

Mechanisms of the InCl₃-Catalyzed Type-I, II and III Cycloisomerizations of 1,6-Enynes

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1. Additional Calculation Details and Results

We computed the energy surface of **b-4** using bigger basis sets (LANL2DZ for In, and 6-311+G(d, p) for all other atoms).¹ The energy barriers and selectivity in Figure S1 were similar to those shown in Figure 2 of text. At this level, the cyclobutyl cation **b-8** was not a minimum.

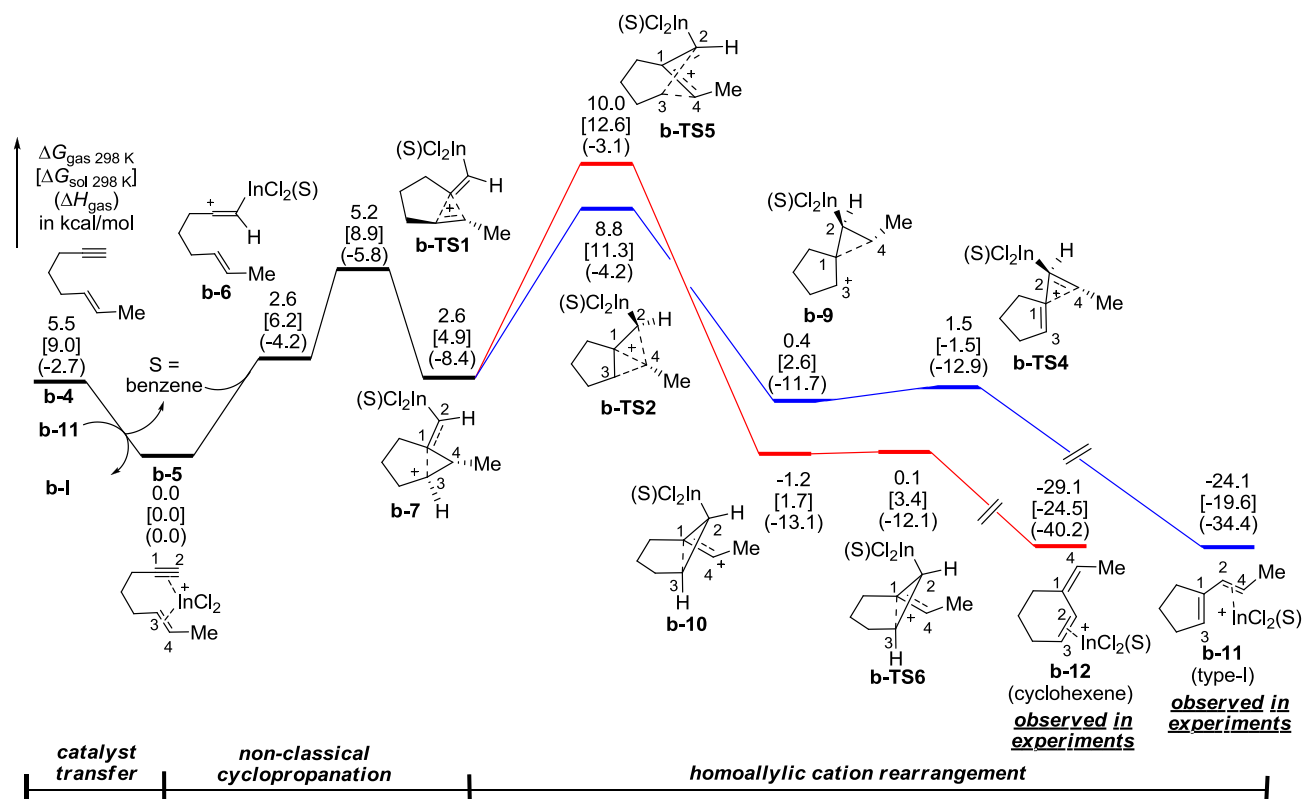


Figure S1. Full energy surface of **b-4** (LANL2DZ for In, and 6-311+G(d, p) for all other atoms)

When InCl_3 was chosen to as the catalytic species, the computed selectivities were not consistent with the experimentally observed ones, as mentioned in the text (section 5 of “Results and Discussion”). The computed energy surfaces using InCl_3 as the catalyst have been summarized in Figures S2, S3 and S4. We found that, all 6/3-bicyclic intermediates (**m-b-10**, **m-c-10**, **m-d-10**) and cyclobutyl cation **m-d-8** were not minima using InCl_3 as the catalytic species.

¹ Full citation of Gaussian 09: Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, J. A., Jr.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, N. J.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, Ö.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J. *Gaussian 09*, Revision A. 02, Gaussian, Inc., Wallingford CT, 2009.

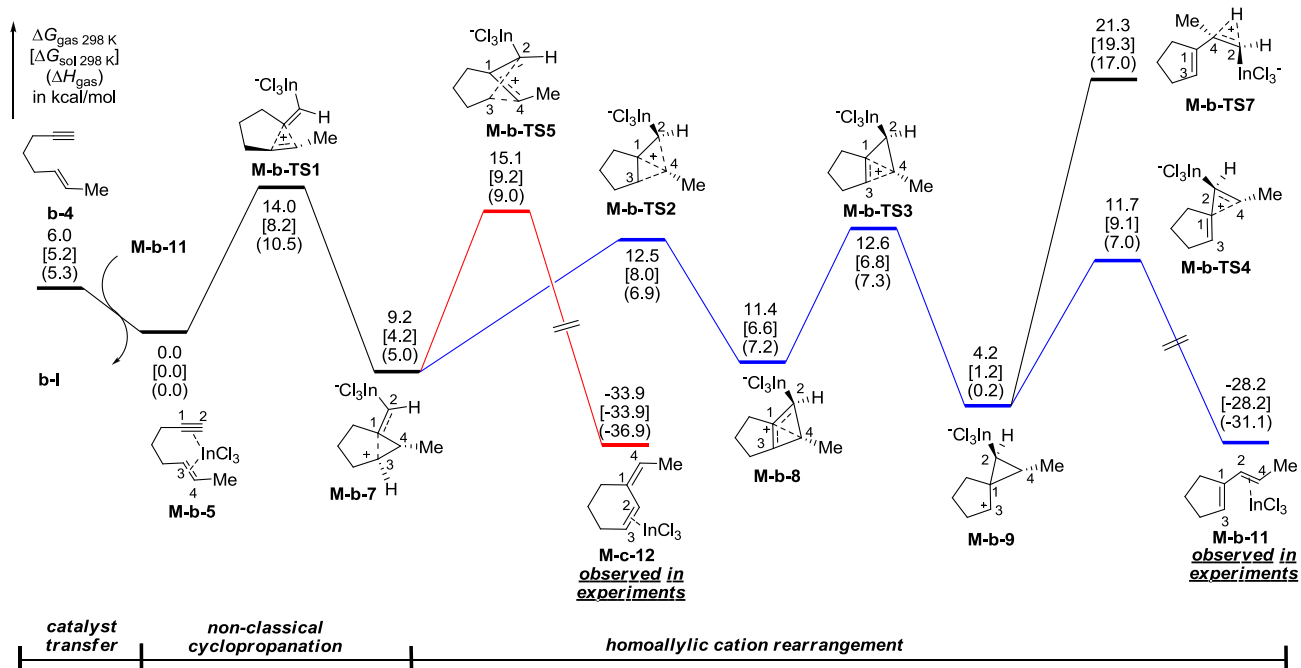


Figure S2. Full energy surface of **b-4**, taking InCl_3 as the catalyst.

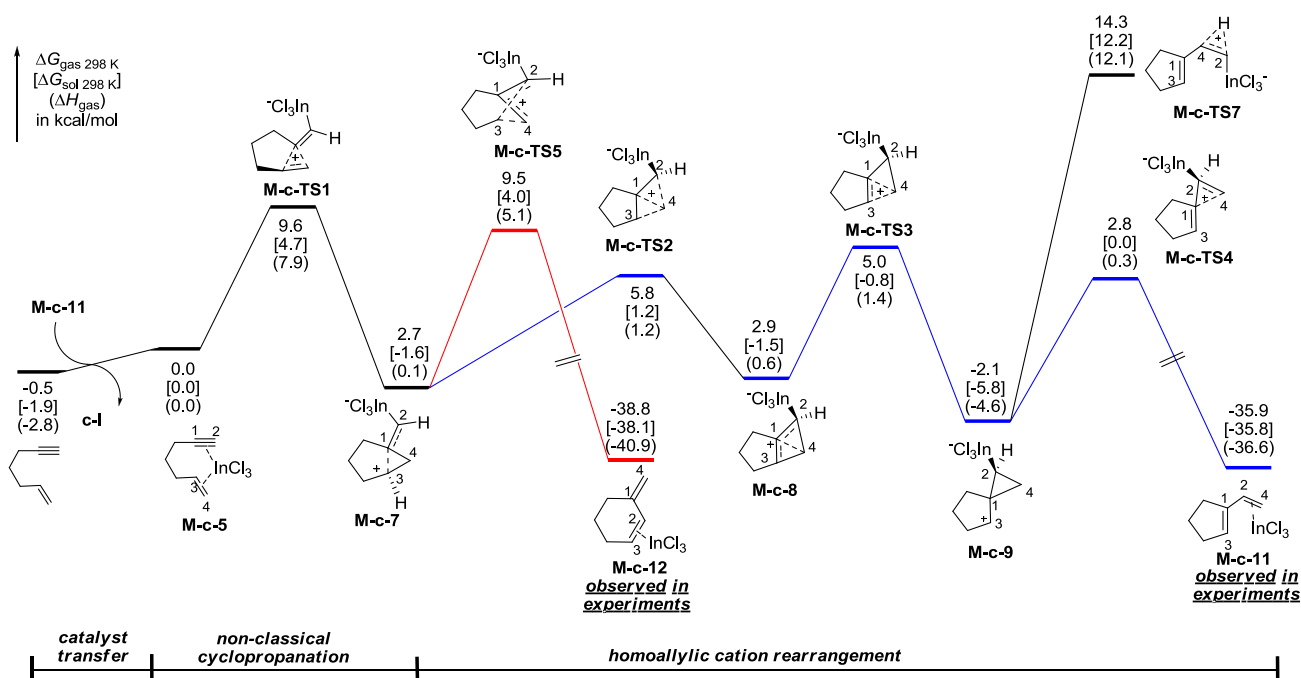


Figure S3. Full energy surface of **c-4**, taking InCl_3 as the catalyst.

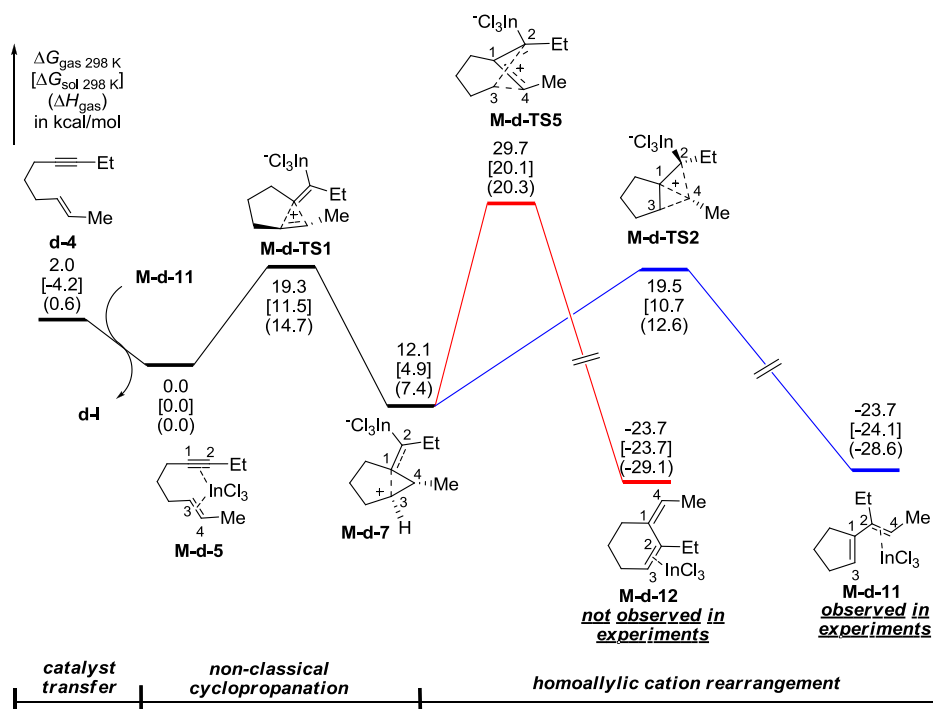


Figure S4. Full energy surface of **d-4**, taking InCl_3 as the catalyst.

Single point energy calculations using BP86, MP2 and MPWPW91 indicated that the calculated energy barriers of cyclopropanation progress by BP86 and MPWPW91 are similar to that from B3LYP calculations, while the MP2 calculations gave higher activation energy than that from B3LYP calculations (Table S1). Calculations by BP86, MP2 and MPWPW91 suggested that a mixture of type-I and type-III dienes should be produced, which is consistent with the experimentally observed results (Table S2).

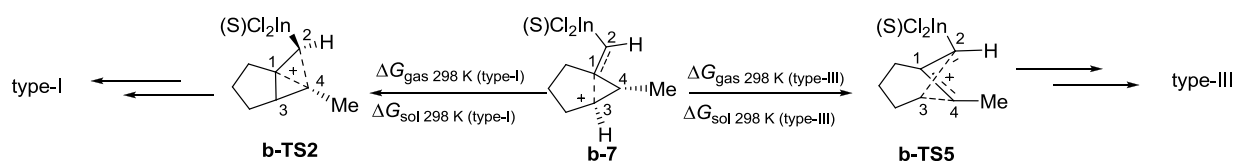
We have also included the dispersion energy in our calculations by using B3LYP-D2, M06 and M06-2X functionals. However, all of them suggested that the **TS2** was more favored than **TS5** by 3.1, 5.1 and 4.8 kcal/mol, respectively, predicting that type-III diene products should be obtained exclusively, with negligible formation of type-I dienes. These predictions disagreed with experiments. Calculations using bigger basis set (M06-2X/6-311+G(d,p)) gave results contradicting with the experimental observation (Table S2). To check whether this discrepancy was caused by the single point energy calculations using the B3LYP optimized structures, we reoptimized all stationary points in Table S2 by the M06-2X functional. It was found that the M06-2X calculated structures were very similar to those obtained from B3LYP optimizations, and the predicted selectivity by M06-2X was wrong again (**TS2** was more favored than **TS5** by 3.4 kcal/mol at this level). Based on these calculation results, we can conclude that B3LYP functional is appropriate for investigating the present system.

Table S1. Cyclopropanation progress calculated with various computational methods.

b-5 + S = benzene $\xrightarrow[\Delta G_{\text{sol 298 K}}]{\Delta G_{\text{gas 298 K}}}$ **b-TS1**

	B3LYP ^a	BP86 ^a	MPWPW91 ^a	MP2 ^a	M06 ^a	M06-2X ^a	B3LYP-D2 ^a
$\Delta G_{\text{gas 298K}}$ kcal/mol	2.9	0.3	0.0	10.5	0.8	4.2	-2.9
$\Delta G_{\text{sol 298K}}$ kcal/mol	6.8	4.2	4.0	14.7	4.8	8.3	1.0

Table S2. The type-I vs. type-III selectivity calculated with various computational methods.



	B3LYP ^a	BP86 ^a	MPWPW91 ^a	MP2 ^a	M06 ^a	M06-2X ^a	M06-2X ^b	M06-2X ^c	B3LYP-D2 ^a
$\Delta\Delta G_{\text{gas 298K}}$ kcal/mol ^d	-0.4	0.6	1.0	-1.1	5.1	4.8	4.7	3.4	3.1
$\Delta\Delta G_{\text{sol 298K}}$ kcal/mol ^e	-0.5	0.7	1.1	-1.3	-5.2	4.8	0.7	4.8	3.0

^a Single point energy was calculated using 6-31G(d) basis set based on the B3LYP/6-31G(d) optimized structures (In atom by the LANL2DZ)

^b Single point energy was calculated using 6-311+G(d,p) basis set based on the B3LYP/6-31G(d) optimized structures (In atom by the LANL2DZ)

^c The structures were optimized by the M06-2X functional using 6-31G(d) basis set (In atom by the LANL2DZ)

^d $\Delta\Delta G_{\text{gas 298K}} = \Delta G_{\text{gas 298K (type-I)}} - \Delta G_{\text{gas 298K (type-III)}}$

^e $\Delta\Delta G_{\text{sol 298K}} = \Delta G_{\text{sol 298K (type-I)}} - \Delta G_{\text{sol 298K (type-III)}}$

2. Computed Energies of All Stationary Points

thermal enthalpy (*H*, in Hartree)

thermal free energy (*G*, in Hartree)

thermal correction to Gibbs free energy (*TCGFE*, in Hartree)

total free energy in solution (*E_{sol}*, in Hartree)

thermal corrected Gibbs free energy in dichloroethane solution (*G_{sol}*, which equals to *E_{sol}* + *TCGFE*, in Hartree)

	<i>TCGFE</i>	<i>H</i>	<i>G</i>	<i>G_{sol}</i>	<i>E_{sol}</i>
benzene	0.073321	-232.137717	-232.170508	-232.171996	-232.245317
b-4	0.13998	-311.795246	-311.841429	-311.84375	-311.98373
b-5	0.136357	-1233.939946	-1233.9991	-1234.045108	-1234.181465
b-6	0.223094	-1466.087549	-1466.167891	-1466.209685	-1466.432779
b-7	0.231838	-1466.1016	-1466.175658	-1466.219381	-1466.451219
b-8	0.233893	-1466.097177	-1466.169393	-1466.21316	-1466.447053
b-9	0.22978	-1466.106295	-1466.181705	-1466.225666	-1466.455446

b-10	0.232908	-1466.108691	-1466.181324	-1466.224225	-1466.457133
b-11	0.228611	-1466.141388	-1466.21886	-1466.259237	-1466.487848
b-12	0.233322	-1466.151461	-1466.224969	-1466.265131	-1466.498453
b-TS1	0.230427	-1466.093357	-1466.16494	-1466.206201	-1466.436628
b-TS2	0.234624	-1466.096569	-1466.167338	-1466.210585	-1466.445209
b-TS3	0.233881	-1466.097942	-1466.169189	-1466.213139	-1466.44702
b-TS4	0.230268	-1466.106522	-1466.180119	-1466.222921	-1466.453189
b-TS5	0.23372	-1466.09515	-1466.166656	-1466.209853	-1466.443573
b-TS6	0.23175	-1466.105533	-1466.177897	-1466.220097	-1466.451847
b-TS7	0.136878	-1233.900403	-1233.957726	-1234.008446	-1234.145324
b-I	0.145442	-311.853279	-311.896002	-311.896932	-312.042374
c-4	0.113963	-272.506216	-272.548621	-272.551068	-272.665031
c-5	0.10993	-1194.647959	-1194.703789	-1194.751824	-1194.861754
c-6	0.197046	-1426.796982	-1426.873687	-1426.916171	-1427.113217
c-7	0.206027	-1426.812771	-1426.883126	-1426.927867	-1427.133894
c-9	0.205341	-1426.817315	-1426.887549	-1426.93142	-1427.136761
c-10	0.205737	-1426.811763	-1426.881974	-1426.925821	-1427.131558
c-11	0.204684	-1426.858744	-1426.93023	-1426.994335	-1427.199019
c-12	0.207712	-1426.858973	-1426.928358	-1426.969618	-1427.17733
c-TS1	0.201786	-1426.799843	-1426.871071	-1426.912994	-1427.11478
c-TS2	0.207834	-1426.807668	-1426.875291	-1426.919939	-1427.127773
c-TS4	0.203518	-1426.804332	-1426.872384	-1426.917551	-1427.121069
c-TS5	0.207881	-1426.803171	-1426.870857	-1426.915962	-1427.123843
c-TS6	0.20602	-1426.81252	-1426.881251	-1426.924677	-1427.130697
c-I	0.119382	-272.563804	-272.602783	-272.603724	-272.723106
DCE	0.029629	-998.946347	-998.981202	-998.982684	-999.012313
d-4	0.192315	-390.372107	-390.4268	-390.437663	-390.629978
d-5	0.18908	-1312.526709	-1312.594087	-1312.661549	-1312.850629
d-6	0.232393	-2311.467095	-2311.557122	-2311.621437	-2311.853383
d-7	0.240753	-2311.472345	-2311.555097	-2311.623034	-2311.863787
d-9	0.240943	-2311.477378	-2311.559522	-2311.626977	-2311.86792
d-10	0.241894	-2311.465549	-2311.546654	-2311.611683	-2311.853577
d-11	0.237871	-2311.514036	-2311.599395	-2311.666039	-2311.90391
d-12	0.243029	-2311.513541	-2311.594784	-2311.656543	-2311.899572
d-TS1	0.238526	-2311.460622	-2311.543714	-2311.609839	-2311.848365
d-TS2	0.243296	-2311.464211	-2311.543609	-2311.612623	-2311.855919
d-TS4	0.23972	-2311.474609	-2311.556675	-2311.622801	-2311.862521
d-TS5	0.24356	-2311.453979	-2311.533225	-2311.601883	-2311.845443
d-TS6	0.242377	-2311.46322	-2311.542401	-2311.608438	-2311.850815
d-TS7	0.188273	-1312.500611	-1312.565351	-1312.640999	-1312.829272
d-I	0.198801	-390.41865	-390.468056	-390.469335	-390.668136
m-b-5	0.129912	-1694.430991	-1694.500479	-1694.507939	-1694.637851
m-b-7	0.137712	-1694.423011	-1694.485888	-1694.501294	-1694.639006
m-b-8	0.137951	-1694.419577	-1694.482315	-1694.497381	-1694.635332
m-b-9	0.136577	-1694.430673	-1694.493804	-1694.505961	-1694.642538
m-b-11	0.136	-1694.480619	-1694.545413	-1694.552882	-1694.688882

m-b-12	0.136772	-1694.489862	-1694.554572	-1694.561953	-1694.698725
m-b-TS1	0.13424	-1694.414321	-1694.478167	-1694.494839	-1694.629079
m-b-TS2	0.139276	-1694.420065	-1694.480532	-1694.495171	-1694.634447
m-b-TS3	0.138268	-1694.419279	-1694.480463	-1694.497173	-1694.635441
m-b-TS4	0.1363	-1694.419777	-1694.481789	-1694.493434	-1694.629734
m-b-TS5	0.139996	-1694.416699	-1694.476469	-1694.493285	-1694.633281
m-b-TS7	0.133846	-1694.403871	-1694.466513	-1694.477199	-1694.611045
m-c-5	0.104346	-1655.135842	-1655.199238	-1655.207626	-1655.311972
m-c-7	0.111948	-1655.135727	-1655.194911	-1655.210134	-1655.322082
m-c-8	0.111028	-1655.134867	-1655.194625	-1655.209969	-1655.320997
m-c-9	0.111068	-1655.143155	-1655.202555	-1655.21686	-1655.327928
m-c-11	0.108675	-1655.194233	-1655.256468	-1655.264725	-1655.3734
m-c-12	0.111792	-1655.201132	-1655.260928	-1655.268361	-1655.380153
m-c-TS1	0.107661	-1655.123298	-1655.183885	-1655.200151	-1655.307812
m-c-TS2	0.113967	-1655.133952	-1655.189992	-1655.20566	-1655.319627
m-c-TS3	0.111922	-1655.133637	-1655.191269	-1655.208904	-1655.320826
m-c-TS4	0.109366	-1655.135401	-1655.194759	-1655.207567	-1655.316933
m-c-TS5	0.113627	-1655.127699	-1655.184017	-1655.201278	-1655.314905
m-c-TS7	0.106805	-1655.116563	-1655.17641	-1655.188195	-1655.295
m-c-I	0.119382	-272.563804	-272.602783	-272.603724	-272.723106
m-d-5	0.18165	-1773.003528	-1773.081257	-1773.092991	-1773.274641
m-d-7	0.189968	-1772.991662	-1773.061986	-1773.085187	-1773.275155
m-d-11	0.190652	-1773.049078	-1773.119053	-1773.131372	-1773.322024
m-d-12	0.192276	-1773.049949	-1773.11902	-1773.130722	-1773.322998
m-d-TS1	0.18822	-1772.980113	-1773.050405	-1773.074724	-1773.262944
m-d-TS2	0.192264	-1772.983455	-1773.050241	-1773.075912	-1773.268176
m-d-TS5	0.195787	-1772.971227	-1773.033908	-1773.060907	-1773.256694
m-d-TS7	0.186149	-1772.985426	-1773.05557	-1773.075775	-1773.261924
m-d-I	0.198801	-390.41865	-390.468056	-390.469335	-390.668136
LANL2DZ for In, and 6-311+G(d, p) for all other atoms					
benzene	0.072671	-232.205758	-232.238566	-232.240234	-232.312905
b-4	0.138563	-311.894906	-311.941117	-311.943728	-312.082291
b-5	0.134888	-1234.097093	-1234.156357	-1234.201991	-1234.336879
b-6	0.220059	-1466.309546	-1466.390771	-1466.432336	-1466.652395
b-7	0.229020	-1466.316301	-1466.390746	-1466.434364	-1466.663384
b-9	0.229072	-1466.321436	-1466.394229	-1466.438021	-1466.667093
b-10	0.230033	-1466.323669	-1466.396805	-1466.439555	-1466.669588
b-11	0.228189	-1466.357733	-1466.433257	-1466.473537	-1466.701726
b-12	0.230122	-1466.366999	-1466.441363	-1466.481355	-1466.711477
b-TS1	0.226316	-1466.312166	-1466.386683	-1466.428108	-1466.654424
b-TS2	0.231636	-1466.309532	-1466.380875	-1466.424159	-1466.655795
b-TS4	0.227603	-1466.323344	-1466.397295	-1466.439865	-1466.667468
b-TS5	0.231729	-1466.307818	-1466.378985	-1466.422125	-1466.653854
b-TS6	0.229321	-1466.322142	-1466.394685	-1466.436765	-1466.666086
b-I	0.143681	-311.945504	-311.988217	-311.989333	-312.133014

