Supporting Information

An effective method to make polymer degrade readily: spatial isomerization

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Part 1. The energies of 16 reactions.

Table S1. The energies of sixteen reactions. And the energy value represents the sum of the total energy and the zero-point vibration energy.

	$\|\Delta E(R \rightarrow TS)$ (eV)$\|$	$\|\Delta E(R \rightarrow P)$ (eV)$\|$
R1/R2	0.60 / 0.80	0.04 / 0.03
R3/R4	0.70 / 0.85	0.13 / 0.22
R5/R6	0.62 / 0.78	0.02 / 0.18
R7/R8	0.71 / 0.84	0.17 / 0.19
R9/R10	0.63/0.78	0.03/0.03
R11/R12	0.70/0.85	0.12/0.23
R13/R14	0.64/0.84	0.04/0.22
R15/R16	0.59/0.83	0.05/0.10

Part 2. The potential energy curves for the degradation of saturated and unsaturated tetramer.

From the Figure S1, it can be seen that the energy barrier for degradation of saturated polymers is much higher than that of unsaturated polymers, which is even above 3ev. This shows that saturated polymers are very difficult to degrade. Therefore, we foucused on the bi-radicals PAMS tetramer in this study.

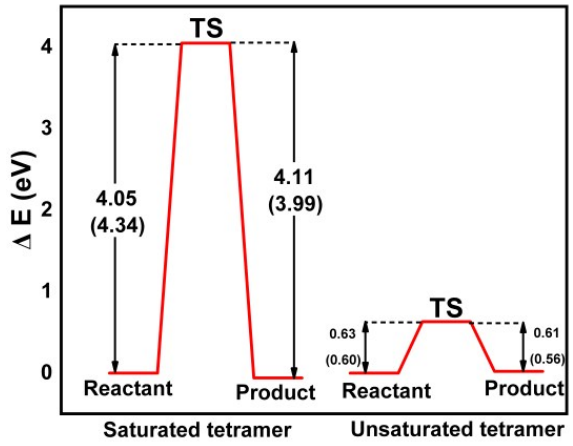


Figure S1. The potential energy curves for the degradation of saturated and unsaturated tetramer. The energy values represent single-point energies (SPE) at the B3LYP-D3/6-311++G (2df, 2pd) level with the correction of ZPE. The brackets energy values represent the sum of the total energy and ZPE at the B3LYP-D3/6-31G* level.

The Part 3 was put at the end for easy reading.

Part 4. Comparison of two functionals on bond properties and thermodynamic stability.

(1) From a geometric structure point of view, the structures obtained by using two different DFT functional are only slightly different in bond length. By taking reactant as an example, on the bottom we give the typical bond length of the C-C bond on the C-unsaturated terminal monomer. It can be found that the bond length of corresponding C-C bond is only 0.01 angstroms different. And the C-C bonds at the junction of the two monomers are both the longest for two functional.

	B3LYP-D3				**PBE-D3**			
Bond length (Å)	a	b	c	d	a	b	c	d
R1	1.60	1.51	1.51	1.43	1.60	1.50	1.51	1.44
R3	1.59	1.51	1.51	1.43	1.59	1.50	1.51	1.44
R5	1.59	1.51	1.51	1.43	1.60	1.51	1.51	1.44
R7	1.59	1.50	1.51	1.43	1.59	1.50	1.51	1.44
R9	1.59	1.51	1.51	1.43	1.60	1.50	1.51	1.44
R11	1.59	1.51	1.51	1.43	1.59	1.50	1.51	1.44
R13	1.59	1.51	1.51	1.43	1.60	1.51	1.51	1.44
R15	1.60	1.51	1.51	1.43	1.60	1.50	1.51	1.44

Bond lengths are in angstroms.

2) From the perspective of energy, also taking the reactants as an example, below we give the energy of the eight isomer reactants. It can be seen that the energy values calculated by the two functionals are indeed different, but in comparison, the energy of the R3 reactant is still the lowest, that is, the relatively stable conformation that researchers think.

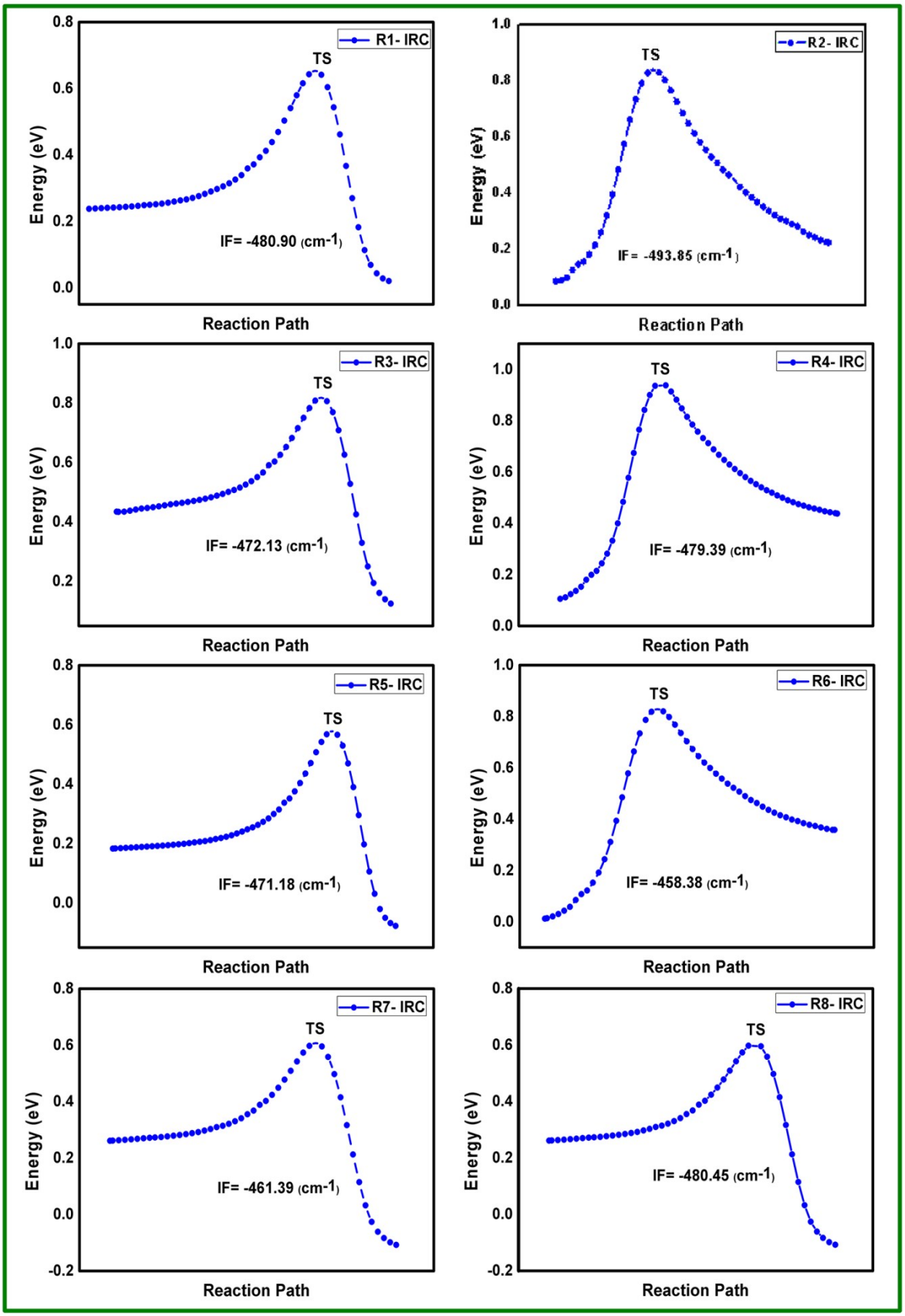
relative energy (KJ/mol)	R1	R3	R5	R7	R9	R11	R13	R15
B3LYP-D3	20.22	0.00	11.29	5.25	17.33	2.89	5.25	15.23
PBE-D3	21.79	0.00	11.03	4.73	17.85	3.41	5.78	15.75

As for energy barrier, it can be seen that there are indeed differences in the values of the energy barrier, but R7 is still the largest. And the energy barriers of other reactions are all smaller than that of R3. These all indicate that isotactic structure and most atactic structures are easier to degrade than syndiotactic structure.

Energy barrier	R1	R3	R5	R7	R9	R11	R13	R15

(KJ/mol)								
PBE-D3	47.44	57.11	52.09	57.42	51.18	56.35	52.27	47.14
B3LYP-D3	51.43	59.77	53.69	60.83	54.37	59.64	56.08	51.42

Part 5. (1) The IRCs of sixteen reactions.



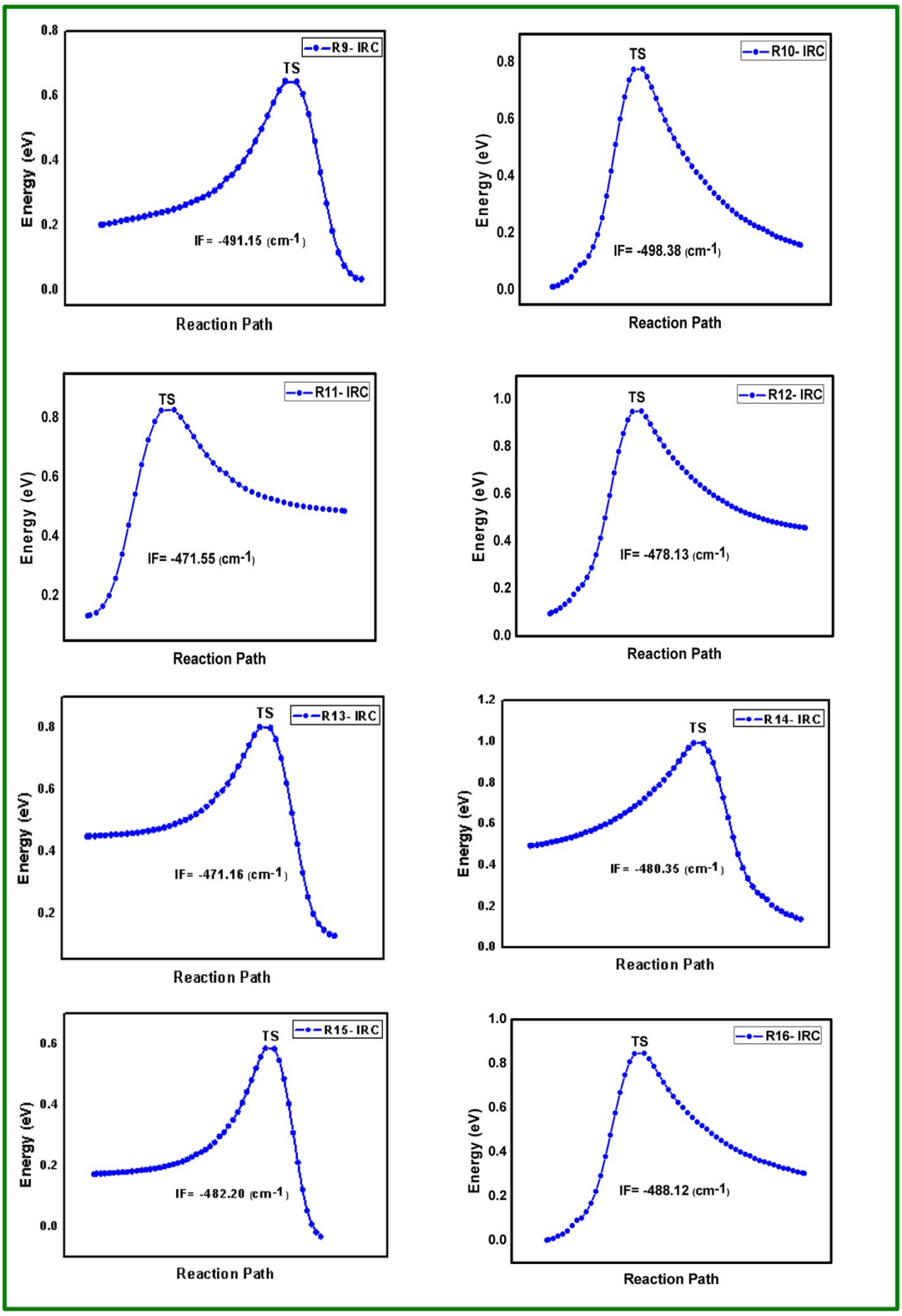


Figure S2. The intrinsic reaction coordinates (IRCs) of nine reactions.

Part 5. (2) The approximate spin-projection (AP) method, energy barrier before and after the approximate spin-projection.

Approximate spin-projection (AP) advocated by Yamaguchi et al [1-3] is an effective way to eliminate spin contamination from the broken-symmetry (BS) solution. According to this scheme, the energies of the pure singlet (ES) is given below

$$E_S = E_{BS} + \frac{< S^2 >_{BS}}{< S^2 >_T - < S^2 >_{BS}}(E_{BS} - E_T)$$

Table S3. The energy barrier before and after the approximate spin-projection.

Energy barrier (KJ/mol)	R1	R3	R5	R7	R9	R11	R13	R15
BS method	51.34	60.31	53.93	60.90	54.38	59.49	56.35	51.43
AP method	51.42	59.77	53.69	60.83	54.37	59.65	56.08	51.42

Part 6. The bond orders and bond lengths of four C-C bonds in eight C-end dissociation reactions.

Table S5 The bond orders and bond lengths (Å) of four C-C bonds (a, b, c, d) in eight C-end dissociation reactions. Here, the "a" represents the broken C-C bond. (The specific location can be seen figure 1)

Bond length (Å)	Bond Length(Å)				Bond Order			
	a	b	c	d	a	b	c	d
R1	1.60	1.51	1.51	1.43	0.93	1.04	1.04	1.26
R3	1.59	1.51	1.51	1.43	0.94	1.04	1.05	1.26
R5	1.59	1.51	1.51	1.43	0.93	1.04	1.04	1.26
R7	1.59	1.50	1.51	1.43	0.94	1.04	1.04	1.26
R9	1.59	1.51	1.51	1.43	0.93	1.04	1.05	1.26
R11	1.59	1.51	1.51	1.43	0.94	1.04	1.05	1.26
R13	1.59	1.51	1.51	1.43	0.93	1.04	1.04	1.26
R15	1.60	1.51	1.51	1.43	0.93	1.04	1.04	1.26

Part 7. The selected frontier MOs of the reactants structures of the R7, R9, R11, R13 and R15.

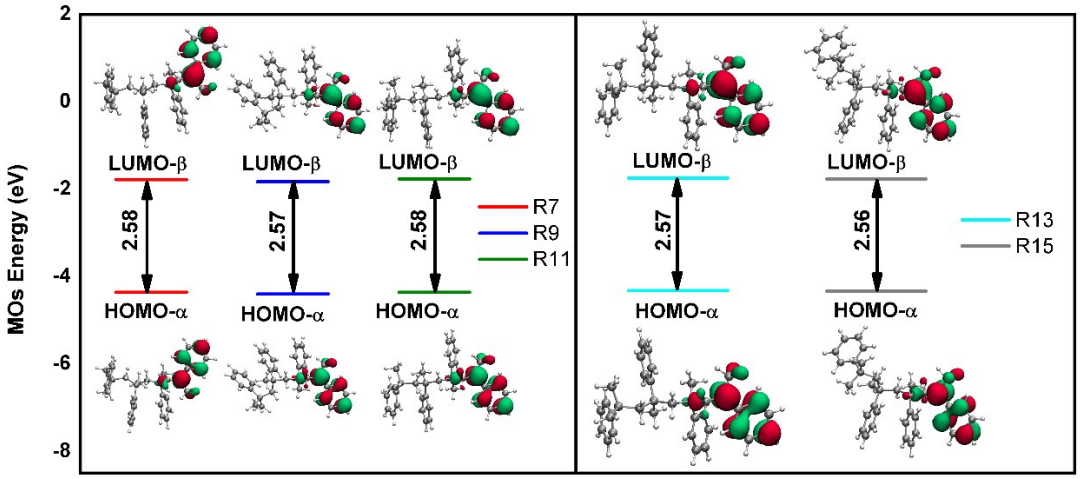


Figure S3. The selected frontier MOs of the stable reactants in R7, R9, R11, R13 and R15 reactions. Isovalue=0.035.

Part 8. The IR spectra for eight spatial structures.

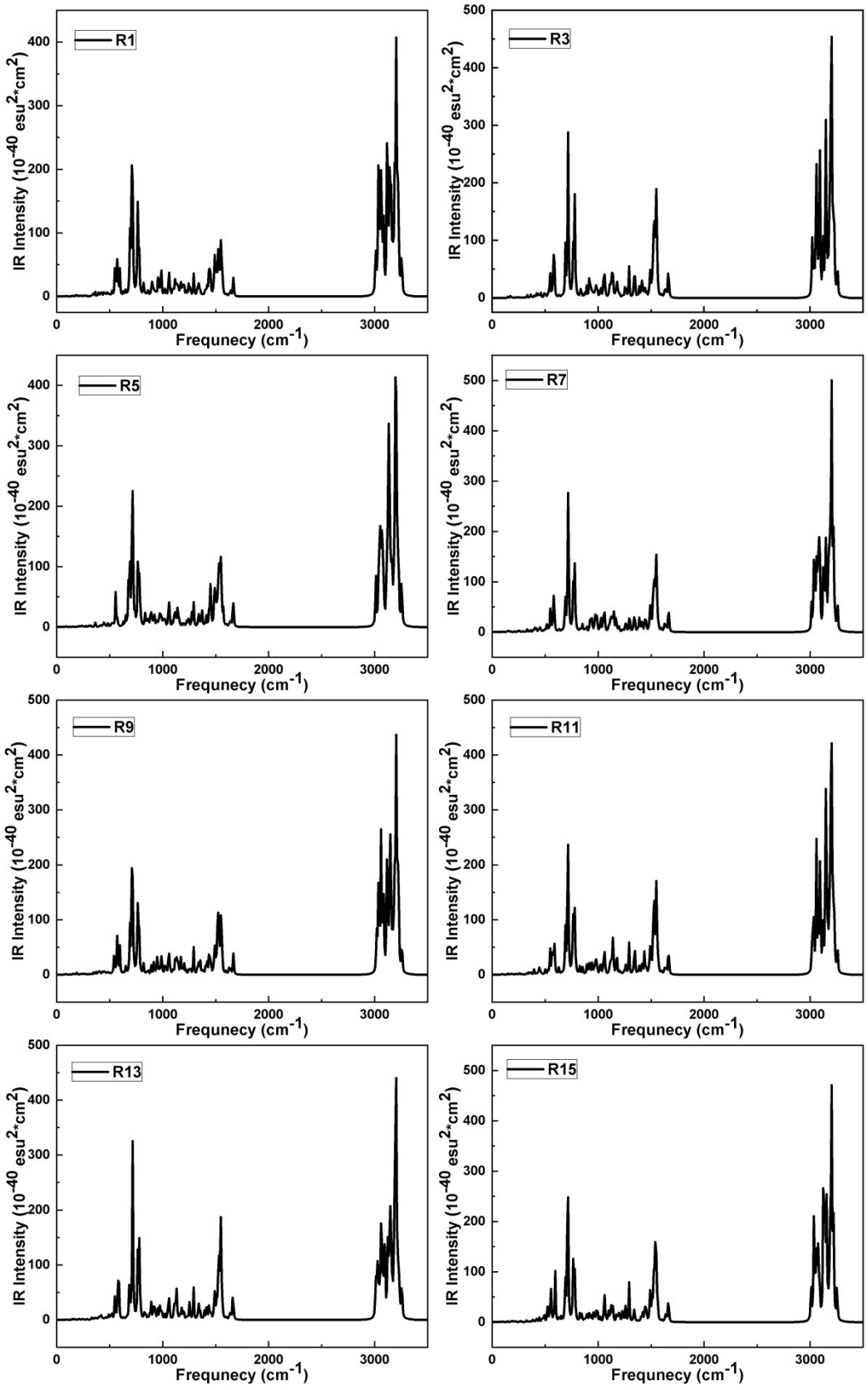


Figure S4. The IR spectra for eight spatial structures.

Part 9. (1) The transition state theory (TST) with Eckart Tunneling corrections.

Reaction rate constants were also calculated in terms of the transition state theory (TST) with Eckart Tunneling corrections. The equation presented for the conventional TST[4] is:

$$k^{TST}(T) = \sigma\frac{k_bT}{h}(\frac{RT}{P^0})^{\Delta n}e^{\frac{-\Delta G^{\neq,0}(T)}{k_bT}}$$

where σ is the reaction path degeneracy, k_b is the Boltzmann's constant, T is the temperature, h is the Planck's constant, R is the ideal gas constant, P^0 is the pressure, $\Delta G^{\neq,0}(T)$ represents the standard Gibbs free energy ($\Delta n = 1$ for gas-phase bimolecular). If the tunneling corrections are considered, then $k^{TST}/_T(T) = \chi(\mathrm{T}) \times k^{TST}(T)$. Where $\chi(\mathrm{T})$ is transmission coefficient. As for Eckart correction, then

$$\chi(\mathrm{T}) = \frac{e^{\frac{\Delta H_f^{\pm,0K}}{k_bT}}}{k_bT}\int_0^{\infty} p(E)e^{-\frac{E}{k_bT}}\,\mathrm{dE}$$

Where $p(E) = 1 - [\frac{cosh[2\pi(\alpha-\beta)+cosh[2\pi\delta]}{cosh[2\pi(\alpha+\beta)+cosh[2\pi\delta]}]$,

$$\alpha = \frac{1}{2\sqrt{C}}\sqrt{E} \qquad \beta = \frac{1}{2\sqrt{C}}\sqrt{E-A} \qquad \delta = \frac{1}{2\sqrt{C}}\sqrt{E-B}$$

$$A = \Delta H_f^{\pm,0K} - \Delta H_r^{\pm,0K} \qquad B = (\sqrt{\Delta H_f^{\pm,0K}} - \sqrt{\Delta H_r^{\pm,0K}})^2$$

$$C = (hIm(v^{\neq}))^2[\frac{B^3}{A^2-B^2}]^2$$

$\Delta H_f^{\pm,0K}, \Delta H_r^{\pm,0K}$ represent the zero-point corrected energy barriers in the reverse and forward direction, $Im(v^{\neq})$ is the imaginary frequency.

Part 9. (2) The curve of synthesis rate constants versus temperature before and after tunneling correction.

