180000
C	0.89430000	-1.58520000	-3.08060000
Cl	-1.10970000	2.03460000	-1.04640000
Cl	-4.14900000	-0.34080000	-1.04150000
Cl	-4.27310000	2.92660000	-0.74990000
Ti	-2.94530000	1.27580000	-0.04240000
O	4.94990000	1.97630000	0.79390000
F	1.49800000	-2.74460000	-3.44380000
F	-0.24540000	-1.48720000	-3.78330000
F	1.71010000	-0.58090000	-3.47440000
Si	6.22000000	1.72090000	-0.30730000
H	6.74830000	0.34410000	-0.15500000
H	5.73070000	1.93920000	-1.68800000
H	7.22860000	2.72610000	0.08320000

Int15

C	-1.69480000	0.45210000	1.97830000
C	-0.33450000	-0.01520000	1.79760000
C	0.80590000	0.76020000	1.79500000
C	-2.76090000	-0.49910000	1.39170000
O	0.82440000	1.98770000	2.29600000
O	-2.04210000	1.51180000	2.48170000

C	-2.42990000	-1.18650000	0.08080000
C	-1.51700000	-0.85170000	-0.84360000
C	-0.59310000	0.32260000	-0.88090000
O	0.64260000	0.12100000	-1.02590000
C	2.02340000	2.77180000	2.15880000
Cl	3.44840000	0.28680000	-1.96940000
H	-0.18710000	-1.03300000	1.46220000
H	1.79610000	3.71450000	2.65560000
H	2.86560000	2.27600000	2.64770000
H	2.26060000	2.94670000	1.10610000
H	-3.68820000	0.07720000	1.29770000
H	-2.96630000	-1.28050000	2.13650000
H	-1.37130000	-1.51730000	-1.69110000
C	-1.11050000	1.69110000	-1.03160000
C	-2.49030000	1.96410000	-1.07500000
C	-0.19180000	2.75210000	-1.16890000
C	-2.93990000	3.27150000	-1.23280000
H	-3.20530000	1.15310000	-1.00220000
C	-0.64670000	4.05360000	-1.32840000
H	0.87000000	2.53140000	-1.16130000
C	-2.02160000	4.31590000	-1.35610000
H	-4.00580000	3.47520000	-1.26300000
H	0.06470000	4.86710000	-1.43580000
H	-2.37530000	5.33560000	-1.47990000
C	-3.24820000	-2.43930000	-0.15790000

Cl	1.54080000	-2.72400000	-0.68560000
Cl	4.22910000	-1.44660000	0.77680000
Ti	2.39910000	-0.70510000	-0.27290000
O	1.90550000	0.32280000	1.21860000
F	-4.56830000	-2.14420000	-0.10330000
F	-3.01270000	-3.02030000	-1.34810000
F	-3.00710000	-3.36160000	0.79980000

TS9

C	0.26750000	1.07110000	1.89590000
C	-0.18360000	-0.28990000	1.54330000
C	0.68230000	-1.46860000	1.72180000
C	1.51650000	1.64380000	1.17680000
O	0.31670000	-2.62730000	1.61940000
O	1.96940000	-1.15040000	2.05150000
O	-0.36800000	1.80560000	2.63430000
C	1.08840000	2.09740000	-0.19240000
C	0.54180000	1.30720000	-1.12950000
H	0.11460000	1.75160000	-2.02640000
C	0.37550000	-0.16000000	-1.07930000
O	-0.79930000	-0.60700000	-1.44760000
Ti	-2.25730000	-0.49990000	-0.24860000
C	2.82760000	-2.26930000	2.32640000
Cl	-2.87060000	-2.30760000	0.83440000

Cl	-3.70110000	-0.57020000	-1.93810000
H	2.42340000	-2.86660000	3.14740000
H	2.93480000	-2.90370000	1.44370000
H	3.78850000	-1.83570000	2.60650000
H	2.29360000	0.87960000	1.11940000
H	1.88380000	2.48570000	1.76490000
Cl	-2.91660000	1.37520000	0.68570000
H	-1.14550000	-0.49390000	2.01820000
C	1.49960000	-1.08360000	-1.17680000
C	2.82710000	-0.60830000	-1.25740000
C	1.25120000	-2.46860000	-1.30110000
C	3.87490000	-1.49620000	-1.46180000
H	3.02260000	0.45610000	-1.19530000
C	2.30620000	-3.34870000	-1.50780000
H	0.23570000	-2.83720000	-1.23260000
C	3.61620000	-2.86610000	-1.58860000
H	4.89180000	-1.12350000	-1.53700000
H	2.10850000	-4.41170000	-1.60430000
H	4.43760000	-3.55720000	-1.75700000
C	1.17580000	3.58410000	-0.45060000
F	0.71930000	3.93580000	-1.66840000
F	2.46780000	3.98240000	-0.37090000
F	0.48190000	4.27760000	0.46770000

Int16

C	-1.30830000	2.07740000	1.06940000
C	-2.05050000	0.80490000	1.05220000
C	-1.78910000	-0.34640000	1.85760000
C	0.21090000	2.05350000	1.39060000
O	-2.18200000	-1.46550000	1.39030000
O	-1.06980000	-0.28790000	2.96510000
O	-1.84590000	3.13130000	0.78250000
C	1.07980000	2.10220000	0.15790000
C	1.63380000	1.04990000	-0.47050000
H	2.31260000	1.23450000	-1.29560000
C	1.43020000	-0.36590000	-0.09850000
O	0.30570000	-0.80700000	0.21480000
Ti	-1.89060000	-0.88800000	-0.56210000
C	-0.66250000	-1.55040000	3.55160000
Cl	-4.05080000	-0.97970000	-1.04630000
Cl	-1.24430000	-2.94250000	-1.22280000
H	-1.54020000	-2.12460000	3.85230000
H	-0.07240000	-2.11890000	2.83040000
H	-0.06450000	-1.27570000	4.41960000
H	0.45760000	1.17060000	1.97870000
H	0.40990000	2.94090000	1.99700000
Cl	-1.25960000	0.52100000	-2.18070000
C	2.59250000	-1.27650000	-0.10380000
C	3.91150000	-0.78720000	-0.15340000

C	2.36960000	-2.66570000	-0.04320000
C	4.98590000	-1.67150000	-0.14190000
H	4.09630000	0.28200000	-0.18170000
C	3.44730000	-3.54400000	-0.04390000
H	1.34950000	-3.03370000	-0.02100000
C	4.75460000	-3.04900000	-0.09100000
H	6.00180000	-1.28930000	-0.17300000
H	3.27140000	-4.61520000	-0.01270000
H	5.59470000	-3.73800000	-0.08970000
C	1.39820000	3.49170000	-0.36960000
F	2.34310000	3.47440000	-1.33420000
F	1.86410000	4.28100000	0.62630000
F	0.30610000	4.07720000	-0.87940000
H	-3.10210000	0.92500000	0.79300000

Int17

C	3.17850000	0.79440000	0.28290000
C	2.04260000	0.06430000	0.53990000
H	2.14550000	-1.01120000	0.52540000
C	0.70160000	0.49890000	0.75290000
C	0.32770000	1.97390000	1.05800000
O	-0.27120000	-0.28040000	0.74860000
Ti	-0.82920000	-2.32790000	0.39610000

Cl	-1.63560000	-4.34080000	-0.17950000
Cl	-2.42030000	-1.89640000	1.97850000
Cl	0.76450000	-3.02300000	1.80570000
O	-2.41330000	-1.37990000	-1.07640000
Si	-3.52620000	-2.31580000	-1.99630000
C	-2.43660000	0.02710000	-1.32290000
C	-3.29920000	0.71100000	-0.37350000
H	-3.80690000	0.07110000	0.33360000
C	-3.44420000	2.04830000	-0.24070000
O	-2.83520000	2.94130000	-1.03790000
Si	-2.76430000	4.60780000	-0.72880000
Cl	0.52830000	-2.16620000	-1.47740000
H	-1.84720000	5.09360000	-1.78540000
H	-4.09150000	5.25070000	-0.88340000
H	-2.19930000	4.90090000	0.60930000
H	-4.32120000	-3.16480000	-1.08520000
H	-4.41380000	-1.34240000	-2.67520000
H	-2.79440000	-3.12380000	-2.99540000
O	-4.19680000	2.67740000	0.69250000
C	-1.71510000	0.49500000	-2.35130000
H	-1.72010000	1.54960000	-2.58920000
H	-1.10550000	-0.17620000	-2.94350000
C	-4.81460000	1.89680000	1.71890000
H	-5.56840000	1.22620000	1.29190000
H	-4.06500000	1.31280000	2.26260000

H	-5.29330000	2.61420000	2.38590000
C	4.45780000	0.12570000	-0.01870000
C	5.67010000	0.72780000	0.36840000
C	4.48710000	-1.11710000	-0.68070000
C	6.88200000	0.09330000	0.11290000
H	5.65310000	1.67290000	0.90090000
C	5.70440000	-1.73870000	-0.94370000
H	3.56220000	-1.57790000	-1.01440000
C	6.90190000	-1.13890000	-0.54570000
H	7.81080000	0.55680000	0.43230000
H	5.71720000	-2.69140000	-1.46460000
H	7.84920000	-1.63030000	-0.74900000
O	3.17790000	2.13390000	0.33410000
Si	3.54790000	3.27980000	-0.86320000
H	2.99220000	4.54500000	-0.34430000
H	5.01400000	3.39790000	-1.04550000
H	2.90740000	2.86500000	-2.13260000
F	-0.94050000	2.06770000	1.46510000
F	0.45940000	2.73680000	-0.05510000
F	1.10690000	2.48560000	2.02310000

