

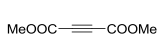
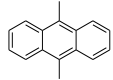
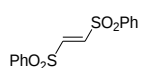
Supporting Information

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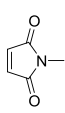
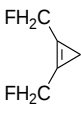
Compared with B3LYP and O3LYP recommended by the referee, M06-2X/6-31+G(d)//B3LYP/6-31G(d) method also performed best for the six representative Diels-Alder reaction activation enthalpies with a precision of 0.8 kcal/mol.

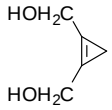
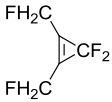
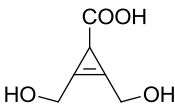
Table S1. Theoretical activation enthalpies of Diels-Alder reactions by different methods

	Dienophile	Diene	$\Delta H_{(exp.)}^{\ddagger a}$	$\Delta H_{(cal.)}^{\ddagger b}$		
				B3LYP	O3LYP	M06-2X
C1			14.3	18.9	21.5	11.5
C2			14.1	22.1	25.8	13.0
C3			13.6	23.0	27.7	10.2
C4			11.6	17.2	20.0	8.8
C5			10.8	17.6	20.2	9.2
C6			7.8	19.3	25.4	5.6
		R		0.4599	0.1056	0.9428
		RMSE		2.3	3.6	0.8

^a J. Sauer, *Chem. Ber.*, 1964, **97**, 3183-3207. ^b basis set: 6-31+g*

Table S2. Calculated activation enthalpies of Diels-Alder and thiol addition reactions of designed alkenes

Entry	Diene	Dienophile	$\Delta G^{\ddagger}(\text{cal})(\text{kcal/mol})$		$\Delta H^{\ddagger}(\text{cal})^b(\text{kcal/mol})$	
			Diels-Alder	Thiol Addition	Diels-Alder	Thiol addition
5-1			20.9	3.4	11.3	-6.9
5-2			21.5	—	11.5	—
5-3			26.8	—	18.0	—
5-4			24.9	20.1	16.2	12.6

<u>5-5</u>			16.6(-65.0) ^a	Not obtained computationally	6.5	Not obtained computationally
<u>5-6</u>			22.3(-57.1) ^a	27.1	13.4	20.3
5-7			29.5	—	21.2	—
<u>5-8</u>			24.2(-49.1) ^a	26.2	15.5	19.0

^a Gibbs free energy of the Diels-Alder reaction ^b activation enthalpy of the Diels-Alder reaction

Energies of Intermediates and Transition States

Table S1. Gibbs Free Energy Corrections and Electronic Energies in Solvate of related compounds and Transition States

Entry	dienophile		diene		TS	
	Thermal		Thermal		Thermal	
	Correction of Gibbs Free Energies (Hartree)	Electronic Energy in solvent (Hartree)	Correction of Gibbs Free Energies (Hartree)	Electronic Energy in solvent (Hartree)	Correction of Gibbs Free Energies (Hartree)	Electronic Energy in solvent (Hartree)
1	0.026813	-379.166142	0.035779	-1075.05374	0.085838	-1454.1991
2	0.026813	-379.166142	0.047488	-615.486706	0.097489	-994.634998
3	0.026813	-379.166142	0.074146	-654.784865	0.123713	-1033.93538
4	0.026813	-379.166142	0.059036	-155.914614	0.109495	-535.066269
5	0.026813	-379.166142	0.085028	-195.214641	0.135299	-574.364996
6	0.026813	-379.166142	0.11262	-234.507575	0.162898	-613.659765
7	0.026813	-379.166142	0.138482	-273.798626	0.189416	-652.954409
8	0.026813	-379.166142	0.112424	-234.511667	0.161589	-613.665221
9	0.026813	-379.166142	0.16545	-313.093609	0.216767	-692.249074
10	0.026813	-379.166142	0.191403	-352.389962	0.242596	-731.548289
11	0.026813	-379.166142	0.09458	-233.317228	0.145067	-612.4686
12	0.034269	-379.166142	0.073017	-194.019336	0.126241	-573.177096
13	0.026813	-379.166142	0.088973	-270.400448	0.139255	-649.549836
14	0.026813	-379.166142	0.043924	-229.937587	0.093756	-609.092536
15	0.039185	-359.315999	0.043924	-229.937587	0.106243	-589.235126
16	0.099161	-534.922996	0.0663	-194.01371	0.189569	-728.930875
17	0.064042	-398.604514	0.0663	-194.01371	0.154931	-592.613502
18	0.091564	-437.900747	0.0663	-194.01371	0.182063	-631.910041
19	0.117984	-477.194242	0.0663	-194.01371	0.208753	-671.203499
20	0.145213	-516.487587	0.0663	-194.01371	0.235352	-710.496677
21	0.139292	-629.56919	0.0663	-194.01371	0.229925	-823.578227
22	0.064042	-398.604514	0.112424	-234.504646	0.199041	-633.100262
23	0.091564	-437.900747	0.112424	-234.504646	0.225962	-672.396695
24	0.117984	-477.194242	0.112424	-234.504646	0.251686	-711.690109
25	0.145213	-516.487587	0.112424	-234.504646	0.278401	-750.9832
26	0.064042	-398.604514	0.09458	-233.310376	0.18246	-631.90458
27	0.091564	-437.900747	0.09458	-233.310376	0.210013	-671.201112
28	0.117984	-477.194242	0.09458	-233.310376	0.236551	-710.494576
29	0.145213	-516.487587	0.09458	-233.310376	0.263201	-749.786854
30	0.012382	-447.365703	0.0663	-194.016076	0.102453	-641.385615
31	0.016318	-355.172578	0.0663	-194.016076	0.106627	-549.18614
32	0.021525	-262.97457	0.0663	-194.016076	0.111024	-456.978507
33	0.020858	-262.973331	0.0663	-194.016076	0.111035	-456.97656

34	0.025101	-170.761778	0.0663	-194.016076	0.11464	-364.759749
35	0.020678	-262.967232	0.0663	-194.016076	0.110413	-456.977831
36	0.101547	-534.147802	0.0663	-194.016076	0.192637	-728.15286
37	0.018277	-1224.2831	0.0663	-194.016076	0.109829	-1418.29964
38	0.185735	-1637.45393	0.0663	-194.016076	0.277929	-1831.463
39	0.113151	-590.271011	0.0663	-194.016076	0.2034	-784.279072
40	0.054846	-381.315667	0.0663	-194.016076	0.14534	-575.321923
41	0.0761	-532.876346	0.0663	-194.016076	0.164891	-726.882545
42	0.034269	-379.165504	0.0663	-194.016076	0.126241	-573.175051
43	0.064042	-398.603156	0.0663	-194.016076	0.154931	-592.610606
44	0.065527	-306.346137	0.0663	-194.016076	0.155475	-500.345638
45	0.100951	-534.140502	0.0663	-194.016076	0.191552	-728.137733
46	0.092548	-383.728896	0.0663	-194.016076	0.18361	-577.734884
47	0.013843	-379.165504	0.19068	-617.903012	0.240026	-997.065408
48	0.001771	-1224.28311	0.19068	-617.903012	0.229797	-1842.18571
49	0.021658	-639.98258	0.19068	-617.903012	0.251882	-1257.88492
50	0.045364	-398.562566	0.19068	-617.903012	0.272063	-1016.45503
51	0.037786	-418.470054	0.19068	-617.903012	0.266132	-1036.36386
52	0.04505	-398.558903	0.19068	-617.903012	0.271909	-1016.45128
53	0.082936	-534.147802	0.19068	-617.903012	0.308373	-1152.03818
54	0.132374	-612.745556	0.19068	-617.903012	0.359812	-1230.63653
55	0.094092	-498.015349	0.19068	-617.903012	0.319123	-1115.90368
56	0.013788	-170.761778	0.19068	-617.903012	0.238933	-788.650207
57	0.057859	-532.883679	0.19068	-617.903012	0.282236	-1150.77089
58	0.051522	-306.346137	0.19068	-617.903012	0.276222	-924.23328
59	0.038318	-210.061097	0.19068	-617.903012	0.263813	-827.947285
60	0.075911	-345.644971	0.19068	-617.903012	0.302417	-963.530291
61	0.027421	-305.089092	0.19068	-617.903012	0.25101	-922.97096
62	0.087645	-309.514591	0.19068	-617.903012	0.314153	-927.399838
63	0.114847	-423.996352	0.19068	-617.903012	0.341479	-1041.88012
64	0.082227	-534.140502	0.19068	-617.903012	0.309641	-1152.02547
65	0.120133	-537.321509	0.19068	-617.903012	0.347435	-1155.20571
66	0.03831	-210.06401	0.19068	-617.903012	0.264412	-827.945972
67	0.076016	-345.647705	0.19068	-617.903012	0.302387	-963.528795
68	0.012382	-447.365703	0.047488	-615.48354	0.08259	-1062.83594
69	0.012382	-447.365703	0.059043	-155.911542	0.094667	-603.269097
70	0.012382	-447.365703	0.08564	-195.210628	0.120239	-642.570187
71	0.012382	-447.365703	0.085028	-195.211108	0.120393	-642.572791
72	0.012382	-447.365703	0.112424	-234.508003	0.14544	-681.871644
3-1	0.064042	-398.604514	0.059036	-155.909812	0.147303	-554.503907
3-2	-0.007087	-475.36419	0.059036	-155.909812	0.073358	-631.246568
3-3	0.028212	-415.498857	0.059036	-155.909812	0.111044	-571.384939
3-4	0.028484	-1426.31147	0.059036	-155.909812	0.11441	-1582.20786
5-2	0.032341	-116.567538	0.059036	-155.909812	0.114052	-272.464498

5-3	0.084141	-195.171115	0.059036	-155.909812	0.166388	-351.060132
5-4	0.066327	-393.586704	0.059036	-155.909812	0.148977	-549.479125
5-5	0.027911	-790.466953	0.059036	-155.909812	0.112988	-946.375053
5-6	0.091966	-345.560168	0.059036	-155.909812	0.175078	-501.457209
5-7	0.048139	-592.028967	0.059036	-155.909812	0.131712	-747.914976
5-8	0.101788	-534.0914	0.059036	-155.909812	0.18647	-689.987
cyc4	0.061329	-155.895139	0.059036	-155.909812	0.142998	-311.777149
cyc5	0.089909	-195.22918	0.059036	-155.909812	0.1729	-351.107101
cyc6	0.118349	-234.531243	0.059036	-155.909812	0.200664	-390.400907
cyc7	0.145699	-273.817645	0.059036	-155.909812	0.228546	-429.689552
cyc8	0.173611	-313.109726	0.059036	-155.909812	0.256491	-468.986607
5-1thioadd	0.064042	-398.604514	0.013537	-438.156643	0.097868	-836.775996
5-4thioadd	0.066327	-393.586704	0.013537	-438.156643	0.097223	-831.728685
5-6thioadd	0.091966	-345.560168	0.013537	-438.156643	0.122705	-783.690799
5-8thioadd	0.101788	-534.0914	0.013537	-438.156643	0.134046	-972.225

Cartesian Coordinates

01-diene

C	-0.55455400	-0.48439700	0.00000600
C	-0.45441900	-1.81693400	0.00115200
H	-1.33803100	-2.44347500	0.00148700
H	0.51519700	-2.29911700	0.00194300
C	0.55455500	0.48440100	0.00000400
C	0.45442500	1.81693900	0.00115100
H	1.33804000	2.44347500	0.00148800
H	-0.51518800	2.29912700	0.00194800
Cl	2.17199100	-0.23428500	-0.00061000
Cl	-2.17199400	0.23428200	-0.00061000

01-dienophile

C	-0.66782300	1.25821500	-0.00030300
C	0.66782200	1.25821600	0.00035100
C	-1.13200700	-0.15883700	-0.00011500
C	1.13200900	-0.15883600	0.00020600
O	2.24568300	-0.59970200	-0.00053000
O	-2.24568400	-0.59970200	-0.00016000
O	0.00000000	-0.97201800	0.00054600
H	-1.36080100	2.08941600	-0.00052000
H	1.36079900	2.08941800	0.00083600

01ts

C	-1.73789200	-0.69506200	0.98239100
C	-1.73813900	0.69449000	0.98242900
C	0.35662000	1.42222000	1.53002800
C	1.18009100	0.71065700	0.67660200
C	1.18033800	-0.71033100	0.67660000
C	0.35706400	-1.42217800	1.52998300
C	-1.71918900	-1.14110800	-0.43489200
C	-1.71963200	1.14063100	-0.43483100
H	0.28618300	2.49933700	1.42665300
H	0.28693600	-2.49930900	1.42654800
O	-1.80404700	2.24075300	-0.90468200
O	-1.80311700	-2.24124200	-0.90480800
H	0.11851300	-1.02187100	2.50695900
H	0.11822200	1.02180100	2.50699700
H	-2.14434600	-1.34080600	1.74962200

H	-2.14478600	1.34005800	1.74970700
Cl	2.00171700	-1.58673100	-0.59103300
Cl	2.00110600	1.58733400	-0.59107300
O	-1.58337100	-0.00018500	-1.23057900

02-diene

C	1.24836700	0.58009500	-0.00036700
C	2.08094700	-0.46685700	0.00036000
H	3.15620800	-0.31907200	-0.00018300
H	1.72082900	-1.49039800	0.00108900
C	-0.21242900	0.54677400	0.00000300
C	-0.98684300	1.63836200	0.00027100
H	-2.06871200	1.58351900	0.00039600
H	-0.52793400	2.62279500	0.00030600
H	1.65551700	1.59056200	-0.00136900
Cl	-0.98330400	-1.04574400	-0.00010800

02ts

C	0.83478800	0.63722000	1.32610800
C	1.65339300	-0.39549500	0.87701300
C	0.32413700	-2.24972500	0.50579600
C	-0.71227600	-1.71739200	-0.23526700
C	-1.50697000	-0.66760200	0.26339400
C	-1.27284100	-0.07020000	1.49174800
C	0.63782000	1.57106200	0.18334800
C	1.96082800	-0.13826100	-0.54835300
H	1.00580700	-2.95777000	0.04455700
H	-1.81753500	0.82464100	1.77282100
O	2.68839000	-0.71399000	-1.30976300
O	0.09708200	2.64070700	0.13985300
H	-0.91728300	-0.68625900	2.30967700
H	0.28699300	-2.27583100	1.58867300
H	0.78081300	1.01216600	2.34003700
H	2.31648700	-1.00346700	1.47768200
Cl	-2.61368600	0.11354600	-0.85545500
O	1.22179800	0.98567100	-0.94044000
H	-0.79406700	-1.96051100	-1.29062300

03-diene

C	0.25958900	0.48512200	-0.00000500
C	0.29474100	1.82322100	-0.00001400

H	1.23051000	2.36895500	-0.00001600	C	0.60203700	0.41058700	0.00000000
H	-0.62204800	2.40152200	-0.00001800	C	0.60203800	1.75119500	0.00000000
C	-0.96240900	-0.34138000	-0.00000100	H	1.55164100	-0.12541000	0.00000000
C	-0.93919500	-1.68288900	-0.00001400	H	1.52370900	2.32501600	0.00000000
H	-1.86519800	-2.24994300	-0.00001500	H	-0.32544100	2.31986900	0.00000000
H	-0.01620000	-2.25026100	-0.00002400				
C	-2.27622700	0.41118900	0.00001400				
H	-2.37073000	1.05439300	0.88337800	04ts			
H	-2.37072400	1.05444800	-0.88331000	C	0.28711700	0.69710800	1.14945000
H	-3.11598600	-0.28839100	-0.00001100	C	0.28894700	-0.69635600	1.14948700
Cl	1.81596400	-0.36837000	0.00000800	C	-1.68347900	-1.44143900	0.32346200
				C	-1.80221200	-0.70528800	-0.84408900
03ts				C	-1.80405900	0.70091300	-0.84392500
C	-1.18397000	-1.03379300	1.10537000	C	-1.68717300	1.43708900	0.32380700
C	-1.74746600	0.23269800	0.97553100	C	1.11405100	1.14271700	0.00210300
C	-0.09583600	1.78423300	1.27687900	C	1.11703400	-1.13992600	0.00218400
C	0.89244900	1.36727700	0.39630600	H	-1.53416900	-2.51605900	0.27628300
C	1.45249400	0.07841300	0.59294800	H	-1.54076600	2.51212300	0.27687500
C	1.01083200	-0.80322800	1.56504300	O	1.47416100	-2.23723500	-0.32920000
C	-1.02434100	-1.58967700	-0.26202400	O	1.46831800	2.24092900	-0.32938600
C	-1.93169200	0.49546100	-0.47052500	H	-2.09807400	1.06657600	1.25673200
H	-0.61605200	2.71836100	1.08752700	H	-2.09537900	-1.07223200	1.25646400
H	1.38154900	-1.82237900	1.57474100	H	0.16691200	1.33888900	2.01210200
O	-2.44727800	1.41813700	-1.04093400	H	0.17025500	-1.33839700	2.01216200
O	-0.68097700	-2.67911500	-0.62789200	O	1.46910100	0.00180400	-0.72566500
O	-1.36242000	-0.57633600	-1.16667100	H	-1.67302000	1.21087200	-1.79560800
H	0.66910600	-0.41658500	2.51725200	H	-1.66975500	-1.21467200	-1.79588500
H	-0.12065900	1.44393500	2.30473300				
H	-1.29208800	-1.70090700	1.95048800	05-diene			
H	-2.35838400	0.74644800	1.70569500	C	-2.53033400	-0.26041300	0.00000000
C	1.18718900	2.16372300	-0.85229000	C	-1.36064300	0.39560200	-0.00000100
H	2.25352300	2.41015700	-0.91093600	C	-0.05301400	-0.24449400	0.00000000
H	0.93786400	1.59871100	-1.75700700	C	1.11458600	0.41948800	0.00000000
H	0.61754200	3.09587700	-0.85895300	C	2.47177100	-0.21736400	0.00000000
Cl	2.53500200	-0.56151400	-0.64076400	H	-1.36259000	1.48639100	0.00000000
				H	-3.48056800	0.26486200	0.00000200
04-diene				H	-2.57379100	-1.34746900	0.00000100
C	-0.60203700	-1.75119500	0.00000000	H	1.09349900	1.51084700	0.00000000
C	-0.60203700	-0.41058700	0.00000000	H	-0.04486300	-1.33590500	-0.00000100
H	0.32544100	-2.31987000	0.00000000	H	3.05501400	0.08739600	0.88004500
H	-1.52370900	-2.32501600	0.00000000	H	2.40407500	-1.31044400	-0.00001400
H	-1.55164000	0.12541000	0.00000000	H	3.05502500	0.08741800	-0.88003000

05ts

C	0.07076400	-0.61498000	1.19672300
C	-1.11282500	0.12545200	1.10903100
C	-0.76913700	2.06187100	0.52027500
C	-0.12704600	1.95559300	-0.71807800
C	1.12226100	1.33783400	-0.87610600
C	1.86826000	0.82933400	0.17325100
C	0.12863300	-1.53630000	0.06834900
C	-1.84788600	-0.40526600	-0.08501700
H	-1.76783700	2.48969000	0.54856800
H	-0.70788900	2.15504700	-1.61573600
O	-2.95346800	-0.15176900	-0.47996900
O	0.91966500	-2.39851400	-0.22188100
O	-1.00475300	-1.28598300	-0.74201800
H	1.70555200	1.22460300	1.17066400
H	-0.17929200	2.24982000	1.41320500
H	-1.69296900	0.45201200	1.96488400
H	0.69711700	-0.75164200	2.06704100
H	1.44989200	1.11090100	-1.88936100
C	3.09523900	-0.00811700	-0.03018300
H	3.90844800	0.30470800	0.63460800
H	2.88092900	-1.06629400	0.17388000
H	3.44493000	0.04876200	-1.06627700

06-diene

C	-2.25437800	-0.61694400	-0.00019900
H	-2.75519600	-1.59098700	-0.00024900
H	-2.59343300	-0.06829500	0.88561200
H	-2.59292700	-0.06843100	-0.88628700
C	1.56197300	0.32398100	-0.00007400
C	2.25604100	-0.82253600	-0.00003400
H	2.11312100	1.26463000	-0.00030000
H	3.34204900	-0.81931600	-0.00022300
H	1.77851500	-1.79808500	0.00009300
C	0.09783900	0.46360800	0.00003900
C	-0.43913400	1.69597100	0.00006300
H	-1.50986700	1.86817000	0.00020400
H	0.19087700	2.58194600	-0.00001800
C	-0.73572400	-0.80354500	0.00022900
H	-0.44619100	-1.40671100	-0.87242100
H	-0.44664500	-1.40613600	0.87344400

06ts

C	-1.74240100	-0.13580700	0.90302800
C	-0.67966000	0.64672900	1.35793600
C	1.19047700	-0.55861000	1.34940500
C	1.23946900	-1.05925000	0.05193000
C	0.18002100	-1.87714000	-0.40009100
C	-0.92144000	-2.19051600	0.37709700
C	-2.03462700	0.27192600	-0.48723000
C	-0.29830500	1.55793400	0.25161600
H	1.93009600	0.15832100	1.68956900
H	0.12618600	-2.08109200	-1.46873000
H	-1.77389300	-2.69211700	-0.07170200
O	0.49685100	2.45940800	0.21684900
O	-2.91285000	-0.05309900	-1.23850500
O	-1.04563100	1.19406400	-0.86945200
H	-0.83587800	-2.30275200	1.45233800
H	0.72427300	-1.13725500	2.13879300
H	-2.51626700	-0.58499100	1.51093800
H	-0.49608600	0.93880300	2.38357300
C	2.24321700	-0.56333500	-0.98022000
H	2.68456000	-1.44946100	-1.45850000
H	1.69437400	-0.04310000	-1.77719100
C	3.35850800	0.34815100	-0.46410700
H	3.94342000	-0.13552200	0.32720100
H	4.04424400	0.59728600	-1.28045600
H	2.95645300	1.28840100	-0.07315000

07-diene

C	2.70341500	-0.33036400	0.11412700
C	1.52287700	-0.34470300	-0.51551900
C	0.31690800	0.42038500	-0.12508500
C	-1.00827200	-0.30017100	-0.35691900
C	-1.12680400	-1.52728100	0.57145100
C	0.41292000	1.65941200	0.38030500
C	-2.24894600	0.59163500	-0.23415300
H	1.40724300	-0.99177500	-1.38756900
H	3.54822600	-0.90682700	-0.25249400
H	2.86309000	0.25175700	1.01826700
H	-0.45624300	2.23171100	0.68718100
H	1.37713400	2.14727700	0.49046100
H	-0.97599000	-0.68080500	-1.39093300
H	-2.18922000	1.46029800	-0.89880100

H	-3.14921800	0.02466100	-0.49629400	C	1.02768700	-1.53227100	-0.00026000
H	-2.37978700	0.95733600	0.79143600	H	2.06561600	-1.85348700	-0.00017400
H	-0.26472800	-2.19516400	0.47128200	H	0.28433500	-2.32228700	-0.00034100
H	-1.18122000	-1.20982500	1.61974600	C	1.79863500	0.81874400	0.00029200
H	-2.03188300	-2.10211500	0.34248200	H	1.73331800	1.46876300	-0.88110900
07ts				H	1.73271700	1.46796600	0.88229700
C	-1.32859600	0.57985900	-1.34176200	H	2.78635500	0.34933100	0.00035500
C	-2.03117300	-0.48531700	-0.78326400	C	-1.79863500	-0.81874400	0.00029200
C	-0.53235300	-2.24656300	-0.54119200	H	-1.73331500	-1.46876900	-0.88110300
C	0.53911800	-1.61933000	0.06574700	H	-1.73272100	-1.46795900	0.88230300
C	1.20907700	-0.51008600	-0.50073000	H	-2.78635600	-0.34933100	0.00034800
C	0.77816000	-0.02572100	-1.73327400	08ts			
C	-1.02177200	1.53025300	-0.24362800	C	-1.22730300	-0.69765900	1.11087400
C	-2.16599000	-0.22812400	0.66349100	C	-1.22722300	0.69777800	1.11087000
H	-1.10539800	-2.98957800	0.00569400	C	0.90551000	1.40119400	1.29788300
H	0.73227700	-1.85430500	1.10865100	C	1.55643800	0.71175900	0.28098300
H	1.20279200	0.89458400	-2.12659900	C	1.55637600	-0.71190300	0.28096700
O	-2.76333300	-0.81778200	1.52205600	C	0.90539300	-1.40130400	1.29785400
O	-0.51135300	2.61815000	-0.26953600	C	-1.40395300	-1.14270700	-0.28897100
O	-1.42628600	0.93389300	0.95113600	C	-1.40382400	1.14283300	-0.28898200
H	0.36592900	-0.69440200	-2.48070100	H	0.80576700	2.48108800	1.23309300
H	-0.62764600	-2.29153300	-1.62008300	H	0.80555000	-2.48118700	1.23303900
H	-2.72396800	-1.14311800	-1.29006900	O	-1.54883500	2.24015900	-0.75641000
C	3.66871300	-0.17287400	-0.13201400	O	-1.54909400	-2.24001800	-0.75639200
H	4.42979300	0.42986100	0.37676400	O	-1.36264900	0.00005800	-1.09950300
H	3.83258700	-1.22304900	0.13876800	H	0.84383600	-0.99870200	2.30184200
H	3.82312800	-0.07711700	-1.21238100	H	0.84392100	0.99857700	2.30186300
C	2.25290300	0.28544100	0.28093600	H	-1.52855200	-1.34065700	1.92709900
C	2.09235000	0.24104100	1.80842900	H	-1.52841600	1.34081300	1.92708600
H	2.13948400	1.33251400	-0.03043300	C	2.03831800	-1.46544400	-0.93914700
H	1.08343600	0.53162100	2.11688900	H	1.47086600	-1.19130300	-1.83686800
H	2.30585800	-0.75556500	2.21364500	H	3.09287600	-1.24405900	-1.14574600
H	2.80182400	0.93462500	2.27269400	H	1.94276900	-2.54496300	-0.79987600
H	-1.41493300	0.93989800	-2.35852200	C	2.03844600	1.46528300	-0.93911600
08-diene				H	3.09298500	1.24381300	-1.14571700
C	-0.70559200	0.22709600	-0.00020600	H	1.47097200	1.19120500	-1.83684300
C	-1.02768600	1.53227100	-0.00026100	H	1.94298500	2.54480800	-0.79982500
H	-2.06561600	1.85348800	-0.00017000	09-diene			
H	-0.28433400	2.32228600	-0.00033600	C	-1.61520500	-0.51164200	0.31467800
C	0.70559200	-0.22709600	-0.00020200	C	-2.83989300	-0.39486900	-0.21171800

