SUPPORTING INFORMATION

Hydrogen abstraction between hydrocarbons: modeling of activation energies and pre-exponential factors

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Transition state geometries and parameters charactering the internal rotations can be found at the end of this document.

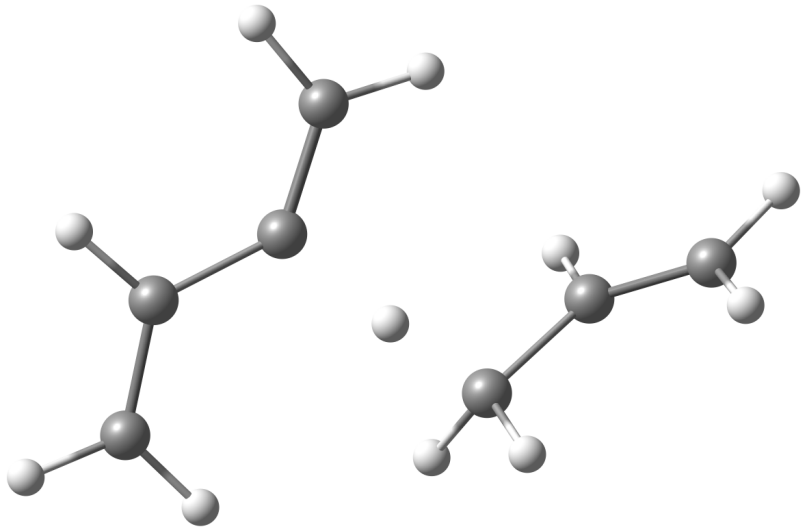
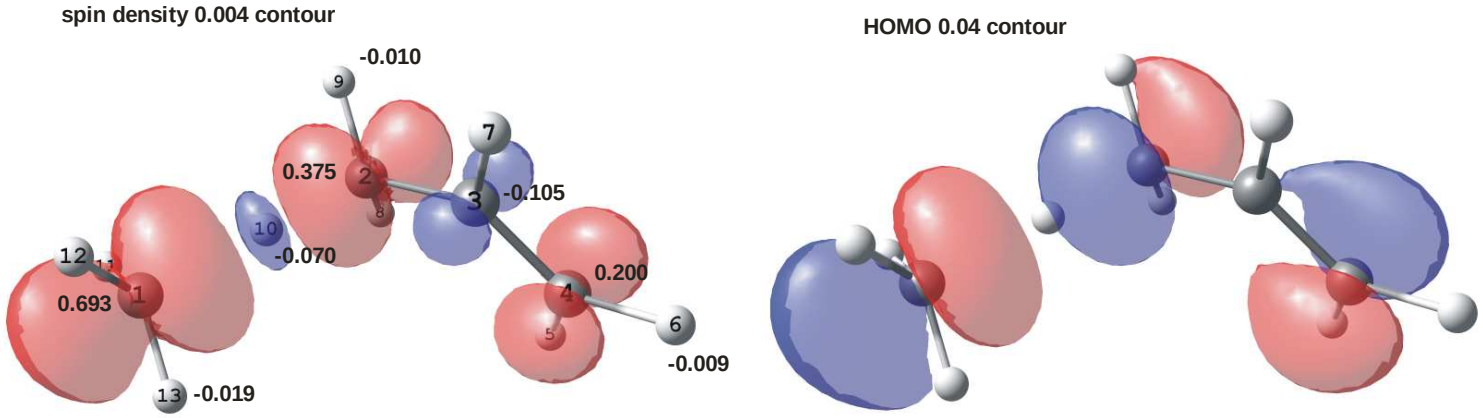


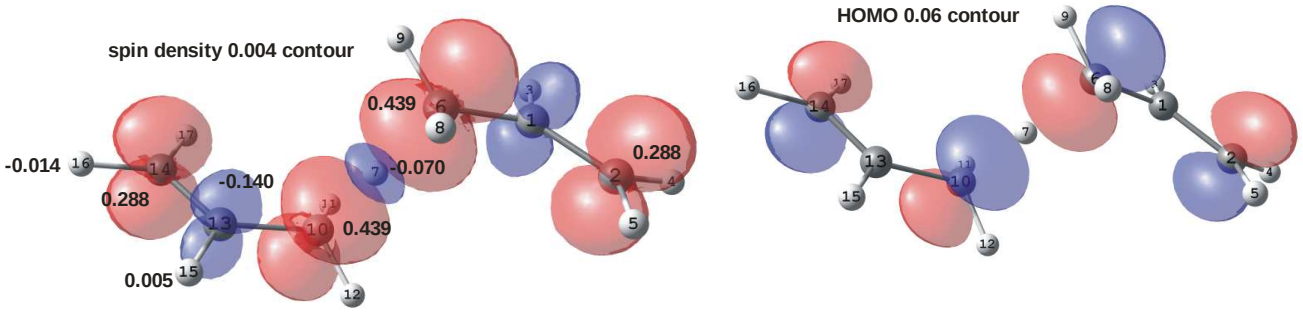
Figure S1: Transition state for the H-abstraction between an allyl radical and 1,3-butadiene.

Figures S2: Spin density plots and HOMO contours for selected reactions from Table 1 and 2, illustrating the resonance stabilization of the transition state relative to the reactions from which the Δ*GAV*° have been determined.

Methyl+propene

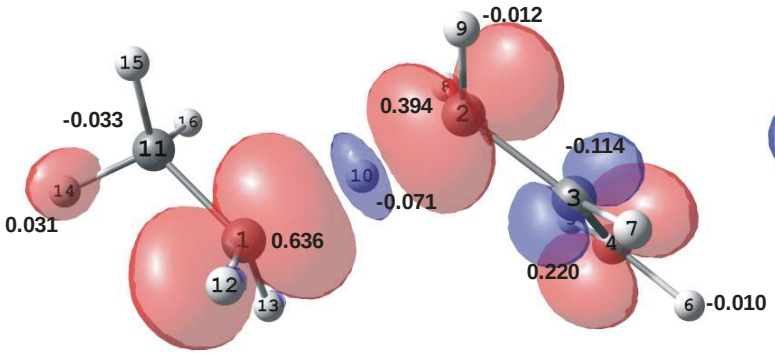


Allyl+propene

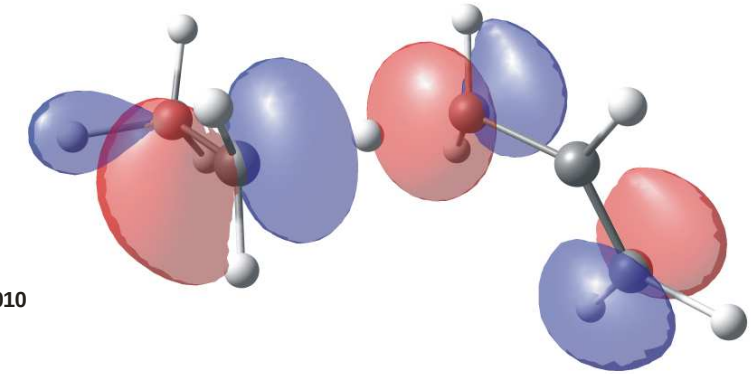


spin densities are not dependent on C2 of Ci geometry

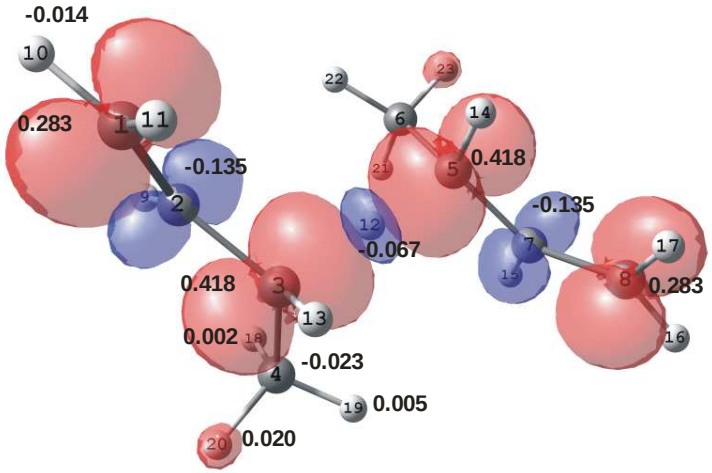
Ethyl+propene

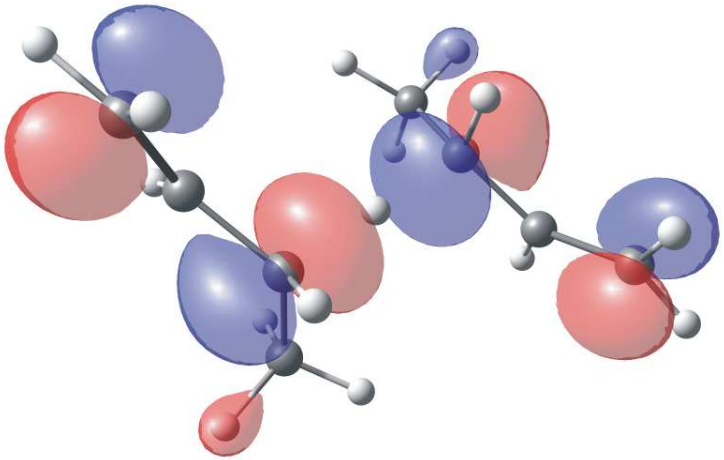


HOMO 0.05 contour

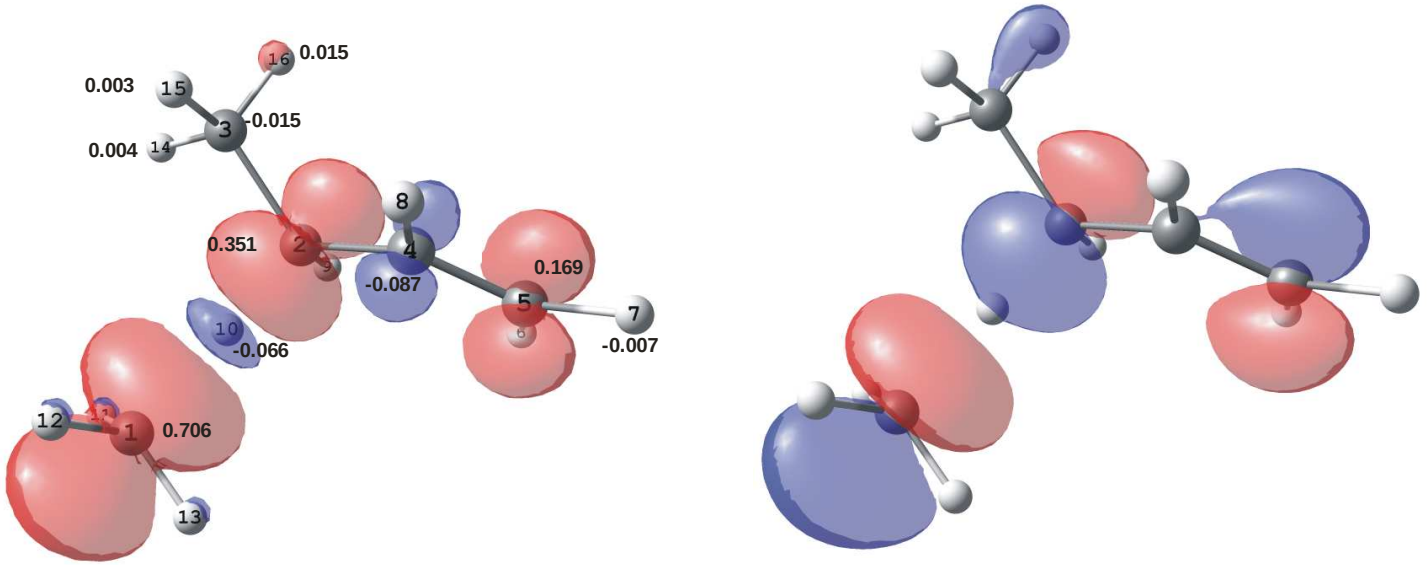


1-buten-3-yl+1-butene





Methyl+1-butene

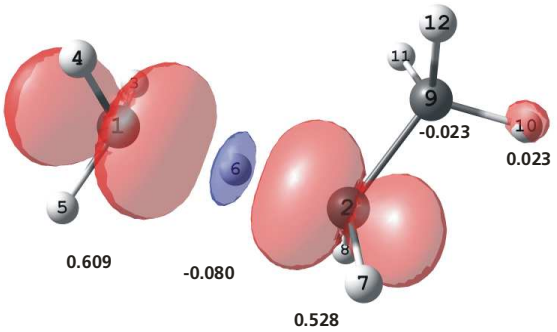


Methyl+ethaan

B3LYP/cbsb7 densities

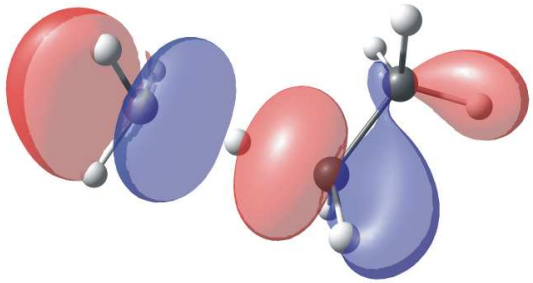
SPIN DENSITIES

Spin density plot (0.006 contour)



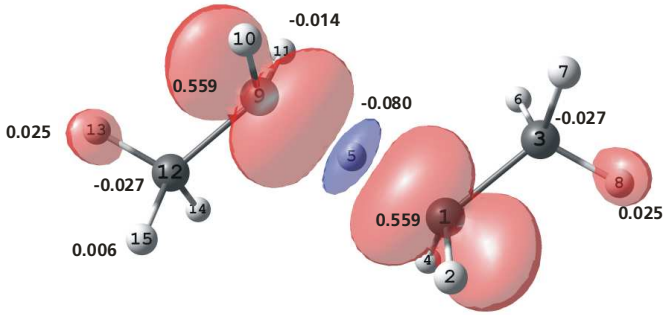
all other spin densities are smaller than 0.02

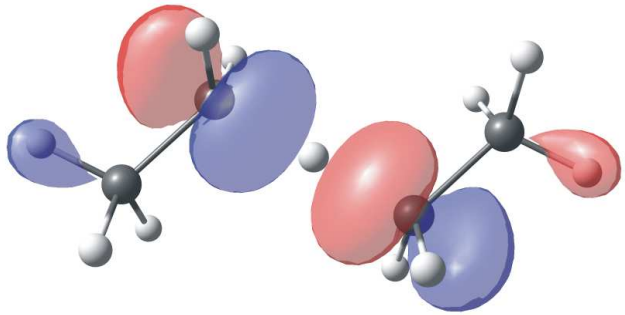
HOMO ORBITALS (0.04 contours)



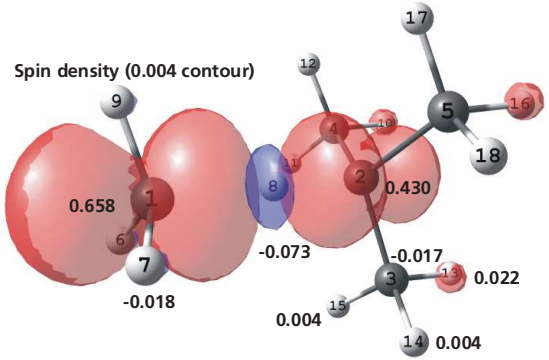
Ethyl+ethane

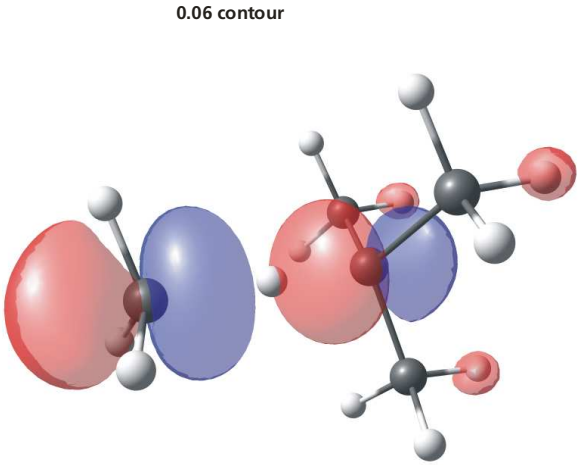
Spin density (0.004 contour)



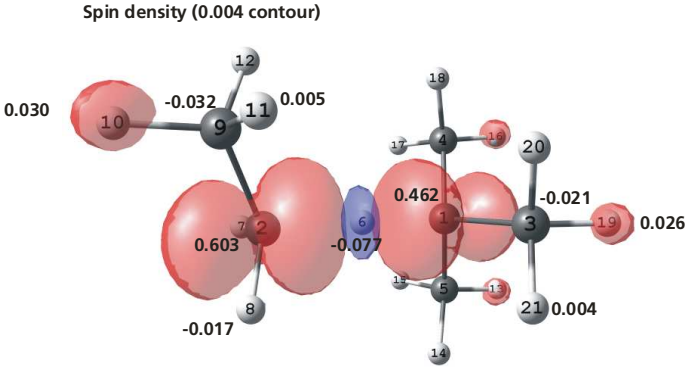


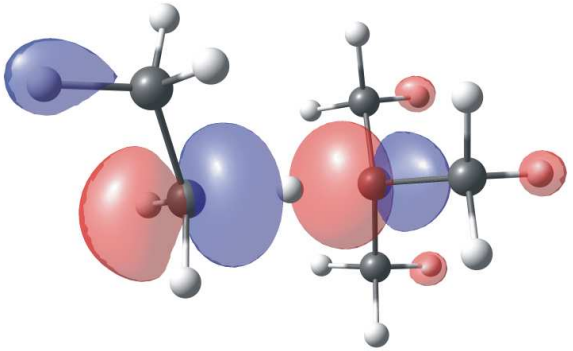
Methyl+isobutane -> methane + tert-butyl





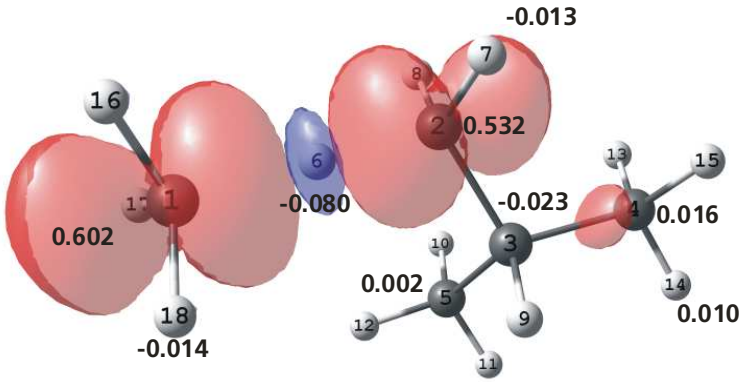
Ethyl+isobutane -> tert-butyl

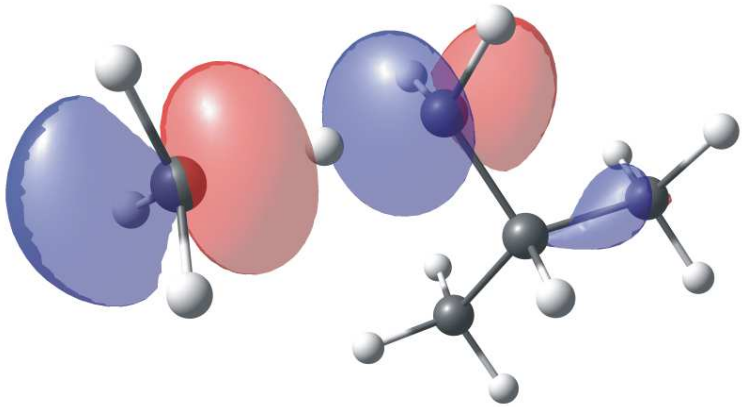




Methyl+isobutane ->isobutyl

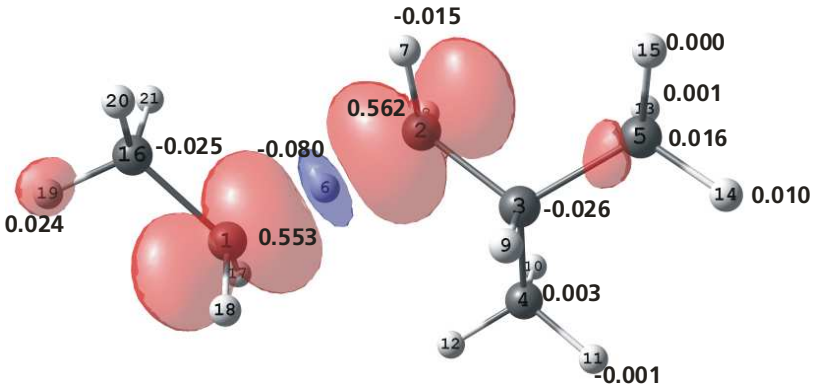
Spin density (0.004 contour)





Ethyl+isobutane -> isobutyl

Spin density (0.004 contour)



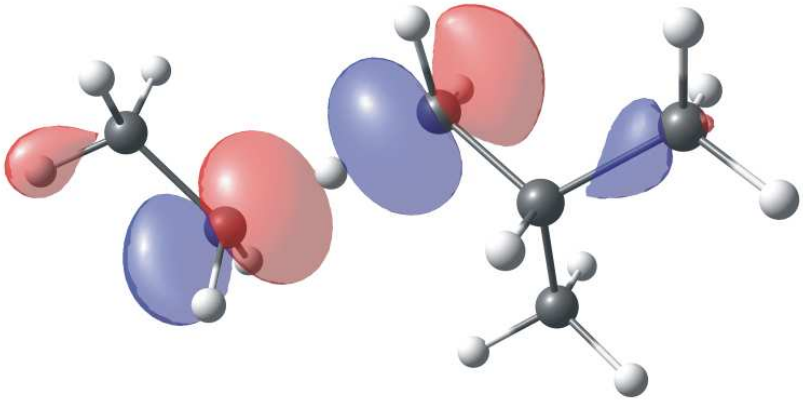
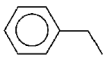
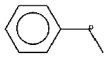
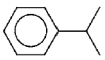
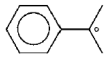


Table S1: Tunneling coefficients, pre-exponential factors [log($m^3mol^{-1}s^{-1}$)], activation energies [$kJmol^{-1}$], rate coefficients [$m^3\ mol^{-1}\ s^{-1}$] and reaction enthalpies [$kJ\ mol^{-1}$] for the training set of H-abstractions at 600 K (Arrhenius parameters exclude tunneling contribution).