TS10

C	-3.47090000	-0.77090000	0.26490000
C	-2.23820000	-0.16100000	0.37440000
H	-2.23390000	0.91930000	0.43570000
C	-0.93980000	-0.72910000	0.37850000

C	-0.65070000	-2.24800000	0.29370000
O	0.09450000	-0.02350000	0.42720000
Ti	0.82720000	1.88450000	0.24840000
Cl	1.98600000	4.01440000	-0.14290000
Cl	1.82110000	1.40820000	2.26310000
Cl	-0.81730000	3.09150000	1.25540000
O	2.53990000	1.51400000	-0.73020000
Si	3.80830000	2.93190000	-1.16340000
C	2.88150000	0.18690000	-1.08560000
C	3.66330000	-0.47890000	-0.05270000
H	4.01850000	0.15800000	0.74400000
C	3.90990000	-1.80450000	0.03380000
O	3.50010000	-2.69770000	-0.88350000
Si	3.53470000	-4.37860000	-0.66860000
Cl	-0.33080000	1.88330000	-1.76610000
H	2.81820000	-4.87540000	-1.86580000
H	4.92140000	-4.90390000	-0.66090000
H	2.81890000	-4.79580000	0.56080000
H	4.75370000	2.57150000	-0.08140000
H	4.03810000	2.20130000	-2.43930000
H	4.18790000	4.32170000	-1.56830000
O	4.58860000	-2.42500000	1.03000000
C	2.48370000	-0.25620000	-2.28950000
H	2.75080000	-1.24890000	-2.62560000
H	1.88680000	0.37510000	-2.93540000

C	5.01520000	-1.65480000	2.15530000
H	5.75320000	-0.90410000	1.85100000
H	4.16170000	-1.16210000	2.63280000
H	5.47390000	-2.36650000	2.84230000
C	-4.69540000	0.03220000	0.11200000
C	-5.91050000	-0.42420000	0.65800000
C	-4.66510000	1.26670000	-0.56640000
C	-7.06620000	0.34090000	0.53440000
H	-5.93410000	-1.35580000	1.21340000
C	-5.82780000	2.01990000	-0.69530000
H	-3.74090000	1.61840000	-1.01440000
C	-7.02780000	1.56140000	-0.14490000
H	-7.99460000	-0.00980000	0.97530000
H	-5.79730000	2.96490000	-1.22900000
H	-7.93170000	2.15580000	-0.24340000
O	-3.59350000	-2.09730000	0.34940000
Si	-4.36530000	-3.22750000	-0.66410000
H	-3.60440000	-4.47810000	-0.48060000
H	-5.77120000	-3.41990000	-0.23890000
H	-4.30270000	-2.73100000	-2.05760000
F	0.66350000	-2.47800000	0.27020000
F	-1.17700000	-2.76000000	-0.84270000
F	-1.17160000	-2.90190000	1.34350000

Int18

C	4.46310000	0.43120000	-0.06170000
C	3.11970000	0.26390000	0.16790000
H	2.80810000	-0.70860000	0.52390000
C	2.03550000	1.18260000	0.00830000
C	2.20740000	2.61930000	-0.55000000
O	0.86080000	0.88740000	0.28290000
Ti	-0.40490000	-0.74730000	1.06850000
Cl	-5.13060000	-2.40870000	-2.90200000
Cl	0.80390000	-0.39750000	2.94670000
Cl	-1.56640000	-2.51260000	1.86440000
O	-1.71940000	0.34060000	0.79170000
Si	-3.08780000	-2.31380000	-2.44260000
C	-2.84490000	1.12120000	0.61900000
C	-4.06570000	0.34270000	0.79020000
H	-3.91790000	-0.69120000	1.07160000
C	-5.33000000	0.79820000	0.63660000
O	-5.62130000	2.06790000	0.31100000
Si	-7.19280000	2.65580000	0.04590000
Cl	0.35510000	-1.83300000	-0.79720000
H	-6.94970000	4.07320000	-0.30670000
H	-7.85610000	1.95670000	-1.07990000
H	-8.02110000	2.57570000	1.27280000
H	-2.68000000	-0.89420000	-2.50150000

H	-2.91450000	-2.88440000	-1.09220000
H	-2.36700000	-3.11280000	-3.46070000
O	-6.46180000	0.07350000	0.78820000
C	-2.64550000	2.41840000	0.32520000
H	-3.48330000	3.08440000	0.17700000
H	-1.63640000	2.80020000	0.22630000
C	-6.36020000	-1.32630000	1.06150000
H	-5.83720000	-1.83860000	0.24730000
H	-5.84030000	-1.49780000	2.01020000
H	-7.38680000	-1.68650000	1.12940000
C	5.40100000	-0.70240000	0.05930000
C	6.70320000	-0.48920000	0.54820000
C	5.00630000	-2.00540000	-0.29770000
C	7.58570000	-1.55740000	0.68460000
H	7.00460000	0.50670000	0.85530000
C	5.89730000	-3.06680000	-0.16870000
H	4.01300000	-2.17810000	-0.70040000
C	7.18630000	-2.84630000	0.32380000
H	8.58250000	-1.38520000	1.07980000
H	5.58640000	-4.06640000	-0.45710000
H	7.87760000	-3.67780000	0.42700000
O	4.97620000	1.63790000	-0.33300000
Si	5.98950000	2.15590000	-1.59560000
H	5.67740000	3.58770000	-1.76920000
H	7.41230000	1.98840000	-1.21690000

H	5.68270000	1.36610000	-2.81090000
F	1.01930000	3.20700000	-0.71130000
F	2.81210000	2.58790000	-1.76120000
F	2.94050000	3.37980000	0.27830000

Int18'

C	2.90340000	0.42080000	0.42410000
C	1.75060000	-0.31490000	0.51890000
H	1.81310000	-1.36370000	0.25720000
C	0.43850000	0.06930000	0.95390000
C	0.07630000	1.51210000	1.40360000
O	-0.50210000	-0.73640000	1.02180000
Ti	-1.48810000	-2.53270000	0.10650000
Cl	-2.58360000	-4.22870000	-0.87000000
Cl	-2.88250000	-2.28940000	1.84480000
O	-1.57000000	-1.38700000	-1.23630000
C	-1.74650000	-0.08560000	-1.63840000
C	-2.98010000	0.49760000	-1.11990000
H	-3.72340000	-0.21140000	-0.78100000
C	-3.22700000	1.81560000	-0.95510000
O	-2.37230000	2.77990000	-1.33250000
Si	-2.45740000	4.39100000	-0.80640000
Cl	0.46790000	-3.62930000	0.40020000
H	-1.20250000	4.97400000	-1.33380000

H	-3.62000000	5.09820000	-1.39510000
H	-2.48610000	4.48480000	0.67200000
O	-4.33620000	2.35190000	-0.39520000
C	-0.79660000	0.46370000	-2.41940000
H	-0.90030000	1.47480000	-2.78750000
H	0.07540000	-0.11370000	-2.70390000
C	-5.30770000	1.47800000	0.18540000
H	-4.84990000	0.85000000	0.95690000
H	-6.06190000	2.12930000	0.62760000
H	-5.76680000	0.84720000	-0.58360000
C	4.14760000	-0.16950000	-0.11070000
C	5.39350000	0.24370000	0.39660000
C	4.11190000	-1.15470000	-1.11490000
C	6.57200000	-0.32090000	-0.08410000
H	5.43010000	0.98050000	1.19180000
C	5.29360000	-1.70900000	-1.59760000
H	3.15990000	-1.46760000	-1.53160000
C	6.52530000	-1.29530000	-1.08350000
H	7.52660000	-0.00540000	0.32670000
H	5.25320000	-2.46190000	-2.37910000
H	7.44570000	-1.73200000	-1.46050000
O	2.96800000	1.68170000	0.88150000
Si	3.43020000	3.11270000	0.09520000
H	2.71870000	4.19020000	0.81040000
H	4.89450000	3.31650000	0.20510000

H	3.03190000	3.03070000	-1.32960000
F	0.75650000	1.86550000	2.50640000
F	0.35190000	2.40750000	0.42240000
F	-1.22810000	1.60780000	1.67230000

TS11

C	2.79140000	0.40540000	0.31730000
C	1.68770000	-0.38590000	0.24180000
H	1.83030000	-1.38600000	-0.15080000
C	0.31520000	-0.16630000	0.67570000
C	-0.10360000	1.06800000	1.51240000
O	-0.41320000	-1.19550000	0.90610000
Ti	-1.47390000	-2.65900000	0.04870000
Cl	-2.82940000	-4.05020000	-1.11030000
Cl	-2.31780000	-3.14810000	2.06360000
O	-2.05870000	-1.22000000	-0.96710000
C	-1.84790000	0.08360000	-1.10520000
C	-3.01520000	0.88800000	-0.84470000
H	-3.90230000	0.32340000	-0.59300000
C	-3.09160000	2.24730000	-0.85300000
O	-2.06190000	3.03880000	-1.14840000
Si	-1.99800000	4.71570000	-0.84150000
Cl	0.42930000	-3.71790000	-0.53840000
H	-0.59790000	5.05030000	-1.17890000

