Table S2. Computed ethene/propene ratios in the decomposition of 1-pentyl radicals as derived from the RRKM/ME models described in the text (see also Figures 3 and 6). Pressure/temperature combinations correspond to approximate average values for the three sets of conditions examined experimentally.

Corresponding Experiments	Temp (K)	Pressure (kPa)	Computed Ethene/Propene Ratio		
			"Best Fit" PES $\alpha = 0.675T$ [a]	*a priori* PES $\alpha = 0.675T$ [b]	*a priori* PES $\alpha = 0.24T$ [a]
Low-Pressure Data Sets	860	71	2.68	5.76	2.65
	900	79	2.97	6.55	2.97
	940	87	3.28	7.37	3.32
	980	95	3.60	8.22	3.69
	1020	103	3.93	9.10	4.11
	1050	109	4.20	9.78	4.44
Mid-Pressure Data Sets	860	154	2.91	6.34	3.04
	900	165	3.24	7.24	3.42
	940	179	3.60	8.18	3.84
	980	196	3.97	9.18	4.29
	1020	215	4.37	10.22	4.80
	1050	232	4.68	11.03	5.20
High-Pressure Data Sets	860	448	3.18	7.00	3.60
	900	494	3.60	8.12	4.13
	940	542	4.05	9.30	4.71
	980	594	4.51	10.54	5.32
	1020	649	4.99	11.82	5.97
	1050	693	5.37	12.80	6.48
Computed High Pressure Limits	860	$1x10^8$	3.56	7.91	5.04
	900	$1x10^8$	4.14	9.42	6.16
	940	$1x10^8$	4.79	11.10	7.44
	980	$1x10^8$	5.48	12.94	8.88
	1020	$1x10^8$	6.24	14.92	10.48
	1050	$1x10^8$	6.84	16.49	11.78

[a] includes tunneling correction [b] no tunneling included

Table S3. Reaction barriers used in our models of the decomposition of *n*-pentyl radicals.

	Reaction	*a priori*		"Best Fit"	
		E_0 kJ mol^{-1}	E_{298} kJ mol^{-1}	E_0 kJ mol^{-1}	E_{298} kJ mol^{-1}
k_1	1-pentyl → ethene + *n*-propyl	121.1	122.8	115.5	116.9
k_{-1}	ethene + *n*-propyl → 1-pentyl	32.7	30.6	26.0	23.6
k_3	2-pentyl → propene + ethyl	119.8	121.2	117.7	118.6
k_{-3}	propene + ethyl → 2-pentyl	33.9	32.0	28.7	26.3
k_6	3-pentyl → 1-butene + methyl	123.0	123.7	124.2	123.6
k_{-6}	1-butene + methyl → 3-pentyl	35.6	31.6	29.3	23.9
k_{4a}	2-pentyl → *(E)*-2-pentene + H	139.2	137.9	141.1	141.4
k_{-4a}	*(E)*-2-pentene + H → 2-pentyl	7.2	1.4	5.6	1.3
k_{4b}	2-pentyl → *(Z)*-2-pentene + H	144.4	144.8	147.2	147.4
k_{-4b}	*(Z)*-2-pentene + H → 2-pentyl	6.4	2.6	6.7	2.7
k_2	1-pentyl → 2-pentyl (*1-4* H transfer, *5ps*)	108.6	105.3	108.0	105.0
k_{-2}	2-pentyl → 1-pentyl (*2-5* H transfer, *5sp*)	120.4	116.12	121.4	117.4
k_5	1-pentyl → 3-pentyl (*1-3* H transfer, *4ps*)	172.2	170.0	157.8	155.6
k_{-5}	3-pentyl → 1-pentyl (*3-5* H transfer, *4sp*)	183.4	179.6	171.1	168.3

Table S4. Rate expressions, $k/s^{-1} = A\,T^{n}\,exp(-E/T)$, from 700-1900 K at selected pressures compatible with the PLOG function in CHEMKIN PRO. Deviations from the RRKM values are given in Table S5. A in s^{-1}, T in Kelvin, E in cal mol^{-1}.

Rate constant	Pressure (bar)	PLOG function	A	n	E
k_1	0.1	PLOG / 0.1	2.02E-13	6.899	8825
	1	PLOG / 1	2.35E+07	1.289	21152
	10	PLOG / 10	6.47E+21	-2.670	31224
	100	PLOG / 100	2.80E+24	-3.256	34426
	1000	PLOG / 1000	6.40E+18	-1.528	32135
k_2	0.1	PLOG / 0.1	2.06E-02	3.305	9137
	1	PLOG / 1	3.45E+09	0.225	16790
	10	PLOG / 10	1.27E+16	-1.515	22019
	100	PLOG / 100	2.41E+15	-1.184	22800
	1000	PLOG / 1000	1.71E+10	0.372	20499
k_{-2}	0.1	PLOG / 0.1	1.09E+12	-0.677	20278
	1	PLOG / 1	5.19E+18	-2.394	25967
	10	PLOG / 10	1.60E+19	-2.358	27939
	100	PLOG / 100	2.33E+13	-0.556	25704
	1000	PLOG / 1000	7.57E+06	1.370	22439
k_3	0.1	PLOG / 0.1	1.52E+12	-0.261	23172
	1	PLOG / 1	5.59E+23	-3.360	31683
	10	PLOG / 10	2.35E+27	-4.198	35685
	100	PLOG / 100	2.20E+22	-2.609	34108
	1000	PLOG / 1000	4.11E+15	-0.606	30776
k_{4a}	0.1	PLOG / 0.1	2.01E-05	4.339	19354
	1	PLOG / 1	5.92E+15	-1.295	32766
	10	PLOG / 10	1.46E+26	-4.024	41100
	100	PLOG / 100	3.87E+22	-2.794	40909
	1000	PLOG / 1000	7.45E+13	-0.187	36722
k_{4b}	0.1	PLOG / 0.1	5.85E-08	5.063	18972
	1	PLOG / 1	5.99E+14	-1.017	33121
	10	PLOG / 10	3.33E+26	-4.128	42256
	100	PLOG / 100	2.59E+23	-3.025	42410
	1000	PLOG / 1000	3.28E+14	-0.361	38160
k_5	0.1	PLOG / 0.1	1.04E-31	11.701	1576
	1	PLOG / 1	2.58E-07	4.853	16385
	10	PLOG / 10	5.79E+12	-0.491	29513
	100	PLOG / 100	6.57E+17	-1.735	34497
	1000	PLOG / 1000	1.64E+11	0.301	31948
k_{-5}	0.1	PLOG / 0.1	1.75E-17	7.973	15507
	1	PLOG / 1	4.11E+03	2.250	28300
	10	PLOG / 10	1.46E+15	-0.900	36754
	100	PLOG / 100	5.41E+11	0.223	36136
	1000	PLOG / 1000	3.16E+03	2.651	31854
k_6	0.1	PLOG / 0.1	4.64E+02	2.761	21728
	1	PLOG / 1	2.33E+17	-1.333	31396
	10	PLOG / 10	5.93E+22	-2.749	35959
	100	PLOG / 100	1.38E+18	-1.319	34218
	1000	PLOG / 1000	1.94E+12	0.402	31125

Table S5. Deviation of the rate constants for beta C-C bond fission derived from the analytical expressions in Table S4 from the RRKM/ME values, expressed as the percent difference.

Pressure (Bar)	Temp (K)	% difference = 100*($k_{analytical}$ - k_{RRKM})/ k_{RRKM})								
		k_1	k_2	k_{-2}	k_3	k_{4a}	k_{4b}	k_5	k_{-5}	k_6
0.1	700	21.5	16.6	15.3	20.1	27.4	28.1	23.2	20.6	19.6
	800	-14.3	-9.9	-7.0	-10.1	-14.4	-15.0	-16.0	-13.3	-11.0
	900	-16.5	-13.5	-13.4	-16.5	-21.2	-21.6	-17.7	-16.8	-16.2
	1000	-7.8	-8.1	-10.4	-11.8	-13.8	-13.6	-7.2	-7.2	-9.6
	1100	3.6	0.3	-2.6	-1.6	0.3	1.0	5.9	5.8	1.7
	1300	18.8	15.0	15.4	19.8	27.3	27.9	20.3	18.7	19.4
	1500	17.0	17.4	21.2	24.8	29.5	28.8	15.4	13.1	18.1
	1700	2.7	5.1	7.8	7.7	6.6	6.0	1.0	0.2	2.9
	1900	-15.8	-16.0	-18.8	-21.2	-24.0	-23.6	-14.7	-12.9	-16.2
1	700	21.0	12.9	7.0	11.2	18.1	19.3	24.3	15.9	11.5
	800	-11.5	-6.4	-1.3	-4.1	-7.6	-8.3	-12.9	-6.4	-4.1
	900	-17.4	-11.7	-7.0	-10.5	-15.6	-16.4	-19.8	-14.6	-10.9
	1000	-11.0	-8.5	-7.8	-9.6	-13.0	-13.4	-12.5	-12.0	-10.0
	1100	0.7	-1.1	-4.2	-3.8	-3.8	-3.6	1.3	-2.3	-3.5
	1300	21.2	13.3	8.1	12.3	19.7	20.9	25.4	19.8	13.9
	1500	21.8	16.1	14.5	18.6	26.6	27.6	24.6	21.2	18.2
	1700	4.6	4.9	6.6	7.1	8.3	8.2	4.1	4.0	5.2
	1900	-19.0	-14.8	-13.3	-16.5	-21.8	-22.4	-20.6	-17.5	-15.6
10	700	10.1	4.4	-1.5	0.9	3.7	4.4	11.6	0.8	-0.2
	800	-3.4	-0.2	3.2	1.6	0.7	0.3	-3.1	3.6	2.5
	900	-9.8	-4.8	1.3	-1.2	-3.9	-4.5	-11.2	-1.4	-0.1
	1000	-9.3	-6.0	-2.0	-3.7	-6.3	-6.8	-11.1	-5.8	-3.3
	1100	-3.7	-3.5	-3.9	-4.2	-5.4	-5.5	-4.7	-6.4	-4.6
	1300	12.0	5.9	-1.4	1.2	4.3	5.0	14.4	2.3	0.1
	1500	17.2	10.4	4.0	7.2	12.4	13.4	20.8	10.9	6.7
	1700	5.8	4.5	4.2	5.0	7.0	7.3	6.8	6.1	4.8
	1900	-15.1	-9.7	-4.2	-7.2	-11.6	-12.4	-17.4	-9.6	-6.4
100	700	-0.5	-2.2	-4.5	-3.5	-4.2	-4.1	-2.3	-7.2	-4.1
	800	1.9	2.6	3.0	2.3	3.1	3.1	4.2	5.5	2.4
	900	0.3	2.0	4.3	3.3	4.0	3.9	1.8	7.2	4.0
	1000	-2.2	-0.5	2.4	1.6	1.6	1.4	-2.3	3.5	2.5
	1100	-3.4	-2.5	-0.6	-0.9	-1.7	-1.8	-4.7	-1.7	-0.4
	1300	-0.6	-2.3	-5.0	-4.1	-4.9	-4.8	-1.9	-7.9	-4.9
	1500	4.4	1.2	-4.0	-2.6	-2.2	-1.9	4.6	-5.4	-4.0
	1700	3.8	2.4	0.3	0.9	1.8	2.0	4.7	1.1	0.4
	1900	-4.6	-1.5	3.7	2.0	1.5	1.2	-4.6	5.1	3.5
1000	700	-2.7	-2.8	-2.5	-1.8	-2.8	-2.8	-5.5	-4.5	-1.6
	800	1.5	1.7	1.3	0.6	1.2	1.1	4.0	2.7	0.4
	900	2.4	2.5	2.1	1.3	2.3	2.3	5.1	3.9	1.1
	1000	1.4	1.6	1.5	1.1	1.8	1.8	2.7	2.6	1.0
	1100	-0.2	-0.1	0.3	0.4	0.5	0.5	-0.7	0.5	0.5
	1300	-2.9	-2.9	-2.2	-1.6	-2.5	-2.5	-5.4	-3.8	-1.2
	1500	-2.6	-2.9	-3.2	-2.5	-3.7	-3.7	-4.9	-5.5	-2.5
	1700	0.0	-0.4	-1.4	-1.1	-1.5	-1.5	-0.4	-2.4	-1.4
	1900	2.3	2.8	3.4	2.5	3.9	3.9	4.9	6.2	2.6