Single point energies

E_{gas}							
	BP86 ^a	MPWPW91 ^a	MP2 ^a	M06 ^a	M06-2X ^a	M06-2X ^b	B3LYP-D2 ^a
Ph	-232.232664	-232.202241	-230.701253	-232.047684	-232.133433		-1466.462685
b-5	-1234.188511	-1234.092739	-1230.501630	-1233.810632	-1233.916568		-1466.466663
b-TS1	-1466.441474	-1466.315650	-1461.206812	-1465.877725	-1466.064060		-1466.462685
b-TS2	-1466.462685	-1466.450174	-1466.325909	-1461.222516	-1465.896663	-1466.084094	-1466.462685
b-TS5	-1466.466663	-1466.450300	-1466.326556	-1461.219782	-1465.903970	-1466.090874	-1466.466663
E_{sol}							
	BP86 ^a	MPWPW91 ^a	MP2 ^a	M06 ^a	M06-2X ^a	M06-2X ^b	B3LYP-D2 ^a
Ph	-232.234213	-232.203800	-230.703339	-232.049316	-232.135218		-232.252761
b-5	-1234.233529	-1234.137705	-1230.550307	-1233.856503	-1233.962776		-1234.221506
b-TS1	-1466.481802	-1466.35928	-1461.250928	-1465.918908	-1466.105579		-1466.493395
b-TS2	-1466.492519	-1466.368208	-1461.268248	-1465.939848	-1466.127477	-1466.346137	-1466.505931
b-TS5	-1466.492759	-1466.368982	-1461.265324	-1465.947208	-1466.134291	-1466.352862	-1466.509860

^a Single point energy was calculated using 6-31G(d) basis set based on the B3LYP/6-31G(d) optimized structures (In atom by the LANL2DZ)

^b Single point energy was calculated using 6-311+G(d,p) basis set based on the B3LYP/6-31G(d) optimized structures (In atom by the LANL2DZ)

^c The structures were optimized by the M06-2X functional using 6-31G(d) basis set (In atom by the LANL2DZ)

3. Coordinates of All Stationary Points

				H	-1.43596800	3.91197300	0.23150400
b-4				H	-1.57724300	2.78422800	-1.13341500
C	0.95665000	-0.67527800	-0.44392500	H	-0.22440300	-1.88388700	-2.47283300
C	1.93469300	-0.29062200	0.38066800				
C	-1.55010200	1.27325000	0.11207800				
C	-1.98515200	-0.04385500	0.58287200	b-6			
C	-1.55197900	-1.22967900	-0.31298500	C	-5.05362900	0.33759600	0.40505100
C	-0.09630100	-1.69894300	-0.11576000	C	-5.19996000	0.92755200	-0.78873600
C	-1.23877700	2.36899500	-0.29031800	C	-1.18139300	-1.59379700	0.78153400
H	0.03656000	-2.04074600	0.92016400	C	-2.46497100	-1.29139600	0.20461300
H	0.04803100	-2.58574000	-0.75266400	C	-3.61627800	-1.60157700	1.21428300
H	-1.72227000	-0.96374000	-1.36368600	C	-4.97063800	-1.14708100	0.62559200
H	-2.21454800	-2.07671100	-0.09355000	C	-0.05116800	-1.80083900	1.24377100
H	-1.61890300	-0.20855200	1.60630600	In	1.33846400	-0.63074300	-0.24397300
H	-3.08170600	-0.03767100	0.65208900	Cl	0.09919500	0.70633000	-1.64406400
H	0.90104700	-0.23173600	-1.43990900	Cl	2.83405700	-2.26714500	-0.85127600
H	1.98341600	-0.73133900	1.37877600	H	-5.16168900	-1.68361000	-0.31228500
C	2.99369200	0.72353300	0.05485100	H	-5.74566200	-1.46768200	1.33532100
H	2.95427400	1.57477000	0.74840400	H	-3.41946000	-1.07757500	2.15645400
H	4.00134300	0.29395000	0.14148900	H	-3.63500300	-2.67465700	1.42940300
H	2.87738600	1.11217800	-0.96263600	H	-2.51520100	-0.22340000	-0.05851700
H	-0.94097100	3.33092100	-0.63966800	H	-2.60417200	-1.86618500	-0.71954800
				H	-5.00044500	0.96021000	1.30098700
b-5				H	-5.27243500	0.29722500	-1.67748900
C	0.81768200	1.78644700	-0.27395300	C	-5.31615500	2.40543900	-1.01931200
C	-0.25426900	2.18652400	0.48206500	H	-4.54447200	2.76086400	-1.71463000
C	1.59148000	-1.23495700	-1.25587400	H	-6.28319600	2.65119500	-1.47691900
C	2.83339900	-0.87138200	-0.57942400	H	-5.22917000	2.97122500	-0.08603400
C	3.13988000	0.64506500	-0.57322300	H	0.54624200	-2.36145800	1.94532500
C	2.20256200	1.51462700	0.28376600	C	1.31947600	2.72484600	1.32368300
C	0.53384700	-1.51370500	-1.80672300	C	1.55443100	1.47545000	1.89387900
In	-0.56426400	-0.38313200	0.09072400	C	2.62312300	0.67299300	1.41772200
Cl	0.17447400	-1.17328100	2.11153300	C	3.47095000	1.16910800	0.38978900
Cl	-2.65182500	-0.44130200	-0.83512400	C	3.21928300	2.42143500	-0.17122400
H	2.14095200	1.13571000	1.31153000	C	2.15062200	3.19385500	0.29854600
H	2.67078900	2.50738500	0.36158500	H	0.50161200	3.34069000	1.68362000
H	3.16531600	1.01709700	-1.60401900	H	0.93815400	1.11911800	2.71421100
H	4.15404000	0.75541800	-0.17762400	H	2.92902800	-0.21231600	1.97640700
H	2.81681800	-1.27931000	0.43994000	H	4.31840400	0.57423200	0.06112100
H	3.63356300	-1.40664900	-1.11059300	H	3.86070700	2.79985700	-0.96048600
H	0.73842900	1.90126900	-1.35905200	H	1.96458900	4.17102500	-0.13664100
H	-0.14643400	2.14881300	1.57002300				
C	-1.49228000	2.84935800	-0.04558400				
H	-2.40577900	2.45748100	0.41223800	b-7			

C	-1.21269700	0.72989300	0.14405900	C	2.72183100	0.83845300	-0.22657900
In	0.60594500	-0.49781700	0.21762500	Cl	-0.87011200	-1.01466400	1.98640000
Cl	1.55388100	-0.21671900	2.30862100	Cl	-0.76421200	2.76926400	0.59986900
C	-2.41348000	0.49498100	-0.44897200	H	5.49663500	-0.51453900	0.15433900
C	-2.85331800	-0.78533300	-1.13371800	H	5.12816100	-1.84730900	-0.93501100
C	-3.72033100	-1.53231800	-0.10487400	H	4.25338700	-2.82946900	1.10728300
C	-4.60287800	-0.46822200	0.62144200	H	3.88491700	-1.25628200	1.79760600
C	-3.81811500	0.80985400	0.71917200	H	1.62713300	-1.84935300	1.09598600
C	-3.57392600	1.64043100	-0.42318400	H	2.23708000	-2.82295200	-0.24085400
Cl	0.37360200	-2.61579000	-0.72276400	H	3.89265000	0.11022400	-1.96953100
H	-5.50773100	-0.27820800	0.03154300	H	2.77806500	0.78358700	0.85913200
H	-4.90461400	-0.81386200	1.61281100	C	3.02831400	2.24561900	-0.76284200
H	-3.06823500	-2.01272700	0.63219900	H	2.28352900	2.94050800	-0.36391600
H	-4.34209300	-2.30756100	-0.55985900	H	4.02259400	2.55002000	-0.42227500
H	-3.42228500	-0.55970800	-2.04308000	H	3.00013900	2.28243200	-1.85415300
H	-1.98706300	-1.38468600	-1.42480100	H	1.30534800	0.66946000	-1.85595600
H	-3.45659700	1.14794400	1.68780500	C	-3.78061500	-1.85831700	-0.25115700
H	-4.20950500	1.44054200	-1.28620100	C	-2.78050900	-2.18138100	-1.17621700
C	-3.17122300	3.09444700	-0.27895100	C	-2.07278300	-1.16645300	-1.81789900
H	-2.59295300	3.28472400	0.62966000	C	-2.35320400	0.18814900	-1.51496400
H	-2.59396700	3.42906300	-1.14537700	C	-3.37892700	0.50254400	-0.59005900
H	-4.07981900	3.70364900	-0.22254900	C	-4.07968700	-0.52458200	0.04352400
H	-1.13445000	1.64675000	0.73104000	H	-4.33139200	-2.65340600	0.24209400
C	3.19172000	-0.33587400	-1.21759700	H	-2.56819000	-3.22101500	-1.40483500
C	2.10412600	0.49777900	-1.57465100	H	-1.32584600	-1.40763200	-2.56940200
C	2.05316700	1.82873100	-1.09392300	H	-1.92593700	0.98301100	-2.12695600
C	3.05166800	2.29777700	-0.24216500	H	-3.61725800	1.54228700	-0.38726700
C	4.11346200	1.45879600	0.11662000	H	-4.86094000	-0.28591400	0.75778700
C	4.18574200	0.14852100	-0.36679300				
H	3.24660600	-1.34482900	-1.61499900				
H	1.42053500	0.17607700	-2.36042600	b-9			
H	1.24925200	2.48621100	-1.41361900	C	1.37569300	0.60048900	-0.68434400
H	3.01460600	3.31616700	0.13149000	In	-0.63267000	0.61171600	0.23998700
H	4.89039100	1.83049800	0.77767300	C	2.46970300	-0.40700000	-0.29499100
H	5.01588600	-0.49110500	-0.08529800	C	2.47232100	-1.29896000	0.94019300
				C	3.89324900	-1.91366300	0.94125400
b-8				C	4.37301100	-1.81087900	-0.53081300
C	1.33189100	0.22137500	-0.86035300	C	3.54401700	-0.70608800	-1.09427100
In	-0.54821600	0.47616700	0.23420500	C	2.41814500	1.41735200	-0.11182100
C	2.32489400	-0.81299900	-0.69980700	Cl	-0.92022600	-0.66564300	2.14891700
C	2.40968900	-1.89692100	0.33413600	Cl	-1.30106200	2.84149600	0.19892600
C	3.86221200	-1.83810500	0.87060400	H	5.44789300	-1.62887200	-0.64671700
C	4.68044600	-1.12805800	-0.23862400	H	4.16449200	-2.73159800	-1.10182900
C	3.64745100	-0.31166100	-0.99754100	H	3.90559800	-2.93879200	1.31668300

H	4.55718600	-1.32234700	1.58022200	H	2.65450500	2.84118800	-1.72091000
H	2.22864400	-0.76767100	1.86498600	H	2.87399700	4.03566100	-0.42237500
H	1.69441300	-2.06348400	0.81644100	H	4.28376900	3.32959600	-1.17973600
H	3.76011000	-0.21792700	-2.04128400	H	1.16768000	1.41240800	-1.28677100
H	2.50194800	1.45998000	0.97429400	C	-2.86893600	2.34714800	0.08652500
C	3.23216700	2.42859400	-0.85230500	C	-2.01322400	1.93307300	-0.93187700
H	2.73206800	3.39503000	-0.68092300	C	-2.12796700	0.62575500	-1.46262700
H	4.24956700	2.52099700	-0.46259400	C	-3.14271200	-0.23828000	-0.98275500
H	3.25208300	2.25730100	-1.93119500	C	-3.99389000	0.19059800	0.03652900
H	1.30416700	0.73293200	-1.76731300	C	-3.85542400	1.47695600	0.56627100
C	-3.29899500	-2.36426700	-0.23300500	H	-2.78097800	3.34752300	0.49824600
C	-2.13568000	-2.60350700	-0.97442400	H	-1.27710600	2.62013600	-1.34049800
C	-1.53745900	-1.56381800	-1.68422600	H	-1.57910900	0.35309400	-2.36459900
C	-2.09703000	-0.26409700	-1.63543200	H	-3.25554800	-1.22650800	-1.41793800
C	-3.28235600	-0.03780600	-0.89421100	H	-4.76665800	-0.47301100	0.41070000
C	-3.87069100	-1.08887200	-0.18979200	H	-4.52187800	1.80634800	1.35757000
H	-3.76281100	-3.17909900	0.31450200				
H	-1.70986900	-3.60137200	-1.00828300	b-11			
H	-0.65997800	-1.75071800	-2.29736900	C	-3.96560600	0.33243900	1.11378100
H	-1.73616100	0.51102800	-2.31184300	C	-3.04732600	0.61430700	-0.06897100
H	-3.72862700	0.95201200	-0.88647200	C	-3.49985100	-0.02340700	-1.18729600
H	-4.77456400	-0.91583500	0.38514700	C	-4.74661300	-0.80198700	-0.92776600
				C	-5.22518400	-0.28580300	0.45470200
				C	-1.88556700	1.44300800	0.01187100
b-10				C	-0.83197600	1.57951200	-0.90176700
C	1.44019600	0.54593500	-0.68400100	H	-0.95789000	1.08726800	-1.87134200
In	-0.37780000	-0.50329700	0.00577800	H	-3.02557300	0.01700900	-2.16432600
Cl	-0.92217300	-0.17277500	2.23365500	H	-5.48802100	-0.69232100	-1.72797700
C	2.57789700	0.89999100	0.33604300	H	-4.48591800	-1.87380200	-0.90437600
C	2.81566600	-0.07879100	1.47559400	H	-5.98603100	0.48767400	0.30925200
C	2.78527700	-1.50869400	0.87991100	H	-5.67148100	-1.07473200	1.06368900
C	3.16190500	-1.39293000	-0.61153000	H	-3.48007400	-0.37870900	1.79606100
C	2.65288500	-0.08125000	-1.14627200	H	-4.19087700	1.23148400	1.69781200
C	3.29761400	2.06488100	0.21433600	In	0.44897900	-0.13506000	0.17728300
Cl	-0.45792700	-2.63437600	-0.94138200	Cl	-0.72500900	-2.12536200	-0.04287000
H	4.24434800	-1.44918600	-0.76560100	Cl	1.28232900	0.73638900	2.14134000
H	2.70805200	-2.20071000	-1.20518200	C	0.01548300	2.84534800	-0.89441100
H	3.78877400	0.13053600	1.93117000	H	0.99170500	2.70105300	-1.36292600
H	2.05489600	0.04451100	2.25384900	H	-0.50230400	3.62785000	-1.46335100
H	3.18660400	0.36032400	-1.98780200	H	0.17536900	3.21939500	0.12169100
H	3.47306300	-2.17572300	1.40537000	H	-1.79952600	2.04193700	0.92230500
H	1.79689900	-1.96606300	0.99192500	C	2.79524800	-1.62010500	-0.53538600
H	3.97429700	2.29015800	1.04084500	C	3.86074900	-1.28338300	0.29928000
C	3.26209300	3.09941200	-0.85114900	C	4.44130300	-0.01301900	0.21244900

C	3.97065400	0.93041600	-0.70945500	H	1.57897500	2.16675800	0.76535100
C	2.90872000	0.60887100	-1.55184000	H	2.72616400	0.55090500	2.27744400
C	2.28698600	-0.66159200	-1.45351500	H	4.50291200	-0.93879800	1.36933500
H	2.35752200	-2.61344400	-0.50175800				
H	4.24508200	-2.01113900	1.00651400				
H	5.27317400	0.24155500	0.86208500	b-I			
H	4.44533600	1.90386300	-0.78008400	C	1.27659100	-1.22259400	0.17553700
H	2.57793500	1.31125800	-2.31100900	C	0.23312000	-0.13937600	-0.06066100
H	1.58502900	-0.98334800	-2.22314300	C	0.81901300	1.07020000	-0.12912900
				C	2.31304100	1.00738900	0.07605100
				C	2.62245500	-0.50395300	-0.08763400
b-12				C	-1.19280800	-0.46432700	-0.15637200
C	-2.06078500	-0.09337700	-1.13538600	C	-2.21513200	0.35503200	0.13742300
In	0.37237100	-0.26856300	0.22340600	H	-1.99675400	1.35638800	0.51047300
Cl	1.02014400	-2.19836700	-0.86280900	H	0.28862400	2.00450400	-0.29344200
C	-3.27436600	0.13871400	-0.40637000	H	2.87153000	1.62990900	-0.63505300
C	-3.59660500	1.57821000	-0.02645500	H	2.58529900	1.37090300	1.08013100
C	-2.33497900	2.41506500	0.24325500	H	2.94252800	-0.69701900	-1.11809300
C	-1.34097400	2.32234500	-0.92540400	H	3.42529700	-0.84863200	0.57180200
C	-1.07957300	0.88029100	-1.33035300	H	1.20759000	-1.59513200	1.20910800
C	-4.13058700	-0.88540000	-0.11671000	H	1.13052100	-2.09568400	-0.47433900
Cl	-0.41341300	-0.21388100	2.39797900	C	-3.66632000	-0.00024400	0.00068300
H	-1.74441900	2.84155900	-1.80741100	H	-4.19407000	0.09575800	0.95982500
H	-0.40651800	2.84429400	-0.68431800	H	-4.17661500	0.67261900	-0.70293300
H	-4.16192700	2.03642400	-0.85038000	H	-3.79784800	-1.02660400	-0.35886500
H	-4.25381800	1.59602700	0.84849100	H	-1.42584800	-1.47977900	-0.48399800
H	-0.37323900	0.69545300	-2.14526900				
H	-5.03980700	-0.61180500	0.42031200				
H	-2.61327500	3.46069300	0.40625900	b-TS1			
H	-1.85722000	2.06685400	1.16724800	C	1.15426500	0.63081000	0.08778800
C	-4.01241000	-2.34032800	-0.41594200	Cl	-1.89634300	0.59439000	2.16354400
H	-4.02280900	-2.90613400	0.52606900	C	2.21716600	-0.07903900	0.07483700
H	-4.89687200	-2.67422400	-0.97486400	C	2.92402200	-1.36221000	0.08272100
H	-3.11884100	-2.62668300	-0.97400400	C	5.01346000	-0.32806700	-0.83032000
H	-1.89143700	-1.07766000	-1.56823800	C	4.28987500	0.97688800	-0.69418400
C	4.25675400	-0.24599700	-0.66095300	C	4.07839600	1.61380900	0.49027600
C	3.56615100	0.60881800	-1.53001000	Cl	-0.49009700	-2.70550800	0.24326900
C	2.56242400	1.43850700	-1.03670100	H	5.61233700	-0.52501900	0.06617000
C	2.22454100	1.39706400	0.34035500	H	5.69757400	-0.29893100	-1.68553900
C	2.94994700	0.54381600	1.21469500	H	3.37251300	-1.53055400	1.07075800
C	3.95267100	-0.28097500	0.70449700	H	2.13993000	-2.12597800	-0.04813800
H	5.04132100	-0.88665000	-1.05193400	H	3.92741000	1.44591700	-1.60971900
H	3.82360400	0.63426800	-2.58399900	H	4.48331300	1.16506200	1.39825000
H	2.05334600	2.13603000	-1.69600900	In	-0.79469000	-0.40362200	0.40436800

C	3.43268100	2.95138700	0.64206900	H	3.04255300	2.33108400	-1.76615500
H	3.00866000	3.31818000	-0.29804800	H	1.39346600	0.79158900	-1.77024100
H	2.65579300	2.93705800	1.41690700	C	-3.83620300	-1.81291800	-0.24754600
H	4.18182700	3.68138200	0.97747900	C	-2.83581100	-2.16441900	-1.16192000
C	3.98572400	-1.46786000	-1.02337300	C	-2.10675300	-1.16970600	-1.81134900
H	3.50643700	-1.39032400	-2.00558500	C	-2.36621600	0.19356900	-1.52664100
H	4.47570700	-2.44437600	-0.97118100	C	-3.39244700	0.53673700	-0.61186600
H	1.08129700	1.71319200	0.07375800	C	-4.11438200	-0.47069100	0.02944500
C	-2.31847300	1.96142300	-1.44948400	H	-4.40352400	-2.59242200	0.25177600
C	-1.76086300	0.73444400	-1.84887100	H	-2.63904700	-3.21019000	-1.37574500
C	-2.47734000	-0.46962400	-1.62986000	H	-1.35804600	-1.43257900	-2.55370000
C	-3.74073300	-0.42767700	-1.01060600	H	-1.92233500	0.97329700	-2.14625200
C	-4.28332900	0.79735400	-0.62647500	H	-3.61467300	1.58283600	-0.42362600
C	-3.57553300	1.98728300	-0.84689900	H	-4.89590200	-0.21036200	0.73580300
H	-1.78109500	2.88662600	-1.63417100				
H	-0.83006900	0.71266400	-2.41132500				
H	-2.09660300	-1.40867000	-2.02342100	b-TS3			
H	-4.29087300	-1.34948900	-0.85016100	C	1.33977500	0.27460000	-0.83531200
H	-5.26048900	0.83081300	-0.15525900	In	-0.56036400	0.49734500	0.22713300
H	-4.01028800	2.93540500	-0.54633200	C	2.34410000	-0.77964900	-0.66512100
				C	2.41212100	-1.85497000	0.38769700
				C	3.88391300	-1.85347200	0.87190600
b-TS2				C	4.68802000	-1.17806500	-0.26879500
C	1.29320400	0.17159800	-0.87996300	C	3.65328500	-0.36854000	-1.01563800
In	-0.57876400	0.46034900	0.23225900	C	2.63563500	0.88647300	-0.18912100
C	2.32595700	-0.73095800	-0.65251000	Cl	-0.87055900	-0.95482300	2.01448600
C	2.40322800	-1.84164800	0.36817100	Cl	-0.83825100	2.79242200	0.53581600
C	3.87387200	-1.87160600	0.84331000	H	5.52499400	-0.56873500	0.08615100
C	4.68775600	-1.24568000	-0.31522200	H	5.10933300	-1.91309000	-0.96784600
C	3.71451900	-0.28421200	-0.99842600	H	4.24555600	-2.85812500	1.09901900
C	3.06386300	0.82652500	-0.18044900	H	3.96630900	-1.26695400	1.79259600
Cl	-0.92802900	-1.00274300	1.99481400	H	1.66621800	-1.74469600	1.17934700
Cl	-0.71586400	2.76479300	0.56454400	H	2.16576200	-2.78566300	-0.14877800
H	5.60108500	-0.74860500	0.02390800	H	3.88964500	0.14034400	-1.94477600
H	4.98280700	-2.00650800	-1.04617000	H	2.70500300	0.81934900	0.89522500
H	4.20807800	-2.88327200	1.08292900	C	3.10671800	2.23603600	-0.73676900
H	3.98365300	-1.27990100	1.75812400	H	2.42705100	2.99692200	-0.33687300
H	1.66287700	-1.76019600	1.16874400	H	4.12316800	2.45870600	-0.40125600
H	2.15965100	-2.75456100	-0.19724700	H	3.06789800	2.27817900	-1.82741000
H	3.93182600	0.03373800	-2.01762700	H	1.28678800	0.67555600	-1.85062400
H	3.10867700	0.73126900	0.90202500	C	-3.73390000	-1.92345100	-0.23365200
C	3.08065000	2.26082600	-0.67680900	C	-2.71598500	-2.24576600	-1.13926300
H	2.27689300	2.85821600	-0.24009200	C	-2.02515300	-1.23066700	-1.79896400
H	4.04015800	2.68015000	-0.34556400	C	-2.34085700	0.12393000	-1.53372500

C	-3.38391300	0.43700700	-0.62815900	H	2.37047400	3.96439900	-0.08249800
C	-4.06758500	-0.59021500	0.02363300	H	1.27256800	3.54367800	-1.43506000
H	-4.27130100	-2.71868900	0.27391000				
H	-2.47632200	-3.28547700	-1.33864900				
H	-1.26427500	-1.47279600	-2.53600600				
H	-1.92460700	0.91324900	-2.16023400	b-TS5			
H	-3.64847200	1.47557800	-0.45399600	C	1.38862800	0.77649200	-0.36706600
H	-4.86216800	-0.35224900	0.72328300	In	-0.42497100	-0.42441900	-0.08662500
				Cl	-1.10500500	-0.66154300	2.11932400
				C	2.44636100	1.01764700	0.58295800
b-TS4				C	2.59140700	0.10802300	1.78297200
C	2.92741400	-0.68550300	0.82301500	C	2.70831700	-1.34967700	1.22690700
C	2.63151700	0.32366900	-0.26842000	C	3.23063200	-1.27614200	-0.22590800
C	3.75746800	0.68619300	-0.93106800	C	2.88274000	0.10192800	-0.77387600
C	4.95486800	-0.07939200	-0.44814700	C	3.66439600	1.42418500	-0.08279000
C	4.47713700	-0.69259100	0.89625200	Cl	-0.29608400	-2.29288700	-1.47837200
C	1.44915400	2.05425500	0.12279700	H	4.31677800	-1.41029400	-0.27507200
C	1.25026800	0.87988700	-0.64406800	H	2.77822300	-2.04938900	-0.85407000
H	1.61893200	1.92553600	1.19249500	H	3.48107100	0.39008600	2.35181700
H	3.78884700	1.38489200	-1.76319100	H	1.71881300	0.20762900	2.43557900
H	5.22555100	-0.84989800	-1.18587100	H	2.96254200	0.30178300	-1.83855600
H	5.83882000	0.56107400	-0.34285600	H	3.35851000	-1.95073600	1.86671000
H	4.87695100	-1.69447100	1.06575800	H	1.72868800	-1.83649100	1.25612300
H	4.81159800	-0.06213400	1.72608600	H	4.57066000	1.17086900	0.46728500
H	2.45971200	-0.43743000	1.78430900	C	3.83051900	2.59775200	-1.02340200
H	2.52521500	-1.66402800	0.52101200	H	2.91778300	2.84652700	-1.57128200
In	-0.41506200	-0.48837700	0.01776700	H	4.12514000	3.47678900	-0.43992800
Cl	-0.90703900	-0.04554400	2.23922800	H	4.62780500	2.39730100	-1.74546600
Cl	-0.03774500	-2.61264400	-0.83353700	H	1.26644200	1.55777700	-1.11732700
H	1.13391700	1.06749100	-1.71525400	C	-2.14503400	0.92053300	-1.36170000
C	-2.48002700	1.50929000	-1.07953200	C	-3.14870500	-0.05743200	-1.15317800
C	-3.37487600	1.85845500	-0.07043300	C	-4.06671800	0.10176900	-0.11456000
C	-4.16311000	0.87270800	0.53668000	C	-4.00505700	1.23384300	0.70382900
C	-4.06497400	-0.46533100	0.14291700	C	-3.02809800	2.21533700	0.49758900
C	-3.17364200	-0.83010900	-0.86724500	C	-2.10581300	2.07115000	-0.53706400
C	-2.35467900	0.15515800	-1.47438700	H	-1.54458500	0.88005500	-2.27123000
H	-1.89961200	2.27424200	-1.58823900	H	-3.20042100	-0.92098400	-1.80931800
H	-3.47454700	2.89526100	0.23496900	H	-4.83116900	-0.65026400	0.05151200
H	-4.86117100	1.15189600	1.31998400	H	-4.72356800	1.35394200	1.50890600
H	-4.68718600	-1.21952100	0.61362800	H	-2.99774100	3.09357300	1.13453300
H	-3.10838800	-1.86110300	-1.20183000	H	-1.37430900	2.85123900	-0.73007400
H	-1.78908000	-0.10135700	-2.37065400				
C	1.43823300	3.45431200	-0.35944800				
H	0.64824300	3.99511100	0.18640400	b-TS6			