H	-2.93080000	5.45390000	-1.72380000
H	-2.28060000	4.99530000	0.58460000
O	-4.19010000	2.96650000	-0.56250000
C	-0.54980000	0.48740000	-1.38970000
H	-0.31260000	1.52980000	-1.54200000
H	0.10240000	-0.25000000	-1.83970000
C	-5.39700000	2.29560000	-0.17720000
H	-5.23250000	1.69940000	0.72580000
H	-6.11810000	3.08790000	0.02180000
H	-5.75620000	1.65710000	-0.99030000
C	4.10920000	-0.05310000	-0.17690000
C	5.28320000	0.34040000	0.49000000
C	4.21650000	-0.89110000	-1.30120000
C	6.52820000	-0.10260000	0.05040000
H	5.21020000	0.97030000	1.37040000
C	5.46360000	-1.32830000	-1.73980000
H	3.32240000	-1.18430000	-1.84250000
C	6.62270000	-0.93690000	-1.06550000
H	7.42540000	0.19860000	0.58380000
H	5.53040000	-1.97080000	-2.61310000
H	7.59460000	-1.27970000	-1.40910000
O	2.76250000	1.60970000	0.94270000
Si	3.09050000	3.13820000	0.31130000
H	2.58180000	4.08670000	1.32400000
H	4.54670000	3.34250000	0.11300000

H	2.39210000	3.30930000	-0.98790000
F	0.57340000	1.08210000	2.67400000
F	0.12090000	2.25190000	0.89040000
F	-1.41170000	1.01930000	1.79920000

Int19

C	-2.75140000	-0.34040000	0.26190000
C	-1.64690000	0.27770000	-0.12920000
H	-1.75180000	0.98000000	-0.93420000
C	-0.21150000	0.24310000	0.35780000
C	0.03030000	-0.37750000	1.74190000
O	0.20090000	1.56940000	0.46800000
Ti	1.44390000	2.69140000	-0.06540000
Cl	1.51560000	2.98850000	-2.31070000
Cl	3.17840000	3.17900000	1.28360000
O	2.50350000	0.93430000	-0.46680000
C	2.13500000	-0.23630000	-0.57710000
C	3.16040000	-1.23080000	-0.65240000
H	4.14780000	-0.82230000	-0.61080000
C	3.02420000	-2.57960000	-0.72060000
O	1.88320000	-3.20770000	-0.77670000
Si	1.63090000	-4.88900000	-0.73810000
Cl	0.29390000	4.58530000	0.36090000
H	0.17260000	-5.00250000	-0.77500000

H	2.24120000	-5.50580000	-1.91910000
H	2.18180000	-5.43620000	0.50440000
O	4.03180000	-3.41970000	-0.73950000
C	0.64910000	-0.49820000	-0.69370000
H	0.41290000	-1.54540000	-0.68590000
H	0.37470000	-0.10260000	-1.66730000
C	5.38330000	-2.98410000	-0.66450000
H	5.55250000	-2.44870000	0.25830000
H	5.97290000	-3.88500000	-0.68590000
H	5.62280000	-2.36210000	-1.51480000
C	-4.05900000	-0.10850000	-0.41880000
C	-5.20800000	0.07550000	0.34690000
C	-4.15830000	-0.06600000	-1.80480000
C	-6.42530000	0.31560000	-0.26360000
H	-5.14130000	0.04690000	1.41870000
C	-5.37920000	0.17060000	-2.41530000
H	-3.28410000	-0.22910000	-2.40820000
C	-6.51410000	0.36390000	-1.64660000
H	-7.30250000	0.46920000	0.33860000
H	-5.44190000	0.19850000	-3.48820000
H	-7.46150000	0.54850000	-2.12010000
O	-2.79900000	-1.16300000	1.33170000
Si	-3.17170000	-2.77760000	1.40960000
H	-2.73200000	-3.23780000	2.73030000
H	-4.61610000	-3.00370000	1.25480000

H	-2.45570000	-3.50140000	0.34210000
F	-0.71450000	0.15060000	2.67640000
F	-0.16360000	-1.69230000	1.72900000
F	1.29800000	-0.20210000	2.09040000

Int20

C	-1.58141200	0.55884500	1.75815800
C	-1.45794700	-0.89033200	1.37804000
C	-0.46746400	-1.78556800	2.05822300
C	-0.33349800	1.48381400	1.73784100
O	-0.67533800	-2.95898900	2.28695200
O	0.70249300	-1.18423600	2.42152300
O	-2.65830000	1.04159100	2.05140400
C	-0.06023700	2.10586300	0.38806100
C	0.72107100	1.59140800	-0.57412600
H	0.91611300	2.15550200	-1.48123100
C	1.33236000	0.24018100	-0.49884000
O	0.58439500	-0.76093000	-0.43676700
Ti	-1.42839600	-1.15549100	-0.83823100
C	1.63225400	-2.03845000	3.10918600
Cl	-1.47468600	-3.32677900	-1.05100400
Cl	-0.85480000	-0.31304400	-2.87801600
H	1.18431600	-2.43667700	4.02274100
H	1.93317500	-2.87300200	2.47071400
H	2.48898500	-1.40588900	3.34544800

H	0.53985000	0.92377000	2.06834000
H	-0.53717600	2.27916100	2.45805700
Cl	-3.52470200	-0.46566500	-0.91192800
H	-2.43741400	-1.35223400	1.52567700
C	2.78360400	0.06918800	-0.53357900
C	3.63752000	1.18585200	-0.45302600
C	3.33189800	-1.22456700	-0.64612200
C	5.01700300	1.01071000	-0.48665100
H	3.21822500	2.18229700	-0.35412800
C	4.71006300	-1.39112200	-0.68223700
H	2.66469300	-2.07717200	-0.71303500
C	5.55212900	-0.27528800	-0.60292400
H	5.67450800	1.87219700	-0.42246900
H	5.13339000	-2.38648000	-0.77631900
H	6.62978400	-0.40982400	-0.63309000
C	-0.70649200	3.45557600	0.14364200
F	-0.36881500	4.32982100	1.11815400
F	-0.33689600	4.00333100	-1.03164600
F	-2.04469700	3.34088200	0.14323900

TS12

C	0.26690000	1.07100000	1.89610000
C	-0.18360000	-0.29010000	1.54300000
C	0.68280000	-1.46850000	1.72160000
C	1.51540000	1.64460000	1.17710000

O	0.31770000	-2.62730000	1.61940000
O	1.96970000	-1.14960000	2.05130000
O	-0.36880000	1.80470000	2.63500000
C	1.08740000	2.09780000	-0.19230000
C	0.54130000	1.30740000	-1.12940000
H	0.11430000	1.75150000	-2.02650000
C	0.37550000	-0.16000000	-1.07910000
O	-0.79910000	-0.60730000	-1.44770000
Ti	-2.25700000	-0.50060000	-0.24870000
C	2.82840000	-2.26820000	2.32630000
Cl	-2.86970000	-2.30880000	0.83390000
Cl	-3.70080000	-0.57100000	-1.93810000
H	2.42470000	-2.86530000	3.14770000
H	2.93570000	-2.90280000	1.44380000
H	3.78930000	-1.83410000	2.60610000
H	2.29310000	0.88100000	1.11980000
H	1.88200000	2.48680000	1.76520000
Cl	-2.91700000	1.37410000	0.68600000
H	-1.14540000	-0.49460000	2.01810000
C	1.50000000	-1.08300000	-1.17670000
C	2.82730000	-0.60720000	-1.25710000
C	1.25220000	-2.46820000	-1.30130000
C	3.87550000	-1.49470000	-1.46150000
H	3.02230000	0.45730000	-1.19480000
C	2.30760000	-3.34780000	-1.50800000

H	0.23680000	-2.83720000	-1.23290000
C	3.61740000	-2.86460000	-1.58860000
H	4.89230000	-1.12150000	-1.53650000
H	2.11030000	-4.41080000	-1.60470000
H	4.43910000	-3.55540000	-1.75700000
C	1.17450000	3.58450000	-0.45070000
F	2.46630000	3.98320000	-0.37060000
F	0.71830000	3.93590000	-1.66870000
F	0.48000000	4.27790000	0.46720000

INt21

C	-0.91150000	1.03420000	-2.02070000
C	-1.01140000	-0.39840000	-1.47090000
C	-2.44910000	-0.92110000	-1.56800000
C	-1.31650000	2.17030000	-1.09450000
O	-2.76350000	-1.90980000	-2.18400000
O	-3.31860000	-0.13220000	-0.90210000
O	-0.54820000	1.23620000	-3.15790000
C	-1.15700000	1.85300000	0.36850000
C	-0.78430000	0.66580000	0.84920000
H	-0.65830000	0.52080000	1.91660000
C	-0.41200000	-0.50500000	-0.03250000
O	1.02160000	-0.40130000	-0.22330000
Ti	2.70380000	-0.01140000	-0.11490000

C	-4.69570000	-0.56170000	-0.94390000
Cl	3.86290000	-1.52250000	-1.22950000
Cl	3.29230000	-0.01960000	2.00740000
H	-5.04780000	-0.60440000	-1.97710000
H	-4.79430000	-1.54940000	-0.48780000
H	-5.24920000	0.18550000	-0.37560000
H	-2.36710000	2.41710000	-1.30210000
H	-0.73060000	3.05460000	-1.36800000
Cl	3.04550000	1.99360000	-0.96110000
H	-0.42690000	-1.04390000	-2.12810000
C	-0.71340000	-1.86170000	0.60040000
C	-1.77030000	-2.00470000	1.50810000
C	0.02640000	-2.99170000	0.22850000
C	-2.07510000	-3.25760000	2.04310000
H	-2.36190000	-1.14120000	1.79720000
C	-0.27740000	-4.24020000	0.76840000
H	0.84550000	-2.89580000	-0.47730000
C	-1.32800000	-4.37700000	1.67780000
H	-2.89400000	-3.35340000	2.75060000
H	0.30890000	-5.10680000	0.47660000
H	-1.56220000	-5.35070000	2.09860000
C	-1.43200000	3.00040000	1.30630000
F	-2.68710000	3.47420000	1.12160000
F	-1.31160000	2.66370000	2.60360000
F	-0.58380000	4.02550000	1.06800000