Table S6. Thermodynamic parameters from our “best fit” model in NASA polynomial format.

```
methyl                                H   3C   1    0    0g    300.00   5000.00 1000.00      1
 2.92073572E+00 6.05451021E-03-2.19235185E-06 3.70311014E-10-2.38399736E-14    2
 1.65607093E+04 4.60228291E+00 3.92826620E+00 2.48844944E-03 2.66130512E-06    3
-2.81470534E-09 8.60893223E-13 1.63419690E+04-3.68606878E-01                   4

ethyl                                 H   5C   2    0    0g    300.00   5000.00 1000.00      1
 3.90951525E+00 1.34062089E-02-5.13263567E-06 9.04770773E-10-6.01924701E-14    2
 1.22896641E+04 3.10220861E+00 2.46706451E+00 1.11842107E-02 9.39798284E-06    3
-1.66774392E-08 6.63357840E-12 1.30536316E+04 1.22101545E+01                   4

n-propyl                              H   7C   3    0    0g    300.00   5000.00 1000.00      1
 6.29444574E+00 1.91252882E-02-7.35197689E-06 1.29996552E-09-8.66859925E-14    2
 8.76186188E+03-7.57384658E+00 7.49525079E-01 3.03514098E-02-9.83414617E-06    3
-6.59334514E-09 4.57311201E-12 1.05520136E+04 2.21979704E+01                   4

1-pentyl                              H  11C   5    0    0g    300.00   5000.00 1000.00      1
 1.18548111E+01 3.02274343E-02-1.17739471E-05 2.10210099E-09-1.41187716E-13    2
 9.82725138E+02-3.45214609E+01-4.49470311E-02 5.01981400E-02-3.04271861E-06    3
-3.04972638E-08 1.55977650E-11 4.96892022E+03 3.02510371E+01                   4

2-pentyl                              H  11C   5    0    0g    300.00   5000.00 1000.00      1
 1.04800446E+01 3.15977348E-02-1.23244136E-05 2.20208257E-09-1.47970732E-13    2
-5.24664670E+01-2.62439327E+01 2.43753578E+00 3.46717680E-02 2.45166588E-05    3
-5.14844006E-08 2.16051976E-11 3.22268382E+03 2.02493152E+01                   4

3-pentyl                              H  11C   5    0    0g    300.00   5000.00 1000.00      1
 1.01241030E+01 3.17615554E-02-1.23394441E-05 2.19840405E-09-1.47407203E-13    2
 1.13356656E+02-2.43636849E+01 1.84063823E+00 4.02186313E-02 9.14893283E-06    3
-3.57099438E-08 1.60386361E-11 3.22534459E+03 2.22208785E+01                   4

ethene                                H   4C   2    0    0g    300.00   5000.00 1000.00      1
 3.56120960E+00 1.14051427E-02-4.36226092E-06 7.68637524E-10-5.11276706E-14    2
 4.43146711E+03 2.12692326E+00 1.32040178E+00 1.24472511E-02 5.58911492E-06    3
-1.41880886E-08 6.13433558E-12 5.33054020E+03 1.50210135E+01                   4

propene                               H   6C   3    0    0g    300.00   5000.00 1000.00      1
 5.42782024E+00 1.77168273E-02-6.83867581E-06 1.21282943E-09-8.10542466E-14    2
-5.39101839E+02-5.07723803E+00 1.33523307E+00 2.26330700E-02 9.40880473E-07    3
-1.40299510E-08 6.52508697E-12 9.81199520E+02 1.78042422E+01                   4

1-butene                              H   8C   4    0    0g    300.00   5000.00 1000.00      1
 7.93087197E+00 2.33452031E-02-9.02765261E-06 1.60318843E-09-1.07249288E-13    2
-4.23020725E+03-1.66008125E+01-6.97135856E-04 4.02892489E-02-1.54483929E-05    3
-6.40611975E-09 5.26550799E-12-1.71672226E+03 2.57645816E+01                   4

E-2-pentene                           H  10C   5    0    0g    300.00   5000.00 1000.00      1
 9.73015325E+00 2.97325593E-02-1.15365764E-05 2.05353801E-09-1.37605432E-13    2
-8.93222482E+03-2.48430499E+01 1.65905781E+00 4.16540688E-02-2.77913456E-06    3
-2.12316461E-08 1.04812566E-11-6.06191361E+03 1.96948613E+01                   4

Z-2-pentene                           H  10C   5    0    0g    300.00   5000.00 1000.00      1
 9.05339120E+00 3.04341464E-02-1.18285722E-05 2.10812102E-09-1.41393713E-13    2
-8.24149239E+03-2.08359496E+01 1.62811664E+00 3.55990026E-02 1.44532705E-05    3
-3.88479034E-08 1.67347871E-11-5.31486120E+03 2.15600555E+01                   4
```

Table S7: ChemRate Input Parameters

General Information

Component
Name=Argon
Atomic composition=Ar1
Type=4
Mass=39.95
Sigma, A=3.542
Epsilon, K=39.95

Component
Name=but1ene
Atomic composition=H8C4
Type=0
Mass=56.1075
Enthalpy(298), 1/cm=-50.1566

Frequencies
Frequency(degeneracy)

3103.95	3029.09	3007.59	2996.22	2987.85
2946.34	2924.72	2899.33	1664.44	1476.06
1466.69	1450.74	1417.78	1378.84	1310.13
1278.39	1253.15	1163.34	1060.32	999.635
987.256	956.303	899.789	830.054	770.701
627.569	415.901	303.055		

Rotors
*Name, Moment of Inertia [amu*A*²], Symmetry, Dimension, Active [Yes/No], Hindrance [1/cm], Minima*

"Ia"	22.3314	1	1	Yes	0	1
"IbIc"	124.278	1	2	No	0	1
"CH3-CH2C2H3 (C1-C2)"	2.86335	3	-1	Yes	1245.56	3
"C2H3-C2H5 (C1-C5)"	7.79095	1	-1	Yes	835.944	2

Electronic
Level(degeneracy)

0

Geometry
N, Symbol, Bond [A], Ref.Atom, Angle, Ref.Atom, Dihedral Angle, Ref.Atom

1	C	0	0	0	0	0	0
2	C	1.5382	1	0	2	0	3
3	H	1.1005	1	108.68	2	0	3
4	H	1.0974	1	109.9	2	116.24	3
5	C	1.5049	1	112.74	2	-121.2	3
6	C	1.3334	5	125.42	1	-119.67	2
7	H	1.0922	5	115.62	1	59.57	2
8	H	1.0869	6	121.89	5	179.59	1
9	H	1.0885	6	121.63	5	-0.6	1
10	H	1.0956	2	110.93	1	-177.25	3
11	H	1.0959	2	111.03	1	-56.95	3
12	H	1.0968	2	111.18	1	62.99	3

Bonds
Atom, Atom, Type (1, 2, 3), Length [A]

C1	C2	1	1.5382
C1	H3	1	1.1005
C1	H4	1	1.0974
C1	C5	1	1.5049
C2	H10	1	1.0956
C2	H11	1	1.0959
C2	H12	1	1.0968
C5	C6	1	1.3334
C5	H7	1	1.0922
C6	H8	1	1.0869
C6	H9	1	1.0885

Comment
g3mp2b3 geom freq 0.96
torsions 235 109
rotors
(1) CH3 14.9 (3)
(1) C2H5 10.0 (2)

Expt So
307.9 (TRC)
308.0 (S&P)
calc 308.0
DfH298 -0.6 kJ webbook

Component
Name=ch3
Atomic composition=H3C1
Type=0
Mass=15.0348
Enthalpy(298), 1/cm=12263.3

Frequencies
Frequency(degeneracy)

3186.18 3185.39 3018.1 1374.03 1373.63
434.448

Rotors
*Name, Moment of Inertia [amu*A*²], Symmetry, Dimension, Active [Yes/No], Hindrance [1/cm], Minima*

"Ia"	3.54492	12	1	Yes	0	1
"IbIc"	1.77246	1	2	No	0	1

Electronic
Level(degeneracy)

0(2)

Geometry
N, Symbol, Bond [A], Ref.Atom, Angle, Ref.Atom, Dihedral Angle, Ref.Atom

1	C	0	0	0	0	0	0
2	H	1.08268	1	0	0	0	0
3	H	1.08277	1	120.012	2	0	0
4	H	1.08277	1	120.012	2	179.939	3

Bonds
Atom, Atom, Type (1, 2, 3), Length [A]

C1	H2	1	1.08268
C1	H3	1	1.08277
C1	H4	1	1.08277

Comment
g3mp2b3 geom freq 0.96
torsions (452 inv)

Component
Name=ethene
Atomic composition=H4C2
Type=0

Mass=28.0538
Enthalpy(298), 1/cm=4380.34

Frequencies
Frequency(degeneracy)

3118.93	3094.4	3041.44	3026.6	1652.01
1434.43	1340.19	1198.3	1027.03	936.256
917.562	801.88			

Rotors
*Name, Moment of Inertia [amu*A*²], Symmetry, Dimension, Active [Yes/No], Hindrance [1/cm], Minima*

"Ia"	3.44063	4	1	Yes	0	1
"IbIc"	18.466	1	2	No	0	1

Electronic
Level(degeneracy)

0

Geometry
N, Symbol, Bond [A], Ref.Atom, Angle, Ref.Atom, Dihedral Angle, Ref.Atom

1	C	0	0	0	0	0	0
2	C	1.33079	1	0	0	0	0
3	H	1.08743	1	121.862	2	0	0
4	H	1.08742	1	116.305	3	180	2
5	H	1.08743	2	121.833	1	0	3
6	H	1.08743	2	121.835	1	180	3

Bonds
Atom, Atom, Type (1, 2, 3), Length [A]

C1	C2	1	1.33079
C1	H3	1	1.08743
C1	H4	1	1.08742
C2	H5	1	1.08743
C2	H6	1	1.08743

Component
Name=ethyl
Atomic composition=H5C2
Type=0
Mass=29.0617
Enthalpy(298), 1/cm=9967.79

Frequencies
Frequency(degeneracy)

3134.88	3042.27	2978.49	2935.88	2847.76
1454.25	1450.24	1433.16	1372.53	1159.19
1031.53	954.632	785.395	439.766	

Rotors
*Name, Moment of Inertia [amu*A*²], Symmetry, Dimension, Active [Yes/No], Hindrance [1/cm], Minima*

"Ia"	4.89188	1	1	Yes	0	1
"IbIc"	23.1858	1	2	No	0	1
"CH2-CH3 (C1-C5)"	1.12222	6	1	Yes	0	1

Electronic
Level(degeneracy)

0(2)

Geometry
N, Symbol, Bond [A], Ref.Atom, Angle, Ref.Atom, Dihedral Angle, Ref.Atom

1	C	0	0	0	0	0	0	0
2	H	1.09731	1	0	0	0	0	0
3	H	1.09677	1	108.006	2	0	0	0
4	H	1.10515	1	106.306	2	113.913	3	0
5	C	1.48948	1	111.796	2	-123.409	3	0
6	H	1.0854	5	120.999	1	153.658	2	0
7	H	1.08553	5	120.887	1	169.87	6	0

Bonds
Atom, Atom, Type (1, 2, 3), Length [A]

C1	H2	1	1.09731
C1	H3	1	1.09677
C1	H4	1	1.10515
C1	C5	1	1.48947
C5	H6	1	1.0854
C5	H7	1	1.08553

Comment
g3mp2b3 geom freq 0.96
torsions 121 (458 inv)
(1) CH2 free (6)*

Component

Name=ethyl#cc-h (ethyl = ethene + h)
Atomic composition=H5C2
Type=1
Mass=43.0886

Frequencies

Frequency(degeneracy)

3125.43	3101.09	3044.43	3031.96	1623.99
1433.04	1328.86	1197.62	1017.17	936.892
911.106	801.033	234.695	197.411	

Rotors

*Name, Moment of Inertia [amu*A*²], Symmetry, Dimension, Active [Yes/No], Hindrance [1/cm], Minima*