H	-3.61231500	-1.13418700	-0.01809700	H	-3.17680900	1.05246900	1.33940400
H	-3.10856800	0.43668700	-0.85836800	H	-2.04857500	2.03276900	0.37164800
C	-0.50823100	0.45807000	0.13308800	H	-3.62016000	1.56727500	-0.29084100
C	-0.76993900	1.77472200	0.13331400	C	-2.18831500	-0.05841700	-0.28130800
H	-0.00608100	2.52725900	-0.02631900	C	-3.28973200	-1.14744100	-0.31714100
H	-1.77704800	2.14131100	0.30937900	H	-2.92895600	-2.07478100	-0.77593200
H	-1.39747900	-1.39795500	0.91044800	H	-3.64397800	-1.38738200	0.69200200
C	0.90654800	-0.12693800	-0.02960500	H	-4.14638300	-0.79477300	-0.90369200
C	1.33326800	-0.82164700	1.28701800	H	2.96940800	-0.98358700	1.33944100
C	0.90327600	-1.16392900	-1.17698600	H	1.57157800	1.09841600	2.28329400
C	1.94944800	0.95658600	-0.35677100				
H	1.34183800	-0.10978100	2.12013400				
H	0.66824700	-1.64893700	1.55688100	10-diene			
H	2.34340900	-1.23609900	1.18301200	C	-1.42390300	0.66599700	1.37682300
H	0.62789300	-0.69341500	-2.12790900	C	-1.35762500	-0.11243600	0.05057900
H	1.89928000	-1.60835600	-1.29310100	C	-2.72021100	-0.01170100	-0.66379400
H	0.19242200	-1.97585500	-0.99098400	C	-0.28760400	0.51910000	-0.89460300
H	2.93416800	0.49458500	-0.49152800	C	1.14391400	0.58930000	-0.39038500
H	1.70095800	1.48960800	-1.28134200	C	1.66844800	1.74522900	0.04908800
H	2.03765000	1.69302300	0.44968700	C	-1.05718600	-1.59568000	0.33824900
				C	1.95748000	-0.64382300	-0.47070800
				C	2.94644600	-0.99673500	0.35993100
09ts				H	-0.62047600	1.53569700	-1.13827900
C	1.50272400	0.67627900	1.28965800	H	-0.29982100	-0.04472500	-1.83980200
C	2.23614000	-0.40252000	0.79640900	H	-2.20040600	0.25032300	2.03058300
C	0.86231800	-2.20446700	0.70094200	H	-0.47078900	0.62373500	1.91409900
C	-0.26841400	-1.70992100	0.07400300	H	-1.66394000	1.72297900	1.20475100
C	-1.02444400	-0.61811700	0.56518200	H	1.70062900	-1.32071600	-1.28711800
C	-0.59354100	-0.01658500	1.74440600	H	3.51433900	-1.90996300	0.20628700
C	1.16852100	1.54586100	0.13868700	H	3.21590200	-0.39336300	1.22322600
C	2.37148100	-0.22084900	-0.66506700	H	1.07432900	2.65353000	0.10575000
H	1.47257400	-2.94876900	0.19759900	H	2.70932600	1.82388500	0.35026200
H	-0.46437200	-2.05093300	-0.93924600	H	-1.00094800	-2.17776700	-0.59047000
H	-1.06192600	0.88727500	2.11475900	H	-0.11077300	-1.72419600	0.87230200
O	2.99086100	-0.84343100	-1.48364900	H	-1.85249200	-2.03316500	0.95451300
O	0.62177400	2.61639600	0.09404600	H	-2.98318300	1.03186500	-0.87706000
O	1.60181500	0.89741100	-1.01983000	H	-2.71156600	-0.55639400	-1.61634100
H	-0.09485800	-0.60853800	2.50292700	H	-3.51867700	-0.43721400	-0.04378800
H	0.95973500	-2.18606500	1.78091500				
C	-1.74968100	0.26339100	-1.73021500				
H	-2.61332800	0.62534600	-2.30031900	10ts			
H	-0.97949700	1.03914700	-1.75322300	C	2.04070000	0.69282600	1.20920000
H	-1.35986300	-0.61499000	-2.25445600	C	2.72937000	-0.42775800	0.74984500
C	-2.78542300	1.22347200	0.32964100	C	1.20968200	-2.17644900	0.64001200

C	0.15370300	-1.58141300	-0.02312900	C	-1.19489500	-0.73245700	0.23953300
C	-0.50379800	-0.41885800	0.44356300	H	-2.03620500	-1.27338400	-0.20943400
C	-0.07457700	0.16549700	1.63339800	H	-1.36113000	-0.76380800	1.33013800
C	1.75867900	1.55014600	0.02979700	H	-2.03767400	1.27099800	0.20957000
C	2.88177600	-0.29411400	-0.71265800				
H	1.77557000	-2.96854800	0.15867300				
H	-0.04034900	-1.88553500	-1.04984200				
H	-0.47888300	1.12720700	1.93619900				
O	3.47959900	-0.96277000	-1.51102700				
O	1.26654200	2.64471800	-0.04067700				
O	2.16214900	0.84810400	-1.10470300				
H	0.31341100	-0.44357300	2.44271800				
H	1.29284400	-2.13911900	1.72042200				
H	3.40907600	-1.04898200	1.31704500				
C	-1.47047300	0.31527700	-0.46463900				
H	2.12891500	1.13837500	2.19143400				
H	-1.31931000	1.39488200	-0.33888800				
H	-1.22612900	0.08824000	-1.51004900				
C	-2.98650800	0.00474500	-0.24798400				
C	-3.77700000	0.84324500	-1.27123000				
H	-4.85438900	0.66484600	-1.17094400				
H	-3.59984200	1.91602200	-1.12827500				
H	-3.49039200	0.59048600	-2.29931000				
C	-3.43156800	0.39309300	1.17316700				
H	-2.90814600	-0.19306200	1.93676300				
H	-3.24329600	1.45534300	1.37324700				
H	-4.50651000	0.21717300	1.29990600				
C	-3.27334500	-1.48912600	-0.48818900				
H	-4.34416900	-1.69822000	-0.37782400				
H	-2.97930300	-1.79341100	-1.50060600				
H	-2.73527200	-2.12519300	0.22367000				
11-diene							
C	0.11453700	-1.42498100	-0.06445100				
C	1.26067500	-0.72549400	-0.10397600				
C	1.25981300	0.72694900	0.10400900				
C	0.11287100	1.42510800	0.06436900				
C	-1.19577100	0.73107400	-0.23950400				
H	2.21028100	1.22855300	0.27198500				
H	0.11734700	-2.50621300	-0.18457400				
H	2.21173800	-1.22599000	-0.27191600				
H	0.11442900	2.50635700	0.18444900				
H	-1.36216500	0.76229200	-1.33009700				
				11-ts			
				C	-0.38179300	0.69697400	-1.05611500
				C	-0.38186300	-0.69700600	-1.05611900
				C	1.31061700	-1.36557900	0.29817500
				C	0.93377800	-0.70133200	1.46106800
				C	0.93405000	0.70181000	1.46086400
				H	1.15762100	-2.44023800	0.23234900
				H	0.42769000	-1.24080900	2.25711600
				H	0.42820100	1.24172100	2.25677000
				C	1.31101900	1.36556900	0.29773700
				C	-1.50848400	1.14183400	-0.20664700
				C	-1.50859500	-1.14178100	-0.20667100
				O	-1.93688100	-2.24232400	0.01589500
				O	-2.06958200	0.00005200	0.37783000
				O	-1.93666000	2.24241700	0.01593100
				H	-0.00554100	-1.34305400	-1.83778900
				C	2.39745600	-0.77939600	-0.57969000
				C	2.39745700	0.77882700	-0.58022200
				H	1.15842800	2.44026900	0.23162500
				H	-0.00551200	1.34297600	-1.83784100
				H	3.35709400	1.14194200	-0.18921600
				H	2.32387300	1.17451600	-1.59869800
				H	2.32436800	-1.17577200	-1.59791000
				H	3.35690100	-1.14223000	-0.18794900
				12-diene			
				C	0.02833100	-0.00020700	-0.01207500
				C	0.03986600	0.00011100	1.33698100
				C	1.43062100	-0.00003000	1.81197400
				C	2.26427300	-0.00037800	0.75129900
				C	1.44818300	-0.00094300	-0.51570100
				H	1.71996400	0.00029800	2.85812500
				H	3.34800800	-0.00045300	0.77254500
				H	1.66254900	-0.87964300	-1.14376300
				H	1.66309600	0.87675400	-1.14495300
				H	-0.84297800	-0.00012000	-0.65708500
				H	-0.82877900	0.00055700	1.98776800

C	-1.09502400	-0.34739500	0.00006100
C	-0.71785400	0.95996200	-0.00004300
C	0.71799200	0.95986600	0.00001900
C	1.09497300	-0.34754500	0.00001900
O	-0.00008200	-1.16102300	-0.00005400
H	-2.05029100	-0.84983100	0.00010200
H	-1.37365900	1.81949400	-0.00007800

H	1.37391600	1.81930700	0.00003400	H	-1.97260900	2.04569000	-0.43965000
H	2.05017000	-0.85011000	0.00003000	H	-1.03219600	1.35684100	2.03951600
				H	-1.03249600	-1.35689200	2.03972200
				C	-1.64709600	-1.07672900	-0.08611200
14ts				H	-1.97298600	-2.04591400	-0.43941500
C	0.21230200	-0.70742900	-1.05105800	C	1.28399100	-1.16814500	-0.11512700
C	0.21183800	0.70719500	-1.05093700	C	1.28368400	1.16827200	-0.11509400
C	-1.62517600	1.07571700	-0.09690200	O	1.65085500	2.29849900	0.13653800
C	-1.32816900	0.68660500	1.24373500	O	1.65153300	-2.29824600	0.13653700
C	-1.32838600	-0.68663600	1.24389800	H	-0.02405800	-1.32135100	-1.91157800
H	-1.95422300	2.04497200	-0.44785700	H	-0.02419400	1.32103500	-1.91167800
H	-1.02045000	1.35476000	2.03671900	O	-2.20105100	-0.00008300	-0.73334000
H	-1.02090700	-1.35472100	2.03703300	N	1.80383100	0.00015200	0.45849700
C	-1.62583300	-1.07594100	-0.09652400	H	2.54254600	0.00023900	1.14951200
H	-1.95484200	-2.04521400	-0.44745500				
C	1.27188200	-1.14200900	-0.10765700				
C	1.27149900	1.14212600	-0.10760500	16-dienophile			
O	1.67238700	2.24157900	0.16165500	C	2.28141100	0.67156500	0.00000800
O	1.78673700	0.00019600	0.51649800	C	1.02506500	1.46295800	-0.00004600
O	1.67323300	-2.24127000	0.16169700	C	-0.26010700	0.70440000	-0.00001800
H	-0.00112500	-1.32648900	-1.91368800	C	-0.26019300	-0.70437800	-0.00001500
H	-0.00130100	1.32605300	-1.91379600	C	1.02486800	-1.46295800	-0.00005000
O	-2.18321700	-0.00014700	-0.74143100	C	2.28136700	-0.67192000	0.00001500
				H	-1.44728700	2.48537000	-0.00001200
15-dienophile				H	3.19937800	1.25328800	0.00002600
C	0.66861300	1.26548900	0.00002300	C	-1.47281300	1.40032200	-0.00000600
C	-0.66861300	1.26550100	0.00006100	C	-1.47291500	-1.40023700	0.00000400
C	1.15773500	-0.15710100	0.00014700	H	3.19919600	-1.25379900	0.00004300
C	-1.15769200	-0.15709500	0.00007100	C	-2.67772400	-0.69951500	0.00001400
O	-2.30011400	-0.56082300	-0.00046400	C	-2.67766700	0.69971400	0.00000800
O	2.30011400	-0.56085000	-0.00047900	H	-1.44740100	-2.48527100	0.00000000
H	1.35543900	2.10227200	-0.00005300	H	-3.61923600	-1.24182600	0.00002500
H	-1.35536000	2.10234100	0.00001500	H	-3.61911800	1.24213000	0.00001600
N	-0.00001400	-0.94016300	0.00094500	O	1.06150100	-2.68793100	0.00002300
H	-0.00024100	-1.95085200	-0.00083900	O	1.06183800	2.68798300	0.00003100
15ts				16ts			
C	0.21201800	-0.70679400	-1.05137700	C	-1.17079200	-0.70548100	-1.17233100
C	0.21170600	0.70663100	-1.05131100	C	-1.17077400	0.70548000	-1.17236600
C	-1.64664700	1.07651700	-0.08636900	C	-2.36288800	1.15424600	0.61879700
C	-1.34221900	0.68794200	1.24816000	C	-1.52077300	0.69935400	1.64921000
C	-1.34235700	-0.68803800	1.24826500	C	-1.52075000	-0.69932000	1.64920400
				H	-2.62118700	2.19570100	0.45994800

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C	0.53509600	0.69815800	-1.23231500	H	1.86883900	-0.87652200	1.20152900
C	0.53506200	-0.69814900	-1.23232200	C	3.56679000	-0.00293000	0.17490500
C	2.21813200	-1.15739200	0.18738400	H	3.81662500	0.87821400	-0.42877700
C	1.66446800	-0.70233400	1.38931100	H	4.21822900	0.00293200	1.05530400
C	1.66449800	0.70229100	1.38930800	H	3.81501900	-0.89323700	-0.41584800
H	2.43141500	-2.19775900	-0.03211100				
H	1.19606900	-1.33108000	2.13836600				
H	1.19612400	1.33106000	2.13836100	19ts			
C	2.21817600	1.15732100	0.18737600	C	1.01059600	0.69814400	-1.23622100
H	2.43150700	2.19767800	-0.03212000	C	1.01059500	-0.69814400	-1.23622100
C	-0.64583000	1.15951900	-0.44619000	C	2.57492200	-1.15737600	0.31293400
C	-0.64588100	-1.15945900	-0.44619600	C	1.92751200	-0.70232400	1.46724500
O	-1.05083500	-2.29214700	-0.25775300	C	1.92751200	0.70232400	1.46724500
O	-1.05073300	2.29222400	-0.25774700	H	2.80494400	-2.19773400	0.11109600
H	0.95692800	1.34205100	-1.99302700	H	1.40116300	-1.33106500	2.17681100
H	0.95686900	-1.34205700	-1.99303400	H	1.40116300	1.33106500	2.17681100
C	2.98705900	-0.00005200	-0.40756900	C	2.57492200	1.15737500	0.31293400
H	3.08937000	-0.00005900	-1.49465200	H	2.80494400	2.19773400	0.11109600
H	4.00243900	-0.00007000	0.02336100	C	-0.22944900	1.15955900	-0.54730600
N	-1.24002700	0.00004100	0.07378700	C	-0.22944900	-1.15955800	-0.54730500
C	-2.44067300	0.00006900	0.90034600	O	-0.64755100	-2.29238200	-0.39098500
H	-2.39200500	-0.88921900	1.53480500	O	-0.64755000	2.29238200	-0.39098500
H	-2.39203500	0.88942800	1.53470400	H	1.49194500	1.34179600	-1.96095800
C	-3.72800600	-0.00006100	0.07267300	H	1.49194400	-1.34179600	-1.96095800
H	-4.60140300	-0.00007800	0.73469200	C	3.38813600	0.00000000	-0.21925600
H	-3.77764300	0.89064400	-0.56142700	H	3.57655900	0.00000000	-1.29478300
H	-3.77749800	-0.89090000	-0.56126500	H	4.36601000	0.00000000	0.29112900
19-dienophile				N	-0.86358700	0.00000000	-0.07689700
C	-2.39788200	-0.66294800	0.30212800	C	-2.12282600	0.00000100	0.65502800
C	-2.39386400	0.67326400	0.30123800	H	-2.12591000	-0.88971200	1.29229200
C	-1.02234700	-1.14830700	-0.06505300	H	-2.12591000	0.88971500	1.29228900
C	-1.01540900	1.14981600	-0.06655000	C	-3.35130300	-0.00000100	-0.26402000
O	-0.62024700	2.29321500	-0.17234600	H	-3.30401800	0.88332100	-0.91228900
O	-0.63417600	-2.29422300	-0.16926100	H	-3.30401800	-0.88332700	-0.91228400
H	-3.20649900	-1.34996400	0.51675600	C	-4.66012400	0.00000100	0.53098900
H	-3.19834500	1.36540000	0.51496500	H	-5.52661200	-0.00000100	-0.13871000
N	-0.25214700	-0.00166100	-0.27860500	H	-4.73627700	-0.88586100	1.17310800
C	1.16160000	-0.00604900	-0.63704300	H	-4.73627800	0.88586600	1.17310400
H	1.33811900	0.87736100	-1.25830700				
H	1.33495900	-0.89911500	-1.24517300	20-dienophile			
C	2.09155900	0.00149200	0.58263500	N	0.63832900	-0.07796000	0.47465800
H	1.87079700	0.88859800	1.18908200	C	1.15850100	1.18241300	0.16188500
				C	2.34930000	0.93337900	-0.72238900

C	2.49259700	-0.38490200	-0.88560800	H	-1.67623300	0.88980200	1.37322100
C	1.40524900	-1.08489200	-0.11771300	C	-2.94511700	-0.00003100	-0.14814100
O	0.72266100	2.24859000	0.54599600	H	-2.91755000	0.88365700	-0.79860800
O	1.21393300	-2.27947800	-0.00945600	H	-2.91748800	-0.88384700	-0.79843400
C	-0.51021600	-0.31672900	1.34527100	C	-4.23849200	-0.00001400	0.67586900
C	-1.79818100	-0.66728200	0.58850100	H	-4.24943500	-0.87914000	1.33580300
C	-2.32011600	0.44541900	-0.32900200	H	-4.24943100	0.87911000	1.33580600
C	-3.63170200	0.06849600	-1.02544200	C	-5.49916900	-0.00001000	-0.19474000
H	2.94362300	1.74643200	-1.11943100	H	-5.53263400	-0.88496000	-0.84172600
H	3.23518200	-0.93338200	-1.45098900	H	-6.40752100	-0.00007900	0.41835100
H	-0.64083400	0.59647200	1.93335100	H	-5.53269600	0.88500800	-0.84162500
H	-0.24158100	-1.13199100	2.02429100				
H	-1.63049400	-1.58579200	0.01146200				
H	-2.56151800	-0.90977300	1.34136200	21-dienophile			
H	-1.56206900	0.68199700	-1.08719600	C	-3.01325200	0.66812500	-0.91444000
H	-2.46029600	1.36454800	0.25575100	C	-3.01337100	-0.66821800	-0.91403200
H	-3.98130500	0.87615500	-1.67816300	C	-1.89731100	1.14937600	-0.02853400
H	-3.50963900	-0.83019500	-1.64249900	C	-1.89746700	-1.14913700	-0.02787500
H	-4.42471300	-0.13705500	-0.29589000	O	-1.58111800	-2.29379900	0.22715500
				O	-1.58073000	2.29407900	0.22590700
20ts				H	-3.66786100	1.35743300	-1.43227900
C	1.38802600	0.69810900	-1.24149600	H	-3.66808700	-1.35773600	-1.43145300
C	1.38799500	-0.69814200	-1.24149300	N	-1.28073200	0.00018100	0.47241300
C	2.99430300	-1.15739600	0.26445500	C	-0.11346400	0.00035500	1.35599500
C	2.37841000	-0.70235400	1.43582000	H	-0.20084500	-0.88747000	1.98754200
C	2.37840500	0.70231400	1.43581400	H	-0.20073800	0.88852000	1.98707000
H	3.21873500	-2.19776100	0.05641400	C	1.20780500	0.00009700	0.61125900
H	1.87139600	-1.33113100	2.15928600	C	1.82079200	-1.20805900	0.25659100
H	1.87138600	1.33109300	2.15927400	C	1.82178000	1.20797200	0.25742800
C	2.99429000	1.15734800	0.26443800	C	3.03175900	-1.20834600	-0.43684800
H	3.21872900	2.19771100	0.05639500	H	1.34105400	-2.14739800	0.51970300
C	0.16764300	1.15950800	-0.51823000	C	3.03277100	1.20775600	-0.43600500
C	0.16758900	-1.15948300	-0.51822500	H	1.34280600	2.14753800	0.52112800
O	-0.24588500	-2.29236100	-0.35027100	C	3.64081500	-0.00041800	-0.78284800
O	-0.24577500	2.29240700	-0.35027800	H	3.50046000	-2.15169400	-0.70446900
H	1.84926300	1.34184300	-1.97913000	H	3.50221500	2.15091900	-0.70297900
H	1.84921200	-1.34190400	-1.97911500	H	4.58576300	-0.00064100	-1.31979600
C	3.79291100	-0.00002400	-0.28959300				
H	3.95179400	-0.00002900	-1.36988800	21ts			
H	4.78441400	-0.00001700	0.19378200	C	1.65911100	0.69801900	-1.23620100
N	-0.45323100	0.00003000	-0.03052000	C	1.65905900	-0.69821500	-1.23610100
C	-1.69176600	0.00009600	0.73631800	C	3.50489900	-1.15746400	-0.03384000
H	-1.67622400	-0.88945800	1.37344000	C	3.10361600	-0.70225900	1.22700400

C	3.10362000	0.70245100	1.22685900	O	-1.53520300	2.29286400	0.05329800
H	3.68910900	-2.19786300	-0.27802700	H	-0.66175700	1.34572600	-2.45788700
H	2.73196100	-1.33075200	2.02870800	H	-0.66303700	-1.32732300	-2.46670200
H	2.73196800	1.33111300	2.02843200	N	-1.51704800	-0.00062300	0.43445700
C	3.50488900	1.15739200	-0.03409000	C	-2.13332800	-0.00824100	1.74634400
H	3.68912900	2.19774000	-0.27847400	H	-2.92334200	-0.76279200	1.77353700
C	0.58461700	1.15996700	-0.31092500	H	-1.40145700	-0.24263800	2.52825100
C	0.58455000	-1.15995900	-0.31075100	H	-2.54694600	0.98564900	1.92672100
O	0.21321300	-2.29379700	-0.06609600	H	1.69677100	-0.98896200	-2.09723600
O	0.21335600	2.29386100	-0.06643200	H	1.69774300	1.00679000	-2.08729100
H	1.98491600	1.34198500	-2.04254100	C	1.89132400	1.46036000	1.36064800
H	1.98486000	-1.34233400	-2.04231900	H	1.78179700	2.53725400	1.21019600
C	4.19377600	-0.00010300	-0.71993600	H	1.13389700	1.14612000	2.08938000
H	4.16070400	-0.00021100	-1.81134000	H	2.86978700	1.28482400	1.82664700
H	5.25455800	-0.00006400	-0.41763500	C	1.88320200	-1.47660100	1.34603400
N	0.05550900	0.00006400	0.27338600	H	2.85723600	-1.30147800	1.82123500
C	-1.03746500	0.00018400	1.24458700	H	1.11904700	-1.17348900	2.07289800
H	-0.90472500	-0.88902000	1.86625600	H	1.77919800	-2.55226900	1.18368700
H	-0.90474100	0.88956900	1.86600000				
C	-2.41516100	0.00007800	0.60730700				
C	-3.05512300	-1.20804900	0.30349700	23ts			
C	-3.05537500	1.20809900	0.30362400	C	-0.00482100	0.69710700	-1.75071100
C	-4.31946500	-1.20797700	-0.28706200	C	-0.00450000	-0.69557600	-1.75105900
H	-2.55055300	-2.14586400	0.51979800	C	1.96177000	-1.40517100	-0.83996300
C	-4.31972100	1.20782500	-0.28693100	C	2.01902800	-0.71323600	0.36067500
H	-2.55101300	2.14600300	0.52002200	C	2.01868500	0.71327500	0.36173600
C	-4.95557500	-0.00012600	-0.58074900	H	1.84412600	-2.48506500	-0.83269200
H	-4.80816600	-2.15140400	-0.51648100	C	1.96124100	1.40696900	-0.83785000
H	-4.80862100	2.15117400	-0.51624900	H	1.84290500	2.48677400	-0.82903700
H	-5.94200600	-0.00020600	-1.03738500	C	-0.88235200	1.15942000	-0.63546700
				C	-0.88184900	-1.15875700	-0.63594800
22ts				O	-1.21334700	-2.29053800	-0.33213700
C	-0.64965700	0.70197700	-1.58827400	O	-1.21445100	2.29089700	-0.33118800
C	-0.64795100	-0.68990500	-1.59242600	H	0.16524000	1.33814200	-2.60578300
C	1.46550700	-1.40071700	-1.12247500	H	0.16540500	-1.33604700	-2.60658600
C	1.77240500	-0.71502300	0.04320900	N	-1.28030900	0.00007700	0.04654200
C	1.77510500	0.71217100	0.05040300	C	-2.17341200	-0.00034100	1.19838900
H	1.35174500	-2.48073400	-1.09706200	H	-1.93378400	-0.88995400	1.78781600
C	1.47134100	1.41051100	-1.10810200	H	-1.93492700	0.88978600	1.78749000
H	1.36010600	2.49048700	-1.07242500	H	2.39137000	-0.99937800	-1.74753200
C	-1.27036900	1.16268400	-0.31289700	H	2.39104900	1.00273800	-1.74601100
C	-1.26934900	-1.15725200	-0.31880300	C	1.86378500	1.46869900	1.66396200
O	-1.53490000	-2.28818800	0.04456200	H	2.73283700	1.30707500	2.31517400
				H	1.77438200	2.54335500	1.48669600