Int22

C	3.23460000	1.24610000	0.34390000
C	2.17370000	0.39550000	0.48640000
H	2.39080000	-0.66240000	0.44400000
C	0.78550000	0.72590000	0.66170000
C	0.27740000	2.13160000	0.83810000
O	-0.07590000	-0.19170000	0.67730000
Ti	-0.45720000	-2.18360000	0.27760000
Cl	-1.23960000	-4.18330000	-0.42010000
Cl	-1.87550000	-2.04290000	2.08690000
Cl	1.31900000	-2.93100000	1.41650000
O	-2.32260000	-1.23500000	-0.89530000
Si	-3.53850000	-2.19270000	-1.64490000
C	-2.49520000	0.17360000	-0.99740000
C	-3.26150000	0.69520000	0.12770000
H	-3.36640000	0.01230000	0.95930000
C	-3.83200000	1.91670000	0.22490000
O	-3.74950000	2.85810000	-0.73260000
Si	-4.58720000	4.33330000	-0.70210000
Cl	0.64400000	-1.77400000	-1.72070000
H	-4.20090000	4.95240000	-1.99050000
H	-6.05500000	4.13030000	-0.65260000
H	-4.14270000	5.19480000	0.42030000
H	-4.11880000	-3.12900000	-0.66100000

H	-4.58070000	-1.23980000	-2.09960000
H	-2.96900000	-2.90180000	-2.81050000
H	0.78840000	2.62850000	1.66820000
H	0.48470000	2.72160000	-0.06170000
H	-0.79870000	2.09970000	1.01190000
O	-4.55930000	2.37140000	1.27520000
C	-1.97550000	0.79870000	-2.06190000
H	-2.08460000	1.86870000	-2.17920000
H	-1.42990000	0.24010000	-2.81270000
C	-4.79660000	1.49590000	2.38000000
H	-5.33940000	0.60220000	2.05420000
H	-3.85270000	1.20050000	2.85030000
H	-5.40310000	2.06730000	3.08310000
C	4.59570000	0.73290000	0.08070000
C	5.71400000	1.35260000	0.66740000
C	4.78710000	-0.39080000	-0.74350000
C	6.99490000	0.85620000	0.43640000
H	5.57510000	2.19390000	1.33960000
C	6.07110000	-0.87660000	-0.97610000
H	3.93210000	-0.86440000	-1.21650000
C	7.17630000	-0.25630000	-0.38830000
H	7.84980000	1.33130000	0.90880000
H	6.20820000	-1.73920000	-1.62150000
H	8.17600000	-0.64050000	-0.57000000
O	3.07980000	2.58040000	0.47480000

Si	3.77510000	3.86310000	-0.39210000
H	2.68370000	4.85410000	-0.52540000
H	4.89240000	4.45420000	0.38000000
H	4.23500000	3.39290000	-1.71870000

TS13

C	3.54020000	1.21880000	0.24050000
C	2.37970000	0.50100000	0.36790000
H	2.47010000	-0.57430000	0.45740000
C	1.03830000	0.99800000	0.38210000
C	0.65960000	2.45200000	0.33690000
O	0.08250000	0.17360000	0.43710000
Ti	-0.54360000	-1.70150000	0.15820000
Cl	-1.67490000	-3.83360000	-0.35370000
Cl	-1.45180000	-1.49290000	2.27260000
Cl	1.20020000	-2.92560000	0.96010000
O	-2.33860000	-1.29820000	-0.67380000
Si	-3.61610000	-2.72570000	-1.06130000
C	-2.76470000	0.02810000	-0.90760000
C	-3.50270000	0.57360000	0.22640000
H	-3.52690000	-0.05950000	1.10140000
C	-4.13220000	1.76680000	0.29050000
O	-4.15330000	2.65800000	-0.71920000
Si	-5.04980000	4.09670000	-0.70800000

Cl	0.46760000	-1.52210000	-1.92500000
H	-4.77410000	4.66150000	-2.04920000
H	-6.50210000	3.84200000	-0.55220000
H	-4.57300000	5.03700000	0.33550000
H	-4.42590000	-2.50650000	0.15900000
H	-4.03410000	-1.88870000	-2.22010000
H	-4.00860000	-4.08210000	-1.55980000
H	1.13030000	3.00200000	1.15750000
H	1.01640000	2.90400000	-0.59510000
H	-0.42640000	2.53800000	0.39340000
O	-4.82330000	2.24620000	1.35590000
C	-2.48100000	0.57590000	-2.10000000
H	-2.80130000	1.58170000	-2.33560000
H	-1.92910000	0.01120000	-2.84070000
C	-4.94570000	1.42750000	2.52040000
H	-5.45570000	0.48840000	2.27990000
H	-3.96070000	1.21120000	2.94760000
H	-5.54170000	2.00680000	3.22620000
C	4.85100000	0.54430000	0.15690000
C	5.97720000	1.10010000	0.79130000
C	4.98330000	-0.67040000	-0.53980000
C	7.20870000	0.45270000	0.72920000
H	5.87690000	2.01250000	1.37150000
C	6.21990000	-1.30700000	-0.60530000
H	4.12380000	-1.09800000	-1.04700000

C	7.33330000	-0.74870000	0.02740000
H	8.06810000	0.88010000	1.23760000
H	6.31360000	-2.23930000	-1.15410000
H	8.29530000	-1.25060000	-0.02280000
O	3.51740000	2.56430000	0.22460000
Si	4.44770000	3.68920000	-0.64800000
H	3.48460000	4.75090000	-1.01510000
H	5.50570000	4.24940000	0.22320000
H	5.02580000	3.04790000	-1.85030000

Int23

C	-4.03950000	0.79440000	-0.35770000
C	-2.70230000	0.55750000	-0.22290000
H	-2.40130000	-0.47830000	-0.14700000
C	-1.62300000	1.51530000	-0.15880000
C	-1.82260000	2.99790000	-0.34470000
O	-0.45270000	1.12670000	0.05980000
Ti	0.69320000	-0.64130000	0.47070000
Cl	0.15170000	-1.16620000	-1.68120000
Cl	1.69740000	-2.64060000	0.84970000
O	2.10390000	0.36590000	0.63740000
C	3.42080000	0.76700000	0.66650000
C	4.27850000	-0.09810000	-0.13690000
H	3.79510000	-0.97640000	-0.54040000
C	5.59160000	0.08170000	-0.39390000

O	6.30570000	1.12510000	0.06410000
Si	7.94970000	1.38190000	-0.26330000
Cl	-0.64300000	-0.77320000	2.31670000
H	8.23100000	2.64330000	0.45970000
H	8.79720000	0.29120000	0.27560000
H	8.19980000	1.56550000	-1.71350000
H	-2.31580000	3.20810000	-1.29850000
H	-2.47100000	3.39840000	0.44230000
H	-0.85040000	3.49200000	-0.30490000
O	6.37460000	-0.73960000	-1.13620000
C	3.71460000	1.85850000	1.39610000
H	4.72900000	2.22520000	1.45850000
H	2.92960000	2.37940000	1.93120000
C	5.79390000	-1.91190000	-1.71010000
H	5.40010000	-2.57080000	-0.92890000
H	4.99110000	-1.64400000	-2.40570000
H	6.60270000	-2.40870000	-2.24660000
C	-5.02390000	-0.30970000	-0.32990000
C	-6.13260000	-0.29380000	-1.19510000
C	-4.85490000	-1.39470000	0.54820000
C	-7.04930000	-1.34290000	-1.18280000
H	-6.25120000	0.51880000	-1.90540000
C	-5.77870000	-2.43670000	0.56020000
H	-4.01360000	-1.40530000	1.23470000
C	-6.87640000	-2.41400000	-0.30350000

H	-7.89280000	-1.32860000	-1.86710000
H	-5.64320000	-3.26510000	1.24930000
H	-7.59380000	-3.22960000	-0.29300000
O	-4.50750000	2.04530000	-0.56300000
Si	-5.89250000	2.81570000	0.04060000
H	-5.45870000	4.20650000	0.30320000
H	-6.96550000	2.81340000	-0.98080000
H	-6.34540000	2.15480000	1.28640000

Int24

C	-2.62080000	-0.54650000	-0.43000000
C	-1.45250000	-1.18190000	-0.24750000
H	-1.48110000	-2.16640000	0.20620000
C	-0.06360000	-0.71470000	-0.65190000
C	0.05940000	-0.52950000	-2.17390000
O	0.82500000	-1.76910000	-0.26270000
Ti	2.52960000	-2.05110000	0.08080000
Cl	3.18880000	-1.53230000	2.18600000
Cl	3.92400000	-2.07370000	-1.69070000
O	2.65860000	0.09330000	-0.18730000
C	1.77420000	0.97510000	-0.06560000
C	2.22140000	2.34020000	-0.12080000
H	3.27630000	2.43830000	-0.34150000
C	1.51660000	3.48190000	0.14520000
O	0.23990000	3.51150000	0.51140000

Si	-0.60220000	4.93240000	0.97880000
Cl	2.43610000	-4.28250000	0.38780000
H	-1.92360000	4.40080000	1.36660000
H	0.07270000	5.56720000	2.13250000
H	-0.71980000	5.86780000	-0.16210000
H	1.08220000	-0.25500000	-2.45000000
H	-0.18920000	-1.46980000	-2.67320000
H	-0.63310000	0.24300000	-2.51740000
O	2.02970000	4.71950000	0.09390000
C	0.32900000	0.56460000	0.13220000
H	-0.34620000	1.37370000	-0.14000000
H	0.18890000	0.36970000	1.20450000
C	3.39980000	4.92370000	-0.28670000
H	3.57800000	4.53360000	-1.29290000
H	3.54340000	6.00350000	-0.27030000
H	4.07050000	4.44320000	0.43140000
C	-3.92230000	-1.11990000	-0.00210000
C	-5.03770000	-1.07640000	-0.85660000
C	-4.05800000	-1.73360000	1.25400000
C	-6.25350000	-1.63510000	-0.46400000
H	-4.94110000	-0.63210000	-1.84270000
C	-5.27300000	-2.29570000	1.64140000
H	-3.20770000	-1.75420000	1.92920000
C	-6.37530000	-2.24610000	0.78540000
H	-7.10310000	-1.60280000	-1.14060000