C	1.50684300	0.48392300	-0.73858200	C	-1.26813700	-0.01021900	1.31391300
In	-0.36609600	-0.52756100	0.01996300	C	-2.58924900	-1.09342900	-0.33495900
Cl	-0.86371500	-0.10323500	2.23746700	H	-0.82493900	0.79800200	1.89914400
C	2.49576300	1.03383100	0.33030000	H	-0.78660300	-1.83418000	2.43312300
C	2.84224600	0.09229000	1.45982200	H	-2.40075300	-1.19000000	2.68026900
C	2.88692000	-1.37215400	0.94252300	H	-1.34673400	-2.76532900	0.28108500
C	3.22536400	-1.39148400	-0.55184600	H	-2.96583800	-2.83538400	0.97437900
C	2.52226700	-0.32946400	-1.30680400	H	-3.66478400	-0.86642700	-0.26510300
C	3.08945300	2.24129800	0.16627400	H	-2.39802700	-1.39542000	-1.37090200
Cl	-0.38398600	-2.69397800	-0.84767700	In	0.99173700	0.12413400	-0.16257100
H	4.30294600	-1.32177200	-0.75795800	Cl	2.48643400	0.51044600	1.50992200
H	2.91489800	-2.34427100	-1.02114100	Cl	0.99510500	-1.47553100	-1.81305000
H	3.80796600	0.38070700	1.88482400	C	-2.44098100	2.65913500	-0.18076100
H	2.09662400	0.17063800	2.26078000	H	-2.00011400	2.95265700	0.77294000
H	2.84126600	-0.16848600	-2.34043200	H	-2.40148000	3.49074200	-0.88673000
H	3.61169200	-1.96570100	1.50530500	H	-3.47937600	2.36086100	-0.02232300
H	1.92133000	-1.86554300	1.10305700	H	-0.12691200	2.61704700	-1.64911200
H	3.72659700	2.56080800	0.99211100				
C	2.94105100	3.24786400	-0.93020000				
H	2.42285300	2.87277300	-1.81677300	benzene			
H	2.39576700	4.12889600	-0.56416000	C	1.06513400	-0.90376700	-0.00000500
H	3.92883600	3.60965900	-1.23977900	C	-0.25025800	-1.37418300	-0.00006900
H	1.15775800	1.24792000	-1.43384800	C	-1.31529500	-0.47052300	0.00005600
C	-2.84529800	2.30310700	0.04751600	C	-1.06505800	0.90385500	-0.00000800
C	-1.99158900	1.87163700	-0.96517900	C	0.25014200	1.37420000	-0.00006200
C	-2.10183300	0.55102200	-1.46658200	C	1.31533500	0.47041800	0.00005700
C	-3.11175400	-0.30780400	-0.96349600	H	1.89357500	-1.60700600	0.00006700
C	-3.95989300	0.13926100	0.05019900	H	-0.44474600	-2.44333400	-0.00007800
C	-3.82533300	1.43838700	0.55037300	H	-2.33850400	-0.83643400	0.00015400
H	-2.76012500	3.31232400	0.43744900	H	-1.89367100	1.60688200	-0.00000700
H	-1.25958900	2.55274500	-1.39062500	H	0.44487700	2.44330000	-0.00001900
H	-1.56254600	0.26441500	-2.37006400	H	2.33846100	0.83658300	0.00006400
H	-3.22350600	-1.30496300	-1.37848000				
H	-4.72826100	-0.51917700	0.44217200	b-I			
H	-4.49013900	1.78185500	1.33706000	C	1.27659100	-1.22259400	0.17553700
				C	0.23312000	-0.13937600	-0.06066100
				C	0.81901300	1.07020000	-0.12912900
b-TS7				C	2.31304100	1.00738900	0.07605100
H	-2.15754200	1.26287000	-1.77590800	C	2.62245500	-0.50395300	-0.08763400
C	-1.68077400	1.38252600	-0.77902800	C	-1.19280800	-0.46432700	-0.15637200
C	-0.30047600	1.72123900	-1.04325500	C	-2.21513200	0.35503200	0.13742300
C	-1.62394700	-1.35108400	1.91934500	H	-1.99675400	1.35638800	0.51047300
C	-2.15314900	-2.15809300	0.70529700	H	0.28862400	2.00450400	-0.29344200
C	-1.81464900	0.13799700	0.07416300	H	2.87153000	1.62990900	-0.63505300

H	2.58529900	1.37090300	1.08013100	H	0.46100100	0.56425600	2.64739700
H	2.94252800	-0.69701900	-1.11809300				
H	3.42529700	-0.84863200	0.57180200				
H	1.20759000	-1.59513200	1.20910800	c-6			
H	1.13052100	-2.09568400	-0.47433900	C	-5.21103500	1.16413300	0.00194200
C	-3.66632000	-0.00024400	0.00068300	C	-5.20287700	1.60929200	-1.25748500
H	-4.19407000	0.09575800	0.95982500	C	-1.62809000	-1.16715100	0.83648200
H	-4.17661500	0.67261900	-0.70293300	C	-2.83403100	-0.77136700	0.15311100
H	-3.79784800	-1.02660400	-0.35886500	C	-4.05992100	-0.80752500	1.12061500
H	-1.42584800	-1.47977900	-0.48399800	C	-5.32179600	-0.28165400	0.40177000
				C	-0.56027000	-1.46636200	1.38458000
				In	1.02649400	-0.67929700	-0.17437700
c-5				Cl	0.02721600	0.63371200	-1.77231300
C	2.16701500	-0.31655500	1.72995100	Cl	2.28990300	-2.56946100	-0.50714000
C	0.84884200	-0.29030100	2.09322900	H	-5.53330200	-0.90489200	-0.47596400
C	2.83015800	0.38300500	-1.21982100	H	-6.16272200	-0.41556000	1.09556800
C	3.46174700	-0.93523000	-1.17358400	H	-3.84245500	-0.19253400	2.00127900
C	4.00010500	-1.31798100	0.22155800	H	-4.22181400	-1.83350100	1.46579800
C	2.90808600	-1.53497700	1.28525100	H	-2.72253200	0.25165000	-0.23646000
C	2.32670400	1.48968300	-1.26304600	H	-3.00861100	-1.43238000	-0.70512000
In	-0.03667600	0.49119100	-0.05781800	H	-5.13131300	1.88051400	0.82146900
Cl	-0.14770100	-1.30621600	-1.49814900	H	-5.30045500	0.93368200	-2.10505700
Cl	-0.23759000	2.78530300	0.24969000	H	-0.05779000	-2.00278300	2.17334300
H	2.20602500	-2.32309400	0.98661800	C	1.41888000	2.80665700	1.02146800
H	3.40393700	-1.90181600	2.20092900	C	1.46744200	1.60713400	1.72868000
H	4.70942400	-0.55587400	0.56461700	C	2.42906000	0.62281800	1.38220800
H	4.56334000	-2.25080000	0.12056100	C	3.36247000	0.88710200	0.34235100
H	2.75237700	-1.68883200	-1.53720600	C	3.29664600	2.09212500	-0.35735400
H	4.29227200	-0.92299200	-1.89158500	C	2.33118600	3.04588100	-0.01398800
H	2.74538500	0.60373800	1.82471400	H	0.68389700	3.56137000	1.28206400
H	0.28595200	-1.22162500	2.14803400	H	0.78819900	1.42760300	2.55704000
H	2.05846500	2.51787800	-1.38719700	H	2.59930500	-0.22720000	2.04408300
C	-3.18249600	-1.99150700	0.56195500	H	4.13014900	0.15355500	0.11267000
C	-2.59016000	-1.07921500	1.43093800	H	4.00303000	2.29392800	-1.15601100
C	-2.48527900	0.27911600	1.06186300	H	2.29030000	3.98524500	-0.55694800
C	-3.02126100	0.71198500	-0.17471700	H	-5.12908200	2.66809700	-1.48884100
C	-3.61377800	-0.21228300	-1.03788800				
C	-3.69158800	-1.55742100	-0.66888100				
H	-3.26685200	-3.03638300	0.84412900	c-7			
H	-2.24319300	-1.40312600	2.40851400	C	1.26646400	-1.03269100	0.11299900
H	-2.17909800	1.02211700	1.79645600	In	-0.42470500	0.36219700	0.27292400
H	-3.00410000	1.76845300	-0.42603500	Cl	-1.44744000	0.02532300	2.31760700
H	-4.02739900	0.11838800	-1.98534600	C	2.45514700	-0.91422900	-0.54455200
H	-4.15903100	-2.27304400	-1.33857100	C	2.99574900	0.32428700	-1.23270900

C	3.94691000	0.98895300	-0.21908500	H	-2.48946600	-0.38011700	1.81238100
C	4.73826800	-0.14592000	0.51142200	H	-2.62692700	1.10779800	0.86910600
C	3.84110400	-1.33872500	0.64264400	In	0.35846400	0.36123800	0.00418800
C	3.48139300	-2.12463200	-0.50764900	Cl	0.72480300	-0.49890300	2.13058500
Cl	0.08875400	2.50670900	-0.48109700	Cl	-0.03471000	2.62684900	-0.34245400
H	5.60820200	-0.42980500	-0.09419700	H	-2.11748800	-2.85341500	-1.05672500
H	5.09099100	0.18756500	1.48984900	C	3.30524100	-1.90819600	-0.36180400
H	3.35350600	1.53466100	0.52178800	C	4.05539500	-1.07451900	0.47654500
H	4.63457100	1.69714600	-0.68840700	C	3.98562200	0.31657500	0.35191300
H	3.52225700	0.05069200	-2.15399500	C	3.16271500	0.88809400	-0.61951700
H	2.18312800	1.00422800	-1.50018800	C	2.38494900	0.05502000	-1.46269800
H	3.46434700	-1.63351800	1.61828700	C	2.47936600	-1.35263800	-1.33716900
H	4.14643800	-2.09571800	-1.36876100	H	3.37762800	-2.98639300	-0.26061300
H	1.13772100	-1.95053600	0.69294600	H	4.69962500	-1.51379200	1.23204000
C	-2.94968800	0.61850900	-1.23510900	H	4.57588500	0.95302200	1.00309700
C	-1.96311100	-0.32281100	-1.61857300	H	3.11922400	1.96603100	-0.74362400
C	-2.09740600	-1.67800300	-1.22929100	H	1.87720400	0.49263100	-2.32283300
C	-3.17671600	-2.06895400	-0.43902800	H	1.92665600	-1.99324700	-2.01885000
C	-4.13693000	-1.12599900	-0.05301900	H	-1.21078600	-0.79640600	-2.07957600
C	-4.02652600	0.21141000	-0.44690000				
H	-2.86338800	1.64969000	-1.56415000				
H	-1.21899500	-0.04205800	-2.36418500	c-10			
H	-1.37206800	-2.41123200	-1.57121300	C	-1.33293300	-1.01365200	-0.67795900
H	-3.28087100	-3.10546200	-0.13437400	In	0.23125200	0.23988800	0.27213600
H	-4.97756000	-1.43734200	0.55949900	Cl	-0.35558100	2.49858000	0.32407200
H	-4.77939200	0.93237600	-0.14540600	C	-2.62655900	-1.26066700	0.20554200
H	3.01136300	-3.09007800	-0.33833600	C	-3.25581400	-0.07230300	0.89714900
				C	-3.99077500	0.71953000	-0.20213700
				C	-3.08662000	0.70636200	-1.47478000
				C	-2.37989400	-0.61409100	-1.56936400
c-9				C	-3.15064200	-2.51071300	0.21875500
C	-2.96927200	0.06700100	0.93763000	Cl	1.05686900	-0.83350900	2.14207500
C	-2.63007900	-0.64779600	-0.37292300	H	-3.67818400	0.88824100	-2.37518700
C	-3.76376600	-0.73266400	-1.15912600	H	-2.33448500	1.49860600	-1.37642200
C	-4.94799400	-0.13399300	-0.49820300	H	-4.21086700	1.74687200	0.09872500
C	-4.51629100	-0.00228100	0.98668500	H	-4.93712100	0.22099300	-0.43667000
C	-1.73821800	-2.05023000	-0.42828300	H	-3.94976600	-0.41020600	1.67246800
C	-1.19314800	-0.84083000	-0.99012000	H	-2.50123400	0.55336900	1.38564500
H	-1.54750200	-2.32332000	0.60782900	H	-2.68726100	-1.30352800	-2.35754600
H	-3.78138400	-1.17364000	-2.15419800	H	-3.93923900	-2.77918000	0.91773800
H	-5.12111700	0.85251100	-0.96707200	H	-2.77171300	-3.30413700	-0.41912400
H	-5.86676100	-0.70594900	-0.67358700	H	-0.89523300	-1.97591900	-0.95317100
H	-4.95817500	0.86858900	1.47422600	C	4.06286500	-0.87992100	-0.14433200
H	-4.84003000	-0.89131000	1.53739000	C	3.23544700	-1.64459200	-0.97608600

C	2.20640000	-1.03031900	-1.68695500	H	-0.17734600	-1.43736500	2.06667200
C	1.98585900	0.36188800	-1.54766900				
C	2.84212300	1.12797800	-0.71783300				
C	3.86964700	0.49890800	-0.01370200	c-12			
H	4.86533900	-1.36367200	0.40411500	C	-2.14225600	-0.17153300	-1.28702300
H	3.40528900	-2.71177500	-1.07758700	In	0.23733200	-0.41164100	0.12964100
H	1.59069100	-1.60848100	-2.37057600	Cl	1.14814300	-1.87784200	-1.39442900
H	1.29727100	0.87380200	-2.22029700	C	-3.39579300	-0.28603000	-0.57302800
H	2.69719900	2.20155200	-0.64344900	C	-3.92315900	0.95348400	0.12841200
H	4.52146000	1.08230900	0.62839400	C	-2.79465300	1.87036900	0.63150600
				C	-1.78660400	2.19384700	-0.48409400
				C	-1.32275800	0.94494000	-1.21330800
c-11				C	-4.05355700	-1.46661600	-0.61741800
C	-4.19244800	-1.29595000	-0.39804900	Cl	-0.62550200	-0.97261000	2.19478300
C	-3.13625800	-0.62923800	0.47744000	H	-2.24849500	2.85267000	-1.23471100
C	-3.51195700	0.65064600	0.78613000	H	-0.93564200	2.76089000	-0.08678800
C	-4.83038700	1.00755800	0.19054600	H	-4.54847700	1.50898300	-0.58488500
C	-5.41688400	-0.35470500	-0.26246700	H	-4.57734900	0.66530600	0.95670500
C	-1.91967200	-1.25422200	0.86873600	H	-0.55428500	1.04632300	-1.98489200
C	-0.84753500	-0.71522800	1.59909200	H	-3.66124700	-2.31936400	-1.16565400
H	-1.00622600	0.20177600	2.16753500	H	-5.00344000	-1.60963400	-0.10985500
H	-2.92280700	1.35208000	1.37001000	H	-1.84388700	-1.00445800	-1.92489800
H	-5.46776600	1.56557600	0.88733900	H	-3.22058900	2.80006500	1.02033400
H	-4.65144600	1.69127100	-0.65715200	H	-2.27866700	1.38526900	1.46895600
H	-6.09253100	-0.73319200	0.51109000	C	4.07226100	0.33744800	-0.57057000
H	-5.98968500	-0.27592400	-1.18872500	C	3.77168700	-0.11145100	0.72058000
H	-3.83720800	-1.34720000	-1.43608200	C	2.66990600	0.40976200	1.39881700
H	-4.41303300	-2.32184600	-0.08546500	C	1.84178700	1.37595900	0.76449100
In	0.50505000	0.07195600	-0.12383400	C	2.17610900	1.83826200	-0.53473100
Cl	-0.51354000	2.05853700	-0.76475400	C	3.27953900	1.30743900	-1.19798200
Cl	1.10352800	-1.61325600	-1.57377900	H	4.93408700	-0.06815400	-1.09169800
H	-1.78695100	-2.28039100	0.52114200	H	4.40066500	-0.85452200	1.19990500
C	3.02749100	1.43000500	-0.00126000	H	2.44513400	0.09585100	2.41413800
C	4.00124400	0.68399100	-0.66689600	H	1.10388000	1.91397300	1.36083900
C	4.41517700	-0.54636500	-0.14518200	H	1.58428600	2.62392200	-0.99619500
C	3.86317400	-1.04642500	1.04143200	H	3.53482200	1.65569400	-2.19364300
C	2.88961100	-0.31508300	1.71780100				
C	2.44394400	0.92391400	1.19090900				
H	2.72197900	2.40241300	-0.37667300	c-I			
H	4.44346100	1.06516500	-1.58160500	C	0.69633200	-1.22315600	0.17782400
H	5.17638600	-1.12014700	-0.66488900	C	-0.35779400	-0.15202400	-0.06336400
H	4.20355700	-1.99670600	1.44006800	C	0.21222800	1.06446800	-0.13235500
H	2.48859400	-0.67481900	2.66127000	C	1.70629100	1.02010400	0.07493600
H	1.82076800	1.58031700	1.79899000	C	2.03464900	-0.48826500	-0.08146700

C	-1.78200900	-0.48581800	-0.16898800	H	4.87054900	0.65230500	-0.68157700
C	-2.80857200	0.32125100	0.13250600	H	5.01235300	-1.73439500	-0.02249000
H	-2.65545400	1.32428700	0.52310700	H	-3.58401000	-2.79986800	1.25718100
H	-0.33059800	1.99073500	-0.30100100				
H	2.25784300	1.64691100	-0.63758700				
H	1.97056700	1.39183200	1.07798100	c-TS2			
H	2.36231600	-0.68129600	-1.10948000	C	1.33094400	0.08741500	-0.98550000
H	2.83817500	-0.82041000	0.58335300	In	-0.50991000	0.49417100	0.17210700
H	0.62829700	-1.59529000	1.21146500	C	2.52645900	-0.41827000	-0.51013800
H	0.56310400	-2.09843700	-0.47176800	C	2.83042800	-1.01482300	0.85597300
H	-2.00293400	-1.49747000	-0.51337600	C	4.36851100	-0.97246200	0.99533800
H	-3.83805700	-0.00022400	0.00275100	C	4.91279200	-0.98805700	-0.45157700
				C	3.84635000	-0.28270300	-1.29008700
				C	3.36420000	1.04311100	-0.86620800
c-TS1				Cl	-0.76543800	-0.85307600	2.03148900
C	-1.23257300	-0.86001900	0.38235200	Cl	-0.63690400	2.81308400	0.29787100
Cl	1.85437300	-0.10163400	2.25315400	H	5.89102300	-0.50807700	-0.54519200
C	-2.32007800	-0.22211600	0.24246500	H	5.01094700	-2.01308700	-0.82443100
C	-3.17849900	0.92652900	-0.01668100	H	4.74968200	-1.80974600	1.58382700
C	-5.22944900	-0.39760700	-0.69215500	H	4.67847800	-0.05922400	1.51462000
C	-4.47721700	-1.62575100	-0.28217800	H	2.29901000	-0.52218000	1.67551500
C	-4.16196500	-1.91736900	0.99806300	H	2.47012600	-2.05117300	0.82569900
Cl	0.09802000	2.55751300	-0.30747900	H	3.81448200	-0.46265900	-2.36263700
H	-5.83615400	-0.02724100	0.14213900	H	3.64354700	1.48453500	0.08560000
H	-5.90697100	-0.61350800	-1.52537100	H	1.33005400	0.37543500	-2.03923300
H	-3.65481600	1.25184100	0.91725300	C	-3.71046800	-1.87135200	-0.03777500
H	-2.47975800	1.72875100	-0.31304700	C	-2.72535100	-2.27667600	-0.94645700
H	-4.11718500	-2.27815100	-1.07772800	C	-2.03587500	-1.32424600	-1.69488000
H	-4.54468700	-1.32906300	1.82926800	C	-2.31861000	0.05264400	-1.51634700
In	0.63689200	0.39964600	0.36839300	C	-3.32954300	0.44906400	-0.60514400
C	-4.22616000	0.70024600	-1.12355000	C	-4.01219600	-0.51678100	0.13547100
H	-3.72223300	0.41716300	-2.05433300	H	-4.24717500	-2.61831100	0.53902700
H	-4.75148000	1.64196600	-1.30861700	H	-2.50896700	-3.33203800	-1.07773600
H	-1.04842700	-1.90122600	0.61249000	H	-1.30235400	-1.63374900	-2.43453600
C	3.04157700	-2.23273400	-0.73504400	H	-1.90981100	0.78800600	-2.20998200
C	1.88245300	-1.76096800	-1.34755100	H	-3.57128300	1.50231900	-0.49803100
C	1.78090700	-0.39379600	-1.70805900	H	-4.78144000	-0.21514000	0.83885400
C	2.87873500	0.47576000	-1.47909300	H	2.97322600	1.73938400	-1.59974200
C	4.03247800	-0.01219700	-0.86484100				
C	4.11063800	-1.35972000	-0.49717700	c-TS4			
H	3.12163200	-3.27782700	-0.45350900	C	-2.98341800	0.18023100	0.90038900
H	1.06475100	-2.43929800	-1.57496400	C	-2.67228700	-0.52632700	-0.40039700
H	0.95722500	-0.05857800	-2.33878300	C	-3.80116300	-0.82523400	-1.09504000
H	2.81575200	1.51297900	-1.79492600	C	-5.02236800	-0.27591700	-0.41982700

C	-4.52813400	0.07262100	1.01077600	H	-4.83698900	-0.24940300	0.96578600
C	-1.37246100	-2.23141900	-0.55667300	H	-3.36232900	-1.98621900	1.62184000
C	-1.29145100	-0.88974200	-0.95180900	H	-1.96030700	-0.92083400	1.74644200
H	-1.26858100	-3.07458800	-1.24277400	H	-3.02130000	0.03820900	-2.26367600
H	-1.56200600	-2.48737000	0.48331000	H	-4.47270800	-2.08806100	-0.79404500
H	-3.81928700	-1.31426400	-2.06521600	H	-3.24184700	-2.18140000	-2.17082300
H	-5.38288700	0.60870500	-0.96637100	H	-1.06312000	-1.16033000	-1.87685500
H	-5.85204700	-0.99337600	-0.42957600	C	2.21619000	-1.48645600	-1.31159800
H	-4.97685100	0.99052700	1.39588200	C	3.07697100	-2.04238900	-0.36727500
H	-4.79456900	-0.73512300	1.69921600	C	3.92630100	-1.21408600	0.37625700
H	-2.46576800	-0.25593800	1.76383000	C	3.92111000	0.17145100	0.18719600
H	-2.64442300	1.22522800	0.82727700	C	3.06299100	0.74261500	-0.75300300
In	0.35564900	0.35595100	0.03250800	C	2.18601400	-0.08294800	-1.49906000
Cl	0.74969900	-0.42800300	2.16973400	H	1.58813500	-2.12824900	-1.92366300
Cl	-0.13302500	2.55549400	-0.50508400	H	3.09919600	-3.11714500	-0.21784200
H	-1.16627600	-0.72745900	-2.02509300	H	4.59757100	-1.65350700	1.10776600
C	2.50668700	-1.41069100	-1.23510700	H	4.58784500	0.80328700	0.76492200
C	3.38519800	-1.84957700	-0.24724800	H	3.06500400	1.81479100	-0.92441700
C	4.11290600	-0.91847900	0.50492700	H	1.64584500	0.34277100	-2.34547900
C	3.96973700	0.45437500	0.27926800				
C	3.09435500	0.90970500	-0.70778900				
C	2.33480600	-0.02263200	-1.46184700	c-TS6			
H	1.97351600	-2.12750400	-1.85368900	C	-1.37076000	-0.88218100	-0.84819300
H	3.51797300	-2.91206600	-0.06991500	In	0.22157300	0.25208000	0.23559000
H	4.79884700	-1.26757800	1.27069500	Cl	-0.33914500	2.50994700	0.43153800
H	4.54599600	1.16615600	0.86135500	C	-2.53348400	-1.34901900	0.11275200
H	2.99787400	1.97139700	-0.91514000	C	-3.20643100	-0.28327000	0.93743300
H	1.79378600	0.32280400	-2.34349500	C	-4.03505000	0.58719800	-0.02569000
				C	-3.18117500	0.87592000	-1.30664200
				C	-2.37988900	-0.32010100	-1.68213900
c-TS5				C	-2.93678600	-2.63329700	0.03767400
C	-1.39305100	-0.69709100	-0.94345000	Cl	0.93156500	-0.98792500	2.04792300
In	0.24583500	0.37824300	0.05581900	H	-3.82241900	1.19018200	-2.13302500
Cl	0.00446700	2.66935100	-0.31989300	H	-2.48210100	1.68971900	-1.06531200
C	-2.46832900	-1.46757900	-0.26726800	H	-4.34264800	1.53206800	0.42970800
C	-2.85568800	-1.13431600	1.15844000	H	-4.93633700	0.04199000	-0.32414300
C	-3.80367400	0.10010100	1.06154800	H	-3.85617800	-0.74466300	1.68735000
C	-3.41935300	0.89797000	-0.20775600	H	-2.47414100	0.33140900	1.47479800
C	-2.78676200	-0.05987100	-1.20693100	H	-2.61643200	-0.81663600	-2.62668700
C	-3.46912200	-1.87235100	-1.15523600	H	-3.64338800	-3.03444900	0.75969700
Cl	0.75413200	-0.37299700	2.19179000	H	-2.52987700	-3.33131800	-0.68789300
H	-4.28881700	1.38922800	-0.65247300	H	-0.89876000	-1.75446400	-1.30705600
H	-2.68503500	1.68353000	0.00807100	C	2.26329200	-0.92021900	-1.71808400
H	-3.75484800	0.71112000	1.96586000	C	3.24835600	-1.59697800	-1.00193600