"Ia"	7.91793	1	1	Yes	0	1
"IbIc"	22.8864	1	2	No	0	1

Electronic

Level(degeneracy)

0(2)

Geometry

N, Symbol, Bond [A], Ref.Atom, Angle, Ref.Atom, Dihedral Angle, Ref.Atom

1	C	0	0	0	0	0	0
2	H	1.08686	1	0	0	0	0
3	H	1.08686	1	116.31	2	0	0
4	H	2.33036	1	84.17	2	80.538	3
5	C	1.33669	1	121.791	2	-176.334	3
6	H	1.08712	5	121.787	1	178.529	2
7	H	1.08712	5	121.788	1	179.077	6

Bonds

Atom, Atom, Type (1, 2, 3), Length [A]

C1	H2	1	1.08686
C1	H3	1	1.08686
C1	C5	1	1.33669
C5	H6	1	1.08712
C5	H7	1	1.08713

Comment

g3mp2b3 geom freq 0.96

-196 img freq

Component
Name=H
Atomic composition=H1
CAS=JCODE = 288
Type=0
Mass=1.00794
Enthalpy(298), 1/cm=18223.6
Beta=unknown
Sigma, A=5.03638
Epsilon, K=412.68

Electronic
Level(degeneracy)

0(2)

Comment

Component
Name=pent1ene
Atomic composition=H10C5
Type=0
Mass=70.1344
Enthalpy(298), 1/cm=-1839.08

Frequencies
Frequency(degeneracy)

3104	3029.11	3008.51	2988.31	2983.72
2951.79	2933.86	2920.22	2912.66	2888.67
1663.83	1477.67	1467.95	1462.11	1449.92
1416.64	1381.94	1346.42	1292.05	1282.91
1260.53	1230.99	1161.08	1079.09	1018.12
1000.9	991.448	920.939	899.702	859.928
848.321	725.953	618.531	418.948	367.94
221.99				

Rotors
*Name, Moment of Inertia [amu*A*²], Symmetry, Dimension, Active [Yes/No], Hindrance [1/cm], Minima*

"Ia"	27.7434	1	1	Yes	0	1
"IbIc"	242.473	1	2	No	0	1
"CHCH4-	14.8965	1	1	Yes	1880.87	3

CH2C2H3 (C1-C2)"						
"C2H3-C2HCH6 (C1-C5)"	8.7823	1	1	Yes	927.897	2
"CH3-C2H2C2H5 (C2-C11)"	2.86232	3	1	Yes	1245.56	3

Electronic
Level(degeneracy)

0

Geometry
N, Symbol, Bond [A], Ref.Atom, Angle, Ref.Atom, Dihedral Angle, Ref.Atom

1	C	0	0	0	0	0	0
2	C	1.5408	1	0	2	0	3
3	H	1.1015	1	108.42	2	0	3
4	H	1.0983	1	109.61	2	-244.12	3
5	C	1.5044	1	113.05	2	-121.39	3
6	C	1.3335	5	125.39	1	-119.14	2
7	H	1.0921	5	115.68	1	-299.92	2
8	H	1.0869	6	121.89	5	-180.47	1
9	H	1.0885	6	121.62	5	-0.7	1
10	H	1.0979	2	108.93	1	180.82	3
11	C	1.5318	2	112.87	1	303.14	3
12	H	1.099	2	109.21	1	65.28	3
13	H	1.0959	11	111.34	2	-179.87	1
14	H	1.0969	11	111.18	2	-59.79	1
15	H	1.0971	11	111.21	2	60	1

Bonds
Atom, Atom, Type (1, 2, 3), Length [A]

C1	C2	1	1.5408
C1	H3	1	1.1015
C1	H4	1	1.0983
C1	C5	1	1.5044
C2	H10	1	1.0979
C2	C11	1	1.5318
C2	H12	1	1.099
C5	C6	1	1.3335
C5	H7	1	1.0921

C6	H8	1	1.0869
C6	H9	1	1.0885
C11	H13	1	1.0959
C11	H14	1	1.0969
C11	H15	1	1.0971

Comment
g3mp2b3 geom freq 0.96
torsions 97, 105, 251
rotors
(1) CH3 14.9 (3)
(1) C2H5 22.5 (3)
(1) C3H7-Cd 11.1 (2)
expt So = 347.4 (S&P)
347.1 TRC

Component
Name=pent1yl
Atomic composition=H11C5
Type=0
Mass=71.1423
Enthalpy(298), 1/cm=4940.43
Beta=unknown
Sigma, A=5.5828
Epsilon, K=388.93

Frequencies
Frequency(degeneracy)

3125.89	3033.6	2985.87	2983.18	2955.46
2930.23	2923.45	2920.56	2912.41	2902.72
2894.34	1480.18	1468.09	1467.82	1456.97
1454.1	1430.96	1382.81	1350.88	1306.61
1291.64	1286.64	1233.01	1225.37	1162.95
1078.16	1036.5	1016.31	955.363	939.254
868.512	830.946	738.127	709.876	502.777
381.271	351.011	173.008		

Rotors
*Name, Moment of Inertia [amu*A*²], Symmetry, Dimension, Active [Yes/No], Hindrance [1/cm], Minima*

"Ia"	28.5015	1	1	Yes	0	1
"IbIc"	260.456	1	2	No	0	1
"C2H5-C3H6 (C1-C2)"	12.1053	1	-1	Yes	1880.87	3

"CH3-C4H8 (C1-C4)"	2.90032	3	-1	Yes	1245.56	3
"C2H4-C3H7 (C2-C3)"	11.9752	1	-1	Yes	1880.87	3
"CH2-C4H9 (C3-C5)"	1.66226	2	1	Yes	0	1

Electronic
Level(degeneracy)

0(2)

Geometry
N, Symbol, Bond [A], Ref.Atom, Angle, Ref.Atom, Dihedral Angle, Ref.Atom

1	C	0	0	0	0	0	0
2	C	1.53404	1	0	0	0	0
3	C	1.55162	2	112.967	1	0	0
4	C	1.5322	1	113.118	2	180.005	3
5	C	1.49141	3	113.768	2	179.99	1
6	H	1.09936	1	109.218	2	57.784	3
7	H	1.09936	1	109.218	2	302.226	3
8	H	1.09889	2	109.635	1	238.112	3
9	H	1.0989	2	109.633	1	121.884	3
10	H	1.0997	3	108.119	2	57.46	1
11	H	1.09966	3	108.13	2	302.53	1
12	H	1.09612	4	111.416	1	179.992	2
13	H	1.09696	4	111.179	1	300.12	2
14	H	1.09696	4	111.178	1	59.865	2
15	H	1.08622	5	120.897	3	84.254	2
16	H	1.08624	5	120.887	3	276.033	2

Bonds
Atom, Atom, Type (1, 2, 3), Length [A]

C1	C2	1	1.53404
C1	C4	1	1.5322
C1	H6	1	1.09936
C1	H7	1	1.09936
C2	C3	1	1.55162
C2	H8	1	1.09889
C2	H9	1	1.0989
C3	C5	1	1.49141
C3	H10	1	1.0997
C3	H11	1	1.09966

C4	H12	1	1.09612
C4	H13	1	1.09696
C4	H14	1	1.09696
C5	H15	1	1.08622
C5	H16	1	1.08624

Collision
Buffer gas, Collision Model, Expression, Alpha0 [/cm], Alpha1 [K/cm], Alpha2

"Argon" 0 0 unknown 0.675 unknown

Comment
g3mp2b3 geom freq 0.96
torsions 246 128 119 87 (inv 524)
rotors
(1) CH3 14.9 (3)
(2) R 22.5 (3)
(1) CH2* free (2)
L-J parameters from interpolation between pentane and pentene
Ia = 28.5015 amu A2; Ib=Ic = 260.456; Iabc = 1933470

Component
Name=pent1yl#cc^h%3 (pent1yl = pent3yl)
Atomic composition=H11C5
Type=1
Mass=71.1423
Enthalpy(298), 1/cm=16886.1

Frequencies
Frequency(degeneracy)

3087.54	2996.72	2992.22	2991.86	2985.67
2979.25	2948.31	2923.49	2912.86	2859.28
1683.54	1473.55	1465.6	1459.37	1449.14
1395.6	1381.7	1348.51	1306.28	1269.66
1242.93	1217.33	1188.21	1143.69	1074.05
1052.04	993.002	961.705	948.949	904.538
854.038	827.293	761.629	709.158	595.465
414.466	352.8	227.895	98	

Rotors
*Name, Moment of Inertia [amu*A*²], Symmetry, Dimension, Active [Yes/No], Hindrance [1/cm], Minima*

"Ia"	42.0087	1	1	Yes	0	1
"IbIc"	221.295	1	2	No	0	1

"C2H5-C3H5 (C3-C4)"	14.4332	1	-1	Yes	2089.86	2
"CH3-C4H7 (C4-C5)"	2.99417	3	-1	Yes	1170.32	3

Electronic
Level(degeneracy)

0(4)

Geometry
N, Symbol, Bond [A], Ref.Atom, Angle, Ref.Atom, Dihedral Angle, Ref.Atom

1	C	0	0	0	0	0	0
2	C	1.5316	1	0	2	0	3
3	C	1.5375	2	92.85	1	0	3
4	C	1.5108	3	119.78	2	-245.91	1
5	C	1.5324	4	113.56	3	192.38	2
6	H	1.0899	1	118.09	2	-109.46	3
7	H	1.0898	1	117.86	2	105.37	3
8	H	1.0943	2	114.51	1	-118.64	3
9	H	1.0953	2	113.49	1	116.64	3
10	H	1.094	3	114.78	2	-101.71	1
11	H	1.4042	3	81.72	2	-358.52	1
12	H	1.0999	4	109.25	3	-44.78	2
13	H	1.104	4	109.19	3	70.08	2
14	H	1.0969	5	111.09	4	-58.87	3
15	H	1.0961	5	110.94	4	-299.25	3
16	H	1.0959	5	111.33	4	-178.9	3

Bonds
Atom, Atom, Type (1, 2, 3), Length [A]

C1	C2	1	1.5316
C1	H6	1	1.0899
C1	H7	1	1.0898
C2	C3	1	1.5375
C2	H8	1	1.0943
C2	H9	1	1.0953
C3	C4	1	1.5108
C3	H10	1	1.094
C4	C5	1	1.5324
C4	H12	1	1.0999
C4	H13	1	1.104
C5	H14	1	1.0969

C5	H15	1	1.0961
C5	H16	1	1.0959

Comment
g3mp2b3 geom freq 0.96
-2032 img freq
99 C2H5-Cd'; 242 CH3-R
25, 14 kJ/mol
electronic set to 4 to account for optically active TS

Component
Name=pent1yl#cc^h%4 (pent1yl = pent2yl)
Atomic composition=H11C5
Type=1
Mass=71.1423
Enthalpy(298), 1/cm=12681.3

Frequencies
Frequency(degeneracy)

3061.3	2984.27	2982.3	2964.82	2956.22
2946.64	2943.67	2921.74	2910.2	2884.36
1577.54	1468.37	1461.09	1456	1453.2
1424.19	1387.48	1374.19	1330.03	1298.54
1266.71	1205.86	1184.73	1145.05	1087.68
1058.53	997.217	966.357	951.628	889.921
862.793	843.664	827.503	776.18	546.592
516.362	458.244	323.337	209.163	69.7

Rotors
*Name, Moment of Inertia [amu*A*²], Symmetry, Dimension, Active [Yes/No], Hindrance [1/cm], Minima*

"Ia"	55.8014	1	1	Yes	0	1
"IbIc"	179.918	1	2	No	0	1
"CH3-C4H7 (C4-C5)"	3.00511	3	-1	Yes	710.552	3

Electronic
Level(degeneracy)

0(4)

Geometry
N, Symbol, Bond [A], Ref.Atom, Angle, Ref.Atom, Dihedral Angle, Ref.Atom