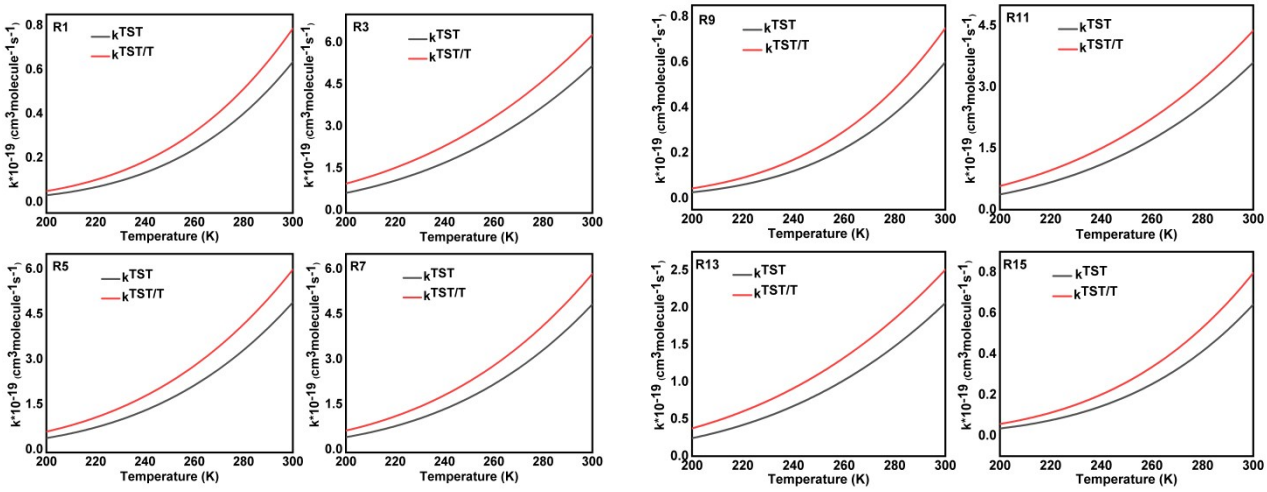


Figure S5. The curve of synthesis rate constants versus temperature before and after tunneling correction.

Part 3.The coordinates of the reactants, TSs and products.

Table S2. The coordinates of the reactants, TSs and products of 16 reactions.

R1/R2	Number	Atom	x (Å)	y (Å)	z (Å)
reactant	1	C	2.608932	-2.010264	0.269541
	2	C	1.941401	-0.933208	-0.306092
	3	C	1.551232	0.182635	0.453906
	4	C	1.878908	0.177854	1.815756
	5	C	2.554162	-0.896619	2.398550
	6	C	2.921611	-1.998602	1.630284
	7	C	-0.082018	1.017143	-1.385498
	8	C	0.878597	1.392518	-0.209156
	9	C	0.167589	2.299824	0.811817
	10	C	5.890658	0.627998	0.533308
	11	C	4.692405	1.140150	0.059686
	12	C	4.230040	2.434433	0.436779
	13	C	5.079740	3.176307	1.311163
	14	C	6.279412	2.656522	1.777793
	15	C	6.698787	1.376612	1.397700
	16	C	2.033907	2.238308	-0.917272
	17	C	2.992336	2.983581	-0.027223
	18	C	2.623259	4.399346	0.344799
	19	C	-1.036043	-3.579294	-0.735361
	20	C	-1.243043	-2.344407	-1.355934
	21	C	-1.263480	-1.151289	-0.622869
	22	C	-1.072541	-1.253868	0.765101
	23	C	-0.855746	-2.476932	1.390500
	24	C	-0.836303	-3.653724	0.640696
	25	C	-1.448431	0.223728	-1.293377
	26	C	-2.514545	1.086015	-0.539913
	27	C	-1.855168	0.074225	-2.777472
	28	H	2.874671	-2.865594	-0.345901
	29	H	1.699554	-0.983581	-1.361778
	30	H	1.614384	1.020529	2.443844
	31	H	2.796101	-0.863820	3.457762
	32	H	3.442161	-2.838085	2.083197
	33	H	-0.340114	1.969554	-1.867227

34	H	0.520536	0.483325	-2.128467
35	H	0.874147	2.757546	1.507303
36	H	-0.357535	3.111970	0.297850
37	H	-0.565695	1.752010	1.407415
38	H	6.196125	-0.370224	0.230178
39	H	4.091273	0.522508	-0.593943
40	H	4.786108	4.169781	1.632158
41	H	6.895036	3.253071	2.446826
42	H	7.636030	0.970528	1.767999
43	H	2.566118	1.554789	-1.587871
44	H	1.534258	2.972348	-1.563460
45	H	3.382218	5.118190	0.002171
46	H	1.668661	4.691349	-0.101044
47	H	2.530248	4.541941	1.431322
48	H	-1.036167	-4.484527	-1.337402
49	H	-1.403879	-2.333050	-2.427213
50	H	-1.073257	-0.361094	1.378430
51	H	-0.689879	-2.506429	2.463878
52	H	-0.668825	-4.612924	1.123416
53	H	-2.289907	1.045305	0.525783
54	H	-2.361270	2.133925	-0.829380
55	H	-2.027977	1.060445	-3.220336
56	H	-1.063190	-0.406414	-3.361454
57	C	-4.067746	0.826174	-0.670502
58	C	-4.646491	1.540876	-1.924527
59	C	-4.247055	-1.386850	0.555342
60	C	-4.432217	-0.666116	-0.634473
61	C	-4.945894	-1.356263	-1.739403
62	C	-5.227515	-2.723633	-1.670960
63	C	-5.008127	-3.428579	-0.489463
64	C	-4.519947	-2.749834	0.629090
65	H	-3.859426	-0.871624	1.428613
66	H	-5.132384	-0.835458	-2.672618
67	H	-5.619922	-3.233832	-2.547120
68	H	-5.217301	-4.493746	-0.437439
69	H	-4.337983	-3.284299	1.557287
70	C	-4.707701	1.506948	0.516179
71	H	-5.715905	1.237426	0.815606
72	H	-4.296019	2.440981	0.890503

73	H	-4.246353	1.155241	-2.865087
74	H	-5.736309	1.436374	-1.953749
75	H	-4.412107	2.609666	-1.878384
76	H	-2.761764	-0.521224	-2.892118

R1	Number	Atom	x (Å)	y (Å)	z (Å)
TS	1	C	3.746104	-3.597189	0.398058
	2	C	2.969725	-2.582089	-0.145521
	3	C	2.556981	-1.469499	0.626288
	4	C	2.975312	-1.440783	1.974785
	5	C	3.749691	-2.461970	2.520328
	6	C	4.145031	-3.546876	1.738155
	7	C	0.912288	-0.629326	-1.182849
	8	C	1.768203	-0.370917	0.047188
	9	C	1.267885	0.699133	0.992571
	10	C	6.844531	-0.838401	1.151525
	11	C	5.749488	-0.357593	0.446177
	12	C	5.298698	0.976534	0.597077
	13	C	6.027239	1.798073	1.491094
	14	C	7.128180	1.314469	2.193117
	15	C	7.545608	-0.008177	2.032312
	16	C	3.373471	0.722663	-0.993530
	17	C	4.140855	1.497524	-0.127592
	18	C	3.717981	2.927858	0.120820
	19	C	-0.175229	-5.210044	-0.728578
	20	C	-0.372124	-3.946469	-1.291536
	21	C	-0.321371	-2.783099	-0.512793
	22	C	-0.067493	-2.944331	0.859810
	23	C	0.141458	-4.197347	1.426523
	24	C	0.087838	-5.343698	0.632589
	25	C	-0.489876	-1.379334	-1.119181
	26	C	-1.489102	-0.511608	-0.290729
	27	C	-0.927901	-1.443108	-2.597524
	28	H	4.032203	-4.441108	-0.224311
	29	H	2.654487	-2.670285	-1.178785
	30	H	2.692846	-0.610643	2.611433
	31	H	4.053873	-2.401466	3.562048
	32	H	4.749450	-4.343315	2.163444
	33	H	0.693095	0.343248	-1.641670

34	H	1.508900	-1.173765	-1.922310
35	H	2.087703	1.150232	1.557631
36	H	0.766423	1.499899	0.440597
37	H	0.549386	0.303949	1.724687
38	H	7.144660	-1.874549	1.020345
39	H	5.220141	-1.039150	-0.207896
40	H	5.730105	2.830057	1.642735
41	H	7.661231	1.975495	2.872137
42	H	8.401466	-0.387092	2.584388
43	H	3.774059	-0.193057	-1.414442
44	H	2.682489	1.246628	-1.648250
45	H	4.505274	3.635934	-0.173400
46	H	2.818478	3.175827	-0.449650
47	H	3.500800	3.122120	1.179965
48	H	-0.232715	-6.090816	-1.363210
49	H	-0.583484	-3.887526	-2.352568
50	H	-0.010770	-2.076017	1.505633
51	H	0.357657	-4.274113	2.488644
52	H	0.247889	-6.325638	1.070012
53	H	-1.214012	-0.597094	0.761598
54	H	-1.313550	0.540377	-0.551816
55	H	-1.079276	-0.431742	-2.989079
56	H	-0.160638	-1.918462	-3.218148
57	C	-3.052870	-0.719489	-0.364108
58	C	-3.654144	0.061966	-1.566728
59	C	-3.257776	-2.975373	0.777306
60	C	-3.458459	-2.201512	-0.376097
61	C	-4.020462	-2.832306	-1.492768
62	C	-4.335082	-4.194001	-1.471971
63	C	-4.100707	-4.952537	-0.327126
64	C	-3.563694	-4.333086	0.803383
65	H	-2.830432	-2.506763	1.658350
66	H	-4.219690	-2.268748	-2.398021
67	H	-4.764770	-4.657701	-2.356454
68	H	-4.335576	-6.013505	-0.312601
69	H	-3.369488	-4.910106	1.703177
70	C	-3.624736	-0.069994	0.873085
71	H	-4.625215	-0.326882	1.207342
72	H	-3.172163	0.837533	1.264912

	73	H	-3.289511	-0.290380	-2.534526
	74	H	-4.746303	-0.018639	-1.566942
	75	H	-3.394774	1.122591	-1.481525
	76	H	-1.854707	-2.004853	-2.723467

R1	Number	Atom	x (Å)	y (Å)	z (Å)
product	1	C	3.088096	-2.414020	0.643521
	2	C	2.155851	-1.409001	0.430043
	3	C	1.809741	-0.481443	1.455932
	4	C	2.454309	-0.662625	2.714552
	5	C	3.387635	-1.670489	2.918465
	6	C	3.720407	-2.554771	1.885525
	7	C	0.356096	0.934981	-0.119510
	8	C	0.891856	0.596898	1.243282
	9	C	0.576809	1.539357	2.375496
	10	C	4.229500	2.344531	1.748107
	11	C	4.065550	1.666149	0.544862
	12	C	3.516828	2.301600	-0.585905
	13	C	3.131432	3.648025	-0.446465
	14	C	3.294739	4.330627	0.759926
	15	C	3.846435	3.683704	1.864899
	16	C	3.803146	0.351450	-2.106827
	17	C	3.315646	1.581298	-1.873319
	18	C	2.507893	2.277565	-2.946951
	19	C	-1.236022	-3.202125	-1.723044
	20	C	-1.234790	-1.804898	-1.741813
	21	C	-1.154000	-1.058657	-0.558954
	22	C	-1.070467	-1.775840	0.647361
	23	C	-1.059967	-3.167260	0.672852
	24	C	-1.145059	-3.892510	-0.516591
	25	C	-1.100800	0.478634	-0.554648
	26	C	-2.131192	1.092455	0.440314
	27	C	-1.277631	1.068788	-1.966885
	28	H	3.321079	-3.101965	-0.165458
	29	H	1.673169	-1.344952	-0.536866
	30	H	2.230890	0.012295	3.533314
	31	H	3.863822	-1.768598	3.891201
	32	H	4.450878	-3.342543	2.047236
	33	H	0.376611	2.029972	-0.217873

34	H	1.035716	0.557101	-0.887205
35	H	1.480582	2.073572	2.705188
36	H	-0.151059	2.295167	2.074114
37	H	0.170865	1.020580	3.255315
38	H	4.639487	1.814173	2.603079
39	H	4.334055	0.617266	0.503503
40	H	2.698222	4.179802	-1.286621
41	H	2.987354	5.370707	0.832584
42	H	3.971714	4.212003	2.806363
43	H	4.391675	-0.202132	-1.384185
44	H	3.618253	-0.150120	-3.052488
45	H	3.000257	3.195160	-3.293370
46	H	2.369207	1.626913	-3.814911
47	H	1.516078	2.562763	-2.574938
48	H	-1.313930	-3.747397	-2.660251
49	H	-1.318188	-1.305498	-2.699671
50	H	-0.995971	-1.240987	1.587481
51	H	-0.980731	-3.684433	1.625531
52	H	-1.141601	-4.979220	-0.501513
53	H	-2.002174	0.589076	1.402366
54	H	-1.838295	2.136196	0.614908
55	H	-1.267419	2.163060	-1.918945
56	H	-0.456714	0.764785	-2.625665
57	C	-3.679021	1.129300	0.136495
58	C	-4.033184	2.380388	-0.716811
59	C	-4.225664	-1.343362	0.265152
60	C	-4.193029	-0.169325	-0.503362
61	C	-4.631545	-0.247491	-1.830756
62	C	-5.056851	-1.460198	-2.380910
63	C	-5.057468	-2.620499	-1.609877
64	C	-4.642120	-2.555203	-0.278070
65	H	-3.892522	-1.305698	1.297760
66	H	-4.646774	0.638746	-2.456160
67	H	-5.387648	-1.491795	-3.416085
68	H	-5.379018	-3.565784	-2.038973
69	H	-4.628909	-3.451749	0.335410
70	C	-4.372196	1.325586	1.462694
71	H	-5.428235	1.094330	1.562474
72	H	-3.909556	1.944196	2.227677

	73	H	-3.547302	2.382891	-1.695527
	74	H	-5.115103	2.442579	-0.874482
	75	H	-3.717236	3.286243	-0.188764
	76	H	-2.214848	0.754051	-2.429722

R3/R4	Number	Atom	x (Å)	y (Å)	z (Å)
reactant	1	C	-2.389861	-1.623640	0.113224
	2	H	-2.165469	-2.322527	-0.704534
	3	H	-2.172713	-2.170339	1.039869
	4	C	-4.551470	-2.769487	0.367342
	5	H	-4.078615	-3.668525	-0.019341
	6	C	-3.949300	-1.414890	0.076811
	7	C	-1.338449	-0.455423	0.041685
	8	C	-1.619734	0.428748	-1.184192
	9	C	-1.341099	0.349532	1.355125
	10	C	-4.418155	-0.427228	1.154686
	11	C	-4.459101	-1.016776	-1.335423
	12	H	-4.097650	-0.041205	-1.663837
	13	H	-4.122910	-1.753976	-2.071529
	14	H	-5.554438	-1.000282	-1.344528
	15	H	-2.300256	0.827758	1.546352
	16	H	-1.129703	-0.312345	2.199667
	17	H	-0.568347	1.121436	1.349726
	18	C	-2.035426	1.761709	-1.065689
	19	H	-2.142729	2.211896	-0.086168
	20	C	-1.511079	-0.098443	-2.482673
	21	H	-1.211555	-1.132886	-2.621987
	22	C	-2.331554	2.534573	-2.191990
	23	H	-2.652893	3.565087	-2.062812
	24	C	-2.216071	1.993225	-3.470967
	25	H	-2.445062	2.593448	-4.347337
	26	C	-1.801671	0.666655	-3.609748
	27	H	-1.709336	0.224059	-4.598375
	28	C	-4.890386	0.857569	0.858053
	29	H	-4.959023	1.189556	-0.171359
	30	C	-4.346162	-0.804473	2.505535
	31	H	-3.990599	-1.800587	2.756264
	32	C	-5.253437	1.743255	1.876438
	33	H	-5.610739	2.737188	1.618701

34	C	-4.705998	0.074878	3.524250
35	H	-5.439077	2.049554	4.004960
36	C	-5.159262	1.359239	3.213640
37	H	-4.631682	-0.241697	4.561556
38	C	2.488879	-1.520369	-0.467013
39	H	2.207292	-1.811236	-1.484865
40	H	2.373294	-2.422443	0.148147
41	C	0.034644	-1.205686	-0.106493
42	H	0.042433	-1.698381	-1.085119
43	H	0.021436	-2.027484	0.617970
44	C	1.406587	-0.467562	0.026943
45	C	3.927822	-1.080935	-0.413230
46	C	4.599352	-0.500723	-1.537525
47	C	4.666631	-1.254655	0.888995
48	C	1.739858	-0.106491	1.485484
49	C	1.462474	0.756206	-0.902052
50	H	2.471656	1.172495	-0.951123
51	H	1.172119	0.474105	-1.917144
52	H	0.776602	1.544089	-0.581606
53	H	4.876048	-0.291121	1.375874
54	H	4.083540	-1.841406	1.601436
55	H	5.632025	-1.758601	0.743933
56	C	5.933377	-0.006261	-1.420896
57	H	6.441392	-0.057662	-0.464269
58	C	3.998053	-0.379615	-2.825769
59	H	2.985332	-0.731973	-2.982341
60	C	6.601031	0.558690	-2.498711
61	H	7.614927	0.927586	-2.363446
62	C	5.982599	0.660085	-3.750123
63	H	6.507700	1.102471	-4.591924
64	C	4.674331	0.183413	-3.898153
65	H	4.177321	0.254033	-4.862627
66	C	2.243921	1.150084	1.847236
67	H	2.372348	1.921055	1.096737
68	C	1.606535	-1.062581	2.506994
69	H	1.234399	-2.055647	2.272975
70	C	2.590425	1.443892	3.169052
71	H	2.975861	2.430748	3.412781
72	C	1.948708	-0.776656	3.826980

	73	H	2.711588	0.711119	5.196166
	74	C	2.444143	0.483676	4.167826
	75	H	1.829343	-1.541350	4.590420
	76	H	-5.579786	-2.840700	0.708464

R3	Number	Atom	x (Å)	y (Å)	z (Å)
TS	1	C	5.558300	3.126643	5.796745
	2	H	5.774112	2.412450	4.989839
	3	H	5.810688	2.605823	6.729476
	4	C	3.420734	1.955131	6.138998
	5	H	3.889588	1.054521	5.751098
	6	C	3.994975	3.309928	5.799646
	7	C	6.577577	4.312605	5.670708
	8	C	6.269292	5.162304	4.430016
	9	C	6.607818	5.151101	6.962312
	10	C	3.545921	4.319187	6.865406
	11	C	3.441474	3.668145	4.393356
	12	H	3.785322	4.637944	4.030228
	13	H	3.762598	2.915301	3.666344
	14	H	2.346274	3.676010	4.415453
	15	H	5.655185	5.635836	7.169534
	16	H	6.842791	4.510230	7.817186
	17	H	7.382659	5.920974	6.913536
	18	C	5.884828	6.506622	4.518777
	19	H	5.813261	6.987992	5.486681
	20	C	6.332189	4.592999	3.146038
	21	H	6.607596	3.548578	3.032404
	22	C	5.573938	7.250899	3.376943
	23	H	5.277113	8.291392	3.482284
	24	C	5.643678	6.668119	2.113091
	25	H	5.403149	7.246035	1.224892
	26	C	6.026618	5.329068	2.004050
	27	H	6.082800	4.854988	1.027411
	28	C	3.058578	5.593967	6.550259
	29	H	2.959555	5.900297	5.515340
	30	C	3.658253	3.976192	8.222558
	31	H	4.026608	2.988444	8.487707
	32	C	2.719522	6.503040	7.556152
	33	H	2.349900	7.488587	7.284044

34	C	3.322624	4.879161	9.228881
35	H	2.593132	6.861892	9.680773
36	C	2.853874	6.153158	8.899301
37	H	3.428107	4.589178	10.271233
38	C	10.675539	2.921832	4.877747
39	H	10.263380	2.991043	3.876300
40	H	10.242395	2.136883	5.491162
41	C	7.981378	3.597427	5.512920
42	H	7.987047	3.075362	4.549464
43	H	8.014800	2.806794	6.268858
44	C	9.236697	4.448363	5.599045
45	C	11.978860	3.317996	5.141147
46	C	12.740218	4.176960	4.230929
47	C	12.584595	2.971906	6.480381
48	C	9.808420	4.767219	6.917838
49	C	9.406084	5.473659	4.500582
50	H	10.454799	5.745629	4.355076
51	H	9.024737	5.093102	3.549638
52	H	8.844634	6.393108	4.718918
53	H	12.623557	3.844191	7.146271
54	H	11.991250	2.210237	6.992809
55	H	13.609396	2.594182	6.371873
56	C	13.880245	4.881784	4.682669
57	H	14.187944	4.796583	5.719091
58	C	12.386410	4.340140	2.869521
59	H	11.535205	3.800623	2.467297
60	C	14.609126	5.709274	3.831741
61	H	15.474750	6.242373	4.217181
62	C	14.233804	5.860029	2.495645
63	H	14.803703	6.504033	1.831593
64	C	13.115959	5.164827	2.021913
65	H	12.815651	5.262153	0.981592
66	C	10.630824	5.901913	7.100336
67	H	10.798284	6.584894	6.276157
68	C	9.633511	3.924406	8.040070
69	H	9.023221	3.031782	7.954959
70	C	11.241041	6.172911	8.324173
71	H	11.865686	7.057297	8.423281
72	C	10.242461	4.194753	9.260093

	73	H	11.532266	5.532076	10.367769
	74	C	11.055721	5.321722	9.414311
	75	H	10.085639	3.518668	10.096964
	76	H	2.408215	1.878044	6.523169

R3	Number	Atom	x (Å)	y (Å)	z (Å)
product	1	C	-1.434420	-1.016601	-0.705380
	2	H	-1.147223	-1.353406	-1.708458
	3	H	-0.858629	-1.644507	-0.018212
	4	C	-3.076572	-2.837032	-0.962555
	5	H	-2.569242	-3.176274	-1.862284
	6	C	-2.942888	-1.399973	-0.517233
	7	C	-0.904490	0.440841	-0.515054
	8	C	-1.367115	1.381822	-1.637799
	9	C	-1.258030	0.974581	0.882489
	10	C	-3.366201	-1.331029	0.961811
	11	C	-3.855475	-0.544623	-1.431998
	12	H	-3.831485	0.515337	-1.162287
	13	H	-3.518669	-0.620382	-2.469502
	14	H	-4.891452	-0.896220	-1.381571
	15	H	-2.329025	1.154297	0.995493
	16	H	-0.972374	0.246085	1.646590
	17	H	-0.724387	1.905163	1.097090
	18	C	-1.920008	2.643424	-1.380875
	19	H	-2.066029	2.974915	-0.359299
	20	C	-1.195278	1.017056	-2.984955
	21	H	-0.753269	0.055684	-3.230594
	22	C	-2.294321	3.500476	-2.420208
	23	H	-2.721248	4.471951	-2.183650
	24	C	-2.122233	3.117124	-3.748365
	25	H	-2.413397	3.781808	-4.557217
	26	C	-1.566695	1.865616	-4.025381
	27	H	-1.420120	1.549416	-5.055220
	28	C	-4.408918	-0.519900	1.425134
	29	H	-4.960196	0.108561	0.734476
	30	C	-2.695717	-2.130728	1.902618
	31	H	-1.897424	-2.788195	1.569103
	32	C	-4.752991	-0.487288	2.779689
	33	H	-5.563670	0.157391	3.109938