H	0.98110600	1.14829700	2.23074600	H	4.51436200	-0.88611300	1.64584100
C	1.86434300	-1.47067300	1.66174000	H	4.51454300	0.88583700	1.64578800
H	2.73200800	-1.30751700	2.31439400	H	5.52738900	-0.00027700	0.49713800
H	0.97996600	-1.15337200	2.22765900				
H	1.77803000	-2.54535100	1.48304400				
C	-3.65180400	-0.00138500	0.80258600	25ts			
H	-3.89140700	-0.89275600	0.21446800	C	1.09372400	0.71588000	-1.78544800
H	-4.28210400	-0.00109200	1.69914000	C	1.08636000	-0.67620800	-1.79872600
H	-3.89233400	0.88895800	0.21328100	C	2.80760400	-1.41109300	-0.50169900
				C	2.61125600	-0.73177600	0.69138200
24ts				C	2.62374900	0.69493100	0.70972000
C	-0.67561700	-0.69573800	-1.79580400	H	2.68247600	-2.48972700	-0.53262000
C	-0.67569900	0.69638400	-1.79559600	C	2.83138700	1.40114200	-0.46522900
C	-2.42828700	1.40626300	-0.51721000	H	2.72384300	2.48208800	-0.46960500
C	-2.24736400	0.71322800	0.67012600	C	0.00163900	1.17629400	-0.87881000
C	-2.24717700	-0.71373300	0.66984300	C	-0.01228000	-1.14164900	-0.90154100
H	-2.31196600	2.48621300	-0.53260100	O	-0.40606000	-2.27372900	-0.68552400
C	-2.42791600	-1.40634800	-0.51777400	O	-0.37977200	2.30802900	-0.64044200
H	-2.31131400	-2.48626300	-0.53357000	H	1.44840200	1.36285500	-2.57699400
C	0.40385000	-1.15883400	-0.87508900	H	1.43022000	-1.31064100	-2.60516400
C	0.40367900	1.15934600	-0.87473000	N	-0.54170000	0.01437400	-0.30969100
O	0.78713800	2.29129800	-0.64061500	C	-1.66288400	0.01162100	0.62018100
O	0.78745200	-2.29081100	-0.64132500	H	-1.55602100	-0.87548100	1.25247800
H	-1.01090400	-1.33640600	-2.60085800	H	-1.56375900	0.90477500	1.24495200
H	-1.01113700	1.33727500	-2.60040700	H	3.42621500	-1.00101700	-1.29056800
N	0.93025900	0.00019500	-0.28529100	H	3.43855400	0.99971300	-1.26717900
C	2.03527100	0.00012300	0.66339500	C	2.19569400	1.43803700	1.95677600
H	1.92263300	0.89040600	1.29023500	H	2.18608900	2.51763000	1.78748200
H	1.92245000	-0.89004600	1.29036800	H	1.19420200	1.14367100	2.29400200
H	-3.02672700	1.00038500	-1.32353900	H	2.88196600	1.23466800	2.78907900
H	-3.02655400	-1.00033900	-1.32389400	C	2.16886800	-1.49958500	1.91814500
C	-1.83465100	-1.46933200	1.91454900	H	2.87886700	-1.36100900	2.74414700
H	-2.54806500	-1.29788300	2.73123200	H	1.18922900	-1.17039600	2.28550300
H	-1.79445200	-2.54505900	1.72627200	H	2.10421000	-2.57027800	1.70918800
H	-0.85033600	-1.15731100	2.28461600	C	-3.02593100	0.00209600	-0.08370400
C	-1.83502200	1.46843600	1.91513500	H	-3.08195500	-0.88447300	-0.72829600
H	-2.54786000	1.29573900	2.73205000	H	-3.09097500	0.88301500	-0.73536400
H	-0.85020600	1.15715800	2.28451000	C	-4.19522900	0.00012100	0.90810700
H	-1.79596800	2.54432000	1.72754300	H	-4.12285800	0.88347000	1.55853600
C	3.41030800	-0.00007700	-0.01727100	H	-4.11133200	-0.87478300	1.56851700
H	3.48030600	0.88327500	-0.66341700	C	-5.56256000	-0.01306800	0.21707500
H	3.48009100	-0.88351400	-0.66332100	H	-5.67846600	-0.90292500	-0.41343200
C	4.55448700	-0.00016100	1.00018800	H	-6.37875800	-0.01364500	0.94837200
				H	-5.68998300	0.86701100	-0.42484000

				O	-1.30236400	-2.29249500	-0.26415200
				O	-1.30229700	2.29256100	-0.26409200
26ts				H	0.79650600	-1.33938000	-1.89204500
C	-0.02325400	-0.69471700	-1.17307600	C	3.05741600	-0.77898200	-0.39376800
C	-0.02497200	0.69725100	-1.17122200	C	3.05743600	0.77888800	-0.39381900
C	-1.55978100	1.36508200	0.39734200	H	1.74828600	2.44255600	0.29312400
C	-1.03628200	0.69638600	1.49545100	H	0.79651600	1.33943300	-1.89203200
C	-1.03645000	-0.70975500	1.49020800	H	3.97720300	1.14156400	0.08462400
H	-1.41685300	2.44004000	0.31636300	H	3.08065600	1.17340400	-1.41537600
H	-0.43521900	1.23416400	2.22396400	H	3.08069000	-1.17356200	-1.41530000
H	-0.43576600	-1.25317100	2.21492000	H	3.97714100	-1.14165900	0.08475300
C	-1.55920000	-1.37064800	0.38691400	N	-1.50595200	0.00003000	0.06174600
C	1.20683900	-1.15671900	-0.46778100	C	-2.74605200	-0.00006400	0.82796000
C	1.20312400	1.16278500	-0.46586800	H	-2.72840100	-0.88955500	1.46380200
O	1.61826900	2.29684600	-0.31153900	H	-2.72841500	0.88921800	1.46410100
O	1.63084800	-2.28752700	-0.31316700	C	-3.99165600	0.00001000	-0.06121200
H	-0.50823900	1.34091200	-1.89417300	H	-4.01089500	-0.89093200	-0.69662100
C	-2.73964800	0.77867200	-0.34957800	H	-4.89588800	0.00037200	0.55804400
C	-2.73847800	-0.77910800	-0.35696000	H	-4.01042700	0.89069200	-0.69700000
H	-1.41668300	-2.44513700	0.29904100				
H	-0.50349700	-1.33701200	-1.89927700	28ts			
H	-3.64886800	-1.14477400	0.13684800	C	0.76596400	0.69606200	-1.18244300
H	-2.78059500	-1.16903100	-1.37966700	C	0.76592500	-0.69610600	-1.18242400
H	-2.78488800	1.17829000	-1.36838100	C	2.23825500	-1.36777400	0.44078800
H	-3.64939700	1.13821600	0.14993300	C	1.67215200	-0.70320100	1.52027400
N	1.83143100	0.00213200	0.01351900	C	1.67208400	0.70297200	1.52035400
C	3.07491800	-0.00215500	0.75921800	H	2.09891400	-2.44246100	0.35062200
H	3.79750500	-0.66439000	0.27457300	H	1.04237800	-1.24356100	2.22207700
H	3.45250900	1.02170600	0.77613700	H	1.04224600	1.24318800	2.22221000
H	2.91614200	-0.35173800	1.78484800	C	2.23815100	1.36771900	0.44095900
27ts				C	-0.48975600	1.15898900	-0.52446600
C	0.32766900	0.69610700	-1.15926600	C	-0.48982700	-1.15893300	-0.52441900
C	0.32765900	-0.69605700	-1.15927800	O	-0.91188700	-2.29259100	-0.38063400
C	1.89259100	-1.36786200	0.37474500	O	-0.91176200	2.29267200	-0.38073000
C	1.39147100	-0.70305000	1.48554900	H	1.27592600	-1.33934300	-1.88724100
C	1.39151400	0.70305800	1.48554300	C	3.44685800	-0.77877200	-0.25642500
H	1.74816000	-2.44258000	0.29314400	C	3.44683000	0.77890300	-0.25627400
H	0.80495300	-1.24333700	2.22396200	H	2.09869500	2.44240100	0.35090200
H	0.80503200	1.24338900	2.22395200	H	1.27607200	1.33925500	-1.88722000
C	1.89266200	1.36783200	0.37473000	H	4.33595900	1.14138100	0.27712000
C	-0.88885600	1.15894400	-0.43119300	H	3.53234600	1.17405600	-1.27426500
C	-0.88888200	-1.15888800	-0.43122400	H	3.53230100	-1.17372200	-1.27450200
				H	4.33604400	-1.14132000	0.27682300

				H	-1.42161100	0.60795600	0.00000000
31-dienophile							
C	-1.10498600	-0.30932200	0.00000000				
C	0.00000000	0.48130700	0.00000000	32ts			
H	-2.08901200	0.15081800	0.00000000	C	0.71939100	-0.80071100	-0.51987000
C	1.33317300	-0.04659300	0.00000000	C	0.71143700	1.45339800	-0.56031000
N	2.42017000	-0.45785100	0.00000000	C	-0.88039600	0.99422300	1.05059600
C	-0.13432300	1.90947900	0.00000000	C	-0.26585200	-1.05820400	0.46369700
N	-0.24146100	3.06687400	0.00000000	C	0.54973800	1.45999800	0.93990000
C	-1.05579900	-1.72896500	0.00000000	H	0.59673200	2.50638900	1.28363300
N	-1.05576300	-2.89277400	0.00000000	H	1.29473000	0.89522500	1.50318800
				C	-0.56192300	1.65506200	-1.11057100
				C	-1.52826800	1.38138800	-0.13419300
31ts				H	1.64647700	1.68542500	-1.05831400
C	-0.62702000	-0.23232300	-0.98043400	H	-1.38730500	0.83500700	1.99655900
C	0.34879700	-1.80160500	-0.19134600	C	2.10203600	-0.96023000	-0.19613600
C	1.28709500	-0.35514300	1.35664500	N	3.23095800	-1.06584400	0.07213300
C	-0.23518500	0.94126400	-0.25066600	C	-1.52399200	-1.61685200	0.07257000
C	0.20227100	-1.38136900	1.26144600	N	-2.55202800	-2.06265500	-0.24387400
H	0.47942200	-2.24382500	1.88983100	H	-2.59805700	1.33814200	-0.30357900
H	-0.79040700	-1.05721800	1.57857300	H	-0.76806500	1.86897600	-2.15384300
C	1.69971500	-1.53984600	-0.53608900	H	0.06110500	-1.32549800	1.46416700
C	2.23752400	-0.62063400	0.37454300	H	0.46884100	-0.95261100	-1.56371300
H	-0.19987600	-2.64499900	-0.60054600				
H	1.40645900	0.33078100	2.18724200	33-dienophile			
C	-1.03638700	1.48064500	0.79913900	C	0.00000000	1.24328200	0.00000000
N	-1.68150900	1.90648700	1.67129800	C	-1.13290400	0.51236200	0.00000000
C	0.77057600	1.78060200	-0.81654100	H	-0.06555600	2.32779100	0.00000000
N	1.60177700	2.43429800	-1.30632300	C	-1.17214000	-0.91279800	0.00000000
H	3.19698500	-0.12667700	0.27661100	N	-1.24555700	-2.07387800	0.00000000
H	2.19149200	-1.88924500	-1.43777800	C	1.31469800	0.69176000	0.00000000
C	-1.98479300	-0.70245100	-0.85976300	N	2.40293100	0.28037200	0.00000000
N	-3.06344500	-1.12631900	-0.76997600	H	-2.09398000	1.01911400	0.00000000
H	-0.25738800	-0.28491800	-2.00052400				
				33ts			
32-dienophile				C	0.49252000	0.70915700	-0.91198800
C	-0.33508600	0.58489500	0.00000000	C	-1.21673900	1.15471300	0.44551600
C	0.33508600	-0.58489500	0.00000000	C	-1.21649400	-1.15472200	0.44514100
C	-0.33508600	-1.84350400	0.00000000	C	0.49232400	-0.70918300	-0.91190000
N	-0.86539600	-2.87927700	0.00000000	C	-0.81608500	-0.00006300	1.32862300
C	0.33508600	1.84350400	0.00000000	H	-1.47739700	-0.00031800	2.21078000
N	0.86539600	2.87927700	0.00000000	H	0.21407100	0.00003800	1.68839700
H	1.42161100	-0.60795600	0.00000000				

C	-2.26701000	0.69983500	-0.36942700			
C	-2.26692400	-0.69977700	-0.36961200			
H	-1.04805100	2.19259300	0.71150300			
H	-1.04793100	-2.19261800	0.71111300			
C	1.49198500	1.46289000	-0.22004800			
N	2.27689800	2.10560300	0.35183600			
C	1.49191400	-1.46287600	-0.21990400			
N	2.27686100	-2.10552300	0.35199700			
H	-2.89455700	-1.32871300	-0.99229200			
H	-2.89471700	1.32887200	-0.99193200			
H	0.07982900	-1.20832300	-1.78139600			
H	0.07949700	1.20806100	-1.78140800			
34-dienophile						
C	0.00000000	0.77492300	0.00000000			
C	1.32213500	0.98401900	0.00000000			
C	-0.58054400	-0.53323900	0.00000000			
N	-1.07182600	-1.58791900	0.00000000			
H	2.03240200	0.16309000	0.00000000			
H	-0.70205400	1.60539400	0.00000000			
H	1.72288400	1.99272700	0.00000000			
34ts						
C	-0.99213200	0.54578700	-0.78854400			
C	0.50987300	-1.30455800	-0.10815300			
C	1.32023200	0.66253300	0.81191700			
C	-0.28425800	1.56825900	-0.13858400			
C	0.54813700	-0.58032700	1.20801800			
H	1.17800900	-1.16074900	1.90338900			
H	-0.41833200	-0.42288100	1.68959200			
C	1.60085900	-0.88088600	-0.85825600			
C	2.12681300	0.28792900	-0.28026600			
H	-0.07914300	-2.19630900	-0.28860000			
H	1.62356000	1.41116300	1.53858200			
C	-2.16611300	-0.02436300	-0.22365800			
N	-3.12396300	-0.49574000	0.24875300			
H	2.93126300	0.88528500	-0.69725600			
H	1.93215200	-1.32223100	-1.79254300			
H	-0.71206800	1.99721400	0.76340200			
H	-0.83739200	0.35854800	-1.84496000			
H	0.26922900	2.27390200	-0.74771700			
35-dienophile						
C	0.00000000	0.40574800	0.00000000			
C	-0.00000100	1.75235500	0.00000000			
C	-1.22550700	-0.34815000	0.00000000			
N	-2.21568200	-0.95617500	0.00000000			
C	1.22550900	-0.34814800	0.00000000			
N	2.21568200	-0.95617500	0.00000000			
H	0.93130800	2.30781100	0.00000000			
H	-0.93131100	2.30780900	0.00000000			
35ts						
C	-1.06729800	0.12316900	0.47550100			
C	0.98218800	-0.38893500	-1.36212800			
C	1.63290200	-0.56434000	0.87029900			
C	-0.18194700	-0.12939300	1.55155800			
C	1.24174100	-1.42934400	-0.31883300			
H	2.12957700	-2.01294600	-0.61580400			
H	0.42844100	-2.14077000	-0.16261300			
C	1.60925600	0.78436100	-0.99828900			
C	2.07738000	0.65992700	0.32867300			
H	0.49102600	-0.58571900	-2.30790500			
H	2.08781700	-0.99411400	1.75912500			
C	-1.30573300	1.46090000	0.04652800			
N	-1.47183400	2.57071200	-0.27118800			
C	-1.86866700	-0.91991400	-0.07174900			
N	-2.50554200	-1.80079900	-0.49590000			
H	0.05687800	0.70769800	2.19882200			
H	-0.32346700	-1.06677900	2.08288600			
H	2.58234400	1.44167200	0.88662600			
H	1.67008900	1.68298100	-1.60088500			
36-dienophile						
C	-4.20829500	0.24316200	0.00012500			
O	-2.85511300	0.72609400	0.00000400			
C	-1.90190000	-0.23115600	-0.00010200			
O	-2.13722900	-1.42281200	0.00000700			
C	-0.54909700	0.38196800	-0.00009500			
C	0.54909700	-0.38196800	-0.00009900			
C	1.90190000	0.23115600	-0.00011700			
O	2.85511300	-0.72609400	0.00000400			
C	4.20829500	-0.24316200	0.00012900			

O	2.13722900	1.42281200	0.00000800	C	-0.59692100	0.30616300	0.00001400
H	0.47436200	-1.46486800	-0.00009600	C	-1.83786900	-0.50604300	0.00000700
H	-0.47436400	1.46486900	-0.00009500	Cl	-3.32483800	0.52120900	-0.00000900
H	-4.83642300	1.13401300	0.00008300	C	0.59692100	-0.30616200	0.00001800
H	-4.39796900	-0.36360500	-0.88941000	C	1.83786900	0.50604300	0.00002700
H	-4.39786600	-0.36343900	0.88979800	Cl	3.32483800	-0.52120900	-0.00001200
H	4.39789800	0.36333600	0.88986500	O	1.90855500	1.69771400	-0.00000800
H	4.83642300	-1.13401400	-0.00003300	O	-1.90855600	-1.69771400	-0.00000300
H	4.39793700	0.36370700	-0.88934200	H	-0.68155100	1.38695000	0.00001500
				H	0.68155100	-1.38695000	0.00001700
36ts				37ts			
C	0.51631700	-0.47917900	0.41930000	C	0.68283200	-0.39344600	-0.30328100
C	0.96481100	1.65085800	0.93308600	C	1.03674700	1.81746300	-0.07911600
C	-0.96248900	1.85428400	-0.32328900	C	-1.07902900	1.59143000	0.82693100
C	-0.63232400	-0.34815700	-0.37560100	C	-0.57937400	-0.53058500	0.31061500
C	-0.51348200	1.89051500	1.11789100	C	0.35067100	1.79180000	1.26367100
H	-0.65300500	2.91649800	1.49761800	H	0.43418800	2.79704100	1.70873900
H	-1.03353200	1.20659600	1.78965100	H	0.74398900	1.07696500	1.98735600
C	1.30189300	2.13133900	-0.34180900	C	0.08698100	2.24930200	-1.01985900
C	0.13430800	2.24794000	-1.10489100	C	-1.19262700	2.12324900	-0.46856400
H	1.66287700	1.56014500	1.75854400	H	2.10940800	1.91991900	-0.20330000
H	-1.99801500	1.96241300	-0.62889500	H	-1.90701700	1.47896600	1.51810800
H	0.09963200	2.47747500	-2.16436100	H	-2.12249900	2.28223600	-1.00223400
H	2.30944500	2.25191500	-0.72315400	H	0.30387600	2.52802000	-2.04516400
H	0.40481100	-0.78099600	1.45469400	C	1.87138500	-0.79744400	0.45381400
H	-0.53093500	-0.44281300	-1.44943500	O	1.97384000	-0.97053400	1.63401800
C	1.79638300	-0.81214600	-0.23353700	C	-1.73244100	-0.79832500	-0.55241700
O	2.03432700	-0.71900300	-1.42422700	O	-1.80736700	-0.67957300	-1.73933900
C	-1.94610500	-0.71555900	0.19095000	Cl	3.34111500	-1.00711700	-0.62329400
O	-2.21267200	-0.82314800	1.37621300	Cl	-3.20452700	-1.33955300	0.40763000
O	2.71673900	-1.22915300	0.67542700	H	0.75274600	-0.43687800	-1.38128000
O	-2.86360100	-0.91075400	-0.78985400	H	-0.63934400	-0.87268700	1.33586700
C	3.99692100	-1.57464100	0.13031800				
H	4.59937200	-1.90103600	0.97907800	38-dienophile			
H	3.90109400	-2.37970100	-0.60356300	C	-5.59072900	-1.09548800	0.24190900
H	4.45808000	-0.71022500	-0.35642600	C	-5.19142400	-0.16321900	1.20252200
C	-4.17429300	-1.27772400	-0.33655400	C	-4.02061200	0.57238600	1.01857700
H	-4.77504300	-1.39162400	-1.23972700	C	-3.26465100	0.35595600	-0.13572500
H	-4.14104200	-2.21716400	0.22208900	C	-3.65485200	-0.56765200	-1.10871800
H	-4.59372100	-0.50019800	0.30823100	C	-4.82748200	-1.29539700	-0.91158100
				S	-1.75219200	1.29178800	-0.37399300
37-dienophile							

O	-1.47253700	1.36436800	-1.81574600	C	-3.53334500	-2.78013600	0.12919200
C	-0.49588700	0.24002800	0.36981400	H	-1.75327600	-1.83263100	0.88481900
C	0.49586800	-0.24004400	-0.36980400	C	-5.27714500	-1.30001000	-0.67001900
S	1.75218900	-1.29178100	0.37399100	H	-4.83942300	0.81986300	-0.52434700
C	3.26464600	-0.35593800	0.13574000	C	-4.79823900	-2.58987200	-0.43344200
C	3.65423400	0.56854200	1.10815700	H	-3.15720900	-3.78385700	0.30347500
C	4.82686000	1.29627700	0.91100100	H	-6.26029500	-1.15355200	-1.10835500
C	5.59073900	1.09547100	-0.24192300	H	-5.40948600	-3.45022700	-0.69217300
C	5.19205600	0.16233300	-1.20194200	C	2.89367400	-1.03411600	-0.09779100
C	4.02122700	-0.57325100	-1.01798700	C	3.15436700	-1.53142300	1.18201200
O	-1.82237800	2.49990000	0.46103800	C	3.92637000	-0.63690600	-0.94738700
O	1.47252700	-1.36440800	1.81574600	C	4.47447100	-1.59634000	1.62681500
O	1.82240200	-2.49987700	-0.46107200	H	2.34060700	-1.88001300	1.81030100
H	0.58129400	-0.07558200	-1.44028000	C	5.24491500	-0.71750100	-0.49571200
H	-0.58127800	0.07550000	1.44028400	H	3.69003200	-0.29128900	-1.94809600
H	3.05531800	0.69791000	2.00348100	C	5.51727400	-1.18790600	0.79029900
H	3.70407400	-1.31751900	-1.74098000	H	4.68988100	-1.97777400	2.62079300
H	5.14643900	2.01603200	1.65888700	H	6.05806100	-0.41725100	-1.15047500
H	5.79467700	0.00251600	-2.09124100	H	6.54450100	-1.24684400	1.13916500
H	6.50354700	1.66571600	-0.39002700	H	2.77400200	2.05970000	-1.55667600
H	-3.70307000	1.31604500	1.74202800	H	0.56645400	3.24234800	-2.43241900
H	-3.05637200	-0.69633700	-2.00442900	S	1.19354200	-0.97799600	-0.69312100
H	-5.79356000	-0.00408500	2.09227200	S	-2.25540900	1.04995400	0.66779200
H	-5.14754600	-2.01446300	-1.65992300	O	-3.01382500	2.22896400	0.20952700
H	-6.50353300	-1.66574200	0.39000700	O	-1.85434900	0.93782300	2.08526600
38ts				O	0.57039800	-2.25566500	-0.29190100
C	0.77303700	2.99363100	-1.39712600	O	1.21802800	-0.56870600	-2.10826700
C	-0.12789900	3.11683300	-0.34140500	39-dienophile			
C	1.78597100	2.05185000	0.42027400	C	-2.99418800	0.65244100	0.14000400
C	1.93970500	2.35956000	-0.93449100	C	-2.99417900	-0.65257300	-0.13937200
C	0.63593900	2.87893700	0.93606800	C	-1.57581000	1.12897400	0.23905400
H	0.06182300	2.45896600	1.76325800	C	-1.57579400	-1.12876900	-0.23992100
H	1.04394000	3.84763600	1.27109400	O	-1.19540100	-2.25486000	-0.47593300
C	-0.76369200	0.87924100	-0.31840000	O	-1.19544200	2.25490300	0.47589000
H	-0.96123900	0.79278000	-1.38124100	H	-3.82690000	1.32832300	0.28667500
C	0.35548900	0.29416700	0.25709900	H	-3.82688400	-1.32866100	-0.28512800
H	0.34814200	0.07407400	1.32074100	N	-0.76223300	0.00007600	-0.00027900
H	-1.08618000	3.61864900	-0.38357100	C	0.66596000	0.00003600	-0.00009800
H	2.57645300	1.66722900	1.05499900	C	1.36270300	-1.06844400	0.57552800
C	-3.23347100	-0.39794800	0.21937200	C	1.36290700	1.06845700	-0.57558300
C	-2.74150900	-1.68300700	0.46508900	C	2.75678300	-1.06597900	0.56447200
C	-4.49240100	-0.19213000	-0.34761700	H	0.81875900	-1.89620700	1.01353300