1	C	0		0	0		0	0		0

2	C	1.5236	1	0	2	0	3
3	C	1.5509	2	105	1	0	3
4	C	1.5282	3	105.15	2	37.55	1
5	C	1.5098	4	119.28	3	-146	2
6	H	1.0975	2	113.45	1	-122.89	3
7	H	1.0977	2	109.65	1	-242.39	3
8	H	1.3644	4	92.45	3	-27.25	2
9	H	1.0902	1	118.38	2	-142	3
10	H	1.0928	1	115.76	2	79.59	3
11	H	1.0961	4	112.98	3	76.64	2
12	H	1.0991	3	109.41	2	-79.57	1
13	H	1.0979	3	112.69	2	161.56	1
14	H	1.1018	5	111.6	4	292.78	3
15	H	1.0973	5	111.31	4	52.22	3
16	H	1.0963	5	111.67	4	172.95	3

Bonds
Atom, Atom, Type (1, 2, 3), Length [A]

C1	C2	1	1.5236
C1	H9	1	1.0902
C1	H10	1	1.0928
C2	C3	1	1.5509
C2	H6	1	1.0975
C2	H7	1	1.0977
C3	C4	1	1.5282
C3	H12	1	1.0991
C3	H13	1	1.0979
C4	C5	1	1.5098
C4	H11	1	1.0961
C5	H14	1	1.1018
C5	H15	1	1.0973
C5	H16	1	1.0963

Comment
g3mp2b3 geom freq 0.96
-1792 mg freq
188 cm-1 CH3-Cd'
8.5 kJ.mol
electronic set to 4 to account for optically active TS

Component
Name=pent1yl#cc-c (pent1yl = ethene + prop1yl)
Atomic composition=H11C5
Type=1

Mass=71.1423
Enthalpy(298), 1/cm=14712.6

Frequencies
Frequency(degeneracy)

3121.94	3099.28	3096.74	3037.81	3028.72
3013.92	2992.49	2983.21	2934.95	2919.57
2903	1546.26	1474.61	1465.42	1454.34
1438.07	1428.91	1373.89	1301.38	1278.17
1265.79	1197.89	1174.25	1071.82	998.703
985.964	909.333	882.004	870.091	823.222
791.756	751.363	728.675	530.088	357.813
356.089	229.668	171		

Rotors
*Name, Moment of Inertia [amu*A*²], Symmetry, Dimension, Active [Yes/No], Hindrance [1/cm], Minima*

"Ia"	30.0078	1	1	Yes	0	1
"IbIc"	319.342	1	2	No	0	1
"C2H4-C3H7 (C2-C3)"	12.0563	1	-1	Yes	501.566	2
"C2H5-C3H6 (C3-C4)"	16.0572	1	-1	Yes	1253.92	2
"CH3-C4H8 (C4-C5)"	2.87599	3	-1	Yes	1253.92	3

Geometry
N, Symbol, Bond [A], Ref.Atom, Angle, Ref.Atom, Dihedral Angle, Ref.Atom

1	C	0	0	0	0	0	0
2	C	1.358	1	0	2	0	3
3	C	2.3372	2	111.27	1	0	3
4	C	1.5005	3	105.33	2	-180	1
5	C	1.5442	4	113.09	3	180	2
6	H	1.0868	1	121.68	2	87.69	3
7	H	1.0868	1	121.68	2	-87.69	3
8	H	1.0865	2	120.66	1	100.33	3
9	H	1.0865	2	120.66	1	-100.33	3
10	H	1.0881	3	98.05	2	58.02	1
11	H	1.0881	3	98.05	2	-58.01	1
12	H	1.0991	4	109.96	3	58.4	2
13	H	1.0991	4	109.96	3	301.6	2
14	H	1.0971	5	110.94	4	180	3

15	H	1.0961	5	111.08	4	59.93	3
16	H	1.0961	5	111.08	4	-59.93	3

Bonds
Atom, Atom, Type (1, 2, 3), Length [A]

C1	C2	1	1.358
C1	H6	1	1.0868
C1	H7	1	1.0868
C2	C3	1	2.3372
C2	H8	1	1.0865
C2	H9	1	1.0865
C3	C4	1	1.5005
C3	H10	1	1.0881
C3	H11	1	1.0881
C4	C5	1	1.5442
C4	H12	1	1.0991
C4	H13	1	1.0991
C5	H14	1	1.0971
C5	H15	1	1.0961
C5	H16	1	1.0961

Collision
Buffer gas, Collision Model, Expression, Alpha0 [/cm], Alpha1 [K/cm], Alpha2

"Argon" 0 0 600 unknown unknown

Comment
g3mp2b3 geom freq 0.96
-343 img freq

Rotors
54 cm-1 corresponds to C3H7--Cd; 73 cm-1 corresponds to C2H5--Cd; 255 cm-1 corresponds to CH3-R

Component
Name=pent1yl#cc-h (pent1yl = pent1ene + h)
Atomic composition=H11C5
Type=1
Mass=71.1423

Frequencies
Frequency(degeneracy)

3113.77	3033.48	3023.11	2989.64	2985.54
2959.03	2938.21	2922.59	2917.67	2910.25

1598.55	1478.19	1469.04	1463.34	1453.75
1410.33	1384.19	1343.48	1289.21	1273.64
1256.68	1231.35	1159.59	1077.17	1014.92
1001.99	985.252	915.739	878.073	859.177
848.143	726.084	615.029	422.669	390.07
366.684	320.677	205.735		

Rotors

*Name, Moment of Inertia [amu*A*²], Symmetry, Dimension, Active [Yes/No], Hindrance [1/cm], Minima*

"Ia"	34.9401	1	1	Yes	0	1
"IbIc"	243.329	1	2	No	0	1
"C2H3-C3H7 (C2-C3)"	9.39795	1	1	Yes	1128.52	2
"C2H5-C3H5 (C3-C4)"	15.8438	1	1	Yes	1170.32	3
"CH3-C4H7 (C4-C5)"	2.91657	3	1	Yes	1203.76	3

Electronic

Level(degeneracy)

0(2)

Geometry

N, Symbol, Bond [A], Ref.Atom, Angle, Ref.Atom, Dihedral Angle, Ref.Atom

1	C	0	0	0	0	0	0
2	C	1.34764	1	0	0	0	0
3	C	1.50906	2	124.525	1	0	0
4	C	1.5415	3	112.283	2	103.366	1
5	C	1.53189	4	112.695	3	178.093	2
6	H	1.08791	1	121.433	2	8.466	3
7	H	1.0863	1	121.75	2	-174.491	3
8	H	1.09067	2	118.564	1	167.752	3
9	H	2.0543	2	98.681	1	-105.809	3
10	H	1.09805	3	109.612	2	-18.603	1
11	H	1.09803	3	109.815	2	-135.448	1
12	H	1.09901	4	109.242	3	56.082	2
13	H	1.09789	4	109.034	3	-59.541	2
14	H	1.09583	5	111.302	4	179.863	3
15	H	1.09691	5	111.202	4	59.773	3
16	H	1.0969	5	111.169	4	-60.025	3

Bonds
Atom, Atom, Type (1, 2, 3), Length [A]

C1	C2	1	1.34764
C1	H6	1	1.08791
C1	H7	1	1.0863
C2	C3	1	1.50906
C2	H8	1	1.09067
C3	C4	1	1.5415
C3	H10	1	1.09805
C3	H11	1	1.09803
C4	C5	1	1.53189
C4	H12	1	1.09901
C4	H13	1	1.09789
C5	H14	1	1.09583
C5	H15	1	1.09691
C5	H16	1	1.0969

Comment
g3mp2b3 geom freq 0.96
-506 img freq
Rotors
90 cm-1 corresponds to CH3-Cd'; 105 cm-1 corresponds to C2H5-R; 250 cm-1 corresponds to CH3-R
13.5, 14, 14.4 kJ/mol

Component
Name=pent2ene-e
Atomic composition=H10C5
Type=0
Mass=70.1344
Enthalpy(298), 1/cm=-2624.86

Frequencies
Frequency(degeneracy)

3011.01	2998.14	2994.25	2987.75	2986.23
2951.1	2943.2	2923.71	2907.93	2896.13
1689.17	1475.89	1466.82	1462.68	1451.61
1449.85	1385.35	1379.33	1332.03	1294.94
1280.84	1238.88	1143.54	1067.75	1047.51
1035.5	997.501	971.731	921.655	856.853
781.922	738.371	469.818	392.438	294.35
167.191				

Rotors
*Name, Moment of Inertia [amu*A*²], Symmetry, Dimension, Active [Yes/No], Hindrance [1/cm], Minima*

"Ia"	29.4173	1	1	Yes	0	1
"IbIc"	247.267	1	2	No	0	1
"CH3-CH2C3H5 (C1-C2)"	2.98654	3	-1	Yes	1245.56	3
"C2H5-C3H5 (C1-C5)"	9.42576	1	-1	Yes	802.506	2
"CH3-C4H7 (C6-C8)"	2.87318	3	-1	Yes	743.99	3

Electronic
Level(degeneracy)

0

Geometry
N, Symbol, Bond [A], Ref.Atom, Angle, Ref.Atom, Dihedral Angle, Ref.Atom

1	C	0	0	0	0	0	0	0
2	C	1.53829	1	0	0	0	0	0
3	H	1.10065	1	108.563	2	0	0	0
4	H	1.09762	1	109.797	2	115.97	3	0
5	C	1.50513	1	112.826	2	-121.422	3	0
6	C	1.33564	5	125.476	1	240.514	2	0
7	H	1.09309	5	118.734	6	180.813	1	0
8	C	1.50242	6	125.335	5	0.377	7	0
9	H	1.09215	6	118.633	5	180.203	7	0
10	H	1.0957	2	110.921	1	182.96	3	0
11	H	1.09613	2	111.136	1	120.381	10	0
12	H	1.09681	2	111.124	1	-119.668	10	0
13	H	1.0987	8	111.338	6	239.136	5	0
14	H	1.09543	8	111.526	6	120.654	13	0
15	H	1.09872	8	111.353	6	-118.708	13	0

Bonds
Atom, Atom, Type (1, 2, 3), Length [A]

C1	C2	1	1.53829
C1	H3	1	1.10065
C1	H4	1	1.09762
C1	C5	1	1.50513
C2	H10	1	1.09571

C2	H11	1	1.09613
C2	H12	1	1.09681
C5	C6	1	1.33564
C5	H7	1	1.09309
C6	C8	1	1.50242
C6	H9	1	1.09215
C8	H13	1	1.0987
C8	H14	1	1.09543
C8	H15	1	1.09872

Comment
g3mp2b3 geom freq 0.96
torsions 94, 210, 215
rotors
(1) CH3 14.9 kJ/mol (sigma = 3) (torsion 251 cm-1)
(1) CH3-Cd 8.9 (3) (torsion 198 cm-1)
(1) C2H5-Cd 9.6 (2) (torsion 76 cm-1)

Expt So 343.2 (TRC)
calc 343.2

Component
Name=pent2ene-z
Atomic composition=H10C5
Type=0
Mass=70.1344
Enthalpy(298), 1/cm=-2215.25

Frequencies
Frequency(degeneracy)

3026.77	3008.43	2999.75	2994.27	2987.59
2961.87	2952.49	2923.82	2912.37	2898.77
1679.84	1476.62	1466.96	1464.54	1453.98
1450.72	1402.15	1379.69	1374.9	1301.36
1263.23	1242.75	1136.45	1059.56	1032.62
1019.18	995.289	973.286	908.354	835.62
768.328	696.496	549.712	453.137	293.282
250.028				

Rotors
*Name, Moment of Inertia [amu*A*²], Symmetry, Dimension, Active [Yes/No], Hindrance [1/cm], Minima*

"Ia"	45.2658	1	1	Yes	0	1
"IbIc"	208.035	1	2	No	0	1
"CH3-	3.01504	3	-1	Yes	1245.56	3

CH2C2HCH4 (C1-C2)"						
"C2H5-C2HCH4 (C1-C5)"	17.1018	1	-1	Yes	434.691	2
"CH3-C4H7 (C6-C9)"	3.05321	3	-1	Yes	334.377	3

Electronic
Level(degeneracy)

0

Geometry
N, Symbol, Bond [A], Ref.Atom, Angle, Ref.Atom, Dihedral Angle, Ref.Atom