34	C	-3.032007	-2.100570	3.254125
35	H	-4.328404	-1.243718	4.755821
36	C	-4.063673	-1.271932	3.702218
37	H	-2.488976	-2.726250	3.958122
38	C	1.260268	-3.288068	1.423103
39	H	0.468536	-3.418229	0.691610
40	H	1.039248	-3.613367	2.435880
41	C	0.666653	0.289372	-0.602759
42	H	0.915220	-0.122276	-1.587917
43	H	0.939537	-0.485029	0.113322
44	C	1.492403	1.522786	-0.377948
45	C	2.449716	-2.747487	1.108844
46	C	2.766310	-2.308974	-0.276963
47	C	3.501257	-2.522852	2.172259
48	C	2.110912	1.804444	0.881819
49	C	1.679318	2.463809	-1.538892
50	H	2.735230	2.731067	-1.681427
51	H	1.317618	2.017618	-2.467401
52	H	1.124956	3.404357	-1.403862
53	H	3.629657	-1.453182	2.378780
54	H	3.221699	-3.009783	3.111175
55	H	4.476598	-2.910569	1.854851
56	C	3.640795	-1.233298	-0.508286
57	H	4.109453	-0.726602	0.328073
58	C	2.167602	-2.922089	-1.392972
59	H	1.522158	-3.782893	-1.246498
60	C	3.871111	-0.758890	-1.799502
61	H	4.530917	0.091829	-1.946462
62	C	3.249141	-1.361440	-2.893304
63	H	3.428802	-0.992005	-3.899295
64	C	2.401257	-2.452901	-2.683304
65	H	1.927066	-2.945546	-3.528364
66	C	2.849760	3.007614	1.089947
67	H	2.920435	3.735875	0.289476
68	C	2.045719	0.908540	1.992212
69	H	1.497709	-0.021924	1.903813
70	C	3.474727	3.282804	2.298872
71	H	4.025268	4.213401	2.414542
72	C	2.677157	1.191652	3.195073

	73	H	3.891205	2.597028	4.309565
	74	C	3.400443	2.379376	3.365198
	75	H	2.602641	0.479509	4.013590
	76	H	-3.858321	-3.466887	-0.550137

R5/R6	Number	Atom	x (Å)	y (Å)	z (Å)
reactant	1	C	-0.940503	2.593065	1.285382
	2	C	0.027356	1.686422	0.859876
	3	C	0.404012	1.585390	-0.492136
	4	C	-0.222143	2.452383	-1.395755
	5	C	-1.191819	3.367030	-0.975989
	6	C	-1.561107	3.441020	0.364946
	7	C	1.294027	-0.816389	-0.252909
	8	C	1.487985	0.584310	-0.925259
	9	C	1.581410	0.454892	-2.454193
	10	C	2.239106	5.347157	0.734612
	11	C	2.471333	4.019462	0.408861
	12	C	3.263825	3.651144	-0.716521
	13	C	3.822930	4.726052	-1.471142
	14	C	3.587527	6.052445	-1.135912
	15	C	2.790528	6.380104	-0.032986
	16	C	2.888630	1.111095	-0.374865
	17	C	3.504144	2.289159	-1.084971
	18	C	4.439559	1.986277	-2.230269
	19	C	0.424002	-5.001724	1.569135
	20	C	0.442914	-4.137857	0.469384
	21	C	0.071523	-2.793423	0.591861
	22	C	-0.299996	-2.342495	1.870664
	23	C	-0.331073	-3.198000	2.966598
	24	C	0.032263	-4.539261	2.822019
	25	C	0.101458	-1.802776	-0.592861
	26	C	-1.233326	-1.007000	-0.723141
	27	C	0.409837	-2.543337	-1.911653
	28	H	-1.208549	2.637659	2.337985
	29	H	0.497795	1.047605	1.601348
	30	H	0.037544	2.425597	-2.447579
	31	H	-1.655680	4.025041	-1.706170
	32	H	-2.316296	4.150796	0.691210
	33	H	2.210227	-1.390551	-0.441419

34	H	1.291061	-0.652085	0.826749
35	H	1.890384	1.394564	-2.918583
36	H	2.319242	-0.307846	-2.723262
37	H	0.625034	0.168026	-2.897874
38	H	1.617744	5.580414	1.595605
39	H	2.022451	3.251811	1.023704
40	H	4.441354	4.511692	-2.335940
41	H	4.027412	6.841643	-1.740948
42	H	2.604532	7.419242	0.223843
43	H	2.770283	1.309132	0.696245
44	H	3.589918	0.270424	-0.449626
45	H	4.096497	2.416245	-3.182487
46	H	5.444432	2.395540	-2.049562
47	H	4.545423	0.909079	-2.383501
48	H	0.715321	-6.040842	1.436534
49	H	0.747281	-4.538429	-0.490385
50	H	-0.601353	-1.308478	2.007793
51	H	-0.652623	-2.819741	3.933105
52	H	0.006712	-5.211286	3.675706
53	H	-1.350421	-0.370762	0.156180
54	H	-1.104018	-0.312006	-1.559304
55	H	0.310413	-1.878653	-2.771167
56	H	1.432020	-2.938218	-1.917269
57	C	-2.626852	-1.694209	-0.937677
58	C	-2.670072	-2.593162	-2.137786
59	C	-3.571826	-1.674088	1.436292
60	C	-3.100551	-2.408978	0.337664
61	C	-3.040034	-3.802622	0.465624
62	C	-3.434341	-4.440109	1.641911
63	C	-3.907889	-3.695474	2.721784
64	C	-3.972685	-2.305899	2.613103
65	H	-3.616161	-0.590483	1.385299
66	H	-2.644204	-4.396893	-0.351237
67	H	-3.357983	-5.521652	1.715666
68	H	-4.215005	-4.190665	3.639225
69	H	-4.334254	-1.708999	3.446944
70	C	-3.604993	-0.514902	-1.269593
71	H	-3.528273	0.296435	-0.536702
72	H	-3.360403	-0.088990	-2.248538

	73	H	-4.640696	-0.867917	-1.291921
	74	H	-3.470620	-3.319773	-2.240456
	75	H	-2.187320	-2.262690	-3.052500
	76	H	-0.279727	-3.376556	-2.068671

R5	Number	Atom	x (Å)	y (Å)	z (Å)
TS	1	C	1.147107	2.926042	-0.621262
	2	C	1.957214	1.865576	-1.009880
	3	C	2.422953	1.732894	-2.341587
	4	C	2.018925	2.732159	-3.254639
	5	C	1.202555	3.791907	-2.865427
	6	C	0.761180	3.901844	-1.546858
	7	C	3.237864	-0.691253	-2.017592
	8	C	3.325587	0.642071	-2.745052
	9	C	3.731190	0.588846	-4.200303
	10	C	4.308410	5.609551	-1.652603
	11	C	4.600211	4.251922	-1.666565
	12	C	5.556727	3.709136	-2.558625
	13	C	6.208857	4.618507	-3.425441
	14	C	5.917173	5.980097	-3.406225
	15	C	4.962987	6.487696	-2.522321
	16	C	5.213043	1.341680	-1.805414
	17	C	5.863307	2.278932	-2.599327
	18	C	6.880643	1.786847	-3.603546
	19	C	2.697095	-5.027221	-0.467877
	20	C	2.609044	-4.087447	-1.499142
	21	C	2.150813	-2.785062	-1.262226
	22	C	1.807205	-2.454429	0.060060
	23	C	1.884111	-3.386852	1.089383
	24	C	2.331238	-4.684756	0.830846
	25	C	2.072867	-1.717153	-2.369526
	26	C	0.716064	-0.951527	-2.379886
	27	C	2.347758	-2.330926	-3.756201
	28	H	0.815359	2.994311	0.411917
	29	H	2.246385	1.133834	-0.262303
	30	H	2.346011	2.684780	-4.286619
	31	H	0.917951	4.541544	-3.599095
	32	H	0.128002	4.730537	-1.242621
	33	H	4.170549	-1.244560	-2.181783

34	H	3.198571	-0.508134	-0.941310
35	H	4.193547	1.526679	-4.521983
36	H	4.450482	-0.217255	-4.372889
37	H	2.869849	0.409614	-4.859407
38	H	3.554966	5.982040	-0.963722
39	H	4.057330	3.602596	-0.991314
40	H	6.953571	4.258717	-4.127140
41	H	6.437545	6.647678	-4.088588
42	H	4.732016	7.549473	-2.510978
43	H	4.690499	1.644846	-0.905332
44	H	5.637491	0.343209	-1.758691
45	H	6.605393	2.040677	-4.636177
46	H	7.869159	2.231152	-3.422531
47	H	6.990732	0.700085	-3.549869
48	H	3.051259	-6.031100	-0.689228
49	H	2.894791	-4.394835	-2.498391
50	H	1.440066	-1.458265	0.287851
51	H	1.582084	-3.102526	2.093684
52	H	2.389797	-5.416399	1.632260
53	H	0.617927	-0.395042	-1.443543
54	H	0.800974	-0.182913	-3.156851
55	H	2.179981	-1.597029	-4.546816
56	H	3.383602	-2.677586	-3.842153
57	C	-0.663623	-1.660942	-2.610564
58	C	-0.729223	-2.407828	-3.910821
59	C	-1.553345	-2.005238	-0.234560
60	C	-1.043483	-2.555611	-1.420004
61	C	-0.851026	-3.943058	-1.461839
62	C	-1.147895	-4.750255	-0.364302
63	C	-1.656171	-4.186998	0.806062
64	C	-1.857453	-2.807964	0.865142
65	H	-1.709520	-0.933970	-0.155156
66	H	-0.428441	-4.394770	-2.353315
67	H	-0.968022	-5.820347	-0.422512
68	H	-1.887116	-4.814013	1.663222
69	H	-2.251717	-2.351851	1.770017
70	C	-1.698019	-0.493933	-2.751295
71	H	-1.624829	0.219857	-1.922602
72	H	-1.510379	0.064402	-3.674482

	73	H	-2.719423	-0.885868	-2.782370
	74	H	-1.499932	-3.156990	-4.065731
	75	H	-0.298168	-1.953102	-4.797614
	76	H	1.684288	-3.176653	-3.955219

R5	Number	Atom	x (Å)	y (Å)	z (Å)
product	1	C	-1.788032	3.764994	0.721410
	2	C	-1.064060	2.703756	0.197352
	3	C	-0.657505	2.673328	-1.169992
	4	C	-1.038254	3.797577	-1.961146
	5	C	-1.765095	4.854382	-1.428928
	6	C	-2.150058	4.852578	-0.083332
	7	C	0.556126	0.418073	-0.916730
	8	C	0.117283	1.605769	-1.726691
	9	C	0.624317	1.714173	-3.140896
	10	C	2.626733	4.014531	-0.898775
	11	C	2.490571	3.080659	0.124259
	12	C	3.342805	1.964442	0.217435
	13	C	4.331102	1.818709	-0.773070
	14	C	4.474380	2.756229	-1.796376
	15	C	3.623551	3.860164	-1.865359
	16	C	2.548781	1.217763	2.445877
	17	C	3.173860	0.945100	1.288724
	18	C	3.727363	-0.438689	1.032807
	19	C	1.774717	-3.849629	0.399994
	20	C	1.129488	-2.995481	-0.499121
	21	C	0.380796	-1.897663	-0.054183
	22	C	0.322984	-1.677921	1.332507
	23	C	0.952173	-2.531070	2.233761
	24	C	1.685562	-3.626432	1.771669
	25	C	-0.298660	-0.914147	-1.021068
	26	C	-1.762903	-0.566426	-0.618308
	27	C	-0.248921	-1.409330	-2.476920
	28	H	-2.072452	3.748717	1.770789
	29	H	-0.790011	1.889102	0.857109
	30	H	-0.756337	3.835995	-3.007515
	31	H	-2.035374	5.691001	-2.068789
	32	H	-2.717616	5.681201	0.330380
	33	H	1.574898	0.152085	-1.224144

34	H	0.637211	0.680159	0.139494
35	H	1.255230	2.606715	-3.263135
36	H	1.233533	0.848686	-3.410101
37	H	-0.187190	1.788909	-3.879075
38	H	1.929056	4.845369	-0.956411
39	H	1.672631	3.196187	0.827051
40	H	5.002614	0.966749	-0.747378
41	H	5.251385	2.618727	-2.544080
42	H	3.727906	4.585299	-2.668200
43	H	2.176091	2.207299	2.692446
44	H	2.406152	0.446899	3.197424
45	H	3.361389	-0.846656	0.083602
46	H	4.823938	-0.426706	0.982485
47	H	3.433542	-1.132999	1.822484
48	H	2.342715	-4.695179	0.019894
49	H	1.210039	-3.209522	-1.558739
50	H	-0.244229	-0.839152	1.721807
51	H	0.860900	-2.344361	3.300451
52	H	2.176308	-4.295931	2.473068
53	H	-1.749597	-0.080032	0.362194
54	H	-2.096593	0.208478	-1.319267
55	H	-0.785701	-0.714127	-3.129343
56	H	0.782146	-1.472473	-2.841406
57	C	-2.905564	-1.638372	-0.551922
58	C	-3.123374	-2.340557	-1.860790
59	C	-2.968407	-2.291986	1.923486
60	C	-2.671551	-2.633050	0.595661
61	C	-2.105593	-3.893330	0.359936
62	C	-1.837827	-4.775861	1.405836
63	C	-2.140463	-4.421089	2.720338
64	C	-2.708391	-3.172552	2.973808
65	H	-3.399425	-1.322735	2.153300
66	H	-1.838204	-4.176104	-0.653090
67	H	-1.380201	-5.737760	1.190958
68	H	-1.931511	-5.106637	3.537330
69	H	-2.949844	-2.879004	3.992506
70	C	-4.217450	-0.823723	-0.297443
71	H	-4.119121	-0.145139	0.557888
72	H	-4.452829	-0.208945	-1.172482

	73	H	-5.059131	-1.497412	-0.108739
	74	H	-3.671852	-3.277412	-1.887006
	75	H	-3.089663	-1.760631	-2.778091
	76	H	-0.713440	-2.393037	-2.586114

R7/R8	Number	Atom	x (Å)	y (Å)	z (Å)
reactant	1	C	0.215545	1.968349	-4.292735
	2	C	1.178444	0.831241	-3.858498
	3	H	0.552815	2.921189	-3.874037
	4	H	0.211794	2.056915	-5.384724
	5	H	-0.809973	1.809980	-3.954027
	6	C	1.371059	0.764228	-2.298248
	7	H	2.209663	0.078846	-2.122655
	8	H	1.736001	1.756025	-1.998944
	9	C	0.243582	0.343267	-1.285772
	10	C	-0.105276	-1.143335	-1.471490
	11	C	0.907606	0.574444	0.125558
	12	H	0.795461	-1.755900	-1.366569
	13	H	-0.834460	-1.468593	-0.726721
	14	H	-0.519261	-1.347788	-2.457943
	15	H	1.942673	0.214813	0.054931
	16	H	0.990424	1.657637	0.269237
	17	C	0.340618	-0.038832	1.456942
	18	C	0.808545	-1.499433	1.620015
	19	C	1.037688	0.796371	2.613275
	20	H	1.900970	-1.547563	1.564786
	21	H	0.519525	-1.897573	2.596643
	22	H	0.412447	-2.163101	0.851910
	23	H	2.104185	0.835869	2.370024
	24	H	0.679249	1.830829	2.544550
	25	C	0.820718	0.301036	4.017302
	26	C	-0.490907	0.642125	4.676122
	27	H	-1.016657	1.428265	4.130664
	28	H	-1.172878	-0.221406	4.707539
	29	H	-0.353217	0.980650	5.711180
	30	C	2.533368	1.188299	-4.424534
	31	H	2.751289	0.985736	-5.468658
	32	H	3.184818	1.875354	-3.890814
	33	C	0.759254	-0.527721	-4.440656

34	C	-0.493704	-0.756592	-5.023088
35	C	1.658592	-1.604621	-4.375751
36	C	-0.845244	-2.022246	-5.501126
37	H	-1.218034	0.046674	-5.093475
38	C	1.312824	-2.868029	-4.849597
39	H	2.642131	-1.445144	-3.941270
40	C	0.052830	-3.084824	-5.413008
41	H	-1.826935	-2.173354	-5.943122
42	H	2.027297	-3.684443	-4.780026
43	H	-0.221734	-4.069161	-5.782754
44	C	-0.989161	1.247973	-1.453070
45	C	-0.866650	2.641638	-1.314125
46	C	-2.256369	0.744092	-1.770139
47	C	-1.956350	3.492232	-1.477942
48	H	0.100729	3.077731	-1.080943
49	C	-3.355149	1.591016	-1.934292
50	H	-2.407651	-0.322672	-1.879435
51	C	-3.213781	2.969532	-1.789325
52	H	-1.823043	4.565376	-1.365589
53	H	-4.326683	1.163751	-2.168758
54	H	-4.068296	3.628723	-1.916692
55	C	-1.183323	0.106423	1.565970
56	C	-2.039422	-0.994731	1.694213
57	C	-1.773282	1.381575	1.545255
58	C	-3.425889	-0.832112	1.780449
59	H	-1.634696	-2.000093	1.725000
60	C	-3.151364	1.552028	1.629490
61	H	-1.148244	2.260730	1.434338
62	C	-3.989708	0.440822	1.746978
63	H	-4.061422	-1.709101	1.875022
64	H	-3.570224	2.553289	1.586186
65	H	-5.067143	0.568386	1.809037
66	C	1.777025	-0.512841	4.707139
67	C	3.068164	-0.812452	4.178732
68	C	1.476527	-1.079523	5.982354
69	C	3.975571	-1.602474	4.869331
70	H	3.361923	-0.412100	3.215279
71	C	2.389179	-1.872591	6.664170
72	H	0.504956	-0.903353	6.430187

	73	C	3.649475	-2.143202	6.119143
	74	H	4.950312	-1.801462	4.430471
	75	H	2.115750	-2.288710	7.630815
	76	H	4.362087	-2.763402	6.655414

R7	Number	Atom	x (Å)	y (Å)	z (Å)
TS	1	C	-5.704004	1.802093	0.949687
	2	C	-4.557337	0.887124	1.451684
	3	H	-5.555229	2.821299	1.316620
	4	H	-5.712051	1.831344	-0.145241
	5	H	-6.686124	1.473085	1.298188
	6	C	-4.398122	0.938912	3.014654
	7	H	-3.516063	0.333712	3.254084
	8	H	-4.116281	1.970868	3.260121
	9	C	-5.520901	0.498673	4.015252
	10	C	-5.852331	-0.990943	3.833066
	11	C	-4.872988	0.722130	5.450865
	12	H	-4.942712	-1.593120	3.916540
	13	H	-6.557658	-1.330442	4.595843
	14	H	-6.286973	-1.195779	2.854346
	15	H	-3.818709	0.430717	5.374989
	16	H	-4.866026	1.801351	5.639997
	17	C	-5.451433	-0.024685	6.645700
	18	C	-4.897728	-1.412802	6.886837
	19	C	-4.322178	1.068553	8.224261
	20	H	-3.830840	-1.450999	6.644067
	21	H	-5.003049	-1.708887	7.934341
	22	H	-5.395421	-2.178308	6.277062
	23	H	-3.371304	0.849207	7.749457
	24	H	-4.767760	2.013616	7.930435
	25	C	-4.627771	0.559184	9.476855
	26	C	-5.871056	1.060650	10.172619
	27	H	-6.263135	1.953218	9.679486
	28	H	-6.675259	0.312658	10.148776
	29	H	-5.677328	1.301822	11.225701
	30	C	-3.274060	1.446646	0.882900
	31	H	-2.972091	1.189624	-0.127543
	32	H	-2.787088	2.292100	1.362102
	33	C	-4.705083	-0.556862	0.940714

34	C	-5.837586	-1.015887	0.256615
35	C	-3.657562	-1.468079	1.154778
36	C	-5.932484	-2.342383	-0.174416
37	H	-6.667565	-0.345614	0.063142
38	C	-3.747290	-2.791462	0.729120
39	H	-2.756928	-1.130360	1.661103
40	C	-4.891699	-3.238201	0.063937
41	H	-6.826370	-2.671759	-0.698153
42	H	-2.921998	-3.474401	0.914397
43	H	-4.966537	-4.269966	-0.268922
44	C	-6.769251	1.385874	3.879733
45	C	-6.652490	2.785445	3.952629
46	C	-8.054389	0.858944	3.700551
47	C	-7.763716	3.618790	3.856943
48	H	-5.674802	3.238854	4.091869
49	C	-9.174264	1.688653	3.603245
50	H	-8.201856	-0.212958	3.647907
51	C	-9.037635	3.072687	3.682536
52	H	-7.634794	4.696564	3.918169
53	H	-10.157535	1.243977	3.473587
54	H	-9.908423	3.718572	3.609346
55	C	-6.839572	0.231916	7.059322
56	C	-7.647650	-0.789911	7.604288
57	C	-7.406405	1.524291	6.985142
58	C	-8.950589	-0.535789	8.032404
59	H	-7.260531	-1.799597	7.685218
60	C	-8.703229	1.777797	7.412395
61	H	-6.822647	2.342329	6.581158
62	C	-9.488951	0.747978	7.940584
63	H	-9.547284	-1.349188	8.438098
64	H	-9.105047	2.783918	7.327515
65	H	-10.504613	0.944987	8.272757
66	C	-3.877554	-0.541079	10.088170
67	C	-2.600432	-0.938991	9.623211
68	C	-4.405884	-1.256393	11.188042
69	C	-1.907475	-1.990561	10.209833
70	H	-2.137765	-0.405811	8.799065
71	C	-3.709896	-2.311194	11.774228
72	H	-5.382099	-0.993872	11.580607

	73	C	-2.456707	-2.689680	11.290290
	74	H	-0.927449	-2.264555	9.827027
	75	H	-4.152338	-2.841984	12.613601
	76	H	-1.912951	-3.511259	11.748338