H	-5.36120000	-2.76420000	2.61770000
H	-7.32320000	-2.68070000	1.09020000
O	-2.65690000	0.66500000	-1.09690000
Si	-3.62430000	2.00000000	-0.78110000
H	-2.83590000	3.15450000	-1.27910000
H	-4.91040000	1.95380000	-1.51840000
H	-3.88260000	2.15100000	0.67380000

TS14

C	2.67700000	0.36980000	0.53870000
C	1.61660000	-0.47340000	0.56590000
H	1.79170000	-1.49330000	0.24290000
C	0.23340000	-0.23250000	0.99650000
C	-0.11710000	0.85050000	1.99360000
O	-0.51720000	-1.29650000	1.05830000
Ti	-1.62860000	-2.50750000	0.03790000
Cl	-3.04250000	-3.58630000	-1.38400000
Cl	-2.55650000	-3.30530000	1.91920000
O	-2.20840000	-0.88100000	-0.71620000
C	-1.82530000	0.38150000	-0.69310000
C	-2.87220000	1.29830000	-0.30290000
H	-3.80250000	0.82120000	-0.02520000
C	-2.82340000	2.65910000	-0.30610000
O	-1.73990000	3.36430000	-0.63830000
Si	-1.68670000	5.06790000	-0.74680000

Cl	0.20520000	-3.59980000	-0.72280000
H	-0.29850000	5.31180000	-1.19420000
H	-2.65440000	5.56390000	-1.75190000
H	-1.92220000	5.69100000	0.57570000
H	-1.20210000	0.95660000	2.05730000
H	0.25310000	0.53370000	2.97760000
H	0.34660000	1.80380000	1.74730000
O	-3.84350000	3.47340000	0.02350000
C	-0.48100000	0.65940000	-0.92420000
H	-0.12900000	1.68160000	-0.93960000
H	0.07560000	-0.06790000	-1.50200000
C	-5.11410000	2.91390000	0.38090000
H	-5.02000000	2.29270000	1.27710000
H	-5.76010000	3.76770000	0.58330000
H	-5.51850000	2.32230000	-0.44610000
C	4.01870000	-0.07120000	0.09190000
C	5.17220000	0.41030000	0.73730000
C	4.16740000	-0.98530000	-0.96640000
C	6.43760000	-0.01490000	0.33670000
H	5.07200000	1.09080000	1.57690000
C	5.43380000	-1.40690000	-1.36320000
H	3.28830000	-1.35100000	-1.48790000
C	6.57280000	-0.92290000	-0.71500000
H	7.31800000	0.35640000	0.85390000
H	5.53130000	-2.10930000	-2.18610000

H	7.55960000	-1.25230000	-1.02790000
O	2.56530000	1.66070000	0.97810000
Si	3.12870000	3.07060000	0.24670000
H	2.13230000	4.10660000	0.61070000
H	4.45490000	3.47030000	0.77540000
H	3.19140000	2.90340000	-1.22640000

Int23'

C	3.23650000	0.00490000	0.41770000
C	2.09900000	-0.73250000	0.26240000
H	1.44280000	-0.45640000	-0.55200000
C	1.64980000	-1.86090000	1.05000000
C	2.45100000	-2.44710000	2.18560000
O	0.55220000	-2.40500000	0.79610000
Ti	-1.13350000	-2.29670000	-0.55630000
Cl	-2.89280000	-2.42100000	-1.95880000
Cl	-2.26960000	-3.07270000	1.24420000
O	-1.00380000	-0.53750000	-0.57150000
C	-1.60620000	0.69900000	-0.62530000
C	-2.61990000	0.86050000	0.41150000
H	-2.79560000	-0.01530000	1.02110000
C	-3.36610000	1.96130000	0.65070000
O	-3.23320000	3.11310000	-0.02860000
Si	-4.22780000	4.47270000	0.18270000
Cl	0.29350000	-3.39960000	-1.93270000

H	-3.69230000	5.42150000	-0.82010000
H	-5.64750000	4.16550000	-0.11170000
H	-4.08840000	5.04740000	1.54240000
H	1.90640000	-3.29910000	2.59550000
H	3.43960000	-2.76250000	1.83740000
H	2.61610000	-1.70050000	2.96970000
O	-4.33600000	2.07270000	1.58980000
C	-1.19030000	1.55500000	-1.57910000
H	-1.63020000	2.53760000	-1.67130000
H	-0.44020000	1.24310000	-2.29660000
C	-4.68520000	0.92170000	2.36260000
H	-3.83880000	0.59810000	2.97820000
H	-5.51080000	1.23590000	3.00150000
H	-5.00210000	0.10090000	1.71080000
C	3.54100000	1.16120000	-0.45500000
C	4.86100000	1.39530000	-0.88060000
C	2.52040000	2.02840000	-0.88210000
C	5.15180000	2.47210000	-1.71570000
H	5.65080000	0.70870000	-0.59160000
C	2.81910000	3.10670000	-1.71170000
H	1.49760000	1.86830000	-0.55410000
C	4.13280000	3.33250000	-2.12940000
H	6.17240000	2.63270000	-2.05100000
H	2.02280000	3.77420000	-2.02790000
H	4.36110000	4.17370000	-2.77780000

O	4.15900000	-0.32830000	1.34910000
Si	5.09330000	0.64840000	2.37140000
H	5.13640000	-0.08910000	3.65440000
H	6.46570000	0.79250000	1.83320000
H	4.45090000	1.97260000	2.54330000

Int25

C	2.74650000	-1.51420000	0.20180000
C	2.92490000	-0.91310000	1.53760000
H	3.47380000	-1.52930000	2.24630000
C	2.54040000	0.31680000	1.94470000
O	-2.42210000	-1.24420000	-0.00600000
Ti	-4.12850000	-1.23010000	0.09930000
O	3.97410000	2.51830000	1.06790000
C	2.79350000	2.52810000	0.72790000
C	2.27360000	3.67040000	-0.02340000
H	3.02990000	4.41750000	-0.22760000
C	1.01060000	3.89610000	-0.47090000
O	-0.01600000	3.06400000	-0.27710000
Si	-1.61100000	3.32640000	-0.83440000
H	-2.31830000	2.13210000	-0.33440000
H	-2.17670000	4.55920000	-0.23840000
H	-1.64600000	3.38650000	-2.31350000
O	0.61190000	4.98400000	-1.16390000
C	1.87340000	1.33780000	1.05670000

C	1.56090000	6.00310000	-1.48970000
H	2.36590000	5.59570000	-2.10980000
H	1.00190000	6.75410000	-2.04790000
H	1.97860000	6.44570000	-0.57960000
C	3.83570000	-2.38890000	-0.32400000
C	3.55220000	-3.24370000	-1.40260000
C	5.13600000	-2.36160000	0.20620000
C	4.54270000	-4.06800000	-1.92610000
H	2.54750000	-3.24780000	-1.81180000
C	6.12970000	-3.18050000	-0.32710000
H	5.37740000	-1.68080000	1.01630000
C	5.83330000	-4.03840000	-1.38830000
H	4.31300000	-4.73350000	-2.75350000
H	7.13530000	-3.14640000	0.08240000
H	6.60760000	-4.68070000	-1.79920000
O	1.72620000	-1.35290000	-0.48910000
Si	-0.68560000	-1.26670000	-0.16030000
H	1.54190000	0.89480000	0.11560000
H	0.96630000	1.71640000	1.54380000
C	2.82120000	0.76290000	3.35450000
H	3.51490000	1.61050000	3.34090000
H	1.89660000	1.10470000	3.83860000
H	3.25350000	-0.03790000	3.96130000
Cl	-4.71980000	-0.43090000	2.07990000
Cl	-4.93360000	0.07200000	-1.50670000

Cl	-4.88490000	-3.29500000	-0.14660000
H	-0.46510000	-0.21330000	-1.16800000
H	-0.26490000	-0.95060000	1.21830000
H	-0.44330000	-2.65130000	-0.60890000

TS15

C	2.52940000	-0.56710000	0.04850000
C	1.91100000	-0.19580000	-1.13090000
H	2.56930000	0.10320000	-1.93850000
C	0.52870000	-0.11300000	-1.41880000
O	0.00300000	1.65030000	-0.30510000
Ti	-1.07810000	2.88910000	-0.17670000
O	0.11920000	-2.66320000	-2.32750000
C	-0.64550000	-2.33330000	-1.42370000
C	-1.69080000	-3.25000000	-0.98350000
H	-1.69040000	-4.18400000	-1.53020000
C	-2.63500000	-3.06150000	-0.02130000
O	-2.71650000	-1.96880000	0.73580000
Si	-3.98440000	-1.59630000	1.82270000
H	-3.60490000	-0.26120000	2.32180000
H	-5.28230000	-1.56590000	1.11090000
H	-4.01600000	-2.58050000	2.93090000
O	-3.60250000	-3.94270000	0.30020000
C	-0.51510000	-0.95330000	-0.73730000
C	-3.71640000	-5.16800000	-0.43030000