C	4.04124300	-0.90372900	-0.07884400	C	-0.31123300	3.08457500	-0.78288500
C	3.85756100	0.46555400	0.13787300	C	-1.62535600	2.28571400	-0.82132300
C	2.87386300	1.15689900	-0.57039700	C	2.16212100	0.43904200	-0.16203000
C	2.05055400	0.46224600	-1.49242800	In	-0.25481500	-0.47706100	0.37980600
H	1.67748400	-1.44076300	-2.47081700	Cl	-1.13205500	0.12941600	2.41469200
H	3.41147600	-2.65681800	-1.16945900	Cl	0.31746300	-2.59089600	-0.29889700
H	4.80993600	-1.43581400	0.47320900	H	-2.11035700	2.28079200	0.16297600
H	4.48345300	0.99367300	0.84980900	H	-2.31348500	2.82099400	-1.49236200
H	2.73886400	2.22521000	-0.43031500	H	0.17047700	3.06715700	-1.76777200
H	1.40506100	1.03022500	-2.16289600	H	-0.56265200	4.13023500	-0.57879400
d-4				H	0.23170700	2.65011500	1.28846200
C	1.62423500	0.85476100	-0.46042500	H	1.52154400	3.37797700	0.34003600
C	1.35541000	1.88612600	0.34476200	H	-0.90060600	0.73369100	-2.25345300
C	-0.52422300	-1.46326500	0.21063300	H	-3.13074600	0.05433900	-0.25644900
C	0.76383200	-2.01562800	0.63955000	C	3.20891900	-0.55211100	-0.42953000
C	1.95563300	-1.69313300	-0.29368400	H	3.26926000	-1.25769600	0.40717000
C	2.55375400	-0.28139700	-0.12891700	H	2.94425400	-1.13451700	-1.31931500
C	-1.60112800	-1.05408500	-0.16140700	C	-2.63637400	-1.37749000	-1.87095000
H	2.92406900	-0.16242900	0.89889000	H	-2.71293700	-2.26484400	-1.23458500
H	3.43893100	-0.22540800	-0.78213100	H	-3.60109500	-1.28307300	-2.39024400
H	1.64630200	-1.85002500	-1.33474300	H	-1.85737700	-1.53751400	-2.62071700
H	2.75097000	-2.42220600	-0.09068400	C	4.57339400	0.15291800	-0.63125000
H	0.99817000	-1.66678500	1.65607100	H	4.86887200	0.70744700	0.26303600
H	0.66606200	-3.10798800	0.71385300	H	5.32864000	-0.61235300	-0.82936900
H	1.15378500	0.81768200	-1.44496100	H	4.54454300	0.83911400	-1.48168800
H	1.82198300	1.91747800	1.33161800				
C	0.43972100	3.02932700	0.01103000	d-6			
H	-0.39972600	3.08626700	0.71838200	C	5.11264100	-0.54648500	0.30400900
H	0.96268000	3.99405300	0.06827300	C	5.16659700	-1.72842700	-0.32113900
H	0.02451800	2.92953100	-0.99784800	C	1.21615400	1.46667500	0.00846900
C	-2.90060600	-0.52541900	-0.58460000	C	2.42118500	0.77486700	-0.44285000
H	-3.62331500	-1.34930900	-0.66995400	C	3.68816700	1.54990100	0.01776100
H	-2.81143600	-0.09999900	-1.59423100	C	4.97015900	0.78616100	-0.38046200
C	-3.45918000	0.54543300	0.37169200	C	0.25388700	2.10727200	0.44114200
H	-2.77517900	1.39735600	0.44237300	In	-1.07116900	0.32127700	-0.58721000
H	-4.42945800	0.90913300	0.01496900	Cl	-0.04382500	-1.39045100	-1.71612500
H	-3.59304000	0.13633600	1.37831400	Cl	-2.85664000	1.62963300	-1.15495100
d-5				H	4.99790500	0.65830700	-1.47019500
C	-1.54668700	0.87895500	-1.38238200	H	5.81960600	1.43260000	-0.11964300
C	-2.43127900	-0.12308200	-1.07784400	H	3.65454200	1.68305500	1.10550100
C	1.34644600	1.33500700	0.05833600	H	3.68907100	2.54732100	-0.43457400
C	0.70071100	2.65135100	0.29720100	H	2.45566600	-0.24382800	-0.03763000
				H	2.41525100	0.68499800	-1.53561400

H	5.19377800	-0.51883500	1.39313300	H	3.10499600	2.00946000	0.96266900
H	5.10359300	-1.74703600	-1.41118700	C	3.84628000	0.11838100	2.60458600
C	5.34869600	-3.05874800	0.35002300	H	4.18955400	1.12357400	2.35726100
H	4.53256900	-3.74831600	0.09651000	H	2.95600400	0.18705200	3.23620900
H	6.27648800	-3.53989300	0.01429600	H	4.63372700	-0.35719500	3.20129000
H	5.39335700	-2.96165500	1.43979200	C	2.04654100	2.88657400	-0.70768300
C	-1.59469300	-2.54983300	1.64941500	H	2.65787600	2.47613600	-1.51739600
H	-0.97826200	-2.93047800	0.83475500	H	1.02563100	3.02883500	-1.07939400
H	-1.33899600	-3.03685200	2.59227400	H	2.43466200	3.87674700	-0.45285100
C	-3.07713800	-2.62870200	1.37132200	C	-4.16069900	-1.33284800	1.27845900
H	-3.34803400	-3.68146500	1.24983400	H	-5.13237400	-1.01650200	1.67123000
H	-3.67541800	-2.18819000	2.16967600	H	-4.05903900	-2.41142700	1.40815500
Cl	-3.51998000	-1.78720700	-0.16500000	C	-3.09796500	-0.56719600	2.03093500
Cl	-1.03950700	-0.79621700	1.89927200	H	-3.11860700	0.50612300	1.84068400
C	-0.55658200	3.18200600	1.07388300	H	-3.13477400	-0.77641500	3.10144900
H	-1.22110200	3.61621500	0.31967800	Cl	-4.14367000	-0.97945700	-0.48359800
H	-1.20261900	2.74992100	1.84730500	Cl	-1.38524200	-1.10973500	1.54256400
C	0.35556200	4.26465200	1.68398000				
H	0.98030500	4.72933100	0.91627900				
H	-0.27124800	5.04000000	2.13419300	d-9			
H	1.00221800	3.84832100	2.46127900	C	-1.23709500	1.61182300	1.46713400
				C	-1.72885300	1.23113200	0.07186200
				C	-2.46515300	2.26355300	-0.45387600
d-7				C	-2.57463900	3.41466000	0.48672900
C	1.60553300	0.60329400	0.25289300	C	-2.11824200	2.82647900	1.84582400
In	-0.48993800	0.57852800	-0.46556000	C	-2.57077500	-0.33069100	-0.17239000
Cl	-1.71163100	2.40007600	0.27712800	C	-1.27552300	-0.01818600	-0.74457300
C	2.32963300	-0.56143100	0.34993500	H	-2.59010400	-0.67182500	0.86418500
C	1.92340500	-1.90327400	-0.26321700	H	-2.90096800	2.27205200	-1.44840700
C	2.91289000	-2.12968300	-1.42164600	H	-1.90224700	4.21426900	0.13107400
C	4.29185700	-1.60586700	-0.93626400	H	-3.57876100	3.85514600	0.49338300
C	4.03848800	-0.48899000	0.06226300	H	-1.58706000	3.55404000	2.46270000
C	3.61379400	-0.76471700	1.39874500	H	-2.99431700	2.49226300	2.41091400
Cl	-0.86224900	-0.46383600	-2.48600400	H	-1.29933300	0.79485000	2.19265500
H	4.85398200	-2.40458000	-0.43899700	H	-0.17932500	1.89779900	1.38780700
H	4.89851400	-1.24101500	-1.76860600	In	0.39530700	-1.15234200	0.15203700
H	2.58526800	-1.54241900	-2.28598100	Cl	-0.21494400	-2.08431900	2.18488100
H	2.96472500	-3.17691200	-1.73044700	Cl	1.77413800	-2.19298200	-1.38428300
H	1.98187600	-2.70989700	0.47630400	C	-3.86383500	-0.56018200	-0.90481600
H	0.89601500	-1.88712200	-0.63611100	H	-4.69792800	-0.17260800	-0.31039200
H	4.37597000	0.51776100	-0.16970500	H	-3.88133800	-0.06441500	-1.87805400
H	3.55679400	-1.82118500	1.65766600	C	-1.13603100	0.12017400	-2.25957800
C	2.09326400	1.98631200	0.55412300	H	-0.25245000	0.71281500	-2.51060300
H	1.42547100	2.42797100	1.30868700	H	-1.00713000	-0.86864100	-2.71319000

H	-2.00187600	0.58445200	-2.74265000	H	-0.95334600	3.10194100	2.67855200
C	-4.04293200	-2.08655100	-1.09441500	C	4.00640400	0.65742100	-1.06784400
H	-4.04126000	-2.61504700	-0.13560200	H	5.05675900	0.78753600	-1.34698400
H	-5.00396200	-2.27632400	-1.58100000	H	3.41491200	0.48844000	-1.96884600
H	-3.25493300	-2.50936500	-1.72557700	C	3.58416800	1.89982300	-0.32145900
C	3.50323000	2.10159000	-0.52931600	H	4.06906000	1.99954200	0.64878000
H	3.56647500	2.84683700	0.26436100	H	3.73111300	2.79553800	-0.92737700
H	4.28103200	2.29615700	-1.27281400	Cl	1.76482400	1.96312200	0.07472900
C	3.68058300	0.69338400	-0.01064500	Cl	3.89899000	-0.81787300	-0.04609900
H	3.55122000	-0.07327100	-0.77539600				
H	4.64865300	0.57993200	0.48136900				
Cl	1.91255200	2.33840900	-1.36024400	d-11			
Cl	2.45361700	0.29257000	1.30928100	C	4.40541500	-0.63804200	-0.64321700
				C	3.33328000	-0.20269000	0.35276000
				C	3.27146600	-1.08519600	1.39180300
d-10				C	4.23505900	-2.21451300	1.24805600
C	-1.71293200	0.56914500	0.52155800	C	5.17238700	-1.76395500	0.09934300
In	0.23561400	-0.42478100	0.09665900	C	2.52405900	0.98440000	0.21815600
Cl	0.75690300	-0.93246600	-2.10079000	C	1.34068900	1.20856500	0.98276600
C	-2.99561600	-0.03088100	-0.76786400	H	1.20031600	0.49156700	1.79933700
C	-2.72374600	-1.42451600	-1.33678200	H	2.60892900	-1.00078200	2.24902100
C	-2.39565400	-2.33207800	-0.13318300	H	4.75596300	-2.44143900	2.18603900
C	-2.99817400	-1.62771600	1.09814600	H	3.66697500	-3.12568900	0.99568100
C	-2.96220300	-0.12304600	0.79532700	H	6.09965700	-1.36501400	0.52161700
C	-3.46938400	0.99729700	-1.53251200	H	5.44447600	-2.58717700	-0.56435800
Cl	0.90638800	-1.56678000	1.98600800	H	3.92782800	-1.00908100	-1.56054300
H	-4.04584800	-1.91725400	1.22936800	H	5.07055600	0.17902400	-0.93921200
H	-2.46962800	-1.86231000	2.02699700	In	-0.16351300	0.29412700	-0.49562100
H	-3.65394500	-1.75758200	-1.81189300	Cl	0.37177300	-1.82085500	-1.27813400
H	-1.94976200	-1.43429700	-2.10885900	Cl	-1.23526300	1.83063600	-1.82712700
H	-3.71706000	0.47776000	1.30954000	C	0.86103700	2.62523300	1.34474400
H	-2.79554600	-3.34113700	-0.26005400	H	1.64233100	3.07405800	1.97391900
H	-1.31295800	-2.48322400	-0.01553400	C	2.96910400	1.99856300	-0.79615200
H	-3.50053100	0.78829200	-2.60377000	H	3.88036300	2.49123300	-0.42558500
C	-4.02811200	2.32414800	-1.15174500	H	3.24736400	1.51703700	-1.73959000
H	-4.34276300	2.38709700	-0.10937600	H	2.22698000	2.77261300	-0.99278000
H	-3.30766400	3.13054400	-1.35547000	H	0.77997600	3.26097200	0.45736800
H	-4.89598900	2.53138500	-1.78890900	C	-0.46785800	2.64788000	2.10748900
C	-1.61362200	2.01664500	0.92477000	H	-0.68014600	3.66017700	2.46266000
H	-0.96526500	2.59234800	0.25581100	H	-1.31373000	2.35528000	1.47228900
H	-2.58726000	2.51009400	0.94908000	H	-0.44532000	1.98925400	2.98362400
C	-1.04332900	2.05592400	2.37124800	C	-4.18926300	-1.35828900	-0.45023700
H	-1.71259900	1.54828800	3.07187900	H	-3.87078200	-0.63751700	-1.20599000
H	-0.05436600	1.59621100	2.45738400	H	-4.65330500	-2.21253700	-0.95486000

C	-3.02932800	-1.89842400	0.35279200	Cl	-3.42193000	-0.97080700	-1.02473200
H	-3.34048500	-2.52696100	1.18669500				
H	-2.29360000	-2.40994100	-0.27113200				
Cl	-2.07876200	-0.52865700	1.20114300				
Cl	-5.44001300	-0.58162300	0.57478900	d-I			
				C	1.50709100	0.60639500	-0.96400100
				C	0.55583200	-0.19905300	-0.08388400
d-12				C	1.25188700	-1.00960700	0.73251800
C	2.29131000	-0.12456100	0.82202900	C	2.74373900	-0.92077000	0.52406800
In	-0.37804400	0.00912000	-0.36401400	C	2.89763100	0.36828200	-0.32357100
Cl	-0.06175900	-2.14439600	-1.13080700	C	-0.92031300	-0.11233500	-0.19142400
C	3.35001500	0.37289400	-0.05521300	C	-1.66017300	-1.23821400	-0.13282500
C	3.56549400	1.88623100	-0.05496600	H	-1.11719700	-2.18012200	-0.05579200
C	2.24869300	2.66630200	-0.11869600	H	0.79852700	-1.68372700	1.45437500
C	1.33647700	2.26022100	1.04007800	H	3.30807900	-0.87491900	1.46454300
C	1.23899300	0.74082900	1.20680500	H	3.11608600	-1.80800100	-0.01277800
C	4.15593300	-0.40190900	-0.83712000	H	3.14076200	1.20814400	0.33765300
Cl	-1.07725400	1.81821200	-1.60632300	H	3.69922500	0.29853000	-1.06577000
H	1.74012400	2.64879400	1.98652700	H	1.46310100	0.23499800	-1.99946300
H	0.34421200	2.71111200	0.93279500	H	1.25571600	1.67264600	-1.01194700
H	4.10227700	2.16433700	0.86361400	C	-3.15539600	-1.38397700	-0.16596600
H	4.21506900	2.16458900	-0.88973500	H	-3.68661600	-0.43083300	-0.22941300
H	0.69928300	0.41938000	2.10029500	H	-3.47009600	-2.00175700	-1.01879000
H	4.89860000	0.15985200	-1.40334600	H	-3.51058900	-1.90129100	0.73643900
H	2.44573300	3.74211900	-0.07134400	C	-1.50542400	1.27939900	-0.35542000
H	1.74944000	2.48397200	-1.07838300	H	-1.02920600	1.77084200	-1.21498700
C	4.19609800	-1.87724200	-1.09482500	H	-2.57066800	1.22180800	-0.59704900
H	4.73139000	-2.07491200	-2.02687600	C	-1.31450200	2.16256600	0.89063100
H	4.74267000	-2.40014600	-0.29679300	H	-0.25509300	2.25547400	1.15467600
H	3.20558100	-2.33536800	-1.16951700	H	-1.71221800	3.17012200	0.72220600
C	2.35778100	-1.52946500	1.38100700	H	-1.83203900	1.73196500	1.75534700
H	2.17197200	-2.23817800	0.56490600				
H	3.40211500	-1.70052900	1.67102300	d-TS1			
C	1.43633800	-1.87862400	2.55383600	C	1.51235000	0.57495900	-0.17750200
H	1.58408600	-1.21167700	3.40991800	Cl	-1.79988000	2.43762100	0.02577600
H	0.37627500	-1.86280200	2.27702100	C	2.20533800	-0.42822800	0.25596300
H	1.65790200	-2.89641600	2.88678300	C	2.18241300	-1.71814500	0.98426900
C	-3.93214700	0.10535100	1.44713800	C	3.90082100	-2.51546200	-0.62521500
H	-4.17740500	-0.89128000	1.81236800	C	4.01838000	-1.03578700	-0.91421300
H	-4.41790500	0.87365900	2.05150400	C	4.60720100	-0.16611300	-0.03229200
C	-4.23613100	0.28939800	-0.02122000	Cl	-1.00298700	-0.71007000	2.45643800
H	-5.31349100	0.17048100	-0.16628000	H	4.69451400	-2.80738000	0.07099000
H	-3.92309000	1.26389300	-0.39918300	H	4.05056000	-3.08730800	-1.54599000
Cl	-2.13104600	0.31497200	1.83058400				

H	2.87834500	-1.69778400	1.83187900	H	-2.15377100	-1.71891800	1.19725600
H	1.18013600	-1.84602400	1.41346500	H	-3.37957900	-0.81034600	2.08634900
H	3.78138600	-0.68421600	-1.91741500	H	-4.21186000	1.45168700	-0.84500900
H	4.88667800	-0.56387600	0.94437500	H	-2.25723200	-0.90009400	-1.47864000
C	1.80281500	1.73028900	-1.11072200	C	-2.24948800	0.97054100	-2.59995700
H	2.71801900	1.51465000	-1.66989000	H	-1.20829300	0.87520200	-2.91959800
H	0.99566500	1.79037800	-1.85077200	H	-2.88756000	0.54117000	-3.37943300
C	1.92109400	3.08713200	-0.39212300	H	-2.49909300	2.02542800	-2.49237500
H	0.97732300	3.37806500	0.07836200	C	-1.49596300	2.36737100	-0.09050800
H	2.69726700	3.06987900	0.37821900	H	-0.75687400	2.64226100	-0.85104900
H	2.17707500	3.86323700	-1.11970900	H	-2.45303300	2.79705700	-0.40738200
In	-0.57966100	0.56016600	0.58475100	C	-1.10613800	2.99865400	1.25790900
C	5.08631300	1.21998000	-0.30724700	H	-0.13427800	2.64678800	1.62063100
H	4.86330900	1.56183300	-1.32014000	H	-1.04546300	4.08573000	1.14857900
H	4.69337600	1.93960300	0.41867400	H	-1.85041900	2.77863900	2.03049300
H	6.17795700	1.22548200	-0.17800200	C	4.55621400	0.26366200	-0.94999400
C	2.52874700	-2.84846800	0.00742700	H	4.63258300	0.39488800	-2.03052600
H	1.75565700	-2.91185900	-0.76647200	H	5.55068700	0.37950700	-0.50660800
H	2.56265300	-3.81253900	0.52270600	C	3.65888900	1.29874400	-0.31398100
C	-3.09881400	-0.36189600	-2.11465900	H	4.01714900	2.31259900	-0.50028400
H	-3.10741800	-0.47436600	-3.20026100	H	3.48715500	1.13236200	0.74967800
H	-3.15530500	0.68915400	-1.83085400	Cl	4.00634600	-1.41582000	-0.62813600
C	-4.15692000	-1.21861200	-1.45997400	Cl	1.95928900	1.29673700	-1.08442300
H	-5.12858800	-0.89270900	-1.84460700				
H	-4.02331400	-2.27819900	-1.68307000	d-TS4			
Cl	-4.18650400	-1.02542400	0.32702800	C	2.76193000	-1.35704400	0.85133500
Cl	-1.38300200	-0.89871800	-1.63668800	C	2.79763000	-0.24772800	-0.18489600
				C	4.03938900	-0.10701700	-0.70996000
				C	4.99589700	-1.12806200	-0.16473400
d-TS2				C	4.25796700	-1.70206200	1.07305900
C	-1.57657500	0.84300600	0.02966300	C	1.94278800	1.64165200	0.25389000
In	0.29501500	-0.22526000	0.48256600	C	1.58470000	0.59488300	-0.64311600
C	-2.80996400	0.21694200	0.38328900	H	1.97296200	1.39078500	1.31577800
C	-3.04826900	-1.10084800	1.07565000	H	4.31316800	0.59607900	-1.49089400
C	-4.18281900	-1.79598600	0.28711000	H	5.19448000	-1.89508900	-0.92843300
C	-4.92310300	-0.65236000	-0.44940800	H	5.97029400	-0.68802100	0.07972300
C	-3.88074000	0.44805700	-0.58992400	H	4.41913500	-2.77455200	1.19957600
C	-2.48856900	0.15214400	-1.32583300	H	4.61885900	-1.20736900	1.97998700
Cl	1.45114200	0.09735700	2.45741400	H	2.25820500	-1.07151400	1.78367100
Cl	0.21039100	-2.30537800	-0.54484300	H	2.20507100	-2.21319900	0.43607100
H	-5.33835800	-0.96223100	-1.41299100	In	-0.27335300	-0.48818500	0.03674400
H	-5.75458900	-0.26213600	0.14887900	Cl	-0.72727200	-0.16125200	2.28827300
H	-4.84517100	-2.36801500	0.93984300	Cl	-0.63078700	-2.38358600	-1.20825700
H	-3.75047700	-2.50266000	-0.42783500	C	1.47392400	0.90526600	-2.13958000

H	2.37358500	1.38692200	-2.53835700	H	5.65123597	1.75681935	-0.71655165
H	1.31497900	-0.01574800	-2.70800800	H	5.41653198	1.75051286	1.02809435
H	0.63338100	1.57886000	-2.34188000	C	1.30488494	2.87048434	-1.08865831
C	2.23751100	3.06158900	-0.05609900	H	1.10836491	3.93176129	-0.91063601
H	3.17407200	3.34525500	0.44091500	H	0.42950995	2.45525846	-1.60320942
H	2.34303900	3.23490000	-1.12918700	H	2.15204994	2.79091156	-1.77870433
C	1.09935000	3.95279200	0.52514500	C	-3.39519800	1.27033057	1.21249428
H	0.14010200	3.73420700	0.04751600	H	-3.01717798	0.45661041	1.83150205
H	0.99448300	3.81631300	1.60556600	H	-3.57591002	2.16675940	1.80820353
H	1.34884100	4.99996100	0.33381500	C	-4.60784500	0.89430376	0.39399218
C	-4.58679500	0.47496400	-0.08592900	H	-4.89195302	1.68339895	-0.30404060
H	-5.43124900	0.63374900	0.59251900	H	-5.43205599	0.72770455	1.09540814
H	-4.92362900	0.62063100	-1.11339600	Cl	-4.37087196	-0.62063297	-0.54006124
C	-3.50528200	1.45489600	0.30293400	Cl	-1.96119902	1.76222191	0.12589241
H	-3.07707800	1.26109600	1.28657800				
H	-3.85079900	2.48690200	0.22078500				
Cl	-4.06042300	-1.23442400	0.09130500	d-TS6			
Cl	-2.06338000	1.39315100	-0.87750500	C	-1.34777900	0.60266800	0.65132300
				In	0.01523000	-1.06217300	-0.12547200
				Cl	0.89296800	-1.07098500	-2.27177400
d-TS5				C	-1.79365200	1.54987400	-0.52872000
C	1.75925901	0.63583304	0.03898107	C	-2.18572500	0.84800700	-1.81908600
In	-0.21686097	-0.35061998	-0.08461420	C	-2.90639800	-0.49723200	-1.54193700
Cl	-0.81309396	-1.25297743	-2.12499245	C	-3.55423100	-0.46077500	-0.15867000
C	2.90408902	0.03066526	-0.63797011	C	-2.68326200	0.16547800	0.86053600
C	2.78057605	-1.41372162	-1.10403551	C	-1.92300600	2.89606300	-0.43089900
C	2.45477609	-2.28539298	0.15589224	Cl	-0.52051600	-3.08596200	0.85610700
C	2.84528007	-1.48990732	1.42557346	H	-4.52395000	0.05955200	-0.15183200
C	2.91665103	-0.01925921	1.03938987	H	-3.79102600	-1.47319400	0.21707600
C	4.18821901	0.36977314	-0.08825803	H	-2.84123700	1.50956300	-2.39165800
Cl	-0.88766593	-1.31184456	1.92941854	H	-1.30004500	0.66646500	-2.44032200
H	3.81762909	-1.80469240	1.81866737	H	-3.14060600	0.32902100	1.84211600
H	2.11314008	-1.63123957	2.22675743	H	-3.65449500	-0.70674800	-2.31089300
H	3.71969606	-1.72737346	-1.56576861	H	-2.20632300	-1.34219600	-1.60517700
H	1.99649005	-1.49586642	-1.86283753	H	-2.19513500	3.35889600	-1.38006700
H	3.09195902	0.74469758	1.79069709	C	-1.70722200	3.88805700	0.68161900
H	2.97911511	-3.24220695	0.10059697	H	-2.40840100	3.74546800	1.51129600
H	1.39095009	-2.54767501	0.18185418	H	-0.69190800	3.84602400	1.09064500
C	1.59931897	2.15329398	0.23758749	H	-1.86416400	4.89989000	0.30120800
H	0.77821297	2.32519576	0.94302654	C	-0.66413700	1.18446900	1.90901500
H	2.47436196	2.60838487	0.70817761	H	0.30285700	1.61153600	1.62781600
H	4.90132804	-0.45021682	-0.17549626	H	-1.26331300	2.01385000	2.29402700
C	4.88921398	1.70108711	0.06974834	C	-0.48919500	0.16997300	3.05000900
H	4.24548295	2.57165612	-0.03244041	H	-1.44642700	-0.25303900	3.37588800