R7	Number	Atom	x (Å)	y (Å)	z (Å)
product	1	C	0.143993	1.425631	-4.182311
	2	C	1.306453	0.591152	-3.587319
	3	H	0.131339	2.422986	-3.735573
	4	H	0.269255	1.537427	-5.264486
	5	H	-0.833187	0.973528	-3.987105
	6	C	1.220405	0.509801	-2.019676
	7	H	2.029627	-0.153221	-1.695065
	8	H	1.493524	1.498680	-1.634567
	9	C	-0.070099	0.035530	-1.277786
	10	C	-0.493183	-1.352791	-1.785346
	11	C	0.351786	-0.065528	0.252331
	12	H	0.361817	-2.035732	-1.787387
	13	H	-1.269618	-1.791473	-1.153633
	14	H	-0.873700	-1.309422	-2.807805
	15	H	1.325065	-0.572657	0.281087
	16	H	0.529723	0.950105	0.617446
	17	C	-0.560119	-0.813829	1.187421
	18	C	-0.323447	-2.296434	1.323812
	19	C	1.590567	2.389425	2.663921
	20	H	0.419439	-2.647052	0.603575
	21	H	0.052678	-2.547692	2.324917
	22	H	-1.238957	-2.883457	1.166241
	23	H	2.263860	2.106502	1.861238
	24	H	1.238057	3.416566	2.649743
	25	C	1.188427	1.535086	3.619529
	26	C	0.207503	1.992456	4.675015
	27	H	0.003972	3.062682	4.580955
	28	H	-0.749973	1.468811	4.576950
	29	H	0.590542	1.800165	5.685007
	30	C	2.588925	1.320666	-3.910722
	31	H	3.100109	1.137239	-4.850380
	32	H	2.868370	2.204297	-3.342356
	33	C	1.397201	-0.810367	-4.221191

34	C	0.458339	-1.303219	-5.135381
35	C	2.483693	-1.638582	-3.893936
36	C	0.584827	-2.582595	-5.683898
37	H	-0.393831	-0.697360	-5.423110
38	C	2.614746	-2.915612	-4.435705
39	H	3.243270	-1.270804	-3.208731
40	C	1.659898	-3.397643	-5.334107
41	H	-0.163655	-2.938910	-6.387202
42	H	3.465510	-3.533424	-4.159259
43	H	1.757283	-4.393170	-5.758834
44	C	-1.213026	1.059308	-1.370859
45	C	-0.962645	2.432533	-1.196102
46	C	-2.548398	0.670423	-1.539736
47	C	-1.992366	3.370726	-1.193191
48	H	0.053461	2.781945	-1.040971
49	C	-3.586899	1.605442	-1.532698
50	H	-2.798368	-0.376006	-1.667959
51	C	-3.316999	2.960860	-1.360157
52	H	-1.759006	4.423549	-1.055072
53	H	-4.611634	1.265005	-1.657183
54	H	-4.124160	3.688265	-1.353559
55	C	-1.550264	-0.180983	2.002989
56	C	-2.285305	-0.923203	2.975903
57	C	-1.853963	1.207990	1.912238
58	C	-3.246821	-0.323201	3.778538
59	H	-2.087095	-1.981360	3.105001
60	C	-2.826155	1.795763	2.707568
61	H	-1.326303	1.825670	1.200591
62	C	-3.534419	1.041339	3.651532
63	H	-3.781468	-0.924361	4.510314
64	H	-3.032206	2.857064	2.592759
65	H	-4.292673	1.506213	4.275529
66	C	1.659767	0.125090	3.689205
67	C	2.786757	-0.320676	2.971513
68	C	0.997111	-0.813785	4.500275
69	C	3.220198	-1.641302	3.048194
70	H	3.347418	0.379286	2.360379
71	C	1.435961	-2.135678	4.586806
72	H	0.112971	-0.521650	5.054649

	73	C	2.548963	-2.559013	3.860642
	74	H	4.094983	-1.952078	2.482737
	75	H	0.899864	-2.836180	5.222120
	76	H	2.891903	-3.587911	3.927507

R9/R10	Number	Atom	x (Å)	y (Å)	z (Å)
reactant	1	C	3.212250	-2.123243	0.229262
	2	C	2.401453	-1.196940	-0.421150
	3	C	1.901503	-0.064457	0.241527
	4	C	2.276564	0.115955	1.579757
	5	C	3.094365	-0.806428	2.236954
	6	C	3.563168	-1.934770	1.567586
	7	C	0.025589	0.342503	-1.509934
	8	C	1.047124	0.970918	-0.505061
	9	C	0.350822	1.953556	0.452974
	10	C	4.185409	5.816518	0.717021
	11	C	4.219494	4.485684	0.324364
	12	C	3.125987	3.875961	-0.361366
	13	C	2.001216	4.715910	-0.617569
	14	C	1.977124	6.045738	-0.223313
	15	C	3.066541	6.613576	0.448619
	16	C	2.031126	1.806618	-1.438690
	17	C	3.182350	2.502786	-0.764035
	18	C	4.442613	1.708293	-0.533521
	19	C	-0.382522	-4.184352	-0.204306
	20	C	-0.776247	-3.064783	-0.942138
	21	C	-0.847563	-1.792615	-0.360725
	22	C	-0.509055	-1.694966	0.998913
	23	C	-0.104180	-2.801086	1.738511
	24	C	-0.039435	-4.059833	1.139333
	25	C	-1.241074	-0.539919	-1.166946
	26	C	-2.306056	0.318192	-0.408347
	27	C	-1.779380	-0.920640	-2.565708
	28	H	3.562039	-3.000084	-0.309011
	29	H	2.134393	-1.379760	-1.456462
	30	H	1.928181	0.981420	2.131743
	31	H	3.360549	-0.638347	3.277642
	32	H	4.191611	-2.658665	2.079300
	33	H	-0.362245	1.186882	-2.096022

34	H	0.606702	-0.252664	-2.222676
35	H	1.070460	2.597511	0.963547
36	H	-0.329893	2.605585	-0.103727
37	H	-0.235051	1.437094	1.216412
38	H	5.039397	6.239826	1.240295
39	H	5.100563	3.897647	0.555784
40	H	1.137119	4.313990	-1.133533
41	H	1.099809	6.649947	-0.441321
42	H	3.043222	7.654980	0.756790
43	H	2.437815	1.107260	-2.180685
44	H	1.415888	2.519769	-1.998768
45	H	4.368921	0.710845	-0.971039
46	H	5.320071	2.207480	-0.968937
47	H	4.651054	1.565435	0.535919
48	H	-0.349627	-5.156870	-0.689081
49	H	-1.041706	-3.208842	-1.982620
50	H	-0.542007	-0.733167	1.496002
51	H	0.170379	-2.674694	2.782119
52	H	0.273389	-4.928481	1.712685
53	H	-1.970909	0.440202	0.621695
54	H	-2.290324	1.327098	-0.840848
55	H	-2.098008	-0.021453	-3.102904
56	H	-1.005524	-1.401051	-3.173572
57	C	-3.830038	-0.091164	-0.328758
58	C	-4.601699	0.397581	-1.587083
59	C	-3.658521	-2.130055	1.170660
60	C	-4.035956	-1.592106	-0.069371
61	C	-4.585452	-2.465089	-1.016526
62	C	-4.717781	-3.830820	-0.750262
63	C	-4.309108	-4.351113	0.475882
64	C	-3.781551	-3.489981	1.440429
65	H	-3.239158	-1.471517	1.924781
66	H	-4.917074	-2.090692	-1.979170
67	H	-5.142525	-4.485183	-1.507466
68	H	-4.402337	-5.414280	0.680925
69	H	-3.452980	-3.878855	2.400196
70	C	-4.412520	0.682100	0.830524
71	H	-5.355787	0.370772	1.268844
72	H	-4.056769	1.687124	1.043845

	73	H	-4.257711	-0.069690	-2.512508
	74	H	-5.672206	0.191510	-1.482194
	75	H	-4.476637	1.480118	-1.696379
	76	H	-2.626223	-1.605067	-2.501322

R9	Number	Atom	x (Å)	y (Å)	z (Å)
TS	1	C	3.991812	-2.283768	-0.027042
	2	C	2.994305	-1.573575	-0.683492
	3	C	2.461500	-0.378891	-0.150040
	4	C	2.995442	0.062409	1.080795
	5	C	3.997058	-0.650010	1.738771
	6	C	4.506114	-1.827740	1.190718
	7	C	0.587815	-0.235983	-1.932682
	8	C	1.443823	0.416426	-0.859666
	9	C	0.802754	1.555531	-0.093249
	10	C	4.929472	4.596389	1.003651
	11	C	4.886534	3.441135	0.227254
	12	C	3.894486	3.253138	-0.764013
	13	C	2.961525	4.304275	-0.941500
	14	C	3.007732	5.456917	-0.166611
	15	C	3.990744	5.613033	0.816555
	16	C	2.700230	1.598571	-2.213286
	17	C	3.853489	2.027973	-1.562466
	18	C	5.059449	1.119927	-1.553579
	19	C	0.238522	-4.694512	-0.401269
	20	C	-0.182359	-3.636787	-1.211527
	21	C	-0.266440	-2.328123	-0.719108
	22	C	0.087582	-2.127314	0.625765
	23	C	0.519030	-3.172543	1.435993
	24	C	0.596606	-4.469128	0.925737
	25	C	-0.679660	-1.139023	-1.603398
	26	C	-1.769555	-0.260365	-0.912606
	27	C	-1.162357	-1.598860	-2.994877
	28	H	4.365499	-3.205578	-0.465183
	29	H	2.604015	-1.974231	-1.611848
	30	H	2.630291	0.976418	1.534379
	31	H	4.380294	-0.278701	2.686194
	32	H	5.284392	-2.385398	1.704462
	33	H	0.212943	0.565167	-2.583895

34	H	1.229226	-0.853753	-2.568991
35	H	1.541992	2.287200	0.243111
36	H	0.078102	2.084756	-0.719089
37	H	0.268107	1.202553	0.800173
38	H	5.700191	4.700934	1.763343
39	H	5.618111	2.661210	0.408511
40	H	2.200112	4.221438	-1.710483
41	H	2.277235	6.244318	-0.334998
42	H	4.026187	6.514898	1.421381
43	H	2.798779	0.803184	-2.946590
44	H	1.887593	2.290680	-2.412607
45	H	4.957584	0.328725	-2.300930
46	H	5.981148	1.677445	-1.764308
47	H	5.189308	0.623418	-0.583026
48	H	0.280745	-5.698658	-0.815682
49	H	-0.461291	-3.856711	-2.235098
50	H	0.046730	-1.132053	1.052214
51	H	0.804466	-2.968951	2.464559
52	H	0.930373	-5.290436	1.554368
53	H	-1.439939	-0.057856	0.107607
54	H	-1.777923	0.715555	-1.415841
55	H	-1.481497	-0.733996	-3.585781
56	H	-0.357849	-2.092140	-3.551118
57	C	-3.280832	-0.707948	-0.815946
58	C	-4.052380	-0.319615	-2.108877
59	C	-3.070266	-2.646208	0.805882
60	C	-3.441754	-2.196465	-0.470702
61	C	-3.942363	-3.142462	-1.373435
62	C	-4.034326	-4.493666	-1.027663
63	C	-3.633818	-4.925490	0.234971
64	C	-3.154589	-3.990882	1.155390
65	H	-2.686402	-1.929673	1.525492
66	H	-4.268054	-2.837484	-2.362256
67	H	-4.421798	-5.206323	-1.751524
68	H	-3.696083	-5.977103	0.501946
69	H	-2.832538	-4.310259	2.142590
70	C	-3.896680	0.114992	0.290088
71	H	-4.829404	-0.202118	0.746310
72	H	-3.576934	1.143090	0.441194

	73	H	-3.676448	-0.823384	-3.002520
	74	H	-5.115637	-0.561180	-2.006368
	75	H	-3.967009	0.759208	-2.276711
	76	H	-1.997876	-2.297218	-2.926096

R9	Number	Atom	x (Å)	y (Å)	z (Å)
product	1	C	3.602851	-1.014721	1.148568
	2	C	2.423771	-0.426440	0.714578
	3	C	1.778769	0.596644	1.469375
	4	C	2.402959	0.964613	2.696481
	5	C	3.588059	0.375693	3.118992
	6	C	4.204922	-0.617675	2.350097
	7	C	0.020655	1.025595	-0.352433
	8	C	0.582666	1.246050	1.023024
	9	C	-0.056557	2.301429	1.887073
	10	C	2.960442	3.990726	0.483261
	11	C	3.381529	2.882380	-0.251269
	12	C	2.886161	2.637722	-1.543359
	13	C	1.972649	3.562882	-2.081905
	14	C	1.549288	4.668937	-1.348969
	15	C	2.039895	4.887825	-0.058652
	16	C	2.512188	0.856221	-3.221744
	17	C	3.309024	1.433529	-2.307131
	18	C	4.671089	0.854953	-1.997323
	19	C	-0.093694	-3.668774	-0.649081
	20	C	-0.532722	-2.408452	-1.062854
	21	C	-0.769220	-1.378850	-0.142587
	22	C	-0.542533	-1.667425	1.214356
	23	C	-0.094809	-2.916802	1.632848
	24	C	0.131824	-3.930356	0.700501
	25	C	-1.198482	0.032296	-0.576877
	26	C	-2.416654	0.550443	0.244678
	27	C	-1.478379	0.114205	-2.089698
	28	H	4.056343	-1.798679	0.547013
	29	H	1.980244	-0.772997	-0.210516
	30	H	1.956339	1.735771	3.314436
	31	H	4.037292	0.692957	4.057109
	32	H	5.130043	-1.079550	2.683350
	33	H	-0.301148	2.002364	-0.740116

34	H	0.813265	0.690620	-1.025004
35	H	0.628211	3.146926	2.049077
36	H	-0.958416	2.705161	1.422233
37	H	-0.335991	1.920727	2.879876
38	H	3.346409	4.141429	1.487903
39	H	4.071807	2.183293	0.207125
40	H	1.607420	3.422997	-3.095006
41	H	0.845124	5.369405	-1.790721
42	H	1.713175	5.752717	0.512646
43	H	2.839482	-0.013161	-3.785076
44	H	1.508264	1.214796	-3.428337
45	H	4.938039	0.071623	-2.712801
46	H	5.446883	1.629658	-2.021430
47	H	4.686966	0.409987	-0.995167
48	H	0.066965	-4.446986	-1.390961
49	H	-0.705166	-2.247329	-2.120264
50	H	-0.701652	-0.898453	1.961754
51	H	0.080819	-3.096061	2.690401
52	H	0.477659	-4.909041	1.022668
53	H	-2.186136	0.411277	1.304413
54	H	-2.471620	1.637341	0.098642
55	H	-1.811674	1.123587	-2.352944
56	H	-0.570587	-0.090465	-2.667941
57	C	-3.882114	0.013164	0.010419
58	C	-4.567762	0.801374	-1.142113
59	C	-3.645825	-2.370106	0.846273
60	C	-3.933130	-1.504859	-0.220647
61	C	-4.249916	-2.079996	-1.457413
62	C	-4.246188	-3.466763	-1.632046
63	C	-3.932082	-4.308776	-0.567510
64	C	-3.635662	-3.751872	0.678386
65	H	-3.402914	-1.947106	1.816218
66	H	-4.503473	-1.452018	-2.304630
67	H	-4.490889	-3.884498	-2.605513
68	H	-3.919659	-5.386865	-0.704051
69	H	-3.381945	-4.393172	1.517858
70	C	-4.665599	0.343090	1.257279
71	H	-5.596794	-0.174523	1.466380
72	H	-4.463423	1.267440	1.792681

	73	H	-4.061720	0.682673	-2.103518
	74	H	-5.606701	0.476843	-1.263174
	75	H	-4.574501	1.869852	-0.902214
	76	H	-2.245225	-0.595863	-2.404863

R11/R12	Number	Atom	x (Å)	y (Å)	z (Å)
reactant	1	C	-0.618035	-1.053763	0.481761
	2	C	0.933069	-1.084391	0.682721
	3	H	-0.831399	-1.677618	-0.393710
	4	H	-1.068587	-1.588854	1.324541
	5	C	1.327093	-2.619399	0.568004
	6	C	2.783310	-2.957549	0.745427
	7	H	0.745965	-3.164925	1.323075
	8	H	0.961679	-2.968698	-0.403614
	9	C	-1.425000	0.286391	0.315728
	10	C	-2.929389	-0.170622	0.338640
	11	C	-4.133537	0.833268	0.490665
	12	H	-3.103840	-0.744932	-0.577365
	13	H	-3.044544	-0.890030	1.160497
	14	C	-5.367469	0.084940	0.045061
	15	H	-6.264418	0.633041	-0.226368
	16	H	-5.461113	-0.977564	0.255401
	17	C	3.682640	-3.095030	-0.361016
	18	C	3.259674	-3.006678	-1.720872
	19	C	5.074592	-3.332709	-0.152330
	20	C	4.151192	-3.147824	-2.774107
	21	H	2.216518	-2.822482	-1.948490
	22	C	5.959774	-3.470232	-1.212666
	23	H	5.460765	-3.396620	0.858890
	24	C	5.511089	-3.381206	-2.535441
	25	H	3.784671	-3.074188	-3.795105
	26	H	7.013169	-3.646014	-1.008179
	27	H	6.206337	-3.489076	-3.363144
	28	C	1.347188	-0.598214	2.083005
	29	C	0.708221	-1.096678	3.231695
	30	C	2.403829	0.301375	2.279083
	31	C	1.096087	-0.709263	4.512476
	32	H	-0.105448	-1.809048	3.131869
	33	C	2.799472	0.693791	3.561050

34	H	2.934074	0.711005	1.427519
35	C	2.147924	0.192915	4.685987
36	H	0.576526	-1.115336	5.376786
37	H	3.622602	1.394879	3.674087
38	H	2.453622	0.497865	5.683124
39	C	-1.107267	0.938200	-1.046267
40	C	-1.249679	0.199583	-2.233432
41	C	-0.667280	2.261956	-1.166637
42	C	-0.957648	0.750379	-3.479184
43	H	-1.596512	-0.829350	-2.193395
44	C	-0.376836	2.822777	-2.411821
45	H	-0.557278	2.882641	-0.285799
46	C	-0.515152	2.070681	-3.576463
47	H	-1.077341	0.146165	-4.375134
48	H	-0.047351	3.857048	-2.465566
49	H	-0.287412	2.506206	-4.545663
50	C	-3.984200	2.088539	-0.381848
51	C	-3.784237	3.368625	0.147898
52	C	-4.055858	1.962499	-1.778532
53	C	-3.635806	4.480708	-0.686480
54	H	-3.741626	3.516681	1.221648
55	C	-3.904987	3.064822	-2.614289
56	H	-4.211992	0.979305	-2.212123
57	C	-3.691556	4.333915	-2.070469
58	H	-3.478556	5.462508	-0.246739
59	H	-3.942136	2.931062	-3.691832
60	H	-3.570397	5.196429	-2.720473
61	C	3.294101	-3.143782	2.151265
62	H	3.964105	-2.327376	2.457975
63	H	2.474808	-3.160140	2.872588
64	H	3.858448	-4.080305	2.257910
65	C	1.656464	-0.315251	-0.434546
66	H	1.295000	-0.640163	-1.413455
67	H	1.479333	0.760309	-0.371125
68	H	2.734632	-0.492157	-0.404231
69	C	-1.121899	1.230169	1.489468
70	H	-1.350582	0.739875	2.440184
71	H	-0.066917	1.510508	1.520206
72	H	-1.711477	2.146278	1.422374

	73	C	-4.370290	1.180966	1.987892
	74	H	-5.256790	1.814573	2.097281
	75	H	-4.543414	0.260061	2.554630
	76	H	-3.525117	1.697007	2.449298

R11	Number	Atom	x (Å)	y (Å)	z (Å)
TS	1	C	-2.527886	0.717060	-0.193293
	2	C	-1.020036	0.842770	-0.050517
	3	H	-2.741101	0.070039	-1.051918
	4	H	-2.937806	0.192164	0.675502
	5	C	-0.547782	-1.326333	-0.160125
	6	C	0.795864	-1.552405	0.099471
	7	H	-1.268920	-1.567556	0.615287
	8	H	-0.936298	-1.383252	-1.171572
	9	C	-3.385465	2.038583	-0.364720
	10	C	-4.873551	1.546733	-0.354486
	11	C	-6.096152	2.530127	-0.208799
	12	H	-5.030626	0.971906	-1.273131
	13	H	-4.977978	0.821854	0.464381
	14	C	-7.312945	1.769095	-0.677682
	15	H	-8.209254	2.306487	-0.971453
	16	H	-7.399665	0.706240	-0.466068
	17	C	1.821022	-1.523089	-0.946662
	18	C	1.501025	-1.561311	-2.326102
	19	C	3.194937	-1.461972	-0.615091
	20	C	2.486916	-1.527839	-3.304166
	21	H	0.463742	-1.625915	-2.637250
	22	C	4.182078	-1.428425	-1.597363
	23	H	3.496454	-1.425363	0.425968
	24	C	3.838679	-1.459199	-2.949738
	25	H	2.200603	-1.559867	-4.352474
	26	H	5.227080	-1.374831	-1.302134
	27	H	4.608595	-1.433606	-3.715911
	28	C	-0.448624	1.178669	1.264181
	29	C	-1.074114	0.803296	2.476320
	30	C	0.796929	1.837470	1.372275
	31	C	-0.492542	1.064592	3.711474
	32	H	-2.025381	0.281987	2.453098
	33	C	1.378296	2.102382	2.611596

34	H	1.318632	2.153222	0.476557
35	C	0.742225	1.716471	3.791837
36	H	-1.003737	0.754024	4.619402
37	H	2.336089	2.615413	2.651784
38	H	1.196442	1.920627	4.757430
39	C	-3.050502	2.697588	-1.715793
40	C	-3.193702	1.970241	-2.910128
41	C	-2.580089	4.011946	-1.819635
42	C	-2.876547	2.524141	-4.147795
43	H	-3.559260	0.947411	-2.880456
44	C	-2.265087	4.576474	-3.057772
45	H	-2.466585	4.622824	-0.932459
46	C	-2.406618	3.836299	-4.229458
47	H	-2.997596	1.929425	-5.049853
48	H	-1.912727	5.603741	-3.099992
49	H	-2.159483	4.274530	-5.192661
50	C	-5.948255	3.795527	-1.066829
51	C	-5.763649	5.071574	-0.521926
52	C	-5.999699	3.683086	-2.465430
53	C	-5.608998	6.192478	-1.343171
54	H	-5.738092	5.209616	0.553680
55	C	-5.842414	4.794259	-3.288414
56	H	-6.144562	2.703434	-2.910785
57	C	-5.643020	6.058844	-2.729263
58	H	-5.463558	7.170734	-0.891690
59	H	-5.863385	4.670772	-4.367622
60	H	-5.516296	6.928197	-3.368980
61	C	1.235909	-1.708045	1.535696
62	H	1.791923	-0.828501	1.885992
63	H	0.374839	-1.820267	2.198873
64	H	1.887015	-2.582325	1.665735
65	C	-0.269759	1.312905	-1.275366
66	H	-0.730924	0.924288	-2.186659
67	H	-0.279549	2.407719	-1.362632
68	H	0.772543	0.982967	-1.260799
69	C	-3.098622	2.972592	0.820327
70	H	-3.340576	2.473495	1.763570
71	H	-2.042101	3.247708	0.865429
72	H	-3.685580	3.890556	0.755364