	Reactie 600 K							Kappa	Forward			Reverse			$\Delta_r H°$
									log*A*	E_a	*k*	log*A*	E_a	*k*	
1	Me°	+	CH_4	⇌	CH_4	+	Me°	2.06	6.766	74.7	3.7E+00	6.766	74.7	3.7E+00	0.0
2	Me°	+		⇌	CH_4	+		1.99	7.012	64.3	5.1E+01	5.964	80.0	2.0E-01	-15.6
3	Me°	+		⇌	CH_4	+		1.90	6.565	54.8	1.2E+02	5.750	82.3	7.4E-02	-27.5
4	Me°	+		⇌	CH_4	+		1.77	6.348	45.6	4.2E+02	5.767	81.0	9.1E-02	-35.5
5	Me°	+		⇌	CH_4	+		1.78	6.409	48.3	2.8E+02	7.358	125.4	4.9E-04	-77.1
6	Me°	+		⇌	CH_4	+		1.60	6.439	41.2	1.1E+03	6.859	131.2	4.4E-05	-90.0
7	Me°	+		⇌	CH_4	+		1.48	6.266	35.2	2.3E+03	6.086	131.9	5.9E-06	-96.7
8	Me°	+		⇌	CH_4	+		1.33	6.468	31.8	6.6E+03	7.358	163.3	1.8E-07	-131.5
9	Me°	+		⇌	CH_4	+		1.24	5.831	26.6	4.0E+03	6.997	166.8	3.7E-08	-140.2
10	Me°	+		⇌	CH_4	+		1.85	6.632	51.3	2.7E+02	6.797	110.2	2.9E-03	-58.9
11	Me°	+		⇌	CH_4	+		1.71	6.511	43.6	8.8E+02	6.331	115.3	3.3E-04	-71.7
12	Me°	+		⇌	CH_4	+		1.56	6.213	36.2	1.8E+03	5.927	117.5	7.8E-05	-81.4
13	Me°	+		⇌	CH_4	+		1.46	6.465	33.5	5.2E+03	6.884	140.4	6.7E-06	-106.9
14	Me°	+		⇌	CH_4	+		1.35	6.163	27.9	7.4E+03	6.549	146.2	8.9E-07	-118.3
15	Me°	+		⇌	CH_4	+		2.03	6.902	74.8	5.0E+00	6.704	54.0	2.1E+02	20.8
16	Me°	+		⇌	CH_4	+		2.01	6.348	65.7	8.6E+00	6.554	57.9	6.6E+01	7.8
17	Me°	+		⇌	CH_4	+		2.00	6.661	65.5	1.8E+01	6.424	86.9	1.4E-01	-21.4
18	Me°	+		⇌	CH_4	+		1.90	6.204	54.6	5.4E+01	5.729	74.3	3.4E-01	-19.8
19	Me°	+		⇌	CH_4	+		1.77	6.315	56.1	4.8E+01	6.731	116.7	6.5E-04	-60.6
20	Me°	+		⇌	CH_4	+		1.61	6.271	47.2	2.3E+02	6.670	118.6	3.5E-04	-71.4
21	Me°	+		⇌	CH_4	+		1.56	5.884	42.0	2.6E+02	5.418	116.4	3.0E-05	-74.4
22	Me°	+		⇌	CH_4	+		1.89	7.105	81.5	1.9E+00	6.735	41.3	2.6E+03	40.2
23	Me°	+		⇌	CH_4	+		1.86	5.681	50.0	4.0E+01	6.695	87.8	2.1E-01	-37.8
24	Me°	+		⇌	CH_4	+		1.93	7.005	54.7	3.4E+02	6.164	80.2	3.0E-01	-25.5
25	Me°	+		⇌	CH_4	+		1.81	6.017	44.7	2.4E+02	5.752	78.3	1.6E-01	-33.6
26	Me°	+		⇌	CH_4	+		1.59	6.730	37.9	4.3E+03	6.741	130.5	3.8E-05	-92.6
27		+		⇌		+		2.36	6.484	88.4	3.0E-09	6.484	88.4	3.0E-09	0.0
28		+		⇌		+		2.30	6.405	78.3	1.4E-07	5.876	91.2	2.3E-10	-12.9

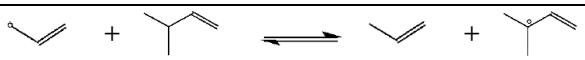
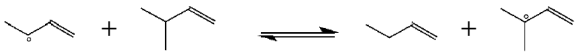
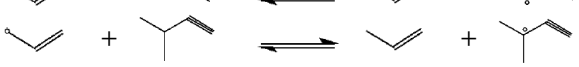
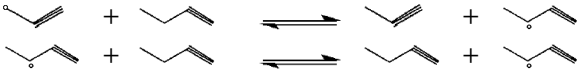
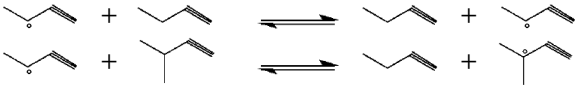
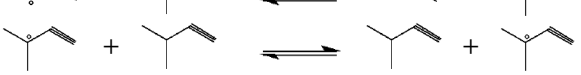
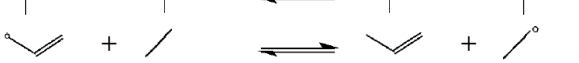
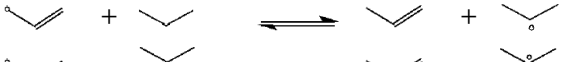
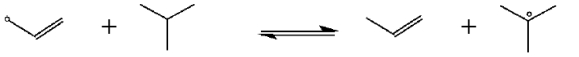
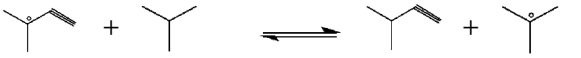
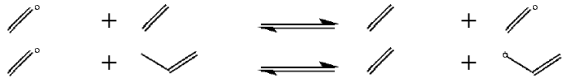
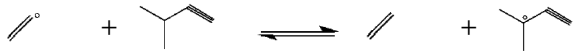
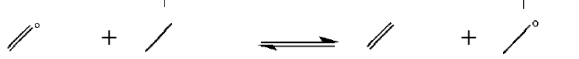
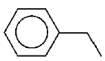
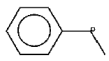
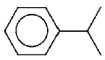
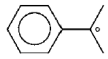
29		2.17	6.268	67.7	6.6E-06	5.140	87.3	1.9E-10	-19.6
30		2.25	5.894	78.9	3.2E-08	5.894	78.9	3.2E-08	0.0
31		2.20	5.536	71.1	3.2E-07	4.936	77.8	5.5E-09	-6.7
32		2.17	**4.589**	68.2	1.1E-07	4.589	68.2	1.1E-07	0.0
33		2.27	7.120	93.5	1.6E-09	6.336	75.3	3.8E-07	18.2
34		2.24	6.620	82.2	4.5E-08	5.492	76.8	2.9E-08	5.4
35		2.19	6.520	71.7	2.4E-06	5.286	76.0	2.5E-08	-4.3
36		2.27	6.614	81.2	6.8E-08	6.614	81.2	6.8E-08	0.0
37		2.22	6.450	69.9	4.3E-06	6.106	82.6	1.2E-08	-12.8
38		2.21	5.623	71.4	3.5E-07	5.623	71.4	3.5E-07	0.0
39		2.16	5.550	60.2	2.5E-05	5.444	69.9	4.1E-07	-9.6
40		2.17	5.005	59.3	1.0E-05	5.005	59.3	1.0E-05	0.0
41		1.94	7.535	111.4	2.7E-12	5.538	49.9	1.4E-03	61.5
42		2.03	7.058	97.7	2.3E-10	5.295	48.1	1.7E-03	49.6
43		2.03	6.770	86.4	1.1E-08	5.241	44.8	5.7E-03	41.6
44		1.96	6.440	104.4	3.6E-12	5.205	41.8	1.6E-02	62.5
45		1.83	5.658	104.1	6.3E-13	5.024	34.9	1.6E-01	69.2
46		1.91	5.073	77.3	7.8E-09	4.778	31.4	3.9E-01	45.9
47		2.13	5.418	61.4	1.1E-05	5.418	61.4	1.1E-05	0.0
48		2.18	4.845	48.5	5.5E-04	4.845	48.5	5.5E-04	0.0
49		1.95	6.839	53.5	6.5E-03	6.839	53.5	6.5E-03	0.0
50		1.43	6.313	28.6	3.1E+01	7.460	126.5	3.8E-15	-97.9
51		1.17	6.079	18.0	**1.0E+03**	5.992	120.2	1.4E-15	-102.2
52		1.79	6.979	43.4	4.7E-01	6.129	79.9	3.0E-08	-36.5
53		1.61	6.546	34.1	6.6E+00	5.929	82.4	6.1E-09	-48.4
54		1.58	7.321	116.3	1.8E-13	6.135	60.6	6.0E-05	55.7

Table S2: Tunneling coefficients, pre-exponential factors [log($m^3mol^{-1}s^{-1}$)], activation energies [$kJmol^{-1}$], rate coefficients [$m^3\ mol^{-1}\ s^{-1}$] and reaction enthalpies [$kJ\ mol^{-1}$] for the training set of H-abstractions at 1000 K (Arrhenius parameters exclude tunneling contribution).

	Reactie 1000K							Kappa	Forward			Reverse			$\Delta_r H°$
									log*A*	E_a	*k*	log*A*	E_a	*k*	
1	Me°	+	CH_4	⇌	CH_4	+	Me°	1.30	7.412	84.4	1.3E+03	7.412	84.4	1.3E+03	0.0
2	Me°	+		⇌	CH_4	+		1.28	7.659	74.0	7.9E+03	6.622	89.8	1.1E+02	-15.8
3	Me°	+		⇌	CH_4	+		1.26	7.212	64.4	8.8E+03	6.429	92.4	5.0E+01	-28.0
4	Me°	+		⇌	CH_4	+		1.23	6.996	55.3	1.6E+04	6.483	91.7	6.0E+01	-36.4
5	Me°	+		⇌	CH_4	+		1.23	7.053	58.0	1.3E+04	8.046	135.7	1.1E+01	-77.7
6	Me°	+		⇌	CH_4	+		1.19	7.086	50.9	3.2E+04	7.556	141.6	1.7E+00	-90.7
7	Me°	+		⇌	CH_4	+		1.16	6.908	44.8	4.3E+04	6.794	142.5	2.6E-01	-97.7
8	Me°	+		⇌	CH_4	+		1.11	7.118	41.6	9.8E+04	8.070	174.0	1.1E-01	-132.4
9	Me°	+		⇌	CH_4	+		1.08	6.471	36.2	4.1E+04	7.831	179.2	3.2E-02	-143.0
10	Me°	+		⇌	CH_4	+		1.25	7.276	61.0	1.5E+04	7.471	120.3	1.9E+01	-59.4
11	Me°	+		⇌	CH_4	+		1.22	7.157	53.3	2.9E+04	7.023	125.7	3.5E+00	-72.4
12	Me°	+		⇌	CH_4	+		1.18	6.859	45.8	3.4E+04	6.640	128.2	1.0E+00	-82.3
13	Me°	+		⇌	CH_4	+		1.15	7.109	43.1	8.3E+04	7.592	151.0	5.9E-01	-107.9
14	Me°	+		⇌	CH_4	+		1.12	6.808	37.5	7.9E+04	7.387	158.7	1.4E-01	-121.2
15	Me°	+		⇌	CH_4	+		1.30	7.543	84.4	1.8E+03	7.398	64.4	1.4E+04	20.1
16	Me°	+		⇌	CH_4	+		1.29	6.985	75.2	1.5E+03	7.268	68.5	6.3E+03	6.7
17	Me°	+		⇌	CH_4	+		1.28	7.297	75.0	3.1E+03	7.101	97.0	1.4E+02	-22.0
18	Me°	+		⇌	CH_4	+		1.26	6.839	64.1	3.9E+03	6.409	84.5	1.2E+02	-20.4
19	Me°	+		⇌	CH_4	+		1.23	7.068	67.4	4.3E+03	7.419	127.0	7.5E+00	-59.6
20	Me°	+		⇌	CH_4	+		1.18	6.913	56.8	1.0E+04	7.368	129.0	5.0E+00	-72.2
21	Me°	+		⇌	CH_4	+		1.18	6.529	51.7	8.0E+03	6.135	127.1	3.7E-01	-75.4
22	Me°	+		⇌	CH_4	+		1.27	7.732	90.9	1.2E+03	7.465	52.2	6.9E+04	38.7
23	Me°	+		⇌	CH_4	+		1.25	6.324	59.6	2.0E+03	7.372	97.9	2.3E+02	-38.3
24	Me°	+		⇌	CH_4	+		1.27	7.648	64.3	2.5E+04	6.849	90.4	1.7E+02	-26.1
25	Me°	+		⇌	CH_4	+		1.25	6.652	54.2	8.3E+03	6.464	88.9	8.3E+01	-34.7
26	Me°	+		⇌	CH_4	+		1.19	7.377	47.6	9.2E+04	7.441	141.0	1.4E+00	-93.3
27		+		⇌		+		1.35	7.160	98.5	1.4E-10	7.160	98.5	1.4E-10	0.0
28		+		⇌		+		1.34	7.083	88.4	6.6E-09	6.560	101.4	1.1E-11	-13.0

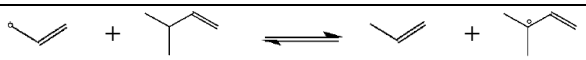
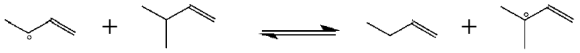
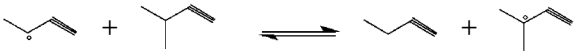
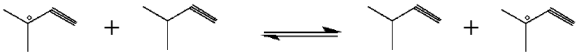
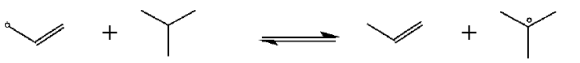
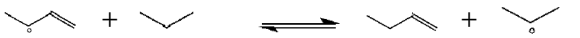
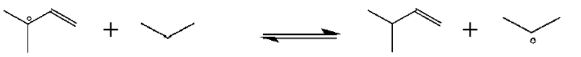
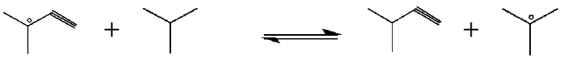
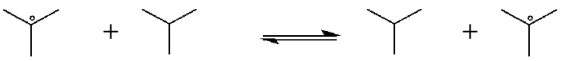
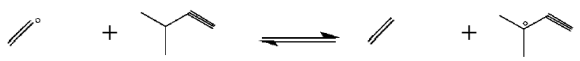
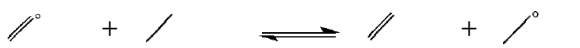
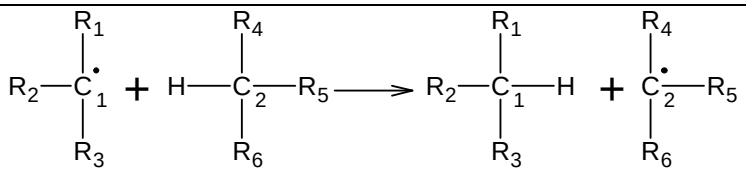
29		1.32	6.937	77.7	3.4E-07	5.829	97.6	9.1E-12	-19.9
30		1.34	6.577	89.1	1.6E-09	6.577	89.1	1.6E-09	0.0
31		1.33	6.206	81.0	1.7E-08	5.622	88.0	2.7E-10	-6.9
32		1.33	5.292	78.7	5.1E-09	5.292	78.7	5.1E-09	0.0
33		1.34	7.800	103.6	7.6E-11	7.001	85.3	1.9E-08	18.4
34		1.34	7.300	92.4	2.2E-09	6.172	87.0	1.4E-09	5.4
35		1.33	7.196	81.8	1.2E-07	5.983	86.4	1.2E-09	-4.6
36		1.34	7.285	91.2	3.4E-09	7.285	91.2	3.4E-09	0.0
37		1.33	7.126	79.9	2.1E-07	6.797	92.9	5.5E-10	-13.0
38		1.33	6.328	81.9	1.6E-08	6.328	81.9	1.6E-08	0.0
39		1.33	6.243	70.6	1.2E-06	6.158	80.5	1.8E-08	-10.0
40		1.34	5.746	70.4	4.2E-07	5.746	70.4	4.2E-07	0.0
41		1.27	8.222	121.6	1.4E-13	6.191	59.7	8.0E-05	61.9
42		1.30	7.742	107.9	1.2E-11	5.965	58.1	9.2E-05	49.8
43		1.30	7.446	96.5	5.7E-10	5.939	55.2	2.8E-04	41.3
44		1.28	7.129	114.6	1.9E-13	5.876	51.9	9.0E-04	62.8
45		1.26	6.358	114.5	3.3E-14	5.690	44.8	9.6E-03	69.7
46		1.29	5.772	87.7	4.0E-10	5.477	41.8	2.0E-02	45.9
47		1.32	6.094	71.5	5.7E-07	6.094	71.5	5.7E-07	0.0
48		1.35	5.547	59.0	2.6E-05	5.547	59.0	2.6E-05	0.0
49		1.29	7.533	63.9	3.3E-04	7.533	63.9	3.3E-04	0.0
50		1.15	7.005	38.9	1.9E+00	8.144	136.7	2.5E-16	-97.8
51		1.06	6.771	28.3	**7.4E+01**	6.697	130.7	9.2E-17	-102.4
52		1.24	7.674	53.8	2.5E-02	6.782	89.7	1.8E-09	-35.9
53		1.20	7.239	44.4	3.8E-01	6.601	92.5	3.8E-10	-48.0
54		1.18	8.002	126.5	1.1E-14	6.812	70.7	3.7E-06	55.8

Table S3: Number of single events n_e, external and internal symmetry numbers σ_e and σ_i, and number of optical isomers n_{opt} for the reactions of Table 1 and 2.