H	0.15825800	-0.67596400	2.79199100	m-b-5			
H	-0.04037900	0.66441600	3.91634900	In	-1.23115400	0.12146500	0.22028700
C	3.63409100	0.05710600	-0.20461500	Cl	-0.90347900	-1.32652100	2.00945200
H	4.58969900	-0.40845100	0.04410000	Cl	-3.00722600	-0.36469800	-1.20222800
H	3.26745300	-0.30011700	-1.16683700	Cl	-0.87768900	2.38028100	0.63872200
C	3.72258100	1.56272500	-0.11478500	C	0.47947800	-1.09655500	-1.29765000
H	3.99853000	1.90368000	0.88382200	C	1.04087500	-0.00933600	-1.28457200
H	4.47612500	1.90052900	-0.83213400	C	1.78206400	1.25763600	-1.36052800
Cl	2.17132600	2.37670900	-0.55929200	H	2.29948500	1.26662300	-2.33074700
Cl	2.46892000	-0.63747800	1.05778100	H	1.05939400	2.08070500	-1.38968300
				C	2.79092700	1.51847700	-0.21628800
				H	3.04473400	2.58389300	-0.26815400
d-TS7				H	2.29540300	1.36237400	0.74795700
C	-0.64407000	1.50388100	0.46483900	C	4.10413400	0.70830800	-0.27370500
C	0.71902200	1.89389200	0.29681300	H	4.78175700	1.12337900	0.48261600
H	0.46995200	1.58744200	1.45101300	H	4.58138600	0.88697900	-1.24963000
C	2.56023400	-0.74651900	-1.75330300	C	3.96553100	-0.77437700	-0.04262400
C	3.36224500	-0.82917300	-0.42852600	H	3.48193900	-1.34952400	-0.83178800
C	1.63761400	0.83218600	-0.23974800	C	4.39428700	-1.41193200	1.04783000
C	2.97293400	0.44526000	0.36648600	H	4.26889400	-2.48400200	1.17266100
C	1.41554000	0.17306400	-1.40838800	H	4.88887900	-0.88386500	1.86092100
H	2.23088900	-1.72138700	-2.12801400	C	0.00319800	-2.48095200	-1.43187000
H	3.14282200	-0.28551300	-2.56403800	H	-0.03858900	-2.97443600	-0.45551600
H	3.05489300	-1.71525100	0.13615800	H	-0.99383300	-2.51178000	-1.88215500
H	4.43889200	-0.90223600	-0.59353700	H	0.69680800	-3.03381900	-2.07517000
H	3.69189900	1.26197000	0.20586000				
H	2.91954400	0.27556700	1.44783600				
In	-0.70029000	-0.70819800	0.19201300	m-b-7			
Cl	0.12146000	-1.87703600	1.98612700	C	0.77589200	0.89390200	0.03942900
Cl	-1.99819900	-1.55291000	-1.49061900	C	1.93154300	0.35952000	0.56267600
C	-1.76100300	2.44547500	0.72675900	C	2.00655400	-1.02301000	1.19819300
C	-2.55068900	2.57516400	-0.61407800	C	2.38205300	-1.97582600	0.04643500
H	-1.42675900	3.43786100	1.04617700	C	3.38970700	-1.20569800	-0.85470600
H	-2.43449700	2.04180400	1.49003800	C	3.03566100	0.26470800	-0.79431600
H	-3.39996900	3.24082000	-0.43798300	C	3.32434200	1.07318000	0.38004000
H	-1.93281800	3.01042700	-1.40470800	H	4.41238100	-1.33366900	-0.47720100
H	-2.93930900	1.61216900	-0.95822000	H	3.36105400	-1.56486700	-1.88630700
C	1.23485900	3.32671800	0.24520700	H	1.48506700	-2.19382700	-0.54238600
H	1.24811100	3.65321500	-0.80058300	H	2.79928500	-2.92463700	0.39641800
H	0.61332000	4.01754200	0.81799200	H	2.76247600	-1.03653000	1.99221000
H	2.25818300	3.38017500	0.62503700	H	1.04713000	-1.28666800	1.65168200
H	0.60348000	0.39649000	-2.10167700	H	2.69321200	0.76708900	-1.69443800
				H	4.03189700	0.62715400	1.07881300
				C	3.41390600	2.58497900	0.29732100

H	2.73564100	3.00539200	-0.45048700	C	-0.36514800	1.33802500	-0.73095400
H	3.18412600	3.04010100	1.26538800	H	-0.91685000	0.34746000	-2.58407200
H	4.43321300	2.87215400	0.01685700	H	-2.75410300	2.25010700	0.33268800
In	-1.28698000	0.05363900	-0.01884700	H	-3.04531300	0.15176900	2.00131100
Cl	-1.03798500	-1.42410500	-1.86111700	H	-4.57999800	0.65864100	1.29927000
Cl	-1.73228000	-1.08476200	1.99399500	H	-3.54102300	-1.94335900	0.91159700
Cl	-2.66166900	1.90507000	-0.43720900	H	-4.57514000	-1.15223200	-0.28211800
H	0.90144500	1.83399000	-0.50384900	H	-2.70376300	-1.38479900	-1.73761900
				H	-1.57553700	-1.54248500	-0.40384400
				Cl	1.14031400	-1.88484800	-1.54268200
m-b-8				Cl	3.04378200	1.03311600	0.35830700
C	0.69483800	0.44699700	-0.96878300	C	-0.22517800	2.72943300	-0.20481800
C	1.90933400	-0.26461900	-0.90559300	H	-0.13487000	2.77633000	0.88473500
C	2.18487900	-1.56939000	-0.20374900	H	0.75297900	3.05868400	-0.59592600
C	3.53037500	-1.37199100	0.53215800	H	-0.98014000	3.44081400	-0.56151200
C	4.24130100	-0.21037200	-0.20945300	In	1.05934300	-0.19230600	0.09419400
C	3.10682800	0.59497200	-0.83142000	Cl	0.08603900	-0.89714800	2.12973700
C	1.95768200	1.17640300	0.07520500	H	-1.63484600	2.00615400	-2.38559300
H	4.87470000	0.39092100	0.45038800				
H	4.88023300	-0.58708100	-1.01715800				
H	4.13322100	-2.28313400	0.54762800				
H	3.33587800	-1.10033200	1.57457400	m-b-11			
H	1.36522000	-1.89443000	0.44156900	C	-3.02883100	0.00812300	1.17075400
H	2.27384500	-2.30338900	-1.02016900	C	-2.25963900	0.75764700	0.09333500
H	3.33503400	1.29068500	-1.63709000	C	-2.88908200	0.67098600	-1.09770200
H	1.90987300	0.79379400	1.09228500	C	-4.14424900	-0.15262800	-1.02008600
C	1.72288600	2.68774900	-0.00701500	C	-1.01507500	1.45840700	0.36943300
H	0.73054000	2.94332000	0.37295300	C	-0.06984500	1.87576900	-0.53415200
H	2.48123900	3.17448700	0.61734900	H	-0.23364900	1.66076300	-1.59244500
H	1.81932200	3.06388800	-1.02807200	H	-2.53705400	1.11995200	-2.02271600
In	-1.23089400	-0.08572300	-0.01369200	H	-4.98289100	0.29528800	-1.56678000
Cl	-2.30188400	-1.81102700	-1.18361300	H	-3.96325100	-1.13612400	-1.48087700
Cl	-2.33872200	1.99568900	0.02515500	H	-2.50339700	-0.92379000	1.41904800
Cl	-0.51036200	-0.74132600	2.16481300	H	-3.11782800	0.58185900	2.10150000
H	0.65239400	1.23646000	-1.71947600	C	-4.40074100	-0.26875500	0.50559400
				H	-4.81662000	-1.23907100	0.78949300
				H	-5.12006900	0.49910900	0.81157600
m-b-9				In	1.10269900	-0.36200100	0.02449400
C	-2.45088300	-0.98375200	-0.74996800	Cl	-0.30867200	-2.16212600	-0.40154800
C	-2.16874700	0.50894200	-0.83131200	Cl	1.76451600	-0.03251500	2.23469100
C	-2.80863800	1.18021000	0.16294100	Cl	2.72346400	-0.02264200	-1.61676800
C	-3.58910100	0.25999400	1.05066600	H	-0.82978800	1.69971200	1.41829300
C	-3.62622300	-1.07224400	0.25860900	C	1.00761300	2.88337400	-0.21091000
C	-1.23466800	1.12053600	-1.88275900	H	0.67142700	3.87770700	-0.53613700

H	1.21171400	2.93080900	0.86336700	C	3.05635600	-2.74378300	-0.08831000
H	1.93998900	2.66810100	-0.74050400	H	2.71714700	-2.91848500	0.93690700
				H	2.28456600	-3.07962200	-0.78715800
				H	3.94427300	-3.36790900	-0.25541100
m-b-12				C	3.10977700	1.95588800	0.11690100
C	-1.41443400	-0.02354500	-1.14211100	H	2.61365300	2.23533100	1.05229800
C	-2.58425800	0.08396200	-0.28249900	H	3.49454400	2.87011200	-0.34507300
C	-2.99780600	1.49649800	0.09983100	In	-1.40405600	-0.00451700	0.02654000
C	-1.77983800	2.41044900	0.31954300	Cl	-2.38057300	-0.63999700	2.06646000
C	-0.87286600	2.43395400	-0.92028700	Cl	-2.20566900	-1.15843700	-1.85820200
C	-0.59855000	1.04102300	-1.43576000	Cl	-1.31928000	2.33878700	-0.29505500
C	-3.27711300	-1.00133900	0.13217300	H	0.77686000	-1.67499800	0.76809800
H	-1.35271300	2.99999200	-1.73408700				
H	0.07017300	2.94960500	-0.70849200				
H	-3.61501700	1.91939800	-0.70754800	m-b-TS2			
H	-3.62647900	1.47303700	0.99614700	C	0.64397100	0.47148800	-0.99220100
H	0.15044700	0.92155600	-2.22088700	C	1.84963000	-0.17045400	-0.78006300
H	-4.14426900	-0.81187600	0.76613400	C	2.06675100	-1.48462800	-0.04916100
H	-2.10946300	3.42704300	0.55855300	C	3.50996800	-1.43092800	0.49851500
H	-1.20787300	2.05153900	1.18521100	C	4.25468200	-0.41047100	-0.39641700
C	-3.00597700	-2.44967600	-0.13101700	C	3.17384300	0.55852500	-0.87346300
H	-3.89881900	-2.93662600	-0.54436800	C	2.30741700	1.24697600	0.13767100
H	-2.16917300	-2.63348700	-0.80855700	H	5.07307000	0.09553800	0.12558400
H	-2.78110700	-2.95907000	0.81569500	H	4.68265800	-0.90205800	-1.27769800
In	1.06199600	-0.20311200	0.12467800	H	3.99301300	-2.41119400	0.49028500
Cl	2.54585500	1.59217000	0.17180800	H	3.50333500	-1.09304800	1.54019400
Cl	1.62931600	-1.97240000	-1.28647600	H	1.31340200	-1.67375400	0.72047500
Cl	0.12044100	-0.76178600	2.17699600	H	1.95373000	-2.27151000	-0.80654700
H	-1.19386500	-0.98231200	-1.60584400	H	3.37434900	1.16012900	-1.75909400
				H	2.29680400	0.86836200	1.15657400
				C	1.95652400	2.71521200	0.03576400
m-b-TS1				H	1.01261200	2.94675100	0.53452000
C	1.73805700	-0.06538800	-0.18875400	H	2.75606000	3.25434500	0.56233300
C	3.69135800	-0.39812700	0.66822700	H	1.93026400	3.08073100	-0.99312800
C	3.43066100	-1.31203700	-0.32545700	In	-1.27948400	-0.07269400	-0.01885000
C	4.26930700	0.96311100	0.40416900	Cl	-1.76515700	-2.31394700	-0.52498500
C	0.70979100	-0.71500700	0.26590600	Cl	-2.84519400	1.51648100	-0.73549300
C	2.10677400	1.24296600	-0.79426800	Cl	-0.59258000	0.22002000	2.24771400
H	4.93099400	0.91922700	-0.46860700	H	0.67854100	1.34995700	-1.63671600
H	4.86443900	1.29722400	1.25966700				
H	2.51810200	1.10592100	-1.80303100				
H	1.17585300	1.81756200	-0.88755300	m-b-TS3			
H	3.47888800	-0.67845800	1.69865200	C	0.69183200	0.64419100	-0.84827100
H	3.72081500	-1.05629800	-1.34418800	C	1.89969400	-0.18716700	-0.81579600

C	2.11072100	-1.47674800	-0.06145500	In	1.12824400	-0.18326400	0.06311100
C	3.51551300	-1.35110600	0.57790700	Cl	2.93927100	1.27538100	-0.22792700
C	4.23781000	-0.23591500	-0.22270900	Cl	0.82556300	-0.95425800	2.25884500
C	3.11099400	0.53624400	-0.86838100	Cl	0.98249800	-1.83270000	-1.61740700
C	1.73925500	1.30731300	0.09376100	H	-1.17790600	2.18205300	-2.22999100
H	4.88425800	0.39646500	0.39485300				
H	4.87042500	-0.64614500	-1.02212500				
H	4.06592100	-2.29454800	0.56474000	m-b-TS5			
H	3.41039100	-1.05322100	1.62596100	C	-1.00396200	0.77074500	0.00398600
H	1.31515000	-1.68868000	0.65705300	C	-2.13715100	0.26314300	-0.76552100
H	2.06598600	-2.26623300	-0.82702500	C	-2.09427400	-1.16235100	-1.27203800
H	3.30154200	1.32469300	-1.58898700	C	-1.77035600	-2.06502500	-0.03931000
H	1.71771200	0.96262000	1.12647000	C	-2.21514900	-1.31312100	1.23382700
C	1.95236900	2.81269100	-0.04356100	C	-2.18193400	0.17426200	0.92087600
H	1.09333700	3.29843100	0.43297700	C	-3.38822100	0.75025500	-0.28880700
H	2.86343100	3.13637800	0.46842300	H	-3.22533400	-1.59672600	1.55116100
H	1.98738900	3.13466400	-1.08692500	H	-1.53341700	-1.51510300	2.06651300
In	-1.22826800	-0.06541400	-0.01766900	H	-3.05626200	-1.42530900	-1.72250900
Cl	-1.70263300	-2.13318100	-1.04728900	H	-1.30982900	-1.25433100	-2.02921800
Cl	-2.81181400	1.63444900	-0.35151500	H	-2.41929500	0.89525700	1.69661500
Cl	-0.63496300	-0.36419500	2.28042800	H	-2.26279400	-3.03636400	-0.13375000
H	0.60043100	1.27361700	-1.73621400	H	-0.69648700	-2.26118600	-0.00099100
				H	-4.23421300	0.08104300	-0.45188600
				C	-3.77105700	2.18657600	-0.03462400
m-b-TS4				H	-2.90994800	2.83190400	0.15325800
C	-2.25748200	-1.04017700	-0.02818200	H	-4.28920500	2.56705600	-0.92316600
C	-2.04789700	0.45926400	-0.13608000	H	-4.46588000	2.26288400	0.80784500
C	-3.22006800	1.12773600	0.04111300	In	1.11565700	0.12459300	-0.00596500
C	-4.34938500	0.19354200	0.37062500	Cl	2.28255300	2.16423200	0.03433900
C	-1.02732000	1.24481200	-1.68530100	Cl	1.40628500	-1.18009500	1.95447200
C	-0.70805900	1.19920900	-0.32145700	Cl	1.49550400	-1.16827300	-1.95579000
H	-1.11722500	0.33383600	-2.27345800	H	-1.02574200	1.84923900	0.16673400
H	-3.32295200	2.20816600	0.05086000				
H	-4.57207400	0.23997400	1.44802200				
H	-5.27854900	0.46848400	-0.14385000	m-b-TS7			
H	-1.75694400	-1.60664900	-0.81967300	H	-1.14047900	1.49726700	-1.67895600
H	-1.81670200	-1.37963300	0.91952500	C	-0.08867100	1.47143400	-0.47220800
C	-0.49119600	2.52245200	0.40932800	C	-1.51246600	1.58338800	-0.56065900
H	-1.22673500	3.28691300	0.12479600	C	-3.37431600	-1.40939800	0.88348100
H	-0.54771100	2.37679700	1.49206700	C	-4.01458300	-1.33658300	-0.52696500
H	0.50242200	2.91592000	0.17418800	C	-2.27362000	-0.38271700	0.81518400
C	-3.79806100	-1.19394400	-0.04989100	C	-2.38757500	0.40736700	-0.26226700
H	-4.14428200	-2.00040900	0.60115400	C	-3.61414600	0.05239700	-1.08884500
H	-4.13312700	-1.42610100	-1.06671500	H	-1.51700000	-0.27616800	1.58671400

H	-2.99322700	-2.40800500	1.12523300	C	2.77619200	1.25018100	0.51466600
H	-4.08907500	-1.14568600	1.67752900	C	3.56181200	-0.02216600	0.93943200
H	-3.58160600	-2.11891700	-1.15903400	C	2.96750800	-1.20502600	0.20596800
H	-5.09771900	-1.48737200	-0.51239500	C	3.19872900	-1.39303800	-1.22906800
H	-4.41306200	0.79549200	-0.94359600	H	4.61804200	0.06546400	0.65278600
H	-3.40993500	0.02330300	-2.16736800	H	3.51458500	-0.17893300	2.01957000
In	1.31442400	-0.17313100	-0.03590200	H	1.89732900	1.34073500	1.16107800
Cl	0.63066800	-2.39524000	0.03183100	H	3.37778300	2.15616000	0.63276200
Cl	3.31453300	0.20031200	-1.16913400	H	3.09862000	1.28487300	-1.65863000
Cl	1.06403000	1.09256500	2.02043900	H	1.42942400	1.62372500	-1.17976900
C	-2.18136900	2.95324300	-0.39034600	H	2.51128600	-2.00996600	0.77246000
H	-2.35569300	3.11958600	0.67763600	H	4.06248600	-0.89867900	-1.66767200
H	-1.55154000	3.76261200	-0.77169900	In	-1.10382500	-0.00731000	0.01670300
H	-3.14754000	2.98666900	-0.90110900	Cl	-0.54181000	0.16726700	2.31773800
H	0.41364200	2.44001800	-0.57130400	Cl	-1.32836100	2.09514100	-1.01860300
				Cl	-2.80764100	-1.54181500	-0.45658400
m-c-5				H	0.72636300	-2.09155600	-0.72017400
In	-1.47857600	0.03134000	-0.01461200	H	2.97962800	-2.37308900	-1.64642800
Cl	-2.35147600	1.81868700	-1.21387600				
Cl	-2.04027700	-0.14383700	2.22910500				
Cl	-1.22252100	-1.97789400	-1.16507200	m-c-8			
C	0.76035400	1.10929700	0.16788500	C	-0.69768600	-0.73689400	-0.97461900
H	0.50880800	2.15171800	0.15827800	C	-1.96295400	-0.14256500	-0.84764200
C	1.40484400	0.07039000	0.21666700	C	-2.31959800	1.13322000	-0.11285500
C	2.07610800	-1.22356800	0.23790700	C	-3.68968800	0.85801400	0.54857000
H	2.22227400	-1.53968500	1.27926400	C	-4.32611000	-0.29205700	-0.27266500
H	1.38186000	-1.94284600	-0.21690900	C	-3.13896700	-1.04644900	-0.85770000
C	3.41936900	-1.26156500	-0.53617400	C	-2.01353000	-1.53474400	0.09320300
H	3.64476600	-2.31965600	-0.71155000	H	-4.98012500	-0.93267100	0.32680800
H	3.28367000	-0.79659200	-1.51853700	H	-4.92440300	0.09861200	-1.10429600
C	4.61878200	-0.61867900	0.19210700	H	-4.32431100	1.74711300	0.57183300
H	5.51457700	-0.80619500	-0.41238700	H	-3.53999200	0.54741400	1.58766700
H	4.76984100	-1.14509400	1.14593400	H	-1.54655800	1.45720700	0.58814100
C	4.49143500	0.86105700	0.44649000	H	-2.39220200	1.90231200	-0.89451800
H	3.77232600	1.16543400	1.20755800	H	-3.29759400	-1.73255500	-1.68683600
C	5.19485600	1.80263800	-0.18495100	H	-1.98781300	-1.25980900	1.14245100
H	5.06436600	2.85886500	0.03391100	In	1.15985500	0.02235000	-0.00586800
H	5.93592400	1.55270500	-0.94182400	Cl	1.51373700	2.18257600	-0.86207300
				Cl	2.82186800	-1.56392700	-0.45600300
				Cl	0.44831400	0.07061900	2.26736000
m-c-7				H	-0.62353600	-1.53898500	-1.71102500
C	0.75978100	-0.99733400	-0.70549800	H	-1.65182100	-2.53245900	-0.12827100
C	1.98910200	-0.45946600	-1.03623900				
C	2.31265500	1.02507900	-0.94055800				

m-c-9				H	0.98143000	1.71098500	1.62664300
C	-2.50301800	-0.56083100	1.03438100	H	-0.66526900	0.25687600	2.61517000
C	-2.18469200	-1.07503800	-0.35956400				
C	-2.84175900	-0.32152000	-1.30642700				
C	-3.58424800	0.82048500	-0.69518400	m-c-12			
C	-3.09131400	0.84947200	0.77565400	C	-1.45328400	-0.56286500	-1.18456900
C	-1.28014400	-2.23641900	-0.71644100	C	-2.61231500	-0.83025100	-0.33561500
C	-0.59306100	-0.98776000	-1.08697500	C	-3.40261800	0.37715300	0.13493400
H	-0.91101900	-2.74304800	0.17429900	C	-2.50052400	1.60141400	0.36928500
H	-2.85803500	-0.54663500	-2.36915900	C	-1.66428400	1.92963300	-0.87787000
H	-3.42587200	1.75962700	-1.23790200	C	-0.99212800	0.70016700	-1.44085400
H	-4.66180500	0.59827700	-0.78050300	C	-2.94653600	-2.10049800	-0.04936700
H	-2.30096900	1.59877700	0.87162300	H	-2.30487500	2.34977200	-1.66916000
H	-3.88856000	1.10518400	1.47749900	H	-0.91408800	2.69610000	-0.65588300
H	-3.24680200	-1.23994300	1.47337500	H	-4.14695600	0.62774100	-0.63584600
H	-1.63805900	-0.55901600	1.70273000	H	-3.96164400	0.12881500	1.04291700
Cl	1.10316400	-0.94403400	2.13431800	H	-0.22555000	0.83530000	-2.20577600
Cl	2.85353000	-0.26990900	-1.36392700	H	-3.80325000	-2.33761400	0.57510900
In	0.99879500	0.10631700	0.02136900	H	-3.10962500	2.46797500	0.64663900
Cl	0.32050100	2.36455700	0.13691100	H	-1.83122000	1.40271100	1.21618900
H	-1.62855200	-2.90795400	-1.50104800	In	0.97355600	-0.07894600	0.13116600
H	-0.62416100	-0.76560500	-2.15481300	Cl	1.83816900	2.08189700	0.20638600
				Cl	2.02750800	-1.55656100	-1.32687000
				Cl	0.21447400	-0.91564600	2.15878800
m-c-11				H	-0.97033700	-1.41496200	-1.66217700
C	3.24043900	1.24389200	0.12777800	H	-2.36911800	-2.94070600	-0.42596300
C	2.30931900	0.23949300	0.79320900				
C	2.73478700	-1.02784900	0.57818600				
C	3.98495900	-1.07409200	-0.24974100	m-c-TS1			
C	1.10858900	0.63638400	1.49333600	C	0.73757800	-1.02031900	0.12019000
C	0.09486200	-0.16504000	1.96150300	C	1.82148700	-0.45017800	-0.29200800
H	0.18083200	-1.25037600	1.95723300	C	2.39122700	0.84644200	-0.73668500
H	2.22662700	-1.92425100	0.92020600	C	4.57635200	0.20225500	0.34715700
H	4.72175100	-1.79085000	0.13286200	C	3.88114300	-1.10384900	0.54553000
H	3.72657200	-1.41357600	-1.26519700	C	3.35210000	-1.81479600	-0.49852700
H	2.75767700	1.66210100	-0.76605700	H	5.16970300	0.17684700	-0.57404000
H	3.48337600	2.09151400	0.77953200	H	5.24814900	0.42496100	1.18135600
C	4.48539300	0.39434900	-0.23314300	H	2.76935400	0.77428300	-1.76479700
H	4.93891000	0.69485900	-1.18122100	H	1.55347600	1.55820900	-0.73955800
H	5.24754100	0.50853100	0.54556100	H	3.67475100	-1.43205600	1.56266100
In	-1.22271800	-0.01238800	-0.13085100	H	3.63716300	-1.59839300	-1.52518700
Cl	-0.28757100	-1.82761300	-1.26306000	C	3.49164600	1.31632200	0.22113100
Cl	-0.83597200	2.08005500	-1.08867100	H	3.05380700	1.52307100	1.20328800
Cl	-3.31388800	-0.33606700	0.83527100	H	3.95423600	2.24006900	-0.14014600