1	C	0	0	0	0	0	0
2	C	1.53874	1	0	0	0	0
3	H	1.10059	1	108.581	2	0	0
4	H	1.09545	1	109.509	2	115.487	3
5	C	1.50601	1	112.437	2	-120.593	3
6	C	1.33863	5	128.305	1	239.893	2
7	H	1.09184	5	117.284	6	180.852	1
8	H	1.09093	6	117.288	5	0.364	7
9	C	1.50368	6	128.054	5	180.062	7
10	H	1.09867	9	110.82	6	240.448	5
11	H	1.09341	9	112.984	6	120.98	10
12	H	1.09851	9	110.788	6	-117.956	10
13	H	1.0957	2	110.963	1	182.937	3
14	H	1.09611	2	111.108	1	120.373	13
15	H	1.09677	2	111.117	1	-119.651	13

Bonds
Atom, Atom, Type (1, 2, 3), Length [A]

C1	C2	1	1.53874
C1	H3	1	1.10059
C1	H4	1	1.09545
C1	C5	1	1.50601
C2	H13	1	1.0957
C2	H14	1	1.09611
C2	H15	1	1.09677
C5	C6	1	1.33863
C5	H7	1	1.09184
C6	H8	1	1.09093

C6	C9	1	1.50368
C9	H10	1	1.09867
C9	H11	1	1.09341
C9	H12	1	1.0985

Comment
g3mp2b3 geom freq 0.96
torsions 57, 140, 220
rotors
(1) CH3 14.9 kJ/mol (sigma = 3) (torsion 250 cm-1)
(1) CH3-Cd 4.0 (3) (torsion 129)
(1) C2H5-Cd 5.2 (3) (torsion 41)

Expt So 347.4 (TRC)
calc 347.4

Component
Name=pent2yl
Atomic composition=H11C5
Type=0
Mass=71.1423
Enthalpy(298), 1/cm=3903.86
Beta=unknown
Sigma, A=5.5828
Epsilon, K=388.93

Frequencies
Frequency(degeneracy)

3037.44	2987.09	2981.43	2977.64	2942.41
2923.45	2919.31	2910.4	2884.53	2837.99
2799.77	1476.78	1468.61	1460.41	1456.79
1445.71	1439.2	1385.21	1380.99	1373.85
1331.22	1280.27	1248.99	1213.19	1137.95
1101.16	1062.84	1023.7	1006.53	955.202
901.329	849.188	829.515	712.979	406.426
386.54	373.919	185.438		

Rotors
*Name, Moment of Inertia [amu*A*²], Symmetry, Dimension, Active [Yes/No], Hindrance [1/cm], Minima*

"Ia"	28.0183	1	1	Yes	0	1
"IbIc"	260.456	1	2	No	0	1
"C2H5-C3H6 (C1-C2)"	12.5348	1	-1	Yes	1880.87	3

"CH3-C4H8 (C1-C4)"	2.8748	3	-1	Yes	1245.56	3
"C2H4-C3H7 (C2-C3)"	10.8264	1	-1	Yes	334.377	2
"CH3-C4H8 (C3-C5)"	2.84639	3	-1	Yes	334.377	3

Electronic
Level(degeneracy)

0(2)

Geometry
N, Symbol, Bond [A], Ref.Atom, Angle, Ref.Atom, Dihedral Angle, Ref.Atom

1	C	0	0	0	0	0	0
2	C	1.53718	1	0	0	0	0
3	C	1.49509	2	113.946	1	0	0
4	C	1.53135	1	113.21	2	180.919	3
5	C	1.49283	3	121.771	2	195.987	1
6	H	1.09817	1	109.009	2	58.452	3
7	H	1.09915	1	108.981	2	303.042	3
8	H	1.10224	2	109.543	1	236.831	3
9	H	1.10898	2	108.385	1	123.202	3
10	H	1.0892	3	117.96	2	31.764	1
11	H	1.09596	4	111.401	1	179.72	2
12	H	1.09711	4	111.221	1	299.806	2
13	H	1.09716	4	111.209	1	59.579	2
14	H	1.09907	5	111.578	3	43.995	2
15	H	1.10602	5	112.293	3	285.034	2
16	H	1.09612	5	111.886	3	165.127	2

Bonds
Atom, Atom, Type (1, 2, 3), Length [A]

C1	C2	1	1.53718
C1	C4	1	1.53135
C1	H6	1	1.09817
C1	H7	1	1.09915
C2	C3	1	1.49509
C2	H8	1	1.10224
C2	H9	1	1.10897
C3	C5	1	1.49283
C3	H10	1	1.0892
C4	H11	1	1.09596

C4	H12	1	1.09711
C4	H13	1	1.09715
C5	H14	1	1.09907
C5	H15	1	1.10602
C5	H16	1	1.09612

Collision
Buffer gas, Collision Model, Expression, Alpha0 [/cm], Alpha1 [K/cm], Alpha2

"Argon" 0 0 unknown 0.675 unknown

Comment
g3mp2b3 geom freq 0.96
torsions 249 127 99 56 (423)
rotors
(1) CH3 14.9 (3)
(1) R 22.5 (3)
(1) CH3-C* 4.0 (3)
(1) R-C* 4.0 (2)

L-J parameters from interpolation between pentane and pentene
Pent2yl Original Ia = 26.3146; Ib=Ic = 268.755; Iabc = 1 900 683.823
K-rotor matching: Set Ib=Ic = 260.456 from 1-pentyl and Ia to 28.0183 to match original Iabc

Component
Name=pent2yl#cc-c (pent2yl = propene + ethyl)
Atomic composition=H11C5
Type=1
Mass=71.1423
Enthalpy(298), 1/cm=13814.8

Frequencies
Frequency(degeneracy)

3107.24	3101.74	3027.47	3023.06	3019.1
2983.42	2974.28	2936.88	2935.85	2895.77
2864.31	1550.86	1461.84	1458.01	1453.35
1446.88	1438.13	1399.99	1375.02	1371.98
1251.14	1179.95	1152.73	1032.51	1016.6
992.39	962.269	904.326	892.139	852.241
799.611	736.733	637.472	511.33	405.435
263.046	200	164.141		

Rotors
*Name, Moment of Inertia [amu*A*²], Symmetry, Dimension, Active [Yes/No], Hindrance [1/cm], Minima*

"Ia" 44.5015 1 1 Yes 0 1

"IbIc"	285.347	1	2	No	0	1
"C2H5-C3H6 (C1-C2)"	16.8852	1	-1	Yes	417.972	2
"CH3-C4H8 (C1-C4)"	2.99255	3	-1	Yes	585.161	3
"CH3-C4H8 (C3-C5)"	3.05032	3	-1	Yes	417.972	3

Electronic
Level(degeneracy)

0(2)

Geometry
N, Symbol, Bond [A], Ref.Atom, Angle, Ref.Atom, Dihedral Angle, Ref.Atom

1	C	0	0	0	0	0	0
2	C	2.3343	1	0	0	0	0
3	C	1.36039	2	111.172	1	0	0
4	C	1.49809	1	105.198	2	179.181	3
5	C	1.49974	3	124.616	2	272.962	1
6	H	1.08749	1	98.066	2	57.237	3
7	H	1.0874	1	98.092	2	301.132	3
8	H	1.08765	2	87.88	1	238.163	3
9	H	1.08604	2	88.212	1	122.263	3
10	H	1.09034	3	118.823	2	88.201	1
11	H	1.10367	4	111.953	1	179.885	2
12	H	1.09722	4	111.784	1	299.445	2
13	H	1.09723	4	111.771	1	60.335	2
14	H	1.09586	5	111.492	3	-6.155	2
15	H	1.09923	5	111.463	3	233.223	2
16	H	1.10033	5	111.708	3	114.463	2

Bonds
Atom, Atom, Type (1, 2, 3), Length [A]

C1	C2	1	2.3343
C1	C4	1	1.49809
C1	H6	1	1.08749
C1	H7	1	1.0874
C2	C3	1	1.36039
C2	H8	1	1.08765
C2	H9	1	1.08604
C3	C5	1	1.49974
C3	H10	1	1.09034

C4	H11	1	1.10367
C4	H12	1	1.09722
C4	H13	1	1.09723
C5	H14	1	1.09586
C5	H15	1	1.09923
C5	H16	1	1.10033

Collision
Buffer gas, Collision Model, Expression, Alpha0 [/cm], Alpha1 [K/cm], Alpha2

"Argon" 0 0 600 unknown unknown

Comment
g3mp2b3 geom freq 0.96
-376 img freq
Rotors

39 cm-1 corresponds to C2H5--Cd; 145 cm-1 corresponds to CH3-CH2'; 171 cm-1 corresponds to CH3-Cd corresponds to 5, 5, 7 kJ/mol

Component
Name=pent2yl#cc-h%1 (pent2yl = pent1ene + h)
Atomic composition=H11C5
Type=1
Mass=71.1423
Enthalpy(298), 1/cm=0

Frequencies
Frequency(degeneracy)

3117.19	3036.86	3020.55	2989.81	2984.78
2952.34	2935.3	2921.4	2913.09	2881.61
1575.7	1477.27	1468.12	1461.33	1448.27
1410.65	1382.61	1344.68	1288.42	1269.96
1255.31	1227.96	1161.51	1073.95	1016.07
1001.23	967.189	941.138	917.968	861.152
846.309	724.823	688.096	454.22	426.441
364.591	334.753	211.614		

Rotors
*Name, Moment of Inertia [amu*A*²], Symmetry, Dimension, Active [Yes/No], Hindrance [1/cm], Minima*

"Ia"	30.0075	1	1	Yes	0	1
"IbIc"	257.478	1	2	No	0	1
"C2H5-C3H5	14.7373	1	1	Yes	1170.32	3

(C1-C2)"						
"CH3-C4H7 (C1-C4)"	2.89203	3	1	Yes	1170.32	3
"C2H3-C3H7 (C2-C3)"	10.0181	1	1	Yes	1421.1	2

Electronic
Level(degeneracy)

0(2)

Geometry
N, Symbol, Bond [A], Ref.Atom, Angle, Ref.Atom, Dihedral Angle, Ref.Atom

1	C	0	0	0	0	0	0
2	C	1.54169	1	0	0	0	0
3	C	1.50026	2	113.11	1	0	0
4	C	1.53161	1	112.824	2	182.182	3
5	C	1.3549	3	125.098	2	235.968	1
6	H	1.09788	1	109.024	2	59.844	3
7	H	1.09896	1	109.166	2	304.266	3
8	H	1.0981	2	109.747	1	237.004	3
9	H	1.1022	2	108.357	1	121.228	3
10	H	1.09109	3	116.161	2	58.579	1
11	H	1.0958	4	111.27	1	179.968	2
12	H	1.09688	4	111.232	1	300.026	2
13	H	1.09698	4	111.2	1	59.868	2
14	H	1.08744	5	121.041	3	8.532	2
15	H	1.98	5	105.857	3	272.047	2
16	H	1.08599	5	121.273	3	174.68	2

Bonds
Atom, Atom, Type (1, 2, 3), Length [A]

C1	C2	1	1.54169
C1	C4	1	1.53161
C1	H6	1	1.09788
C1	H7	1	1.09896
C2	C3	1	1.50026
C2	H8	1	1.0981
C2	H9	1	1.1022
C3	C5	1	1.3549
C3	H10	1	1.09109
C4	H11	1	1.0958
C4	H12	1	1.09688

C4	H13	1	1.09698
C5	H14	1	1.08744
C5	H16	1	1.08599

Collision
Buffer gas, Collision Model, Expression, Alpha0 [/cm], Alpha1 [K/cm], Alpha2

"Argon" 0 0 600 unknown unknown

Comment
g3mp2b3 geom freq 0.96
-771 img freq
Rotors
99 cm-1 corresponds to C3H7-Cd'; 110 cm-1 corresponds to C2H5-R; 249 cm-1 corresponds to CH3-R corresponds to 17, 14, 14 kJ/mol

Component
Name=pent2yl#cc-h%3e (pent2yl = pent2ene-e + h)
Atomic composition=H11C5
Type=1
Mass=71.1423
Enthalpy(298), 1/cm=0

Frequencies
Frequency(degeneracy)

3020.12	3011.13	2995.09	2992.77	2987.71
2954.11	2951.64	2923.81	2922.04	2908.28
1630.31	1476.12	1466.27	1458.23	1454.87
1447.42	1383.06	1377.72	1326.92	1293.95
1274.85	1236.93	1143.22	1069.89	1043.12
1026.73	996.061	972.239	920.046	851.453
777.53	750.031	474.787	414.18	353.872
290.464	268.285	163.957		