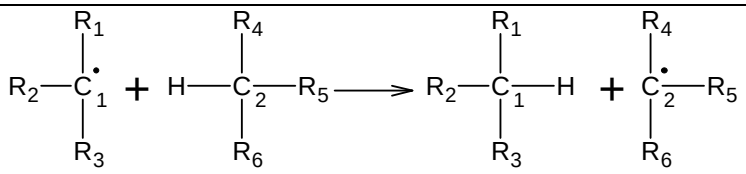
Nr.	Reactant 1			Reactant 2			TS			Product 1			Product 1			n_e	
	σ_e	σ_i	n_{opt}	σ_e	σ_i	n_{opt}	σ_e	σ_i	n_{opt}	σ_e	σ_i	n_{opt}	σ_e	σ_i	n_{opt}	forward	reverse
1	12	1	1	6	1	1	3	3	1	6	1	1	12	1	1	8	8
2	6	3	1	6	1	1	1	9	1	1	6	1	12	1	1	12	8
3	2	9	1	6	1	1	1	27	1	1	9	1	12	1	1	4	4
4	3	27	1	6	1	1	3	81	1	3	27	1	12	1	1	2	4
5	1	3	1	6	1	1	1	3	2	2	1	1	12	1	1	12	16
6	1	3	1	6	1	1	1	9	2	1	3	1	12	1	1	4	8
7	1	9	1	6	1	1	1	27	2	1	9	1	12	1	1	4	8
8	2	1	1	6	1	1	1	3	1	2	1	1	12	1	1	4	8
9	1	3	1	6	1	1	1	9	1	1	6	1	12	1	1	2	8
10	3	1	1	6	1	1	1	3	1	2	1	1	12	1	1	6	8
11	1	3	1	6	1	1	1	9	2	1	3	1	12	1	1	4	8
12	1	9	1	6	1	1	1	27	1	2	9	1	12	1	1	2	8
13	2	1	1	6	1	1	1	3	1	2	1	1	12	1	1	4	8
14	1	3	1	6	1	1	1	9	1	1	6	1	12	1	1	2	8
15	4	1	1	6	1	1	1	3	1	1	1	1	12	1	1	8	4
16	1	3	1	6	1	1	1	9	1	1	3	1	12	1	1	2	4
17	2	1	1	6	1	1	1	3	1	1	1	1	12	1	1	4	4
18	1	1	1	6	1	1	1	3	1	1	1	1	12	1	1	2	4
19	1	6	1	6	1	1	1	3	1	1	1	1	12	1	1	12	4
20	1	6	1	6	1	1	1	9	2	1	3	1	12	1	1	8	8
21	1	18	1	6	1	1	1	27	1	1	9	1	12	1	1	4	4
22	12	1	1	6	1	1	1	6	1	2	1	1	12	1	1	12	4
23	1	1	1	6	1	1	1	3	2	1	1	1	12	1	1	4	8
24	6	1	1	6	1	1	1	3	1	1	1	1	12	1	1	12	4
25	1	3	1	6	1	1	1	9	1	1	3	1	12	1	1	2	4
26	2	1	1	6	1	1	1	3	2	1	1	1	12	1	1	8	8
27	1	3	1	2	1	1	1	1	2	2	1	1	1	3	1	12	12
28	2	1	1	1	3	1	1	3	2	1	3	1	1	3	1	4	6
29	2	1	1	1	9	1	1	9	2	1	3	1	1	9	1	4	6
30	1	3	1	1	3	1	1	9	2	1	3	1	1	3	1	2	2
31	1	3	1	1	9	1	1	27	2	1	3	1	1	9	1	2	2
32	1	9	1	1	9	1	1	81	2	1	9	1	1	9	1	2	2
33	2	1	1	3	1	1	1	1	2	1	3	1	2	1	1	12	12
34	2	1	1	1	3	1	1	3	2	1	3	1	1	3	1	4	6
35	2	1	1	1	9	1	1	9	2	1	3	1	2	9	1	4	12
36	2	1	1	3	1	1	1	1	1	3	1	1	2	1	1	6	6
37	2	1	1	1	3	1	1	3	2	3	1	1	1	3	1	4	6
38	1	3	1	1	3	1	1	9	2	1	3	1	1	3	1	2	2
39	1	3	1	1	9	1	1	27	2	1	3	1	2	9	1	2	4
40	2	9	1	1	9	1	1	81	1	1	9	1	2	9	1	2	2
41	2	1	1	6	3	1	1	3	2	1	3	1	1	6	1	24	12
42	2	1	1	2	9	1	1	9	2	1	3	1	1	9	1	8	6
43	2	1	1	3	27	1	1	81	2	1	3	1	3	27	1	4	6
44	2	9	1	1	3	1	1	27	2	1	9	1	1	3	1	4	2
45	2	9	1	1	9	1	1	81	2	1	9	1	1	9	1	4	2

46	3	27	1	2	9	1	1	729	1	3	27	1	1	9	1	2	1
47	2	9	1	1	9	1	1	81	1	1	9	1	2	9	1	2	2
48	3	27	1	3	27	1	3	2187	1	3	27	1	3	27	1	1	1
49	4	1	1	1	1	1	1	1	1	1	1	1	4	1	1	4	4
50	1	3	1	1	1	1	1	1	2	2	1	1	4	1	1	6	16
51	1	1	1	1	9	1	1	9	1	4	1	1	2	9	1	1	8
52	1	1	1	6	3	1	1	3	1	4	1	1	1	6	1	6	8
53	1	1	1	2	9	1	1	9	1	4	1	1	1	9	1	2	4
54	2	1	1	2	1	1	1	1	2	1	3	1	1	1	1	8	6

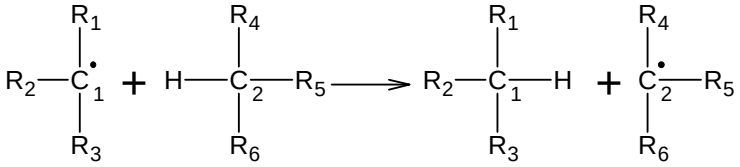
Tables S4: Group additive values between 400-1300 K.



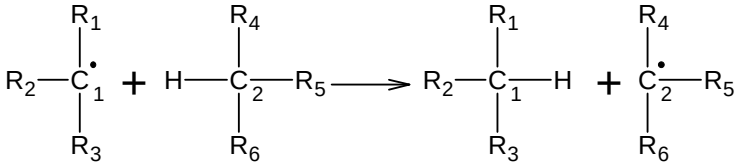
Nr.	Group	400 K				500 K			
		C_1 contribution		C_2 contribution		C_1 contribution		C_2 contribution	
		$\Delta GAV^{o}_{\log A}$	$\Delta GAV^{o}_{E_a}$	$\Delta GAV^{o}_{\log A}$	$\Delta GAV^{o}_{E_a}$	$\Delta GAV^{o}_{\log A}$	$\Delta GAV^{o}_{E_a}$	$\Delta GAV^{o}_{\log A}$	$\Delta GAV^{o}_{E_a}$
	Reference reaction:								
	$CH_3^{\bullet} + CH_4$	5.453	70.9	5.453	70.9	5.662	72.6	5.662	72.6
1	C_i-$(C)(H)_2$	-0.832	+4.9	+0.053	-10.6	-0.814	+5.1	+0.065	-10.4
2	C_i-$(C)_2(H)$	-0.781	+6.9	+0.072	-20.3	-0.741	+7.3	+0.092	-20.0
3	C_i-$(C)_3$	-0.826	+5.1	+0.143	-29.5	-0.748	+5.8	+0.173	-29.2
4	C_i-$(C_d)(H)_2$	+0.205	+49.9	-0.548	-26.6	+0.259	+50.4	-0.537	-26.4
5	C_i-$(C_d)(C)(H)$	-0.006	+55.5	-0.058	-33.9	+0.056	+56.1	-0.035	-33.6
6	C_i-$(C_d)(C)_2$	-0.795	+56.1	-0.232	-39.8	-0.725	+56.8	-0.208	-39.6
7	C_i-$(C_d)_2(H)$	+0.465	+87.4	-0.035	-43.3	+0.544	+88.1	-0.008	-43.0
8	C_i-$(C_d)_2(C)$	+0.002	+89.9	-0.363	-48.4	+0.137	+91.1	-0.341	-48.1
9	C_i-$(C_t)(H)_2$	-0.025	+35.0	-0.023	-23.6	+0.009	+35.3	-0.013	-23.4
10	C_i-$(C_t)(C)(H)$	-0.520	+39.8	+0.017	-31.4	-0.469	+40.3	+0.037	-31.2
11	C_i-$(C_t)(C)_2$	-0.955	+41.7	+0.011	-38.9	-0.886	+42.3	+0.038	-38.6
12	C_i-$(C_t)_2(H)$	+0.007	+64.6	-0.026	-41.5	+0.074	+65.2	-0.007	-41.3
13	C_i-$(C_t)_2(C)$	-0.444	+69.3	-0.037	-47.2	-0.312	+70.5	-0.010	-46.9
14	$C_{i,d}$-(H)	+0.151	-21.6	+0.120	-0.1	+0.205	-21.1	+0.132	+0.1
15	$C_{i,d}$-(C)	-0.025	-17.9	+0.164	-9.3	+0.044	-17.3	+0.181	-9.0
16	$C_{i,d}$-(C_d)	-0.105	+11.5	+0.173	-9.5	-0.065	+11.9	+0.192	-9.2
17	$C_{i,d}$-(C_t)	-0.784	-0.9	+0.022	-20.4	-0.758	-0.6	+0.038	-20.2
18	C_i-$(C_B)(H)_2$	+0.182	+41.2	-0.729	-19.6	+0.235	+41.7	-0.671	-19.0
19	C_i-$(C_B)(C)(H)$	-0.192	+43.0	-0.521	-27.8	-0.133	+43.5	-0.502	-27.5
20	C_i-$(C_B)(C)_2$	-1.171	+40.5	-0.618	-33.1	-1.096	+41.2	-0.591	-32.8
21	$C_{i,B}$	+0.126	-34.8	+0.150	+6.6	+0.214	-33.9	+0.163	+6.8
22	$C_{i,cyclo\text{-}5}$-(H)	-0.140	+12.4	-0.805	-25.0	-0.097	+12.8	-0.789	-24.8
23	$C_{i,cyclo\text{-}6}$-(H)	-0.377	+4.7	+0.035	-20.3	-0.330	+5.2	+0.055	-20.1
24	$C_{i,cyclo\text{-}6}$-(C)	-0.836	+2.4	-0.173	-30.3	-0.760	+3.1	-0.153	-30.1
25	$C_{i,cycloallylic\text{-}6}$-$(C_d)(H)$	-0.131	+54.8	-0.067	-37.1	-0.065	+55.4	-0.045	-36.9



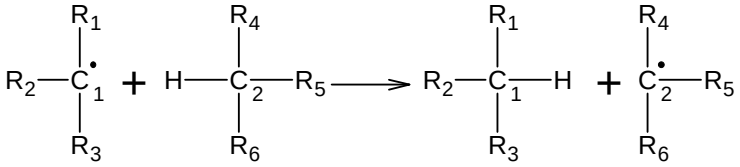
Nr.	Group	600 K				700 K			
		C_1 contribution		C_2 contribution		C_1 contribution		C_2 contribution	
		$\Delta GAV^{o}_{\log A}$	$\Delta GAV^{o}_{E_a}$	$\Delta GAV^{o}_{\log A}$	$\Delta GAV^{o}_{E_a}$	$\Delta GAV^{o}_{\log A}$	$\Delta GAV^{o}_{E_a}$	$\Delta GAV^{o}_{\log A}$	$\Delta GAV^{o}_{E_a}$
	Reference reaction:								
	$CH_3^{\bullet} + CH_4$	5.863	74.7	5.863	74.7	6.050	77.0	6.050	77.0
1	C_i-$(C)(H)_2$	-0.802	+5.3	+0.070	-10.4	-0.797	+5.3	+0.071	-10.4
2	C_i-$(C)_2(H)$	-0.715	+7.6	+0.100	-19.9	-0.700	+7.8	+0.101	-19.9
3	C_i-$(C)_3$	-0.698	+6.3	+0.184	-29.1	-0.667	+6.7	+0.187	-29.1
4	C_i-$(C_d)(H)_2$	+0.291	+50.7	-0.533	-26.4	+0.309	+51.0	-0.533	-26.4
5	C_i-$(C_d)(C)(H)$	+0.093	+56.5	-0.026	-33.5	+0.115	+56.8	-0.024	-33.5
6	C_i-$(C_d)(C)_2$	-0.680	+57.2	-0.199	-39.5	-0.654	+57.6	-0.199	-39.5
7	C_i-$(C_d)_2(H)$	+0.591	+88.6	+0.003	-42.9	+0.620	+89.0	+0.007	-42.8
8	C_i-$(C_d)_2(C)$	+0.231	+92.1	-0.333	-48.1	+0.297	+92.9	-0.333	-48.1
9	C_i-$(C_t)(H)_2$	+0.031	+35.5	-0.009	-23.4	+0.043	+35.7	-0.009	-23.4
10	C_i-$(C_t)(C)(H)$	-0.435	+40.6	+0.046	-31.1	-0.415	+40.9	+0.047	-31.0
11	C_i-$(C_t)(C)_2$	-0.839	+42.8	+0.049	-38.5	-0.810	+43.2	+0.051	-38.5
12	C_i-$(C_t)_2(H)$	+0.118	+65.7	0.000	-41.2	+0.145	+66.0	+0.001	-41.2
13	C_i-$(C_t)_2(C)$	-0.217	+71.5	-0.001	-46.8	-0.149	+72.3	+0.001	-46.8
14	$C_{i,d}$-(H)	+0.239	-20.7	+0.136	+0.1	+0.259	-20.5	+0.134	+0.1
15	$C_{i,d}$-(C)	+0.089	-16.8	+0.184	-9.0	+0.117	-16.5	+0.182	-9.0
16	$C_{i,d}$-(C_d)	-0.041	+12.2	+0.196	-9.2	-0.028	+12.4	+0.193	-9.2
17	$C_{i,d}$-(C_t)	-0.736	-0.4	+0.040	-20.1	-0.722	-0.2	+0.037	-20.2
18	C_i-$(C_B)(H)_2$	+0.266	+42.0	-0.627	-18.6	+0.283	+42.3	-0.594	-18.2
19	C_i-$(C_B)(C)(H)$	-0.096	+43.9	-0.495	-27.5	-0.074	+44.2	-0.495	-27.5
20	C_i-$(C_B)(C)_2$	-1.047	+41.7	-0.581	-32.7	-1.017	+42.1	-0.579	-32.6
21	$C_{i,B}$	+0.270	-33.4	+0.163	+6.8	+0.304	-32.9	+0.157	+6.7
22	$C_{i,cyclo\text{-}5}$-(H)	-0.071	+13.1	-0.784	-24.7	-0.057	+13.3	-0.784	-24.7
23	$C_{i,cyclo\text{-}6}$-(H)	-0.301	+5.5	+0.063	-20.0	-0.284	+5.7	+0.063	-20.0
24	$C_{i,cyclo\text{-}6}$-(C)	-0.713	+3.6	-0.147	-30.0	-0.684	+3.9	-0.149	-30.0
25	$C_{i,cycloallylic\text{-}6}$-$(C_d)(H)$	-0.025	+55.8	-0.036	-36.8	-0.002	+56.1	-0.034	-36.7



Nr.	Group	800 K				900 K			
		C_1 contribution		C_2 contribution		C_1 contribution		C_2 contribution	
		$\Delta GAV^{o}_{\log A}$	$\Delta GAV^{o}_{E_a}$	$\Delta GAV^{o}_{\log A}$	$\Delta GAV^{o}_{E_a}$	$\Delta GAV^{o}_{\log A}$	$\Delta GAV^{o}_{E_a}$	$\Delta GAV^{o}_{\log A}$	$\Delta GAV^{o}_{E_a}$
	Reference reaction:								
	$CH_3^{\bullet} + CH_4$	6.219	79.5	6.219	79.5	6.371	81.9	6.371	81.9
1	C_i-$(C)(H)_2$	-0.793	+5.3	+0.071	-10.4	-0.791	+5.4	+0.071	-10.4
2	C_i-$(C)_2(H)$	-0.691	+7.8	+0.102	-20.0	-0.685	+8.0	+0.102	-19.9
3	C_i-$(C)_3$	-0.648	+6.9	+0.187	-29.2	-0.635	+7.2	+0.187	-29.1
4	C_i-$(C_d)(H)_2$	+0.321	+51.0	-0.533	-26.5	+0.329	+51.2	-0.534	-26.4
5	C_i-$(C_d)(C)(H)$	+0.129	+56.9	-0.024	-33.6	+0.139	+57.1	-0.024	-33.5
6	C_i-$(C_d)(C)_2$	-0.637	+57.7	-0.199	-39.6	-0.625	+58.0	-0.201	-39.5
7	C_i-$(C_d)_2(H)$	+0.638	+89.2	+0.008	-42.9	+0.650	+89.4	+0.008	-42.8
8	C_i-$(C_d)_2(C)$	+0.347	+93.6	-0.334	-48.2	+0.387	+94.3	-0.336	-48.1
9	C_i-$(C_t)(H)_2$	+0.051	+35.7	-0.009	-23.5	+0.057	+35.9	-0.010	-23.4
10	C_i-$(C_t)(C)(H)$	-0.402	+41.0	+0.047	-31.1	-0.393	+41.2	+0.047	-31.1
11	C_i-$(C_t)(C)_2$	-0.791	+43.4	+0.051	-38.6	-0.779	+43.6	+0.050	-38.5
12	C_i-$(C_t)_2(H)$	+0.162	+66.2	+0.001	-41.3	+0.174	+66.4	0.000	-41.3
13	C_i-$(C_t)_2(C)$	-0.097	+73.0	+0.001	-46.9	-0.057	+73.7	+0.000	-46.9
14	$C_{i,d}$-(H)	+0.272	-20.4	+0.133	0.0	+0.282	-20.1	+0.132	+0.1
15	$C_{i,d}$-(C)	+0.136	-16.3	+0.179	-9.2	+0.149	-16.0	+0.177	-9.1
16	$C_{i,d}$-(C_d)	-0.019	+12.4	+0.190	-9.4	-0.013	+12.6	+0.188	-9.3
17	$C_{i,d}$-(C_t)	-0.712	-0.1	+0.034	-20.3	-0.706	+0.1	+0.032	-20.3
18	C_i-$(C_B)(H)_2$	+0.295	+42.3	-0.566	-17.9	+0.303	+42.5	-0.541	-17.4
19	C_i-$(C_B)(C)(H)$	-0.059	+44.3	-0.496	-27.6	-0.049	+44.5	-0.497	-27.5
20	C_i-$(C_B)(C)_2$	-0.998	+42.3	-0.579	-32.7	-0.984	+42.6	-0.580	-32.7
21	$C_{i,B}$	+0.327	-32.7	+0.151	+6.6	+0.343	-32.4	+0.147	+6.6
22	$C_{i,cyclo\text{-}5}$-(H)	-0.048	+13.3	-0.785	-24.8	-0.042	+13.5	-0.786	-24.8
23	$C_{i,cyclo\text{-}6}$-(H)	-0.273	+5.7	+0.063	-20.1	-0.266	+5.9	+0.062	-20.1
24	$C_{i,cyclo\text{-}6}$-(C)	-0.666	+4.1	-0.152	-30.2	-0.654	+4.4	-0.154	-30.1
25	$C_{i,cycloallylic\text{-}6}$-$(C_d)(H)$	+0.013	+56.2	-0.033	-36.8	+0.023	+56.4	-0.033	-36.8