	73	C	-6.354874	2.860421	1.288575
	74	H	-7.249177	3.483697	1.393420
	75	H	-6.525175	1.932213	1.844183
	76	H	-5.520596	3.380803	1.764870

R11	Number	Atom	x (Å)	y (Å)	z (Å)
product	1	C	0.641326	-0.370200	0.180276
	2	C	1.940726	0.325560	0.471175
	3	H	0.742690	-0.920171	-0.760329
	4	H	0.435469	-1.126351	0.938514
	5	C	-0.075458	-3.793251	2.126556
	6	C	1.198087	-3.807729	1.698427
	7	H	-0.324009	-4.009009	3.161973
	8	H	-0.907012	-3.553515	1.470260
	9	C	-0.651130	0.533220	0.086461
	10	C	-1.824265	-0.479412	-0.126874
	11	C	-3.337198	-0.066645	0.009856
	12	H	-1.694626	-0.920851	-1.120248
	13	H	-1.674393	-1.307408	0.579335
	14	C	-4.139628	-1.138505	-0.686512
	15	H	-5.158475	-0.937142	-1.002697
	16	H	-3.816487	-2.175188	-0.630507
	17	C	1.545931	-3.526989	0.280317
	18	C	0.649382	-3.821024	-0.763354
	19	C	2.767155	-2.917115	-0.054488
	20	C	0.941212	-3.479196	-2.081669
	21	H	-0.281448	-4.332735	-0.537936
	22	C	3.060212	-2.572178	-1.374062
	23	H	3.479256	-2.667053	0.724540
	24	C	2.146705	-2.843061	-2.393368
	25	H	0.230195	-3.716476	-2.868848
	26	H	4.000171	-2.076960	-1.601450
	27	H	2.374569	-2.572439	-3.420769
	28	C	2.511144	0.358413	1.784776
	29	C	1.984500	-0.397369	2.876090
	30	C	3.662397	1.152015	2.072050
	31	C	2.571857	-0.369663	4.133281
	32	H	1.119578	-1.032758	2.726667
	33	C	4.236874	1.179399	3.335640

34	H	4.093363	1.769129	1.291264
35	C	3.703349	0.417562	4.381566
36	H	2.142592	-0.969828	4.932189
37	H	5.109455	1.804291	3.510621
38	H	4.156910	0.438297	5.368440
39	C	-0.511633	1.476209	-1.120852
40	C	-0.306306	0.943604	-2.406455
41	C	-0.548401	2.870046	-1.002673
42	C	-0.150622	1.763175	-3.521014
43	H	-0.258809	-0.133261	-2.543620
44	C	-0.398538	3.698634	-2.117906
45	H	-0.715472	3.331254	-0.036814
46	C	-0.197556	3.152320	-3.383214
47	H	0.007813	1.315931	-4.499383
48	H	-0.446611	4.777009	-1.990197
49	H	-0.080591	3.796710	-4.250507
50	C	-3.641173	1.286142	-0.649611
51	C	-3.988407	2.430782	0.077388
52	C	-3.566217	1.396929	-2.047259
53	C	-4.227688	3.649293	-0.564938
54	H	-4.076169	2.387784	1.157689
55	C	-3.798547	2.607952	-2.692177
56	H	-3.298150	0.521908	-2.631585
57	C	-4.129651	3.744962	-1.951219
58	H	-4.492375	4.522816	0.025788
59	H	-3.708550	2.666988	-3.773297
60	H	-4.308300	4.693268	-2.451159
61	C	2.334898	-4.054291	2.664424
62	H	2.889253	-3.127257	2.857351
63	H	1.961237	-4.418041	3.626123
64	H	3.047253	-4.786264	2.266151
65	C	2.636643	1.006561	-0.677498
66	H	2.292247	0.602431	-1.632119
67	H	2.431373	2.087424	-0.705970
68	H	3.725288	0.881442	-0.631938
69	C	-0.789278	1.294198	1.413916
70	H	-0.880752	0.586095	2.243860
71	H	0.095982	1.906591	1.608925
72	H	-1.664093	1.947596	1.421238

	73	C	-3.774750	-0.107876	1.501581
	74	H	-4.843556	0.111794	1.595623
	75	H	-3.600049	-1.110701	1.905611
	76	H	-3.225514	0.598904	2.128219

R13/R14	Number	Atom	x (Å)	y (Å)	z (Å)
reactant	1	C	-2.751769	2.992569	0.488019
	2	C	-1.307044	2.633294	0.254641
	3	C	-0.937977	1.083203	0.245720
	4	H	-0.934213	3.065981	-0.680736
	5	H	-0.715844	3.091269	1.058445
	6	C	0.623831	1.034179	0.306385
	7	H	1.016301	1.475221	-0.616029
	8	H	0.922458	1.733367	1.094128
	9	C	1.411985	-0.307465	0.541350
	10	C	2.902408	0.081245	0.219305
	11	C	4.139768	-0.853297	0.487288
	12	H	2.926883	0.326043	-0.850326
	13	H	3.121806	1.020801	0.745421
	14	C	5.324483	-0.153347	-0.136220
	15	H	6.224610	-0.716179	-0.364138
	16	H	5.395304	0.930706	-0.102638
	17	C	-3.703812	3.175469	-0.564793
	18	C	-5.072542	3.459723	-0.276665
	19	C	-3.356192	3.092774	-1.944059
	20	C	-6.010940	3.626636	-1.285957
	21	H	-5.399855	3.539596	0.754145
	22	C	-4.300863	3.257352	-2.945467
	23	H	-2.335543	2.875445	-2.227663
	24	C	-5.638942	3.524523	-2.631371
	25	H	-7.045184	3.836116	-1.023371
	26	H	-3.992189	3.171537	-3.984271
	27	H	-6.376837	3.650604	-3.418799
	28	C	-1.503962	0.486183	-1.053945
	29	C	-2.683279	-0.269811	-1.071124
	30	C	-0.897697	0.754324	-2.293946
	31	C	-3.234000	-0.736704	-2.267049
	32	H	-3.196002	-0.500370	-0.144954
	33	C	-1.438207	0.288021	-3.490267

34	H	0.009579	1.349038	-2.336794
35	C	-2.616167	-0.461652	-3.484457
36	H	-4.154765	-1.313633	-2.240416
37	H	-0.938987	0.514779	-4.429062
38	H	-3.043949	-0.823746	-4.415344
39	C	1.296251	-0.765410	2.005078
40	C	1.566318	0.127996	3.056122
41	C	0.972139	-2.084033	2.352161
42	C	1.520593	-0.274557	4.388867
43	H	1.840734	1.155286	2.835442
44	C	0.926495	-2.495733	3.687053
45	H	0.762003	-2.812451	1.578460
46	C	1.200547	-1.594438	4.714265
47	H	1.741303	0.443260	5.174886
48	H	0.674315	-3.527475	3.919078
49	H	1.165853	-1.913120	5.752520
50	C	3.972087	-2.225280	-0.180578
51	C	3.742444	-3.402165	0.543566
52	C	4.013801	-2.314598	-1.581400
53	C	3.537583	-4.620511	-0.109753
54	H	3.699502	-3.377586	1.626102
55	C	3.810028	-3.526622	-2.237429
56	H	4.199050	-1.414401	-2.161752
57	C	3.565599	-4.688994	-1.502180
58	H	3.355446	-5.517847	0.476434
59	H	3.840102	-3.563921	-3.323451
60	H	3.403496	-5.636239	-2.009589
61	C	-3.184478	3.191860	1.920317
62	H	-3.983005	2.498219	2.220848
63	H	-2.351722	3.041113	2.612021
64	H	-3.575335	4.206518	2.087335
65	C	-1.537487	0.422248	1.498765
66	H	-1.347705	-0.653270	1.517620
67	H	-1.090305	0.847036	2.401882
68	H	-2.617270	0.576333	1.558481
69	C	0.914644	-1.381380	-0.444829
70	H	-0.144225	-1.603028	-0.291409
71	H	1.024175	-1.025645	-1.472565
72	H	1.473929	-2.311746	-0.362256

	73	C	4.470269	-0.981621	1.999640
	74	H	4.601000	0.013848	2.435725
	75	H	3.688548	-1.486008	2.569257
	76	H	5.405593	-1.537011	2.129437

R13	Number	Atom	x (Å)	y (Å)	z (Å)
TS	1	C	-3.083508	0.228076	-0.034599
	2	C	-1.792332	-0.051328	-0.463524
	3	C	-1.362350	-2.234428	-0.357821
	4	H	-1.535428	-0.012816	-1.515989
	5	H	-0.976346	0.204673	0.205976
	6	C	0.151293	-2.145016	-0.243972
	7	H	0.568340	-1.710760	-1.158493
	8	H	0.395783	-1.434081	0.551488
	9	C	0.961828	-3.475754	0.039599
	10	C	2.460645	-3.058386	-0.164344
	11	C	3.684991	-3.983681	0.184881
	12	H	2.561518	-2.797493	-1.225730
	13	H	2.626209	-2.123794	0.389856
	14	C	4.905844	-3.268683	-0.343577
	15	H	5.821224	-3.823727	-0.524721
	16	H	4.969684	-2.185476	-0.280884
	17	C	-4.247403	0.173664	-0.919776
	18	C	-5.549273	0.429235	-0.426923
	19	C	-4.136044	-0.137810	-2.296475
	20	C	-6.666841	0.371659	-1.255957
	21	H	-5.693420	0.675375	0.619511
	22	C	-5.252702	-0.198708	-3.119867
	23	H	-3.167850	-0.362105	-2.726350
	24	C	-6.529583	0.055345	-2.608827
	25	H	-7.651205	0.573062	-0.840500
	26	H	-5.124278	-0.458517	-4.167241
	27	H	-7.402152	0.005611	-3.254617
	28	C	-1.957817	-2.669896	-1.631469
	29	C	-3.201485	-3.339420	-1.673943
	30	C	-1.346964	-2.389229	-2.878403
	31	C	-3.799080	-3.696151	-2.880588
	32	H	-3.712565	-3.587634	-0.751331
	33	C	-1.947759	-2.738565	-4.082170

34	H	-0.393973	-1.870960	-2.907703
35	C	-3.183367	-3.394764	-4.095336
36	H	-4.758818	-4.206166	-2.868496
37	H	-1.449525	-2.497367	-5.017982
38	H	-3.652826	-3.667689	-5.036314
39	C	0.722192	-3.946272	1.481453
40	C	0.909353	-3.061917	2.558283
41	C	0.346875	-5.261161	1.787660
42	C	0.732615	-3.469315	3.878224
43	H	1.219472	-2.038686	2.367580
44	C	0.170674	-5.677860	3.110415
45	H	0.197803	-5.981919	0.992951
46	C	0.360772	-4.785175	4.163583
47	H	0.890016	-2.759054	4.685989
48	H	-0.117937	-6.706355	3.312319
49	H	0.222953	-5.107646	5.192053
50	C	3.575054	-5.351329	-0.502376
51	C	3.289109	-6.532355	0.194480
52	C	3.727668	-5.432067	-1.895904
53	C	3.136873	-7.746775	-0.480020
54	H	3.159632	-6.513406	1.270251
55	C	3.576445	-6.640196	-2.573057
56	H	3.957500	-4.528129	-2.454169
57	C	3.274865	-7.806789	-1.866317
58	H	2.908805	-8.647433	0.084576
59	H	3.692203	-6.671217	-3.653498
60	H	3.153422	-8.750904	-2.390615
61	C	-3.303837	0.524687	1.431236
62	H	-3.979368	-0.199719	1.905679
63	H	-2.358781	0.501290	1.981039
64	H	-3.750796	1.517707	1.578253
65	C	-2.088885	-2.607967	0.913393
66	H	-2.042317	-3.689380	1.101893
67	H	-1.635598	-2.117599	1.778909
68	H	-3.142259	-2.316612	0.873640
69	C	0.540701	-4.532961	-0.998198
70	H	-0.524511	-4.764008	-0.914419
71	H	0.709140	-4.150709	-2.009229
72	H	1.101100	-5.461442	-0.903151

	73	C	3.902417	-4.121534	1.716794
	74	H	3.994883	-3.128622	2.168438
	75	H	3.083043	-4.633897	2.223119
	76	H	4.828221	-4.673490	1.912382

R13	Number	Atom	x (Å)	y (Å)	z (Å)
product	1	C	0.740430	3.049871	-2.030256
	2	C	0.752586	2.195212	-3.066882
	3	C	-2.470642	-0.792729	0.380233
	4	H	-0.101326	1.578143	-3.328255
	5	H	1.637849	2.074540	-3.684858
	6	C	-1.290851	0.090940	0.671406
	7	H	-1.129439	0.794647	-0.145690
	8	H	-1.524197	0.711655	1.544421
	9	C	0.095479	-0.631388	0.943248
	10	C	1.128988	0.538382	1.022109
	11	C	2.666942	0.315520	1.246133
	12	H	1.023614	1.100702	0.089603
	13	H	0.800167	1.228608	1.808941
	14	C	3.279719	1.694988	1.318311
	15	H	4.311772	1.853104	1.021561
	16	H	2.799569	2.464609	1.918602
	17	C	-0.465183	3.237912	-1.179482
	18	C	-0.344001	3.650381	0.159702
	19	C	-1.759071	2.983558	-1.671319
	20	C	-1.463828	3.761859	0.983313
	21	H	0.636835	3.856244	0.574998
	22	C	-2.877268	3.085736	-0.847632
	23	H	-1.892549	2.701538	-2.710663
	24	C	-2.735142	3.471689	0.487108
	25	H	-1.339384	4.068666	2.018664
	26	H	-3.860757	2.862028	-1.250895
	27	H	-3.607050	3.550794	1.130489
	28	C	-2.916350	-1.050797	-0.955345
	29	C	-4.031122	-1.903417	-1.213305
	30	C	-2.285686	-0.480738	-2.101917
	31	C	-4.478665	-2.151117	-2.504074
	32	H	-4.543377	-2.379545	-0.384401
	33	C	-2.740577	-0.732898	-3.387287

34	H	-1.426759	0.164858	-1.973455
35	C	-3.843456	-1.568194	-3.606747
36	H	-5.331722	-2.808284	-2.655479
37	H	-2.228712	-0.277622	-4.232399
38	H	-4.196310	-1.764372	-4.615284
39	C	-0.010755	-1.406161	2.264351
40	C	-0.250650	-0.719978	3.468414
41	C	0.086841	-2.802187	2.330183
42	C	-0.376469	-1.392506	4.681180
43	H	-0.340319	0.362662	3.461493
44	C	-0.038583	-3.484239	3.544636
45	H	0.264633	-3.377224	1.428986
46	C	-0.269392	-2.784876	4.727015
47	H	-0.558447	-0.828791	5.592823
48	H	0.043961	-4.568180	3.559243
49	H	-0.366700	-3.313812	5.671256
50	C	3.317328	-0.430549	0.069129
51	C	3.992700	-1.648600	0.213801
52	C	3.247293	0.129367	-1.217064
53	C	4.559870	-2.294808	-0.888885
54	H	4.074508	-2.116123	1.188616
55	C	3.807305	-0.512004	-2.318977
56	H	2.728742	1.071087	-1.361399
57	C	4.467217	-1.733105	-2.161042
58	H	5.074082	-3.242137	-0.747211
59	H	3.725481	-0.057838	-3.303581
60	H	4.904498	-2.237662	-3.018522
61	C	1.988256	3.819516	-1.657613
62	H	2.428369	3.430852	-0.728607
63	H	2.750000	3.735340	-2.438119
64	H	1.770266	4.881643	-1.495040
65	C	-3.187008	-1.417938	1.549086
66	H	-3.041375	-2.507780	1.586499
67	H	-2.820008	-1.019919	2.497216
68	H	-4.271217	-1.243515	1.506033
69	C	0.404376	-1.548643	-0.252316
70	H	-0.412974	-2.253006	-0.431576
71	H	0.531093	-0.951954	-1.159854
72	H	1.326460	-2.114884	-0.110754

	73	C	2.952041	-0.373557	2.605410
	74	H	2.472124	0.184269	3.414465
	75	H	2.561333	-1.393775	2.640400
	76	H	4.029141	-0.403187	2.802269

R15/R16	Number	Atom	x (Å)	y (Å)	z (Å)
reactant	1	C	2.093528	-2.969500	-0.885995
	2	C	1.675666	-1.642732	-0.845895
	3	C	1.510260	-0.958656	0.370420
	4	C	1.802284	-1.660768	1.546526
	5	C	2.229945	-2.990021	1.513440
	6	C	2.376327	-3.653792	0.298082
	7	C	0.074195	0.914804	-0.709047
	8	C	1.118648	0.525344	0.389121
	9	C	0.650954	0.983554	1.782062
	10	C	5.836978	-1.439229	0.270936
	11	C	4.780662	-0.547078	0.167426
	12	C	4.612216	0.525048	1.091121
	13	C	5.603649	0.637768	2.111690
	14	C	6.659354	-0.258752	2.205902
	15	C	6.788216	-1.309173	1.290106
	16	C	2.421192	1.361264	-0.005436
	17	C	3.522927	1.450444	1.017684
	18	C	3.469386	2.611085	1.981780
	19	C	-1.557603	-3.172416	-2.254265
	20	C	-1.561391	-1.778404	-2.157059
	21	C	-1.474472	-1.128372	-0.917530
	22	C	-1.388290	-1.942471	0.223874
	23	C	-1.382868	-3.331842	0.135901
	24	C	-1.468193	-3.958565	-1.108055
	25	C	-1.419834	0.407866	-0.812550
	26	C	-2.250769	0.946824	0.394525
	27	C	-1.933106	1.076479	-2.111098
	28	H	2.188925	-3.471593	-1.844967
	29	H	1.456117	-1.143319	-1.782971
	30	H	1.706510	-1.175834	2.510957
	31	H	2.453808	-3.502129	2.445773
	32	H	2.703996	-4.689534	0.271048
	33	H	0.004642	2.010610	-0.676757

34	H	0.530936	0.690928	-1.679715
35	H	1.461795	0.939011	2.512271
36	H	0.298725	2.019862	1.744831
37	H	-0.163438	0.364462	2.163153
38	H	5.916489	-2.250517	-0.448169
39	H	4.059895	-0.693941	-0.625558
40	H	5.535576	1.435582	2.843269
41	H	7.390013	-0.140571	3.002566
42	H	7.612941	-2.012014	1.369333
43	H	2.791952	0.954912	-0.952862
44	H	2.084064	2.383243	-0.223953
45	H	2.589367	3.234493	1.802937
46	H	3.430055	2.288470	3.032266
47	H	4.356372	3.255307	1.888867
48	H	-1.626360	-3.639500	-3.233693
49	H	-1.632272	-1.202551	-3.072561
50	H	-1.296589	-1.493618	1.205816
51	H	-1.296568	-3.924182	1.042546
52	H	-1.461180	-5.042773	-1.180759
53	H	-1.981133	0.392056	1.293730
54	H	-1.916370	1.973356	0.581624
55	H	-1.988086	2.161095	-1.982233
56	H	-1.263938	0.880780	-2.955469
57	C	-3.817734	0.961457	0.373109
58	C	-4.397756	-0.427040	0.033024
59	C	-5.332369	1.825741	-1.545068
60	C	-4.391045	2.074770	-0.537407
61	C	-3.999742	3.409755	-0.331090
62	C	-4.504045	4.445710	-1.113603
63	C	-5.430655	4.176527	-2.124156
64	C	-5.843679	2.861852	-2.331428
65	H	-5.667586	0.813270	-1.740363
66	H	-3.291049	3.644366	0.458180
67	H	-4.175843	5.466029	-0.931520
68	H	-5.826498	4.982019	-2.736737
69	H	-6.566844	2.633787	-3.110526
70	C	-4.269701	1.318332	1.770096
71	H	-3.659680	1.953282	2.406570
72	H	-5.314019	1.188569	2.039602

	73	H	-4.153456	-0.745975	-0.983714
	74	H	-3.988738	-1.177195	0.713697
	75	H	-5.487861	-0.428201	0.145003
	76	H	-2.931949	0.731090	-2.384164

R15	Number	Atom	x (Å)	y (Å)	z (Å)
TS	1	C	3.039048	-4.405221	-1.419186
	2	C	2.540956	-3.109553	-1.388948
	3	C	2.339203	-2.419981	-0.169262
	4	C	2.671929	-3.112114	1.015621
	5	C	3.166414	-4.414149	0.984653
	6	C	3.357835	-5.071369	-0.230471
	7	C	0.941435	-0.534375	-1.247587
	8	C	1.854402	-1.030967	-0.136456
	9	C	1.655567	-0.400884	1.224651
	10	C	6.631651	-2.900624	0.513237
	11	C	5.695950	-1.977780	0.064141
	12	C	5.545726	-0.713974	0.685750
	13	C	6.401996	-0.434168	1.777914
	14	C	7.342634	-1.359632	2.222323
	15	C	7.464583	-2.601783	1.596294
	16	C	3.673420	0.023952	-0.811750
	17	C	4.555899	0.264485	0.237553
	18	C	4.432060	1.567059	0.995211
	19	C	-0.778203	-4.463251	-2.974171
	20	C	-0.781516	-3.076933	-2.799187
	21	C	-0.665906	-2.497975	-1.526924
	22	C	-0.551264	-3.374011	-0.434610
	23	C	-0.546732	-4.756356	-0.600653
	24	C	-0.659393	-5.312091	-1.875657
	25	C	-0.583381	-0.972975	-1.340046
	26	C	-1.327013	-0.482833	-0.062049
	27	C	-1.117819	-0.215679	-2.576129
	28	H	3.168947	-4.904570	-2.375726
	29	H	2.283584	-2.631485	-2.327237
	30	H	2.539162	-2.632789	1.978469
	31	H	3.411149	-4.913457	1.918636
	32	H	3.743975	-6.086686	-0.254471
	33	H	0.928904	0.562431	-1.203332