Rotors
*Name, Moment of Inertia [amu*A*²], Symmetry, Dimension, Active [Yes/No], Hindrance [1/cm], Minima*

"Ia"	38.2082	1	1	Yes	0	1
"IbIc"	243.991	1	2	No	0	1
"C2H5-C3H5 (C1-C2)"	11.0625	1	1	Yes	1387.67	2
"CH3-C4H7 (C1-C4)"	3.03988	3	1	Yes	919.538	3
"CH3-C4H7	2.93794	3	1	Yes	618.598	3

(C3-C5)"

Electronic
Level(degeneracy)

0(2)

Geometry
N, Symbol, Bond [A], Ref.Atom, Angle, Ref.Atom, Dihedral Angle, Ref.Atom

1	C	0	0	0	0	0	0
2	C	1.50891	1	0	0	0	0
3	C	1.34834	2	124.71	1	0	0
4	C	1.53859	1	112.229	2	105.389	3
5	C	1.49903	3	125.16	2	184.555	1
6	H	1.09746	1	109.666	2	226.717	3
7	H	1.09735	1	109.514	2	343.282	3
8	H	1.09159	2	115.981	1	190.817	3
9	H	2.09903	2	98.536	1	104.772	3
10	H	1.09156	3	118.443	2	7.421	1
11	H	1.09611	4	110.943	1	178.415	2
12	H	1.09576	4	111.03	1	298.737	2
13	H	1.09672	4	111.176	1	58.561	2
14	H	1.09504	5	111.629	3	3.506	2
15	H	1.09895	5	111.124	3	242.947	2
16	H	1.09857	5	111.232	3	124.401	2

Bonds
Atom, Atom, Type (1, 2, 3), Length [A]

C1	C2	1	1.50891
C1	C4	1	1.53859
C1	H6	1	1.09746
C1	H7	1	1.09735
C2	C3	1	1.34834
C2	H8	1	1.09159
C3	C5	1	1.49903
C3	H10	1	1.09156
C4	H11	1	1.09611
C4	H12	1	1.09576
C4	H13	1	1.09672
C5	H14	1	1.09504
C5	H15	1	1.09895
C5	H16	1	1.09857

Collision
Buffer gas, Collision Model, Expression, Alpha0 [/cm], Alpha1 [K/cm], Alpha2

"Argon"	0	0	600	unknown	unknown

Comment
g3mp2b3 geom freq 0.96
-369 img freq
Rotors
92 cm-1 corresponds to C2H5-Cd'; 179 cm-1 corresponds to CH3-Cd'; 214 cm-1 corresponds to CH3-R corresponds to 16.6, 7.4, 11 kJ/mol

Component
Name=pent2yl#cc-h%3z (pent2yl = pent2ene-z + h)
Atomic composition=H11C5
Type=1
Mass=71.1423
Enthalpy(298), 1/cm=16222.3

Frequencies
Frequency(degeneracy)

3036.38	3017.95	3008.22	2996.06	2989.5
2967.61	2950.83	2932.62	2924.3	2910.59
1619.05	1478.37	1467.52	1465.44	1451.23
1450.6	1399.57	1379.93	1370.89	1300.63
1258.73	1237.9	1137.52	1057.62	1025.52
1018.76	990.634	970.789	905.513	830.006
767.191	719.666	546.522	488.589	351.381
297.034	257.032	255		

Rotors
*Name, Moment of Inertia [amu*A*²], Symmetry, Dimension, Active [Yes/No], Hindrance [1/cm], Minima*

"Ia"	58.3608	1	1	Yes	0	1
"IbIc"	199.099	1	2	No	0	1
"C2H5-C3H5 (C1-C2)"	18.2019	1	-1	Yes	1145.24	2
"CH3-C4H7 (C1-C4)"	3.06284	3	-1	Yes	919.538	3
"CH3-C4H7 (C3-C5)"	3.07306	3	-1	Yes	334.377	3

Electronic
Level(degeneracy)

0(2)

Geometry
N, Symbol, Bond [A], Ref.Atom, Angle, Ref.Atom, Dihedral Angle, Ref.Atom

1	C	0	0	0	0	0	0
2	C	1.51009	1	0	0	0	0
3	C	1.35114	2	127.313	1	0	0
4	C	1.53932	1	111.966	2	100.247	3
5	C	1.50018	3	127.617	2	8.188	1
6	H	1.09706	1	109.003	2	220.982	3
7	H	1.09539	1	110.82	2	337.548	3
8	H	1.09031	2	114.784	1	190.936	3
9	H	2.10726	2	97.312	1	104.605	3
10	H	1.09026	3	117.227	2	185.255	1
11	H	1.09616	4	110.924	1	177.099	2
12	H	1.09569	4	111.083	1	297.433	2
13	H	1.09659	4	111.161	1	57.21	2
14	H	1.09321	5	112.977	3	-3.915	2
15	H	1.09852	5	110.702	3	234.98	2
16	H	1.09906	5	110.711	3	117.184	2

Bonds
Atom, Atom, Type (1, 2, 3), Length [A]

C1	C2	1	1.51009
C1	C4	1	1.53932
C1	H6	1	1.09706
C1	H7	1	1.09539
C2	C3	1	1.35114
C2	H8	1	1.09031
C3	C5	1	1.50018
C3	H10	1	1.09026
C4	H11	1	1.09616
C4	H12	1	1.09569
C4	H13	1	1.09659
C5	H14	1	1.09321
C5	H15	1	1.09852
C5	H16	1	1.09906

Collision
Buffer gas, Collision Model, Expression, Alpha0 [/cm], Alpha1 [K/cm], Alpha2

"Argon" 0 0 600 unknown unknown

Comment
g3mp2b3 geom freq 0.96
-387 img freq
Rotors

64 cm-1 corresponds to C2H5-Cd'; 128 cm-1 corresponds to CH3-Cd'; 231 cm-1 corresponds to CH3-R corresponds to 13.7, 4, 11 kJ/mol

Component
Name=pent3yl
Atomic composition=H11C5
Type=0
Mass=71.1423
Enthalpy(298), 1/cm=3878.78
Beta=unknown
Sigma, A=5.5828
Epsilon, K=388.93

Frequencies
Frequency(degeneracy)

3022.36	2993.32	2993.08	2986.92	2986.72
2925.28	2924.64	2897.06	2891.24	2812.21
2807.15	1474.05	1473.61	1467.02	1466.89
1447.41	1436.8	1385.05	1382.02	1377.34
1328.83	1245.44	1240.66	1226.1	1136.92
1102.75	1056.06	1009.59	1008.7	993.58
914.706	848.22	758.852	731.877	401.96
388.76	376.985	174.295		

Rotors
*Name, Moment of Inertia [amu*A*²], Symmetry, Dimension, Active [Yes/No], Hindrance [1/cm], Minima*

"Ia"	31.4485	2	1	Yes	0	1
"IbIc"	260.456	1	2	No	0	1
"C2H5-C3H6 (C1-C2)"	10.8037	1	-1	Yes	334.377	2
"CH3-C4H8 (C1-C4)"	2.94759	3	-1	Yes	1245.56	3
"C2H5-C3H6 (C2-C3)"	10.8267	1	-1	Yes	334.377	2
"CH3-C4H8 (C3-C5)"	2.94715	3	-1	Yes	1245.56	3

Electronic
Level(degeneracy)

0(2)

Geometry
N, Symbol, Bond [A], Ref.Atom, Angle, Ref.Atom, Dihedral Angle, Ref.Atom

1	C	0	0	0	0	0	0
2	C	1.4954	1	0	0	0	0
3	C	1.4954	2	122.043	1	0	0
4	C	1.5349	1	113.682	2	194.589	3
5	C	1.5348	3	113.692	2	166.055	1
6	H	1.1079	1	110.162	2	72.422	3
7	H	1.1013	1	109.586	2	317.775	3
8	H	1.0906	2	118.002	1	196.148	3
9	H	1.1014	3	109.581	2	42.867	1
10	H	1.1079	3	110.16	2	288.249	1
11	H	1.0957	4	111.327	1	181.149	2
12	H	1.0967	4	110.941	1	301.104	2
13	H	1.0959	4	111.024	1	60.737	2
14	H	1.0967	5	110.943	3	58.951	2
15	H	1.0959	5	111.024	3	299.317	2
16	H	1.0957	5	111.329	3	178.91	2

Bonds
Atom, Atom, Type (1, 2, 3), Length [A]

C1	C2	1	1.4954
C1	C4	1	1.5349
C1	H6	1	1.1079
C1	H7	1	1.1013
C2	C3	1	1.4954
C2	H8	1	1.0906
C3	C5	1	1.5348
C3	H9	1	1.1014
C3	H10	1	1.1079
C4	H11	1	1.0957
C4	H12	1	1.0967
C4	H13	1	1.0959
C5	H14	1	1.0967
C5	H15	1	1.0959
C5	H16	1	1.0957

Collision
Buffer gas, Collision Model, Expression, Alpha0 [/cm], Alpha1 [K/cm], Alpha2

"Argon" 0 0 unknown 0.675 unknown

Comment
g3mp2b3 geom freq 0.96
torisons 246 cm-1, 245cm-1, 57 cm-1, 47cm-1, (inv 418 cm-1)
rotors
(2) CH3 14.9 kJ/mol (sigma = 3)
(2) R-C* 4.0 kJ/mol (sigma = 2)

Original Ia = 30.5783; Ib=Ic = 264.136; Iabc = 2 133 381.529
K Rotor Matching: Set Ib=Ic = 260.456 from 1-pentyl and Ia to 31.4485 to match original Iabc

Component
Name=pent3yl#cc-c (pent3yl = but1ene + ch3)
Atomic composition=H11C5
Type=1
Mass=71.1423
Enthalpy(298), 1/cm=14211

Frequencies
Frequency(degeneracy)

3152.77	3144	3112.86	3033.65	3013.96
2996.79	2994.78	2987.05	2939.62	2923.92
2882.06	1554.51	1475.47	1466.65	1450.3
1407.54	1393.71	1389.21	1377.67	1301.17
1259.24	1243.69	1162.92	1050.12	989.627
976.998	929.45	887.014	829.138	766.432
745.069	677.141	466.698	456.881	405.137
352.578	325	320		

Rotors
*Name, Moment of Inertia [amu*A*²], Symmetry, Dimension, Active [Yes/No], Hindrance [1/cm], Minima*

"Ia"	41.9431	1	1	Yes	0	1
"IbIc"	278.942	1	2	No	0	1
"C2H5-C3H6 (C1-C2)"	17.7326	1	-1	Yes	1086.73	2
"CH3-C4H8 (C1-C4)"	2.94934	3	-1	Yes	1086.73	3
"CH3-C4H8 (C3-C5)"	3.25919	3	-1	Yes	167.189	3

Electronic
Level(degeneracy)

0(4)

Geometry
N, Symbol, Bond [A], Ref.Atom, Angle, Ref.Atom, Dihedral Angle, Ref.Atom

1	C	0	0	0	0	0	0
2	C	1.50229	1	0	0	0	0
3	C	1.3577	2	124.933	1	0	0
4	C	1.53911	1	112.848	2	125.007	3
5	C	2.3645	3	109.803	2	87.805	1
6	H	1.10189	1	109.649	2	245.98	3
7	H	1.09785	1	109.639	2	362.369	3
8	H	1.0914	2	116.076	1	176.529	3
9	H	1.08712	3	120.558	2	-11.428	1
10	H	1.08562	3	120.856	2	187.521	1
11	H	1.09612	4	111.105	1	178.035	2
12	H	1.09565	4	110.952	1	298.423	2
13	H	1.09673	4	111.077	1	58.108	2
14	H	1.08466	5	100.575	3	60.34	2
15	H	1.08473	5	100.572	3	300.173	2
16	H	1.08599	5	99.209	3	180.259	2

Bonds
Atom, Atom, Type (1, 2, 3), Length [A]