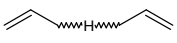
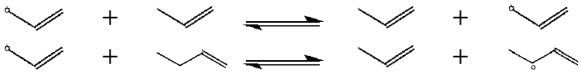
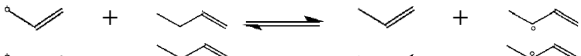
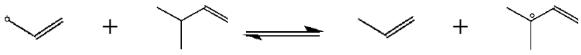
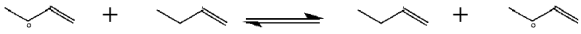
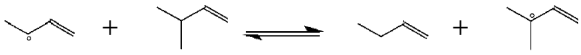
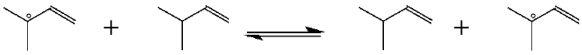
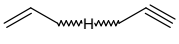
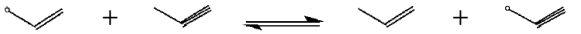
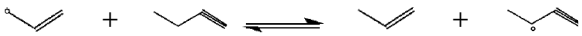
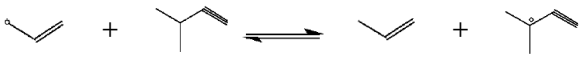
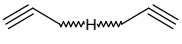
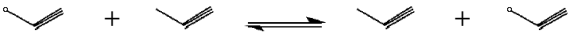
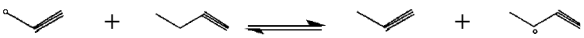
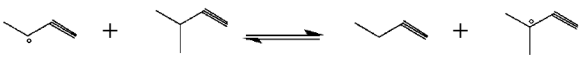
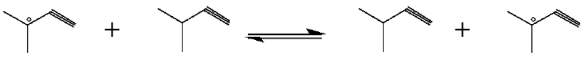
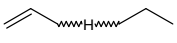
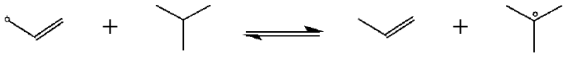
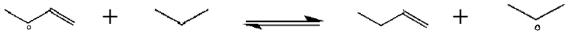
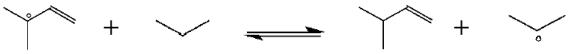
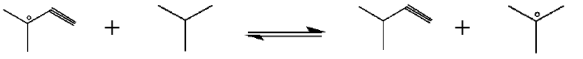
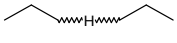
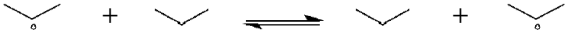
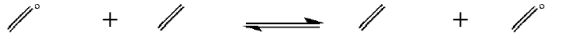
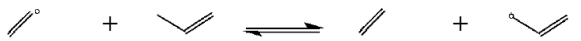


Nr.	Group	1000 K				1100 K			
		C_1 contribution		C_2 contribution		C_1 contribution		C_2 contribution	
		$\Delta GAV^{o}_{\log A}$	$\Delta GAV^{o}_{E_a}$	$\Delta GAV^{o}_{\log A}$	$\Delta GAV^{o}_{E_a}$	$\Delta GAV^{o}_{\log A}$	$\Delta GAV^{o}_{E_a}$	$\Delta GAV^{o}_{\log A}$	$\Delta GAV^{o}_{E_a}$
	Reference reaction:								
	$CH_3^{\bullet} + CH_4$	6.509	84.4	6.509	84.4	6.633	86.9	6.633	86.9
1	C_i-$(C)(H)_2$	-0.790	+5.4	+0.071	-10.4	-0.789	+5.4	+0.071	-10.4
2	C_i-$(C)_2(H)$	-0.682	+8.0	+0.101	-20.0	-0.680	+8.0	+0.101	-20.0
3	C_i-$(C)_3$	-0.628	+7.3	+0.186	-29.1	-0.623	+7.4	+0.186	-29.1
4	C_i-$(C_d)(H)_2$	+0.333	+51.3	-0.535	-26.4	+0.337	+51.4	-0.536	-26.5
5	C_i-$(C_d)(C)(H)$	+0.144	+57.2	-0.025	-33.5	+0.148	+57.3	-0.025	-33.5
6	C_i-$(C_d)(C)_2$	-0.618	+58.1	-0.203	-39.6	-0.614	+58.2	-0.204	-39.6
7	C_i-$(C_d)_2(H)$	+0.658	+89.6	+0.007	-42.8	+0.664	+89.7	+0.006	-42.9
8	C_i-$(C_d)_2(C)$	+0.419	+94.8	-0.339	-48.2	+0.446	+95.4	-0.341	-48.2
9	C_i-$(C_t)(H)_2$	+0.059	+35.9	-0.011	-23.4	+0.061	+35.9	-0.011	-23.5
10	C_i-$(C_t)(C)(H)$	-0.389	+41.3	+0.046	-31.1	-0.386	+41.3	+0.046	-31.1
11	C_i-$(C_t)(C)_2$	-0.772	+43.8	+0.049	-38.6	-0.767	+43.8	+0.048	-38.6
12	C_i-$(C_t)_2(H)$	+0.180	+66.6	-0.002	-41.3	+0.185	+66.6	-0.003	-41.3
13	C_i-$(C_t)_2(C)$	-0.025	+74.3	-0.002	-46.9	+0.002	+74.8	-0.004	-46.9
14	$C_{i,d}$-(H)	+0.287	-20.0	+0.131	0.0	+0.292	-20.0	+0.132	0.0
15	$C_{i,d}$-(C)	+0.157	-15.9	+0.175	-9.2	+0.164	-15.8	+0.175	-9.2
16	$C_{i,d}$-(C_d)	-0.010	+12.6	+0.186	-9.4	-0.008	+12.6	+0.185	-9.4
17	$C_{i,d}$-(C_t)	-0.702	+0.1	+0.029	-20.3	-0.700	+0.1	+0.028	-20.4
18	C_i-$(C_B)(H)_2$	+0.308	+42.6	-0.520	-17.0	+0.312	+42.7	-0.500	-16.6
19	C_i-$(C_B)(C)(H)$	-0.044	+44.6	-0.499	-27.6	-0.039	+44.7	-0.501	-27.6
20	C_i-$(C_B)(C)_2$	-0.976	+42.7	-0.582	-32.7	-0.970	+42.8	-0.583	-32.8
21	$C_{i,B}$	+0.354	-32.2	+0.144	+6.5	+0.362	-32.0	+0.142	+6.4
22	$C_{i,cyclo\text{-}5}$-(H)	-0.040	+13.5	-0.787	-24.8	-0.038	+13.5	-0.788	-24.8
23	$C_{i,cyclo\text{-}6}$-(H)	-0.262	+6.0	+0.060	-20.1	-0.259	+6.0	+0.059	-20.1
24	$C_{i,cyclo\text{-}6}$-(C)	-0.647	+4.5	-0.158	-30.2	-0.643	+4.6	-0.159	-30.3
25	$C_{i,cycloallylic\text{-}6}$-$(C_d)(H)$	+0.029	+56.6	-0.035	-36.8	+0.034	+56.6	-0.036	-36.8



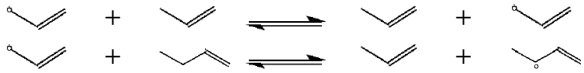
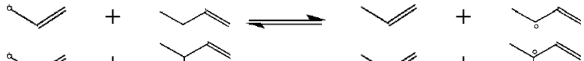
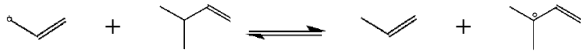
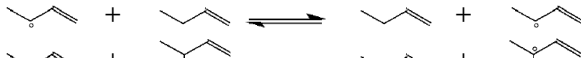
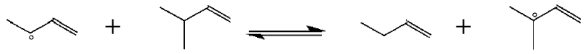
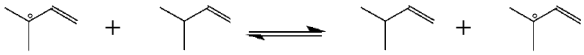
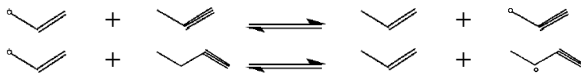
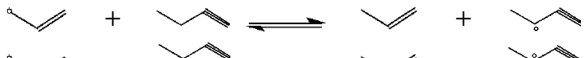
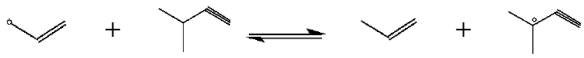
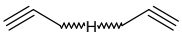
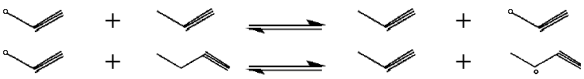
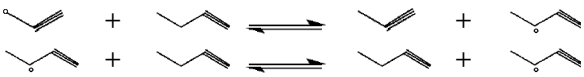
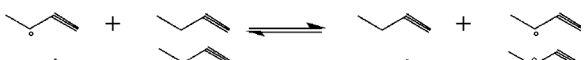
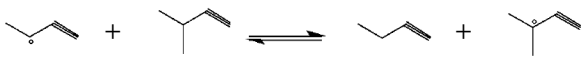
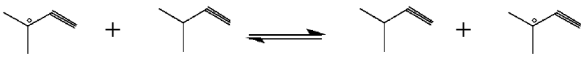
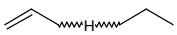
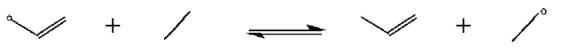
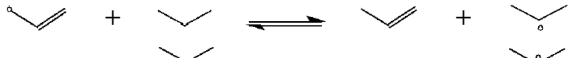
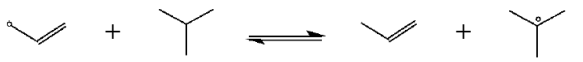
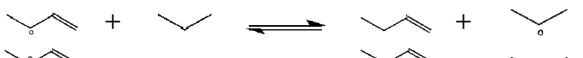
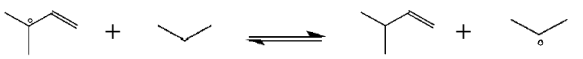
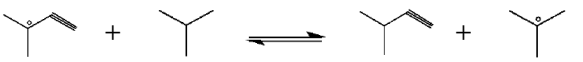
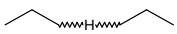
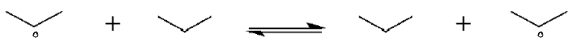
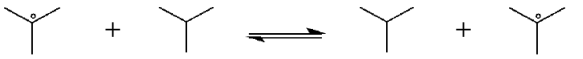
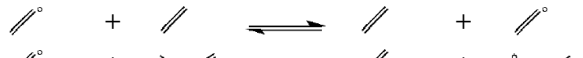
Nr.	Group	1200 K				1300 K			
		C_1 contribution		C_2 contribution		C_1 contribution		C_2 contribution	
		$\Delta GAV^{o}_{\log A}$	$\Delta GAV^{o}_{E_a}$	$\Delta GAV^{o}_{\log A}$	$\Delta GAV^{o}_{E_a}$	$\Delta GAV^{o}_{\log A}$	$\Delta GAV^{o}_{E_a}$	$\Delta GAV^{o}_{\log A}$	$\Delta GAV^{o}_{E_a}$
	Reference reaction:								
	$CH_3^{\bullet} + CH_4$	6.746	89.4	6.746	89.4	6.849	91.9	6.849	91.9
1	C_i-$(C)(H)_2$	-0.789	+5.4	+0.071	-10.4	-0.789	+5.4	+0.072	-10.4
2	C_i-$(C)_2(H)$	-0.679	+8.0	+0.101	-20.0	-0.679	+8.0	+0.101	-20.0
3	C_i-$(C)_3$	-0.621	+7.4	+0.186	-29.2	-0.619	+7.4	+0.185	-29.2
4	C_i-$(C_d)(H)_2$	+0.340	+51.4	-0.537	-26.5	+0.342	+51.4	-0.538	-26.6
5	C_i-$(C_d)(C)(H)$	+0.150	+57.3	-0.026	-33.6	+0.152	+57.3	-0.027	-33.6
6	C_i-$(C_d)(C)_2$	-0.611	+58.2	-0.206	-39.7	-0.609	+58.2	-0.207	-39.7
7	C_i-$(C_d)_2(H)$	+0.667	+89.7	+0.005	-42.9	+0.670	+89.8	+0.004	-43.0
8	C_i-$(C_d)_2(C)$	+0.470	+95.9	-0.344	-48.3	+0.490	+96.3	-0.346	-48.4
9	C_i-$(C_t)(H)_2$	+0.062	+36.0	-0.012	-23.5	+0.063	+35.9	-0.012	-23.5
10	C_i-$(C_t)(C)(H)$	-0.384	+41.3	+0.045	-31.1	-0.383	+41.3	+0.045	-31.2
11	C_i-$(C_t)(C)_2$	-0.765	+43.9	+0.047	-38.6	-0.763	+43.9	+0.047	-38.7
12	C_i-$(C_t)_2(H)$	+0.188	+66.7	-0.004	-41.4	+0.191	+66.7	-0.005	-41.5
13	C_i-$(C_t)_2(C)$	+0.025	+75.3	-0.005	-47.0	+0.045	+75.7	-0.006	-47.0
14	$C_{i,d}$-(H)	+0.295	-19.9	+0.132	0.0	+0.297	-19.9	+0.133	0.0
15	$C_{i,d}$-(C)	+0.167	-15.7	+0.174	-9.2	+0.170	-15.7	+0.174	-9.3
16	$C_{i,d}$-(C_d)	-0.006	+12.7	+0.185	-9.4	-0.005	+12.6	+0.184	-9.5
17	$C_{i,d}$-(C_t)	-0.699	+0.1	+0.027	-20.4	-0.699	+0.1	+0.027	-20.5
18	C_i-$(C_B)(H)_2$	+0.315	+42.7	-0.482	-16.3	+0.317	+42.7	-0.466	-15.9
19	C_i-$(C_B)(C)(H)$	-0.037	+44.8	-0.502	-27.7	-0.035	+44.8	-0.503	-27.7
20	C_i-$(C_B)(C)_2$	-0.966	+42.9	-0.584	-32.8	-0.964	+42.9	-0.585	-32.9
21	$C_{i,B}$	+0.368	-31.9	+0.140	+6.4	+0.373	-31.8	+0.139	+6.3
22	$C_{i,cyclo\text{-}5}$-(H)	-0.038	+13.5	-0.788	-24.8	-0.038	+13.5	-0.788	-24.9
23	$C_{i,cyclo\text{-}6}$-(H)	-0.258	+6.0	+0.058	-20.2	-0.257	+6.0	+0.058	-20.2
24	$C_{i,cyclo\text{-}6}$-(C)	-0.640	+4.6	-0.161	-30.3	-0.639	+4.6	-0.163	-30.4
25	$C_{i,cycloallylic\text{-}6}$-$(C_d)(H)$	+0.037	+56.7	-0.037	-36.9	+0.039	+56.7	-0.037	-36.9

Table S5: Resonance stabilization energies and effects of resonance on the pre-exponential factor, according to Eqs. 17 and 18, and remaining deviations between group additive prediction and ab initio value after correcting the group additive predictions with the resonance corrections (600 K).

	Reaction (600 K)	Resonance effect		Remaining deviations	
		$\Delta E^{o}_{\text{resonance}}$	$\Delta \log \tilde{A}_{\text{resonar}}$	$E_{a,\text{pred}}$ -$E_{a,\text{AI}}$	$\log A_{\text{pred}}$ -$\log A_{\text{AI}}$
		kJ mol^{-1}		kJ mol^{-1}	
	1. 				
27		-10.6	-0.216	0.6	0.014
28		-13.6	-0.325	0.3	0.071
29		-18.2	-0.288	1.6	-0.018
30		-18.8	-0.337	1.9	-0.019
31		-20.6	-0.522	0.1	0.064
32		-24.2	-0.695	-0.2	0.085
	2. 				
33		-8.5	-0.104	-1.5	-0.098
34		-12.1	-0.181	-1.2	-0.073
35		-15.2	-0.284	-1.4	-0.022
	3. 				
36		-5.6	-0.049	-0.1	0.046
37		-9.3	-0.091	0.3	0.036
38		-12.8	-0.152	0.2	-0.005
39		-16.5	-0.228	0.3	-0.031
40		-19.6	-0.368	-0.5	-0.043
	4. 				
41		-3.6	-0.069	0.3	0.017
42		-7.8	-0.099	1.2	-0.005
43		-9.8	-0.169	-0.1	0.013
44		-6.9	-0.218	-0.3	0.014
45		-7.8	-0.226	0.0	-0.078
46		-11.0	-0.436	-0.7	-0.020
	5. 				
47		-0.8	-0.131	-0.4	-0.069
48		-3.4	-0.504	0.7	0.054
	6. No resonance stabilization				
49		-0.5	0.000	0.5	0.000
50		1.0	-0.033	-1.0	0.033

51		+				+		2.6	-0.071	-2.6	0.071
52		+				+		-0.1	0.030	0.1	-0.030
53		+				+		0.1	0.044	-0.1	-0.044
54		+				+		0.2	0.069	-0.2	-0.069
				MD						-0.1	-0.004
				MAD						0.7	0.041

Table S6: Resonance stabilization energies and effects of resonance on the transition state, according to Eqs. 17 and 18, and remaining deviations between group additive prediction and ab initio value after correcting the group additive predictions with the resonance corrections (1000 K).

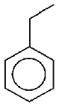
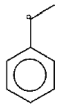
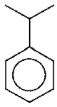
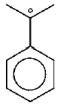
	Reaction (1000 K)	$\Delta E^{o}_{\text{resonance}}$	$\Delta \log \tilde{A}_{\text{resonance}}$	$\log A_{\text{pred}} - \log A_{\text{AI}}$ $E_{a,\text{pred}} - E_{a,\text{AI}}$	$\log A_{\text{pred}} - \log A_{\text{AI}}$
		kJ mol^{-1}		kJ mol^{-1}	
	1. 				
27		-10.8	-0.227	+0.7	+0.015
28		-13.8	-0.337	+0.3	+0.072
29		-18.5	-0.305	+1.6	-0.013
30		-19.0	-0.352	+1.8	-0.017
31		-21.0	-0.545	+0.1	+0.072
32		-24.2	-0.697	-0.7	+0.069
	2. 				
33		-8.6	-0.111	-1.5	-0.101
34		-12.2	-0.191	-1.3	-0.074
35		-15.3	-0.298	-1.6	-0.020
	3. 				
36		-5.6	-0.051	+0.1	+0.059
37		-9.3	-0.091	+0.4	+0.046
38		-12.7	-0.140	+0.1	-0.009
39		-16.5	-0.227	+0.2	-0.026
40		-19.2	-0.340	-1.1	-0.068
	4. 				
41		-3.7	-0.072	+0.3	+0.019
42		-7.9	-0.105	+1.1	-0.001
43		-10.1	-0.185	-0.1	+0.026
44		-7.0	-0.227	-0.4	+0.019
45		-8.0	-0.236	-0.0	-0.074
46		-11.3	-0.452	-0.7	-0.013
	5. 				
47		-0.9	-0.136	-0.3	-0.068
48		-3.6	-0.521	+0.9	+0.062
	6. No resonance stabilization				
49		-0.5	0.003	+0.5	-0.003
50		1.0	-0.034	-1.0	+0.034
51		2.5	-0.074	-2.5	+0.074

52		+				+		-0.2	0.028	+0.2	-0.028
53		+				+		0.0	0.040	-0.0	-0.040
54		+				+		0.2	0.070	-0.2	-0.070
				MD						-0.1	-0.002
				MAD						0.7	0.043

Table S7: Applied groups and resonance corrections for the reactions of Table 4.

Reaction	Groups		Number of resonance corrections			
	C_1	C_2	C-1	C-2	C-3	C-4
27	5	5	1	-	-	-
28	5	6	1	-	1	-
29	5	7	1	-	2	-
30	6	6	1	-	2	1
31	6	7	1	-	3	2
32	7	7	1	-	4	4
33	5	10	1	-	-	-
34	5	11	1	-	1	-
35	5	12	1	-	2	-
36	10	10	-	1	-	-
37	10	11	-	1	1	-
38	11	11	-	1	2	1
39	11	12	-	1	3	2
40	12	12	-	1	4	4
41	5	2	-	-	1	-
42	5	3	-	-	2	-
43	5	4	-	-	3	-
44	6	3	-	-	2	2
45	7	3	-	-	2	4
46	12	4	-	-	3	6
47	3	3	-	-	-	4
48	4	4	-	-	-	9
49	15	15	-	-	-	-
50	15	5	-	-	-	-
51	15	12	-	-	-	-
52	15	2	-	-	-	-
53	15	3	-	-	-	-
54	5	17	-	-	-	-

Table S8: Tunneling coefficients for all reactions from Table 1 and 4 (300-1000K).