C	2.75698500	1.06587900	-0.56423600	C	0.67155300	-1.26944300	0.00005500
H	0.81912200	1.89625600	-1.01371400	C	1.44479900	0.00001000	0.00019600
C	3.45894800	-0.00007600	0.00019500	C	0.67162900	1.26948500	0.00006900
H	3.29333500	-1.90097000	1.00635500	C	-0.67151800	1.26951000	-0.00008500
H	3.29369600	1.90082400	-1.00601100	C	-1.44480800	0.00002600	-0.00027300
H	4.54535000	-0.00011900	0.00031000	H	-1.25987800	-2.18284600	-0.00010000
39ts				H	1.25993900	-2.18284700	0.00014600
C	-1.78318500	-0.22476300	-1.38523000	H	1.25998500	2.18291200	0.00015200
C	-1.77464100	1.08615000	-0.91076000	H	-1.25982400	2.18295800	-0.00014100
C	-2.86585900	0.89227200	1.02845200	O	2.66960300	-0.00007400	-0.00009700
C	-1.94489700	0.13830400	1.76676800	O	-2.66974300	-0.00005400	0.00018000
C	-1.96192600	-1.18562500	1.30019600	40ts			
H	-3.12985800	1.92037400	1.25070200	C	-0.13927100	0.70492900	-1.07685000
H	-1.24268800	0.54105700	2.48811100	C	-0.13933600	-0.70496100	-1.07687200
H	-1.27829900	-1.96852200	1.60919700	C	1.70670100	-1.15448800	0.04278700
C	-2.89289700	-1.29082500	0.26010000	C	1.37780700	-0.69974500	1.33131500
H	-3.17801300	-2.22340200	-0.21430600	C	1.37777100	0.69972600	1.33128200
C	-0.41555700	-0.78591800	-1.23365600	H	1.87310700	-2.19588500	-0.21084400
C	-0.39973100	1.40532500	-0.44205000	H	1.05056600	-1.32933100	2.15141400
O	0.02013900	2.46805600	-0.02811000	H	1.05050600	1.32933500	2.15135400
O	-0.00253500	-1.86895500	-1.59589900	C	1.70660400	1.15442600	0.04271200
H	-2.43990800	-0.63339800	-2.14191900	H	1.87302700	2.19581500	-0.21093800
H	-2.41947400	1.89267100	-1.23468000	C	-1.11214900	1.46091800	-0.25629800
C	-3.80451100	-0.08989900	0.36510600	C	-1.11222100	-1.46089000	-0.25630400
H	-4.26944100	0.24340100	-0.56500000	O	-1.27432800	-2.67244700	-0.36603100
H	-4.61340900	-0.32989200	1.07541500	O	-1.27416900	2.67248500	-0.36603200
N	0.35133400	0.20865900	-0.56789100	H	0.22063500	1.24620400	-1.94702800
C	1.71026700	0.04526600	-0.16639800	H	0.22057900	-1.24626900	-1.94702600
C	2.14188900	-1.18882800	0.33817200	C	2.38573400	-0.00003900	-0.65935200
C	2.61429300	1.11016400	-0.27379400	H	2.32994600	-0.00008500	-1.74932100
C	3.46976800	-1.35195000	0.72812700	H	3.45101600	0.00002000	-0.37489600
H	1.44723600	-2.01649400	0.40477100	C	-1.91055500	-0.67244300	0.72178900
C	3.93675700	0.93596500	0.13314800	C	-1.91052800	0.67252900	0.72178300
H	2.27847000	2.06528800	-0.65474000	H	-2.53235600	1.25318100	1.39890900
C	4.37249100	-0.29176400	0.63235400	H	-2.53240700	-1.25306000	1.39892200
H	3.79624900	-2.31471200	1.11213400	41-dienophile			
H	4.62976800	1.76906800	0.05198400	C	-0.01829100	-0.03363500	0.10725600
H	5.40564400	-0.42211500	0.94243800	C	-0.00377600	-0.02864600	1.31935100
40-dienophile				C	0.06999300	-0.04343800	-1.34645900
C	-0.67150500	-1.26944700	-0.00008100	O	1.13404300	0.00804900	-1.91589000

O	-1.08784600	-0.11372700	-2.03206600	44-dienophile		
C	0.00121900	0.06952300	2.76687800	C	-2.49182300	-0.01308800 0.00002200
O	-0.18370900	1.10529300	3.36812700	C	-1.31706000	-0.64638000 -0.00000800
O	0.23182400	-1.12851400	3.32899300	C	-0.04361800	0.11761900 -0.00004700
C	-2.33905400	-0.16019700	-1.32579000	O	1.01691400	-0.72527700 -0.00000900
H	-2.47931500	0.73454800	-0.71208900	C	2.30316800	-0.08855800 0.00002300
H	-3.10284600	-0.19836200	-2.10269400	O	0.06069500	1.32782200 -0.00000300
H	-2.40471600	-1.05428400	-0.69846900	H	-3.43292700	-0.55459300 0.00004600
C	0.26286300	-1.12954800	4.77064400	H	-2.53036300	1.07258800 0.00002100
H	0.45800900	-2.16403800	5.05135300	H	-1.23964300	-1.72957100 -0.00000800
H	1.05698000	-0.47249800	5.13347500	H	3.03227100	-0.89942100 0.00005100
H	-0.69584200	-0.79205300	5.17216200	H	2.42291900	0.53653400 -0.88917500
				H	2.42286900	0.53654900 0.88921700
41ts				44ts		
C	0.42783000	-0.38336300	0.20913900	C	0.19558900	-0.36885900 -0.96146700
C	1.51992600	2.10107900	0.15869600	C	-1.01338000	1.22401800 0.52982200
C	-0.80007700	2.07738900	0.33955500	C	-2.24334200	-0.73323400 0.38675500
C	-0.73863500	0.06956100	0.17570900	C	-0.73259500	-1.40912400 -0.85106100
C	0.44143200	2.24009800	1.19424200	H	0.17738900	0.31240700 -1.80273000
H	0.45271800	3.27552200	1.57678100	H	-1.34271900	-1.65860300 -1.71220700
H	0.52497700	1.56840700	2.04938000	H	-0.45586500	-2.25525000 -0.22746500
C	0.98222700	2.36555800	-1.08111900	C	-1.31246800	-0.00648700 1.33668000
C	-0.43075600	2.40943500	-0.97242600	H	-1.89744800	0.29197800 2.22366600
H	2.57379100	1.99876900	0.39118200	H	-0.44139600	-0.56813200 1.67763400
H	-1.80423500	2.22371700	0.71990400	C	-2.06832300	1.42705000 -0.35356800
H	-1.12406200	2.53898500	-1.79595000	C	-2.84752800	0.25909100 -0.41025800
H	1.53898800	2.44467900	-2.00854500	H	-0.27096100	1.96491500 0.80458500
C	-2.13514800	-0.35441200	-0.02056400	H	-2.74902400	-1.65324200 0.66664800
O	-3.06612000	0.37926100	-0.29048800	C	1.41628400	-0.37658900 -0.15617800
O	-2.25471400	-1.69025300	0.12744600	O	1.64876400	-1.10429000 0.79985300
C	1.69368700	-1.01903100	0.37750400	O	2.31061700	0.55344600 -0.59691500
O	2.25257500	-1.16441000	1.45299700	C	3.54425900	0.60077900 0.12803600
O	2.20195200	-1.44788200	-0.80665600	H	4.05889400	-0.36356200 0.08568300
C	-3.58293900	-2.20517800	-0.06590000	H	4.14224100	1.37300800 -0.35858100
H	-4.27714300	-1.75940400	0.65154500	H	3.37154300	0.85729500 1.17766600
H	-3.93406400	-1.99310400	-1.07935500	H	-3.68842700	0.09949900 -1.07779700
H	-3.50080500	-3.28027200	0.09547800	H	-2.21025600	2.30657800 -0.97317500
C	3.47436200	-2.10486900	-0.70940500	45-dienophile		
H	4.23188200	-1.42779400	-0.30393500	C	-2.65924700	-1.55373800 -0.35395600
H	3.40850200	-2.98625600	-0.06572300	O	-1.78576300	-0.48359700 -0.75653100
H	3.72844000	-2.39458400	-1.72974700			

C	-1.66654500	0.51761700	0.12857600	H	2.99916300	-1.87915800	-2.04238900
O	-2.31743100	0.63126400	1.14372200	H	3.69457700	-2.04037500	-0.39321900
C	-0.68518000	1.55844900	-0.32311900	H	1.16966700	3.65282200	1.05394300
C	0.64513400	1.42064500	-0.35351500	H	-1.46213400	3.66289500	0.68173900
C	1.34002700	0.17201400	0.04772600				
O	2.65976000	0.25817400	-0.23497600				
C	3.43906000	-0.89371700	0.12420900				
O	0.82463000	-0.79551700	0.57130200				
H	1.27760100	2.24819300	-0.65981200				
H	-1.12977900	2.51921200	-0.57267100				
H	-2.68658600	-2.24022300	-1.20030700				
H	-2.25232600	-2.05001600	0.53064700				
H	-3.65906800	-1.17328200	-0.13026600				
H	3.37128300	-1.08191900	1.19907600				
H	3.08610400	-1.77792600	-0.41337700				
H	4.46371000	-0.65424300	-0.16095400				
45ts							
C	-0.70894300	0.21042100	0.92004200				
C	-1.09965200	1.96477400	-0.68266800				
C	1.18521500	1.90821900	-0.31559400				
C	0.68806100	0.32811400	1.03378000				
H	-1.33044300	0.70404800	1.65536700				
H	1.03141400	0.80015600	1.94867000				
C	0.15920600	1.48448500	-1.34493500				
H	0.32668200	2.09067800	-2.25207600				
H	0.18075700	0.43430100	-1.63240200				
C	-0.75885000	3.01296900	0.17124300				
C	0.63150900	3.00440000	0.36979000				
H	-2.09805500	1.75947700	-1.05253500				
H	2.24963900	1.76711900	-0.46673600				
C	-1.37199500	-0.86092800	0.16801200				
O	-0.84602200	-1.64750800	-0.60375200				
O	-2.70759000	-0.88170000	0.43435900				
C	-3.44421700	-1.91394000	-0.23271200				
H	-3.06519700	-2.90184800	0.04401200				
H	-4.47765000	-1.79626100	0.09640200				
H	-3.37381100	-1.80378700	-1.31886000				
C	1.62580000	-0.79878500	0.67361600				
O	2.05109000	-1.55786700	1.51933900				
O	1.98617800	-0.85740200	-0.62171000				
C	2.77483500	-2.00255400	-0.98237500				
H	2.20032500	-2.91730100	-0.81701200				
				46-dienophile			
				C	-3.07645900	-0.78319600	0.00006600
				C	-1.92466800	0.20165700	-0.00006000
				O	-2.10207600	1.40936900	-0.00002200
				C	-0.54827900	-0.38563000	-0.00014900
				C	0.54827900	0.38563000	0.00011800
				C	1.92466800	-0.20165700	0.00002300
				C	3.07645900	0.78319700	-0.00006300
				O	2.10207600	-1.40936900	0.00004200
				H	0.43587600	1.46796600	0.00035100
				H	-0.43587600	-1.46796600	-0.00038400
				H	-3.02051600	-1.43568500	-0.88092000
				H	-3.02025300	-1.43578300	0.88096800
				H	-4.02651600	-0.24620000	0.00022600
				H	3.01983200	1.43643900	-0.88044300
				H	3.02093700	1.43502900	0.88144400
				H	4.02651500	0.24620100	-0.00100800
				46ts			
				C	-0.46253500	-0.73793900	-0.40622000
				C	-1.01899700	1.38265700	-0.95017900
				C	0.88536300	1.67845300	0.32236200
				C	0.67280000	-0.52993800	0.39601100
				C	0.44974700	1.68040500	-1.12227900
				H	0.55374600	2.70596600	-1.51462000
				H	1.00686000	1.00814900	-1.77648800
				C	-1.39110000	1.84854900	0.31952800
				C	-0.23797300	2.02195700	1.09285800
				H	-1.70190700	1.27126500	-1.78622400
				H	1.90989200	1.86517900	0.62877500
				H	-0.22508800	2.26031000	2.15087400
				H	-2.40669000	1.92531200	0.69037500
				H	-0.30420300	-1.02777400	-1.44140800
				H	0.53278900	-0.61443900	1.46896400
				C	-1.73802200	-1.13881000	0.23430500
				O	-1.93406900	-0.99635400	1.43524200
				C	2.02716500	-0.84051000	-0.13032900

O	2.27405800	-0.88612000	-1.33023300	47ts	C	2.59778000	-0.70360000	2.40715600
C	-2.79696400	-1.74920900	-0.67120900	C	1.60693100	-1.39922200	1.73941500	
H	-2.97146700	-1.12704400	-1.55714000	C	0.56046500	-0.71233700	1.08183800	
H	-2.45915500	-2.72975300	-1.03130100	C	0.56048200	0.71200500	1.08200200	
H	-3.72886900	-1.87549600	-0.11642900	C	1.60696600	1.39871700	1.73972900	
C	3.10612400	-1.11767200	0.90461000	C	2.59779900	0.70291900	2.40731200	
H	2.89316700	-2.06462300	1.41737500	C	-0.48192300	-1.39191800	0.33561100	
H	4.07985800	-1.18734000	0.41566400	C	-0.48188900	1.39176600	0.33595200	
H	3.12750500	-0.33758900	1.67476100	C	-1.76559400	0.71169600	0.28083200	
				C	-1.76561400	-0.71181000	0.28064000	
47-diene				C	-2.99644000	-1.39686400	0.16963600	
C	3.66564100	0.73090700	-0.09288700	H	-3.01205500	-2.48117400	0.17850300	
C	2.47920700	1.41249500	-0.04163700	C	-4.19127800	-0.70276300	0.09106400	
C	1.21446900	0.73824000	0.01833500	C	-4.19125600	0.70276800	0.09124400	
C	1.22301300	-0.71124200	0.02126200	C	-2.99639700	1.39681600	0.16999600	
C	2.49131000	-1.37838700	-0.02992000	H	3.38104800	-1.24622000	2.92872100	
C	3.67275200	-0.68876600	-0.08586700	H	1.62270300	-2.48331500	1.73858700	
C	-0.01227400	1.43879600	0.06307700	H	1.62276400	2.48280900	1.73915400	
C	0.01227600	-1.43879300	0.06308900	H	3.38107800	1.24540500	2.92900100	
C	-1.21445500	-0.73823600	0.01832200	H	-5.13024100	-1.24649000	0.03569100	
C	-1.22300000	0.71124400	0.02126000	H	-5.13020300	1.24653900	0.03601400	
C	-2.49130200	1.37838700	-0.02987400	H	-3.01198100	2.48112400	0.17914900	
H	-2.51652100	2.46165600	-0.04579500	C	0.12958000	0.70457800	-1.69529300	
C	-3.67274000	0.68876400	-0.08583300	C	0.12964000	-0.70408900	-1.69549800	
C	-3.66562600	-0.73091400	-0.09292000	H	-0.62073600	1.33047900	-2.15823900	
C	-2.47919300	-1.41249800	-0.04168600	H	-0.62065300	-1.32990400	-2.15862100	
H	4.60387700	1.27672000	-0.14599100	C	1.54370900	1.13770000	-1.71329500	
H	2.50290900	2.49516300	-0.07114500	C	1.54376300	-1.13717600	-1.71346700	
H	2.51652800	-2.46165400	-0.04590600	O	2.34653500	0.00027900	-1.60345300	
H	4.61617000	-1.22617300	-0.13230100	O	2.02501700	2.23921800	-1.78755200	
H	-4.61616200	1.22616800	-0.13221800	O	2.02513100	-2.23866000	-1.78785200	
H	-4.60386200	-1.27672100	-0.14606300	C	-0.43160600	-2.89728000	0.21129400	
H	-2.50287100	-2.49516600	-0.07124800	H	-0.66536800	-3.37793700	1.17086500	
C	0.05418400	-2.95153500	0.13444200	H	-1.15051800	-3.26143500	-0.52673100	
H	-0.88628500	-3.37757700	0.48458700	H	0.55787100	-3.23086000	-0.10865800	
H	0.27699800	-3.40406100	-0.84156500	C	-0.43162600	2.89715900	0.21205300	
H	0.82536200	-3.29218400	0.83179400	H	-1.15055100	3.26149200	-0.52587000	
C	-0.05423400	2.95153600	0.13438300	H	-0.66541800	3.37752800	1.17176000	
H	-0.82514700	3.29216800	0.83204900	H	0.55784000	3.23087000	-0.10779900	
H	0.88634700	3.37767700	0.48408500					
H	-0.27751700	3.40398700	-0.84155100	48-dienophile	C	0.59691000	-0.30621000	0.00005400

C	1.83782600	0.50597600	0.00007700	C	1.82553100	-1.48372500	-1.89587800
Cl	3.32465800	-0.52121000	-0.00003300	H	1.41537800	-2.49297800	-1.81935500
C	-0.59690900	0.30621100	0.00002600	H	2.01578300	-1.27751100	-2.95791600
C	-1.83782500	-0.50597500	0.00000700	H	2.78599300	-1.48869700	-1.37949200
Cl	-3.32465900	0.52121000	-0.00002200	C	-1.84422100	2.36402800	0.45717700
O	-1.90847000	-1.69773400	-0.00000100	H	-1.41955400	2.77714200	1.37456900
O	1.90846900	1.69773500	-0.00001600	H	-2.05808800	3.20106700	-0.22128500
H	0.68124600	-1.38702700	0.00006100	H	-2.79392900	1.89980500	0.72485800
H	-0.68124500	1.38702700	0.00002000				
48ts				49-dienophile			
C	-2.34785000	-1.47692700	-3.00820900	C	1.09894800	1.80465200	-0.01028600
C	-1.01237500	-1.46495300	-2.64478400	N	1.56582600	2.87028800	-0.03267400
C	-0.51693100	-0.49826000	-1.74274700	C	0.58527000	0.47498000	0.00646700
C	-1.41914900	0.44626300	-1.17857900	C	1.65232200	-0.60785100	0.10925100
C	-2.78329000	0.39157700	-1.54063500	O	2.03192900	-1.02804100	-1.10304600
C	-3.23787700	-0.54262300	-2.45438100	C	-0.74908200	0.22252400	0.00176800
C	0.87597500	-0.45231600	-1.32569500	C	-1.23678200	-1.19739700	0.01009800
C	-0.89634100	1.38701800	-0.20363900	O	-2.57646500	-1.26206200	0.01175800
C	0.48945800	1.79009500	-0.38238500	C	-1.70788700	1.28247600	-0.00974900
C	1.39139400	0.85702900	-0.96550300	N	-2.49141300	2.14148600	-0.02233300
C	2.74879300	1.21754000	-1.11392000	O	2.13424900	-0.93271600	1.16276900
H	3.44850600	0.51839500	-1.55713500	O	-0.50052600	-2.15841000	0.01481500
C	3.19633900	2.46947500	-0.73078900	H	2.72824600	-1.70126300	-0.97112900
C	2.30659200	3.38915500	-0.15251800	H	-2.81934800	-2.20763000	0.02051500
C	0.97837600	3.04772600	0.03408800				
H	-2.70629300	-2.21109900	-3.72416600	49ts			
H	-0.33786500	-2.19191200	-3.08312300	C	3.12345700	-1.55563400	-1.97866400
H	-3.48302500	1.10458500	-1.12011000	C	2.09499700	-0.64753700	-2.17416800
H	-4.28591900	-0.55436000	-2.73927000	C	0.95130500	-0.66286400	-1.35583600
H	4.23883400	2.73804800	-0.87501700	C	0.86921700	-1.62908100	-0.31414300
H	2.65960000	4.37130200	0.14886500	C	1.95490100	-2.51004100	-0.09807500
H	0.30320500	3.76969700	0.47928000	C	3.05938700	-2.48526500	-0.92885700
C	-0.40384800	-0.14278200	1.36438400	C	-0.15986400	0.29386800	-1.49720100
C	0.43394300	-1.12610900	0.75749100	C	-0.33298100	-1.68192200	0.47963900
H	0.05647600	0.56236700	2.04409000	C	-1.55926000	-1.24927600	-0.14685400
H	-0.02259000	-2.06118700	0.45999000	C	-1.48082300	-0.28818000	-1.19112800
C	-1.76386400	-0.57467600	1.69356100	C	-2.66837600	0.13270300	-1.81403000
O	-2.44497000	-1.38122900	1.13422000	H	-2.63510000	0.86797100	-2.60836500
C	1.80317500	-1.20452700	1.27398300	C	-3.89600000	-0.39100200	-1.43145000
O	2.48352400	-0.32753500	1.71530900	C	-3.97574800	-1.32213000	-0.38681400
Cl	-2.43166400	0.29588000	3.18303000	C	-2.82335500	-1.73316900	0.25993000
Cl	2.48241200	-2.92269400	1.19366000	H	3.98515800	-1.54324300	-2.64026700

H	2.17209200	0.07208700	-2.97948100				
H	1.90223400	-3.24525900	0.69703500				
H	3.87199600	-3.18895700	-0.77314900	50ts			
H	-4.79936200	-0.06580300	-1.93928700	C	1.93484100	3.34610400	-0.35652900
H	-4.93964600	-1.71648700	-0.07936000	C	0.75467100	2.96361200	0.25455000
H	-2.89220500	-2.45053800	1.06899100	C	0.14433800	1.72751300	-0.05582300
C	0.02785700	0.63476200	1.38430700	C	0.78328500	0.85664400	-0.98313800
C	0.06738900	1.45370700	0.16834400	C	2.00576600	1.25741400	-1.56856500
C	1.30679500	0.29600600	2.02495900	C	2.56372600	2.48797700	-1.27511000
O	2.39887600	0.42685200	1.49795400	C	-1.08874600	1.27718100	0.56306000
C	1.33610300	2.34547500	0.08180500	C	0.16811800	-0.43161500	-1.23626400
O	1.50632600	3.25294600	0.85811500	C	-1.28088500	-0.47199000	-1.15758500
C	-0.12181800	1.24718700	-2.68285100	C	-1.92634900	0.41102100	-0.24704800
H	0.85873400	1.70153100	-2.80731800	C	-3.33112800	0.35028800	-0.11050600
H	-0.37224800	0.70340800	-3.60215500	H	-3.83325900	1.01145400	0.58638900
H	-0.84792500	2.05445700	-2.56489400	C	-4.08003300	-0.52647000	-0.87508200
C	-0.40565700	-2.55345300	1.70464000	C	-3.44402000	-1.39606200	-1.77742600
H	-1.14847100	-2.17051100	2.40876600	C	-2.06624100	-1.38003000	-1.90352800
H	-0.69762800	-3.57640000	1.42900500	H	2.37398900	4.31313500	-0.12764900
H	0.54971200	-2.60380800	2.22742300	H	0.27588300	3.63920300	0.95476400
C	-1.15158000	0.58756000	2.17699700	H	2.49910300	0.60687100	-2.28256700
N	-2.12386500	0.49435700	2.81445800	H	3.48943800	2.79132000	-1.75617800
O	2.16209400	2.09158800	-0.94594500	H	-5.16147700	-0.54365500	-0.77407700
H	2.90887400	2.71151800	-0.83757000	H	-4.03420600	-2.08250900	-2.37823300
O	1.16528400	-0.21861300	3.27217200	H	-1.59005100	-2.05528700	-2.60607200
H	2.07242800	-0.37851100	3.59225800	C	0.48331600	-1.25447400	0.85021700
C	-1.07584500	2.33117600	0.00157700	C	-0.17739700	-0.37194200	1.74379300
N	-1.97469000	3.03835800	-0.20628200	C	1.95925700	-1.25272700	0.90214800
				O	2.65084500	-0.34995300	1.33538800
				C	-1.73455300	2.14065200	1.62400300
50-dienophile				H	-0.99061100	2.53679300	2.32008400
C	-3.19528500	-0.35311500	-0.00003200	H	-2.25593700	2.99537000	1.17214900
O	-1.82626700	-0.79713000	0.00001900	H	-2.46306900	1.57435000	2.20852000
C	-0.90267600	0.18341900	0.00004600	C	0.86675100	-1.42021500	-2.14368400
O	-1.15991700	1.37026900	0.00000600	H	0.48256100	-2.43282800	-1.99968800
C	0.46822200	-0.39240500	0.00000900	H	0.71641800	-1.15104000	-3.19815600
C	1.53019800	0.42872400	-0.00001700	H	1.94011200	-1.45679500	-1.95539500
C	2.87693600	-0.03936200	-0.00002800	O	2.47430300	-2.40599000	0.39984600
N	3.98272800	-0.40185800	0.00000800	C	-1.35082400	-0.81888000	2.42429400
H	1.37334400	1.50528100	-0.00001200	N	-2.31986700	-1.15447500	2.97819700
H	0.56882100	-1.47251100	0.00001200	H	0.01540100	-2.20006800	0.60361900
H	-3.79561800	-1.26249400	-0.00043800	H	0.46155200	0.29747600	2.31321800
H	-3.40040200	0.24670300	0.89041800	C	3.90552800	-2.50753000	0.45858600
H	-3.40014100	0.24735300	-0.89010000	H	4.25124000	-2.45874400	1.49479100