34	H	1.383365	-0.786282	-2.218022
35	H	2.568887	-0.453066	1.824194
36	H	1.383113	0.654480	1.125863
37	H	0.860210	-0.893638	1.800605
38	H	6.701573	-3.865856	0.018849
39	H	5.055258	-2.256034	-0.763248
40	H	6.332016	0.519596	2.289418
41	H	7.982153	-1.109045	3.065160
42	H	8.195014	-3.326090	1.946625
43	H	3.889703	-0.740870	-1.549009
44	H	3.123366	0.875087	-1.203238
45	H	3.630925	2.186090	0.581297
46	H	4.213135	1.411981	2.060437
47	H	5.362026	2.150449	0.946253
48	H	-0.869574	-4.875313	-3.976157
49	H	-0.875685	-2.449073	-3.677983
50	H	-0.433055	-2.978462	0.567363
51	H	-0.436576	-5.398333	0.268903
52	H	-0.651964	-6.390461	-2.009553
53	H	-1.008543	-1.087652	0.789323
54	H	-0.961423	0.527505	0.153918
55	H	-1.151171	0.859113	-2.376468
56	H	-0.472919	-0.367990	-3.448260
57	C	-2.891153	-0.439675	0.008269
58	C	-3.518598	-1.795252	-0.376779
59	C	-4.465227	0.553023	-1.797740
60	C	-3.483652	0.731296	-0.813783
61	C	-3.063015	2.046704	-0.548283
62	C	-3.578182	3.132336	-1.252464
63	C	-4.545511	2.933907	-2.240945
64	C	-4.987796	1.639168	-2.505321
65	H	-4.824828	-0.441538	-2.036605
66	H	-2.322957	2.226480	0.226439
67	H	-3.226792	4.135909	-1.026053
68	H	-4.950232	3.778246	-2.792355
69	H	-5.742982	1.465854	-3.267963
70	C	-3.258429	-0.152404	1.445043
71	H	-2.598187	0.428740	2.082709
72	H	-4.288611	-0.277636	1.766123

	73	H	-3.330457	-2.060732	-1.420481
	74	H	-3.095264	-2.590714	0.240623
	75	H	-4.601907	-1.779842	-0.212253
	76	H	-2.129290	-0.528173	-2.843959

R15	Number	Atom	x (Å)	y (Å)	z (Å)
product	1	C	2.404033	-3.511588	-0.833987
	2	C	1.694872	-2.364425	-0.509186
	3	C	1.487099	-1.972631	0.845841
	4	C	2.030237	-2.836258	1.842116
	5	C	2.740682	-3.981463	1.507433
	6	C	2.940748	-4.331603	0.166790
	7	C	0.396566	0.261336	0.186947
	8	C	0.807692	-0.764771	1.205762
	9	C	0.648748	-0.408009	2.660992
	10	C	4.402136	-0.084577	2.233392
	11	C	4.159294	-0.105264	0.863979
	12	C	3.761716	1.055460	0.172058
	13	C	3.605961	2.233754	0.925384
	14	C	3.847261	2.256740	2.299890
	15	C	4.250420	1.098347	2.962623
	16	C	3.732930	-0.017373	-2.074873
	17	C	3.485625	1.045397	-1.291037
	18	C	2.883540	2.293702	-1.899591
	19	C	-1.443919	-2.286279	-3.185089
	20	C	-1.300350	-1.075606	-2.501784
	21	C	-1.356772	-1.013891	-1.101167
	22	C	-1.563969	-2.222046	-0.413823
	23	C	-1.707150	-3.431850	-1.088907
	24	C	-1.647491	-3.472505	-2.482609
	25	C	-1.101179	0.294753	-0.338429
	26	C	-2.038785	0.480871	0.889550
	27	C	-1.169469	1.528555	-1.260631
	28	H	2.535043	-3.774543	-1.880747
	29	H	1.280294	-1.767263	-1.310991
	30	H	1.907070	-2.589024	2.890736
	31	H	3.146300	-4.608286	2.298121
	32	H	3.497018	-5.228082	-0.092527
	33	H	0.597967	1.254614	0.612329

34	H	1.031971	0.181946	-0.698903
35	H	1.629966	-0.262323	3.136912
36	H	0.089895	0.521792	2.786004
37	H	0.125812	-1.187687	3.232264
38	H	4.690992	-1.004632	2.733959
39	H	4.246041	-1.049325	0.339325
40	H	3.293149	3.151829	0.440338
41	H	3.718258	3.184904	2.850668
42	H	4.437574	1.112950	4.033088
43	H	4.161118	-0.942322	-1.705922
44	H	3.500977	0.008235	-3.135770
45	H	2.676275	2.148520	-2.963472
46	H	1.942131	2.563567	-1.404869
47	H	3.556632	3.155378	-1.805513
48	H	-1.395089	-2.295811	-4.271180
49	H	-1.140578	-0.173518	-3.081435
50	H	-1.587592	-2.228984	0.669839
51	H	-1.854093	-4.346940	-0.521378
52	H	-1.756453	-4.415424	-3.011662
53	H	-1.957816	-0.408950	1.521509
54	H	-1.616723	1.295834	1.487609
55	H	-1.093580	2.445465	-0.668239
56	H	-0.343110	1.529481	-1.980057
57	C	-3.571226	0.785871	0.728857
58	C	-4.267404	-0.257787	-0.181252
59	C	-4.471832	2.541153	-0.948452
60	C	-3.813289	2.228791	0.246835
61	C	-3.374610	3.297390	1.046700
62	C	-3.561466	4.622274	0.657933
63	C	-4.206338	4.915590	-0.546126
64	C	-4.664115	3.868177	-1.343389
65	H	-4.834849	1.749781	-1.595034
66	H	-2.885439	3.084428	1.993893
67	H	-3.206936	5.426576	1.297727
68	H	-4.354145	5.947288	-0.853899
69	H	-5.174880	4.078462	-2.279749
70	C	-4.183987	0.655720	2.103207
71	H	-5.100325	1.185649	2.343421
72	H	-3.873454	-0.150816	2.762540

73	H	-3.877165	-0.242755	-1.203397
74	H	-4.102420	-1.264980	0.209701
75	H	-5.346878	-0.076121	-0.214551
76	H	-2.106554	1.581425	-1.818514

CH2-unsaturated end degradation reaction

R2	Number	Atom	x (Å)	y (Å)	z (Å)
TS	1	C	3.169187	-3.456791	1.165348
	2	C	2.581710	-2.511000	0.330248
	3	C	2.165612	-1.259012	0.813475
	4	C	2.385522	-0.989200	2.170074
	5	C	2.982998	-1.929999	3.012011
	6	C	3.376146	-3.170355	2.516442
	7	C	0.637033	-0.801146	-1.231289
	8	C	1.583092	-0.205498	-0.138298
	9	C	0.889723	0.936801	0.626244
	10	C	6.498126	-0.813764	1.127178
	11	C	5.347713	-0.430816	0.454504
	12	C	4.918859	0.927838	0.417932
	13	C	5.750858	1.869263	1.095423
	14	C	6.902684	1.476757	1.763509
	15	C	7.289360	0.131898	1.790671
	16	C	2.799586	0.405405	-0.974602
	17	C	3.729756	1.348675	-0.258002
	18	C	3.386869	2.817959	-0.311770
	19	C	-0.138496	-5.148055	0.260944
	20	C	-0.321192	-4.044023	-0.573401
	21	C	-0.556378	-2.763955	-0.052191
	22	C	-0.594026	-2.633661	1.343669
	23	C	-0.409289	-3.730142	2.183711
	24	C	-0.183421	-4.998099	1.646337
	25	C	-0.742472	-1.544988	-0.968079
	26	C	-1.768539	-0.565174	-0.417096
	27	C	-1.207367	-1.969370	-2.387255
	28	H	3.457804	-4.422848	0.760020
	29	H	2.431168	-2.766368	-0.712942
	30	H	2.098705	-0.032342	2.590222
	31	H	3.143423	-1.684050	4.058598

32	H	3.835784	-3.905817	3.171182
33	H	0.391300	0.031343	-1.904007
34	H	1.231852	-1.493462	-1.839665
35	H	1.607307	1.530144	1.197452
36	H	0.380913	1.610445	-0.071433
37	H	0.147297	0.558813	1.332366
38	H	6.778217	-1.864028	1.140370
39	H	4.755930	-1.195266	-0.030298
40	H	5.481967	2.919966	1.099437
41	H	7.506403	2.225461	2.270898
42	H	8.188729	-0.172867	2.318599
43	H	3.348054	-0.437403	-1.409627
44	H	2.358436	0.950199	-1.819686
45	H	4.173631	3.398740	-0.816171
46	H	2.453402	2.988264	-0.854938
47	H	3.266162	3.261833	0.686871
48	H	0.034753	-6.127753	-0.177570
49	H	-0.296577	-4.199177	-1.645762
50	H	-0.758880	-1.661528	1.791881
51	H	-0.433056	-3.588804	3.260820
52	H	-0.039685	-5.854885	2.299164
53	H	-1.559810	-0.127901	0.550083
54	H	-2.072870	0.186665	-1.144267
55	H	-1.440629	-1.078825	-2.981553
56	H	-0.425217	-2.515812	-2.924375
57	C	-3.806597	-1.215376	0.201727
58	C	-4.441149	0.134046	-0.125769
59	C	-3.657895	-3.660400	-0.450022
60	C	-4.101954	-2.353951	-0.728044
61	C	-4.829981	-2.156444	-1.913600
62	C	-5.086715	-3.210248	-2.792407
63	C	-4.623926	-4.494399	-2.507859
64	C	-3.909791	-4.711479	-1.326920
65	H	-3.070015	-3.857017	0.438202
66	H	-5.202615	-1.170033	-2.166226
67	H	-5.650261	-3.021958	-3.702775
68	H	-4.816513	-5.314490	-3.194393
69	H	-3.532412	-5.702508	-1.088873
70	C	-3.643603	-1.483165	1.560386

	71	H	-3.463431	-2.477155	1.948843
	72	H	-3.585792	-0.665684	2.273744
	73	H	-4.251665	0.461593	-1.151158
	74	H	-5.528688	0.080488	0.011715
	75	H	-4.056572	0.907627	0.546201
	76	H	-2.098886	-2.594926	-2.350381

R2	Number	Atom	x (Å)	y (Å)	z (Å)
product	1	C	2.409601	-1.823324	1.167879
	2	C	1.993585	-0.900241	0.213745
	3	C	1.604926	0.403011	0.568276
	4	C	1.665031	0.743857	1.924698
	5	C	2.091026	-0.174676	2.887743
	6	C	2.464635	-1.463301	2.516438
	7	C	0.243266	0.807118	-1.589854
	8	C	1.204006	1.413002	-0.515633
	9	C	0.582090	2.685588	0.084016
	10	C	5.922069	0.576905	1.218588
	11	C	4.871083	0.964492	0.401307
	12	C	4.563160	2.337635	0.176715
	13	C	5.411423	3.286379	0.823508
	14	C	6.463495	2.888859	1.637250
	15	C	6.730416	1.531158	1.848102
	16	C	2.516948	1.816841	-1.323405
	17	C	3.474645	2.764310	-0.648500
	18	C	3.262251	4.238961	-0.890509
	19	C	-0.754646	-3.402028	-0.102039
	20	C	-0.833001	-2.263392	-0.903577
	21	C	-1.109316	-1.002498	-0.356071
	22	C	-1.292420	-0.923694	1.030979
	23	C	-1.211376	-2.056874	1.839870
	24	C	-0.949264	-3.306261	1.276657
	25	C	-1.183469	0.252097	-1.240812
	26	C	-2.069302	1.301854	-0.633920
	27	C	-1.845392	-0.102922	-2.613811
	28	H	2.682671	-2.828433	0.858031
	29	H	1.958067	-1.209910	-0.825426
	30	H	1.381410	1.736962	2.251993
	31	H	2.131177	0.126249	3.931541

32	H	2.791011	-2.180698	3.264623
33	H	0.085616	1.596880	-2.337518
34	H	0.772360	0.006704	-2.121848
35	H	1.293020	3.219990	0.719307
36	H	0.276047	3.369784	-0.715071
37	H	-0.304283	2.452090	0.679820
38	H	6.109884	-0.482840	1.371698
39	H	4.262858	0.195526	-0.054420
40	H	5.233450	4.347682	0.688696
41	H	7.082531	3.644183	2.115606
42	H	7.551437	1.223498	2.489784
43	H	3.018981	0.890005	-1.622324
44	H	2.178126	2.291164	-2.253952
45	H	4.140974	4.703003	-1.362520
46	H	2.405598	4.414562	-1.546540
47	H	3.077471	4.797237	0.038593
48	H	-0.543320	-4.366306	-0.557985
49	H	-0.683544	-2.370322	-1.972775
50	H	-1.483638	0.040110	1.489650
51	H	-1.345170	-1.958391	2.913814
52	H	-0.887028	-4.191150	1.904447
53	H	-2.926447	1.014037	-0.036328
54	H	-2.066016	2.297880	-1.066627
55	H	-2.010099	0.811152	-3.194681
56	H	-1.209325	-0.761458	-3.217267
57	C	-5.209375	-0.210706	0.501805
58	C	-5.861743	1.129070	0.236552
59	C	-4.237289	-2.283803	-0.579952
60	C	-5.061293	-1.143843	-0.648734
61	C	-5.728223	-0.899138	-1.863794
62	C	-5.592530	-1.759843	-2.953686
63	C	-4.781644	-2.890456	-2.860009
64	C	-4.104185	-3.144405	-1.665155
65	H	-3.657433	-2.485424	0.313102
66	H	-6.365837	-0.028078	-1.968634
67	H	-6.121861	-1.541533	-3.877638
68	H	-4.669888	-3.559252	-3.709265
69	H	-3.443661	-4.002192	-1.579442
70	C	-4.783621	-0.509235	1.740476

	71	H	-4.320190	-1.456071	1.993983
	72	H	-4.890350	0.203171	2.553583
	73	H	-5.351186	1.663750	-0.574330
	74	H	-6.911496	1.015291	-0.062833
	75	H	-5.838493	1.760125	1.129382
	76	H	-2.808289	-0.596445	-2.460820

R4	Number	Atom	x (Å)	y (Å)	z (Å)
TS	1	C	5.892925	3.112740	6.037081
	2	H	5.897146	2.421655	5.194904
	3	H	5.942042	2.598257	6.996147
	4	C	3.334381	2.043912	6.385202
	5	H	3.278715	1.263855	5.631694
	6	C	3.678231	3.343585	6.027370
	7	C	6.882769	4.279977	5.914852
	8	C	6.525521	5.104017	4.665927
	9	C	6.860663	5.122063	7.203246
	10	C	3.549560	4.434817	7.046122
	11	C	3.452326	3.716186	4.567967
	12	H	4.037457	4.577342	4.248423
	13	H	3.712128	2.876569	3.916448
	14	H	2.390910	3.946484	4.406287
	15	H	5.874440	5.544065	7.393780
	16	H	7.125450	4.497121	8.060985
	17	H	7.585975	5.937687	7.163261
	18	C	6.072992	6.427438	4.748692
	19	H	5.992655	6.914529	5.712752
	20	C	6.590922	4.522727	3.388279
	21	H	6.918564	3.493040	3.279792
	22	C	5.702664	7.141211	3.605358
	23	H	5.354335	8.166167	3.705740
	24	C	5.776970	6.547953	2.346443
	25	H	5.489606	7.102342	1.457157
	26	C	6.225188	5.229097	2.244402
	27	H	6.285873	4.746681	1.272112
	28	C	3.225949	5.747753	6.667963
	29	H	3.057486	5.986056	5.624316
	30	C	3.767836	4.186453	8.414091

31	H	4.052334	3.190620	8.739977
32	C	3.135763	6.771056	7.614389
33	H	2.888832	7.778604	7.289146
34	C	3.675556	5.203492	9.358958
35	H	3.298211	7.304342	9.700168
36	C	3.361744	6.507342	8.964399
37	H	3.862862	4.981412	10.406414
38	C	10.742786	3.338139	5.352871
39	H	10.441894	2.956260	4.371548
40	H	10.693375	2.482613	6.038870
41	C	8.284354	3.571006	5.758544
42	H	8.278184	3.030049	4.806083
43	H	8.327282	2.791700	6.527316
44	C	9.627931	4.375599	5.806630
45	C	12.157212	3.850881	5.319209
46	C	12.759123	4.372668	4.128360
47	C	12.944350	3.824230	6.604253
48	C	9.975858	4.846119	7.228969
49	C	9.603181	5.535999	4.799442
50	H	10.590708	5.991836	4.692497
51	H	9.297592	5.175387	3.813937
52	H	8.891734	6.312195	5.090590
53	H	13.112581	4.833932	7.006341
54	H	12.418552	3.265496	7.380895
55	H	13.932405	3.364415	6.465615
56	C	14.065637	4.946864	4.156622
57	H	14.605321	5.002096	5.095396
58	C	12.111135	4.353709	2.857329
59	H	11.116446	3.933490	2.766722
60	C	14.665406	5.456200	3.013105
61	H	15.660231	5.889840	3.081080
62	C	14.002718	5.419756	1.780943
63	H	14.474713	5.818976	0.887673
64	C	12.719786	4.861996	1.719161
65	H	12.189575	4.825522	0.770616
66	C	10.413173	6.149818	7.499357
67	H	10.478317	6.878353	6.699683
68	C	9.922017	3.949611	8.310182
69	H	9.603336	2.924361	8.146136

	70	C	10.771564	6.545169	8.791271
	71	H	11.104044	7.565652	8.964136
	72	C	10.277056	4.336575	9.600478
	73	H	10.982121	5.948450	10.855340
	74	C	10.704882	5.642326	9.850271
	75	H	10.220602	3.615629	10.412207
	76	H	3.199999	1.733856	7.415555

R4	Number	Atom	x (Å)	y (Å)	z (Å)
product	1	C	-1.927273	-2.148713	0.361970
	2	H	-1.700867	-3.070102	-0.167772
	3	H	-2.937776	-2.014135	0.733828
	4	C	-6.210870	-2.295985	0.486165
	5	H	-6.504651	-3.027581	-0.261221
	6	C	-5.573969	-1.166592	0.137425
	7	C	-1.008237	-0.953365	0.255013
	8	C	-1.517754	-0.147268	-0.964087
	9	C	-1.124884	-0.150981	1.566972
	10	C	-5.136412	-0.165965	1.149269
	11	C	-5.283417	-0.864616	-1.315505
	12	H	-4.230376	-0.610303	-1.468659
	13	H	-5.530545	-1.721283	-1.949217
	14	H	-5.874744	-0.011165	-1.671873
	15	H	-2.166943	0.110422	1.770035
	16	H	-0.759822	-0.753760	2.402652
	17	H	-0.532950	0.767781	1.547106
	18	C	-2.014561	1.158249	-0.854887
	19	H	-2.032275	1.655028	0.106990
	20	C	-1.545907	-0.747990	-2.235543
	21	H	-1.193056	-1.768549	-2.353662
	22	C	-2.507202	1.841607	-1.970068
	23	H	-2.885283	2.854087	-1.850321
	24	C	-2.518228	1.234480	-3.224386
	25	H	-2.902020	1.765260	-4.091357
	26	C	-2.032912	-0.070016	-3.350889
	27	H	-2.040228	-0.563499	-4.319465
	28	C	-4.943543	1.181412	0.798582
	29	H	-5.105579	1.502525	-0.224247
	30	C	-4.876082	-0.534889	2.483146

31	H	-4.963970	-1.576673	2.776100
32	C	-4.533111	2.123020	1.742967
33	H	-4.395210	3.158346	1.441325
34	C	-4.466530	0.403087	3.427360
35	H	-3.964108	2.471711	3.796303
36	C	-4.293893	1.740955	3.063006
37	H	-4.262106	0.084838	4.446218
38	C	2.899858	-1.475934	-0.416330
39	H	2.631014	-1.890695	-1.393910
40	H	2.949437	-2.330485	0.271055
41	C	0.438695	-1.503781	0.033873
42	H	0.447486	-2.025293	-0.931434
43	H	0.583665	-2.290396	0.783089
44	C	1.685728	-0.565594	0.047709
45	C	4.253698	-0.818280	-0.463903
46	C	4.787944	-0.236987	-1.658818
47	C	5.049670	-0.763649	0.814721
48	C	2.001946	-0.040454	1.458629
49	C	1.512020	0.574341	-0.969635
50	H	2.442616	1.129658	-1.110393
51	H	1.216379	0.171023	-1.942412
52	H	0.731898	1.274956	-0.663910
53	H	5.099120	0.255334	1.225602
54	H	4.599414	-1.388022	1.588973
55	H	6.083875	-1.102063	0.665203
56	C	6.028298	0.469603	-1.642554
57	H	6.568961	0.580456	-0.709101
58	C	4.132809	-0.321935	-2.923624
59	H	3.185681	-0.842160	-3.004856
60	C	6.560577	1.038930	-2.791133
61	H	7.505750	1.573294	-2.732161
62	C	5.893053	0.934863	-4.016916
63	H	6.312302	1.381385	-4.914098
64	C	4.674171	0.247399	-4.066843
65	H	4.140975	0.156867	-5.010096
66	C	2.296600	1.306804	1.707004
67	H	2.271196	2.027339	0.897849
68	C	2.063692	-0.923744	2.550242
69	H	1.856326	-1.979599	2.402840

	70	C	2.628293	1.755796	2.988679
	71	H	2.849381	2.808711	3.144886
	72	C	2.392714	-0.483474	3.830339
	73	H	2.933711	1.212472	5.055565
	74	C	2.676976	0.864710	4.058590
	75	H	2.428203	-1.195762	4.650829
	76	H	-6.481154	-2.523332	1.512902

R6	Number	Atom	x (Å)	y (Å)	z (Å)
TS	1	C	1.084035	1.970433	-0.315319
	2	C	2.123546	1.257302	-0.906771
	3	C	2.377725	1.327306	-2.289400
	4	C	1.565632	2.181035	-3.045675
	5	C	0.523682	2.904192	-2.458929
	6	C	0.268848	2.796941	-1.093030
	7	C	3.431381	-0.993742	-2.414233
	8	C	3.506069	0.487529	-2.909341
	9	C	3.502278	0.546651	-4.445332
	10	C	4.044903	5.070345	-0.770887
	11	C	4.346528	3.806397	-1.255147
	12	C	5.082676	3.621362	-2.461003
	13	C	5.508300	4.810082	-3.126675
	14	C	5.203796	6.071428	-2.633434
	15	C	4.466377	6.218158	-1.452945
	16	C	4.902014	1.039404	-2.383551
	17	C	5.395524	2.328517	-2.989450
	18	C	6.272194	2.220654	-4.213377
	19	C	2.098906	-5.191732	-0.671561
	20	C	2.239072	-4.321771	-1.758366
	21	C	2.058562	-2.941576	-1.610929
	22	C	1.729429	-2.464533	-0.330340
	23	C	1.592871	-3.324123	0.755297
	24	C	1.779107	-4.698444	0.590895
	25	C	2.202021	-1.942184	-2.780876
	26	C	0.905880	-1.169292	-2.941188
	27	C	2.519413	-2.663788	-4.107516
	28	H	0.909833	1.878263	0.753635
	29	H	2.742959	0.628338	-0.274867