In	-1.27386300	-0.00257800	0.02531000	H	-1.57082100	1.29794100	0.76173900
Cl	-2.16977700	-0.55891700	2.12294800	H	-2.33698600	1.87902800	-0.71387500
Cl	-2.35797300	-0.96565900	-1.81721700	H	-3.23977600	-1.77559100	-1.66352800
Cl	-0.86507900	2.31241100	-0.23952300	H	-1.69244100	-1.37769300	1.13788600
H	0.67228000	-2.02433700	0.52507400	In	1.13646000	0.01615800	-0.01856400
H	2.85524900	-2.76480200	-0.33512200	Cl	1.31719900	2.16934700	-0.96584700
				Cl	2.93164200	-1.42818500	-0.44160600
				Cl	0.51927000	0.14657900	2.28938200
m-c-TS2				H	-0.56750000	-1.48713200	-1.76590800
C	0.75435400	-0.68820900	0.85183200	H	-1.87208500	-2.65089200	-0.17854800
C	2.04263500	-0.14260600	0.79653100				
C	2.46901300	1.21678300	0.28078100				
C	3.84535300	0.99014300	-0.38517000	m-c-TS4			
C	4.41936900	-0.29164400	0.27145300	C	-2.35595500	0.66263100	0.57541900
C	3.19176800	-1.08686900	0.70053100	C	-2.06622200	-0.52801500	-0.31556800
C	2.09752600	-1.38018000	-0.33834000	C	-3.19205100	-0.95709800	-0.94817600
H	5.07496200	-0.85577400	-0.39896800	C	-4.36529100	-0.06790500	-0.65033000
H	4.99990100	-0.04953100	1.16934700	C	-1.06981400	-2.15164500	0.34878600
H	4.51078700	1.84814100	-0.26328200	C	-0.70171400	-1.16749000	-0.58008900
H	3.71743500	0.84149100	-1.46270800	H	-1.22521600	-1.89019000	1.39352500
H	1.71960300	1.68858700	-0.36011400	H	-3.22190000	-1.78032500	-1.65668500
H	2.56162400	1.84563000	1.17757800	H	-4.55622600	0.59760900	-1.50652800
H	3.30336900	-1.88704600	1.42919600	H	-5.29007400	-0.63682200	-0.49451000
H	2.12660500	-0.95481700	-1.33538800	H	-1.90197800	0.57982700	1.56844500
In	-1.18032500	0.03227700	0.00066800	H	-1.91100300	1.55258400	0.10869000
Cl	-0.90383800	2.21687000	-0.84539100	C	-3.90361100	0.71966600	0.60608700
Cl	-2.73521800	-0.16201900	1.74037000	H	-4.28220300	1.74451300	0.62239700
Cl	-1.38517600	-1.57219500	-1.73076400	H	-4.27542300	0.21786000	1.50607100
H	0.67070800	-1.60531100	1.43969100	In	1.12620000	0.10734200	-0.01941500
H	1.64275400	-2.36261900	-0.28544100	Cl	2.89420000	-1.19438200	-0.82645600
				Cl	0.79738600	2.15647700	-1.11223300
				Cl	0.96467900	0.21616900	2.33240000
m-c-TS3				H	-1.19510000	-3.20731300	0.09874600
C	-0.69875400	-0.88244700	-0.86731300	H	-0.55324000	-1.52885200	-1.59865700
C	-1.99010200	-0.18705000	-0.78734300				
C	-2.32794600	1.05475500	0.01284800				
C	-3.72905900	0.77732700	0.60774100	m-c-TS5			
C	-4.34559700	-0.32496400	-0.29131200	C	0.95710500	1.15845600	-0.06878200
C	-3.14864900	-0.97633300	-0.93426400	C	2.18662900	0.96195200	0.72760200
C	-1.68447200	-1.61317500	0.07714800	C	2.51194900	-0.40788900	1.26978400
H	-4.97969300	-1.03562200	0.24822500	C	2.38985200	-1.39327300	0.06349500
H	-4.96248800	0.09775100	-1.09785900	C	2.61168600	-0.59227800	-1.23706200
H	-4.35121500	1.67401900	0.65125800	C	2.18264300	0.84308500	-0.98712300
H	-3.62393500	0.40616100	1.63244100	C	3.23613300	1.77007500	0.26342700

H	3.65619000	-0.61110200	-1.56749000	Cl	3.19972100	1.04096700	-0.79249000
H	1.99560500	-0.99308400	-2.05011900	Cl	1.67134400	-2.45618700	0.12663400
H	3.52019600	-0.41153600	1.69529100	C	-0.35881700	0.99270300	-1.05919200
H	1.79296500	-0.67269300	2.05093400	C	-0.69470800	-0.15274600	-1.33494100
H	2.31504400	1.57899300	-1.77522500	C	-1.13845100	-1.49387300	-1.73634000
H	3.10488200	-2.21397300	0.16342200	H	-1.64635100	-1.38530200	-2.70576300
H	1.39482200	-1.84345600	0.05837500	H	-0.24971700	-2.10748000	-1.92299100
H	4.27060000	1.48176600	0.44101900	C	-2.05636000	-2.23096200	-0.73159900
In	-0.94575000	0.01826000	0.00864200	H	-2.04568400	-3.28843000	-1.02161200
Cl	-2.59040300	1.68932500	-0.10768100	H	-1.61419300	-2.17740500	0.26899400
Cl	-0.90966000	-1.41896000	-1.88032000	C	-3.52504200	-1.75678000	-0.68698000
Cl	-0.96758500	-1.22701600	2.02533900	H	-4.07667300	-2.45699600	-0.04719900
H	0.72147200	2.21540200	-0.21876900	H	-3.95283000	-1.85879500	-1.69638500
H	3.06400900	2.79721500	-0.04369100	C	-3.74411800	-0.35372900	-0.18281100
m-c-TS7				H	-3.44444400	0.45914500	-0.84585800
				C	-4.27663900	-0.04836300	1.00424600
				H	-4.58389100	-0.86200500	1.66460200
				C	-0.21042700	2.45147600	-0.87420000
				H	-0.28128500	2.68109700	0.19575900
H	1.06421500	-1.44664000	-1.94406600	H	0.79306000	2.75242400	-1.19588000
C	0.05634800	-1.53480500	-0.71311400	C	-4.49645600	1.34153500	1.52827400
C	1.46144700	-1.71765100	-0.86384200	H	-5.55607500	1.51780800	1.75762500
C	3.70912500	0.75648100	0.93416800	H	-3.94102300	1.50496600	2.46140700
C	4.44291000	0.64900400	-0.42875900	H	-4.17628200	2.10093800	0.80612600
C	2.44543800	-0.03225900	0.71451700	C	-1.28105300	3.23068400	-1.66135200
C	2.49184000	-0.74882800	-0.41922000	H	-2.28833100	2.96552500	-1.32603600
C	3.81892500	-0.58104000	-1.13947600	H	-1.13666200	4.30387200	-1.50210800
H	1.63346600	-0.05682000	1.43455900	H	-1.20690600	3.02824600	-2.73396100
H	3.50273900	1.79273300	1.22571300	m-d-7			
H	4.28999300	0.31183600	1.75605400				
H	4.24121700	1.54826000	-1.01992600				
H	5.52782500	0.56474100	-0.32123500				
H	4.43829200	-1.48348000	-1.02124900				
H	3.70396800	-0.42307100	-2.21964000	C	0.67856200	0.71528600	-0.23800800
In	-1.23925400	0.13030100	-0.00953400	C	1.81470500	-0.03088000	0.06657300
Cl	-0.33535600	2.26884600	0.16712600	C	1.83899000	-1.56428600	0.15638900
Cl	-3.24979600	-0.00560300	-1.17857400	C	2.94369500	-1.98697800	-0.83162200
Cl	-1.09452900	-1.24805400	1.95207400	C	4.03506100	-0.88857900	-0.76148400
H	-0.50526600	-2.44769800	-0.94010500	C	3.32586800	0.40414800	-0.35550000
H	1.82540100	-2.74822100	-0.97924500	C	2.98345500	0.64118300	1.02763700
m-d-5				H	4.79976700	-1.13890900	-0.01679300
				H	4.54594000	-0.75948700	-1.72002400
				H	2.52302200	-2.01545000	-1.84307100
				H	3.34410200	-2.98158800	-0.61422900
				H	2.05517500	-1.90412600	1.17542600
In	1.50775200	-0.14125900	0.28464900	H	0.87625000	-1.99341400	-0.12753000
Cl	0.78892800	0.70136100	2.33084600				

H	3.39047600	1.26667300	-1.01356000	H	-4.85660200	-1.23450300	0.14503400
H	3.24168900	-0.15648000	1.72258500	H	-5.15381000	0.49697900	0.29553900
C	0.70394300	2.11749600	-0.73581900	In	0.97054300	-0.65683400	-0.04076300
H	-0.01108900	2.71989900	-0.15983500	Cl	0.13918300	-1.86161200	1.78833200
H	1.68376700	2.60231900	-0.69186100	Cl	3.26456400	-0.26317200	0.10894700
C	2.86386000	1.98464300	1.70511300	Cl	0.16908600	-1.36712700	-2.11929600
H	2.72715500	2.81760900	1.01483000				
H	2.05111500	1.99019700	2.43772600				
H	3.80075700	2.15824400	2.24955300	m-d-12			
C	0.22150300	2.12310200	-2.21616900	C	-1.51452400	0.29361800	0.87908200
H	0.86376200	1.50038700	-2.84667900	C	-2.54424500	-0.30228500	-0.00679600
H	-0.80847500	1.76911300	-2.30262200	C	-2.91734900	-1.73124600	0.36235600
H	0.26077100	3.15123900	-2.58900600	C	-1.66269700	-2.61432600	0.44419200
In	-1.36154600	-0.18316700	0.11263200	C	-0.67636700	-2.05721300	1.47812600
Cl	-1.67996900	-1.89971100	-1.47167700	C	-0.58979400	-0.53806700	1.48134100
Cl	-1.16447700	-0.96021000	2.33468700	C	-3.11924900	0.29965200	-1.06979700
Cl	-2.86651200	1.61628300	-0.10398200	H	-0.99896800	-2.33433800	2.49393100
				H	0.31675400	-2.50715100	1.36233300
				H	-3.42929000	-1.73924900	1.33682900
m-d-11				H	-3.62293300	-2.13369000	-0.37153700
C	-3.16668100	-0.07702500	0.97919100	H	0.03041200	-0.11477000	2.27082400
C	-2.18573400	0.73420500	0.13926600	H	-3.87850300	-0.29160900	-1.58222800
C	-2.59492500	0.78957300	-1.14759700	H	-1.93587100	-3.64051300	0.71555100
C	-3.86079900	0.01785600	-1.38558100	H	-1.18716300	-2.65563300	-0.54097700
C	-0.96539400	1.34814600	0.67411600	C	-2.85299100	1.63492600	-1.70688000
C	0.10811700	1.69081600	-0.13420900	H	-3.01546500	1.56167000	-2.78737900
H	-0.03602000	1.55682300	-1.20948200	H	-3.54867400	2.40068100	-1.33500800
H	-2.07591500	1.31114900	-1.94569800	H	-1.83513200	1.99903100	-1.55197800
H	-4.57532000	0.55753500	-2.01883200	C	-1.60565000	1.76778500	1.23985900
H	-3.61722800	-0.91378100	-1.91931200	H	-1.31560500	2.37662100	0.37769700
H	-2.71430700	-1.04057300	1.24879600	H	-2.67257700	1.97427000	1.39567800
H	-3.43460800	0.41603700	1.92031200	C	-0.80620200	2.23640600	2.45928900
C	1.21686400	2.66848000	0.25225200	H	-1.06541700	1.67117100	3.36145200
H	0.75497900	3.54732100	0.72296300	H	0.27427000	2.16186000	2.29945900
C	-0.93225600	1.61050500	2.15744200	H	-1.02646400	3.29138000	2.65003200
H	-1.77564100	2.25504600	2.43608500	In	1.16037500	0.00613400	-0.26944600
H	-1.04646300	0.67212400	2.71175700	Cl	0.66962300	-1.29508900	-2.13986300
H	-0.00648000	2.08985700	2.47865800	Cl	2.88830600	-0.78132200	1.08822100
H	1.89140000	2.24001700	1.00253600	Cl	1.25305200	2.29665800	-0.72815000
C	2.03871400	3.11597600	-0.96236200				
H	2.79762700	3.84486400	-0.66114700				
H	2.55671000	2.26923600	-1.42375300	m-d-TS1			
H	1.40184100	3.58711000	-1.72041000	C	0.67241100	0.74686700	-0.04255100
C	-4.39206000	-0.24984200	0.04558700	C	1.58743700	-0.13574100	0.24531700

C	1.76047200	-1.62291900	0.26910400	H	-3.35301600	1.72287800	0.25059000
C	3.95459700	-1.12738500	-0.82320300	H	-1.61633600	-0.23176000	-1.53474300
C	3.60769500	0.26199600	-0.34699500	C	-2.01009800	1.87959600	-1.92310300
C	3.42344600	0.55535900	0.98572700	H	-1.15222100	1.97010900	-2.59905200
H	4.65626200	-1.58136800	-0.11348300	H	-2.90097600	1.67534400	-2.52397800
H	4.45471600	-1.08187000	-1.79510500	H	-2.13583100	2.82963600	-1.40303000
H	2.16515700	-1.97187100	1.22667000	In	1.20969500	-0.26194500	-0.09570400
H	0.77752900	-2.08873100	0.15030100	Cl	1.77578700	-1.32854100	1.93331300
H	3.56827000	1.07321600	-1.07144900	Cl	2.80583300	1.27130600	-0.89729400
H	3.55897600	-0.25943300	1.69556400	Cl	0.58148300	-1.88277400	-1.73961400
C	0.74404800	2.19542500	-0.43710500	C	-0.48147400	2.33105800	0.65143400
H	0.07323100	2.77974500	0.20380500	H	0.16693300	2.83774500	-0.07243500
H	1.75590800	2.59133600	-0.30518900	H	-1.42802000	2.89119500	0.67343400
C	0.31867600	2.39655300	-1.90673800	C	0.15833900	2.40565400	2.04456400
H	0.95510200	1.81924800	-2.58591700	H	-0.46443400	1.90843200	2.79741300
H	-0.71943600	2.09363600	-2.06871000	H	1.14550900	1.93296300	2.06699200
H	0.40343300	3.45605300	-2.17002600	H	0.28494800	3.45087900	2.34573300
In	-1.41502900	-0.14248500	0.10231300				
Cl	-2.87013900	1.70092500	0.05884900				
Cl	-1.47178000	-1.34358900	2.13011300	m-d-TS5			
Cl	-1.55812700	-1.58655800	-1.76239900	C	-0.98134500	0.55179000	0.09384800
C	3.38131300	1.91971800	1.61069000	C	-2.04543300	-0.07852400	-0.72144400
H	3.45431000	2.72570500	0.87735200	C	-1.72182800	-1.38936600	-1.43206300
H	2.47596700	2.06127400	2.20945000	C	-1.86653000	-2.52664500	-0.37630400
H	4.23494200	2.00518200	2.29556700	C	-1.66206300	-1.90459100	1.02645900
C	2.67435800	-2.00202700	-0.90313100	C	-1.93703500	-0.41218300	0.91814400
H	2.14169100	-1.80562400	-1.83934500	C	-3.38112200	0.00864100	-0.25830400
H	2.93443200	-3.06505200	-0.88109100	H	-2.32007500	-2.36136100	1.77224300
				H	-0.63383500	-2.04212800	1.37828200
				H	-2.40873000	-1.53622100	-2.27197200
m-d-TS2				H	-0.70685000	-1.35988400	-1.82836100
C	-0.68352400	0.88147300	0.18350700	H	-2.37563900	0.12811500	1.75144600
C	-1.86903800	0.14534300	0.66397500	H	-2.86924000	-2.96383300	-0.43993500
C	-2.02032600	-1.33562100	0.92529800	H	-1.14600400	-3.32308200	-0.57126000
C	-3.38154800	-1.72323500	0.29900600	C	-1.06811000	2.02909200	0.53809100
C	-4.17306900	-0.39529300	0.18650100	H	-0.19123500	2.24539100	1.15903200
C	-3.10138000	0.66873900	0.21503300	H	-1.92303900	2.21533800	1.20001300
C	-1.70840700	0.70715500	-0.99040600	H	-3.98721600	-0.86062900	-0.52036500
H	-4.80397400	-0.33625400	-0.70675000	C	-4.22294200	1.17495800	0.18615200
H	-4.83478700	-0.23620500	1.04953200	H	-3.67061300	2.09762800	0.34191600
H	-3.91212200	-2.47685300	0.88545100	H	-4.96310200	1.35238300	-0.60544300
H	-3.21211000	-2.14681600	-0.69612100	H	-4.78753900	0.92966000	1.09250200
H	-1.18340900	-1.93458500	0.56068800	C	-1.10143300	3.00150600	-0.64879700
H	-2.02481600	-1.43046000	2.02201700	H	-1.10726000	4.03646600	-0.29066800

H	-0.22164700	2.87345100	-1.28608500	H	3.15222100	0.99949200	-1.61995100
H	-1.99455800	2.85131800	-1.26832200	H	4.14536000	0.73564900	-0.20333300
In	1.20142500	0.00755100	0.00737600	H	2.79600400	-1.28134600	0.43026600
Cl	2.31848100	1.56139000	-1.36568900	H	3.59366000	-1.42369400	-1.12442800
Cl	1.69795000	0.21407100	2.31885200	H	0.73979100	1.91061800	-1.36281100
Cl	1.65202800	-2.20961700	-0.71369900	H	-0.12431800	2.15587200	1.56361200
b-4 (Figure S1)				C	-1.47265700	2.86609200	-0.03906400
C	0.95665000	-0.67527800	-0.44392500	H	-2.38500300	2.48656900	0.42570300
C	1.93469300	-0.29062200	0.38066800	H	-1.40293600	3.92549500	0.23821800
C	-1.55010200	1.27325000	0.11207800	H	-1.56733800	2.80309900	-1.12360500
C	-1.98515200	-0.04385500	0.58287200	H	-0.24799100	-1.88311400	-2.47589100
C	-1.55197900	-1.22967900	-0.31298500	b-6(Figure S1)			
C	-0.09630100	-1.69894300	-0.11576000	C	5.12156600	0.01347100	-0.38688400
C	-1.23877700	2.36899500	-0.29031800	C	5.30271400	0.88511900	0.60827100
H	0.03656000	-2.04074600	0.92016400	C	1.05340100	-1.58556100	-0.71186100
H	0.04803100	-2.58574000	-0.75266400	C	2.29881700	-1.21431300	-0.08994200
H	-1.72227000	-0.96374000	-1.36368600	C	3.49375000	-1.90112900	-0.82019100
H	-2.21454800	-2.07671100	-0.09355000	C	4.83588200	-1.45074900	-0.20805800
H	-1.61890300	-0.20855200	1.60630600	C	-0.01766900	-1.89246800	-1.22398900
H	-3.08170600	-0.03767100	0.65208900	In	-1.45957500	-0.63026200	0.21445400
H	0.90104700	-0.23173600	-1.43990900	Cl	-0.30931200	0.41045200	1.90391100
H	1.98341600	-0.73133900	1.37877600	Cl	-3.21548800	-2.10769700	0.32367100
C	2.99369200	0.72353300	0.05485100	H	4.86462000	-1.71569100	0.85392200
H	2.95427400	1.57477000	0.74840400	H	5.61842000	-2.04147800	-0.69849100
H	4.00134300	0.29395000	0.14148900	H	3.46220500	-1.64500800	-1.88287300
H	2.87738600	1.11217800	-0.96263600	H	3.39015700	-2.98564700	-0.74095400
H	-0.94097100	3.33092100	-0.63966800	H	2.43226700	-0.12736200	-0.12726300
b-5(Figure S1)				H	2.28387300	-1.51045900	0.96383900
C	0.82287200	1.79275800	-0.28057200	H	5.21097800	0.36183000	-1.41637200
C	-0.23984900	2.19222000	0.47859400	H	5.23579300	0.52393800	1.63461100
C	1.55916500	-1.23278400	-1.25306400	C	5.63668200	2.33665600	0.44245600
C	2.80736700	-0.87845700	-0.58841500	H	4.90594700	2.97208900	0.95416900
C	3.12954400	0.63223300	-0.58984200	H	6.60988400	2.56180700	0.89124500
C	2.20660200	1.51308000	0.26757600	H	5.67363400	2.62753900	-0.60967900
C	0.53233200	-1.53217200	-1.83223800	H	-0.64837400	-2.45873100	-1.88180600
In	-0.56814500	-0.38480600	0.10252300	C	-0.79031100	2.85516200	-1.00634000
Cl	0.19008100	-1.17279700	2.11696300	C	-1.09671500	1.70492500	-1.72405600
Cl	-2.64683200	-0.43511400	-0.84530700	C	-2.30440100	1.01627700	-1.46641400
H	2.15082000	1.14271700	1.29624400	C	-3.21056700	1.52676700	-0.50367700
H	2.68135900	2.50082000	0.33632300	C	-2.88743700	2.67884200	0.20777500
				C	-1.68375100	3.33856800	-0.04672200
				H	0.13292600	3.38644200	-1.20238200

H	-0.42864200	1.34770900	-2.49930000				
H	-2.63514200	0.23067700	-2.14212400	b-9(Figure S1)			
H	-4.16132700	1.02989800	-0.34587000	C	1.41400300	0.71192800	-0.60770800
H	-3.57700200	3.06938300	0.94587900	In	-0.65285600	0.67214100	0.19462400
H	-1.44121500	4.23968200	0.50407900	C	2.44956100	-0.37832900	-0.28858100
				C	2.36307000	-1.40124400	0.83265900
				C	3.75036900	-2.08554100	0.80682400
b-7(Figure S1)				C	4.30150300	-1.81968700	-0.61754900
C	-1.23130100	0.71802000	0.17718600	C	3.54268000	-0.61937200	-1.07038100
In	0.59710000	-0.50074500	0.23878700	C	2.41661400	1.45687100	0.10215900
Cl	1.62585000	-0.20431000	2.28787400	Cl	-0.94652700	-0.46927500	2.18511300
C	-2.42092900	0.46921600	-0.41220000	Cl	-1.43397100	2.84513000	-0.08514200
C	-2.87194000	-0.80183400	-1.09682000	H	5.38397300	-1.66877700	-0.66077700
C	-3.80296000	-1.51348400	-0.10252600	H	4.09213000	-2.65150300	-1.30722100
C	-4.69461200	-0.42207700	0.56785400	H	3.69673700	-3.14724800	1.04453700
C	-3.88985200	0.83564400	0.69281300	H	4.40993800	-1.62042400	1.54308100
C	-3.57829900	1.65050700	-0.43333800	H	2.11282500	-0.96857600	1.80286300
Cl	0.36120400	-2.61073400	-0.71959200	H	1.55592900	-2.10469700	0.59862100
H	-5.56275700	-0.22121900	-0.06727000	H	3.81610400	-0.03247900	-1.94092900
H	-5.05032000	-0.75109200	1.54406600	H	2.46297300	1.34769600	1.18382500
H	-3.20075700	-1.99980200	0.66860300	C	3.27152400	2.53138400	-0.47021000
H	-4.41988200	-2.27711000	-0.57706000	H	2.77887400	3.47658700	-0.19622900
H	-3.39468600	-0.56956600	-2.02938700	H	4.26831200	2.55711500	-0.02770600
H	-2.01530100	-1.42813400	-1.34730800	H	3.33361000	2.49897400	-1.55761600
H	-3.55463600	1.16387900	1.67195600	H	1.39187000	0.96466400	-1.66840900
H	-4.16431000	1.45166300	-1.32780800	C	-2.47247900	-2.76076600	-0.30941300
C	-3.14802400	3.09190400	-0.28271500	C	-1.48894200	-2.31834300	-1.18689400
H	-2.60760400	3.27558900	0.64698600	C	-1.57670100	-1.03322900	-1.74318900
H	-2.53027500	3.40775400	-1.12463400	C	-2.66452000	-0.19765500	-1.41020200
H	-4.04348800	3.71911000	-0.26950900	C	-3.64543800	-0.65374000	-0.51774400
H	-1.15797800	1.63592200	0.75851700	C	-3.54660600	-1.92999300	0.02555000
C	3.17062700	-0.33282900	-1.26913000	H	-2.41061600	-3.75592000	0.11414400
C	2.10787700	0.54249700	-1.57950800	H	-0.67177900	-2.97327800	-1.46523500
C	2.11088200	1.85592200	-1.06341800	H	-0.87447700	-0.72348600	-2.51101200
C	3.14066600	2.26922300	-0.22529100	H	-2.78598000	0.76073600	-1.90256300
C	4.17975400	1.38982200	0.08654500	H	-4.48214800	-0.01313000	-0.26738900
C	4.19759600	0.09499800	-0.43225900	H	-4.30766400	-2.28442900	0.71003300
H	3.18731500	-1.32914900	-1.69483900				
H	1.39484900	0.26334000	-2.35129900	b-10(Figure S1)			
H	1.32735200	2.54941400	-1.34802800	C	1.46201300	0.52257300	-0.70237900
H	3.14522600	3.27605800	0.17400600	In	-0.36115800	-0.51877400	-0.00346000
H	4.98147800	1.71761400	0.73751700	Cl	-0.91396900	-0.15511700	2.21582900
H	5.01105400	-0.57719700	-0.18903500	C	2.57808300	0.92511600	0.32657700
				C	2.81398000	-0.01715400	1.49295600