H	4.14828300	-3.47619100	0.02017900	H	-0.49427300	-0.57844400	-2.47017400
H	4.37597400	-1.69880000	-0.10712600	C	1.35713900	1.76937600	-1.09387700
				C	1.62632500	-0.33599400	-1.89827800
				O	2.29096100	0.76051900	-1.36157100
51-dienophile				O	1.71185300	2.87210100	-0.75762200
C	-0.38565200	-1.22737500	0.00015000	O	2.22710600	-1.26587000	-2.37194900
C	0.80620200	-0.61374000	-0.00007500	C	-0.18882300	-2.83379500	-0.95705400
C	-1.45533700	-0.20027400	0.00006900	H	-0.36199700	-3.66984800	-0.26691500
C	0.53589200	0.86309900	0.00000900	H	-0.91934200	-2.91289300	-1.76641200
O	1.32290100	1.76862900	0.00000700	H	0.80132400	-2.95047500	-1.40187200
O	-2.64704600	-0.32387900	-0.00012100	C	-0.51766100	2.38276800	1.54617100
O	-0.83680200	1.05613700	0.00003500	H	-1.33876900	2.95863000	1.11517200
H	-0.60952200	-2.28661200	0.00015100	H	-0.64496000	2.38937800	2.63760300
C	2.19828100	-1.14300000	-0.00005800	H	0.41115600	2.90797700	1.30926100
H	2.74426400	-0.77846100	-0.87807900	C	-1.11006400	2.15243500	-1.71624900
H	2.74408600	-0.77881500	0.87823300	H	-0.99880100	3.12772500	-1.23557800
H	2.21242800	-2.23547200	-0.00024200	H	-1.08345300	2.31925600	-2.80176600
				H	-2.09447900	1.74329000	-1.47035800
51ts				52-dienophile			
C	2.83184800	-1.55880700	1.88038800	C	1.79848200	1.58811300	0.00000900
C	1.84200800	-1.97750300	1.00810900	O	0.65600100	0.71315500	-0.00001200
C	0.73182900	-1.15228700	0.72957500	C	0.92733200	-0.60109300	-0.00002700
C	0.65308000	0.13331000	1.33490700	O	2.04599200	-1.07533600	0.00001000
C	1.69940400	0.55420700	2.18893200	C	-0.29235500	-1.45107000	0.00000200
C	2.76195500	-0.28486300	2.47001300	C	-1.57951200	-1.06105100	0.00000600
C	-0.30463500	-1.50720900	-0.23499300	C	-2.07720000	0.27775900	-0.00001000
C	-0.48416800	0.97086900	1.01655800	N	-2.57956400	1.32712300	0.00000800
C	-1.71942400	0.27910900	0.71206500	H	-2.35471400	-1.82470100	0.00002300
C	-1.63539400	-0.99454300	0.08037000	H	-0.06807100	-2.51263400	0.00002100
C	-2.82492800	-1.66840200	-0.26491600	H	2.40778100	1.41588400	0.89083300
H	-2.77490000	-2.64276800	-0.73824600	H	2.40778300	1.41592500	-0.89082100
C	-4.06412100	-1.12204100	0.02919500	H	1.38774700	2.59716100	0.00003200
C	-4.14986000	0.13379100	0.65201200				
C	-2.99628200	0.82841800	0.97439800	52ts			
H	3.66828300	-2.21514900	2.10305500	C	-1.36143400	3.01661900	1.74334400
H	1.91527800	-2.95532000	0.54607900	C	-0.35280000	2.83229200	0.81598900
H	1.65768400	1.53585300	2.64729000	C	0.19713700	1.54998600	0.59225100
H	3.54549100	0.04370900	3.14689300	C	-0.33504700	0.43465400	1.30002700
H	-4.96911600	-1.67020100	-0.21751800	C	-1.38841900	0.64733300	2.21782900
H	-5.12134800	0.55939700	0.88752400	C	-1.87932000	1.91835200	2.45125100
H	-3.07657500	1.79122300	1.46709300	C	1.23975800	1.30066500	-0.38273400
C	0.00079200	1.22617700	-1.30604700				
C	0.16421800	-0.11424000	-1.74494300				

C	0.19263700	-0.87881800	0.98666700	C	0.54909700	-0.38196800	-0.00011300
C	1.59666300	-0.92600000	0.60537500	C	1.90190000	0.23115600	-0.00011900
C	2.13267400	0.19049200	-0.09340500	O	2.85511300	-0.72609400	0.00000000
C	3.47658900	0.14699900	-0.52724200	C	4.20829500	-0.24316200	0.00013600
H	3.90119500	0.99642800	-1.05133600	O	2.13722900	1.42281200	0.00001800
C	4.27489400	-0.95199100	-0.25934900	H	0.47436200	-1.46486800	-0.00011300
C	3.74430600	-2.05650100	0.42828700	H	-0.47436400	1.46486900	-0.00011800
C	2.42265400	-2.04741000	0.84107800	H	-4.83642300	1.13401300	0.00008800
H	-1.75600100	4.01287700	1.92195900	H	-4.39797400	-0.36361200	-0.88939700
H	0.03542400	3.68703000	0.27409400	H	-4.39786100	-0.36343200	0.88981100
H	-1.80128400	-0.18997300	2.76943200	H	4.39789300	0.36332900	0.88987800
H	-2.67207700	2.06664600	3.17915500	H	4.83642300	-1.13401400	-0.00003000
H	5.31398800	-0.95652600	-0.57682300	H	4.39794200	0.36371500	-0.88932900
H	4.37219900	-2.91709200	0.64201100				
H	2.02816600	-2.90479400	1.37558800				
C	-0.53236700	-1.00132200	-1.11290700	53ts			
C	-0.02449700	0.13370700	-1.80410700	C	2.49974700	-1.85412400	-2.66099300
C	-1.98234800	-1.13742600	-0.85961100	C	1.16257200	-1.51849500	-2.55205000
O	-2.76661900	-0.22979200	-0.67253900	C	0.58591100	-1.23049900	-1.29433400
C	1.74603500	2.44895000	-1.22557500	C	1.41375700	-1.24866700	-0.13668900
H	0.91937800	3.03520900	-1.63266000	C	2.78356300	-1.56518600	-0.27973100
H	2.37941700	3.12163100	-0.63172500	C	3.31496000	-1.88098300	-1.51654000
H	2.34216100	2.09222700	-2.06975900	C	-0.81228900	-0.87788700	-1.12964200
C	-0.40433200	-2.09383900	1.66406500	C	0.81229700	-0.87768500	1.12975200
H	-0.16405300	-3.01231000	1.12317700	C	-0.58589700	-1.23029500	1.29450000
H	-0.01927900	-2.19452000	2.68784900	C	-1.41374600	-1.24865200	0.13686200
H	-1.49200000	-2.03171100	1.72315500	C	-2.78355300	-1.56515000	0.27995600
O	-2.34304500	-2.45088900	-0.83945000	H	-3.42390000	-1.59113100	-0.59502100
C	-0.85942700	1.19158200	-2.28564000	C	-3.31494600	-1.88075000	1.51681700
N	-1.43481100	2.10481900	-2.72395000	C	-2.49972600	-1.85371600	2.66126100
H	-0.01383900	-1.93708300	-1.28358800	C	-1.16255200	-1.51810200	2.55226200
C	-3.74134700	-2.68963000	-0.61926000	H	2.91864700	-2.10016300	-3.63290500
H	-4.33941500	-2.22365200	-1.40703600	H	0.54467100	-1.50836200	-3.44321300
H	-3.86004600	-3.77365800	-0.63847100	H	3.42390900	-1.59103200	0.59525000
H	-4.05818600	-2.28526800	0.34629100	H	4.36458500	-2.14833800	-1.60266100
H	0.83317200	-0.04591600	-2.44574900	H	-4.36457000	-2.14808900	1.60298500
				H	-2.91862200	-2.09960600	3.63321400
				H	-0.54464600	-1.50782800	3.44342100
53-dienophile				C	0.41536900	1.26346700	0.57111700
C	-4.20829500	0.24316200	0.00013300	C	-0.41538000	1.26338500	-0.57132500
O	-2.85511300	0.72609400	0.00000000	C	1.80554600	1.72965900	0.39002100
C	-1.90190000	-0.23115600	-0.00010400	O	2.43142000	1.72545700	-0.65326000
O	-2.13722900	-1.42281200	0.00001600	C	-1.80555000	1.72958100	-0.39027300
C	-0.54909700	0.38196800	-0.00010900	O	-2.43138700	1.72553600	0.65302500

C	-1.68072700	-0.79818300	-2.36678400	H	-4.81606800	0.59766600	1.64184200
H	-1.20212000	-0.20519900	-3.14987100	H	-5.86577600	-0.59673300	0.85074800
H	-1.87171800	-1.80099400	-2.77313200	H	-4.24571000	-1.07187500	1.39709700
H	-2.64414000	-0.33190700	-2.15850500				
C	1.68071200	-0.79780300	2.36690000				
H	1.20207200	-0.20473800	3.14990500	54ts			
H	1.87172800	-1.80055900	2.77336800	C	1.68459300	-2.10802000	-3.23802400
H	2.64411800	-0.33152400	2.15859000	C	0.42754600	-1.76920700	-2.77143900
O	-2.32782300	2.18892700	-1.56140600	C	0.21319600	-1.48120500	-1.40449400
O	2.32778000	2.18919800	1.56108600	C	1.32329800	-1.50233400	-0.51437300
C	-3.66203100	2.70695400	-1.46768300	C	2.60261900	-1.82193700	-1.02225700
H	-3.92312500	3.02911800	-2.47664200	C	2.77893300	-2.13758600	-2.35685600
H	-4.35580100	1.93727300	-1.11798800	C	-1.08786800	-1.12838700	-0.86643100
H	-3.69947100	3.55213200	-0.77458200	C	1.08790000	-1.12793500	0.86700500
C	3.66199600	2.70719600	1.46732400	C	-0.21317000	-1.48033500	1.40530100
H	3.69947100	3.55225100	0.77407300	C	-1.32328700	-1.50192900	0.51520000
H	3.92305200	3.02953700	2.47623600	C	-2.60263700	-1.82105800	1.02330800
H	4.35577400	1.93744800	1.11779400	H	-3.45570400	-1.84961800	0.35404100
H	0.04531500	1.48707900	-1.52656000	C	-2.77896400	-2.13582300	2.35811600
H	-0.04534300	1.48729200	1.52631300	C	-1.68461100	-2.10580200	3.23925000
				C	-0.42753100	-1.76742300	2.77243200
54-dienophile				H	1.82433900	-2.35408100	-4.28711700
C	5.16790600	-0.96801900	0.11546900	H	-0.40813800	-1.75660100	-3.46253500
C	4.18145400	0.18409000	0.13028800	H	3.45567100	-1.85016200	-0.35295800
O	2.85347200	-0.37891600	0.01804800	H	3.76547800	-2.40706600	-2.72392900
C	1.83647200	0.50830800	0.00940900	H	-3.76553200	-2.40496200	2.72537900
O	1.98099900	1.71228800	0.08897500	H	-1.82437100	-2.35116900	4.28850400
C	0.53316100	-0.19554100	-0.10976500	H	0.40816200	-1.75444400	3.46351000
C	-0.61595600	0.48840700	-0.14390100	C	0.56132400	1.01162200	0.42856500
C	-1.91830900	-0.21695100	-0.26432000	C	-0.56123500	1.01149500	-0.42913500
O	-2.93370300	0.67373100	-0.28829300	C	1.84425900	1.47024400	-0.14524400
C	-4.27071100	0.12834200	-0.40317300	O	2.14027000	1.45848600	-1.32578800
C	-4.82908400	-0.25760000	0.95844200	C	-1.84419800	1.47035500	0.14444200
O	-2.05710800	-1.42246200	-0.33622200	O	-2.14020400	1.45924500	1.32499200
H	0.53731200	-1.27942500	-0.16928000	C	-2.25995900	-1.05125900	-1.82068600
H	4.34000000	0.87573400	-0.70348700	H	-2.01024700	-0.46779500	-2.71020400
H	4.23796300	0.76544900	1.05635000	H	-2.55929600	-2.05562800	-2.15062100
H	-0.62102800	1.57227200	-0.08474400	H	-3.12728300	-0.57628200	-1.36128000
H	5.09004200	-1.53787500	-0.81587600	C	2.26005800	-1.05024900	1.82113700
H	6.18961700	-0.58212300	0.19944000	H	2.01054500	-0.46592400	2.71014700
H	4.98666400	-1.64919400	0.95294600	H	2.55915700	-2.05439400	2.15196600
H	-4.85000800	0.93330400	-0.86168000	H	3.12747200	-0.57590100	1.36124500
H	-4.24189400	-0.73055100	-1.07812300	O	-2.68369200	1.92777000	-0.82400900
				O	2.68369800	1.92825500	0.82295300

C	-3.94805500	2.44495300	-0.35739600	C	3.02494600	-0.46663200	-0.23442200
H	-4.47673100	1.65727600	0.18972200	C	4.22616600	-1.08081900	-0.65094300
H	-3.75761400	3.26003000	0.34872500	C	4.55881300	-2.35726800	-0.23152400
C	3.94807400	2.44517000	0.35607200	C	0.91240800	-0.55976000	1.02953200
H	3.75765700	3.25949800	-0.35091400	C	2.58646300	0.83928400	-0.71139300
H	4.47698000	1.65701600	-0.19014200	C	1.77342300	1.59953100	0.22596500
C	4.72540800	2.91802300	1.57055600	C	0.89350300	0.87506600	1.08418300
H	5.69259800	3.32695400	1.25800400	C	0.01538500	1.59878800	1.93136100
H	4.17697500	3.70012400	2.10535100	H	-0.66354900	1.06227500	2.58510400
H	4.90956900	2.09212500	2.26557800	C	0.03952900	2.97776700	1.96863800
C	-4.72570400	2.91647600	-1.57219300	C	0.91941300	3.68945000	1.13239600
H	-4.90992500	2.08984600	-2.26632900	C	1.75505400	3.01120800	0.26455500
H	-5.69287300	3.32561600	-1.25984800	H	3.94444500	-4.08027200	0.92827100
H	-4.17748100	3.69809200	-2.10791000	H	1.82625600	-3.07085700	1.65314300
H	0.39330700	1.24048900	1.47456300	H	4.91558000	-0.53717700	-1.28786900
H	-0.39322500	1.23981100	-1.47525800	H	5.50168200	-2.80006900	-0.54106300
55-dienophile				H	-0.62234300	3.51348100	2.64330900
C	-3.35701400	0.25130300	0.09983500	H	0.94161500	4.77533700	1.16662000
C	-2.87795400	-1.04447200	0.30205000	H	2.42525400	3.57628800	-0.37407400
C	-1.51732400	-1.31746600	0.16686800	C	1.11965600	0.20192600	-2.00123400
C	-0.64165600	-0.28632700	-0.17144200	C	0.13244900	-0.57589700	-1.37471400
C	-1.10275700	1.01337900	-0.38442100	C	-1.16693900	0.01494900	-1.08285100
C	-2.46734400	1.27115600	-0.24256400	O	-1.43718600	1.20026100	-1.08703300
O	0.68794700	-0.66697800	-0.36101200	C	-0.11388100	-1.35976700	1.79489100
C	1.72899000	0.10906200	0.07718300	H	-0.23595400	-2.35847100	1.36859800
O	1.60837400	1.16921800	0.64769700	H	0.18130100	-1.48032900	2.84719800
C	3.01040600	-0.55971300	-0.25709400	H	-1.09313700	-0.87923000	1.77641000
C	4.17532800	0.00068200	0.07637700	C	3.50361200	1.60584900	-1.64797000
H	5.12363900	-0.47351400	-0.15716500	H	2.97616800	2.43560400	-2.12566100
H	4.19897600	0.95444500	0.59585600	H	4.36787600	2.02089500	-1.11340000
H	2.94880500	-1.51153100	-0.77558900	H	3.88360400	0.96433300	-2.44766800
H	-1.12201500	-2.31731100	0.31601400	O	-2.08251200	-0.98192900	-0.77841000
H	-0.41190800	1.80492000	-0.64272600	H	0.81751900	1.19098400	-2.33409800
H	-3.56166200	-1.84674600	0.56547700	H	1.81621000	-0.30968800	-2.65869100
H	-2.83373700	2.28141600	-0.40308400	H	0.19652000	-1.65690500	-1.36982800
H	-4.41671200	0.46478200	0.20698500	C	-3.41610200	-0.71030600	-0.50113500
55ts				C	-4.15714000	0.30143800	-1.11881000
C	3.68170200	-3.07872500	0.59884900	C	-4.02401400	-1.59060400	0.39775700
C	2.48933900	-2.50974300	1.00334100	C	-5.51353600	0.42497500	-0.81194600
C	2.13950000	-1.19194400	0.61513800	H	-3.68072400	0.98263600	-1.80971000
				C	-5.38015600	-1.45604800	0.69041000
				H	-3.42499500	-2.37608400	0.84812200
				C	-6.13110300	-0.44461300	0.08844400
				H	-6.09084900	1.21307100	-1.28829400

H	-5.84813000	-2.14453500	1.38905800	H	0.37831200	3.17702700	1.44120000
H	-7.18768700	-0.33658800	0.31696000	H	-0.71801000	3.54984600	0.10377500
				H	-1.34871000	2.89331900	1.62068200
				H	0.86197000	0.93300700	2.45007800
56-dienophile				H	-0.93924400	0.66740300	2.58832700
C	0.00000000	0.77492300	0.00000000	H	-0.67510700	-1.68926200	1.98583400
C	1.32213500	0.98401900	0.00000000	C	1.44906600	-1.63135000	1.95304300
C	-0.58054400	-0.53323900	0.00000000	N	2.49114300	-2.15815600	1.97411600
N	-1.07182600	-1.58791900	0.00000000				
H	2.03240200	0.16309100	0.00000000	57-dienophile			
H	-0.70205400	1.60539400	0.00000000	C	-0.60230200	0.19145800	-0.06123900
H	1.72288400	1.99272700	0.00000000	C	0.60230800	0.19148800	0.06121300
				C	-2.03502100	0.24896000	-0.27883600
56ts				O	-2.56229200	0.97813600	-1.09046800
C	-3.75941700	-0.83930900	-0.81617400	O	-2.67940100	-0.60702200	0.53291000
C	-2.49457100	-1.39159400	-0.87682500	C	2.03501200	0.24881300	0.27895600
C	-1.34880400	-0.63424400	-0.52535700	O	2.56224100	0.97743500	1.09111400
C	-1.52190100	0.70800300	-0.07551400	O	2.67943300	-0.60664700	-0.53330900
C	-2.82884600	1.23900100	-0.00048900	C	-4.11338500	-0.61934200	0.38887100
C	-3.92778500	0.48684800	-0.37678000	H	-4.39123200	-0.90555700	-0.62855000
C	-0.01295700	-1.17213800	-0.57312500	H	-4.46676500	-1.35702800	1.10875000
C	-0.34001200	1.42699800	0.38041000	H	-4.52646600	0.36785000	0.61042800
C	0.89332900	1.10194100	-0.31929700	C	4.11340400	-0.61910800	-0.38915900
C	1.06645600	-0.24150600	-0.76589900	H	4.46680800	-1.35643600	-1.10939300
C	2.30864200	-0.62114500	-1.33438000	H	4.52654500	0.36818100	-0.61018000
H	2.45691900	-1.64310300	-1.66428000	H	4.39116100	-0.90585500	0.62813500
C	3.32197300	0.30102200	-1.50451500				
C	3.14221600	1.63095300	-1.08164500	57ts			
C	1.95630800	2.01749600	-0.48306600	C	2.33894300	-1.91270400	2.82968800
H	-4.62295700	-1.42685600	-1.11558300	C	2.39354200	-1.63344200	1.47800200
H	-2.37548700	-2.40949500	-1.23237400	C	1.21502700	-1.36426400	0.74151900
H	-2.97677000	2.26154700	0.33027700	C	-0.03693500	-1.35777700	1.42435200
H	-4.92171900	0.92433600	-0.33833500	C	-0.05925600	-1.61352500	2.81636700
H	4.25883900	-0.00146900	-1.96362800	C	1.10329400	-1.90088900	3.50435700
H	3.93768300	2.35750900	-1.22364800	C	1.22618900	-1.04052100	-0.66685200
H	1.83664200	3.04643800	-0.16112000	C	-1.22653500	-1.03918200	0.66851300
C	-0.00379000	0.36015600	2.13119800	C	-1.21545400	-1.36514800	-0.73933900
C	0.17141700	-1.01685900	1.89415500	C	0.03651000	-1.36006200	-1.42218000
C	0.21078200	-2.63807600	-0.85068900	C	0.05877400	-1.61804200	-2.81378100
H	-0.58056700	-3.25425000	-0.41682600	H	1.00311200	-1.61240600	-3.34638900
H	0.23661300	-2.84348600	-1.93023400	C	-1.10384500	-1.90620700	-3.50131800
H	1.16061300	-2.97268600	-0.42493300	C	-2.33949800	-1.91664000	-2.82663600
C	-0.51661000	2.83668200	0.91361300				

C	-2.39403500	-1.63521600	-1.47539600	H	3.03227100	-0.89942100	0.00005100
H	3.25170200	-2.14272900	3.37246000	H	2.42291900	0.53653400	-0.88917500
H	3.35229200	-1.64821700	0.97166500	H	2.42286900	0.53654900	0.88921700
H	-1.00358700	-1.60679800	3.34897600				
H	1.06317500	-2.11914500	4.56794500				
H	-1.06377800	-2.12616800	-4.56455700	58ts			
H	-3.25231100	-2.14730500	-3.36904600	C	3.71515300	-1.76686700	0.81616500
H	-3.35279000	-1.64896300	-0.96904000	C	2.37584500	-1.74917600	1.15598000
C	-0.54736500	1.12595800	0.30191700	C	1.51536600	-0.72585200	0.68536800
C	0.54777400	1.12522300	-0.30385200	C	2.04695200	0.27530700	-0.17882300
C	-1.58991500	1.88272800	0.97253900	C	3.41404300	0.21976900	-0.52927100
O	-1.60825600	2.14023900	2.16068400	C	4.23935400	-0.77297200	-0.03046800
C	1.59056700	1.88067800	-0.97562100	C	0.11575400	-0.66557500	1.02642100
O	1.60918500	2.13607200	-2.16421700	C	1.11749300	1.24793700	-0.73663200
C	2.54944200	-0.93446600	-1.39104100	C	0.01773900	1.62508500	0.13643800
H	3.29410500	-0.42172700	-0.77818800	C	-0.50749100	0.62972600	1.01264000
H	2.94426000	-1.92956200	-1.63683900	C	-1.63870500	0.94537200	1.80720700
H	2.44708700	-0.37193500	-2.32112200	H	-2.04709900	0.19715900	2.47821600
C	-2.54974400	-0.93152600	1.39253900	C	-2.20168100	2.20504900	1.77385300
H	-3.29427400	-0.41960900	0.77884200	C	-1.67516100	3.18914900	0.91677300
H	-2.94484500	-1.92608800	1.64004400	C	-0.59814400	2.89594400	0.10123200
H	-2.44718700	-0.36745300	2.32166500	H	4.36420900	-2.54479600	1.20901800
O	2.57032000	2.24235900	-0.11250200	H	1.98696800	-2.51442700	1.81937700
O	-2.56981800	2.24298700	0.10898800	H	3.83409000	0.98118100	-1.17799700
C	3.63264000	3.01750000	-0.69311900	H	5.29460700	-0.78102200	-0.29000000
H	4.31970300	3.22608200	0.12747800	H	-3.05099200	2.43695400	2.41067000
H	4.13602100	2.45456900	-1.48403900	H	-2.11601000	4.18212000	0.89471500
H	3.24384400	3.94842100	-1.11430400	H	-0.20485500	3.66642600	-0.55304100
C	-3.63191100	3.01928500	0.68846800	C	0.12120200	-0.03687300	-2.02076800
H	-3.24293300	3.95099500	1.10773600	C	-0.49599000	-1.10220100	-1.34888100
H	-4.31923300	3.22633100	-0.13230200	C	-1.94635900	-1.07157500	-1.15400200
H	-4.13505700	2.45789900	1.48063500	O	-2.67031800	-0.10246400	-1.30986500
				C	-0.50599700	-1.79572100	1.81111200
58-dienophile				H	-0.14912900	-2.76646900	1.45882400
C	-2.49182300	-0.01308800	0.00002200	H	-0.26349000	-1.71876900	2.88082800
C	-1.31706000	-0.64638000	-0.00000800	H	-1.59248400	-1.80118000	1.71254500
C	-0.04361800	0.11761900	-0.00004700	C	1.65627000	2.28532200	-1.70508400
O	1.01691400	-0.72527700	-0.00000900	H	0.84436000	2.79272700	-2.23267100
C	2.30316800	-0.08855800	0.00002300	H	2.24978100	3.05072300	-1.18803800
O	0.06069500	1.32782200	-0.00000300	H	2.29550700	1.82581900	-2.46411300
H	-3.43292700	-0.55459300	0.00005000	O	-2.42797800	-2.29051900	-0.76356000
H	-2.53036300	1.07258800	0.00001800	C	-3.84995500	-2.35205600	-0.60250900
H	-1.23964300	-1.72957100	-0.00000600	H	-4.06742500	-3.37508900	-0.29105300
				H	-4.18999100	-1.64001000	0.15486600