H	-2.81800000	-5.77970000	-0.29880000
H	-4.58080000	-5.67950000	-0.00720000
H	-3.88030000	-4.96800000	-1.49400000
C	3.97770000	-0.83070000	0.13540000
C	4.59760000	-0.91390000	1.39670000
C	4.76610000	-1.02320000	-1.01730000
C	5.96520000	-1.15010000	1.50110000
H	4.00180000	-0.79920000	2.29460000
C	6.13100000	-1.26270000	-0.90840000
H	4.30830000	-1.01300000	-2.00030000
C	6.73680000	-1.32050000	0.35020000
H	6.42850000	-1.20340000	2.48200000
H	6.72320000	-1.41280000	-1.80630000
H	7.80400000	-1.50630000	0.43200000
O	1.85620000	-0.70150000	1.19470000
Si	1.23450000	0.45290000	2.29760000
H	-0.28840000	-1.12060000	0.31430000
H	-1.47930000	-0.44020000	-0.77470000
C	0.16130000	0.40410000	-2.77490000
H	0.27730000	-0.43690000	-3.47280000
H	-0.87940000	0.73300000	-2.80800000
H	0.81480000	1.22090000	-3.09080000
Cl	-0.38040000	4.60650000	-1.45820000
Cl	-3.05760000	2.08000000	-0.93610000
Cl	-1.23170000	3.46970000	2.00460000

H	-0.23250000	0.32740000	2.32040000
H	1.75370000	1.78460000	1.94140000
H	1.78640000	0.01350000	3.60580000

Int26

C	-3.09970000	0.39010000	-1.29650000
C	-2.95090000	-0.20370000	0.01660000
C	-3.50230000	-1.40060000	0.39570000
C	-2.27850000	1.70310000	-1.51980000
O	-4.29540000	-2.08890000	-0.41090000
O	-3.77700000	-0.05060000	-2.21730000
C	-1.03270000	1.39130000	-2.30850000
C	0.21850000	1.27300000	-1.78860000
C	0.68030000	1.51570000	-0.42660000
O	1.50900000	0.72720000	0.09660000
C	-4.77180000	-3.38080000	-0.00140000
Cl	2.93580000	-0.86020000	2.11630000
H	-2.32980000	0.30980000	0.74100000
H	-5.36830000	-3.73250000	-0.84280000
H	-3.93850000	-4.06400000	0.18290000
H	-5.39090000	-3.30400000	0.89620000
H	-2.05560000	2.17030000	-0.56120000
H	-2.92540000	2.37120000	-2.09870000
H	0.98940000	0.83690000	-2.42050000
C	0.30960000	2.70850000	0.36970000

C	-0.10890000	3.90090000	-0.24690000
C	0.46510000	2.67010000	1.76770000
C	-0.38650000	5.02680000	0.52380000
H	-0.19070000	3.94450000	-1.32780000
C	0.17110000	3.79320000	2.53400000
H	0.81820000	1.75580000	2.23330000
C	-0.25470000	4.97210000	1.91380000
H	-0.69720000	5.94870000	0.04120000
H	0.28180000	3.75520000	3.61380000
H	-0.47430000	5.85110000	2.51350000
C	-1.26880000	1.06190000	-3.75640000
H	-1.61630000	1.96030000	-4.28550000
H	-0.36700000	0.69260000	-4.25130000
H	-2.07410000	0.32410000	-3.84720000
Cl	0.67740000	-2.00920000	-0.69040000
Cl	3.82010000	0.13400000	-1.55210000
Cl	3.82430000	-2.91320000	-0.33060000
Ti	2.60810000	-1.05770000	-0.08370000
O	-3.30470000	-1.96740000	1.59490000
Si	-2.25850000	-1.49090000	2.84730000
H	-2.44090000	-2.54230000	3.86880000
H	-0.86730000	-1.43140000	2.35270000
H	-2.68420000	-0.16910000	3.37050000

Int27

C	-0.05780000	2.26950000	1.03300000
C	-0.44010000	0.86840000	0.98260000
C	0.16080000	-0.16820000	1.66270000
C	-0.47870000	3.07790000	-0.21350000
O	0.93340000	0.03750000	2.72290000
O	0.58250000	2.81240000	1.92370000
C	-0.44190000	2.39820000	-1.57310000
C	0.28230000	1.30920000	-1.90690000
C	1.25740000	0.52930000	-1.10420000
O	1.12290000	-0.72720000	-1.02040000
C	1.60280000	-1.08790000	3.31750000
Cl	1.68820000	-3.64410000	-0.96560000
H	-1.11360000	0.55630000	0.19630000
H	2.15160000	-0.67000000	4.16110000
H	0.87830000	-1.82920000	3.66380000
H	2.29460000	-1.55480000	2.61150000
H	0.13820000	3.98550000	-0.22150000
H	-1.50970000	3.42370000	-0.04610000
H	0.10880000	0.85690000	-2.88240000
C	2.51520000	1.12280000	-0.61790000
C	2.85580000	2.45920000	-0.89440000
C	3.41680000	0.31870000	0.10830000
C	4.06020000	2.98490000	-0.43630000
H	2.18460000	3.07260000	-1.48380000

C	4.61830000	0.84700000	0.56030000
H	3.16210000	-0.71860000	0.29480000
C	4.93990000	2.18270000	0.29290000
H	4.31550000	4.01780000	-0.65260000
H	5.30940000	0.22220000	1.11840000
H	5.88050000	2.59450000	0.64810000
C	-1.37320000	3.00510000	-2.59330000
H	-1.17750000	4.08030000	-2.70090000
H	-1.27430000	2.53560000	-3.57590000
H	-2.41600000	2.90840000	-2.26400000
Cl	-4.58030000	2.40800000	0.17670000
Cl	-1.47340000	-1.82240000	-2.03800000
Cl	-1.29690000	-3.92670000	0.50490000
Ti	-0.01770000	-2.31960000	-0.40960000
O	0.04290000	-1.40760000	1.23130000
Si	-4.77070000	0.53540000	1.08550000
H	-3.91440000	-0.42140000	0.35290000
H	-4.34240000	0.66410000	2.49640000
H	-6.19490000	0.13730000	1.00620000

Int27’

C	2.23940000	1.14140000	1.47210000
C	0.85240000	0.66720000	1.03280000
C	0.20500000	-0.53440000	1.68220000

C	2.61760000	2.47380000	0.83570000
O	-0.96210000	-0.83450000	1.40260000
O	0.92110000	-1.23050000	2.53070000
O	2.96510000	0.56350000	2.24830000
C	2.13680000	2.64270000	-0.59180000
C	1.33970000	1.74670000	-1.18700000
H	1.03240000	1.87730000	-2.22160000
C	0.79450000	0.49440000	-0.53660000
O	-0.58220000	0.40090000	-0.89050000
Ti	-2.20420000	0.14870000	-0.22500000
C	0.28730000	-2.39330000	3.12130000
Cl	-3.06760000	-1.91470000	-0.38380000
Cl	-3.40250000	1.11920000	-1.84050000
H	-0.60250000	-2.09170000	3.67710000
H	0.01220000	-3.10150000	2.33770000
H	1.04220000	-2.81270000	3.78400000
H	3.70710000	2.58030000	0.90370000
H	2.19890000	3.27730000	1.46440000
Cl	-2.78430000	1.52490000	1.45600000
H	0.17020000	1.50640000	1.23120000
C	2.63240000	3.87170000	-1.30730000
H	3.72930000	3.88330000	-1.35840000
H	2.24060000	3.93070000	-2.32660000
H	2.33230000	4.78230000	-0.77160000
C	1.53350000	-0.77280000	-1.00650000

C	2.93310000	-0.77520000	-1.09310000
C	0.83630000	-1.94460000	-1.32610000
C	3.62040000	-1.92660000	-1.47440000
H	3.49360000	0.12860000	-0.87750000
C	1.52660000	-3.09470000	-1.71440000
H	-0.24560000	-1.96460000	-1.28560000
C	2.91890000	-3.09200000	-1.78690000
H	4.70500000	-1.90760000	-1.53420000
H	0.96680000	-3.99120000	-1.96610000
H	3.45380000	-3.98750000	-2.09110000

Ts16

C	0.17390000	2.04020000	1.31650000
C	0.06460000	0.61120000	1.55190000
C	1.17470000	-0.27120000	1.90400000
C	1.28050000	2.55790000	0.34440000
O	1.06420000	-1.44310000	2.23230000
O	2.40290000	0.34150000	1.87850000
O	-0.66640000	2.85700000	1.68620000
C	0.58150000	2.67170000	-0.98090000
C	0.13100000	1.57170000	-1.63940000
H	-0.60050000	1.69540000	-2.43750000
C	0.35190000	0.18240000	-1.27260000
O	-0.70330000	-0.60710000	-1.35860000
Ti	-2.10960000	-0.64340000	-0.14130000

C	3.49660000	-0.46730000	2.33080000
Cl	-2.02650000	-2.21590000	1.38020000
Cl	-3.60320000	-1.47390000	-1.55170000
H	3.31720000	-0.82020000	3.34980000
H	3.64310000	-1.33170000	1.67870000
H	4.37170000	0.18430000	2.30190000
H	2.12520000	1.87230000	0.32830000
H	1.61290000	3.53770000	0.69500000
Cl	-3.12870000	1.19540000	0.48130000
H	-0.83510000	0.34470000	2.10200000
C	1.64950000	-0.48370000	-1.23450000
C	2.80940000	0.18170000	-1.68700000
C	1.73550000	-1.84300000	-0.86250000
C	4.02050000	-0.49400000	-1.76110000
H	2.73950000	1.21350000	-2.01260000
C	2.95100000	-2.51210000	-0.94430000
H	0.85460000	-2.35900000	-0.50230000
C	4.09350000	-1.84180000	-1.39200000
H	4.90520000	0.02150000	-2.12280000
H	3.00850000	-3.55670000	-0.65440000
H	5.04000000	-2.37100000	-1.46030000
C	0.17240000	4.04800000	-1.41200000
H	1.05590000	4.68350000	-1.55700000
H	-0.41660000	4.04560000	-2.33340000
H	-0.41820000	4.50340000	-0.60650000