	Reaction							κ(*T*)							
								300	400	500	600	700	800	900	1000
1	Me°	+	CH_4	⇌	CH_4	+	Me°	49.1	6.1	2.9	2.1	1.7	1.5	1.4	1.3
2	Me°	+		⇌	CH_4	+		34.9	5.4	2.8	2.0	1.7	1.5	1.4	1.3
3	Me°	+		⇌	CH_4	+		22.7	4.7	2.6	1.9	1.6	1.4	1.3	1.3
4	Me°	+		⇌	CH_4	+		13.2	3.8	2.3	1.8	1.5	1.4	1.3	1.2
5	Me°	+		⇌	CH_4	+		15.6	4.0	2.3	1.8	1.5	1.4	1.3	1.2
6	Me°	+		⇌	CH_4	+		8.2	3.0	2.0	1.6	1.4	1.3	1.2	1.2
7	Me°	+		⇌	CH_4	+		5.3	2.4	1.8	1.5	1.3	1.2	1.2	1.2
8	Me°	+		⇌	CH_4	+		3.3	1.9	1.5	1.3	1.2	1.2	1.1	1.1
9	Me°	+		⇌	CH_4	+		2.4	1.6	1.4	1.2	1.2	1.1	1.1	1.1
10	Me°	+		⇌	CH_4	+		20.3	4.4	2.5	1.9	1.6	1.4	1.3	1.2
11	Me°	+		⇌	CH_4	+		11.6	3.5	2.2	1.7	1.5	1.4	1.3	1.2
12	Me°	+		⇌	CH_4	+		6.9	2.8	1.9	1.6	1.4	1.3	1.2	1.2
13	Me°	+		⇌	CH_4	+		5.1	2.4	1.7	1.5	1.3	1.2	1.2	1.2
14	Me°	+		⇌	CH_4	+		3.4	2.0	1.5	1.4	1.2	1.2	1.1	1.1
15	Me°	+		⇌	CH_4	+		30.9	5.5	2.8	2.0	1.7	1.5	1.4	1.3
16	Me°	+		⇌	CH_4	+		28.6	5.3	2.8	2.0	1.7	1.5	1.4	1.3
17	Me°	+		⇌	CH_4	+		36.4	5.5	2.8	2.0	1.7	1.5	1.4	1.3
18	Me°	+		⇌	CH_4	+		22.4	4.7	2.6	1.9	1.6	1.4	1.3	1.3
19	Me°	+		⇌	CH_4	+		16.5	4.0	2.3	1.8	1.5	1.4	1.3	1.2
20	Me°	+		⇌	CH_4	+		9.1	3.1	2.0	1.6	1.4	1.3	1.2	1.2
21	Me°	+		⇌	CH_4	+		7.3	2.8	1.9	1.6	1.4	1.3	1.2	1.2
22	Me°	+		⇌	CH_4	+		15.6	4.3	2.5	1.9	1.6	1.4	1.3	1.3
23	Me°	+		⇌	CH_4	+		19.1	4.4	2.5	1.9	1.6	1.4	1.3	1.3
24	Me°	+		⇌	CH_4	+		24.2	4.8	2.6	1.9	1.6	1.4	1.3	1.3
25	Me°	+		⇌	CH_4	+		14.5	4.0	2.4	1.8	1.5	1.4	1.3	1.2
26	Me°	+		⇌	CH_4	+		7.6	2.9	2.0	1.6	1.4	1.3	1.2	1.2

27		+				+		144.9	9.3	3.6	2.4	1.9	1.6	1.5	1.4
28		+				+		102.3	8.3	3.5	2.3	1.8	1.6	1.4	1.3
29		+				+		56.1	6.8	3.1	2.2	1.8	1.5	1.4	1.3
30		+				+		78.4	7.7	3.3	2.2	1.8	1.6	1.4	1.3
31		+				+		57.5	7.0	3.2	2.2	1.8	1.6	1.4	1.3
32		+				+		44.6	6.5	3.1	2.2	1.8	1.5	1.4	1.3
33		+				+		94.5	8.1	3.4	2.3	1.8	1.6	1.4	1.3
34		+				+		78.1	7.6	3.3	2.2	1.8	1.6	1.4	1.3
35		+				+		56.8	6.9	3.2	2.2	1.8	1.5	1.4	1.3
36		+				+		92.1	8.0	3.4	2.3	1.8	1.6	1.4	1.3
37		+				+		65.3	7.3	3.3	2.2	1.8	1.6	1.4	1.3
38		+				+		55.3	7.0	3.2	2.2	1.8	1.6	1.4	1.3
39		+				+		38.8	6.3	3.1	2.2	1.8	1.5	1.4	1.3
40		+				+		32.7	6.1	3.1	2.2	1.8	1.6	1.4	1.3
41		+				+		25.1	5.0	2.7	1.9	1.6	1.4	1.3	1.3
42		+				+		27.7	5.4	2.8	2.0	1.7	1.5	1.4	1.3
43		+				+		23.8	5.2	2.8	2.0	1.7	1.5	1.4	1.3
44		+				+		19.4	4.8	2.6	2.0	1.6	1.5	1.4	1.3
45		+				+		12.0	3.9	2.4	1.8	1.6	1.4	1.3	1.3
46		+				+		11.1	4.0	2.5	1.9	1.6	1.5	1.4	1.3
47		+				+		37.2	6.1	3.0	2.1	1.7	1.5	1.4	1.3
48		+				+		26.1	5.8	3.0	2.2	1.8	1.6	1.4	1.3
49		+				+		20.0	4.7	2.6	2.0	1.6	1.5	1.4	1.3
50		+				+		4.3	2.2	1.7	1.4	1.3	1.2	1.2	1.1
51		+				+		1.8	1.4	1.3	1.2	1.1	1.1	1.1	1.1
52		+				+		13.3	3.9	2.3	1.8	1.5	1.4	1.3	1.2
53		+				+		6.8	2.9	2.0	1.6	1.4	1.3	1.2	1.2
54		+				+		8.9	3.0	2.0	1.6	1.4	1.3	1.2	1.2

Table S9: Number of single events n_e, external and internal symmetry numbers σ_e and σ_i, and number of optical isomers n_{opt} for the reactions of Table 8.

	Reactant 1			Reactant 2			TS			Product 1			Product 2			n_e	
nr	σ_e	σ_i	n_{opt}	σ_e	σ_i	n_{opt}	σ_e	σ_i	n_{opt}	σ_e	σ_i	n_{opt}	σ_e	σ_i	n_{opt}	forward	reverse
1	1	3	1	6	1	1	1	9	1	1	3	1	12	1	1	2	4
2	2	9	1	6	1	1	1	9	1	1	6	1	12	1	1	12	8
3	2	9	1	6	1	1	1	9	2	1	3	1	12	1	1	24	8
4	2	9	1	6	1	1	1	9	2	1	3	1	12	1	1	24	8
5	2	9	1	6	1	1	1	9	2	1	6	1	12	1	1	24	16
6	2	9	1	6	1	1	1	9	1	1	6	1	12	1	1	12	8
7	2	9	1	6	1	1	1	27	2	1	9	1	12	1	1	8	8
8	3	27	1	6	1	1	1	27	1	1	18	1	12	1	1	18	8
9	12	81	1	6	1	1	1	243	1	1	162	1	12	1	1	24	8
10	4	81	1	6	1	1	1	81	2	1	27	1	12	1	1	48	8
11	1	2187	1	6	1	1	1	2187	1	1	###	1	12	1	1	6	8
12	2	9	1	1	6	1	1	27	1	1	9	1	6	3	1	4	6
13	1	3	1	1	6	1	1	9	2	1	3	1	6	3	1	4	12
14	2	1	1	1	6	1	1	3	2	1	1	1	6	3	1	8	12
15	3	27	1	2	1	1	1	9	2	1	18	1	1	3	1	36	12
16	2	1	1	2	1	1	1	1	2	2	1	1	1	3	1	8	12
17	2	1	1	3	27	1	1	81	1	2	1	1	3	27	1	2	2
18	2	1	1	3	27	1	1	81	1	2	1	1	3	27	1	2	2
19	2	9	1	1	9	1	1	81	2	1	9	1	2	9	1	4	4

Table S10: Applied number of resonance corrections for the reactions of Table 8.

Reaction	Groups		Number of resonance corrections:			
	C_1	C_2	C-1	C-2	C-3	C-4
1	0	15	-	-	-	-
2	0	2	-	-	-	-
3	0	5	-	-	-	-
4	0	5	-	-	-	-
5	0	5	-	-	-	-
6	0	2	-	-	-	-
7	0	3	-	-	-	-
8	0	2	-	-	-	-
9	0	2	-	-	-	-
10	0	5	-	-	-	-
11	0	2	-	-	-	-
12	2	3	-	-	-	2
13	2	11	-	-	1	1
14	2	26	-	-	1	1
15	5	2	-	-	1	-
16	5	8	2	-	-	-
17	4	13	-	-	6	-
18	4	8	-	-	6	-
19	3	16	-	-	-	2

Table S11: Tunneling coefficients, pre-exponential factors [log($m^3mol^{-1}s^{-1}$)], activation energies [$kJmol^{-1}$] and rate coefficients [$m^3\ mol^{-1}\ s^{-1}$] for the validation set of H-abstractions of Table 8 at 300 K, both the ab initio calculated and the group additivity obtained values.

	Reaction (300 K)	Ab initio				Group additivity			
		κ	log*A*	E_a	*k*	κ	log*A*	E_a	*k*
1f	CH_3° +  ⇌ CH_4 + 	21.59	5.669	70.2	5.7E-06	22.19	5.642	69.3	8.3E-06
1r			5.843	45.4	1.8E-01		5.925	47.5	1.0E-01
2f	CH_3° +  ⇌ CH_4 + 	37.49	5.774	58.1	1.6E-03	42.71	6.364	58.9	5.5E-03
2r			5.259	72.5	1.5E-06		5.305	74.4	9.6E-07
3f	CH_3° +  ⇌ CH_4 + 	12.38	5.839	37.2	2.8E+00	16.91	6.067	42.9	6.7E-01
3r			5.754	117.3	2.6E-14		6.268	118.9	6.3E-14
4f	CH_3° +  ⇌ CH_4 + 	13.94	6.054	42.3	6.5E-01	16.91	6.067	42.9	6.7E-01
4r			6.122	120.0	2.2E-14		6.268	118.9	6.3E-14
5f	CH_3° +  ⇌ CH_4 + 	15.26	6.025	42.4	6.4E-01	16.91	6.067	42.9	6.7E-01
5r			6.268	113.2	5.2E-13		6.569	118.9	1.3E-13
6f	CH_3° +  ⇌ CH_4 + 	36.94	5.880	58.7	1.6E-03	42.71	6.364	58.9	5.5E-03
6r			5.304	73.2	1.3E-06		5.305	74.4	9.6E-07
7f	CH_3° +  ⇌ CH_4 + 	23.10	6.083	48.2	1.1E-01	24.32	6.181	49.0	1.1E-01
7r			5.190	74.3	3.9E-07		5.321	76.1	2.8E-07
8f	CH_3° +  ⇌ CH_4 + 	37.96	5.973	58.2	2.5E-03	42.71	6.540	58.9	8.3E-03
8r			5.248	71.2	2.6E-06		5.305	74.4	9.6E-07
9f	CH_3° +  ⇌ CH_4 + 	40.64	6.641	57.3	1.8E-02	42.71	6.665	58.9	1.1E-02
9r			5.045	68.4	5.4E-06		5.305	74.4	9.6E-07
10f	CH_3° +  ⇌ CH_4 + 	12.67	5.498	38.1	9.0E-01	16.91	6.368	42.9	1.3E+00
10r			6.351	121.6	1.8E-14		6.268	118.9	6.3E-14
11f	CH_3° +  ⇌ CH_4 + 	40.06	5.395	56.6	1.3E-03	42.71	6.063	58.9	2.8E-03
11r			4.687	70.3	1.1E-06		5.305	74.4	9.6E-07
12f	 +  ⇌  + 	36.32	4.978	53.6	1.5E-03	30.92	4.916	53.2	1.4E-03
12r			5.178	65.2	2.3E-05		5.115	64.7	2.2E-05
13f	 +  ⇌  + 	18.50	4.923	38.8	2.6E-01	13.33	4.850	38.9	1.6E-01
13r			5.722	94.3	3.6E-10		5.648	94.4	2.1E-10
14f	 +  ⇌  + 	12.63	5.406	33.0	5.5E+00	9.50	5.066	33.2	1.8E+00
14r			6.343	109.0	2.7E-12		6.002	109.2	9.4E-13
15f	 +  ⇌  + 	21.84	6.133	105.3	1.4E-11	18.30	6.877	104.7	8.2E-11
15r			4.605	42.3	3.9E-02		4.839	44.2	2.5E-02
16f	 +  ⇌ +	43.91	5.784	53.9	1.0E-02	35.45	5.802	55.5	4.8E-03
16r			5.708	108.2	3.1E-12		5.726	109.8	1.4E-12
17f	+ ⇌ +	4.55	4.362	14.1	3.5E+02	2.89	4.168	11.7	4.0E+02
17r			5.351	85.5	1.3E-09		5.156	83.1	1.4E-09

18f		4.07	4.212	13.6	2.7E+02	2.58	4.144	9.8	6.9E+02
18r			5.649	109.4	1.5E-13		5.581	105.7	3.9E-13
19f		10.00	4.859	62.3	9.7E-06	7.80	5.022	65.9	2.8E-06
19r			5.531	26.3	8.2E+01		5.640	29.7	2.3E+01

Table S12: Tunneling coefficients, pre-exponential factors [log($m^3mol^{-1}s^{-1}$)], activation energies [$kJmol^{-1}$] and rate coefficients [$m^3\ mol^{-1}\ s^{-1}$] for the validation set of H-abstractions of Table 8 at 1000 K, both the ab initio calculated and the group additivity obtained values.

	Reaction (1000 K)	Ab initio				Group additivity			
		κ	log*A*	E_a	*k*	κ	log*A*	E_a	*k*
1f	$CH_3°$ +  ⇌ CH_4 + 	1.27	6.965	85.2	4.1E+02	1.27	6.941	84.4	4.3E+02
1r			7.356	62.6	1.5E+04		7.398	64.4	1.4E+04
2f	$CH_3°$ +  ⇌ CH_4 + 	1.29	7.068	73.3	2.2E+03	1.31	7.659	74.0	8.1E+03
2r			6.584	88.0	1.2E+02		6.622	89.8	1.1E+02
3f	$CH_3°$ +  ⇌ CH_4 + 	1.22	7.131	52.2	3.1E+04	1.25	7.354	58.0	2.6E+04
3r			7.262	134.4	2.1E+00		7.745	135.7	5.7E+00
4f	$CH_3°$ +  ⇌ CH_4 + 	1.22	7.334	57.3	2.7E+04	1.25	7.354	58.0	2.6E+04
4r			7.624	137.1	3.5E+00		7.745	135.7	5.7E+00
5f	$CH_3°$ +  ⇌ CH_4 + 	1.23	7.310	57.5	2.5E+04	1.25	7.354	58.0	2.6E+04
5r			7.988	132.8	1.4E+01		8.046	135.7	1.1E+01
6f	$CH_3°$ +  ⇌ CH_4 + 	1.29	7.175	73.8	2.7E+03	1.31	7.659	74.0	8.1E+03
6r			6.628	88.6	1.3E+02		6.622	89.8	1.1E+02
7f	$CH_3°$ +  ⇌ CH_4 + 	1.27	7.412	63.6	1.5E+04	1.27	7.513	64.4	1.8E+04
7r			6.605	90.6	9.3E+01		6.730	92.4	1.0E+02
8f	$CH_3°$ +  ⇌ CH_4 + 	1.29	7.270	73.4	3.5E+03	1.31	7.835	74.0	1.2E+04
8r			6.586	86.8	1.4E+02		6.622	89.8	1.1E+02
9f	$CH_3°$ +  ⇌ CH_4 + 	1.30	8.001	73.1	2.0E+04	1.31	7.960	74.0	1.6E+04
9r			6.373	83.9	1.3E+02		6.622	89.8	1.1E+02
10f	$CH_3°$ +  ⇌ CH_4 + 	1.22	6.785	53.1	1.2E+04	1.25	7.655	58.0	5.3E+04
10r			7.904	139.2	5.2E+00		7.745	135.7	5.7E+00
11f	$CH_3°$ +  ⇌ CH_4 + 	1.30	6.704	71.8	1.2E+03	1.31	7.358	74.0	4.1E+03
11r			6.007	85.8	4.4E+01		6.622	89.8	1.1E+02
12f	 +  ⇌  + 	1.30	6.374	69.5	7.1E+02	1.29	6.321	69.2	6.5E+02
12r			6.627	81.7	3.0E+02		6.574	81.4	2.7E+02
13f	 +  ⇌  + 	1.27	6.343	54.9	3.8E+03	1.23	6.264	55.0	3.0E+03
13r			7.246	111.5	3.3E+01		7.166	111.6	2.7E+01
14f	 +  ⇌  + 	1.24	6.822	49.1	2.2E+04	1.21	6.484	49.3	9.8E+03
14r			7.922	126.7	2.5E+01		7.584	126.9	1.1E+01
15f	 +  ⇌  + 	1.27	7.650	122.3	2.3E+01	1.25	8.417	121.9	1.4E+02
15r			5.972	58.0	1.1E+03		6.210	60.0	1.5E+03
16f	 +  ⇌ +	1.30	7.333	71.2	5.3E+03	1.31	7.328	72.6	4.5E+03
16r			7.291	125.9	6.7E+00		7.287	127.3	5.7E+00
17f	+ ⇌ +	1.20	5.980	32.0	2.4E+04	1.13	5.862	30.0	2.2E+04
17r			6.977	103.5	4.5E+01		6.859	101.4	4.1E+01
18f	+ ⇌ +	1.17	5.834	31.6	1.8E+04	1.12	5.871	28.4	2.7E+04

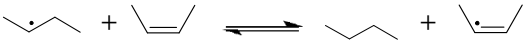
18r		7.300	127.6	5.1E+00		7.336	124.4	7.7E+00
19f		1.27	6.369	79.2	2.2E+02	1.20	6.503	82.6	1.9E+02
19r			7.246	45.2	9.6E+04		7.268	48.0	7.0E+04

Table S13: Experimental validation set: source and kinetic parameters ($k=A(T/298)^n\exp(-E_a/RT)$).

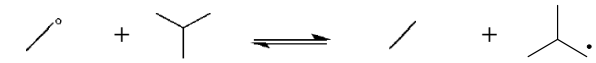
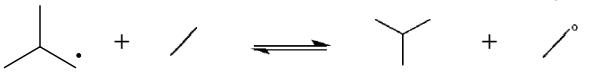
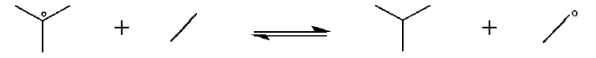
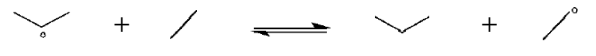
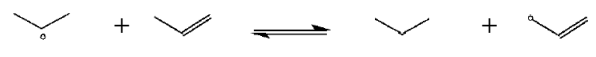
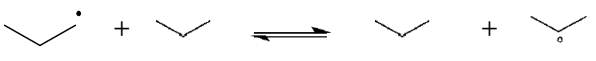
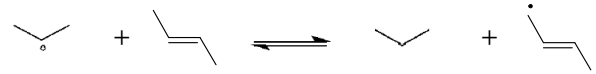
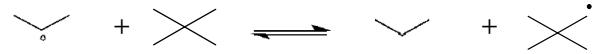
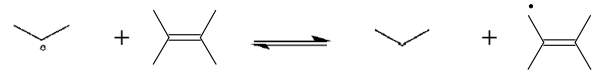
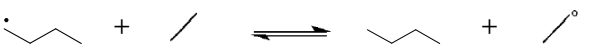
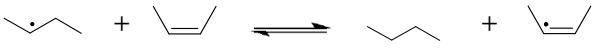
	Reaction	Source	T K	A m^3/mole s	n	Ea kJ mol^{-1}
	Other					
1		1990TSA1-68	300-2500	1.49E+03	3.65	38.25
2		1990TSA1-68	300-2500	1.97E+02	3.46	24.94
3		1979PAP/PRI 3178-3181	464-701	1.20E+05		40.24
4		1971LOU469	653-784	1.00E+05		66.93
5		1990TSA1-68	300-2500	4.13E+02	3.7	40.91
6		1990TSA1-68	300-2500	2.09E+01	5.17	37.91
	Rate coefficients derived from complex reaction mechanisms					
7		1989ZHA/AHO1541-1549	650-770	1.58E+05		39.99
8		1958JAM/STE289	298-500	1.84E+08		38.5
9		1976SZI/MAR897	496-578	1.00E+05		54.04
10		1976SZI/MAR897	496-548	5.01E+03		32.01
11		1969BER/WOO3305-3311	301-399	7.94E+03		38.91
12		1995SER/FIS1303-1312	489-542	2.82E+05		46.89
13		1979SZI/MAR369	512-571	3.16E+04		55.04
14		1992KOR/SER2445-2450	490-540	6.17E+06		57.04
15		1985RIC/MAR389-399	717-917	1.26E+06		63.61
16		1966LIN/BAC2369	823-999	5.00E+05		62.77
17		1983COL/RIC5	773-794	2.51E+05		33.51

Table S14: Experimental validation set: Number of single events n_e, external and internal symmetry numbers σ_e and σ_i, and number of optical isomers n_{opt} for the reactions of Table 9.