30	H	1.725637	2.282577	-4.112571
31	H	-0.089816	3.553433	-3.078199
32	H	-0.545082	3.354515	-0.637855
33	H	4.331782	-1.506617	-2.777182
34	H	3.535428	-0.979274	-1.327525
35	H	3.678155	1.562119	-4.810177
36	H	4.295576	-0.092333	-4.847070
37	H	2.551839	0.204644	-4.861404
38	H	3.472088	5.163085	0.148439
39	H	3.998739	2.945366	-0.701464
40	H	6.075928	4.736889	-4.047778
41	H	5.542066	6.951724	-3.174755
42	H	4.226285	7.206757	-1.071689
43	H	4.845312	1.108867	-1.291636
44	H	5.646112	0.261401	-2.596459
45	H	5.828084	2.703030	-5.096419
46	H	7.248513	2.701642	-4.055356
47	H	6.458867	1.176551	-4.478295
48	H	2.246115	-6.258805	-0.819997
49	H	2.490461	-4.741971	-2.725553
50	H	1.550289	-1.404472	-0.182862
51	H	1.316522	-2.920873	1.725292
52	H	1.668884	-5.374044	1.435045
53	H	0.603520	-0.552761	-2.107818
54	H	0.775203	-0.680015	-3.903090
55	H	2.616055	-1.943692	-4.922705
56	H	3.460698	-3.221013	-4.046824
57	C	-1.035645	-2.275916	-2.972387
58	C	-0.738122	-3.450077	-3.648267
59	C	-1.470647	-1.125137	-0.751070
60	C	-1.335964	-2.311221	-1.496455
61	C	-1.533753	-3.524071	-0.818328
62	C	-1.811167	-3.555669	0.547301
63	C	-1.913811	-2.370677	1.275724
64	C	-1.745987	-1.152558	0.614448
65	H	-1.335889	-0.160783	-1.230643
66	H	-1.474765	-4.460122	-1.361767
67	H	-1.947048	-4.514067	1.041559
68	H	-2.130031	-2.394758	2.340593

	69	H	-1.829219	-0.216408	1.161083
	70	C	-1.769216	-1.189406	-3.753932
	71	H	-1.550154	-0.181115	-3.390926
	72	H	-1.499549	-1.225824	-4.814182
	73	H	-2.852880	-1.340343	-3.669959
	74	H	-0.340908	-4.322242	-3.142496
	75	H	-0.743237	-3.473407	-4.733823
	76	H	1.720010	-3.359181	-4.376294

R6	Number	Atom	x (Å)	y (Å)	z (Å)
product	1	C	-0.733815	1.753728	1.449691
	2	C	0.330373	1.090265	0.843783
	3	C	0.621910	1.249514	-0.522677
	4	C	-0.205836	2.109440	-1.255943
	5	C	-1.277691	2.775761	-0.656469
	6	C	-1.549534	2.603370	0.699921
	7	C	1.846897	-0.980576	-0.738481
	8	C	1.830057	0.528211	-1.141239
	9	C	1.871868	0.668679	-2.671039
	10	C	1.947428	4.969571	1.365815
	11	C	2.367776	3.775749	0.799291
	12	C	3.115806	3.742904	-0.412802
	13	C	3.427061	5.008952	-0.993702
	14	C	3.003511	6.199467	-0.418867
	15	C	2.256231	6.195631	0.764519
	16	C	3.156358	1.155822	-0.531189
	17	C	3.548460	2.524356	-1.026862
	18	C	4.448739	2.585581	-2.236601
	19	C	0.259954	-5.301967	0.616166
	20	C	0.621000	-4.393664	-0.384476
	21	C	0.419004	-3.017609	-0.220048
	22	C	-0.160745	-2.584426	0.985700
	23	C	-0.519191	-3.483308	1.985461
	24	C	-0.312074	-4.853627	1.805263
	25	C	0.757780	-1.970850	-1.317329
	26	C	-0.547510	-1.312720	-1.681741
	27	C	1.324143	-2.654659	-2.580456
	28	H	-0.924415	1.602680	2.508443
	29	H	0.954768	0.450098	1.459437

30	H	-0.027568	2.267848	-2.312763
31	H	-1.897194	3.437237	-1.256537
32	H	-2.380837	3.124752	1.166996
33	H	2.823997	-1.386033	-1.030541
34	H	1.834215	-1.041842	0.351715
35	H	1.960514	1.713333	-2.980319
36	H	2.737299	0.131807	-3.074040
37	H	0.967376	0.255234	-3.126007
38	H	1.369523	4.944862	2.286288
39	H	2.105329	2.850470	1.293326
40	H	3.998263	5.052449	-1.914632
41	H	3.255532	7.142395	-0.898244
42	H	1.922780	7.128950	1.209569
43	H	3.064885	1.137652	0.560295
44	H	3.971273	0.462389	-0.775445
45	H	3.970467	3.077504	-3.096387
46	H	5.367794	3.151793	-2.027178
47	H	4.744402	1.585257	-2.563785
48	H	0.430253	-6.364323	0.458790
49	H	1.060485	-4.781186	-1.296382
50	H	-0.362934	-1.528935	1.136829
51	H	-0.985359	-3.112230	2.893259
52	H	-0.595748	-5.560075	2.580973
53	H	-1.092859	-0.725591	-0.955366
54	H	-1.109215	-1.692575	-2.529245
55	H	1.544079	-1.913773	-3.351636
56	H	2.252052	-3.194848	-2.363075
57	C	-3.547942	-2.537888	-0.683535
58	C	-2.997024	-3.725687	-0.974138
59	C	-3.420061	-0.697984	1.037117
60	C	-3.624667	-2.051347	0.719145
61	C	-3.899901	-2.941486	1.771747
62	C	-3.945255	-2.503709	3.093472
63	C	-3.722978	-1.157765	3.396106
64	C	-3.462736	-0.258890	2.360702
65	H	-3.197796	0.021330	0.255025
66	H	-4.089627	-3.985591	1.541992
67	H	-4.163345	-3.212809	3.888168
68	H	-3.763039	-0.812683	4.425935

	69	H	-3.290555	0.791141	2.577809
	70	C	-4.082661	-1.629319	-1.766268
	71	H	-3.471269	-0.722747	-1.862598
	72	H	-4.080578	-2.130805	-2.738957
	73	H	-5.105571	-1.301600	-1.543963
	74	H	-2.536456	-4.350184	-0.214893
	75	H	-2.949184	-4.088248	-1.997786
	76	H	0.604017	-3.365785	-2.999998

R8	Number	Atom	x (Å)	y (Å)	z (Å)
TS	1	C	-5.438043	2.095150	0.328089
	2	C	-4.469223	0.922266	0.396174
	3	H	-4.959212	3.007167	0.696470
	4	H	-5.732779	2.270675	-0.715016
	5	H	-6.341814	1.936302	0.914368
	6	C	-4.206103	0.753306	2.600727
	7	H	-3.350741	0.080553	2.550297
	8	H	-3.904675	1.792647	2.722478
	9	C	-5.301902	0.277759	3.564568
	10	C	-5.577919	-1.216963	3.331222
	11	C	-4.674936	0.512231	4.999394
	12	H	-4.655469	-1.791724	3.461087
	13	H	-6.322641	-1.595522	4.034284
	14	H	-5.938872	-1.404443	2.320758
	15	H	-3.629499	0.180353	4.949078
	16	H	-4.627509	1.595421	5.154865
	17	C	-5.267377	-0.137613	6.305378
	18	C	-4.759668	-1.585602	6.458956
	19	C	-4.638026	0.702868	7.496337
	20	H	-3.665109	-1.599114	6.444535
	21	H	-5.072880	-2.013759	7.415005
	22	H	-5.105658	-2.243718	5.662284
	23	H	-3.563790	0.770594	7.297157
	24	H	-5.019707	1.728582	7.423160
	25	C	-4.902490	0.184825	8.883367
	26	C	-6.242236	0.499919	9.497074
	27	H	-6.756849	1.288012	8.943878
	28	H	-6.914593	-0.371626	9.491477
	29	H	-6.146475	0.824905	10.541200

30	C	-3.149182	1.197598	0.053176
31	H	-2.768345	2.213099	0.108625
32	H	-2.431542	0.422080	-0.190326
33	C	-5.021693	-0.441806	0.114226
34	C	-6.375288	-0.624634	-0.212556
35	C	-4.209635	-1.588648	0.189006
36	C	-6.897463	-1.899573	-0.442256
37	H	-7.039538	0.229614	-0.274525
38	C	-4.727275	-2.859350	-0.041339
39	H	-3.165063	-1.489862	0.468691
40	C	-6.079239	-3.024804	-0.355556
41	H	-7.950949	-2.008594	-0.687407
42	H	-4.076006	-3.726239	0.036484
43	H	-6.486557	-4.017372	-0.527462
44	C	-6.560885	1.139225	3.365152
45	C	-6.492027	2.534505	3.521025
46	C	-7.792898	0.593629	2.985977
47	C	-7.603897	3.348237	3.320655
48	H	-5.550869	3.000305	3.799533
49	C	-8.912987	1.403946	2.784125
50	H	-7.897991	-0.475820	2.853139
51	C	-8.827479	2.784697	2.951263
52	H	-7.513959	4.424028	3.449336
53	H	-9.857403	0.946229	2.501235
54	H	-9.699057	3.414633	2.794674
55	C	-6.797517	-0.041732	6.359233
56	C	-7.622345	-1.171117	6.435497
57	C	-7.426515	1.214630	6.333551
58	C	-9.015663	-1.053596	6.467666
59	H	-7.187026	-2.163571	6.467745
60	C	-8.811589	1.340310	6.364447
61	H	-6.825451	2.114443	6.261714
62	C	-9.617888	0.201523	6.430363
63	H	-9.626159	-1.951476	6.522745
64	H	-9.260540	2.328370	6.319291
65	H	-10.700466	0.294357	6.449984
66	C	-3.964094	-0.628863	9.598160
67	C	-2.644838	-0.893714	9.124164
68	C	-4.312680	-1.228822	10.845440

	69	C	-1.756298	-1.684277	9.838417
	70	H	-2.313469	-0.464485	8.185632
	71	C	-3.418641	-2.022352	11.551066
	72	H	-5.306810	-1.078972	11.251402
	73	C	-2.130219	-2.259592	11.059014
	74	H	-0.758710	-1.856033	9.441414
	75	H	-3.728872	-2.465025	12.494524
	76	H	-1.432285	-2.880310	11.613675

R8	Number	Atom	x (Å)	y (Å)	z (Å)
product	1	C	0.039667	2.311629	-4.921506
	2	C	0.960486	1.167593	-5.282272
	3	H	0.564191	3.269672	-4.984835
	4	H	-0.817714	2.361624	-5.605734
	5	H	-0.360017	2.201191	-3.909512
	6	C	1.743682	0.795777	-1.959451
	7	H	2.575147	0.139884	-2.196094
	8	H	1.822211	1.831262	-2.265483
	9	C	0.654027	0.313228	-1.087785
	10	C	0.445107	-1.192671	-1.327837
	11	C	1.196493	0.583206	0.417126
	12	H	1.376180	-1.732512	-1.127288
	13	H	-0.336310	-1.601877	-0.682950
	14	H	0.173276	-1.378807	-2.368269
	15	H	2.248942	0.275789	0.427070
	16	H	1.194494	1.669372	0.542491
	17	C	0.533559	-0.070404	1.680115
	18	C	1.069540	-1.503564	1.871690
	19	C	1.081057	0.825088	2.917230
	20	H	2.160254	-1.482210	1.955971
	21	H	0.684726	-1.960990	2.785979
	22	H	0.818235	-2.154625	1.034823
	23	H	2.161232	0.911561	2.771523
	24	H	0.661639	1.828974	2.792856
	25	C	0.724851	0.272111	4.243081
	26	C	-0.665360	0.538430	4.753572
	27	H	-1.131957	1.367847	4.218212
	28	H	-1.333890	-0.327835	4.623361
	29	H	-0.663483	0.782597	5.823757

30	C	2.169264	1.413758	-5.812677
31	H	2.521680	2.431733	-5.952870
32	H	2.840223	0.626141	-6.141179
33	C	0.455205	-0.215825	-5.066425
34	C	-0.921538	-0.467615	-4.935897
35	C	1.327401	-1.318888	-4.983450
36	C	-1.407667	-1.764239	-4.759486
37	H	-1.627341	0.354603	-4.961768
38	C	0.844906	-2.612972	-4.812630
39	H	2.399768	-1.156370	-5.024762
40	C	-0.529469	-2.845711	-4.703023
41	H	-2.478494	-1.924810	-4.662559
42	H	1.544650	-3.442127	-4.746304
43	H	-0.906464	-3.854906	-4.561091
44	C	-0.613895	1.140272	-1.362596
45	C	-0.581642	2.540249	-1.241445
46	C	-1.815210	0.554743	-1.778573
47	C	-1.701982	3.322337	-1.513558
48	H	0.336391	3.032118	-0.930458
49	C	-2.942001	1.333352	-2.051380
50	H	-1.888439	-0.519499	-1.888935
51	C	-2.894763	2.720163	-1.920856
52	H	-1.642039	4.402909	-1.410166
53	H	-3.862767	0.846026	-2.361981
54	H	-3.772391	3.324889	-2.133113
55	C	-0.996598	-0.008097	1.635794
56	C	-1.797149	-1.157105	1.659253
57	C	-1.650910	1.233044	1.557691
58	C	-3.191813	-1.073247	1.594712
59	H	-1.340430	-2.138361	1.724325
60	C	-3.037246	1.324996	1.493361
61	H	-1.067630	2.146455	1.519540
62	C	-3.818850	0.167304	1.510916
63	H	-3.783400	-1.985166	1.611165
64	H	-3.505610	2.301424	1.410191
65	H	-4.902122	0.234623	1.456560
66	C	1.598797	-0.578711	4.983912
67	C	2.965194	-0.797422	4.622840
68	C	1.148355	-1.261282	6.157148

	69	C	3.798165	-1.612935	5.371492
	70	H	3.374846	-0.307720	3.746858
	71	C	1.989980	-2.078539	6.897039
	72	H	0.116845	-1.155552	6.473450
	73	C	3.324149	-2.265765	6.517146
	74	H	4.832193	-1.744654	5.062138
	75	H	1.602387	-2.582581	7.779135
	76	H	3.980080	-2.907016	7.098722

R10	Number	Atom	x (Å)	y (Å)	z (Å)
TS	1	C	3.461571	-2.821259	0.070016
	2	C	2.676501	-1.901659	-0.619781
	3	C	2.173753	-0.748976	0.005520
	4	C	2.519290	-0.542017	1.347552
	5	C	3.313270	-1.456856	2.043789
	6	C	3.785007	-2.604814	1.411195
	7	C	0.317955	-0.369909	-1.765850
	8	C	1.348467	0.275795	-0.786448
	9	C	0.658328	1.301884	0.129532
	10	C	4.501516	5.142478	0.271754
	11	C	4.531222	3.794868	-0.059201
	12	C	3.447461	3.164141	-0.741441
	13	C	2.336856	4.001371	-1.060860
	14	C	2.317178	5.347987	-0.728025
	15	C	3.396835	5.936295	-0.057966
	16	C	2.354356	1.056242	-1.742243
	17	C	3.499356	1.773553	-1.079455
	18	C	4.745491	0.978611	-0.783613
	19	C	0.030957	-4.849596	-0.463957
	20	C	-0.387347	-3.725410	-1.179475
	21	C	-0.539658	-2.478989	-0.559559
	22	C	-0.255413	-2.407273	0.813588
	23	C	0.169657	-3.520567	1.532714
	24	C	0.314474	-4.754370	0.896318
	25	C	-0.952945	-1.226307	-1.349796
	26	C	-1.950670	-0.367715	-0.579059
	27	C	-1.589827	-1.601032	-2.711825
	28	H	3.813055	-3.714292	-0.439698
	29	H	2.432394	-2.104094	-1.657317

30	H	2.167669	0.339540	1.871263
31	H	3.558236	-1.267329	3.086001
32	H	4.394633	-3.322757	1.953192
33	H	-0.074707	0.456622	-2.373254
34	H	0.875484	-1.003324	-2.465924
35	H	1.382413	1.950458	0.628354
36	H	-0.005332	1.945515	-0.456848
37	H	0.053140	0.817847	0.899246
38	H	5.347643	5.581590	0.794787
39	H	5.400908	3.210264	0.219261
40	H	1.480332	3.584527	-1.577750
41	H	1.450870	5.949298	-0.993009
42	H	3.376801	6.990796	0.202176
43	H	2.767227	0.318749	-2.442762
44	H	1.755960	1.747118	-2.346657
45	H	4.674688	-0.034158	-1.184914
46	H	5.639419	1.453436	-1.212437
47	H	4.922490	0.874783	0.296101
48	H	0.128873	-5.802780	-0.977461
49	H	-0.606930	-3.843188	-2.234037
50	H	-0.342664	-1.461976	1.336376
51	H	0.400478	-3.418368	2.589515
52	H	0.646341	-5.626308	1.453816
53	H	-1.760565	-0.235426	0.478249
54	H	-2.187076	0.576653	-1.068965
55	H	-1.956921	-0.698069	-3.211432
56	H	-0.863750	-2.067011	-3.386016
57	C	-4.076264	-0.964884	-0.341871
58	C	-4.628165	-0.304758	-1.600976
59	C	-3.421227	-3.146674	0.759257
60	C	-3.999303	-2.463517	-0.324701
61	C	-4.514711	-3.235723	-1.378145
62	C	-4.443151	-4.630673	-1.355056
63	C	-3.858199	-5.288049	-0.274640
64	C	-3.349293	-4.535249	0.786369
65	H	-2.979865	-2.582129	1.573140
66	H	-4.980303	-2.752013	-2.230382
67	H	-4.849054	-5.200515	-2.187200
68	H	-3.791844	-6.372588	-0.260266

	69	H	-2.866294	-5.028227	1.624767
	70	C	-4.355402	-0.307385	0.856186
	71	H	-4.267540	-0.795972	1.820370
	72	H	-4.570454	0.757346	0.863884
	73	H	-4.110817	-0.619234	-2.508691
	74	H	-5.692082	-0.548198	-1.718813
	75	H	-4.548021	0.783973	-1.525579
	76	H	-2.425526	-2.290156	-2.580346

R10	Number	Atom	x (Å)	y (Å)	z (Å)
product	1	C	3.232701	-1.958250	0.831172
	2	C	2.544519	-1.087648	-0.008577
	3	C	1.970943	0.100696	0.472982
	4	C	2.133304	0.386949	1.834374
	5	C	2.828735	-0.479444	2.682660
	6	C	3.380962	-1.657772	2.187142
	7	C	0.243801	0.352704	-1.436658
	8	C	1.262344	1.066151	-0.489429
	9	C	0.572824	2.220180	0.258129
	10	C	4.481751	5.933940	0.210545
	11	C	4.487394	4.554702	0.055000
	12	C	3.451152	3.873390	-0.652023
	13	C	2.413180	4.694326	-1.185221
	14	C	2.417720	6.072568	-1.027748
	15	C	3.449886	6.710636	-0.328824
	16	C	2.358314	1.682575	-1.458969
	17	C	3.476747	2.449724	-0.805453
	18	C	4.655475	1.664496	-0.289745
	19	C	0.184959	-3.977064	-0.075737
	20	C	-0.217238	-2.843570	-0.781895
	21	C	-0.612243	-1.673153	-0.119468
	22	C	-0.590939	-1.680994	1.281418
	23	C	-0.191511	-2.810727	1.994875
	24	C	0.198218	-3.968103	1.319400
	25	C	-1.016287	-0.415284	-0.904290
	26	C	-1.934957	0.469511	-0.112347
	27	C	-1.831242	-0.824960	-2.176167
	28	H	3.646017	-2.878324	0.426835
	29	H	2.439519	-1.351269	-1.055994

30	H	1.715611	1.293946	2.255020
31	H	2.933574	-0.226800	3.734940
32	H	3.916263	-2.336530	2.845715
33	H	-0.132049	1.126786	-2.120809
34	H	0.793077	-0.354408	-2.070222
35	H	1.297050	2.855622	0.774152
36	H	0.029997	2.855659	-0.449497
37	H	-0.150206	1.847577	0.988840
38	H	5.289148	6.411546	0.760435
39	H	5.297916	3.984879	0.495564
40	H	1.595054	4.238889	-1.730827
41	H	1.607849	6.659831	-1.453836
42	H	3.448698	7.790023	-0.206339
43	H	2.792839	0.851364	-2.029055
44	H	1.828573	2.305056	-2.188419
45	H	4.606993	0.621054	-0.606919
46	H	5.607843	2.083546	-0.642613
47	H	4.694490	1.654604	0.809115
48	H	0.485215	-4.869745	-0.619011
49	H	-0.219205	-2.880733	-1.866156
50	H	-0.865096	-0.781328	1.822684
51	H	-0.170620	-2.778849	3.080929
52	H	0.515628	-4.847719	1.873237
53	H	-2.678164	0.038537	0.548987
54	H	-2.113453	1.481008	-0.464599
55	H	-2.228425	0.069721	-2.668266
56	H	-1.208616	-1.350393	-2.910176
57	C	-5.339358	-0.613227	0.495937
58	C	-5.659597	0.477333	-0.501424
59	C	-3.899120	-2.671039	0.661553
60	C	-4.845630	-1.908263	-0.044971
61	C	-5.274122	-2.388054	-1.295348
62	C	-4.787510	-3.590864	-1.808355
63	C	-3.849435	-4.334543	-1.090411
64	C	-3.406013	-3.867608	0.148165
65	H	-3.503688	-2.297795	1.600445
66	H	-5.998875	-1.823256	-1.873564
67	H	-5.138139	-3.942482	-2.775394
68	H	-3.454945	-5.260862	-1.499327

	69	H	-2.644159	-4.409555	0.699273
	70	C	-5.477578	-0.405385	1.814583
	71	H	-5.287554	-1.186146	2.545179
	72	H	-5.806004	0.554493	2.203674
	73	H	-4.808546	0.650089	-1.171660
	74	H	-6.517305	0.210922	-1.132120
	75	H	-5.901250	1.416841	0.004253
	76	H	-2.667526	-1.473405	-1.903358

R12	Number	Atom	x (Å)	y (Å)	z (Å)
TS	1	C	-2.974271	1.417570	-0.150135
	2	C	-1.427779	1.255191	0.033689
	3	H	-3.205321	1.084211	-1.167509
	4	H	-3.472381	0.695940	0.507132
	5	C	-1.100489	-0.193508	-0.530775
	6	C	0.336830	-0.631794	-0.450814
	7	H	-1.719476	-0.910025	0.024878
	8	H	-1.461367	-0.219913	-1.564371
	9	C	-3.703829	2.801279	0.064859
	10	C	-5.192024	2.434840	0.040246
	11	C	-6.835490	3.927548	-0.223487
	12	H	-5.501817	1.853200	-0.824832
	13	H	-5.552039	2.006653	0.975544
	14	C	-7.881220	3.164409	0.283157
	15	H	-8.502500	2.538171	-0.347609
	16	H	-8.051975	3.104203	1.354328
	17	C	1.255028	-0.466992	-1.537939
	18	C	0.864186	0.030465	-2.816826
	19	C	2.634866	-0.801502	-1.391128
	20	C	1.774040	0.174615	-3.853962
	21	H	-0.168323	0.307376	-2.994101
	22	C	3.538741	-0.650858	-2.433753
	23	H	2.997289	-1.171720	-0.438607
	24	C	3.121471	-0.163007	-3.677370
	25	H	1.431739	0.556051	-4.812873
	26	H	4.582159	-0.913445	-2.276680
	27	H	3.831127	-0.046267	-4.491531
	28	C	-1.011286	1.289933	1.513895
	29	C	-1.687473	0.505510	2.464516