C1	C2	1	1.50229
C1	C4	1	1.53911
C1	H6	1	1.10189
C1	H7	1	1.09785
C2	C3	1	1.3577
C2	H8	1	1.0914
C3	C5	1	2.3645
C3	H9	1	1.08712
C3	H10	1	1.08562
C4	H11	1	1.09612
C4	H12	1	1.09564
C4	H13	1	1.09673
C5	H14	1	1.08466
C5	H15	1	1.08473
C5	H16	1	1.08599

Collision
Buffer gas, Collision Model, Expression, Alpha0 [/cm], Alpha1 [K/cm], Alpha2

"Argon" 0 0 600 unknown unknown

Comment
g3mp2b3 geom freq 0.96
-362 img freq
64 cm-1 corresponds to C2H5-Cd; 86 cm-1 corresponds to CH3--Cd; 237 cm-1 corresponds to CH3-R

Component
Name=pent3yl#cc-h%2e (pent3yl = pent2ene-e + h)
Atomic composition=H11C5
Type=1
Mass=71.1423
Enthalpy(298), 1/cm=15720.8

Frequencies
Frequency(degeneracy)

3025.17	3006.1	2997.95	2995.94	2989.36
2971.95	2948.62	2925.52	2916.62	2895.85
1628.26	1475.52	1467.43	1462.64	1451.63
1450.25	1384.95	1380.2	1332.55	1286.36
1275.51	1235.66	1144.25	1064.47	1047.11
1029.93	996.562	970.662	920.306	858.204
792.446	744.017	466.685	415.416	342.349
332.374	290.842	190.4		

Rotors
*Name, Moment of Inertia [amu*A*²], Symmetry, Dimension, Active [Yes/No], Hindrance [1/cm], Minima*

"Ia"	34.7529	1	1	Yes	0	1
"IbIc"	252.753	1	2	No	0	1
"CH3-C4H7 (C1-C4)"	2.92673	3	-1	Yes	710.552	3
"C2H5-C3H5 (C2-C3)"	11.0029	1	-1	Yes	1295.71	2
"CH3-C4H7 (C3-C5)"	3.00583	3	-1	Yes	902.819	3

Electronic
Level(degeneracy)

0(2)

Geometry
N, Symbol, Bond [A], Ref.Atom, Angle, Ref.Atom, Dihedral Angle, Ref.Atom

1	C	0	0	0	0	0	0
2	C	1.34865	1	0	0	0	0
3	C	1.50179	2	125.336	1	0	0
4	C	1.50601	1	124.695	2	184.469	3
5	C	1.53873	3	112.795	2	123.326	1
6	H	2.08534	1	96.905	2	79.437	3
7	H	1.09068	1	118.372	2	354.191	3
8	H	1.09235	2	118.528	1	182.011	3
9	H	1.09727	3	109.714	2	0.439	1
10	H	1.10086	3	109.184	2	244.236	1
11	H	1.09554	4	111.58	1	226.077	2
12	H	1.09519	4	111.418	1	347.041	2
13	H	1.09871	4	110.577	1	107.016	2
14	H	1.09663	5	111.133	3	58.03	2
15	H	1.09566	5	111.029	3	298.212	2
16	H	1.09586	5	110.975	3	177.912	2

Bonds
Atom, Atom, Type (1, 2, 3), Length [A]

C1	C2	1	1.34865
C1	C4	1	1.50601
C1	H7	1	1.09068
C2	C3	1	1.50179
C2	H8	1	1.09235
C3	C5	1	1.53873
C3	H9	1	1.09727
C3	H10	1	1.10086
C4	H11	1	1.09554
C4	H12	1	1.09519
C4	H13	1	1.09871
C5	H14	1	1.09663
C5	H15	1	1.09566
C5	H16	1	1.09586

Collision
Buffer gas, Collision Model, Expression, Alpha0 [/cm], Alpha1 [K/cm], Alpha2

"Argon"	0	0	600	unknown	unknown	

Comment
g3mp2b3 geom freq 0.96

-421 img freq
89 cm-1 corresponds to C2H5-Cd'; 192 cm-1 corresponds to CH3-Cd'; 213 cm-1 corresponds to CH3-R
15.5, 8.5, 10.8 kJ/mol

Component

Name=pent3yl#cc-h%2z (pent3yl = pent2ene-z + h)
Atomic composition=H11C5
Type=1
Mass=71.1423

Frequencies
Frequency(degeneracy)

3038.78	3015.12	3010.43	2995.9	2990.91
2976.97	2965	2925.45	2918.85	2895.29
1616.5	1475.37	1466.88	1464.78	1454.16
1449.81	1401.8	1378.77	1373.58	1299.37
1256.39	1239.74	1136.8	1053.89	1028.96
1019.87	991.401	969.514	905.856	834.317
771.958	724.316	554.148	464.531	359.508
313.702	275.807	196.332		

Rotors
*Name, Moment of Inertia [amu*A*²], Symmetry, Dimension, Active [Yes/No], Hindrance [1/cm], Minima*

"Ia"	50.08	1	1	Yes	0	1
"IbIc"	214.617	1	2	No	0	1
"CH3-C4H7 (C1-C4)"	3.0672	3	1	Yes	417.972	3
"C2H5-C3H5 (C2-C3)"	17.472	1	1	Yes	702.193	2
"CH3-C4H7 (C3-C5)"	3.02367	3	1	Yes	961.335	3

Electronic
Level(degeneracy)

0(2)

Geometry
N, Symbol, Bond [A], Ref.Atom, Angle, Ref.Atom, Dihedral Angle, Ref.Atom

1	C	0	0	0	0	0	0
2	C	1.35161	1	0	0	0	0
3	C	1.50254	2	128.045	1	0	0
4	C	1.50736	1	127.353	2	353.047	3

5	C	1.53952	3	112.413	2	123.593	1
6	H	2.08853	1	96.849	2	97.534	3
7	H	1.08951	1	117.038	2	183.396	3
8	H	1.09118	2	117.132	1	182.099	3
9	H	1.09505	3	111.026	2	0.472	1
10	H	1.10095	3	108.767	2	243.859	1
11	H	1.09892	4	110.252	1	257.508	2
12	H	1.09321	4	112.839	1	378.055	2
13	H	1.09514	4	110.871	1	139.115	2
14	H	1.09658	5	111.146	3	57.479	2
15	H	1.09564	5	111.059	3	297.664	2
16	H	1.09584	5	110.937	3	177.376	2

Bonds
Atom, Atom, Type (1, 2, 3), Length [A]

C1	C2	1	1.35161
C1	C4	1	1.50736
C1	H7	1	1.08951
C2	C3	1	1.50254
C2	H8	1	1.09118
C3	C5	1	1.53952
C3	H9	1	1.09505
C3	H10	1	1.10095
C4	H11	1	1.09892
C4	H12	1	1.09321
C4	H13	1	1.09514
C5	H14	1	1.09658
C5	H15	1	1.09564
C5	H16	1	1.09584

Collision
Buffer gas, Collision Model, Expression, Alpha0 [/cm], Alpha1 [K/cm], Alpha2

"Argon" 0 0 600 unknown unknown

Comment
g3mp2b3 geom freq 0.96
-423 img freq
52 cm-1 corresponds to C2H5-Cd'; 143 cm-1 corresponds to CH3-Cd'; 220 cm-1 corresponds to CH3-R
8.4, 5, 11.5 kJ/mol

Component
Name=prop1yl

Atomic composition=H7C3
Type=0
Mass=43.0886
Enthalpy(298), 1/cm=8359.44

Frequencies
Frequency(degeneracy)

3125.85	3033.32	2996.73	2987.54	2939.32
2922.32	2905.22	1475.38	1464.16	1454.14
1432.46	1369.21	1292.63	1272.71	1161.26
1060.86	993.699	865.651	865.441	722.958
502.726	321.65			

Rotors
*Name, Moment of Inertia [amu*A*²], Symmetry, Dimension, Active [Yes/No], Hindrance [1/cm], Minima*

"Ia"	16.1788	1	1	Yes	0	1
"IbIc"	60.6625	1	2	No	0	1
"CH3-C2H4 (C1-C2)"	2.68163	3	-1	Yes	1245.56	3
"CH2-C2H5 (C2-C3)"	1.59216	2	1	Yes	0	1

Electronic
Level(degeneracy)

0(2)

Geometry
N, Symbol, Bond [A], Ref.Atom, Angle, Ref.Atom, Dihedral Angle, Ref.Atom

1	C	0	0	0	0	0	0
2	C	1.54791	1	0	0	0	0
3	C	1.49286	2	113.383	1	0	0
4	H	1.0957	1	110.971	2	59.891	3
5	H	1.0957	1	110.971	2	-59.885	3
6	H	1.09688	1	110.805	2	180.002	3
7	H	1.09876	2	108.413	1	122.374	3
8	H	1.09879	2	108.406	1	-122.368	3
9	H	1.08628	3	120.868	2	84.069	1
10	H	1.0863	3	120.858	2	-83.824	1

Bonds
Atom, Atom, Type (1, 2, 3), Length [A]

C1	C2	1	1.54791
C1	H4	1	1.0957
C1	H5	1	1.0957
C1	H6	1	1.09688
C2	C3	1	1.49286
C2	H7	1	1.09876
C2	H8	1	1.09879
C3	H9	1	1.08628
C3	H10	1	1.0863

Collision
Buffer gas, Collision Model, Expression, Alpha0 [/cm], Alpha1 [K/cm], Alpha2

"Argon" 0 0 600 unknown unknown

Comment
g3mp2b3 geom freq 0.96
torsions 252 cm-1, 80 cm-1, (524 cm-1 inv)
rotors
(1) CH2* free (2)
(1) CH3 14.9 (3)

Component
Name=prop1yl#cc-c (prop1yl = ethene + ch3)
Atomic composition=H7C3
Type=1
Mass=43.0886
Enthalpy(298), 1/cm=0
Beta=unknown
Sigma, A=4
Epsilon, K=200
Critical T=unknown
Critical P=unknown
Acentric factor=unknown
Status=0
Concentration, %=100
Init distr.type=0
Init distr.T=unknown
Subtruct reactions=0
Use cut-off noise=0
Cut-off noise parameter=0.5
Optically active=0

Frequencies
Frequency(degeneracy)

3157.18	3146.57	3125.53	3101.19	3041.44
3032.07	2998.44	1552.14	1430.02	1394.06

1388.57	1273.47	1198.2	986.065	907.475
832.227	793.635	751.011	477.783	459.697
334.386	208.487			

Rotors
*Name, Moment of Inertia [amu*A*²], Symmetry, Dimension, Active [Yes/No], Hindrance [1/cm], Minima*

"Ia"	18.2189	1	1	Yes	0	1
"IbIc"	87.3102	1	2	No	0	1
"CH3-C2H4 (C1-C2)"	2.86126	3	1	Yes	183.908	3

Electronic
Level(degeneracy)

0(2)

Geometry
N, Symbol, Bond [A], Ref.Atom, Angle, Ref.Atom, Dihedral Angle, Ref.Atom

1	C	0	0	0	0	0	0
2	C	2.3641	1	0	2	0	3
3	C	1.3556	2	109.97	1	0	3
4	H	1.0844	1	100.26	2	60.09	3
5	H	1.0844	1	100.27	2	-59.95	3
6	H	1.086	1	99.14	2	-179.93	3
7	H	1.0861	2	87.46	1	122.01	3
8	H	1.0861	2	87.46	1	-122.01	3
9	H	1.0868	3	121.68	2	-272.12	1
10	H	1.0868	3	121.68	2	-87.88	1

Bonds
Atom, Atom, Type (1, 2, 3), Length [A]

C1	C2	1	2.3641
C1	H4	1	1.0844
C1	H5	1	1.0844
C1	H6	1	1.086
C2	C3	1	1.3556
C2	H7	1	1.0861
C2	H8	1	1.0861
C3	H9	1	1.0868
C3	H10	1	1.0868

Collision
Buffer gas, Collision Model, Expression, Alpha0 [/cm], Alpha1 [K/cm], Alpha2

"Argon" 0 0 600 unknown unknown

Comment
g3mp2b3 geom freq 0.96
-360 img freq
98 cm-1 corresponds to CH3--Cd
2.1 kJ/mol

Component
Name=prop1yl#cc-c (prop1yl = propene + h)
Atomic composition=H7C3
Type=1
Mass=43.0886