	Reactant 1			Reactant 2			TS			n_e	Groups		Resonance corrections			
nr	σ_e	σ_i	n_{opt}	σ_e	σ_i	n_{opt}	σ_e	σ_i	n_{opt}	forward	C_1	C_2	C-1	C-2	C-3	C-4
1	3	27	1	1	6	1	1	27	1	18	2	2	-	-	-	1
2	3	27	1	1	6	1	1	243	1	2	2	4	-	-	-	3
3	1	6	1	1	6	1	1	3	1	12	2	19	-	-	2	-
4	1	6	1	2	1	1	1	1	2	24	5	19	2	-	-	-
5	1	18	1	6	3	1	1	27	1	12	2	2	-	-	-	1
6	3	27	1	6	3	1	1	243	1	6	4	2	-	-	-	3
7	10	1	1	1	6	1	1	3	1	20	2	23	-	-	-	2
8	2	1	1	1	6	1	1	3	2	8	2	26	-	-	1	1
9	2	9	1	6	3	1	1	27	1	12	3	2	-	-	-	2
10	1	3	1	2	9	1	1	9	2	12	3	5	-	-	2	-
11	2	9	1	1	6	1	1	27	1	4	2	3	-	-	-	3
12	2	9	1	2	9	1	1	27	2	24	3	5	-	-	2	-
13	12	81	1	2	9	1	1	729	1	24	3	2	-	-	-	2
14	4	81	1	2	9	1	1	243	2	48	3	5	-	-	2	-
15	2	9	1	1	3	1	1	9	2	12	6	5	1	-	1	-
16	6	3	1	1	6	1	1	9	1	12	2	2	-	-	-	1
17	2	9	1	1	9	1	1	81	2	4	3	16	-	-	-	2

Transition state geometries and parameters for internal rotation

Description of information given:
Following information is displayed below:
- geometry of the transition state [Å]
- imaginary frequency in the transition state[cm^{-1}]
- Parameters for internal rotation about the transitional C-H-C bond:
  - Fourier expansion coefficients (see separate section) of the potential energy surface for internal rotation [kJ mol^{-1}]
  - indication of free rotor calculation (F)
  - barrier to internal rotation [kJ mol^{-1}]
  - symmetry number for internal rotation
  - reduced moment of inertia Im,red [amu $bohr^2$]
  - frequency of the harmonic contrubition that is replaced by an internal rotational contribution [cm^{-1}]

Notation of Fourier expansion coefficients:
Fourier expansions of the potential energy profiles for internal rotation. E.g., the notation
```
cos   1.2   0.5 0.25
```
means that the Fourier expansion for internal rotation about the transitional bond can be written as

$$V(\phi) = \sum_{k=1}^{n} \frac{1}{2} A_k (1 - \cos(k\phi)) + \sum_{k=1}^{n} B_k \sin(k\phi)$$

With A_1=1.2, A_2=0.5, A_3=0.25, A_4= 0.0, A_5= 0.0, A_6=0.0 *A*nd B_i=0 for all *i*
In the standard notation the sinus coefficients are not written as in general they are negligible; if there are significant sinus coefficients present for a certain potential energy profile, the notation continuous on the next line with the prefix *sin*. E.g., in the notation
```
cos    0.74   -0.35    1.07
sin    0.42    0.17   -0.05
```
the second line describes the sinus coefficients B_1 to B_3.
In case an internal rotation is treated as a free rotor, the notation is completed by an "F", e.g.:
```
cos    0.00    0.00    0.30 F
```
In case only a an "F" is present without expansion coefficients, the free rotor approximation has been applied without determination of the potential energy surface.

Nomenclature
The nomenclature for the hydrogen abstraction
R1+R2H −>R1H+R2
in following tables is the composition of the transition state denoted as radical1/radical2.

ΔGAV° training set reactions of Table 1

```
methyl/methyl
 C  0.000000  0.000000  1.347599
 C  0.000000  0.000000 -1.347599
 H  0.000000  1.049672  1.632870
 H  0.909043 -0.524836  1.632870
 H -0.909043 -0.524836  1.632870
 H  0.000000  0.000000  0.000000
 H  0.000000 -1.049672 -1.632870
 H -0.909043  0.524836 -1.632870
 H  0.909043  0.524836 -1.632870
ImagFreq  1637i
Internal rotation:
cos   0.00   0.00   0.31 F
barrier   0.31
symmetry     3
Im,red   5.95
freq  39.3  (from HO analysis)

ethyl/methyl
 C -0.947999  1.727019  0.000000
 C  0.892135 -0.254856  0.000000
 H -1.523408  1.572691  0.909968
 H -1.523408  1.572691 -0.909968
 H -0.373801  2.650634  0.000000
 H  0.000000  0.722840  0.000000
 H  1.478693 -0.060765 -0.899173
 H  1.478693 -0.060765  0.899173
 C  0.153074 -1.574917  0.000000
 H  0.847028 -2.424608  0.000000
 H -0.483530 -1.678097  0.883585
 H -0.483530 -1.678097 -0.883585
ImagFreq  1629i
Internal rotation:
cos   0.00   0.00   0.30 F
barrier   0.30
symmetry     3
Im,red  10.29
freq  24.9  (from HO analysis)

iso-propyl/methyl
 C  0.124553 -2.224584  0.000000
 C -0.455044  0.426952  0.000000
 C  0.124553  0.987342  1.283511
 C  0.124553  0.987342 -1.283511
 H  1.211315 -2.262201  0.000000
 H -0.328017 -2.609304  0.910733
 H -0.188683 -0.849031  0.000000
 H -0.328017 -2.609304 -0.910733
 H -1.548711  0.430210  0.000000
 H -0.077324  2.062586 -1.375729
 H  1.211375  0.858183 -1.316847
 H -0.298835  0.497890 -2.165032
 H -0.077324  2.062586  1.375729
 H -0.298835  0.497890  2.165032
```

```
 H  1.211375  0.858183  1.316847
ImagFreq  1570i
Internal rotation:
cos   0.00   0.00   0.29 F
barrier   0.29
symmetry     3
Im,red  11.37
freq  12.5  (from HO analysis)

tert-butyl/methyl
 C  0.000000  0.000000  2.376398
 C  0.000000  0.000000 -0.348639
 C -1.271441 -0.734067 -0.742782
 C  0.000000  1.468134 -0.742782
 C  1.271441 -0.734067 -0.742782
 H -0.912033  0.526563  2.645400
 H  0.000000 -1.053125  2.645400
 H  0.000000  0.000000  0.938009
 H  0.912033  0.526563  2.645400
 H  0.000000  1.580271 -1.835721
 H -0.885114  1.985342 -0.360587
 H  0.885114  1.985342 -0.360587
 H -1.368555 -0.790136 -1.835721
 H -1.276800 -1.759202 -0.360587
 H -2.161914 -0.226140 -0.360587
 H  1.368555 -0.790136 -1.835721
 H  2.161914 -0.226140 -0.360587
 H  1.276800 -1.759202 -0.360587
ImagFreq  1481i
Internal rotation:
cos   0.00   0.00   0.30 F
barrier   0.30
symmetry     3
Im,red  11.63
freq  29.2  (from HO analysis)

allyl/methyl
 C -2.397949 -0.473731  0.022922
 C -0.046176  0.909157 -0.203452
 C  1.054371  0.178483  0.439884
 C  1.957731 -0.577189 -0.196441
 H  1.957133 -0.672979 -1.278123
 H  2.728784 -1.115366  0.342401
 H  1.102997  0.238624  1.525855
 H  0.053832  1.013420 -1.284814
 H -0.295853  1.861756  0.266312
 H -1.123339  0.256049 -0.070140
 H -3.093459  0.130666 -0.552035
 H -2.588730 -0.498425  1.091996
 H -2.149224 -1.434064 -0.418934
ImagFreq  1478i
Internal rotation:
cos  -0.00  -0.00   0.28 F
barrier   0.28
symmetry     3
Im,red  11.18
freq  35.3  (from HO analysis)

but-1-en-3-yl/methyl
 C -2.150193 -1.283160  0.067936
 C -0.021520  0.402282 -0.359855
 C -0.542965  1.777435  0.035565
 C  1.147018 -0.093422  0.391484
 C  2.162913 -0.794628 -0.122868
 H  2.213025 -1.028639 -1.182091
 H  2.977065 -1.153563  0.496114
 H  1.148126  0.116479  1.461115
 H  0.111799  0.300110 -1.440564
 H -0.971848 -0.388632 -0.137740
 H -2.846407 -0.990649 -0.712423
 H -2.467362 -1.045287  1.079107
 H -1.704927 -2.265749 -0.055022
 H -1.478807  2.008895 -0.480095
 H -0.731458  1.833778  1.112145
 H  0.179275  2.562215 -0.214126
ImagFreq  1366i
Internal rotation:
cos  -0.00  -0.00   0.29 F
barrier   0.30
symmetry     3
Im,red  11.76
freq  33.5  (from HO analysis)

3-methylbut-1-en-3-yl/methyl
 C  2.230726 -1.324572 -0.004888
 C  0.039900  0.356239 -0.015863
 C  0.520434  1.555852 -0.831750
 C -1.066155 -0.385559 -0.672615
 C -2.143181 -0.918889 -0.088221
 H -2.882205 -1.460868 -0.667201
 H -2.331410 -0.831716  0.975875
 H -0.953562 -0.511504 -1.749171
 C -0.152880  0.675772  1.460116
 H  1.010108 -0.427830 -0.041759
 H  1.825838 -2.225699  0.445067
 H  2.494544 -1.410430 -1.054612
 H  2.941207 -0.777916  0.607498
 H  1.447527  1.965238 -0.420261
 H  0.706325  1.281373 -1.874078
 H -0.229417  2.355598 -0.827540
 H  0.741340  1.153023  1.869708
 H -0.994788  1.362222  1.607880
 H -0.348586 -0.224548  2.047920
ImagFreq  1246i
Internal rotation:
cos  -0.00  -0.00   0.29 F
barrier   0.30
symmetry     3
Im,red  11.87
freq  23.1  (from HO analysis)

penta-1,4-dien-3-yl/methyl
 C  2.387947  1.153588  0.000000
 C -0.030916 -0.245805  0.000000
 H  1.005218  0.412287  0.000000
 H  0.343102 -1.273140  0.000000
 H  2.071753  2.191559  0.000000
 C -0.738277  0.095621  1.260547
 C -0.738277  0.095621 -1.260547
 C -0.738277 -0.645587  2.369612
 C -0.738277 -0.645587 -2.369612
 H  2.830283  0.791266  0.921711
 H  2.830283  0.791266 -0.921711
 H -1.271366  1.045526  1.263754
 H -1.271366  1.045526 -1.263754
 H -0.226038 -1.601835  2.415691
 H -0.226038 -1.601835 -2.415691
 H -1.254681 -0.323862  3.266549
```

```
 H -1.254681 -0.323862 -3.266549
ImagFreq  1078i
Internal rotation:
cos  -0.00  -0.00   0.24 F
barrier   0.24
symmetry     3
Im,red  12.02
freq  34.7  (from HO analysis)

3-methylpenta-1,4-dien-3-
yl/methyl
 C  2.009359  1.849543  0.000000
 H  0.810894  0.808186  0.000000
 C -0.045902 -0.064815  0.000000
 C  0.743880 -1.366393  0.000000
 H  0.077255 -2.234702  0.000000
 H  1.462573  2.786439  0.000000
 H  2.519838  1.594444  0.922200
 H  2.519838  1.594444 -0.922200
 H  1.386099 -1.431845  0.880791
 H  1.386099 -1.431845 -0.880791
 C -0.837358  0.215227  1.237442
 C -0.837358  0.215227 -1.237442
 C -0.837358 -0.487565  2.371024
 C -0.837358 -0.487565 -2.371024
 H -1.462114  1.105938  1.184979
 H -1.462114  1.105938 -1.184979
 H -1.442453 -0.179793  3.216088
 H -1.442453 -0.179793 -3.216088
 H -0.250443 -1.389685  2.499444
 H -0.250443 -1.389685 -2.499444
ImagFreq  954i
Internal rotation:
cos  -0.00  -0.00   0.26 F
barrier   0.26
symmetry     3
Im,red  12.06
freq  18.8  (from HO analysis)

propargyl/methyl
 C  2.274966 -0.517337  0.000000
 C  0.000000  0.979626  0.000000
 C -1.151130  0.132588  0.000000
 C -2.088307 -0.626329  0.000000
 H -2.926103 -1.278944  0.000000
 H  1.058312  0.261200  0.000000
 H  3.069470  0.223555  0.000000
 H  2.188500 -1.096325  0.914841
 H  2.188500 -1.096325 -0.914841
 H  0.104073  1.587773  0.899766
 H  0.104073  1.587773 -0.899766
ImagFreq  1538i
Internal rotation:
cos   0.00   0.00   0.28 F
barrier   0.28
symmetry     3
Im,red  11.11
freq  40.3  (from HO analysis)

but-1-yn-3-yl/methyl
 C  2.176793 -1.098672 -0.118360
 C -0.011717  0.423421  0.492718
 C  0.199075  1.740543 -0.250188
 C -1.192585 -0.313436  0.142291
 C -2.159430 -0.957252 -0.181453
 H -3.019348 -1.516410 -0.456818
 H  0.983847 -0.305680  0.210853
 H  0.088955  0.534587  1.575902
 H  0.185563  1.584540 -1.331200
 H -0.589024  2.459276 -0.006437
 H  1.159922  2.184038  0.022730
 H  1.999526 -2.019032  0.429903
 H  2.110604 -1.189661 -1.198487
 H  3.007134 -0.499281  0.243507
ImagFreq  1445i
Internal rotation:
cos   0.00   0.00   0.27 F
barrier   0.27
symmetry     3
Im,red  11.74
freq  36.8  (from HO analysis)

3-methylbut-1-yn-3-yl/methyl
 C  2.106528  1.379077 -0.001372
 C -0.021789 -0.357649  0.001161
 C  0.168889 -1.168171  1.284749
 C  0.172820 -1.176727 -1.276392
 C -1.223470  0.439461 -0.003347
 C -2.209049  1.133779 -0.007179
 H  0.926134  0.463533 -0.000127
 H  2.962773  0.711290  0.001998
 H -3.082825  1.737569 -0.010537
 H  1.956461  1.945276  0.912684
 H  1.959081  1.939389 -0.919474
 H  0.085847 -0.533016  2.168943
 H  0.092503 -0.547494 -2.165060
 H -0.589289 -1.954636  1.362617
 H -0.585126 -1.963700 -1.351332
 H  1.153463 -1.644127  1.290949
 H  1.157403 -1.652705 -1.276387
ImagFreq  1327i
Internal rotation:
cos   0.00   0.00   0.25 F
barrier   0.26
symmetry     3
Im,red  11.87
freq  23.1  (from HO analysis)

penta-1,4-diyn-3-yl/methyl
 C  1.887413  1.760890  0.000000
 C -0.490260  0.347351  0.000000
 C -0.536073 -0.416385  1.226491
 C -0.536073 -1.021267  2.265961
 C -0.536073 -0.416385 -1.226491
 C -0.536073 -1.021267 -2.265961
 H -1.227682  1.156073  0.000000
 H  0.581366  0.974950  0.000000
 H  2.605448  0.947611  0.000000
 H  1.812088  2.328951 -0.921243
 H  1.812088  2.328951  0.921243
 H -0.550243 -1.567078 -3.177295
 H -0.550243 -1.567078  3.177295
ImagFreq  1254i
Internal rotation:
cos   0.00   0.00   0.23 F
barrier   0.23
symmetry     3
Im,red  11.99
```

```
freq  13.1  (from HO analysis)

3-methylpenta-1,4-diyn-3-
yl/methyl
 H -2.291476  0.905671  0.000000
 C -1.269237  1.290493  0.000000
 C -0.256620  0.130194  0.000000
 H  0.845832  0.682921  0.000000
 C  2.199677  1.425294  0.000000
 H  2.877188  0.578284  0.000000
 H -1.129689  1.908013  0.889179
 H -1.129689  1.908013 -0.889179
 C -0.288112 -0.663980  1.213756
 C -0.288112 -0.663980 -1.213756
 C -0.288112 -1.282866  2.245341
 C -0.288112 -1.282866 -2.245341
 H -0.297546 -1.843210  3.147707
 H -0.297546 -1.843210 -3.147707
 H  2.147350  1.994893  0.921777
 H  2.147350  1.994893 -0.921777
ImagFreq  1123i
Internal rotation:
cos   0.00   0.00   0.21 F
barrier   0.21
symmetry     3
Im,red  12.05
freq  14.0  (from HO analysis)

vinyl/methyl
 C  0.795516  1.724663  0.000000
 C -0.788529 -0.442058  0.000000
 C -0.201970 -1.621687  0.000000
 H  0.880211 -1.725301  0.000000
 H  0.000000  0.675273  0.000000
 H  1.805652  1.320309  0.000000
 H -0.771442 -2.550625  0.000000
 H -1.853138 -0.229657  0.000000
 H  0.554309  2.272249  0.908660
 H  0.554309  2.272249 -0.908660
ImagFreq  1587i
Internal rotation:
cos   0.00   0.00   0.20 F
barrier   0.20
symmetry     3
Im,red   9.28
freq  29.0  (from HO analysis)

prop-1-en-2-yl/methyl
 C -2.220949 -0.124304  0.000000
 C  0.458765  0.123455  0.000000
 C  0.902957  1.366646  0.000000
 C  1.197316 -1.168455  0.000000
 H -2.585489  0.900481 -0.000172
 H -2.466009 -0.668442  0.909551
 H -2.465980 -0.668737 -0.909383
 H -0.877813 -0.013525  0.000003
 H  1.969845  1.592852 -0.000003
 H  0.229007  2.217858  0.000000
 H  2.281663 -1.006328 -0.000005
 H  0.943125 -1.769107  0.879875
 H  0.943118 -1.769108 -0.879872
ImagFreq  1618i
Internal rotation:
cos   0.00   0.00   0.26 F
barrier   0.26
symmetry     3
Im,red  11.22
freq  21.1  (from HO analysis)

buta-1,3-dien-2-yl/methyl
 C  2.053145 -1.098168  0.000000
 C  0.000000  0.639684  0.000000
 C  0.371723  1.914204  0.000000
 C -1.334737  0.082056  0.000000
 C -1.630204 -1.222165  0.000000
 H  1.011461 -0.262226  0.000000
 H -0.360519  2.721718  0.000000
 H  1.416007  2.208984  0.000000
 H -2.149941  0.809058  0.000000
 H -2.657089 -1.566978  0.000000
 H -0.855303 -1.980494  0.000000
 H  2.928100 -0.451721  0.000000
 H  1.953861 -1.686001  0.909897
 H  1.953861 -1.686001 -0.909897
ImagFreq  1614i
Internal rotation:
cos  -0.01  -0.01   0.74 F
barrier   0.75
symmetry     3
Im,red  11.56
freq  48.3  (from HO analysis)

but-1-en-3-yn-2-yl/methyl
 C -2.182486 -1.090543  0.000000
 C  0.000000  0.482917  0.000000
 C -0.288458  1.780669  0.000000
 C  1.226682 -0.184295  0.000000
 C  2.231738 -0.857590  0.000000
 H  3.131476 -1.422199  0.000000
 H -1.036536 -0.307080  0.000000
 H  0.487921  2.540896  0.000000
 H -1.317227  2.124849  0.000000
 H -3.003292 -0.378320  0.000000
 H -2.093600 -1.672544  0.913255
 H -2.093600 -1.672544 -0.913255
ImagFreq  1574i
Internal rotation:
cos F
barrier   0.00
symmetry     3
Im,red  11.62
freq  -4.5  (from HO analysis)

benzyl/methyl
 C  0.426988 -0.307787  1.203621
 C  0.429587  0.416750  0.000000
 C  0.426988 -0.307787 -1.203621
 C  0.426988 -1.698401 -1.204192
 C  0.426596 -2.401662  0.000000
 C  0.426988 -1.698401  1.204192
 C  0.382235  1.893071  0.000000
 C -2.206527  2.765529  0.000000
 H  0.786119  2.358035  0.899608
 H -0.828865  2.279909  0.000000
 H  0.786119  2.358035 -0.899608
 H -2.109823  3.847482  0.000000
 H -2.612112  2.342495 -0.914505
 H -2.612112  2.342495  0.914505
```

```
 H  0.430457  0.230849 -2.145994
 H  0.430825 -2.236153 -2.146103
 H  0.429062 -3.485709  0.000000
 H  0.430825 -2.236153  2.146103
 H  0.430457  0.230849  2.145994
ImagFreq  1477i
Internal rotation:
cos  -0.01  -0.01   0.25 F
barrier   0.26
symmetry     3
Im,red  11.89
freq  21.2  (from HO analysis)

1-phenyleth-1-yl/methyl
 C  1.929983  0.921780  0.866228
 C  0.580282  1.005762  0.535444
 C -0.009934  0.079686 -0.339597
 C  0.808351 -0.934799 -0.865231
 C  2.155870 -1.020824 -0.534838
 C  2.725448 -0.090907  0.334554
 C -1.458144  0.111213 -0.678622
 C -2.815717 -1.430276  1.142508
 C -2.184666  1.447253 -0.649011
 H -2.052181 -0.611089  0.162765
 H -1.653372 -0.432978 -1.606102
 H -3.810513 -1.502768  0.712906
 H -2.249925 -2.356941  1.154843
 H -2.749283 -0.841776  2.052793
 H  0.375880 -1.660857 -1.546798
 H  2.764983 -1.811325 -0.959712
 H  3.776669 -0.153892  0.591867
 H  2.362503  1.652331  1.541376
 H -0.017299  1.803556  0.960638
 H -3.232757  1.318667 -0.930758
 H -2.168970  1.902427  0.344788
 H -1.734565  2.161316 -1.347224
ImagFreq  1363i
Internal rotation:
cos  -0.01  -0.01   0.24 F
barrier   0.26
symmetry     3
Im,red  11.98
freq  35.8  (from HO analysis)

2-phenylprop-2-yl/methyl
 C  2.960373 -0.227110 -0.139123
 C  2.379230  0.991415 -0.475342
 C  1.003291  1.176159 -0.349540
 C  0.170940  0.151430  0.124840
 C  0.777988 -1.073700  0.454356
 C  2.148693 -1.262102  0.324831
 C -1.318327  0.313811  0.253188
 C -1.877406 -0.067821  1.624393
 C -1.893038  1.634513 -0.243113
 C -2.458109 -1.522031 -1.443866
 H  0.580408  2.136412 -0.616363
 H  0.165224 -1.896361  0.805845
 H  2.996815  1.806248 -0.837609
 H  2.585772 -2.220469  0.583696
 H  4.030138 -0.371796 -0.238953
 H -1.565750  2.475510  0.380156
 H -1.563388  0.659108  2.382950
 H -2.985096  1.606630 -0.204403
 H -2.971095 -0.079810  1.605018
 H -1.602369  1.846860 -1.274946
 H -1.538336 -1.051720  1.953596
 H -1.808081 -0.541252 -0.526982
 H -1.811018 -1.482316 -2.314852
 H -3.456042 -1.120341 -1.593051
 H -2.418989 -2.454085 -0.887855
ImagFreq  1320i
Internal rotation:
cos   0.03   0.03   0.18 F
barrier   0.21
symmetry     3
Im,red  11.99
freq  38.4  (from HO analysis)

phenyl/methyl
 C -1.210495 -1.432223  0.000000
 C -0.001448 -2.127025  0.000000
 C  1.208281 -1.433523  0.000000
 C  1.213445 -0.035636  0.000000
 C  0.000000  0.630845  0.000000
 C -1.214195 -0.034385  0.000000
 C  0.002562  3.316169  0.000000
 H  1.052324  3.603201  0.000000
 H -0.518099  3.612436  0.908331
 H -0.518099  3.612436 -0.908331
 H -0.000152  2.009791  0.000000
 H  2.151902  0.509471  0.000000
 H -2.151974  0.511956  0.000000
 H  2.146945 -1.977794  0.000000
 H -2.149714 -1.975539  0.000000
 H -0.002029 -3.211293  0.000000
ImagFreq  1561i
Internal rotation:
cos F
barrier   0.00
symmetry     6
Im,red  11.43
freq  12.7  (from HO analysis)

cyclopentyl/methyl
 C  1.217849 -0.866342 -0.630890
 C  0.338478 -1.162108  0.596772
 C -0.403661  0.151700  0.844243
 C  0.425131  1.283209  0.214317
 C  1.663664  0.588807 -0.405625
 C -2.760370  0.006146 -0.488192
 H  2.495734  0.607455  0.306434
 H  2.009681  1.077477 -1.319683
 H  0.706574  2.046350  0.945231
 H -0.153362  1.798236 -0.561729
 H -0.732623  0.318089  1.870853
 H  0.616480 -0.937701 -1.544278
 H  2.055929 -1.559677 -0.736505
 H -0.336231 -2.011099  0.449854
 H  0.973726 -1.407232  1.458318
 H -1.524114  0.081404  0.206682
 H -3.186193  1.000988 -0.383743
 H -2.495802 -0.254864 -1.509974
 H -3.316348 -0.767897  0.034789
ImagFreq  1533i
Internal rotation:
cos   0.00   0.00   0.41 F
barrier   0.42
symmetry     3
```

```
Im,red  11.64
freq  43.8  (from HO analysis)

cyclohexyl/methyl
 C -0.595927  0.664620  0.000000
 H -0.439335  1.962284  0.000000
 H -1.685817  0.556428  0.000000
 C  0.038248  0.120997  1.269939
 C  0.038248  0.120997 -1.269939
 C  0.038248 -1.421679  1.271400
 C  0.038248 -1.421679 -1.271400
 C  0.692835 -1.982378  0.000000
 H  1.076155  0.473618  1.338207
 H  1.076155  0.473618 -1.338207
 H -0.481389  0.500297  2.155549
 H -0.481389  0.500297 -2.155549
 H  0.554351 -1.796051  2.162099
 H  0.554351 -1.796051 -2.162099
 H -0.996680 -1.780885  1.334488
 H -0.996680 -1.780885 -1.334488
 H  0.640766 -3.076130  0.000000
 H  1.759375 -1.721943  0.000000
 C -0.243660  3.352879  0.000000
 H  0.835910  3.484077  0.000000
 H -0.726604  3.699392 -0.910593
 H -0.726604  3.699392  0.910593
ImagFreq  1581i
Internal rotation:
cos   0.02   0.02   0.36 F
barrier   0.39
symmetry     3
Im,red  11.63
freq  21.3  (from HO analysis)

1-methylcyclohex-1-yl/methyl
 C  1.977455 -1.352878 -0.000113
 C  0.741912 -0.469587  0.000000
 C -2.178406  0.097140  0.002315
 C  1.857761  2.021610 -0.005332
 H  1.051347  2.750038 -0.005570
 H  1.215634  0.733538 -0.002557
 H  1.699729 -2.415425  0.001889
 H -3.040791  0.771726  0.002225
 H -2.581356 -0.924317  0.004394
 C -1.339103  0.307960 -1.264666
 C -1.336223  0.311976  1.266706
 C -0.092542 -0.589659 -1.271642
 C -0.089645 -0.585621  1.273694
 H -1.941976  0.113234 -2.157548
 H -1.937061  0.120087  2.161571
 H -1.029655  1.358388 -1.321260
 H -1.026651  1.362578  1.319262
 H -0.408867 -1.639697 -1.382885
 H -0.405713 -1.635299  1.388989
 H  0.529673 -0.368370 -2.146422
 H  0.534557 -0.361558  2.146349
 H  2.595195 -1.176819 -0.886016
 H  2.597209 -1.174011  0.883818
 H  2.449702  2.018685 -0.917234
 H  2.451776  2.021577  0.905225
ImagFreq  1502i
Internal rotation:
cos F
barrier   0.00
symmetry     3
Im,red  11.83
freq -16.6  (from HO analysis)

cyclohex-1-en-3-yl/methyl
 C -0.839682 -1.288612 -0.363286
 C  0.004185 -1.057895  0.898193
 C  0.683077  0.307591  0.859461
 C -0.173331  1.397956  0.348468
 C -1.337193  1.186092 -0.283695
 C -1.898528 -0.189255 -0.537398
 C  2.902010 -0.015214 -0.744774
 H -1.924708  2.035202 -0.622439
 H  0.175668  2.417571  0.490654
 H -2.325628 -0.235197 -1.545900
 H  1.175246  0.565632  1.801421
 H -2.742754 -0.366308  0.144810
 H  1.676674  0.198469  0.100280
 H -1.317144 -2.272517 -0.330332
 H  0.751185 -1.850604  1.009671
 H -0.178315 -1.287384 -1.237093
 H -0.643603 -1.113851  1.783508
 H  3.586790 -0.538775 -0.084073
 H  2.535100 -0.599735 -1.583162
 H  3.188263  1.003527 -0.989158
ImagFreq  1363i
Internal rotation:
cos  -0.00  -0.00   0.13
sin  -0.00   0.00   0.04 F
barrier   0.16
symmetry     3
Im,red  11.86
freq  32.1  (from HO analysis)
```