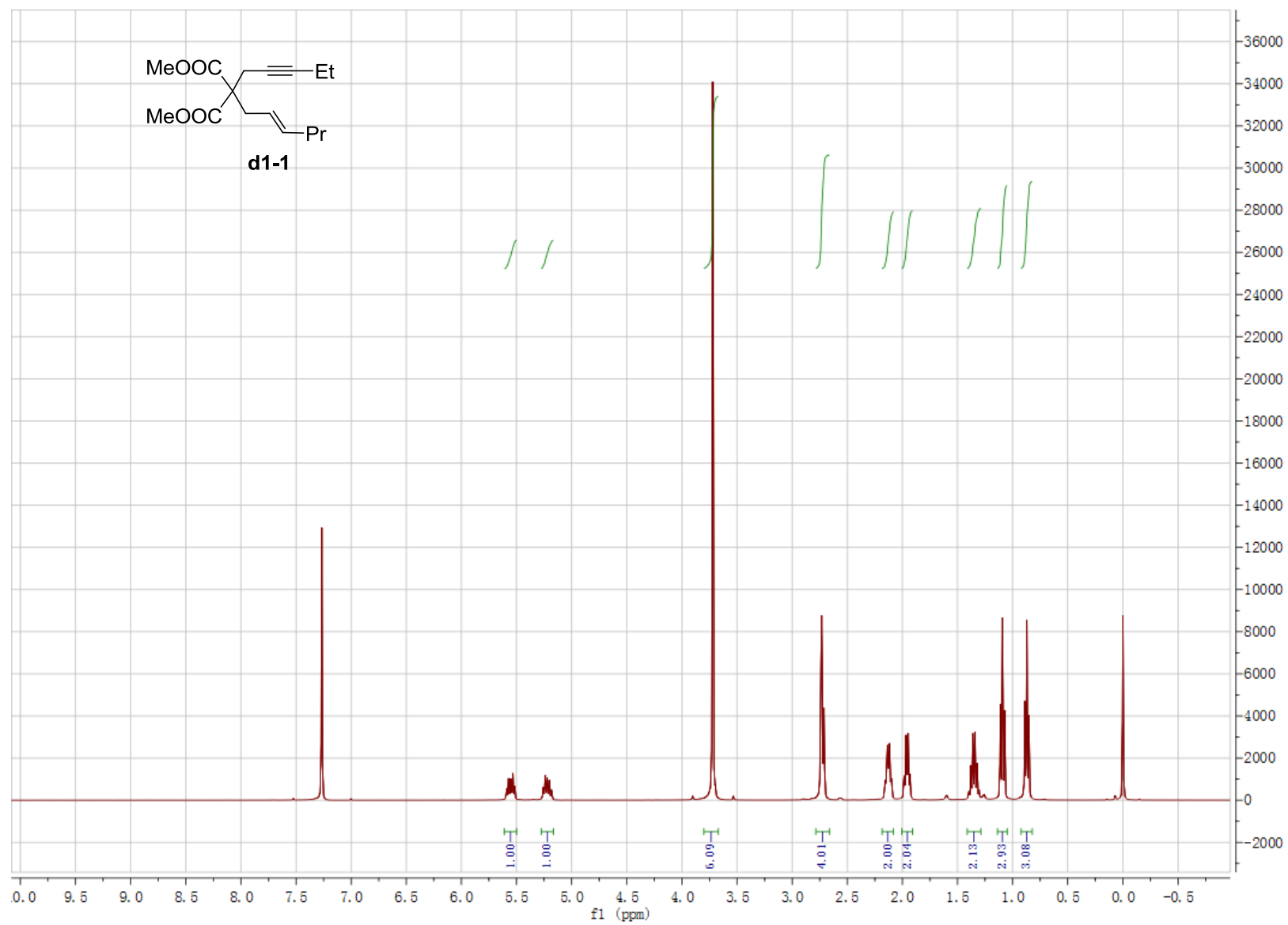
C	2.78479400	-1.46393500	0.94584100	H	-4.48591800	-1.87380200	-0.90437600
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C	2.67474900	-0.11700100	-1.13266600	H	-5.67148100	-1.07473200	1.06368900
C	3.26950600	2.09831500	0.18283000	H	-3.48007400	-0.37870900	1.79606100
Cl	-0.45981400	-2.64302000	-0.96084400	H	-4.19087700	1.23148400	1.69781200
H	4.26447100	-1.45780900	-0.67752400	In	0.44897900	-0.13506000	0.17728300
H	2.74259200	-2.22922200	-1.11139600	Cl	-0.72500900	-2.12536200	-0.04287000
H	3.78472500	0.20588300	1.94074300	Cl	1.28232900	0.73638900	2.14134000
H	2.05507700	0.12953900	2.26534000	C	0.01548300	2.84534800	-0.89441100
H	3.21674900	0.29599300	-1.98048500	H	0.99170500	2.70105300	-1.36292600
H	3.46057100	-2.11476100	1.50084700	H	-0.50230400	3.62785000	-1.46335100
H	1.79607800	-1.91338100	1.06446600	H	0.17536900	3.21939500	0.12169100
H	3.92222800	2.36394000	1.01436000	H	-1.79952600	2.04193700	0.92230500
C	3.22766400	3.09648000	-0.91242800	C	2.79524800	-1.62010500	-0.53538600
H	2.65368800	2.79201600	-1.78660600	C	3.86074900	-1.28338300	0.29928000
H	2.79898800	4.02984500	-0.52350200	C	4.44130300	-0.01301900	0.21244900
H	4.24714300	3.35171300	-1.22017000	C	3.97065400	0.93041600	-0.70945500
H	1.19157900	1.36413100	-1.33561800	C	2.90872000	0.60887100	-1.55184000
C	-2.88443200	2.34432800	0.09172800	C	2.28698600	-0.66159200	-1.45351500
C	-2.04924400	1.92782800	-0.93866200	H	2.35752200	-2.61344400	-0.50175800
C	-2.16952000	0.62148200	-1.45806300	H	4.24508200	-2.01113900	1.00651400
C	-3.16509000	-0.24239800	-0.95261900	H	5.27317400	0.24155500	0.86208500
C	-3.99836700	0.18886500	0.07602800	H	4.44533600	1.90386300	-0.78008400
C	-3.85577100	1.47574400	0.59462900	H	2.57793500	1.31125800	-2.31100900
H	-2.79309800	3.34583700	0.49391700	H	1.58502900	-0.98334800	-2.22314300
H	-1.32921500	2.61642700	-1.36667000	b-12(Figure S1)			
H	-1.63287400	0.34287300	-2.36206400				
H	-3.28363200	-1.23170200	-1.37830900				
H	-4.75990500	-0.47417900	0.46741300				
H	-4.50739400	1.80663000	1.39458200				
b-11(Figure S1)				C	2.03283200	0.23412800	-1.11568000
				In	-0.37038900	0.18512200	0.30125500
				Cl	-0.96266600	2.26627500	-0.49951500
				C	3.28660300	0.02005100	-0.45316700
				C	3.71711800	-1.42191600	-0.23396600
C	-3.96560600	0.33243900	1.11378100	C	2.52866500	-2.36303500	0.01150000
C	-3.04732600	0.61430700	-0.06897100	C	1.46440500	-2.22745800	-1.08721800
C	-3.49985100	-0.02340700	-1.18729600	C	1.11412000	-0.77758000	-1.36676900
C	-4.74661300	-0.80198700	-0.92776600	C	4.08595100	1.06567900	-0.10394900
C	-5.22518400	-0.28580300	0.45470200	Cl	0.33485200	-0.30725800	2.44400900
C	-1.88556700	1.44300800	0.01187100	H	1.83539600	-2.65623600	-2.02746900
C	-0.83197600	1.57951200	-0.90176700	H	0.57443900	-2.81309400	-0.83601700
H	-0.95789000	1.08726800	-1.87134200	H	4.26346800	-1.75559700	-1.12466300
H	-3.02557300	0.01700900	-2.16432600	H	4.41927800	-1.47831500	0.60006800
H	-5.48802100	-0.69232100	-1.72797700	H	0.36776200	-0.56956700	-2.13551200
				H	5.03434000	0.80760300	0.36484700

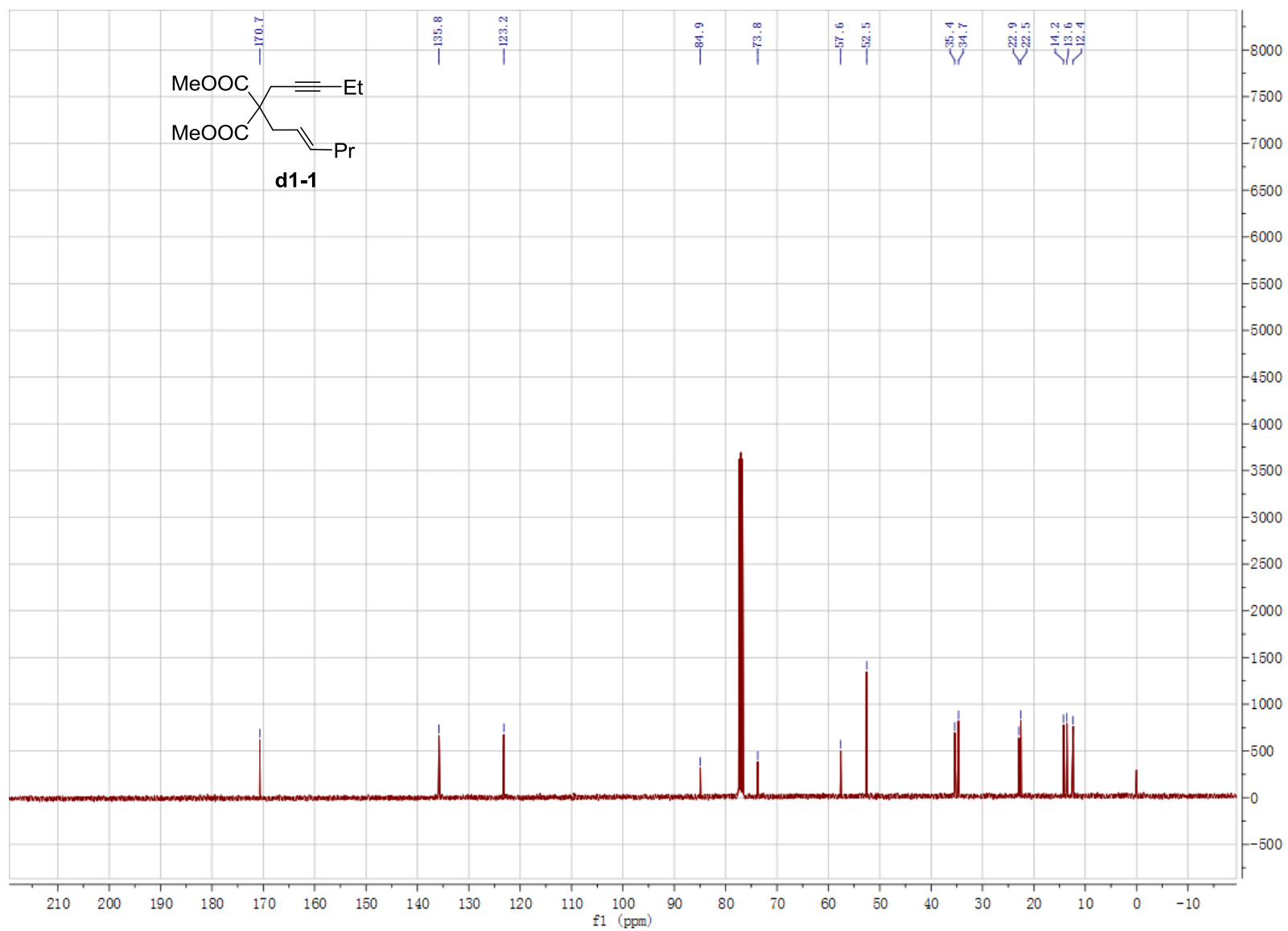
H	2.87899700	-3.39634300	0.05270900	b-TS1(Figure S1)			
H	2.08615600	-2.14427600	0.98763600	C	1.19780100	0.65906800	0.10497500
C	3.85578800	2.52696200	-0.25857200	Cl	-1.91384200	0.73247100	2.11345300
H	3.88487000	3.00529300	0.72762700	C	2.28127100	-0.02261600	0.06187600
H	4.68145400	2.97003700	-0.82687200	C	2.92903400	-1.34066000	0.04307300
H	2.91656300	2.79759300	-0.73877500	C	4.94474800	-0.31214100	-0.98882300
H	1.79265300	1.23509400	-1.46202300	C	4.20815700	0.97023800	-0.75631300
C	-4.24266800	0.43666500	-0.73414700	C	4.04600100	1.54336000	0.46956600
C	-3.56077300	-0.31925800	-1.69184800	Cl	-0.46990000	-2.67968600	0.37651300
C	-2.61011200	-1.25019200	-1.29173300	H	5.62080500	-0.51412500	-0.15383400
C	-2.31765700	-1.41324200	0.08146200	H	5.54917000	-0.24257600	-1.89616800
C	-3.02991200	-0.65611100	1.04293300	H	3.42320600	-1.52360400	1.00374900
C	-3.98132000	0.27099600	0.62669400	H	2.11630600	-2.07463900	-0.04241300
H	-4.98733000	1.15663700	-1.05235000	H	3.81775800	1.49279000	-1.62739000
H	-3.78558200	-0.19093200	-2.74352600	H	4.48721600	1.04551700	1.33127800
H	-2.11413100	-1.87404800	-2.02678300	In	-0.73816000	-0.36913900	0.46560100
H	-1.71446700	-2.25614600	0.41119500	C	3.44612300	2.88442500	0.71478500
H	-2.84549500	-0.81963100	2.09854300	H	2.97283800	3.30076500	-0.17641900
H	-4.52471400	0.85356400	1.36021500	H	2.73182700	2.86309500	1.54276700
b-I(Figure S1)				H	4.24289400	3.57378200	1.01858600
				C	3.92373500	-1.46761100	-1.11499000
				H	3.39325200	-1.40587300	-2.06894200
				H	4.42826300	-2.43427600	-1.07979500
				H	1.12483200	1.73961800	0.09339800
				C	-3.03031300	2.06358900	-1.30555800
				C	-1.94870000	1.33834300	-1.79289700
				C	-1.97643000	-0.07274700	-1.76201600
				C	-3.12031900	-0.73917900	-1.26955400
				C	-4.19727400	-0.00058300	-0.78753500
C	1.27659100	-1.22259400	0.17553700	C	-4.14959300	1.39361900	-0.80636100
C	0.23312000	-0.13937600	-0.06066100	H	-3.01150000	3.14636100	-1.32507400
C	0.81901300	1.07020000	-0.12912900	H	-1.09632600	1.85138600	-2.22399200
C	2.31304100	1.00738900	0.07605100	H	-1.20999400	-0.64223100	-2.28180300
C	2.62245500	-0.50395300	-0.08763400	H	-3.15824400	-1.82215900	-1.28348300
C	-1.19280800	-0.46432700	-0.15637200	H	-5.07315000	-0.50958100	-0.40481400
C	-2.21513200	0.35503200	0.13742300	H	-4.99114400	1.96355900	-0.43087500
H	-1.99675400	1.35638800	0.51047300	b-TS2(Figure S1)			
H	0.28862400	2.00450400	-0.29344200	C	1.31521000	0.17483100	-0.87341300
H	2.87153000	1.62990900	-0.63505300	In	-0.55578300	0.48470800	0.23765100
H	2.58529900	1.37090300	1.08013100	C	2.32311900	-0.76546100	-0.66071500
H	2.94252800	-0.69701900	-1.11809300	C	2.39864700	-1.86623700	0.36053400
H	3.42529700	-0.84863200	0.57180200	C	3.86298900	-1.87900400	0.85298600
H	1.20759000	-1.59513200	1.20910800				
H	1.13052100	-2.09568400	-0.47433900				
C	-3.66632000	-0.00024400	0.00068300				
H	-4.19407000	0.09575800	0.95982500				
H	-4.17661500	0.67261900	-0.70293300				
H	-3.79784800	-1.02660400	-0.35886500				
H	-1.42584800	-1.47977900	-0.48399800				

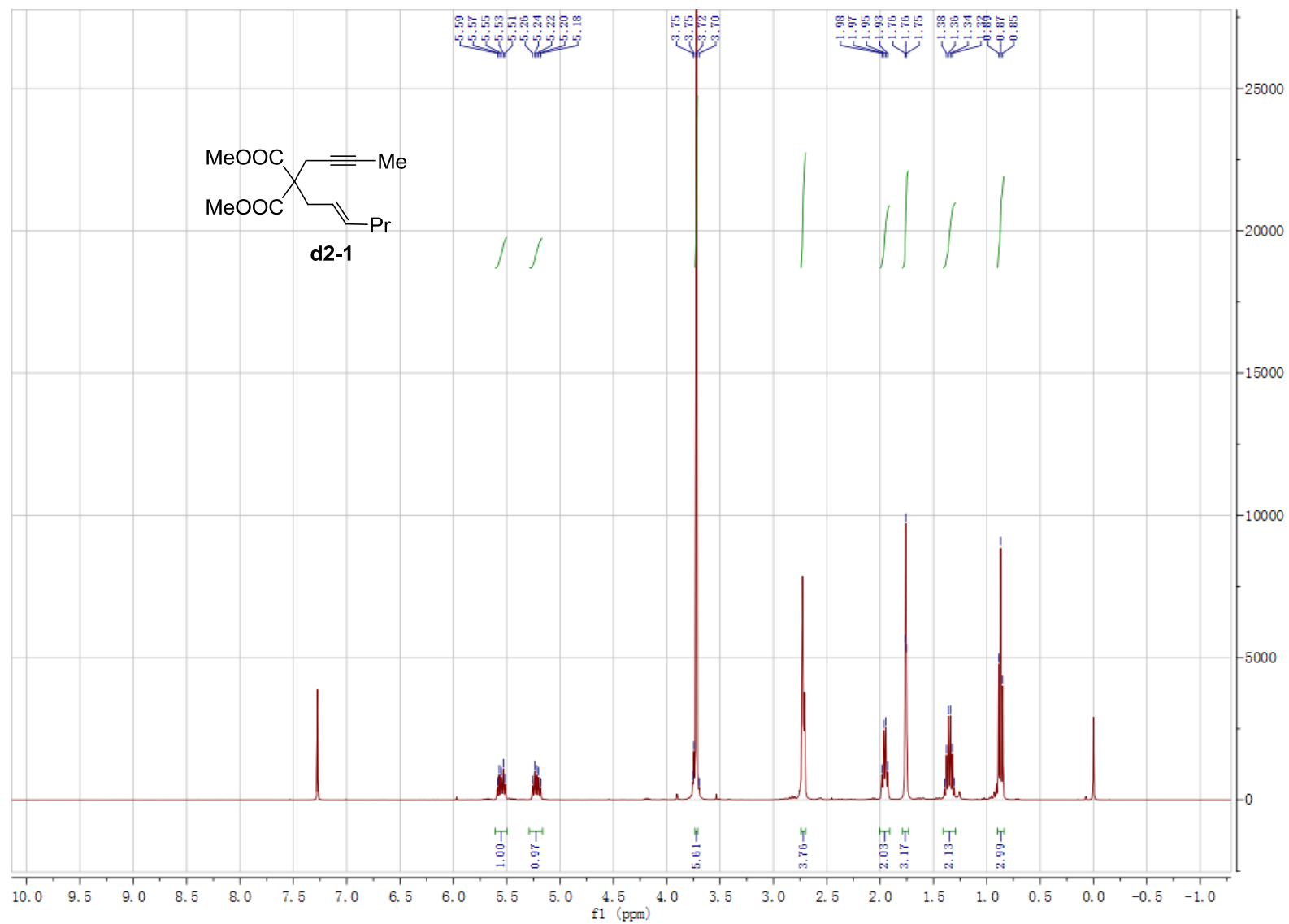
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C	3.69933200	-0.30475200	-0.99354800	H	4.82532900	-0.02029400	1.70885300
C	3.00311900	0.81582000	-0.19416100	H	2.47095800	-0.38865800	1.80533100
Cl	-0.91930200	-0.99044300	1.98762900	H	2.52212600	-1.64008700	0.57005600
Cl	-0.73845800	2.78816700	0.53892000	In	-0.40707600	-0.48657500	0.01995900
H	5.57284300	-0.71337500	0.06687000	Cl	-0.93050800	0.00701800	2.22395000
H	5.01594600	-1.98701500	-1.00977400	Cl	-0.03922800	-2.62107400	-0.81006800
H	4.20714200	-2.88454900	1.09168500	H	1.15368600	1.06634500	-1.71685600
H	3.95027200	-1.29192900	1.76997900	C	-2.53024700	1.48745800	-1.12352600
H	1.64790100	-1.79839400	1.14870100	C	-3.41211300	1.86145800	-0.11603000
H	2.17280700	-2.77748400	-0.21265400	C	-4.18306300	0.89227800	0.53075400
H	3.92487700	0.01829800	-2.00631200	C	-4.07953100	-0.45307800	0.17776700
H	3.04620700	0.72937300	0.88652400	C	-3.19880900	-0.84180300	-0.82854000
C	3.07641200	2.24662000	-0.70114400	C	-2.40114900	0.12721500	-1.47711200
H	2.28910300	2.86805400	-0.27459300	H	-1.96817600	2.24078400	-1.66441800
H	4.04394200	2.63911500	-0.37016400	H	-3.51592600	2.90472500	0.15626000
H	3.04157900	2.30766400	-1.78848100	H	-4.87214600	1.18995600	1.31214600
H	1.40451300	0.75680900	-1.78735200	H	-4.68865800	-1.19542900	0.67836000
C	-3.81660700	-1.85873600	-0.24574300	H	-3.13297700	-1.88028600	-1.13123700
C	-2.82597700	-2.17771000	-1.17715800	H	-1.84051200	-0.15364700	-2.36565500
C	-2.12470400	-1.16243400	-1.81880300	C	1.55638000	3.43607500	-0.37246100
C	-2.40215100	0.18716100	-1.51055400	H	0.71846600	3.97416300	0.09755500
C	-3.41576200	0.49774800	-0.57774900	H	2.45487600	3.94628500	-0.01208400
C	-4.11218300	-0.52869500	0.05429000	H	1.47884300	3.52250300	-1.45535600
H	-4.36372000	-2.65352400	0.24725600				
H	-2.61673200	-3.21420200	-1.41203100				
H	-1.38906000	-1.40296700	-2.57834000	b-TS5(Figure S1)			
H	-1.97773000	0.98252700	-2.11876900	C	1.40076400	0.78545000	-0.36155800
H	-3.65437700	1.53430100	-0.37024500	In	-0.41093800	-0.42132400	-0.07629900
H	-4.88747600	-0.29262600	0.77254200	Cl	-1.11939900	-0.60421200	2.12476600
				C	2.46464400	1.01412600	0.57991300
				C	2.61681300	0.09693500	1.77076900
b-TS4(Figure S1)				C	2.72526900	-1.35491100	1.20418600
C	2.92948800	-0.65990000	0.84963600	C	3.24906000	-1.26844100	-0.24521100
C	2.63588900	0.32464000	-0.26333100	C	2.89950800	0.11002400	-0.78217200
C	3.75673200	0.64332700	-0.95195000	C	3.67722000	1.43372500	-0.08392200
C	4.94456200	-0.12608400	-0.46054600	Cl	-0.27470500	-2.30313900	-1.44808200
C	4.47729900	-0.67996500	0.91092700	H	4.33345100	-1.39865900	-0.29246200
C	1.50115500	2.04332400	0.11640200	H	2.80328900	-2.03776700	-0.87854000
C	1.25335600	0.87671000	-0.64722800	H	3.51120400	0.37159700	2.33104400
H	1.64261800	1.91384500	1.18835700	H	1.75454900	0.19633700	2.43305000
H	3.78898800	1.31651200	-1.80194200	H	2.96713600	0.32396800	-1.84151800
H	5.18453300	-0.92713400	-1.17277000	H	3.37006800	-1.96448600	1.83683300
H	5.84134200	0.49693100	-0.39582600	H	1.74681300	-1.83916300	1.22675500