H	-4.35736700	-2.12522900	-1.54491200	C	-0.15626500	2.25416200	-1.54976200
H	-0.00811300	-2.06546200	-1.26341700	H	0.71592200	2.87880900	-1.34298700
H	-0.53895200	0.71720800	-2.43941300	H	-0.27600200	2.20678700	-2.64144200
H	1.00862000	-0.25275700	-2.60750800	H	-1.03372400	2.76474700	-1.14147200
59-dienophile				C	0.28166000	-2.71625400	1.40913500
C	-0.95354200	1.34126800	0.00000000	H	-0.60063900	-2.85965100	2.03859200
C	-0.39478700	0.12209500	0.00000000	H	0.37628900	-3.59605600	0.76002900
H	-2.03359600	1.45584800	0.00000000	H	1.15019000	-2.69681400	2.07290000
H	-0.35513900	2.24626600	0.00000000	H	-0.94989900	-0.44531900	2.46104400
C	1.03992000	0.00270500	0.00000000	H	0.86242500	-0.35483600	2.61426900
N	2.19550600	-0.13224100	0.00000000	C	-1.26681300	1.98662900	1.49232300
C	-1.17154500	-1.17395800	0.00000000	N	-2.26265400	2.58693500	1.37667100
H	-0.92666200	-1.77679900	-0.88213100	C	1.21870200	2.14788200	1.71306900
H	-0.92666200	-1.77679900	0.88213100	H	2.10960100	1.54866800	1.50132600
H	-2.24676500	-0.97549500	0.00000000	H	1.19970500	2.99478000	1.02064300
59ts				H	1.32389000	2.55804800	2.72739400
C	3.67440300	0.18448700	-1.25260800	60-dienophile			
C	2.45164800	0.81317900	-1.39013600	C	-1.36364400	1.58039200	-0.00001300
C	1.27528300	0.26086700	-0.82037800	C	-1.14481900	0.25942900	-0.00001200
C	1.38000700	-0.94759500	-0.06769400	C	-2.24021900	-0.77408500	0.00004900
C	2.64601700	-1.55485100	0.07632000	C	0.24144400	-0.29923400	-0.00009100
C	3.77260100	-1.01031200	-0.51660800	O	1.20741400	0.64925100	0.00000500
C	-0.01550400	0.87964300	-0.94734800	C	2.55200800	0.14982900	0.00004600
C	0.17625500	-1.43736900	0.59595900	O	0.48456800	-1.49094700	-0.00003000
C	-1.06809600	-1.18797700	-0.12407200	H	-2.37443700	1.98012200	0.00003200
C	-1.17100100	0.03030800	-0.85761700	H	-0.54737000	2.29364700	-0.00006200
C	-2.41619800	0.37376600	-1.44307000	H	3.19247400	1.03251800	0.00012700
H	-2.51275300	1.30508300	-1.98918600	H	2.73713800	-0.45954800	0.88896900
C	-3.50043500	-0.47691000	-1.35560200	H	2.73722500	-0.45944800	-0.88892700
C	-3.38839900	-1.69030700	-0.65326300	H	-2.16232800	-1.42667400	-0.87681200
C	-2.19775500	-2.02828200	-0.03280000	H	-2.16220000	-1.42670800	0.87687400
H	4.55832500	0.60969200	-1.72012400	H	-3.22498800	-0.29832400	0.00012800
H	2.38559300	1.72449900	-1.97473600	60ts			
H	2.73948600	-2.47929300	0.63627700	C	3.74249300	-1.36965300	1.13021400
H	4.73212300	-1.51043600	-0.41700000	C	2.40111100	-1.35778300	1.46303500
H	-4.44018700	-0.20769200	-1.82938100	C	1.50361000	-0.44144100	0.85754400
H	-4.23893300	-2.36402100	-0.59386600	C	2.00269500	0.45124900	-0.13779500
H	-2.13188300	-2.96508700	0.51001300	C	3.37221700	0.40212600	-0.47345300
C	-0.02230700	-0.04601800	2.06183600	C	4.23337300	-0.47993800	0.15800400
C	-0.02896300	1.29487900	1.60748300	C	0.10630400	-0.38620300	1.19329200

C	1.03645900	1.30176600	-0.82719900	O	0.28635000	1.46492900	0.00033500
C	-0.07736700	1.75591500	-0.00211400	O	0.75039700	-0.75643100	-0.00062100
C	-0.57379100	0.86098900	0.99086000	C	2.15304100	-0.43341300	0.00068800
C	-1.72714800	1.23244900	1.72852000	H	2.66921000	-1.39334700	0.00043900
H	-2.11704800	0.56194600	2.48696900	H	2.41299300	0.14589000	-0.88907800
C	-2.33525600	2.45559700	1.53106700	H	2.41162900	0.14468600	0.89163000
C	-1.83225200	3.34322700	0.56297700	H	-3.66770500	-0.67336800	0.00200200
C	-0.73494000	2.98831700	-0.20114700				
H	4.41804700	-2.06211500	1.62519200				
H	2.03746800	-2.03913800	2.22468700	61ts			
H	3.76883300	1.08252700	-1.21932800	C	-1.41034700	3.32115400	-1.28948800
H	5.28983100	-0.48082200	-0.09662100	C	-1.30463700	1.96587900	-1.52643700
H	-3.20143300	2.73321400	2.12555600	C	-0.33391900	1.17836100	-0.85490000
H	-2.30660000	4.30932100	0.41286400	C	0.51693500	1.80770700	0.10353700
H	-0.36303600	3.68438300	-0.94534300	C	0.36823400	3.19250000	0.34471400
C	0.09669900	-0.08218800	-1.95801800	C	-0.56511000	3.94034300	-0.34823000
C	-0.42822200	-1.18284900	-1.24650500	C	-0.18427200	-0.23125100	-1.08557900
C	-1.87254900	-1.15283400	-0.97369000	C	1.43642400	0.96593200	0.84758300
O	-2.61237800	-0.19691600	-1.14781900	C	1.95301000	-0.19065500	0.13720500
C	-0.48293400	-1.42511100	2.11519000	C	1.09634200	-0.82161900	-0.81436900
H	-0.08199500	-2.41930100	1.90341300	C	1.53006700	-2.02056900	-1.43574200
H	-0.26390700	-1.19956400	3.16902000	H	0.88459700	-2.51474000	-2.15335500
H	-1.56733100	-1.48687000	2.00627600	C	2.77493900	-2.55119400	-1.16532500
C	1.55911000	2.25200500	-1.89213400	C	3.62550300	-1.91714600	-0.23901600
H	0.74231300	2.65389900	-2.49724800	C	3.21274600	-0.76913200	0.41134200
H	2.09540800	3.09923300	-1.44583800	H	-2.14225700	3.91183200	-1.83357600
H	2.24552900	1.74585300	-2.57589500	H	-1.95288700	1.50358600	-2.26279300
O	-2.33730600	-2.34791200	-0.49585900	H	1.01250900	3.68557700	1.06471100
C	-3.75092400	-2.39775000	-0.27400600	H	-0.64401200	5.00911100	-0.16818900
H	-3.95508300	-3.40252100	0.09995400	H	3.09972400	-3.45731700	-1.66917600
H	-4.05987900	-1.64572400	0.45745500	H	4.60888200	-2.33143200	-0.03352200
H	-4.29652800	-2.21979900	-1.20550500	H	3.87909100	-0.29552700	1.12424300
H	-0.62979800	0.60326300	-2.38319000	C	0.01369600	-0.04695300	1.97595900
H	0.95740700	-0.28266500	-2.59199900	C	-0.85890200	-0.68024000	1.35030500
C	0.31867500	-2.49342800	-1.20630700	C	-1.93751400	-1.55536900	1.00262800
H	1.39960200	-2.32399400	-1.21961000	O	-1.83616300	-2.75471100	0.80325400
H	0.07115900	-3.09243800	-0.32632500	C	-1.17714900	-0.97024000	-1.94801500
H	0.07033500	-3.10683000	-2.08506300	H	-2.18358000	-0.56380200	-1.82738700
				H	-0.91305100	-0.90322000	-3.01278600
				H	-1.21630300	-2.02827300	-1.67658300
61-dienophile				C	2.30153900	1.60533200	1.91718100
C	-2.63344200	-0.40998500	0.00129900	H	2.74766100	0.84847200	2.56815200
C	-1.46339100	-0.11336800	-0.00176900	H	3.11886700	2.19141100	1.47791400
C	-0.07622500	0.30812400	-0.00066800	H	1.71525100	2.27587000	2.55157200

O	-3.11372700	-0.87707000	0.89409100	H	2.26271700	-2.56954300	1.84663500
C	-4.25134800	-1.69438100	0.58258000	H	4.13293200	0.62996600	-1.45049000
H	-5.09704300	-1.00703100	0.53455900	H	5.51541200	-1.21166600	-0.59776000
H	-4.11695000	-2.20414100	-0.37561300	H	-2.31037200	2.80742000	2.56371800
H	-4.41358800	-2.44608100	1.36025300	H	-1.33535800	4.41452300	0.92283300
H	0.37479700	0.20920000	2.95722400	H	0.41441400	3.67744800	-0.63473300
62-dienophile				C	0.27946400	-0.10387400	-1.95722100
C	1.78092600	-1.04609900	0.00014900	C	-0.41549700	-1.07549800	-1.21367000
C	0.40651300	-1.28140500	0.00001100	C	-0.18665100	-1.64131600	1.97394400
C	-0.51518200	-0.22055400	-0.00013800	H	0.12887600	-2.65288200	1.70469700
C	-0.00891900	1.09239900	-0.00019900	H	0.04338700	-1.49735400	3.03964200
C	1.36214300	1.32963300	-0.00006600	H	-1.27378600	-1.60099300	1.86137700
C	2.26531200	0.26189900	0.00011300	C	2.03104000	2.07861000	-1.88047100
H	2.47213400	-1.88486500	0.00028900	H	1.22565100	2.63677000	-2.36577000
H	0.03510400	-2.30388700	0.00003800	H	2.72974700	2.80749700	-1.44930000
H	-0.69417000	1.93515300	-0.00038600	H	2.56246100	1.53242100	-2.66465100
H	1.73026900	2.35237100	-0.00013000	H	-0.29796500	0.68844300	-2.42657900
H	3.33542900	0.45059800	0.00019700	H	1.10825900	-0.45230200	-2.56584300
C	-1.95472500	-0.52933600	-0.00024700	H	0.04925100	-2.05226600	-1.11280100
C	-2.97732700	0.33500600	0.00031900	C	-1.84718900	-1.04019200	-0.92946000
H	-2.18631200	-1.59470200	-0.00080300	C	-2.61882600	0.13960800	-0.99440500
H	-4.00438300	-0.01697400	0.00016500	C	-2.51391600	-2.23600100	-0.58423700
H	-2.84051600	1.41305600	0.00097800	C	-3.98755900	0.11611200	-0.73991200
62ts				H	-2.14093700	1.08395700	-1.23567000
C	3.95486600	-2.01559500	0.67146500	C	-3.88378500	-2.25788000	-0.33508600
C	2.65362900	-1.87085500	1.11434900	H	-1.94221200	-3.16003200	-0.53147500
C	1.83968700	-0.80052300	0.66353600	C	-4.63121300	-1.08028100	-0.41325500
C	2.38152500	0.11586100	-0.28630200	H	-4.55638500	1.04085000	-0.79604300
C	3.70674500	-0.06692500	-0.73626900	H	-4.36975900	-3.19716000	-0.08291900
C	4.48869200	-1.10484700	-0.25809300	H	-5.70065800	-1.09431800	-0.22130200
C	0.48453700	-0.60518200	1.10874800	63-dienophile			
C	1.48789300	1.13477500	-0.82267100	C	-0.86679600	-1.03563500	-0.00003800
C	0.50657300	1.64950000	0.12034200	C	0.50852700	-1.27755400	0.00004900
C	-0.03038600	0.73459400	1.07607200	C	1.44955000	-0.23902100	0.00019500
C	-1.07383900	1.17804000	1.92858800	C	0.95301800	1.08120800	0.00026500
H	-1.49994600	0.49207900	2.65285500	C	-0.40702200	1.34064200	0.00020600
C	-1.53007800	2.48166000	1.88105900	C	-1.33224700	0.28276900	0.00005800
C	-0.98414400	3.38645300	0.95275800	H	-1.55485000	-1.87330900	-0.00010200
C	0.00271400	2.96805000	0.07573000	H	0.85821100	-2.30770200	-0.00006500
H	4.56857900	-2.82862200	1.05034600	H	1.64499200	1.91841100	0.00044700
				H	-0.78600400	2.35802500	0.00026800
				C	2.88249400	-0.56483000	0.00021500

C	3.91859800	0.28440700	-0.00045800	H	0.38629300	0.81258200	-2.42152500
H	3.09968300	-1.63351200	0.00067700	H	1.61457800	-0.51612100	-2.56574300
H	4.94024600	-0.08278400	-0.00039100	H	0.33889500	-1.95614100	-1.12223300
H	3.79768700	1.36446300	-0.00114900	C	-1.39652800	-0.69109700	-0.93710600
O	-2.64703100	0.64737800	-0.00022700	C	-2.00686200	0.58307700	-1.00620100
C	-3.62753300	-0.37768600	-0.00010200	C	-2.22589500	-1.77402400	-0.58866600
H	-4.59312900	0.13132100	-0.00043500	C	-3.35934600	0.75198100	-0.75634700
H	-3.55094000	-1.01014600	-0.89456900	H	-1.40952500	1.45573100	-1.25101600
H	-3.55119000	-1.00960000	0.89478900	C	-3.58970500	-1.61927400	-0.33974100
				H	-1.79382500	-2.77045300	-0.52928500
				C	-4.16691000	-0.34700700	-0.42471100
63ts				H	-3.81932900	1.73403900	-0.80920300
C	4.21849700	-2.48956600	0.65268000	H	-4.18551500	-2.48927500	-0.08715900
C	2.95256200	-2.16467400	1.10247400	O	-5.48745100	-0.07157200	-0.20533700
C	2.29579300	-0.98743000	0.66101600	C	-6.34930000	-1.14813100	0.12207100
C	2.95943300	-0.15070100	-0.28533600	H	-7.34175000	-0.71107900	0.24810200
C	4.24346300	-0.51649400	-0.74228400	H	-6.38286300	-1.89782000	-0.67993300
C	4.87251800	-1.65807600	-0.27437100	H	-6.04830400	-1.63806100	1.05802400
C	0.98347500	-0.60518200	1.11081800				
C	2.21647000	0.98751800	-0.81404000				
C	1.31998800	1.63016600	0.13494400	64-dienophile			
C	0.65979800	0.79304900	1.08469100	C	3.43905800	-0.89371700	0.12420900
C	-0.31283800	1.37178600	1.94000700	O	2.65975800	0.25817500	-0.23497600
H	-0.82950700	0.74613500	2.65992900	C	1.34002500	0.17201500	0.04772700
C	-0.58356900	2.72646100	1.90076600	O	0.82462900	-0.79551600	0.57130500
C	0.08482200	3.55239900	0.97895400	C	0.64513200	1.42064600	-0.35351300
C	1.00524600	3.00619800	0.09970300	C	-0.68518100	1.55845100	-0.32311900
H	4.71220500	-3.38383200	1.02402100	C	-1.66654700	0.51761700	0.12857300
H	2.46968400	-2.80461800	1.83358800	O	-1.78575900	-0.48359900	-0.75653100
H	4.76081000	0.11713700	-1.45528500	C	-2.65923800	-1.55374300	-0.35395400
H	5.87215300	-1.90743800	-0.62012700	O	-2.31743600	0.63126500	1.14371700
H	-1.31228600	3.15343000	2.58468700	H	-1.12978000	2.51921400	-0.57267000
H	-0.11981000	4.61954200	0.95555500	H	4.46370700	-0.65424500	-0.16096000
H	1.51249800	3.65629300	-0.60577300	H	3.37128600	-1.08191600	1.19907700
C	0.844476300	-0.05545900	-1.95419800	H	3.08609800	-1.77792600	-0.41337300
C	0.01469200	-0.92396300	-1.22048200	H	-2.25232700	-2.05000500	0.53066200
C	0.16934600	-1.54092600	1.96742400	H	-3.65906600	-1.17329400	-0.13028500
H	0.35496900	-2.58658100	1.70754200	H	-2.68655800	-2.24024000	-1.20029600
H	0.39491200	-1.42276600	3.03731000	H	1.27760000	2.24819500	-0.65980800
H	-0.90149200	-1.35946800	1.83360600				
C	2.88891100	1.85117700	-1.86571500	64ts			
H	2.17489000	2.53191300	-2.33701800	C	-4.39344200	1.02835300	-0.23142300
H	3.69419300	2.45890900	-1.43268000	C	-3.21231600	1.44388100	0.35943100
H	3.32478900	1.23967400	-2.66078300				

C	-2.08869000	0.58977800	0.41530700	H	3.20863400	-2.84724700	-1.07049400
C	-2.17527700	-0.70287300	-0.17132400	H	3.89887500	-1.63732800	-2.17574200
C	-3.38246800	-1.09259600	-0.79521100				
C	-4.47865300	-0.24789400	-0.81373100				
C	-0.80855600	0.99482300	0.97782000	65-dienophile			
C	-0.99334400	-1.54612700	-0.13945800	C	4.14631900	-0.33188500	0.00018300
C	-0.11863900	-1.36921600	0.99949000	C	3.22963000	-1.38873500	-0.00019200
C	-0.01962600	-0.06836900	1.57108000	C	1.86286700	-1.13254600	-0.00034100
C	0.86776400	0.13543200	2.65216900	C	1.37815800	0.18995200	-0.00015300
H	0.95755400	1.12003700	3.09616900	C	2.31371900	1.24052300	0.00020900
C	1.59920100	-0.91202900	3.17872700	C	3.68349700	0.98439700	0.00038600
C	1.49830100	-2.19726600	2.61605100	C	-0.04693500	0.52117500	-0.00034100
C	0.66847800	-2.41641900	1.53293700	C	-1.09182800	-0.32689500	0.00004900
H	-5.25573900	1.68951300	-0.24105600	C	-2.47123400	0.19808300	-0.00009400
H	-3.16128100	2.43138700	0.80554500	O	-2.79345200	1.37173000	-0.00046000
H	-3.46334800	-2.07738800	-1.24236500	O	-3.37018400	-0.81948500	0.00037900
H	-5.40678800	-0.57511300	-1.27429700	C	-4.74627700	-0.41622300	0.00024800
H	2.25410900	-0.74090900	4.02863800	H	-0.28893800	1.58329100	-0.00058900
H	2.07098600	-3.02036700	3.03515800	H	-5.32372900	-1.34152700	-0.00062000
H	0.59427600	-3.41251100	1.10988200	H	-4.97448600	0.17794100	0.88960900
C	0.18092900	-0.20018100	-1.55403900	H	-4.97394200	0.17937200	-0.88827500
C	0.17902200	1.10015800	-0.97905900	H	-0.98257900	-1.40658900	0.00055500
C	1.37620500	1.89866700	-0.58704300	H	1.16438400	-1.96409100	-0.00065600
O	2.31274700	1.59011600	0.11718500	H	1.95461800	2.26687400	0.00037100
C	-0.68588000	2.39846100	1.53456900	H	3.58473000	-2.41574000	-0.00038900
H	-1.06227500	3.14188800	0.82684000	H	4.38802900	1.81157200	0.00066600
H	-1.25842200	2.50201100	2.46608600	H	5.21351600	-0.53614200	0.00025800
H	0.35365600	2.64954900	1.75373200				
C	-1.03936500	-2.88332400	-0.84301000				
H	-0.04346400	-3.30695300	-0.97844300	65ts			
H	-1.64175600	-3.60292900	-0.27142900	C	0.17651100	0.45719400	-0.07379100
H	-1.47825300	-2.79390000	-1.83955200	C	0.11695500	0.26291200	1.29711200
O	1.24427000	3.15331000	-1.11624100	C	1.27737400	-0.04802100	2.03862400
C	2.31547500	4.05494800	-0.81007100	C	2.52800200	-0.13344800	1.36181400
H	2.06489900	4.98988100	-1.31321700	C	2.56622100	0.10378300	-0.03232400
H	2.39752700	4.21166600	0.26962200	C	1.40988700	0.37807900	-0.74168900
H	3.26795100	3.66477700	-1.17962100	C	1.28024700	-0.20474000	3.48677300
H	-0.58668400	1.74641100	-1.39509600	C	3.71097600	-0.39361100	2.14974800
H	-0.57436000	-0.36139700	-2.31452300	C	3.52708400	-1.19874400	3.33636600
C	1.33433700	-1.09371200	-1.80892300	C	2.27596600	-1.12686100	4.01127600
O	1.33229700	-1.92067400	-2.70838600	C	2.07933700	-1.90774300	5.17124400
O	2.35797200	-0.94445600	-0.95050600	H	1.12829700	-1.86976500	5.69091300
C	3.48839000	-1.79502100	-1.17442300	C	3.06900900	-2.75551900	5.63614700
H	4.21453100	-1.51429800	-0.41143100	C	4.30848700	-2.81815400	4.97652300

C	4.53802600	-2.04079600	3.85659200	H	-0.05597000	1.56433600	0.00003600
H	-0.73200200	0.67079500	-0.63044900	C	1.50185000	0.09158900	-0.00011700
H	-0.84201100	0.32761300	1.80009500	N	2.62501000	-0.21427500	0.00011400
H	3.51205600	0.04956300	-0.55994800	C	-2.33217400	-0.00625900	0.00006300
H	1.45909700	0.53629500	-1.81570600	H	-2.46906900	1.07938500	0.00015300
H	2.88771500	-3.37220700	6.51204100	H	-2.84169500	-0.42043900	-0.87990600
H	5.08619600	-3.48428900	5.34076700	H	-2.84167200	-0.42060400	0.87995700
H	5.49358400	-2.11116700	3.34811300				
C	3.59021300	1.65124300	3.27315900				
C	2.30372800	1.66669900	3.87530100	66ts			
C	2.27455400	1.69883600	5.35628900	C	-3.57974800	-1.15718300	-1.10005800
O	3.06398200	1.16226100	6.10912600	C	-2.30213500	-1.66384100	-0.94983700
C	-0.03970400	-0.06922500	4.21928900	C	-1.21286100	-0.81479000	-0.63869600
H	-0.56977600	0.83949200	3.92376200	C	-1.45419300	0.57727600	-0.44380800
H	-0.69277500	-0.92571700	4.00409000	C	-2.77444500	1.06372500	-0.58186400
H	0.10008400	-0.02099800	5.30067400	C	-3.81673000	0.21706200	-0.91733000
C	5.06239400	-0.38205100	1.47664600	C	0.13790900	-1.30034800	-0.47471400
H	5.87153200	-0.31517500	2.20922200	C	-0.33299500	1.40357100	-0.02723000
H	5.22240900	-1.29783900	0.89023400	C	0.96312600	1.01181400	-0.56067600
H	5.16828100	0.46906800	0.80122000	C	1.20246600	-0.37404000	-0.78133900
O	1.22634400	2.45246700	5.79735600	C	2.48126100	-0.79233200	-1.21873900
C	1.16542700	2.64855100	7.21684000	H	2.67544600	-1.84677600	-1.37934300
H	0.33059300	3.33134900	7.38319700	C	3.48041100	0.12909500	-1.47060300
H	0.99398700	1.70243000	7.73818100	C	3.24300200	1.49822200	-1.25951800
H	2.09652500	3.08826100	7.58542100	C	2.01126200	1.92868300	-0.79702800
H	1.54000300	2.28896700	3.42105800	H	-4.39819900	-1.81975000	-1.36790800
H	4.40071800	1.36329200	3.93685100	H	-2.12845000	-2.72267700	-1.10964200
C	3.97072800	2.54925000	2.17655700	H	-2.97405400	2.12193400	-0.45272000
C	3.04305200	3.10898800	1.27549900	H	-4.81884500	0.61740100	-1.04528800
C	5.33214100	2.86724300	1.99659900	H	4.45000400	-0.20665700	-1.82722600
C	3.46369400	3.94076500	0.24032400	H	4.02796300	2.22258200	-1.45952700
H	1.98588400	2.88475700	1.37659200	H	1.84680800	2.98927200	-0.64085200
C	5.75172400	3.69602900	0.95938000	C	-0.11537900	0.57118900	1.95743000
H	6.06367600	2.45313500	2.68643400	C	0.20339200	-0.80467800	1.82873400
C	4.81823600	4.23673600	0.07206200	C	0.41414200	-2.78420200	-0.51449600
H	2.72701300	4.35494400	-0.44328100	H	-0.37247600	-3.35194400	-0.01080400
H	6.80934000	3.91817600	0.84349600	H	0.47559100	-3.15007800	-1.54902700
H	5.14245500	4.88038300	-0.74095000	H	1.36051600	-3.01924200	-0.02092600
				C	-0.56212200	2.88247600	0.21986400
66-dienophile				H	0.23313200	3.30844400	0.83903500
C	-0.88528500	-0.38619700	-0.00005500	H	-0.57869100	3.44079100	-0.72551300
C	0.13038300	0.49219100	-0.00004300	H	-1.50843800	3.07556200	0.72732100
H	-0.65531100	-1.45070200	-0.00012500	H	0.71989800	1.23071300	2.18081400
				C	1.52662100	-1.27605000	2.04951400