Resonance training set reactions of Table 3

```
28  allyl/allyl
 C -2.237154  0.391826  0.352256
 C -3.185069 -0.432715 -0.128936
 H -2.342553  0.755153  1.373066
 H -4.038560 -0.727050  0.469964
 H -3.134582 -0.825729 -1.139793
 C -1.040335  0.802419 -0.360388
 H  0.000000  0.000000  0.000000
 H -1.047159  0.638734 -1.437786
 H -0.616042  1.765965 -0.082546
 C  1.040335 -0.802419  0.360388
 H  1.047159 -0.638734  1.437786
 H  0.616042 -1.765965  0.082546
 C  2.237154 -0.391826 -0.352256
 C  3.185069  0.432715  0.128936
 H  2.342553 -0.755153 -1.373066
 H  4.038560  0.727050 -0.469964
 H  3.134582  0.825729  1.139793
ImagFreq  1776i
Internal rotation:
cos  -0.25  -0.15   0.71 F
barrier   0.86
symmetry     1
Im,red  97.24
freq  20.1  (from HO analysis)

29  allyl/but-1-en-3-yl
```

```
 C -3.029026  0.964979  0.167493
 C -2.171536  0.061493 -0.334940
 C -0.998064 -0.469411  0.350789
 C -0.545455 -1.876517  0.012704
 C  1.130199  1.052496 -0.420384
 C  2.305476  0.675829  0.340497
 C  3.265280 -0.175522 -0.070500
 H -2.327811 -0.288081 -1.355468
 H -3.860012  1.344377 -0.415204
 H -2.925574  1.344199  1.179602
 H  0.051053  0.291073 -0.029028
 H -0.983195 -0.249023  1.421016
 H  1.153788  0.819681 -1.484739
 H  0.708352  2.033899 -0.210021
 H  2.389494  1.097213  1.340972
 H  4.103453 -0.435010  0.564944
 H  3.239247 -0.623985 -1.058844
 H  0.453500 -2.076475  0.408294
 H -1.226757 -2.624948  0.434569
 H -0.516785 -2.033002 -1.070056
ImagFreq  1752i
Internal rotation:
cos   0.74  -0.35   1.07
sin   0.42   0.17  -0.05
barrier   1.87
symmetry     1
Im,red  132.40
freq  18.9  (from HO analysis)

30  allyl/3-methylbut-1-en-3-yl
 C -0.993533 -0.395621  0.158142
 C -1.167944  1.015088  0.527074
 C -1.899344  1.937565 -0.117914
 C  1.441134 -0.481788 -1.070378
 C  2.492053 -0.313677 -0.088665
 C  3.039336  0.864200  0.272656
 C -1.896782 -0.947677 -0.929808
 C -0.784156 -1.335571  1.335982
 H  0.221588 -0.418500 -0.413706
 H  1.368775 -1.458666 -1.544544
 H  1.292697  0.345649 -1.763180
 H -0.609254  1.331943  1.406525
 H -1.932643  2.964099  0.227829
 H -2.489983  1.702922 -0.996139
 H  2.827146 -1.213657  0.424027
 H  3.800085  0.923593  1.041711
 H  2.744936  1.794511 -0.202859
 H -0.436872 -2.317973  1.002307
 H -0.046750 -0.935737  2.037561
 H -1.720242 -1.486105  1.888199
 H -1.600414 -1.964740 -1.200367
 H -2.940399 -0.984361 -0.593586
 H -1.863260 -0.338092 -1.836310
ImagFreq  1700i
Internal rotation:
cos  -0.45   0.19   1.23
sin   0.64   0.17  -0.24
barrier   2.68
symmetry     1
Im,red  159.25
freq  15.9  (from HO analysis)

31  but-1-en-3-yl/but-1-en-3-yl
 C -1.801874 -0.779896 -0.026307
 C -2.122836 -1.435180 -1.156272
 H -1.819873 -1.331040  0.913194
 H -2.399750 -2.482555 -1.145336
 H -2.123032 -0.937205 -2.121116
 C -1.363853  0.605817  0.053296
 H  0.000000  0.546280  0.000000
 C -1.644580  1.372953  1.330827
 H -1.554616  1.178566 -0.857148
 C  1.363935  0.605710 -0.053285
 C  1.801767 -0.780063  0.026246
 H  1.554689  1.178340  0.857234
 C  1.644875  1.372923 -1.330724
 H -1.107874  2.325514  1.352110
 H -2.713058  1.596016  1.435948
 H -1.342424  0.797762  2.211360
 C  2.122526 -1.435485  1.156190
 H  1.819795 -1.331126 -0.913302
 H  2.399307 -2.482894  1.145194
 H  2.122686 -0.937592  2.121077
 H  2.713400  1.595795 -1.435757
 H  1.342663  0.797878 -2.211333
 H  1.108349  2.325587 -1.351941
ImagFreq  1728i
Internal rotation:
cos  -0.82   2.08  -0.18
sin  -1.74   0.45  -0.17
barrier   4.99
symmetry     1
Im,red  233.27
freq  14.2  (from HO analysis)

32  but-1-en-3-yl/3-methylbut-1-
en-3-yl
 C -2.077005  0.186609 -0.596180
 C -2.972066  0.934243  0.070902
 H -2.127578  0.189220 -1.684842
 H -3.711097  1.523851 -0.458764
 H -3.002962  0.977159  1.153506
 C -1.003283 -0.636970 -0.030156
 H  0.133142  0.084901 -0.226744
 C -0.686875 -1.899664 -0.818962
 C -0.989665 -0.830624  1.474513
 C  1.307836  0.772973 -0.437815
 C  0.922687  2.202822 -0.113452
 H  1.411792  0.576885 -1.507748
 C  2.335318  0.136746  0.372529
 C  3.184614 -0.823249 -0.039622
 H  2.389930  0.459593  1.412182
 H  3.904229 -1.271393  0.634993
 H  3.185463 -1.178167 -1.065592
 H  0.272689 -2.325067 -0.513375
 H -1.456602 -2.664924 -0.655704
 H -0.644796 -1.700370 -1.893668
 H  1.696314  2.906496 -0.444086
 H -0.013031  2.484864 -0.602291
 H  0.791969  2.343062  0.963854
 H -0.068316 -1.327314  1.789659
 H -1.058680  0.119342  2.010499
 H -1.831841 -1.455462  1.797574
ImagFreq  1721i
Internal rotation:
cos   3.74  -0.57   1.90
sin  -0.53  -0.56   0.78
barrier   5.99
```

```
symmetry     1
Im,red  275.32
freq  16.3  (from HO analysis)

33  3-methylbut-1-en-3-yl/3-
methylbut-1-en-3-yl
 C  2.133269 -0.248352 -0.677844
 C  3.052415 -1.036509 -0.092682
 H  2.048184 -0.293850 -1.763142
 H  3.677161 -1.696493 -0.682928
 H  3.216070 -1.044348  0.978731
 C  1.198154  0.670183 -0.023362
 H  0.000000  0.000000  0.000000
 C  0.834890  1.902445 -0.839053
 C  1.417179  0.958142  1.450777
 C -1.198154 -0.670183  0.023362
 C -0.834890 -1.902445  0.839053
 C -1.417179 -0.958142 -1.450777
 C -2.133269  0.248352  0.677844
 C -3.052415  1.036509  0.092682
 H -2.048184  0.293850  1.763142
 H -3.677161  1.696493  0.682928
 H -3.216070  1.044348 -0.978731
 H -0.066127  2.383042 -0.448843
 H  1.645894  2.641732 -0.806446
 H  0.660557  1.652948 -1.889234
 H -1.645894 -2.641732  0.806446
 H  0.066127 -2.383042  0.448843
 H -0.660557 -1.652948  1.889234
 H  0.578621  1.527423  1.860813
 H  1.521988  0.043776  2.039388
 H  2.326203  1.554376  1.600436
 H -2.326203 -1.554376 -1.600436
 H -1.521988 -0.043776 -2.039388
 H -0.578621 -1.527423 -1.860813
ImagFreq  1708i
Internal rotation:
cos   4.90  -1.60   3.93
barrier   8.83
symmetry     1
Im,red  324.97
freq  28.3  (from HO analysis)

34  allyl/propargyl
 C -0.912985 -0.865597  0.094642
 C -2.165207 -0.201258  0.423777
 C -3.034638  0.300139 -0.470378
 C  1.136294  0.924671  0.191241
 C  2.352091  0.232867 -0.026549
 C  3.354668 -0.415222 -0.217083
 H  4.249241 -0.963079 -0.382636
 H  0.087413  0.016897  0.165813
 H  0.829594  1.604399 -0.602697
 H  1.009765  1.354057  1.184455
 H -2.383624 -0.073268  1.482463
 H -3.937357  0.811823 -0.158756
 H -2.869509  0.200765 -1.538850
 H -0.555841 -1.602425  0.812945
 H -0.811021 -1.202769 -0.936636
ImagFreq  1742i
Internal rotation:
cos   0.49   0.49   0.07
sin  -0.26   0.11   0.01
barrier   1.08

symmetry     1
Im,red  95.33
freq  10.2  (from HO analysis)

35  allyl/but-1-yn-3-yl
 C -3.170610 -0.972463 -0.041515
 C -2.201344 -0.299990  0.220804
 C -1.023062  0.451610  0.484183
 C -0.839558  1.762507 -0.262790
 H -4.034336 -1.551332 -0.257800
 H -0.778110  0.512503  1.546426
 H -1.543866  2.521320  0.094618
 H  0.172946  2.147113 -0.116106
 H -1.009762  1.630034 -1.333719
 H  0.032219 -0.313859  0.059476
 C  1.087463 -1.062712 -0.332678
 C  2.257692 -0.213965 -0.470816
 C  3.194344 -0.019481  0.476617
 H  0.675029 -1.472977 -1.253167
 H  1.119838 -1.792004  0.476340
 H  2.353477  0.332181 -1.407470
 H  4.029266  0.652731  0.319355
 H  3.153751 -0.538750  1.429219
ImagFreq  1740i
Internal rotation:
cos   1.75   0.44   0.39
barrier   2.31
symmetry     1
Im,red  132.02
freq  23.3  (from HO analysis)

36  allyl/3-methylbut-1-yn-3-yl
 C -1.216154 -1.234570 -0.005640
 C -2.386473 -0.502222  0.437144
 C -3.278426  0.108033 -0.368365
 C  0.953533  0.413833  0.022543
 C  2.081616 -0.457582 -0.083588
 C  3.001936 -1.234583 -0.174979
 H  3.822080 -1.904597 -0.255262
 H -0.119799 -0.417513  0.026117
 C  0.695536  1.290358 -1.196937
 C  0.810477  1.127749  1.360715
 H -2.527582 -0.418489  1.513336
 H -4.117960  0.662916  0.032770
 H -3.194977  0.054635 -1.449458
 H -0.852564 -2.017007  0.658308
 H -1.202494 -1.528510 -1.054689
 H -0.289819  1.758937 -1.127216
 H  1.444818  2.087883 -1.266466
 H  0.740711  0.709126 -2.120072
 H -0.178475  1.587814  1.442235
 H  0.943768  0.437045  2.195839
 H  1.560024  1.921667  1.459196
ImagFreq  1722i
Internal rotation:
cos   2.08  -0.00   0.86
barrier   3.00
symmetry     1
Im,red  149.45
freq  23.1  (from HO analysis)

37  propargyl/propargyl
 C  0.528079  1.251719  0.000000
 H  1.132532  1.223063  0.906066
```

```
 H  1.132532  1.223063 -0.906066
 C -0.528079  2.197200  0.000000
 H  0.000000  0.000000  0.000000
 C -0.528079 -1.251719  0.000000
 H -1.132532 -1.223063 -0.906066
 H -1.132532 -1.223063  0.906066
 C  0.528079 -2.197200  0.000000
 C  1.471098 -2.952806  0.000000
 H  2.283579 -3.636902  0.000000
 C -1.471098  2.952806  0.000000
 H -2.283579  3.636902  0.000000
ImagFreq  1742i
Internal rotation:
cos   2.21   0.53   0.10
barrier   2.31
symmetry     1
Im,red  92.84
freq   9.2  (from HO analysis)

38  propargyl/but-1-yn-3-yl
 C  1.144538 -1.146041  0.303870
 H  0.902385 -1.297892  1.355052
 H  0.958653 -2.031324 -0.302902
 H  0.092817 -0.344925 -0.089622
 C  2.360601 -0.468791  0.045498
 C  3.365133  0.158239 -0.199622
 H  4.263309  0.686529 -0.405012
 C -0.910824  0.464679 -0.457011
 C -2.118624 -0.249426 -0.209873
 C -0.675991  1.742253  0.335103
 H -0.681126  0.561211 -1.520512
 C -3.112289 -0.890919  0.035441
 H -3.997743 -1.441480  0.237990
 H -1.365565  2.531000  0.016449
 H -0.832489  1.575010  1.403011
 H  0.344496  2.101911  0.185106
ImagFreq  1717i
Internal rotation:
cos   3.34   0.41   0.41
sin   0.52   0.07  -0.09
barrier   3.78
symmetry     1
Im,red  125.83
freq  19.8  (from HO analysis)

39  but-1-yn-3-yl/but-1-yn-3-yl
 C  1.095079 -0.656545  0.472016
 H  0.848535 -0.660961  1.535921
 C  1.013221 -2.027321 -0.181810
 H  0.000000  0.000000  0.000000
 C  2.221621  0.154936  0.160294
 C  3.147625  0.868819 -0.146366
 H  3.975096  1.484240 -0.400550
 C -1.095079  0.656545 -0.472016
 C -2.221621 -0.154936 -0.160294
 C -1.013221  2.027321  0.181810
 H -0.848535  0.660961 -1.535921
 C -3.147625 -0.868819  0.146366
 H -3.975096 -1.484240  0.400550
 H -1.774937  2.701105 -0.224929
 H -1.174106  1.956776  1.259907
 H -0.033312  2.476630  0.005463
 H  1.174106 -1.956776 -1.259907
 H  1.774937 -2.701105  0.224929
 H  0.033312 -2.476630 -0.005463
ImagFreq  1722i
Internal rotation:
cos   6.04  -0.60   1.07
barrier   7.11
symmetry     1
Im,red  214.93
freq  14.8  (from HO analysis)

40  but-1-yn-3-yl/3-methylbut-1-
yn-3-yl
 C  1.033452 -0.571524  0.092713
 C  0.817973 -0.940214  1.556245
 C  0.958817 -1.747801 -0.874953
 H -0.083891  0.118187 -0.210032
 C  2.103653  0.345056 -0.151789
 C  2.977432  1.149345 -0.374096
 H  3.758312  1.843663 -0.564569
 C -1.239832  0.801684 -0.523252
 C -2.319635 -0.092963 -0.291691
 C -1.171360  2.061268  0.325740
 H -1.041544  0.973766 -1.583152
 C -3.207915 -0.881286 -0.062593
 H -4.002979 -1.559830  0.125676
 H -1.963499  2.764860  0.046909
 H -1.294542  1.827522  1.385460
 H -0.210347  2.562543  0.189365
 H  1.055195 -1.416667 -1.910883
 H  1.764701 -2.463508 -0.675023
 H  0.005410 -2.270617 -0.763463
 H  0.831677 -0.056082  2.196418
 H -0.141781 -1.448188  1.682375
 H  1.607774 -1.617049  1.902978
ImagFreq  1701i
Internal rotation:
cos   6.50  -0.07   1.62
sin   1.20   0.30  -0.01
barrier   8.29
symmetry     1