30	C	0.078494	2.045644	1.966467
31	C	-1.302258	0.483416	3.803207
32	H	-2.527704	-0.110453	2.157574
33	C	0.471868	2.027379	3.307758
34	H	0.637876	2.662331	1.272871
35	C	-0.216490	1.248239	4.235194
36	H	-1.850413	-0.134755	4.509769
37	H	1.321792	2.627559	3.622831
38	H	0.087195	1.234113	5.278414
39	C	-3.390878	3.774097	-1.086666
40	C	-3.611014	3.385060	-2.418275
41	C	-2.890697	5.063756	-0.866937
42	C	-3.321602	4.234237	-3.482419
43	H	-4.033681	2.409145	-2.634266
44	C	-2.603476	5.924141	-1.931108
45	H	-2.702639	5.410305	0.143256
46	C	-2.808952	5.511331	-3.245171
47	H	-3.516957	3.903833	-4.498486
48	H	-2.210935	6.916746	-1.724520
49	H	-2.584028	6.176730	-4.074338
50	C	-6.776389	4.143111	-1.707695
51	C	-6.426528	5.388171	-2.250253
52	C	-7.098566	3.108388	-2.605433
53	C	-6.410597	5.595514	-3.630118
54	H	-6.153054	6.209120	-1.597742
55	C	-7.079587	3.311107	-3.982332
56	H	-7.354495	2.125254	-2.219863
57	C	-6.737342	4.561254	-4.504909
58	H	-6.128887	6.570475	-4.018745
59	H	-7.329528	2.490083	-4.649767
60	H	-6.719374	4.721857	-5.579573
61	C	0.810455	-1.249975	0.839839
62	H	1.497006	-0.587961	1.387600
63	H	-0.025089	-1.454037	1.512119
64	H	1.344236	-2.194320	0.666086
65	C	-0.666440	2.289975	-0.810479
66	H	-1.036547	2.286191	-1.839022
67	H	-0.799561	3.304500	-0.428506
68	H	0.403286	2.068061	-0.841792

	69	C	-3.345104	3.374207	1.448519
	70	H	-3.556225	2.631281	2.223242
	71	H	-2.284766	3.623897	1.527562
	72	H	-3.925671	4.269695	1.678651
	73	C	-6.309696	5.046925	0.661793
	74	H	-6.982494	5.913476	0.612887
	75	H	-6.265972	4.721706	1.704987
	76	H	-5.315395	5.378517	0.357532

R12	Number	Atom	x (Å)	y (Å)	z (Å)
product	1	C	-0.426857	-1.114250	0.886658
	2	C	1.131024	-1.209795	0.951166
	3	H	-0.710156	-1.298780	-0.156347
	4	H	-0.841798	-1.958122	1.451047
	5	C	1.484416	-2.593425	0.256511
	6	C	2.944255	-2.953640	0.182213
	7	H	0.955601	-3.382997	0.806269
	8	H	1.035324	-2.570283	-0.741991
	9	C	-1.218139	0.159376	1.351976
	10	C	-2.685249	-0.191518	1.265818
	11	C	-4.907450	2.600233	-0.186450
	12	H	-3.430644	0.591024	1.169097
	13	H	-3.021068	-1.185637	1.551125
	14	C	-5.809174	1.988129	0.596410
	15	H	-6.416913	1.162827	0.236289
	16	H	-5.977447	2.306979	1.621594
	17	C	3.751787	-2.667541	-0.965844
	18	C	3.222528	-2.112479	-2.169082
	19	C	5.155014	-2.929338	-0.961531
	20	C	4.026914	-1.849711	-3.268237
	21	H	2.165345	-1.884463	-2.236737
	22	C	5.952622	-2.660068	-2.065172
	23	H	5.620626	-3.336715	-0.071036
	24	C	5.400536	-2.119304	-3.232031
	25	H	3.580600	-1.427849	-4.165475
	26	H	7.018341	-2.870430	-2.016518
	27	H	6.027281	-1.909811	-4.094240
	28	C	1.649667	-1.257353	2.397707
	29	C	1.098015	-2.160561	3.323020

30	C	2.709561	-0.454594	2.840337
31	C	1.572764	-2.251721	4.629361
32	H	0.283149	-2.812173	3.021214
33	C	3.191853	-0.540989	4.149793
34	H	3.175467	0.252559	2.164010
35	C	2.626169	-1.438128	5.053045
36	H	1.119441	-2.960727	5.317573
37	H	4.014861	0.098614	4.458694
38	H	2.999132	-1.505684	6.071410
39	C	-0.966967	1.357881	0.418483
40	C	-1.316831	1.250408	-0.936675
41	C	-0.415661	2.569942	0.853976
42	C	-1.104478	2.298091	-1.829597
43	H	-1.784728	0.339607	-1.296703
44	C	-0.197841	3.625339	-0.037135
45	H	-0.138466	2.702165	1.893889
46	C	-0.537060	3.493642	-1.383323
47	H	-1.406928	2.184640	-2.866124
48	H	0.235786	4.552836	0.328493
49	H	-0.371855	4.315524	-2.074926
50	C	-4.653153	2.136065	-1.577319
51	C	-4.403355	3.047444	-2.616108
52	C	-4.624786	0.764278	-1.881868
53	C	-4.152821	2.606171	-3.915163
54	H	-4.408925	4.113538	-2.411321
55	C	-4.364128	0.320336	-3.177220
56	H	-4.763365	0.043297	-1.081924
57	C	-4.127910	1.239907	-4.202098
58	H	-3.971022	3.331932	-4.703786
59	H	-4.334086	-0.746377	-3.384445
60	H	-3.921969	0.895033	-5.211871
61	C	3.562708	-3.619602	1.384580
62	H	4.242472	-2.944665	1.925238
63	H	2.800538	-3.930154	2.101991
64	H	4.145406	-4.507168	1.103741
65	C	1.782097	-0.079716	0.136296
66	H	1.331980	-0.024465	-0.859077
67	H	1.639870	0.896012	0.603873
68	H	2.854113	-0.249116	0.007204

	69	C	-0.921288	0.503034	2.833897
	70	H	-1.124271	-0.364498	3.467858
	71	H	0.123812	0.782640	2.994457
	72	H	-1.560213	1.327238	3.168702
	73	C	-4.091317	3.769840	0.313017
	74	H	-4.304352	4.683599	-0.256290
	75	H	-4.305982	3.979144	1.365433
	76	H	-3.019899	3.568865	0.205197

R14	Number	Atom	x (Å)	y (Å)	z (Å)
TS	1	C	-2.999525	-0.535096	0.106530
	2	C	-1.539421	-0.834823	-0.109306
	3	C	-1.117927	-2.371607	-0.130153
	4	H	-1.169852	-0.380163	-1.035439
	5	H	-0.974945	-0.365735	0.707098
	6	C	0.446934	-2.366453	-0.073937
	7	H	0.823572	-1.906906	-0.993605
	8	H	0.727915	-1.669652	0.722138
	9	C	1.275249	-3.694730	0.146737
	10	C	2.722800	-3.273657	-0.142186
	11	C	4.500419	-4.570184	0.199789
	12	H	2.922888	-3.098943	-1.198747
	13	H	3.098279	-2.469886	0.489893
	14	C	5.455801	-3.780886	-0.431913
	15	H	5.704259	-3.886684	-1.482134
	16	H	5.925543	-2.957815	0.098421
	17	C	-3.944055	-0.389706	-0.959384
	18	C	-5.331999	-0.196123	-0.689587
	19	C	-3.569987	-0.421980	-2.333583
	20	C	-6.262983	-0.068639	-1.711507
	21	H	-5.680093	-0.158338	0.336817
	22	C	-4.506829	-0.296921	-3.347945
	23	H	-2.532881	-0.566065	-2.603589
	24	C	-5.864007	-0.121110	-3.051905
	25	H	-7.312431	0.070095	-1.462774
	26	H	-4.176687	-0.341189	-4.382737
	27	H	-6.595678	-0.026350	-3.849454
	28	C	-1.663930	-2.982112	-1.431430
	29	C	-2.814238	-3.781674	-1.449504

30	C	-1.070012	-2.686940	-2.671076
31	C	-3.347887	-4.266068	-2.646154
32	H	-3.317151	-4.033230	-0.523407
33	C	-1.593268	-3.170643	-3.868132
34	H	-0.186014	-2.057953	-2.712617
35	C	-2.741546	-3.964841	-3.863223
36	H	-4.246421	-4.877081	-2.620524
37	H	-1.104188	-2.922310	-4.806813
38	H	-3.155964	-4.340699	-4.794718
39	C	1.183487	-4.178905	1.605115
40	C	1.458253	-3.298772	2.665587
41	C	0.886749	-5.508523	1.933541
42	C	1.437004	-3.723363	3.992483
43	H	1.712126	-2.263652	2.456470
44	C	0.865619	-5.941565	3.262340
45	H	0.680710	-6.227926	1.150614
46	C	1.139649	-5.052673	4.300332
47	H	1.658521	-3.015247	4.787026
48	H	0.633574	-6.980935	3.481008
49	H	1.123728	-5.388544	5.333630
50	C	4.021057	-5.814917	-0.482804
51	C	3.639368	-6.947846	0.253771
52	C	3.917949	-5.884906	-1.884587
53	C	3.162994	-8.096578	-0.382194
54	H	3.696061	-6.936642	1.336013
55	C	3.446299	-7.028991	-2.520334
56	H	4.172540	-5.017072	-2.485430
57	C	3.060576	-8.144552	-1.771552
58	H	2.869898	-8.955413	0.216495
59	H	3.365667	-7.045967	-3.604190
60	H	2.683290	-9.035343	-2.266246
61	C	-3.463172	-0.371766	1.533489
62	H	-4.222077	-1.114449	1.819786
63	H	-2.632325	-0.475819	2.236104
64	H	-3.917969	0.615912	1.699274
65	C	-1.685012	-3.063265	1.121008
66	H	-1.456510	-4.131288	1.128276
67	H	-1.246128	-2.630680	2.024728
68	H	-2.769074	-2.949333	1.189732

	69	C	0.833388	-4.773590	-0.857993
	70	H	-0.214164	-5.050721	-0.717988
	71	H	0.932752	-4.396671	-1.879213
	72	H	1.443753	-5.672310	-0.778263
	73	C	4.537162	-4.574607	1.722402
	74	H	4.759191	-3.572388	2.100922
	75	H	3.600298	-4.898973	2.172964
	76	H	5.333380	-5.245789	2.070542

R14	Number	Atom	x (Å)	y (Å)	z (Å)
product	1	C	-3.035001	3.028042	0.394397
	2	C	-1.577569	2.821298	0.072089
	3	C	-1.042504	1.320483	0.084339
	4	H	-1.316741	3.258501	-0.898247
	5	H	-0.989120	3.369756	0.818761
	6	C	0.515613	1.443921	0.090485
	7	H	0.821217	1.958922	-0.827589
	8	H	0.772239	2.135368	0.900998
	9	C	1.461484	0.197398	0.243079
	10	C	2.866283	0.692972	-0.011079
	11	C	5.281131	-1.915257	1.297110
	12	H	3.049957	1.384184	-0.830178
	13	H	3.719073	0.181146	0.421383
	14	C	6.380344	-1.237134	0.927581
	15	H	6.778682	-1.262124	-0.081792
	16	H	6.936523	-0.641140	1.645377
	17	C	-4.071501	3.037118	-0.592289
	18	C	-5.443638	3.149443	-0.215367
	19	C	-3.810138	2.944081	-1.989768
	20	C	-6.462138	3.145038	-1.158608
	21	H	-5.708568	3.229442	0.833237
	22	C	-4.833938	2.938240	-2.924915
	23	H	-2.790988	2.859975	-2.341089
	24	C	-6.171740	3.035631	-2.523379
	25	H	-7.495138	3.225073	-0.828412
	26	H	-4.586746	2.852337	-3.980043
	27	H	-6.971513	3.027594	-3.258715
	28	C	-1.571678	0.624844	-1.180078
	29	C	-2.604567	-0.320460	-1.136705

30	C	-1.072640	0.971402	-2.448412
31	C	-3.116909	-0.894736	-2.303062
32	H	-3.030700	-0.618274	-0.186089
33	C	-1.576106	0.401292	-3.614913
34	H	-0.280826	1.709614	-2.534176
35	C	-2.606983	-0.538666	-3.549175
36	H	-3.923696	-1.619554	-2.230609
37	H	-1.163870	0.694291	-4.577295
38	H	-3.005787	-0.983749	-4.456693
39	C	1.416166	-0.371028	1.673914
40	C	1.795508	0.447165	2.750979
41	C	1.029016	-1.685591	1.963138
42	C	1.758857	-0.014985	4.065533
43	H	2.134035	1.460615	2.552282
44	C	0.992301	-2.156048	3.278908
45	H	0.755403	-2.360921	1.161544
46	C	1.349943	-1.322797	4.337963
47	H	2.056883	0.644138	4.876982
48	H	0.684544	-3.180943	3.471308
49	H	1.320846	-1.688345	5.360890
50	C	4.482789	-2.723967	0.335044
51	C	3.580782	-3.702228	0.789717
52	C	4.583436	-2.531898	-1.056661
53	C	2.835654	-4.472837	-0.104119
54	H	3.449155	-3.864377	1.853475
55	C	3.845182	-3.302500	-1.950078
56	H	5.225876	-1.748587	-1.445595
57	C	2.966757	-4.282167	-1.479170
58	H	2.148387	-5.222499	0.279737
59	H	3.940320	-3.124096	-3.017921
60	H	2.382302	-4.876752	-2.175849
61	C	-3.390802	3.247951	1.844699
62	H	-4.070243	2.476847	2.235908
63	H	-2.500031	3.240303	2.478279
64	H	-3.897604	4.212741	1.994298
65	C	-1.526554	0.630812	1.370668
66	H	-1.239649	-0.421780	1.396944
67	H	-1.083154	1.110144	2.248824
68	H	-2.613217	0.687335	1.470355

	69	C	1.158148	-0.888604	-0.819059
	70	H	0.149122	-1.298693	-0.713809
	71	H	1.227258	-0.458872	-1.821736
	72	H	1.880887	-1.704110	-0.747891
	73	C	4.822492	-1.886832	2.737877
	74	H	5.408157	-1.169508	3.319584
	75	H	3.766419	-1.614777	2.818441
	76	H	4.940358	-2.870333	3.211630

R16	Number	Atom	x (Å)	y (Å)	z (Å)
TS	1	C	2.510080	-4.294906	-1.342910
	2	C	2.117723	-2.960743	-1.294859
	3	C	1.972418	-2.278683	-0.074839
	4	C	2.257387	-2.990703	1.096823
	5	C	2.659503	-4.327851	1.055821
	6	C	2.786280	-4.989226	-0.162990
	7	C	0.533978	-0.394405	-1.118378
	8	C	1.603652	-0.789221	-0.051135
	9	C	1.167271	-0.321466	1.348375
	10	C	6.288330	-2.809537	-0.190908
	11	C	5.245041	-1.902930	-0.301291
	12	C	5.096998	-0.816696	0.609359
	13	C	6.095011	-0.705574	1.623704
	14	C	7.137415	-1.616760	1.724943
	15	C	7.246003	-2.680870	0.822407
	16	C	2.905474	0.030454	-0.478081
	17	C	4.020994	0.123494	0.529765
	18	C	3.991038	1.298788	1.476870
	19	C	-1.139766	-4.437844	-2.705624
	20	C	-1.125844	-3.047971	-2.563313
	21	C	-1.028484	-2.441673	-1.302958
	22	C	-0.947991	-3.290578	-0.187635
	23	C	-0.958696	-4.676492	-0.321328
	24	C	-1.057011	-5.261061	-1.584838
	25	C	-0.967850	-0.911997	-1.152115
	26	C	-1.723219	-0.426384	0.077938
	27	C	-1.569558	-0.198266	-2.390767
	28	H	2.590480	-4.794962	-2.304297
	29	H	1.903226	-2.452309	-2.228483

30	H	2.175704	-2.507821	2.063603
31	H	2.878685	-4.848110	1.984761
32	H	3.093902	-6.030930	-0.196074
33	H	0.458549	0.700406	-1.081626
34	H	0.947035	-0.621086	-2.108741
35	H	1.988233	-0.380481	2.066574
36	H	0.832048	0.720496	1.314021
37	H	0.345279	-0.924450	1.738697
38	H	6.352448	-3.630984	-0.899942
39	H	4.519047	-2.048399	-1.089776
40	H	6.042015	0.102445	2.345230
41	H	7.873397	-1.499501	2.516834
42	H	8.060261	-3.395182	0.907201
43	H	3.259355	-0.391625	-1.425044
44	H	2.573217	1.051960	-0.705671
45	H	3.121172	1.934430	1.291726
46	H	3.949667	0.992326	2.532126
47	H	4.888725	1.925900	1.371507
48	H	-1.216890	-4.872800	-3.699095
49	H	-1.190614	-2.438645	-3.457801
50	H	-0.839880	-2.871948	0.806039
51	H	-0.875468	-5.299750	0.564709
52	H	-1.064044	-6.342382	-1.692438
53	H	-1.615808	-1.004126	0.987161
54	H	-1.628913	0.642579	0.256256
55	H	-1.670481	0.873573	-2.195974
56	H	-0.935888	-0.316051	-3.276140
57	C	-3.952822	-0.464418	0.152793
58	C	-4.167887	-1.900442	-0.304134
59	C	-5.026945	0.364377	-1.984981
60	C	-4.302002	0.629858	-0.812589
61	C	-3.924706	1.962316	-0.567569
62	C	-4.249759	2.982984	-1.457368
63	C	-4.966255	2.699781	-2.623175
64	C	-5.355003	1.385476	-2.878845
65	H	-5.340556	-0.649568	-2.210058
66	H	-3.352308	2.199033	0.324935
67	H	-3.936545	4.001851	-1.243755
68	H	-5.215766	3.493796	-3.321721

	69	H	-5.916854	1.148418	-3.778773
	70	C	-4.117431	-0.201868	1.508514
	71	H	-4.020908	-0.998541	2.240805
	72	H	-4.256685	0.803326	1.891755
	73	H	-3.711367	-2.109624	-1.273579
	74	H	-3.736999	-2.601477	0.415092
	75	H	-5.242230	-2.115290	-0.379125
	76	H	-2.563973	-0.578339	-2.628941

R16	Number	Atom	x (Å)	y (Å)	z (Å)
product	1	C	1.783050	-2.747233	-0.805777
	2	C	1.618514	-1.365688	-0.783102
	3	C	1.621172	-0.642832	0.421826
	4	C	1.811544	-1.368000	1.604320
	5	C	1.986520	-2.753883	1.588848
	6	C	1.972227	-3.452665	0.384704
	7	C	0.461698	1.423415	-0.619641
	8	C	1.505470	0.887892	0.412210
	9	C	1.195417	1.455041	1.808448
	10	C	5.794739	-1.868889	0.094946
	11	C	4.905231	-0.807951	0.020807
	12	C	4.976132	0.294037	0.921412
	13	C	6.027461	0.251713	1.886017
	14	C	6.915926	-0.813038	1.950295
	15	C	6.809543	-1.887318	1.059529
	16	C	2.902026	1.473022	-0.083441
	17	C	4.059842	1.392607	0.876980
	18	C	4.255982	2.559022	1.814619
	19	C	-1.793194	-2.348421	-2.023583
	20	C	-1.567521	-0.974678	-1.910112
	21	C	-1.394241	-0.366552	-0.658773
	22	C	-1.474542	-1.185792	0.477065
	23	C	-1.689838	-2.558119	0.370637
	24	C	-1.849605	-3.149104	-0.883247
	25	C	-1.080976	1.130808	-0.523489
	26	C	-1.685089	1.692047	0.732259
	27	C	-1.716104	1.932139	-1.705448
	28	H	1.755107	-3.274480	-1.755640
	29	H	1.470287	-0.846910	-1.724047

30	H	1.829008	-0.858449	2.560372
31	H	2.137964	-3.283165	2.526175
32	H	2.103177	-4.531365	0.370656
33	H	0.555997	2.518010	-0.606649
34	H	0.777829	1.119409	-1.624603
35	H	1.996050	1.241689	2.520528
36	H	1.084099	2.543619	1.756970
37	H	0.263340	1.045629	2.207007
38	H	5.692002	-2.695414	-0.603653
39	H	4.126513	-0.839106	-0.728764
40	H	6.138446	1.063031	2.597121
41	H	7.699507	-0.808949	2.704308
42	H	7.503079	-2.721738	1.116299
43	H	3.140875	0.984686	-1.034875
44	H	2.733331	2.532355	-0.318919
45	H	3.496465	3.329349	1.656966
46	H	4.201606	2.263973	2.872618
47	H	5.239933	3.030622	1.674154
48	H	-1.922907	-2.790798	-3.008313
49	H	-1.523137	-0.379743	-2.816057
50	H	-1.339354	-0.745656	1.459241
51	H	-1.723093	-3.166566	1.270238
52	H	-2.017228	-4.219304	-0.969844
53	H	-2.607759	1.281540	1.127215
54	H	-1.392935	2.687356	1.054133
55	H	-1.619243	3.007091	-1.522711
56	H	-1.216501	1.716054	-2.657873
57	C	-5.162849	0.097356	0.475616
58	C	-5.005650	-1.310361	-0.052827
59	C	-5.466089	0.932503	-1.879016
60	C	-5.215753	1.201126	-0.521227
61	C	-4.988594	2.542919	-0.157771
62	C	-5.028947	3.565888	-1.100188
63	C	-5.288373	3.279679	-2.443084
64	C	-5.504775	1.956702	-2.826499
65	H	-5.632386	-0.087730	-2.206822
66	H	-4.746541	2.787931	0.870879
67	H	-4.840283	4.589738	-0.787912
68	H	-5.310526	4.077211	-3.180706

69	H	-5.701266	1.715351	-3.867919
70	C	-5.256876	0.314888	1.797989
71	H	-5.193880	-0.507798	2.504292
72	H	-5.419211	1.299570	2.225131
73	H	-4.163628	-1.384172	-0.747737
74	H	-4.831695	-2.017353	0.761963
75	H	-5.907713	-1.634367	-0.588905
76	H	-2.777500	1.699241	-1.807164

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