Frequencies
Frequency(degeneracy)

3115.89	3036.4	3032.01	3002.35	2976.61
2919.72	1602.64	1463.56	1451.02	1410.54
1375.68	1269.95	1153.78	1033.84	990.514
918.142	888.288	876.905	572.194	410.842
385.073	338.04	185.059		

Rotors
*Name, Moment of Inertia [amu*A*²], Symmetry, Dimension, Active [Yes/No], Hindrance [1/cm], Minima*

"Ia"	15.8658	1	1	Yes	0	1
"IbIc"	61.2236	1	2	No	0	1
"CH3-C2H3 (C1-C2)"	2.61339	1	1	Yes	0	1

Electronic
Level(degeneracy)

0(2)

Geometry
N, Symbol, Bond [A], Ref.Atom, Angle, Ref.Atom, Dihedral Angle, Ref.Atom

1	C	0	0	0	0	0	0	0
2	C	1.50652	1	0	0	0	0	0
3	C	1.34754	2	124.465	1	0	0	0
4	H	1.09493	1	111.379	2	14.96	3	
5	H	1.09852	1	110.271	2	-104.876	3	

6	H	1.09513	1	111.628	2	136.133	3
7	H	1.08983	2	116.058	1	168.799	3
8	H	2.04701	2	97.723	1	-105.779	3
9	H	1.08618	3	121.64	2	175.13	1
10	H	1.08775	3	121.507	2	-7.705	1

Bonds
Atom, Atom, Type (1, 2, 3), Length [A]

C1	C2	1	1.50652
C1	H4	1	1.09493
C1	H5	1	1.09852
C1	H6	1	1.09513
C2	C3	1	1.34754
C2	H7	1	1.08983
C3	H9	1	1.08618
C3	H10	1	1.08775

Collision
Buffer gas, Collision Model, Expression, Alpha0 [/cm], Alpha1 [K/cm], Alpha2

"Argon" 0 0 600 unknown unknown

Comment
g3mp2b3 geom freq 0.96
-522 img freq

Component
Name=propene
Atomic composition=H6C3
Type=0
Mass=42.0806
Enthalpy(298), 1/cm=1646.81

Frequencies
Frequency(degeneracy)

3105.59	3030.48	3019.08	2991.99	2955.92
2911.03	1668.97	1462.99	1449.18	1414.39
1377.58	1284.72	1155.1	1038.59	993.846
917.487	898.676	895.535	565.254	406.839

Rotors
*Name, Moment of Inertia [amu*A*²], Symmetry, Dimension, Active [Yes/No], Hindrance [1/cm], Minima*

"Ia" 10.8069 1 1 Yes 0 1

"IbIc"	58.4197	1	2	No	0	1
"CH3-C2H3 (C1-C5)"	2.36607	3	-1	Yes	752.349	3

Electronic
Level(degeneracy)

0

Geometry
N, Symbol, Bond [A], Ref.Atom, Angle, Ref.Atom, Dihedral Angle, Ref.Atom

1	C	0	0	0	0	0	0
2	H	1.0985	1	0	2	0	3
3	H	1.0985	1	106.56	2	0	3
4	H	1.0952	1	108.11	2	116	3
5	C	1.5021	1	111.17	2	-121.27	3
6	C	1.3333	5	125.24	1	-120.76	2
7	H	1.0912	5	115.89	1	59.25	2
8	H	1.0868	6	121.82	5	-180	1
9	H	1.0885	6	121.65	5	0	1

Bonds
Atom, Atom, Type (1, 2, 3), Length [A]

C1	H2	1	1.0985
C1	H3	1	1.0985
C1	H4	1	1.0952
C1	C5	1	1.5021
C5	C6	1	1.3333
C5	H7	1	1.0912
C6	H8	1	1.0868
C6	H9	1	1.0885

Collision
Buffer gas, Collision Model, Expression, Alpha0 [/cm], Alpha1 [K/cm], Alpha2

"Argon"	0	0	600	unknown	unknown

Comment
g3mp2b3 geom freq 0.96
torsions 211 cm-1
rotors
(1) CH3 9.0 (3)
expt So
267.0 (S&P)

266.7 (TRC)
calc 266.8

Component

Name=pent2yl#cc^h%2 (pent2yl = pent3yl)
Atomic composition=H11C5
Type=1
Mass=71.1423
Enthalpy(298), 1/cm=18390.8

Frequencies

Frequency(degeneracy)

3046.07	3033.88	2991.62	2982.24	2981.83
2938.59	2936.71	2919.44	2900.2	2864.47
2098.66	1473.15	1464.87	1463.61	1453.62
1450.49	1390.8	1378.19	1368.58	1311.84
1292.58	1262.54	1209.8	1165.28	1123.55
1045.83	1018.08	1013.25	971.789	898.202
835.509	747.877	718.371	631.842	420.481
337.015	282.433	99.4358		

Rotors

*Name, Moment of Inertia [amu*A*²], Symmetry, Dimension, Active [Yes/No], Hindrance [1/cm], Minima*

"Ia"	45.0428	1	1	Yes	0	1
"IbIc"	227.711	1	2	No	0	1
"CH3-C4H8 (C1-C7)"	2.99068	3	-1	Yes	794.146	3
"C2H5-C2HCH5 (C2-C3)"	10.5622	1	-1	Yes	1086.73	3
"CH3-C3HCH7 (C3-C4)"	3.09144	3	-1	Yes	919.538	3

Electronic

Level(degeneracy)

0(2)

Geometry

N, Symbol, Bond [A], Ref.Atom, Angle, Ref.Atom, Dihedral Angle, Ref.Atom

1	C	1.5014	1	121.19	2	150.29	3
2	H	1.0884	1	115.92	2	-7.19	3
3	H	1.0888	2	115.83	1	-156.69	3
4	H	1.0979	3	110.03	2	-202.63	1
5	H	1.0999	3	109.44	2	-318.81	1

6	H	1.0961	4	110.79	3	-301.99	2
7	H	1.0963	4	111.06	3	-61.65	2
8	H	1.0957	7	111.92	1	-198.57	2
9	H	1.1034	7	111.68	1	-77.83	2
10	H	1.098	7	111.26	1	41.11	2
11	C	0	0	0	0	0	0
12	C	1.499	1	0	2	0	3
13	C	1.5057	2	121.23	1	0	3
14	C	1.5418	3	113.04	2	-80.14	1
15	H	1.0971	4	111.25	3	-181.83	2
16	H	1.3039	1	54.93	2	-105.07	3

Bonds
Atom, Atom, Type (1, 2, 3), Length [A]

C1	H2	1
C1	H6	1
C1	H7	1
C1	H8	1
H2	H3	1
H2	H6	1
H2	H9	1
H3	H4	1
H3	H10	1
H3	C11	1
H4	H5	1
H4	C12	1
H4	C13	1
H7	C14	1
H7	H15	1
H7	H16	1

Comment
g3mp2b3 geom freq 0.96
-1913 img freq
Replaced torsions with rotors
CH3 213 cm-1, 11 kJ/mol
CH3-Cd' 199 cm-1, 9.5 kJ/mol
C2H5-Cd' 125 cm-1, 13 kJ/mol

Component
Name=pent1yl#cc^h%2 (pent1yl = pent2yl)
Atomic composition=H11C5
Type=1
Mass=71.1423

Enthalpy(298), 1/cm=18498.6

Frequencies
Frequency(degeneracy)

3143.63	3044.08	3037.58	2984.8	2981.33
2949.76	2925.81	2918.11	2914.64	2890.44
2122.87	1476.29	1468.5	1460.46	1447.65
1393.97	1380.24	1353.1	1333.3	1290.56
1272.23	1244.9	1217.61	1145.21	1136.55
1061.57	1000.87	969.583	891.71	840.139
832.523	722.775	705.576	691.336	459.075
365.364	316.689	211.254		

Rotors
*Name, Moment of Inertia [amu*A*²], Symmetry, Dimension, Active [Yes/No], Hindrance [1/cm], Minima*

"Ia"	37.7223	1	1	Yes	0	1
"IbIc"	235.575	1	2	No	0	1
"C2H4-C3H7 (C2-C3)"	10.254	1	-1	Yes	835.944	3
"C2H5-C3H6 (C3-C4)"	16.4185	1	-1	Yes	1003.13	3
"CH3-C4H8 (C4-C5)"	2.92776	3	-1	Yes	1170.32	3

Electronic
Level(degeneracy)

0(2)

Geometry
N, Symbol, Bond [A], Ref.Atom, Angle, Ref.Atom, Dihedral Angle, Ref.Atom

1	C	0	0	0	0	0	0
2	C	1.4967	1	0	2	0	3
3	C	1.5047	2	120.82	1	0	3
4	C	1.5445	3	113.26	2	-80.35	1
5	C	1.532	4	112.97	3	-181.73	2
6	H	1.2972	2	55.08	1	105.64	3
7	H	1.0846	1	119.97	2	155.03	3
8	H	1.0852	1	118.97	2	-6.9	3
9	H	1.0881	2	116.1	1	-156.21	3
10	H	1.0989	3	110.14	2	-202.74	1
11	H	1.1009	3	109.49	2	40.92	1

12	H	1.0981	4	108.84	3	-304.07	2
13	H	1.0986	4	109.04	3	-59.54	2
14	H	1.0962	5	111.45	4	179.61	3
15	H	1.0972	5	111.22	4	59.48	3
16	H	1.0972	5	111.2	4	299.74	3

Bonds
Atom, Atom, Type (1, 2, 3), Length [A]

C1	C2	1	1.4967
C1	H6	1	1.30386
C1	H7	1	1.0846
C1	H8	1	1.0852
C2	C3	1	1.5047
C2	H6	1	1.2972
C2	H9	1	1.0881
C3	C4	1	1.5445
C3	H10	1	1.0989
C3	H11	1	1.1009
C4	C5	1	1.532
C4	H12	1	1.0981
C4	H13	1	1.0986
C5	H14	1	1.0962
C5	H15	1	1.0972
C5	H16	1	1.0972

Comment
g3mp2b3 geom freq 0.96
-1906 img freq
Replaced torsions with rotors
CH3 247 cm-1, 14 kj/mol
C2H5 94 cm-1, 12 kj/mol
C3H7-Cd' 109 cm-1, 10 kJ/mol

Reactions:

pent1yl ----> pent1yl#cc-c (pent1yl = ethene + prop1yl)# ----> ethene + prop1yl
Degeneracy=1
Threshold, 1/cm=9653.4

pent2yl <---> pent1yl#cc^h%4 (pent1yl = pent2yl)# <---> pent1yl
Degeneracy=1
Threshold, 1/cm=9031.23

pent3yl <---> pent1yl#cc^h%3 (pent1yl = pent3yl)# <---> pent1yl
Degeneracy=1
Threshold, 1/cm=13191.8

pent2yl ----> pent2yl#cc-c (pent2yl = propene + ethyl)# ----> ethyl + propene
Degeneracy=1
Threshold, 1/cm=9836

pent3yl ----> pent3yl#cc-c (pent3yl = but1ene + ch3)# ----> but1ene + ch3
Degeneracy=1
Threshold, 1/cm=10386.2

pent1yl <---> pent1yl#cc^h%4 (pent1yl = pent2yl)# <---> pent2yl
Degeneracy=1
Threshold, 1/cm=7916.61

pent1yl <---> pent1yl#cc^h%3 (pent1yl = pent3yl)# <---> pent3yl
Degeneracy=1
Threshold, 1/cm=12036.4

pent2yl ----> pent3yl#cc-h%2e (pent3yl = pent2ene-e + h)# ----> pent2ene-e + H
Degeneracy=1
Threshold, 1/cm=11790.6

pent1yl ----> pent1yl#cc^h%2 (pent1yl = pent2yl)# ----> pent2yl 1,2 shift
Degeneracy=1
Threshold, 1/cm=13801.4

pent2yl ----> pent2yl#cc^h%2 (pent2yl = pent3yl)# ----> pent3yl
Degeneracy=1
Threshold, 1/cm=14537.4

pent2yl ----> pent2yl#cc-h%3z (pent2yl = pent2ene-z + h)# ----> pent2ene-z + H
Degeneracy=1
Threshold, 1/cm=12301