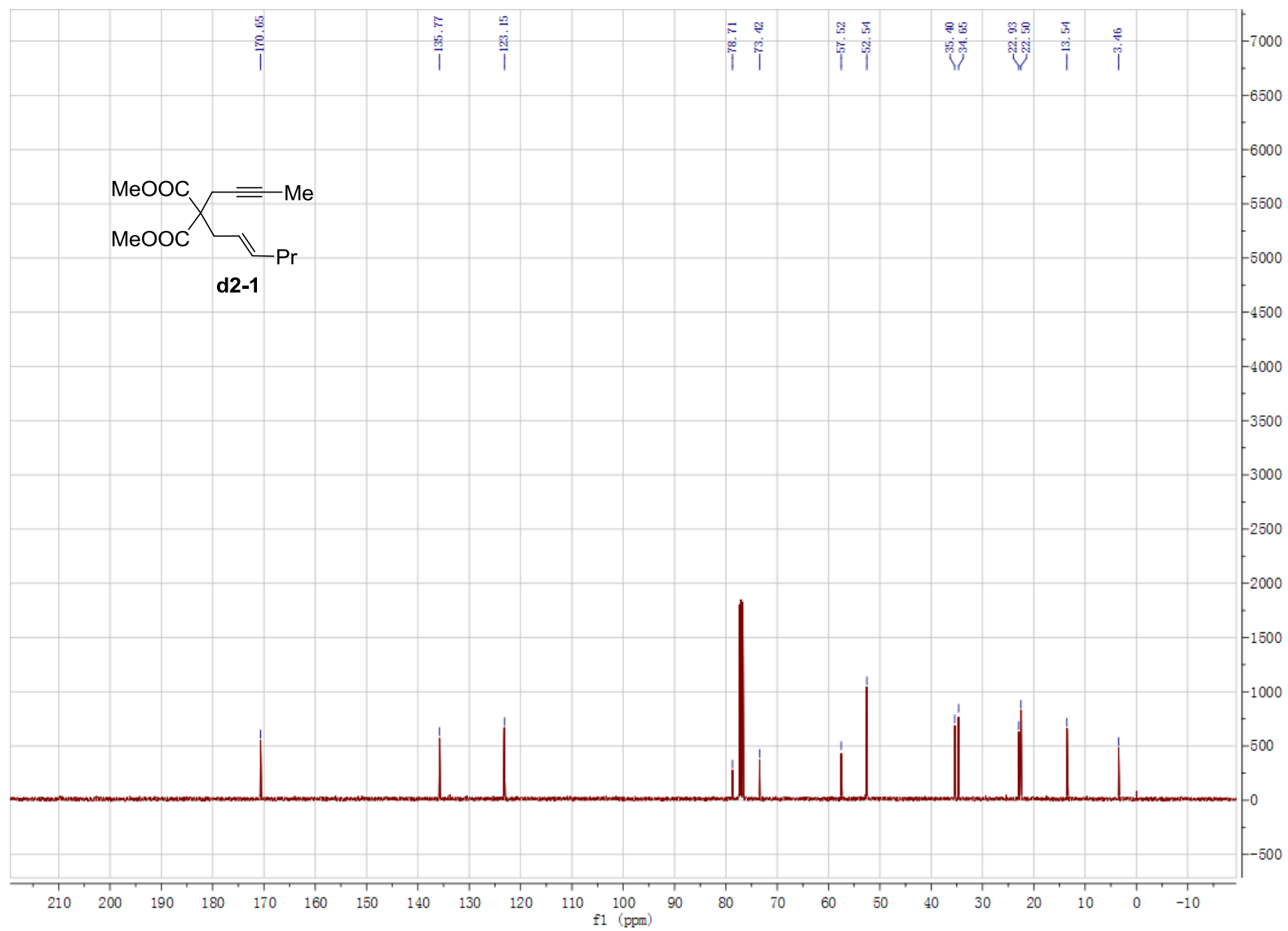
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C	3.83300200	2.61273500	-1.01432300	C	-2.86063000	2.30481300	0.04003700
H	2.91983900	2.85819900	-1.55771600	C	-2.03200300	1.86147100	-0.98426200
H	4.12097000	3.48759300	-0.42560400	C	-2.15107200	0.53859600	-1.46346000
H	4.62976200	2.42547600	-1.73685000	C	-3.13993400	-0.31416500	-0.92370500
H	1.28123200	1.56853300	-1.10631900	C	-3.96567000	0.14450200	0.09891300
C	-2.19021300	0.88413600	-1.37602300	C	-3.82406300	1.44758400	0.57681800
C	-3.17171300	-0.10333400	-1.13998500	H	-2.76969400	3.31801100	0.41174500
C	-4.08847500	0.06595000	-0.10642800	H	-1.31757200	2.53946100	-1.43765800
C	-4.04288800	1.21463500	0.68395500	H	-1.62691100	0.23762400	-2.36764200
C	-3.08467300	2.20375900	0.45192200	H	-3.25965100	-1.31550200	-1.32027700
C	-2.16592400	2.04990200	-0.58047800	H	-4.72143300	-0.50907900	0.51654100
H	-1.58907300	0.82877900	-2.28085700	H	-4.47044900	1.79990300	1.37186600
H	-3.21299700	-0.98134900	-1.77366400				
H	-4.83909800	-0.69232700	0.07879700	benzene (Figure S1)			
H	-4.75973400	1.34169000	1.48649300	C	-1.13051000	0.81673300	-0.00021900
H	-3.06625700	3.09541500	1.06643700	C	-1.27260600	-0.57069200	0.00005600
H	-1.45316600	2.83838300	-0.79536700	C	-0.14210200	-1.38734300	0.00017000
				C	1.13049200	-0.81672500	-0.00040400
				C	1.27259500	0.57069200	0.00020000
				C	0.14209500	1.38735600	0.00003300
b-TS6(Figure S1)				H	-2.00949900	1.45180000	-0.00015000
C	1.51681500	0.46907200	-0.74525500	H	-2.26209700	-1.01437700	0.00030800
In	-0.35165800	-0.53990800	0.01042100	H	-0.25227400	-2.46616900	0.00028200
Cl	-0.86012000	-0.08541100	2.21950400	H	2.00950400	-1.45176400	-0.00002400
C	2.49845800	1.04229100	0.32073000	H	2.26216200	1.01423000	0.00031600
C	2.83423100	0.12799200	1.47360900	H	0.25241900	2.46615900	0.00024900
C	2.87467700	-1.34515600	0.98925100				
C	3.24073100	-1.38772300	-0.49702100				
C	2.56918100	-0.32385400	-1.27125900				
C	3.07807500	2.25225900	0.14351300				
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H	4.32026900	-1.34457900	-0.68227000				
H	2.91718500	-2.33644700	-0.96183100				
H	3.79768400	0.42101800	1.89396800				
H	2.08694500	0.23138600	2.26626700				
H	2.93557500	-0.14373200	-2.28344600				
H	3.58350000	-1.93203100	1.57377500				
H	1.90622300	-1.82816000	1.14702500				
H	3.69617700	2.59445300	0.97237200				
C	2.93622800	3.23137200	-0.97366000				
H	2.44199500	2.83205800	-1.85968100				
H	2.37291600	4.10891000	-0.63418700				
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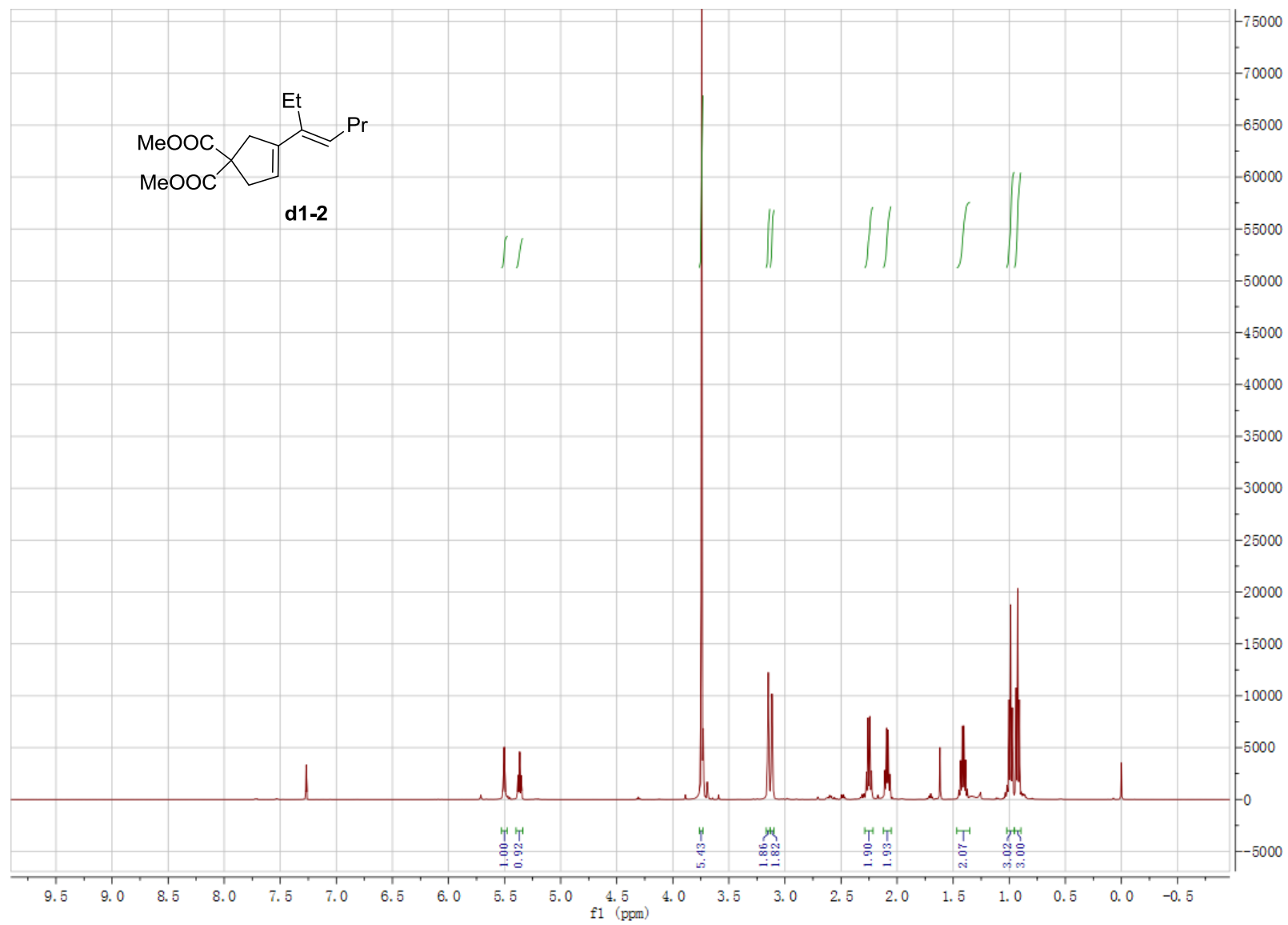
4. NMR Spectra

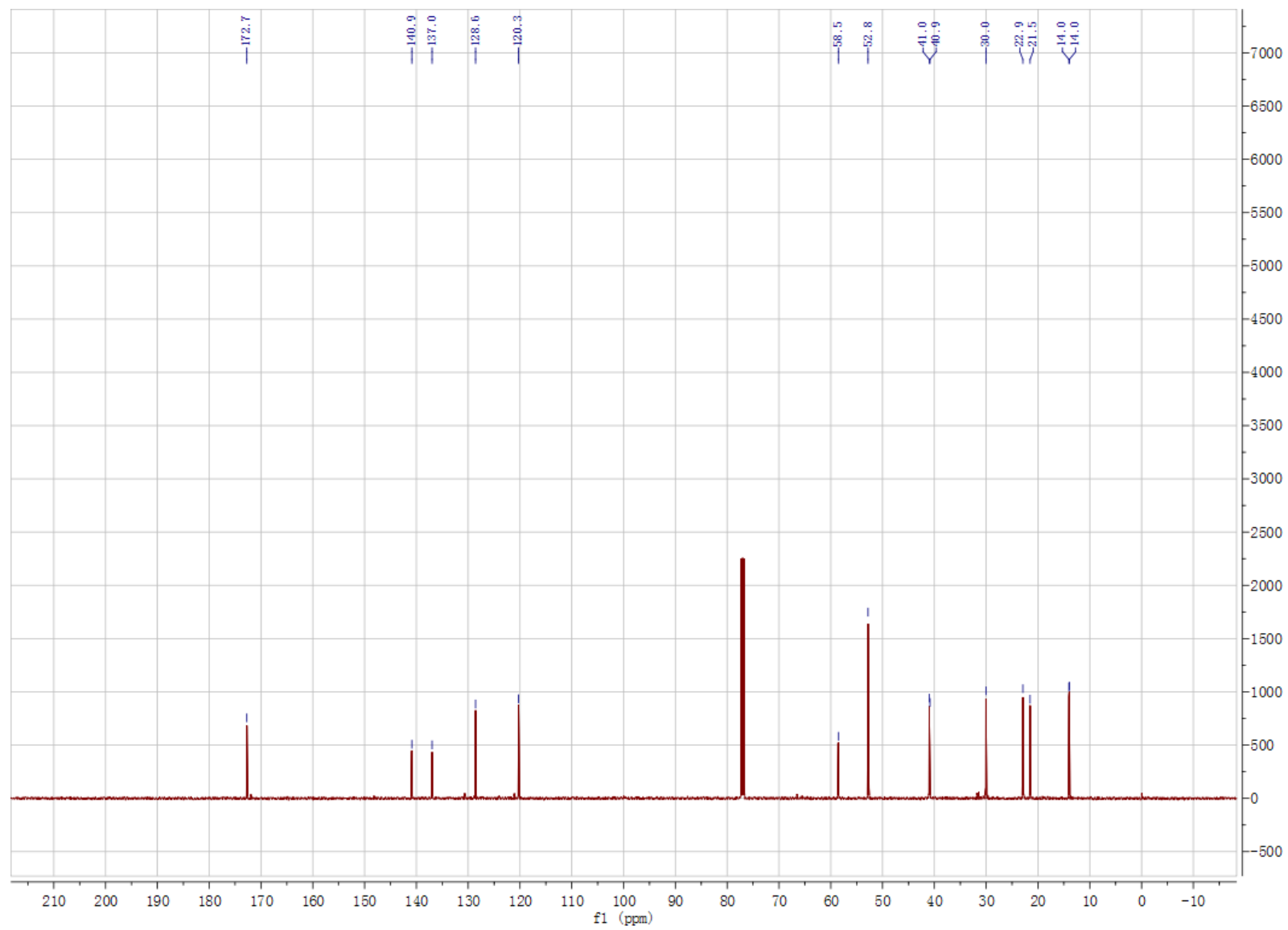


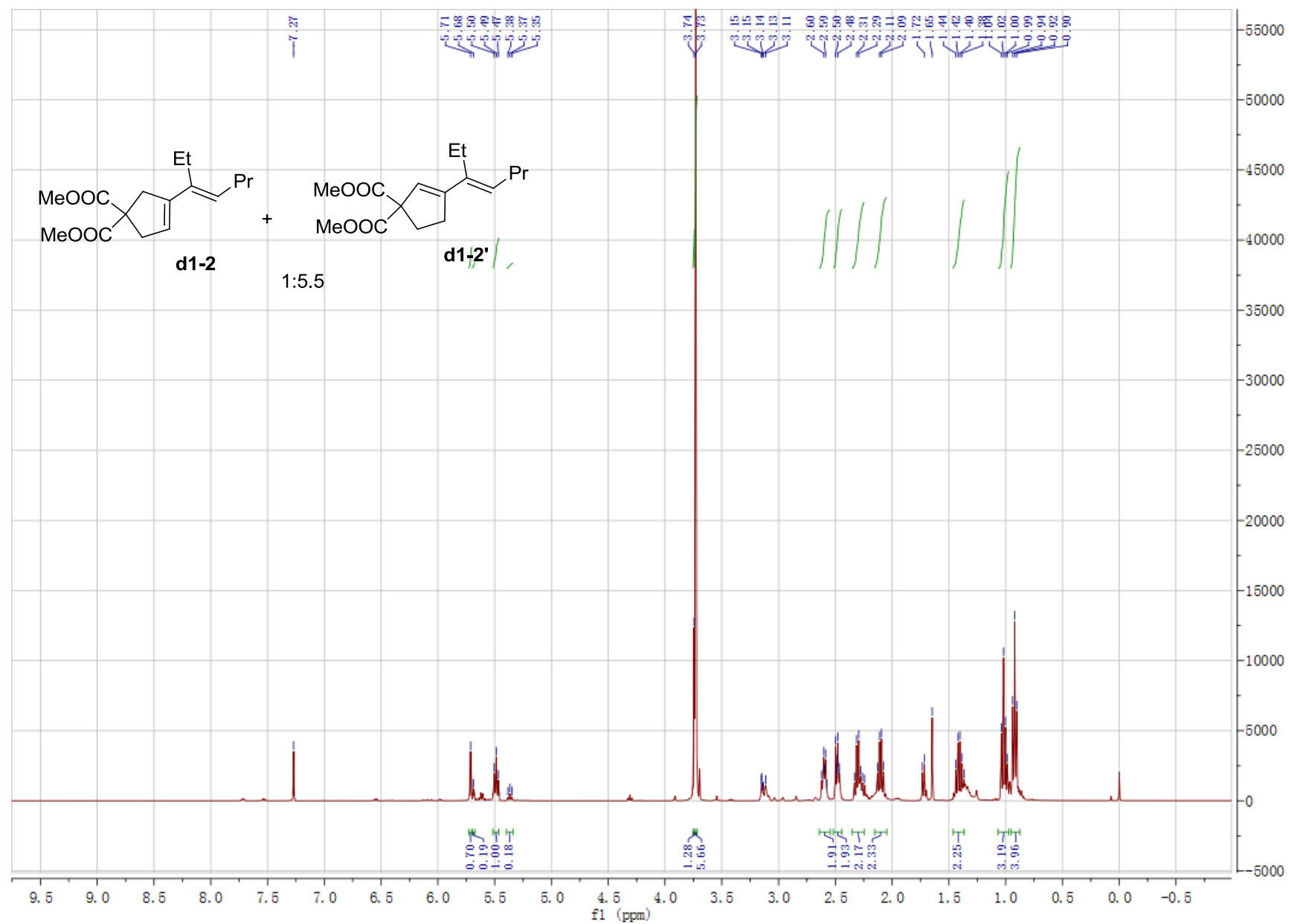


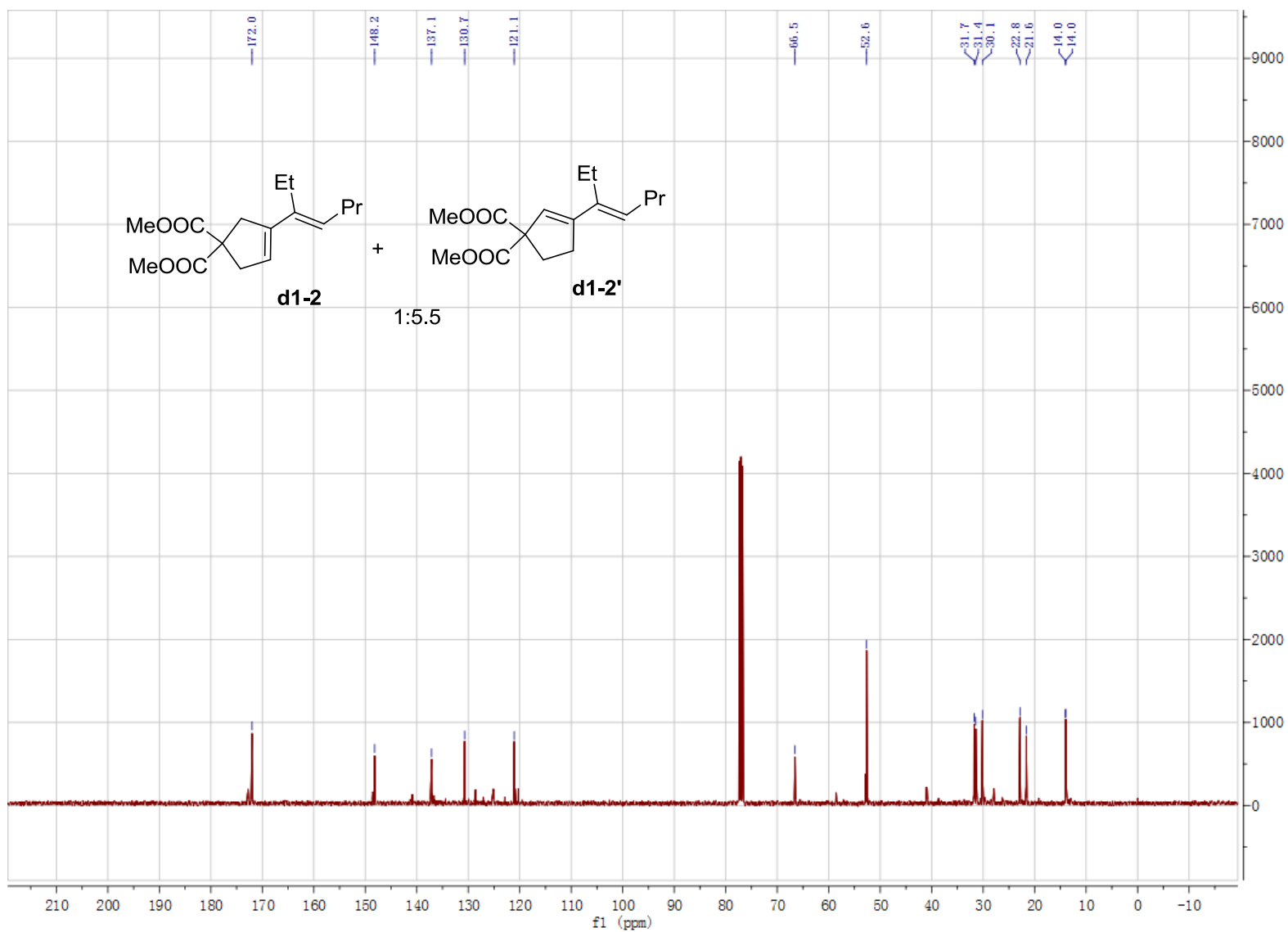


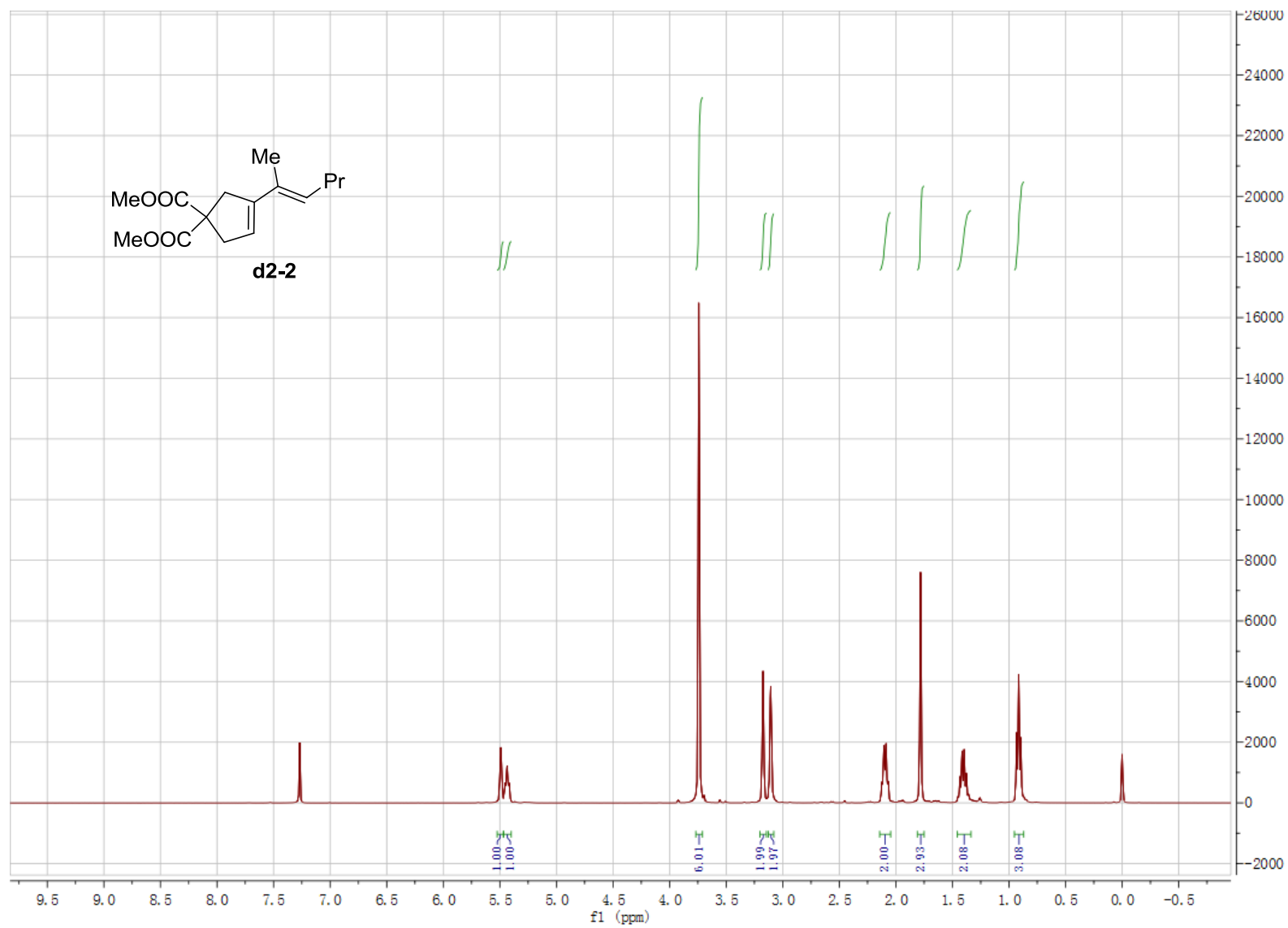


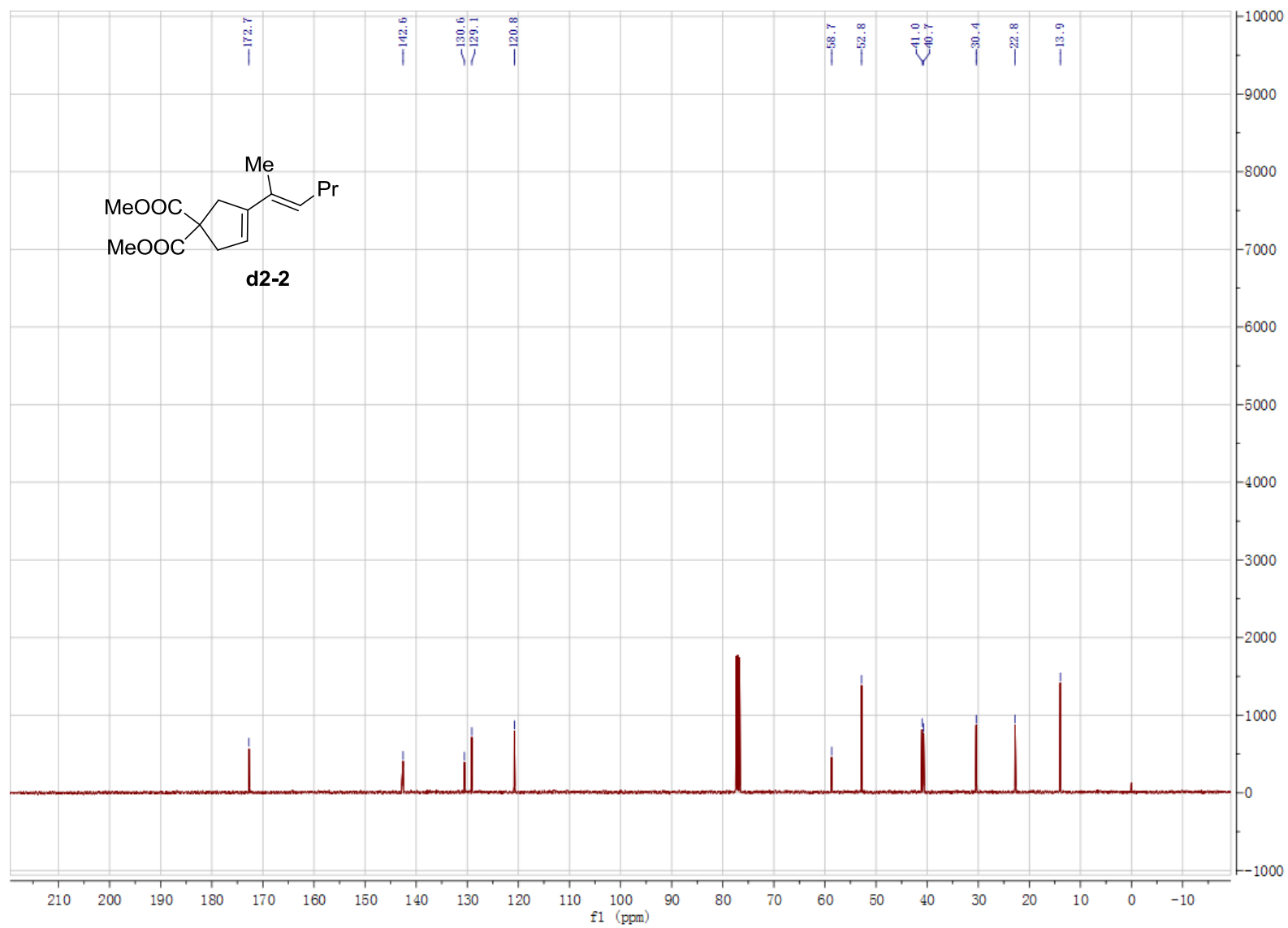












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