N	2.60705700	-1.68642200	2.21249200	H	-3.81994900	1.13520900	0.81454100
H	-0.57777300	-1.53187400	2.03546700	H	-5.28850200	-0.49480500	-0.28535800
C	-1.41694800	0.92237400	2.64634000	H	3.30976300	2.45517200	-2.24446000
H	-1.68671600	1.97481500	2.52664600	H	2.38582200	4.13356200	-0.64907600
H	-2.24481000	0.31146500	2.27191200	H	0.39353800	3.60994400	0.67941500
H	-1.32651600	0.73283200	3.72445300	C	-0.19407000	-0.24757500	1.89547200
67-dienophile				C	0.48658000	-1.18439800	1.08716900
C	2.88476800	-0.25356500	0.00013000	C	1.94978000	-1.10182900	1.00808500
O	1.54570800	-0.76685900	-0.00004400	O	2.63097100	-0.13649700	1.30658700
C	0.56750800	0.17377300	-0.00019200	C	0.60290800	-1.71609700	-1.97770400
O	0.79231800	1.36897500	-0.00000200	H	0.19251000	-2.69166300	-1.70513800
C	-0.76785000	-0.46295100	-0.00009900	H	0.41176600	-1.56107400	-3.04908200
C	-1.88079800	0.28104400	0.00000600	H	1.68223200	-1.77242100	-1.83152600
C	-3.27831300	-0.25241000	0.00009000	C	-1.60319300	2.29045400	1.59030400
H	-1.75896500	1.36393100	0.00002800	H	-0.81873600	2.65514500	2.25989400
H	3.53594200	-1.12849800	0.00040500	H	-2.01251000	3.15845900	1.05635900
H	3.06378600	0.35805200	-0.88866300	H	-2.40207200	1.88655400	2.21449700
H	3.06344300	0.35836600	0.88877200	O	2.49623800	-2.26969300	0.55416100
H	-3.30056200	-1.34663900	0.00004800	C	3.92845400	-2.28233400	0.50034900
H	-3.83045700	0.10583600	0.87928300	H	4.19994900	-3.26892100	0.12129900
H	-3.83059300	0.10590700	-0.87898900	H	4.30165200	-1.49872100	-0.16487600
H	-0.79868900	-1.54923700	-0.00012600	H	4.35467600	-2.12600700	1.49569400
67ts				H	0.05561400	-2.16827900	0.93343900
C	-3.67329600	-1.52057000	-1.29847400	H	0.44962000	0.48563400	2.37555300
C	-2.30906300	-1.56401800	-1.52144600	C	-1.35973200	-0.74255700	2.72500100
C	-1.44212300	-0.61421400	-0.93024400	H	-1.95486500	0.07031100	3.14988200
C	-1.98985700	0.37196300	-0.05836900	H	-2.02609400	-1.38580600	2.14175400
C	-3.38505500	0.38108200	0.16720100	H	-0.98062800	-1.33638100	3.56794200
C	-4.21539800	-0.53731800	-0.45196300	68-diene			
C	-0.01287700	-0.61140400	-1.15085100	C	1.24836700	0.58009500	-0.00036700
C	-1.05910400	1.25904700	0.62021100	C	2.08094700	-0.46685700	0.00036000
C	0.11805100	1.62757600	-0.15184100	H	3.15620800	-0.31907200	-0.00018300
C	0.64828100	0.66911600	-1.06081400	H	1.72082900	-1.49039800	0.00108900
C	1.81850900	0.98508200	-1.79061200	C	-0.21242900	0.54677400	0.00000300
H	2.22667700	0.26236700	-2.48954000	C	-0.98684300	1.63836200	0.00027100
C	2.42776300	2.21814800	-1.65562700	H	-2.06871200	1.58351900	0.00039600
C	1.90638100	3.16425600	-0.75633600	H	-0.52793400	2.62279500	0.00030600
C	0.78245600	2.86569200	-0.00697400	H	1.65551700	1.59056200	-0.00136900
H	-4.32573800	-2.24090000	-1.78452000	Cl	-0.98330400	-1.04574400	-0.00010800
H	-1.90476200	-2.31848500	-2.18789800	68ts			

C	1.29879700	-0.46028200	0.29455600	C	1.50490300	-0.61374000	-1.45836600
C	0.12100200	-1.79322500	-1.32803200	H	2.57435500	-0.49688700	-1.31015900
C	-0.87220100	0.87610100	-1.19227100	H	-1.04907000	-0.08615200	-2.07844400
C	0.63592600	0.83089500	0.27728000	H	1.04659300	0.14914400	-2.07793200
C	-1.17855300	-1.53988600	-0.93359000	C	1.44462800	-0.23903600	1.31302900
C	-1.68406600	-0.23165400	-0.90882400	N	2.08016500	-0.81887500	2.09491300
H	0.54641000	-2.78236600	-1.18884800	C	-1.35691900	-0.55522000	1.31157800
H	-1.28247800	1.87371100	-1.07198300	N	-1.84794400	-1.26197700	2.09314100
C	1.04754900	-1.36780600	1.37394600	C	-1.57855700	1.42808200	-0.07464500
N	0.84421300	-2.11548800	2.24219700	N	-2.25246300	2.30668100	-0.42947800
C	2.54526400	-0.61427900	-0.39284400	C	1.22028300	1.74388500	-0.07342900
N	3.53675200	-0.76303500	-0.98424700	N	1.68227400	2.75025400	-0.42810200
C	1.37960800	1.94475700	-0.27223600				
N	1.94050600	2.84728600	-0.74161500				
C	-0.16688800	1.17908600	1.43007000				
N	-0.82674600	1.46928100	2.34086100				
H	-1.76128900	-2.32613600	-0.46302700				
Cl	-3.24860700	0.03554900	-0.19663400				
H	-0.14209000	0.78072500	-1.98934900				
H	0.64407400	-1.15881200	-2.03272700				
69-diene				70-diene			
C	-1.84882700	-0.10916700	-0.00007900	C	0.83363700	-0.67891400	0.00001600
C	-0.60893500	0.40062500	-0.00008000	C	1.98621100	0.00509600	-0.00001100
C	0.60886800	-0.40025900	0.00004400	H	0.87168600	-1.76835200	0.00003800
C	1.84892500	0.10894900	0.00008800	H	2.94392100	-0.50686500	-0.00000700
H	-2.72942000	0.52602200	-0.00007100	H	2.02059400	1.09096600	-0.00004100
H	-2.02251000	-1.18317800	0.00001600	C	-0.51594900	-0.10061900	0.00000800
H	-0.47441000	1.48289200	-0.00007700	C	-1.58891700	-0.91015100	-0.00001100
H	0.47388300	-1.48249300	0.00009100	H	-2.60257900	-0.51918200	-0.00001700
H	2.02327400	1.18283200	0.00003800	H	-1.48526100	-1.99248700	-0.00002200
H	2.72899700	-0.52696200	0.00016600	C	-0.66052000	1.40200800	0.00000500
				H	-0.18098400	1.84638000	0.88144600
				H	-0.18091200	1.84638000	-0.88139800
				H	-1.71322900	1.69864100	-0.00003900
69ts				70ts			
C	0.67544000	0.47264900	0.32545200	C	1.02693800	-0.47739400	0.29933200
C	-0.76479400	0.30988300	0.32429400	C	-0.06327300	-1.70571700	-1.39821600
C	-1.32762200	-0.93235100	-1.46025600	C	-1.11430800	0.91558500	-1.24438600
C	-0.47445200	-2.02410400	-1.31718600	C	0.38837000	0.82331200	0.30518800
C	0.91533400	-1.86768800	-1.31593400	C	-1.38436500	-1.47832100	-1.05175000
H	-2.39664800	-1.05619400	-1.31456800	C	-1.94033900	-0.18818600	-0.97634000
H	-0.88909200	-2.97450900	-0.99097900	H	0.36698500	-2.69636200	-1.28571400
H	1.53017700	-2.70215100	-0.98844900	C	0.71432300	-1.41406000	1.33928000
				N	0.45548200	-2.18276400	2.17350500
				C	2.31419600	-0.61913100	-0.31489600
				N	3.34033100	-0.75820900	-0.84598100
				C	1.14655000	1.94640900	-0.19402500
				N	1.72282100	2.85989700	-0.62291100

C	-0.48311200	1.14123500	1.41210500	H	-1.37582600	0.43307900	-1.63374700
N	-1.21565900	1.40114400	2.27637200	H	0.57655000	-0.07714700	-2.19889700
H	-0.33940400	0.84668900	-1.99992000	H	-2.01734600	-2.36571400	-0.51625400
H	0.47509700	-1.04602700	-2.06819800	H	0.24535200	-2.95644800	-1.15027500
H	-1.95951200	-2.30289300	-0.63599800	C	-3.18867300	0.11552000	-0.43634400
C	-3.30392000	0.02109200	-0.36980400	H	-3.50965400	-0.53417000	0.38278700
H	-3.21179800	0.45818700	0.63358900	H	-3.16646400	1.15380600	-0.08968000
H	-3.90272800	0.71324000	-0.97168600	H	-3.94694600	0.06801900	-1.23259500
H	-3.85014300	-0.92169800	-0.27830900				
H	-1.50567500	1.91944200	-1.09958000				
				72-diene			
				C	-0.70559200	0.22709600	-0.00020600
71-diene				C	-1.02768600	1.53227100	-0.00026100
C	0.05304900	-0.24490100	0.00031200	H	-2.06561600	1.85348800	-0.00017000
C	-1.11453200	0.41919000	-0.00013100	H	-0.28433400	2.32228600	-0.00033600
C	1.36059900	0.39564300	0.00021000	C	0.70559200	-0.22709600	-0.00020200
C	2.53039200	-0.26017300	-0.00024600	C	1.02768700	-1.53227100	-0.00026000
H	1.36203900	1.48640300	0.00052200	H	2.06561600	-1.85348700	-0.00017400
H	3.48072700	0.26492200	-0.00024500	H	0.28433500	-2.32228700	-0.00034100
H	2.57385100	-1.34724600	-0.00056000	C	1.79863500	0.81874400	0.00029200
C	-2.47182500	-0.21707000	-0.00009400	H	1.73331800	1.46876300	-0.88110900
H	-3.05479900	0.08730700	0.88029200	H	1.73271700	1.46796600	0.88229700
H	-3.05536700	0.08842100	-0.87972400	H	2.78635500	0.34933100	0.00035500
H	-2.40481700	-1.31020500	-0.00076600	C	-1.79863500	-0.81874400	0.00029200
H	0.04509800	-1.33625900	0.00071000	H	-1.73331500	-1.46876900	-0.88110300
H	-1.09283000	1.51052900	-0.00053400	H	-1.73272100	-1.46795900	0.88230300
				H	-2.78635600	-0.34933100	0.00034800
71ts				72ts			
C	1.17590500	0.06157000	0.08254300	C	0.95900900	-0.72547500	0.28602500
C	0.87904600	-0.96451100	-1.64987400	C	-0.49765700	-1.38891900	-1.27616800
C	-1.86499200	-0.29217300	-0.99095500	C	-0.49766400	1.38891100	-1.27616600
C	-0.07292600	0.61204000	0.58220700	C	0.95902300	0.72547300	0.28598700
C	-0.08763800	-1.93746300	-1.33077200	C	-1.66223900	-0.70870500	-0.90970000
C	-1.39341800	-1.59871600	-0.97075800	C	-1.66222700	0.70868300	-0.90967000
H	1.88551400	-1.29864000	-1.88771200	H	-0.45404300	-2.46908400	-1.16830600
C	1.79492300	-0.97557000	0.88703700	C	0.32583600	-1.40795800	1.38375000
N	2.29409100	-1.82622600	1.49988100	N	-0.21198500	-1.96507700	2.25153900
C	2.13314800	1.01195600	-0.45193700	C	2.07893400	-1.41215600	-0.29995300
N	2.90190200	1.74770100	-0.91744300	N	2.95471700	-1.98730900	-0.80456500
C	-0.44052000	1.95019300	0.25333000	C	2.07894400	1.41208400	-0.30008200
N	-0.78905000	3.02274400	-0.04051400	N	2.95472300	1.98717000	-0.80477800
C	-0.71576600	0.02729200	1.71437000	C	0.32591500	1.40804600	1.38369500
N	-1.26490000	-0.44187600	2.62854600				

N	-0.21186100	1.96524100	2.25146300	F	-1.10877900	0.00000000	-0.72395700
H	0.18216700	0.98846300	-2.01834500	F	-1.10881200	0.00000000	2.04984600
H	0.18219700	-0.98841500	-2.01829600				
C	-2.80491000	1.46932600	-0.28269900				
H	-2.88984100	1.24743200	0.78901500	3-2ts			
H	-2.67182000	2.54795400	-0.39037300	C	1.25761200	1.43089400	-0.63857400
H	-3.75995600	1.19584500	-0.74637000	C	-0.80307200	0.68899100	0.09164400
C	-2.80496000	-1.46934000	-0.28278500	C	-0.80308400	-0.68897700	0.09164000
H	-2.88997500	-1.24742100	0.78891600	C	1.25757600	-1.43092600	-0.63857500
H	-3.75997200	-1.19587200	-0.74653800	C	2.11314700	-0.70845600	0.15949400
H	-2.67186200	-2.54797000	-0.39042400	C	2.11316200	0.70840200	0.15949600
H	-0.45407600	2.46907600	-1.16828900	H	0.91296800	1.05391800	-1.59547800
				H	1.16317700	2.50588100	-0.51127300
3-1ts				H	1.16311900	-2.50591300	-0.51128100
C	0.28196700	0.69641000	-1.30928200	H	0.91293700	-1.05393800	-1.59547600
C	0.27886600	-0.69456500	-1.31065000	H	2.64250100	-1.21822500	0.96178600
C	1.99406200	-1.44816400	0.00189800	H	2.64252400	1.21815800	0.96179100
C	1.79977700	-0.71274700	1.15637900	F	-1.46342200	-1.34519300	-0.87320900
C	1.80304200	0.69647300	1.16120400	F	-1.46337800	1.34523600	-0.87320600
H	1.83745200	-2.52265600	0.00627300	F	-0.77270100	-1.34150900	1.25871800
H	1.42336300	-1.22386300	2.03998800	F	-0.77264000	1.34152700	1.25871700
H	1.42922500	1.20332200	2.04831600				
C	2.00138400	1.43852900	0.01185800	3-3-dienophile			
H	1.84917100	2.51358800	0.02255200	C	2.11381300	0.04384900	-0.00001000
C	-0.81950700	1.16298300	-0.41413600	C	0.98074800	-0.65149800	-0.00002500
C	-0.82633700	-1.15531600	-0.41608000	H	0.96181200	-1.73790400	-0.00006300
O	-1.23020400	-2.28333800	-0.20602000	H	3.07811200	-0.45469900	-0.00001600
O	-1.21118600	2.29533500	-0.20449900	C	-0.37458200	-0.01725700	-0.00001200
H	0.63690600	1.33609500	-2.10665000	H	2.11576200	1.12921300	0.00004300
H	0.62877200	-1.33332800	-2.11101800	F	-1.08729600	-0.39754900	1.08628000
N	-1.35826500	0.00326700	0.16448800	F	-0.32257800	1.32995800	-0.00007200
C	-2.47265400	-0.00006900	1.09320000	F	-1.08741000	-0.39765000	-1.08617200
H	-2.17078400	-0.40870300	2.06270900				
H	-2.80069900	1.03356400	1.21513700	3-3ts			
H	-3.28962000	-0.61022600	0.69773900	C	2.52862100	0.91551400	-0.03558500
H	2.62352800	-1.07390700	-0.79782100	C	0.44026600	1.62185900	-0.38305300
H	2.62804800	1.06606600	-0.79083300	C	-0.35563900	0.57702700	-0.82861200
				C	0.99446800	-1.33150800	-0.96143600
3-2-dienophile				C	1.58760200	-1.31488400	0.28397600
C	0.00000700	0.00000000	0.00017400	C	2.34159300	-0.21538500	0.73812400
C	-0.00000700	0.00000000	1.32574200	H	2.60168000	0.83685500	-1.11473200
F	1.10877900	0.00000000	2.04987300	H	3.02253900	1.78681300	0.38705800
F	1.10881200	0.00000000	-0.72393000				

H	0.31505900	-2.13190600	-1.23560200	H	-0.80466000	-2.96391400	2.07349000
H	1.43261100	-0.79475500	-1.79474300	H	-1.24388600	0.06375800	2.44322800
H	1.29239200	-2.06631000	1.01299200	H	0.78629400	0.47928600	2.41865900
H	2.58754800	-0.17047100	1.79756700	C	1.45727000	1.46936000	-0.10252000
C	-1.41976800	0.02688700	0.06765000	C	-1.53845900	1.33343700	0.22018000
H	-0.59125400	0.48424800	-1.88409500	C	1.51178200	-0.99355500	-0.71140000
H	0.80237500	2.35383600	-1.09706800	C	-1.49403500	-0.92296900	-0.94564000
H	0.33539600	1.97539800	0.63597000	F	2.74135200	-1.17241300	-0.18265500
F	-1.88191200	-1.18091500	-0.33680200	F	0.90308500	-2.19062700	-0.63413500
F	-0.99851600	-0.10222400	1.34693400	F	1.69154500	-0.70322000	-2.01570600
F	-2.50859500	0.84416400	0.10167500	F	-0.92233100	-0.98116900	-2.16597700
3-4-dienophile				F	-1.59739600	-2.18708700	-0.49358400
C	0.67092300	0.00002200	-0.00018200	F	-2.75833800	-0.49559200	-1.14131700
C	-0.67074700	0.00006300	-0.00010900	F	-2.76034400	1.09770100	0.74509200
C	-1.51935900	1.26661600	0.17343300	F	-1.73810900	2.02324000	-0.91833600
C	1.51939100	1.26673500	-0.17345400	F	-0.91930700	2.15057200	1.10096700
C	-1.51916100	-1.26666500	-0.17346800	F	1.57707500	2.14262700	1.05959500
C	1.51927500	-1.26669800	0.17343000	F	0.85655400	2.29497500	-0.98014600
F	-2.64162000	-0.95379700	-0.84920800	F	2.71508900	1.28373700	-0.54828600
F	-0.88134400	-2.19434100	-0.90519700	cyc3			
F	-1.87018400	-1.80798300	1.00030100	C	0.79270900	-0.20517400	0.00000000
F	0.88172000	-2.19400600	0.90582500	C	-0.68117900	-0.52719200	0.00000000
F	1.86975800	-1.80859100	-1.00031800	C	0.00000000	0.81878500	0.00000000
F	2.64196300	-0.95362400	0.84860100	H	-1.15916800	-0.89757800	0.91274000
F	2.64201100	0.95395300	-0.84878400	H	-1.15916800	-0.89757800	-0.91274000
F	1.87006600	1.80831100	1.00034900	H	-0.14357600	1.88898300	0.00000000
F	0.88160500	2.19426200	-0.90552600	H	1.79273600	-0.61234000	0.00000000
F	-1.87059800	1.80814000	-1.00023800	cyc3ts			
F	-0.88189600	2.19437000	0.90529800	C	0.83313200	1.46464100	-0.53861600
F	-2.64169400	0.95325700	0.84913000	C	-1.40935300	0.66977100	-0.38107000
3-4ts				C	-1.40932400	-0.66983600	-0.38113800
C	-0.72399200	0.05115400	-0.01679700	C	0.83338600	-1.46458800	-0.53864200
C	-1.42262500	-0.92588900	2.04352100	C	1.40661900	-0.71216300	0.45241800
C	1.37756900	-0.37584200	2.12210500	C	1.40651800	0.71232100	0.45241100
C	0.70106100	0.11076800	-0.00213000	H	-1.76703700	1.52348700	-0.93584500
C	-0.49037200	-1.93121200	2.20136500	H	0.70512300	1.08050000	-1.54406000
C	0.88801700	-1.66138500	2.27029000	H	0.76854700	2.54492400	-0.44107300
H	-2.46247200	-1.16756100	1.85601300	H	0.76895400	-2.54488200	-0.44106000
H	2.44673700	-0.20160600	2.08052300	H	0.70539300	-1.08051600	-1.54411500
H	1.58080300	-2.49787400	2.22462900	H	-1.76711800	-1.52341500	-0.93600700
				H	1.72505500	-1.21090200	1.36619400

H	1.72490700	1.21111000	1.36617500	C	-0.66700400	1.07642400	-0.04562700
C	-1.58905800	-0.00013500	0.93997100	C	0.66834000	1.07555200	-0.04565100
H	-0.73503900	-0.00025600	1.63347100	C	1.23654800	-0.31858600	0.10080900
H	-2.56030800	-0.00011700	1.44431500	C	-0.00084700	-1.22750500	-0.13217000
cyc4				H	-1.66407200	-0.45534000	1.10617100
C	-0.69952800	0.78627900	-0.00013400	H	-2.04891200	-0.52558100	-0.60761400
C	0.81462000	0.67026300	-0.00002700	H	2.04795400	-0.52795300	-0.60808100
C	0.81461900	-0.67026400	-0.00015500	H	1.66402000	-0.45774100	1.10586400
C	-0.69952800	-0.78627900	0.00028600	H	1.29439400	1.96235200	-0.10181200
H	-1.14599200	1.24714900	0.88972300	H	-1.29175600	1.96409500	-0.10233700
H	-1.14594600	1.24671300	-0.89024200	H	-0.00107800	-1.57827600	-1.17034700
H	-1.14575600	-1.24670900	0.89049200	H	-0.00137700	-2.11444900	0.50912100
H	-1.14618600	-1.24714900	-0.88947400	cyc5ts			
H	1.60139000	-1.42052100	-0.00024700	C	0.61687100	-0.69831400	-0.98998000
H	1.60139100	1.42051900	-0.00007300	C	0.61687200	0.69831300	-0.98998100
cyc4ts				C	-1.45079700	1.42785500	-0.39539800
C	0.97807500	0.69601000	0.75883700	C	-1.73781700	0.70427400	0.74869900
C	0.97548200	-0.70132000	0.75626100	C	-1.73781700	-0.70427400	0.74869800
C	-1.17275200	-1.43680800	0.47265600	H	-1.34203100	2.50855200	-0.34270400
C	-1.59591500	-0.70354700	-0.61822500	H	-1.74390500	1.21763900	1.70898900
C	-1.59230600	0.70838000	-0.61879900	H	-1.74390400	-1.21763900	1.70898800
H	-1.08305400	-2.51798700	0.40095000	C	-1.45079700	-1.42785400	-0.39539900
H	-1.74127000	-1.21342400	-1.56911600	H	-1.34203100	-2.50855200	-0.34270600
H	-1.73474300	1.21822500	-1.57014800	C	1.53547300	-1.22077600	0.10687600
C	-1.16595300	1.44028900	0.47177500	C	1.53547500	1.22077600	0.10687400
H	-1.07070600	2.52093800	0.39930900	H	0.48863300	-1.26648200	-1.90662100
C	1.67226400	0.78066400	-0.59720300	H	0.48863300	1.26648100	-1.90662200
C	1.66730900	-0.78355700	-0.60102700	C	1.70632400	0.00000000	1.03818500
H	1.04700900	1.38445200	1.59605400	H	2.50248900	1.50571400	-0.33781300
H	1.04277000	-1.39326200	1.59068200	H	1.15545900	2.10439400	0.63103200
H	2.66967300	-1.22796300	-0.57129600	H	2.66284000	0.00000000	1.57128500
H	1.09771000	-1.25096600	-1.41214100	H	0.90948500	0.00000100	1.78879700
H	2.67767800	1.21782100	-0.56302600	H	2.50248800	-1.50571600	-0.33781100
H	1.10772900	1.25641400	-1.40697900	H	1.15545600	-2.10439300	0.63103500
H	-1.30682000	-1.05933500	1.48037900	H	-1.74816700	1.05352600	-1.36864200
H	-1.30320400	1.06441300	1.47967400	H	-1.74816700	-1.05352400	-1.36864300
cyc5				cyc6			
C	-1.23689800	-0.31707000	0.10081200	C	-0.66618700	1.30604600	-0.05726500
				C	0.66607400	1.30610900	0.05711200
				C	1.49889800	0.04787400	0.11085500