Int28

C	-1.87930000	2.20170000	0.46200000
C	-2.24570000	0.80880000	0.74020000
C	-1.72420000	-0.00840000	1.79530000
C	-0.45760000	2.67920000	0.84500000
O	-1.67620000	-1.26050000	1.57900000
O	-1.20620000	0.50970000	2.89640000
O	-2.62340000	2.95730000	-0.14560000
C	0.40260000	2.82610000	-0.38670000
C	1.29670000	1.89300000	-0.79620000
H	1.94930000	2.13940000	-1.62930000
Ti	-1.38700000	-1.02880000	-0.45900000
C	-0.49590000	-0.39770000	3.77670000
Cl	-3.40260000	-1.86020000	-0.92270000
Cl	-0.19710000	-2.94120000	-0.62590000
H	-1.18200000	-1.14780000	4.17380000
H	0.31460000	-0.88580000	3.23190000
H	-0.10850000	0.23290000	4.57590000
H	-0.00260000	2.00460000	1.56700000
H	-0.57770000	3.66250000	1.31320000
Cl	-1.11330000	0.09480000	-2.37670000
C	2.86930000	0.02380000	-0.11140000
C	4.00080000	0.84330000	-0.28550000
C	3.04670000	-1.34230000	0.17790000
C	5.28010000	0.30600000	-0.18120000

H	3.87840000	1.90360000	-0.48120000
C	4.32790000	-1.87580000	0.27230000
H	2.17300000	-1.97140000	0.30500000
C	5.44500000	-1.05450000	0.09350000
H	6.14810000	0.94590000	-0.31110000
H	4.45740000	-2.93360000	0.48180000
H	6.44450000	-1.47390000	0.16950000
C	0.23590000	4.11550000	-1.13490000
H	0.52880000	4.96950000	-0.50910000
H	0.81380000	4.14020000	-2.06260000
H	-0.82920000	4.24820000	-1.36410000
C	1.49850000	0.57320000	-0.20000000
O	0.54050000	-0.11690000	0.23730000
H	-3.25420000	0.54250000	0.42900000

TS17

C	1.87620000	2.31500000	-0.23110000
O	2.21450000	1.21190000	0.37250000
Ti	2.55770000	-0.65080000	-0.11160000
Cl	2.62450000	-2.94090000	-0.44780000
Cl	2.67470000	-0.98280000	2.13620000
O	1.13250000	-0.52180000	-1.27770000
C	-0.19850000	-0.54930000	-1.30060000
C	-0.78330000	-1.68530000	-0.64390000
H	-0.07480000	-2.34250000	-0.15870000

C	-2.09330000	-2.07140000	-0.64550000
O	-3.06990000	-1.41030000	-1.26580000
Si	-4.69590000	-1.93080000	-1.33460000
Cl	4.47240000	-0.19100000	-1.17950000
H	-5.33230000	-0.86470000	-2.13790000
H	-4.80400000	-3.23910000	-2.01860000
H	-5.29260000	-1.98420000	0.02000000
O	-2.56400000	-3.17300000	-0.04160000
C	-0.85330000	0.53470000	-1.87700000
H	-0.28850000	1.16230000	-2.55280000
H	-1.92480000	0.49610000	-2.01090000
C	-1.66670000	-4.02970000	0.68630000
H	-1.20100000	-3.47950000	1.50890000
H	-2.29090000	-4.83410000	1.07390000
H	-0.89780000	-4.43270000	0.02090000
C	0.58580000	2.71850000	-0.53830000
C	-0.71540000	2.15730000	-0.30040000
H	0.54260000	3.60580000	-1.16220000
O	-1.72310000	2.88120000	-0.90130000
Si	-2.22120000	4.44000000	-0.50340000
H	-1.22690000	5.44880000	-0.95040000
H	-3.49170000	4.62140000	-1.24040000
H	-2.42880000	4.56940000	0.96040000
C	3.03550000	3.21810000	-0.57580000
H	3.73980000	2.67850000	-1.21860000

H	2.71920000	4.13990000	-1.06920000
H	3.57740000	3.46950000	0.34350000
C	-1.18010000	1.43610000	0.91740000
C	-2.53820000	1.07260000	1.01670000
C	-0.33550000	1.17440000	2.00760000
C	-3.03250000	0.46840000	2.16760000
H	-3.20030000	1.26760000	0.18050000
C	-0.83550000	0.56330000	3.15880000
H	0.71000000	1.44500000	1.96830000
C	-2.18070000	0.20970000	3.24630000
H	-4.08460000	0.20220000	2.22620000
H	-0.16100000	0.36960000	3.98740000
H	-2.56610000	-0.26130000	4.14660000

Int29

C	1.61380000	0.50100000	-2.13950000
O	2.27390000	0.01380000	-1.05310000
Ti	2.19790000	-1.40660000	0.02940000
Cl	2.00740000	-1.25160000	2.28090000
Cl	4.40920000	-1.82070000	0.06060000
O	0.14220000	-0.99310000	0.05960000
C	-1.05760000	-0.66910000	-0.04310000
C	-2.03970000	-1.65490000	0.32470000
H	-1.61350000	-2.58910000	0.66530000
C	-3.40280000	-1.54290000	0.27870000

O	-4.04120000	-0.45580000	-0.13580000
Si	-5.74620000	-0.27790000	-0.21470000
Cl	1.61930000	-3.30260000	-1.05050000
H	-5.89410000	1.09490000	-0.73810000
H	-6.32120000	-1.27100000	-1.14920000
H	-6.33720000	-0.40160000	1.13650000
O	-4.26110000	-2.50470000	0.64040000
C	-1.44000000	0.71390000	-0.53090000
C	-3.77130000	-3.76430000	1.13140000
H	-3.17670000	-3.61400000	2.03690000
H	-4.66240000	-4.34850000	1.35810000
H	-3.17500000	-4.26620000	0.36420000
C	0.49950000	1.24630000	-2.06020000
H	0.07040000	1.57450000	-3.00200000
O	-1.01220000	2.88410000	-1.38430000
Si	-1.70980000	4.13690000	-0.53370000
H	-0.73170000	5.05280000	0.10570000
H	-2.48230000	4.88400000	-1.55720000
H	-2.65440000	3.65370000	0.51650000
C	2.28060000	0.13340000	-3.43840000
H	2.31260000	-0.95630000	-3.55750000
H	1.75330000	0.56730000	-4.29180000
H	3.31730000	0.49000000	-3.44310000
C	0.54000000	2.17000000	0.33730000
C	0.16590000	1.92700000	1.66390000

C	1.67210000	2.96680000	0.10010000
C	0.90470000	2.45650000	2.72520000
H	-0.69690000	1.31050000	1.89350000
C	2.41000000	3.49470000	1.15550000
H	1.97120000	3.16890000	-0.92360000
C	2.02810000	3.24100000	2.47550000
H	0.60350000	2.24120000	3.74630000
H	3.28600000	4.10310000	0.94780000
H	2.60620000	3.64770000	3.30060000
C	-0.30390000	1.72110000	-0.86040000
H	-2.03040000	0.59590000	-1.44720000
H	-2.13660000	1.15770000	0.18890000

Int29'

C	-0.58490000	1.02430000	-0.96740000
C	-0.97530000	2.37760000	-0.94180000
C	-2.15810000	2.88280000	-0.41050000
C	0.75550000	0.67400000	-1.57190000
O	-3.21890000	2.23670000	-0.01940000
O	-2.21140000	4.20440000	-0.27090000
O	-1.32140000	0.07890000	-0.53970000
C	1.83530000	0.06550000	-0.58190000
C	2.47670000	-1.14180000	-1.21340000
C	1.69310000	-2.18840000	-1.54400000
C	2.14940000	-3.47940000	-2.15420000

O	0.36410000	-2.10560000	-1.32800000
Ti	-0.73620000	-1.84750000	0.12520000
C	-3.42150000	4.80580000	0.23000000
Cl	0.12460000	-3.72510000	1.10200000
H	-0.26450000	3.12350000	-1.27240000
H	-4.26770000	4.57240000	-0.42070000
H	-3.63010000	4.46060000	1.24510000
H	-3.22100000	5.87670000	0.22450000
H	3.23020000	-3.47850000	-2.32050000
H	1.88670000	-4.31400000	-1.49490000
H	1.64100000	-3.64560000	-3.11150000
H	1.19330000	1.55110000	-2.05080000
H	0.54210000	-0.05800000	-2.35240000
O	1.11720000	-0.40570000	0.63250000
Si	1.96040000	-0.62370000	2.12470000
H	1.49140000	-1.86110000	2.76110000
H	3.40790000	-0.72290000	1.81770000
H	1.72100000	0.54420000	3.00310000
H	3.54890000	-1.21250000	-1.33650000
Cl	-1.44120000	-1.03800000	2.19210000
Cl	-2.64420000	-2.69870000	-0.69220000
C	2.79190000	1.20630000	-0.21630000
C	2.34790000	2.22590000	0.64260000
C	4.06190000	1.33300000	-0.79350000
C	3.16360000	3.31590000	0.94320000

H	1.35690000	2.16530000	1.08010000
C	4.87650000	2.42780000	-0.49700000
H	4.42690000	0.58760000	-1.49100000
C	4.43520000	3.42000000	0.37720000
H	2.80140000	4.08520000	1.61960000
H	5.86020000	2.49960000	-0.95290000
H	5.07240000	4.26830000	0.61090000
Si	-4.02310000	0.75880000	-0.44600000
H	-3.82860000	-0.22200000	0.62300000
H	-5.42980000	1.24020000	-0.45050000
H	-3.65010000	0.37990000	-1.82090000