C	0.69826600	-1.19221400	-0.31893300	cyc7			
C	-0.69814200	-1.19228400	0.31892700	C	0.35473100	-1.56907100	-0.31896300
C	-1.49891300	0.04773600	-0.11081700	C	1.54797900	-0.65078500	-0.15628100
H	2.38666200	0.16393600	-0.52641300	C	1.54791800	0.65093000	0.15626500
H	0.59290000	-1.19184900	-1.41287100	C	-0.86737800	-1.18520300	0.53407400
H	1.24478500	-2.10595400	-0.05507300	C	0.35458000	1.56909400	0.31898700
H	-1.24458500	-2.10608000	0.05509300	C	-1.69189600	-0.00008500	-0.00001800
H	-0.59274500	-1.19190400	1.41286000	C	-0.86749400	1.18513900	-0.53406400
H	-1.88894600	-0.09051800	-1.13205300	H	0.06762900	-1.64422500	-1.38026800
H	-2.38662500	0.16373300	0.52654100	H	0.06747200	1.64417700	1.38029500
H	1.88883600	-0.09033400	1.13213600	H	-0.51208400	-0.96035800	1.54808300
H	-1.19974900	2.25463100	-0.11224200	H	-2.35372100	0.34858200	0.80491600
H	1.19949300	2.25473600	0.11275300	H	0.67421800	-2.58151300	-0.03779100
				H	-1.52981300	-2.05543700	0.63033000
cyc6ts				H	0.67396500	2.58157900	0.03785400
C	-0.23389200	-0.69878900	0.86655300	H	-2.35362800	-0.34884000	-0.80499100
C	-0.23389300	0.69877700	0.86656000	H	-1.53001400	2.05531100	-0.63028500
C	1.87145800	1.43245800	0.37527700	H	-0.51217800	0.96036900	-1.54808100
C	2.18622700	0.70477800	-0.75800300	H	2.51880600	-1.13135900	-0.28193100
C	2.18626200	-0.70473400	-0.75800800	H	2.51870000	1.13160400	0.28187300
H	1.77127400	2.51365900	0.31735500				
H	2.22650600	1.21688500	-1.71803300	cyc7ts			
H	2.22656700	-1.21683300	-1.71804100	C	-0.13514500	0.84937500	0.97794600
C	1.87153800	-1.43244000	0.37526400	C	-0.10445500	-0.53262700	1.21890500
H	1.77139100	-2.51364400	0.31733600	C	-1.95831000	-1.44093900	0.25030100
C	-1.05095500	-1.36557300	-0.22095600	C	-2.11077200	-0.76306300	-0.94897100
C	-1.05099300	1.36556800	-0.22092400	C	-2.23500000	0.63638100	-0.98763100
H	-0.14284700	-1.21950300	1.81664500	H	-1.76025500	-2.50979200	0.24591500
H	-0.14286500	1.21947400	1.81666400	H	-1.92722700	-1.29213400	-1.88291400
H	-0.57661400	-1.19497500	-1.19617900	H	-2.14845000	1.13658200	-1.95061700
H	-1.08873100	-2.45166400	-0.07963400	C	-2.16757500	1.39260000	0.17189900
H	-1.08879200	2.45165500	-0.07957300	H	-2.14726400	2.47832800	0.10939200
H	-0.57666500	1.19500700	-1.19616000	C	0.76126100	1.56044200	-0.02932800
C	-2.48422600	-0.77785700	-0.25787500	C	0.95495300	-1.50179000	0.70283900
C	-2.48424700	0.77781600	-0.25783000	H	-0.42420400	1.45998600	1.83020500
H	-3.00725800	-1.16307400	-1.14214300	H	-0.48798300	-0.82957000	2.19514700
H	-3.03928700	-1.14866800	0.61219400	H	0.55077200	-2.52026300	0.73412700
H	-3.00732300	1.16307000	-1.14205600	H	1.78853000	-1.50322100	1.42645200
H	-3.03928800	1.14856200	0.61228100	H	0.40623900	1.38429800	-1.05241800
H	2.12511000	1.05571500	1.35950100	H	0.66474500	2.64020900	0.13745300
H	2.12514700	-1.05568800	1.35949500	C	1.52124200	-1.22317200	-0.69793400
				C	2.24761800	1.15559400	0.05873200
				H	2.51675300	1.01275900	1.11346900

H	2.87702400	1.97975500	-0.30280700	H	2.00282300	2.07727600	-1.04716800
C	2.58774400	-0.11326400	-0.74885500	H	0.06978400	2.57724800	0.49066500
H	1.96597900	-2.14604600	-1.09265200	H	2.59994200	-2.26269000	0.72011000
H	0.69068200	-0.97972500	-1.37038900	H	0.14946700	-2.41320400	0.92619800
H	3.54677000	-0.51302600	-0.39106800	H	2.39714100	2.62872200	0.57122900
H	2.74776400	0.16048800	-1.80092700	H	0.51717700	1.21883900	1.49672100
H	-2.56726400	1.00723700	1.10307700	C	2.71698200	-0.64054900	-0.70617200
H	-2.46198000	-1.08309000	1.14113800	H	2.18600100	-0.32301300	-1.61291200
cyc8				H	3.68289500	-1.03362300	-1.04980300
C	1.86631200	0.51025100	0.06007500	C	2.96470000	0.59191600	0.19355200
C	1.39066300	-0.83842500	0.65024300	H	2.97848400	0.28873400	1.25110500
C	-1.72877100	0.78357100	-0.04766200	H	3.97229500	0.97664200	-0.01197600
C	0.58009200	-1.65401400	-0.32092900	C	-3.25995000	0.63751600	-0.41108800
C	-1.65660400	-0.69792700	0.39149800	C	-3.22529700	-0.75683800	-0.24875700
C	-0.74972200	-1.57312800	-0.44515200	C	-2.35511300	1.46345700	0.23278400
H	2.65728000	0.32329100	-0.67956800	C	-2.27077500	-1.36739300	0.55006200
H	0.79829800	-0.63807800	1.55151000	H	-2.32073800	2.52264400	-0.01113900
H	-1.96225800	0.82923400	-1.12085800	H	-2.19343600	-2.45210900	0.55775100
H	-2.67251600	-1.11123000	0.35649700	H	-0.57144900	-1.25592800	-1.24958000
H	2.33561200	1.08720900	0.86954200	H	-0.53027800	1.10361300	-1.41063100
H	2.27085000	-1.40477400	0.98119400	H	-3.85849700	1.04610100	-1.22407300
H	-2.58404200	1.24110800	0.46924800	H	-3.79920700	-1.37008100	-0.94193500
H	-1.35341000	-0.73280000	1.44712400	H	-1.92701100	-0.89151200	1.46234700
C	0.77646600	1.36619700	-0.61129600	H	-1.99119600	1.22023600	1.22456100
H	0.47568400	0.89554500	-1.55530700	5-3-dienophile			
H	1.24590300	2.31922700	-0.88877700	C	0.64976600	0.03872800	-0.00064400
C	-0.48973700	1.66035300	0.23098700	C	-0.00029600	1.40158000	0.00003300
H	-0.24676500	1.61872000	1.30335100	C	-0.64936200	0.03819800	0.00026600
H	-0.79383000	2.69834000	0.04246200	H	-0.00162800	2.01150100	-0.91251600
H	1.13254000	-2.30250900	-1.00150400	H	0.00027600	2.01099400	0.91293900
H	-1.23553800	-2.16454800	-1.22148900	C	-1.95645000	-0.65799200	0.00004600
cyc8ts				H	-1.83611500	-1.74686700	-0.00134200
C	1.96137700	-1.80816000	-0.05120100	H	-2.54778000	-0.37745000	0.88163900
C	0.60167500	-1.46912900	0.59839800	H	-2.54846800	-0.37522700	-0.88039700
C	1.99417100	1.77361900	0.01003900	C	1.95655500	-0.65775200	0.00012200
C	-0.32937300	-0.71825200	-0.33557400	H	2.54707000	-0.37795800	0.88249900
C	0.52727400	1.58062100	0.45987500	H	1.83551700	-1.74654800	-0.00222300
C	-0.31547200	0.68231000	-0.43204100	H	2.54985300	-0.37500700	-0.87953600
H	1.80515800	-2.58598200	-0.81220300	5-3ts			
H	0.76945900	-0.88661800	1.51146400	C	-1.21896000	-1.45312200	-0.60288200
				C	0.90137600	-0.67629700	0.15041900

C	0.90157200	0.67622900	0.15049700	C	-2.41199900	0.71216900	-0.17399600
C	-1.21908600	1.45323600	-0.60285500	C	-2.41198700	-0.71219100	-0.17399600
C	-2.06075100	0.71099800	0.18537500	H	-0.71861000	-1.07874600	-1.45475300
C	-2.06070900	-0.71097500	0.18536000	H	-1.38867800	-2.53953100	-0.57674200
H	-0.83177900	-1.06948300	-1.53988000	H	-1.38872100	2.53952600	-0.57674000
H	-1.17435500	-2.53303000	-0.49172400	H	-0.71862600	1.07875200	-1.45475100
H	-1.17454300	2.53313500	-0.49164400	H	-3.18020600	1.21300100	0.41280400
H	-0.83179300	1.06965400	-1.53981900	H	-3.18018600	-1.21303600	0.41280500
H	-2.61830700	1.21385300	0.97369400	C	-0.10901900	0.00000200	1.87612900
H	-2.61822100	-1.21389100	0.97367000	C	1.33059900	-1.81860500	0.36064700
C	0.68729400	-0.00003300	1.46383500	H	0.86661000	-2.77938000	0.60864700
H	-0.32500000	0.00004200	1.89354600	H	2.25893900	-1.72472700	0.94632900
H	1.48162300	-0.00016000	2.22115000	C	1.33058700	1.81861700	0.36064400
C	1.72808400	-1.80473500	-0.37548800	H	0.86658900	2.77939000	0.60863200
H	1.36084600	-2.78181500	-0.04550600	H	2.25892500	1.72475200	0.94633200
H	1.75909800	-1.80499300	-1.47141700	H	0.46877700	0.00000300	2.80839700
H	2.76455400	-1.70515100	-0.01897400	H	-1.19688100	0.00000000	2.03290800
C	1.72828800	1.80469500	-0.37546700	F	1.67747800	-1.83803300	-0.98765100
H	1.75930400	1.80497800	-1.47139700	F	1.67747400	1.83803600	-0.98765300
H	1.36116300	2.78182300	-0.04547700				
H	2.76476200	1.70505700	-0.01898200				
				5-5-dienophile			
				C	-1.92805300	-0.16711700	-0.00004200
5-4-dienophile				F	-1.72756800	-1.49572400	0.00010000
C	-1.95598500	-0.03908200	-0.00005000	C	-0.64671300	0.57610300	-0.00000700
F	-1.81074700	-1.41692800	0.00006700	C	0.00000000	1.93789600	0.00000600
C	-0.64824700	0.64260000	-0.00001600	C	0.64671300	0.57610300	0.00000800
C	0.00000000	2.00419100	0.00001100	C	1.92805300	-0.16711700	0.00004100
C	0.64824900	0.64260100	-0.00000800	F	1.72756800	-1.49572400	-0.00010700
C	1.95598600	-0.03908300	0.00004300	H	0.00001400	2.52932200	-0.91768100
F	1.81074500	-1.41692900	-0.00005600	H	-0.00001400	2.52931400	0.91769800
H	0.00000800	2.60884700	-0.91418600	F	2.65788300	0.14814000	-1.08889900
H	-0.00000800	2.60881700	0.91422700	F	2.65770000	0.14792600	1.08916600
H	-2.53512100	0.25485100	-0.88730400	F	-2.65788200	0.14813600	1.08890000
H	2.53525000	0.25497700	-0.88708400	F	-2.65770100	0.14793100	-1.08916600
H	-2.53524000	0.25499400	0.88707700				
H	2.53511500	0.25486200	0.88729600				
				5-5ts			
5-4ts				C	-1.47908900	2.06094800	-0.59401500
C	-1.38953700	-1.45904200	-0.69420500	C	-0.66849200	-0.04948200	0.43676100
C	0.43025200	-0.67295600	0.65814600	C	0.66849200	-0.04948200	0.43676100
C	0.43025000	0.67296200	0.65814700	C	1.47908900	2.06094900	-0.59401500
C	-1.38956300	1.45903700	-0.69420600	C	0.71565600	2.92005400	0.14041100
				C	-0.71565700	2.92005400	0.14041100

H	-1.08904900	1.53193100	-1.45600900	H	1.43691700	-2.57156500	-0.67720200
H	-2.55702400	2.03765600	-0.47622800	H	1.54664400	2.51096600	-0.54957700
H	2.55702400	2.03765700	-0.47622700	H	0.80673800	1.10089300	-1.44961400
H	1.08905000	1.53193200	-1.45600900	H	0.80312900	-1.06677100	-1.52346500
H	1.20921300	3.55161000	0.87694600	H	-0.27562400	0.00045400	2.80736700
H	-1.20921500	3.55160900	0.87694500	H	1.36360600	-0.04305000	1.97765500
C	0.00000000	0.23355300	1.74151300	H	3.27905400	-1.29891800	0.29669400
C	-1.77320800	-0.90197100	-0.06056400	H	3.33813500	1.12328500	0.33224800
C	1.77320800	-0.90197100	-0.06056400	C	-1.26893200	1.76875700	0.33589600
H	0.00000000	-0.52578900	2.52765700	H	-0.80251200	2.75555700	0.26412100
H	0.00000000	1.26731400	2.10238600	H	-1.98337900	1.81875500	1.18135400
F	-1.72162600	-1.03823400	-1.40363800	C	-1.37109000	-1.69188200	0.38237800
F	1.72162600	-1.03823500	-1.40363800	H	-0.95905300	-2.70231300	0.26654200
F	-2.99472600	-0.41838700	0.25310600	H	-2.05907100	-1.72275100	1.23813300
F	-1.69434700	-2.14003700	0.48166200	O	-1.92689600	1.54191300	-0.89667600
F	1.69434800	-2.14003700	0.48166300	H	-2.26908800	0.62589700	-0.86439200
F	2.99472600	-0.41838600	0.25310500	O	-2.19205300	-1.36185800	-0.75025400
				H	-1.64979800	-1.48022100	-1.54658600
5-6-dienophile				5-7-dienophile			
C	-1.86214900	-0.08991400	-0.00305800	C	-0.70918100	1.93245600	-0.00001800
O	-1.52005700	-1.47329300	-0.03732700	F	-2.07111000	1.69593200	0.00002100
C	-0.64955400	0.76330000	-0.00941100	C	0.04925400	0.66134100	-0.00000500
C	0.64937800	0.76340800	0.00685200	C	1.33934000	-0.00000600	0.00000000
C	1.86210200	-0.08962200	0.00407800	C	0.04924900	-0.66134400	-0.00000200
O	1.52005200	-1.47313100	0.03743500	C	-0.70919600	-1.93245300	0.00001200
C	-0.00010500	2.12666900	0.00036300	F	-2.07112400	-1.69591800	-0.00001600
H	0.00516200	2.73469000	-0.91153700	H	-0.44757400	2.52267100	-0.88832000
H	-0.00548900	2.73240900	0.91380300	H	-0.44755700	-2.52271200	-0.88825000
H	-2.47836400	0.09728300	-0.89073600	H	-0.44753000	2.52271700	0.88824100
H	2.49200200	0.15093500	-0.86894700	H	-0.44758700	-2.52267300	0.88831000
H	-2.48912100	0.15086900	0.87203000	F	2.16409000	-0.00000900	-1.09291400
H	2.47531100	0.09772700	0.89379500	F	2.16408300	-0.00000100	1.09291900
H	0.85694000	-1.61781900	-0.65934500				
H	-0.85443700	-1.61774300	0.65713000	5-7ts			
5-6ts				C	-1.04579000	-1.45798800	-1.38121000
C	-0.32242300	-0.66288200	0.65397600	C	0.48377000	-0.69000200	0.21439800
C	1.46232700	-1.48950000	-0.77274200	C	0.48376800	0.69000400	0.21439300
C	2.51110000	-0.77155900	-0.26662100	C	-1.04579900	1.45797500	-1.38121800
C	2.54169900	0.65254200	-0.24146800	C	-2.12172400	0.70928500	-0.97380700
C	1.51786400	1.43567800	-0.70304200	C	-2.12172000	-0.70930300	-0.97380300
C	-0.28049100	0.68740000	0.65826200	H	-0.30774300	-1.08250300	-2.07884800
C	0.27259400	-0.01033100	1.85705500	H	-1.05883400	-2.53673300	-1.25183400
				H	-1.05884800	2.53672100	-1.25184700

H	-0.30774900	1.08249100	-2.07885400	H	1.93672300	-0.88655200	2.50045300
H	-2.93122800	1.20936000	-0.44718100	H	2.39824200	0.18771400	1.09389500
H	-2.93122100	-1.20937900	-0.44717400	H	2.44684100	0.23062200	-1.07670900
C	1.58169200	0.00000000	-0.43188900	H	-0.37598700	-1.89239600	-0.04713200
C	0.32755600	1.79910100	1.20511200	H	1.98153700	-2.80683400	-1.31184100
H	0.53934300	2.77378600	0.75291900	H	1.98701700	-2.88042300	1.10979500
H	1.02590800	1.64709500	2.04065500	C	-0.14299700	1.20046100	1.77875000
C	0.32756100	-1.79909100	1.20512500	H	0.14421500	0.81079700	2.75900900
H	0.53934700	-2.77378000	0.75293900	H	-1.21799500	1.44421000	1.82159300
H	1.02591600	-1.64707900	2.04066500	C	-0.25215900	1.28038200	-1.69233000
F	-0.96062400	-1.82152500	1.72068700	H	0.04476500	0.97096400	-2.70180100
F	-0.96063000	1.82153900	1.72067000	H	-1.32988000	1.47444400	-1.70192200
F	1.77052400	-0.00000400	-1.79892300	O	0.65347500	2.34787700	1.54745700
F	2.84508800	0.00000400	0.11156000	H	0.43143900	2.66251100	0.64811000
5-8-dienophile				O	0.36253700	2.53253400	-1.35481800
C	0.32761600	-0.64838800	-0.44048200	H	1.31896900	2.43715000	-1.48959200
C	-0.97660500	-0.00777400	-0.87494500	C	-2.26507300	-0.78409400	0.00143100
C	0.32749600	0.64409200	-0.45739500	O	-2.91482100	0.24568400	-0.00424500
C	1.09642000	1.87743600	-0.15858400	O	-2.85004500	-2.00752100	0.01775700
C	1.10793000	-1.87608100	-0.14841000	H	-3.81200000	-1.84295800	0.02637600
H	-1.27880100	-0.01604200	-1.92511700	5-1TAts			
H	1.19279700	2.50770600	-1.04998900	N	-1.32282900	0.26052500	0.24195300
H	0.56109000	2.47211300	0.59926300	C	-1.19629100	-1.07564700	-0.33350200
O	2.41979700	1.55698400	0.25437400	C	-0.05152200	-1.03161800	-1.17382800
H	2.34493800	0.91206500	0.97860600	C	0.56247300	0.24870400	-1.09903600
H	0.61342100	-2.46723500	0.63050200	C	-0.40957700	1.12293400	-0.32041800
H	1.16725600	-2.51288300	-1.04620400	O	-2.03352500	-1.95023800	-0.08032200
O	2.39869900	-1.54675000	0.35305500	O	-0.43599000	2.34480100	-0.22383000
H	2.80218900	-0.92510000	-0.27633700	C	-2.46521400	0.68034700	1.00747700
C	-2.17834500	-0.00302200	0.01943100	S	2.38081700	0.36408800	0.14052300
O	-3.32620000	-0.01322900	-0.37057400	C	2.16107900	-1.18465200	1.06289800
O	-1.85732800	0.01504400	1.34255600	H	-3.08455000	-0.20778400	1.16005400
H	-2.70971600	0.01539700	1.81629900	H	-2.16732300	1.09407800	1.97989800
5-8ts				H	-3.04419300	1.45059900	0.47912700
C	0.01726900	0.22906300	-0.65907500	H	1.94446400	-1.00744500	2.12250000
C	2.08109700	-0.69988900	-1.49764300	H	1.30596000	-1.71809100	0.61132300
C	2.12684400	-1.86653200	-0.78303400	H	3.04887900	-1.82308900	0.98353100
C	2.12511800	-1.90818100	0.64021800	H	1.02658500	0.72817100	-1.95640000
C	2.05975800	-0.78739200	1.42555300	H	0.28733800	-1.88243300	-1.75039600
C	0.03704300	0.18680500	0.68233700	5-2TAts			
C	-0.77654500	-0.87370000	-0.01299600	C	-1.49828700	1.09438100	0.13739200
H	1.97481100	-0.71937100	-2.57871200	S	-1.26733100	-0.69736400	-0.00902500

C	0.98228700	-0.51789600	-0.42461700	H	3.23065000	-0.88514900	-1.03356300
C	1.88355100	-0.08717700	0.69737600	O	2.16703200	0.90019600	-1.29101000
C	1.52055400	0.74159000	-0.50005500	H	1.36905400	0.59018000	-1.75959000
H	1.44946600	0.14393200	1.68148000	S	-1.71923100	-0.64763700	-0.80929900
H	2.85980700	-0.59847400	0.80317200	C	-3.10032200	0.39616700	-0.18231200
H	2.12206700	1.22452800	-1.26535500	H	-3.86898500	0.51530800	-0.95904600
H	1.05974800	-1.42496900	-1.01710700	H	-3.58879600	-0.03770300	0.70152600
H	-0.49078800	1.54358500	-0.03816700	H	-2.73714600	1.39705000	0.08256000
H	-2.19700200	1.49024100	-0.61271600				
H	-1.85462700	1.39358600	1.13252000				
5-4TAts				5-8TAts			
S	-2.03669500	-0.40662100	-0.92027800	C	0.55801000	0.60928800	-0.90457600
C	0.05201400	-0.03835900	0.25880400	C	0.77783500	-0.86122800	-0.72979500
C	0.33978100	-1.26440100	1.10896200	C	-0.25725200	0.01299600	0.00519300
C	1.12349200	-0.79634000	-0.06068700	C	-0.46311500	0.24111500	1.47987500
C	2.43868100	-0.78430100	-0.66419000	C	1.35931300	1.85819400	-0.92787500
H	2.40944000	-0.32770500	-1.66190900	H	0.39664700	-1.57881500	-1.46271100
H	2.87832500	-1.78809500	-0.74589700	H	-1.28301000	-0.36126100	1.88436800
F	3.43871400	-0.02182700	0.06894200	H	0.46463400	-0.06698800	1.99313000
H	0.71337900	-1.12224700	2.13838100	O	-0.77029900	1.59875100	1.78601000
H	-0.36788000	-2.09936400	1.02762300	H	-0.24998300	2.14782300	1.16647700
C	-0.11965400	1.37712200	0.68089500	H	2.20127500	1.87141200	-0.21448300
H	0.50355400	1.54558000	1.57676600	H	1.78757000	2.07317500	-1.92439100
F	0.32536800	2.27035000	-0.30123200	O	0.51723800	2.96570600	-0.52125000
H	-1.15799900	1.63365300	0.91132800	H	-0.34478200	2.76791200	-0.93033200
H	-2.61895500	-0.43096700	1.45885900	S	-2.34943900	-0.38768500	-0.84797000
C	-3.17121300	-0.28752100	0.51860300	C	-3.30851000	-1.45487300	0.30245300
H	-3.94706000	-1.06437600	0.47708500	H	-4.23363300	-1.79261000	-0.18439600
H	-3.68102000	0.68554900	0.57849800	H	-2.74207600	-2.35125700	0.58739800
5-6TAts				H	-3.59075900	-0.92364000	1.22118400
C	1.29425100	-0.94000100	-0.05330900	C	1.96101700	-1.42824300	-0.03853700
C	0.76755000	-1.75315200	1.07290600	O	2.44717400	-2.53284900	-0.23315300
C	0.16207000	-0.46933500	0.55789100	O	2.56973100	-0.57464200	0.85641200
C	-0.07778100	0.77413000	1.35918000	H	3.31060500	-1.10200400	1.20670100
C	2.53188400	-0.23959700	-0.46847100	SMe			
H	0.25216800	-2.70561800	0.89225100	S	0.00000000	0.00000000	0.71486200
H	1.22640000	-1.72149500	2.08214600	C	0.00000000	0.00000000	-1.12950900
H	-1.10156300	0.83769800	1.74670600	H	0.00000000	1.01948000	-1.55357800
H	0.59538700	0.70402700	2.24209500	H	0.88289600	-0.50974000	-1.55357800
O	0.16651800	1.98487800	0.65014600	H	-0.88289600	-0.50974000	-1.55357800
H	0.87143600	1.78165300	0.00281900				
H	3.12476500	0.19637000	0.36246700				