TS18

C	-0.86140000	0.89060000	-0.95840000
C	-1.59960000	2.09350000	-0.98590000
C	-2.86700000	2.28680000	-0.44450000
C	0.49280000	0.88250000	-1.65530000
O	-3.70100000	1.39920000	0.01320000
O	-3.27790000	3.55040000	-0.37170000
O	-1.30780000	-0.18400000	-0.46410000
C	1.80360000	0.58040000	-0.88720000
C	2.61680000	-0.45650000	-1.44810000
C	2.05020000	-1.67720000	-1.74290000
C	2.81200000	-2.83430000	-2.31890000
O	0.79010000	-1.89530000	-1.46860000

Ti	-0.16110000	-1.86760000	0.23030000
C	-4.60250000	3.82450000	0.12580000
Cl	1.18150000	-3.52420000	1.02950000
H	-1.12890000	2.98350000	-1.38260000
H	-5.35760000	3.33320000	-0.49260000
H	-4.70050000	3.49160000	1.16140000
H	-4.70390000	4.90740000	0.06140000
H	3.84540000	-2.56640000	-2.55430000
H	2.80170000	-3.66460000	-1.60340000
H	2.31240000	-3.18580000	-3.22890000
H	0.64810000	1.85240000	-2.13520000
H	0.38440000	0.14000000	-2.44850000
O	1.10940000	-0.32530000	0.66000000
Si	1.90050000	-0.09940000	2.14580000
H	1.86660000	-1.32690000	2.96210000
H	3.32110000	0.23610000	1.86080000
H	1.29040000	1.03050000	2.89240000
H	3.69500000	-0.37120000	-1.46900000
Cl	-1.16790000	-1.45810000	2.27770000
Cl	-1.84060000	-3.16150000	-0.61860000
C	2.45960000	1.81530000	-0.34470000
C	1.69820000	2.75040000	0.38060000
C	3.81330000	2.10650000	-0.58080000
C	2.27250000	3.92210000	0.86620000
H	0.65310000	2.54680000	0.58720000

C	4.38440000	3.28680000	-0.10670000
H	4.43100000	1.42720000	-1.15580000
C	3.61960000	4.19670000	0.62290000
H	1.66630000	4.61960000	1.43720000
H	5.43180000	3.49190000	-0.30900000
H	4.06820000	5.11260000	0.99720000
Si	-4.08290000	-0.26130000	-0.34240000
H	-3.61250000	-1.10370000	0.75740000
H	-5.56770000	-0.17340000	-0.32610000
H	-3.64530000	-0.56710000	-1.71580000

Int30

C	0.48960000	1.05200000	-0.81920000
C	1.08490000	2.34220000	-0.76090000
C	0.51890000	3.48510000	-0.21610000
C	1.27990000	-0.01660000	-1.59890000
O	-0.73360000	3.68460000	0.10210000
O	1.34570000	4.50520000	0.01030000
O	-0.63680000	0.78720000	-0.33410000
C	1.99040000	-1.13550000	-0.84810000
C	1.49560000	-2.39720000	-0.75110000
C	0.18380000	-2.83230000	-1.20810000
C	-0.04750000	-4.28940000	-1.51030000
O	-0.77000000	-2.04220000	-1.33520000
Ti	-1.92720000	-0.92720000	0.17070000

C	0.79480000	5.75750000	0.46240000
Cl	-3.11340000	-2.84580000	0.44750000
H	2.10800000	2.45160000	-1.09630000
H	0.07290000	6.14780000	-0.25940000
H	0.31440000	5.63740000	1.43580000
H	1.65180000	6.42600000	0.53990000
H	0.87370000	-4.87620000	-1.53790000
H	-0.71570000	-4.68800000	-0.73490000
H	-0.58280000	-4.37970000	-2.46030000
H	2.03750000	0.50300000	-2.19290000
H	0.54770000	-0.45590000	-2.28110000
O	-0.57010000	-1.35550000	1.29270000
Si	-0.03120000	-1.40880000	2.86080000
H	-1.08130000	-1.90200000	3.78660000
H	1.13720000	-2.33260000	2.92900000
H	0.42390000	-0.06050000	3.29930000
H	2.12660000	-3.16920000	-0.31890000
Cl	-3.05150000	0.30420000	1.71180000
Cl	-3.10570000	-0.15630000	-1.69550000
C	3.36590000	-0.87430000	-0.34990000
C	3.65640000	0.26970000	0.41480000
C	4.40740000	-1.78080000	-0.61920000
C	4.94120000	0.48440000	0.91140000
H	2.86850000	0.97580000	0.65310000
C	5.69460000	-1.55400000	-0.13650000

H	4.21060000	-2.65210000	-1.23690000
C	5.96550000	-0.42260000	0.63490000
H	5.13970000	1.36290000	1.51900000
H	6.48710000	-2.26040000	-0.36750000
H	6.96790000	-0.24780000	1.01540000
Si	-2.18430000	3.31530000	-0.77980000
H	-3.04670000	2.50110000	0.07680000
H	-2.76450000	4.67010000	-0.98100000
H	-1.77420000	2.75780000	-2.08070000

12

C	-0.27220000	0.80770000	0.36430000
C	-1.68000000	0.79620000	0.40300000
H	-2.15650000	1.74940000	0.58710000
C	-2.50570000	-0.28750000	0.12170000
C	0.37890000	2.17830000	0.66040000
O	-2.08340000	-1.53570000	0.05030000
O	0.48290000	-0.15810000	0.09830000
Si	-0.97930000	-2.50090000	0.94810000
H	-1.82380000	-3.66080000	1.32650000
H	0.11210000	-2.93440000	0.06490000
H	-0.56400000	-1.76070000	2.15540000
C	-3.94660000	-0.11960000	-0.13110000
C	-4.49200000	1.12430000	-0.50440000

C	-4.80270000	-1.23060000	-0.00850000
C	-5.85820000	1.25360000	-0.72940000
H	-3.84580000	1.98260000	-0.65440000
C	-6.16920000	-1.09430000	-0.22890000
H	-4.38680000	-2.19290000	0.26720000
C	-6.70040000	0.14730000	-0.58730000
H	-6.26580000	2.21520000	-1.02630000
H	-6.82090000	-1.95630000	-0.12230000
H	-7.76720000	0.25150000	-0.76350000
Ti	2.58900000	-0.30960000	-0.28900000
Cl	4.60620000	0.59600000	-0.33660000
Cl	1.91560000	0.63720000	-2.25140000
Cl	2.88000000	-2.38450000	-0.94900000
Cl	2.57970000	-0.60740000	1.97620000
F	0.09390000	2.56240000	1.91400000
F	-0.07360000	3.11890000	-0.18090000
F	1.72180000	2.11050000	0.53730000

TS2

C	-0.67960000	0.33270000	0.00050000
C	0.39830000	-0.55540000	-0.22130000
H	0.23670000	-1.59320000	-0.46530000
C	1.67950000	-0.10640000	0.02640000
O	2.02010000	1.09830000	0.31230000
O	-0.47280000	1.57780000	0.24980000
C	-2.09010000	-0.11090000	0.00300000
C	-2.44990000	-1.46920000	-0.05870000
C	-3.10390000	0.86190000	0.07220000
C	-3.79070000	-1.84250000	-0.05660000
H	-1.68860000	-2.24100000	-0.09220000
C	-4.44280000	0.48460000	0.07150000
H	-2.82090000	1.90720000	0.12140000
C	-4.78940000	-0.86750000	0.00640000
H	-4.05700000	-2.89450000	-0.10040000
H	-5.21740000	1.24430000	0.12050000
H	-5.83540000	-1.16180000	0.00650000
Si	1.05070000	2.65460000	-0.17650000
H	2.30520000	3.33530000	0.27310000
H	1.07940000	2.47250000	-1.65160000
H	0.08070000	3.75220000	0.14450000
C	2.86090000	-1.08030000	0.01810000
F	2.47160000	-2.33840000	-0.27540000
F	3.45660000	-1.09950000	1.22120000

F	3.76910000	-0.70390000	-0.89600000

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C	0.93730000	0.95090000	0.23810000
C	2.29850000	0.59270000	-0.16760000
H	2.93820000	1.35980000	-0.57970000
C	2.83640000	-0.64450000	-0.06610000
O	2.31260000	-1.74760000	0.45640000
O	0.13250000	0.08840000	0.63040000
Si	1.52170000	-2.00120000	1.94550000
H	2.28100000	-3.13450000	2.53090000
H	1.69580000	-0.80810000	2.80490000
H	0.12060000	-2.41020000	1.75930000
Ti	-2.57120000	-0.86470000	-0.27340000
Cl	-2.70710000	-0.74720000	1.91180000
Cl	-1.15990000	-2.32690000	-1.07660000
Cl	-2.48490000	1.06440000	-1.29840000
Cl	-4.52130000	-1.66590000	-0.85350000
C	0.54500000	2.38980000	0.20560000
C	-0.48530000	2.81100000	1.06360000
C	1.16430000	3.33350000	-0.63120000
C	-0.87710000	4.14550000	1.09440000
H	-0.95900000	2.07880000	1.70900000
C	0.75580000	4.66560000	-0.61360000

H	1.94260000	3.03030000	-1.32410000
C	-0.25920000	5.07530000	0.25350000
H	-1.66540000	4.46200000	1.77140000
H	1.22990000	5.38340000	-1.27680000
H	-0.56890000	6.11660000	0.27300000
C	4.24260000	-0.92490000	-0.58350000
F	5.03270000	-1.33630000	0.42860000
F	4.21860000	-1.89810000	-1.50920000
F	4.81330000	0.16250000	-1.13710000