Im,red  260.93
freq  24.2  (from HO analysis)

41  3-methylbut-1-yn-3-yl/3-
methylbut-1-yn-3-yl
 C -0.245300  1.343997  0.000000
 H  0.000000  0.000000  0.000000
 C  0.245300 -1.343997  0.000000
 C  1.048365  1.950132  0.000000
 C -1.048365 -1.950132  0.000000
 C  2.159171  2.427191  0.000000
 C -2.159171 -2.427191  0.000000
 C -1.048365  1.533488  1.281810
 C -1.048365  1.533488 -1.281810
 C  1.048365 -1.533488 -1.281810
 C  1.048365 -1.533488  1.281810
 H  3.127725  2.863040  0.000000
 H -3.127725 -2.863040  0.000000
 H -1.426669  2.560505  1.350176
 H -1.426669  2.560505 -1.350176
 H  1.426669 -2.560505 -1.350176
 H  1.426669 -2.560505  1.350176
 H  1.906457 -0.856292 -1.297317
 H  1.906457 -0.856292  1.297317
 H -0.438368  1.343938  2.166895
```

```
 H -0.438368  1.343938 -2.166895
 H -1.906457  0.856292  1.297317
 H -1.906457  0.856292 -1.297317
 H  0.438368 -1.343938  2.166895
 H  0.438368 -1.343938 -2.166895
ImagFreq  1699i
Internal rotation:
cos   8.09  -0.51   3.59
barrier  11.69
symmetry     1
Im,red  323.87
freq  26.5  (from HO analysis)

42  allyl/ethyl
 C  1.832036  0.475185  0.481449
 C  2.172353 -0.815676 -0.215598
 C -0.714669  1.107910 -0.280380
 C -1.493821 -0.119274 -0.464911
 C -2.314689 -0.664236  0.444956
 H -2.494759 -0.188726  1.404430
 H -2.836625 -1.594468  0.253705
 H -1.354829 -0.640997 -1.410357
 H -1.048442  1.739820  0.543816
 H -0.549185  1.688131 -1.188852
 H  0.488933  0.805107  0.067469
 H  1.711112  0.415983  1.562237
 H  2.395088  1.354159  0.170422
 H  3.163019 -1.185892  0.081242
 H  1.450653 -1.601653  0.025612
 H  2.187773 -0.694919 -1.302826
ImagFreq  1590i
Internal rotation:
cos   0.88   0.13   0.25
sin  -0.39  -0.18   0.17
barrier   1.29
symmetry     1
Im,red  55.68
freq  30.7  (from HO analysis)

43  allyl/iso-propyl
 C -1.558043 -0.044077  0.388843
 C -1.677717 -1.234277 -0.530865
 C  1.057434 -0.050928  1.169731
 C  1.901123 -0.445252  0.042687
 C  2.536863  0.395319 -0.789637
 H  3.119710  0.031554 -1.627595
 H  2.499691  1.471231 -0.647593
 H  1.980568 -1.514187 -0.148862
 H  1.047893 -0.748581  2.007486
 H  1.187922  0.979749  1.501859
 H -0.198745 -0.067073  0.801665
 C -1.757089  1.317653 -0.230673
 H -2.065711 -0.171992  1.347157
 H -2.689954 -1.314126 -0.952094
 H -0.984062 -1.152397 -1.374296
 H -1.467547 -2.172645 -0.010007
 H -2.783352  1.439046 -0.606083
 H -1.577689  2.121207  0.488971
 H -1.084148  1.467584 -1.081123
ImagFreq  1643i
Internal rotation:
cos F
barrier   0.00
symmetry     1
Im,red  106.02
freq -13.2  (from HO analysis)

44  allyl/tert-butyl
 C  1.144893  1.346610 -0.830694
 C  1.234698  0.095136  0.016082
 C  1.261971  0.346661  1.508157
 C  2.232576 -0.932132 -0.473680
 C -1.185977 -1.094139 -0.387891
 C -2.224275 -0.386089  0.353701
 C -3.029595  0.568352 -0.143384
 H  2.166649 -1.862721  0.098138
 H  2.079079 -1.170727 -1.530509
 H  3.262805 -0.560055 -0.371130
 H  0.309527  1.980476 -0.520123
 H  2.062867  1.946737 -0.742595
 H  1.014868  1.107127 -1.890349
 H  1.222017 -0.588411  2.075176
 H  2.185076  0.867418  1.802573
 H  0.421526  0.972227  1.823206
 H -0.014324 -0.513886 -0.171084
 H -1.269238 -1.032119 -1.473528
 H -0.983195 -2.110954 -0.051468
 H -2.317575 -0.635944  1.409463
 H -3.757825  1.076449  0.477545
 H -2.988012  0.857992 -1.189049
ImagFreq  1653i
Internal rotation:
cos  -0.00  -0.00   0.94 F
barrier   0.94
symmetry     3
Im,red  128.63
freq  16.7  (from HO analysis)

45  but-1-en-3-yl/iso-propyl
 C -1.899931 -0.307948 -0.241892
 C -2.683789 -1.106413  0.497036
 H -1.935752 -0.409643 -1.326744
 H -3.339563 -1.838688  0.040770
 H -2.694925 -1.046486  1.581202
 C -0.943500  0.677407  0.277272
 H  0.217635  0.092217  0.318600
 C -0.735615  1.933416 -0.555615
 H -1.099843  0.893207  1.337815
 C  1.503231 -0.551391  0.401592
 H  1.322138 -1.162782  1.288123
 C  1.601362 -1.353482 -0.872401
 C  2.532107  0.532061  0.612870
 H  2.508109 -1.975423 -0.886125
 H  0.746070 -2.024226 -0.991683
 H  1.647743 -0.702408 -1.752039
 H  3.539814  0.108124  0.735131
 H  2.576194  1.214520 -0.242241
 H  2.321810  1.123831  1.508393
 H  0.084038  2.541479 -0.164114
 H -0.501212  1.684932 -1.595543
 H -1.635454  2.559446 -0.564707
ImagFreq  1617i
Internal rotation:
cos  -1.27   0.41   0.74
sin  -0.60   0.16   0.20
barrier   2.51
symmetry     1
Im,red  160.63
```

```
freq  18.6  (from HO analysis)

46  3-methylbut-1-en-3-yl/iso-
propyl
 C  1.620840 -0.780192  0.387705
 C  2.481659 -1.360277 -0.459689
 H  1.438557 -1.274531  1.341652
 H  2.975572 -2.290523 -0.203658
 H  2.728014 -0.931833 -1.424557
 C  0.844401  0.458156  0.171449
 H -0.347328  0.048776 -0.124996
 C  0.644180  1.279797  1.441856
 C  1.240281  1.298040 -1.034038
 C -1.680809 -0.389851 -0.515321
 H -1.459188 -0.668632 -1.547543
 C -1.957678 -1.569925  0.382111
 C -2.604211  0.796918 -0.391338
 H -2.908338 -2.057594  0.121309
 H -1.172808 -2.327091  0.304582
 H -2.033746 -1.265251  1.431567
 H -3.627347  0.540262 -0.704755
 H -2.669301  1.148130  0.643793
 H -2.278849  1.634819 -1.014007
 H -0.085320  2.079655  1.286400
 H  0.292962  0.657664  2.270310
 H  1.584719  1.748093  1.758230
 H  0.566936  2.151879 -1.147848
 H  2.259024  1.689712 -0.925518
 H  1.204457  0.720468 -1.961371
ImagFreq  1573i
Internal rotation:
cos  -0.63   0.44   1.05
sin  -0.97  -0.20   0.37
barrier   3.32
symmetry     1
Im,red  175.31
freq  18.5  (from HO analysis)

47  tert-butyl/3-methylbut-1-yn-
3-yl
 C  2.923107 -0.766339  0.000000
 C  1.736529 -0.992030  0.000000
 C  0.319220 -1.216872  0.000000
 C -0.206991 -1.864097  1.279973
 C -0.206991 -1.864097 -1.279973
 H  3.969135 -0.582895  0.000000
 H -0.216050 -0.002531  0.000000
 H -1.300670 -1.870318 -1.285479
 H  0.134041 -2.903058 -1.359117
 H  0.141292 -1.331909 -2.167366
 H -1.300670 -1.870318  1.285479
 H  0.134041 -2.903058  1.359117
 H  0.141292 -1.331909  2.167366
 C -0.766712  1.301548  0.000000
 C -2.269615  1.114782  0.000000
 C -0.206991  1.904420  1.271495
 C -0.206991  1.904420 -1.271495
 H -0.501427  2.960725 -1.363580
 H  0.885771  1.867452 -1.284043
 H -0.576102  1.387176 -2.161831
 H -2.782331  2.089003  0.000000
 H -2.611971  0.572936 -0.886486
 H -2.611971  0.572936  0.886486
 H -0.501427  2.960725  1.363580
 H -0.576102  1.387176  2.161831
 H  0.885771  1.867452  1.284043
ImagFreq  1656i
Internal rotation:
cos   0.03   0.03   2.85
barrier   2.89
symmetry     3
Im,red  249.99
freq  24.7  (from HO analysis)

48  iso-propyl/iso-propyl
 C -0.290004  1.330823  0.000000
 C  0.290004  1.889787  1.281958
 H -1.383194  1.318797  0.000000
 C  0.290004  1.889787 -1.281958
 H -0.144026  1.414218 -2.165761
 H  0.105703  2.969732 -1.368972
 H  1.375410  1.746578 -1.322035
 H  1.375410  1.746578  1.322035
 H  0.105703  2.969732  1.368972
 H -0.144026  1.414218  2.165761
 H  0.000000  0.000000  0.000000
 C  0.290004 -1.330823  0.000000
 C -0.290004 -1.889787 -1.281958
 H  1.383194 -1.318797  0.000000
 C -0.290004 -1.889787  1.281958
 H -0.105703 -2.969732 -1.368972
 H -1.375410 -1.746578 -1.322035
 H  0.144026 -1.414218 -2.165761
 H -0.105703 -2.969732  1.368972
 H  0.144026 -1.414218  2.165761
 H -1.375410 -1.746578  1.322035
ImagFreq  1700i
Internal rotation:
cos   0.79  -0.53   0.74
barrier   1.53
symmetry     1
Im,red  117.80
freq  18.2  (from HO analysis)

49  tert-butyl/tert-butyl
 H  0.000000  0.000000  0.000000
 C  0.000000  0.000000  1.370519
 C  0.000000  0.000000 -1.370519
 C -1.269896 -0.733175  1.762378
 C  1.269896 -0.733175  1.762378
 C  0.000000  1.466349  1.762378
 C  1.269896  0.733175 -1.762378
 C  0.000000 -1.466349 -1.762378
 C -1.269896  0.733175 -1.762378
 H  0.000000  1.580547  2.856793
 H  0.885487  1.985681  1.383962
 H -0.885487  1.985681  1.383962
 H -1.368794 -0.790273  2.856793
 H -2.162394 -0.225986  1.383962
 H -1.276907 -1.759695  1.383962
 H  1.368794 -0.790273  2.856793
 H  1.276907 -1.759695  1.383962
 H  2.162394 -0.225986  1.383962
 H -1.368794  0.790273 -2.856793
 H -2.162394  0.225986 -1.383962
 H -1.276907  1.759695 -1.383962
 H  1.368794  0.790273 -2.856793
 H  1.276907  1.759695 -1.383962
```

```
 H  2.162394  0.225986 -1.383962
 H  0.000000 -1.580547 -2.856793
 H  0.885487 -1.985681 -1.383962
 H -0.885487 -1.985681 -1.383962
ImagFreq  1718i
Internal rotation:
cos  -0.04  -0.04   1.80
barrier   1.81
symmetry     3
Im,red  202.87
freq  17.4  (from HO analysis)

50  vinyl/vinyl
 C  0.283644  1.303565  0.490272
 C -0.283644  2.025340 -0.455358
 C -0.283644 -1.303565  0.490272
 C  0.283644 -2.025340 -0.455358
 H  0.978012  1.637630  1.254866
 H -0.092267  3.092526 -0.560488
 H -0.970193  1.586561 -1.174493
 H  0.000000  0.000000  0.541267
 H -0.978012 -1.637630  1.254866
 H  0.092267 -3.092526 -0.560488
 H  0.970193 -1.586561 -1.174493
ImagFreq  1582i
Internal rotation:
cos  -0.13   1.60   0.33
sin   0.21   0.40  -0.22
barrier   2.36
symmetry     1
Im,red  22.71
freq  39.2 (from rotation
profile)

51  allyl/vinyl
 C -2.005790  0.417297 -0.082683
 C -2.163307 -0.881269  0.037753
 C  0.631310  1.178890 -0.088677
 C  1.423294  0.063825  0.457067
 C  2.119917 -0.817729 -0.270252
 H  2.172793 -0.744719 -1.352310
 H  2.664139 -1.632418  0.193244
 H  1.403896 -0.055949  1.538810
 H  0.834825  1.398769 -1.137858
 H  0.658596  2.086473  0.517373
 H -0.567866  0.873828 -0.069587
 H -2.738218  1.210170 -0.189259
 H -3.148525 -1.350174  0.045594
 H -1.312180 -1.552063  0.134743
ImagFreq  1190i
Internal rotation:
cos   1.17   1.85   0.76
barrier   2.91
symmetry     1
Im,red  33.23
freq  50.0 (from rotation
profile)

52  vinyl/3-methylbut-1-yn-3-yl
 C  1.015722  2.280419 -0.000001
 C  0.866709  1.084095  0.000000
 C  0.664385 -0.346585  0.000000
 C  1.158097 -1.025370  1.281295
 C  1.158111 -1.025373 -1.281288
 H  1.158120  3.333019 -0.000001
 H -0.548858 -0.508195 -0.000006
 H  0.879411 -2.082764 -1.281094
 H  2.248364 -0.960451 -1.358309
 H  0.727079 -0.554611 -2.166791
 H  0.879396 -2.082761  1.281101
 H  2.248349 -0.960448  1.358328
 H  0.727055 -0.554605  2.166791
 C -2.076606 -0.692515 -0.000007
 C -2.753945  0.432469 -0.000001
 H -2.412857 -1.723637 -0.000010
 H -3.845280  0.452351  0.000001
 H -2.255611  1.399260  0.000002
ImagFreq  933i
Internal rotation:
cos   1.48   1.72   0.85
barrier   2.93
symmetry     1
Im,red  47.68
freq  40.1 (from rotation
profile)

53  vinyl/ethyl
 C -1.353761 -0.426447  0.393781
 C -2.247833  0.178666 -0.361083
 C  1.146318  0.587426  0.390835
 C  2.046885 -0.360243 -0.373284
 H  1.399017  0.701152  1.446329
 H  1.010638  1.561991 -0.081205
 H -0.046105  0.094023  0.414130
 H -1.496451 -1.296759  1.027066
 H -3.281078 -0.162925 -0.425216
 H -1.998039  1.051796 -0.959421
 H  3.073687  0.021311 -0.428115
 H  2.091615 -1.343237  0.104220
 H  1.697065 -0.503761 -1.399276
ImagFreq  1511i
Internal rotation:
cos   0.05   0.22   0.22
sin  -0.07   0.08  -0.08 F
barrier   0.45
symmetry     1
Im,red  30.31
freq  23.6  (from HO analysis)

54  vinyl/iso-propyl
 C  0.261272 -0.910679  0.000000
 H  1.355364 -0.899262  0.000000
 H -0.019352  0.327470  0.000000
 C -0.304163  1.743118  0.000000
 C  0.719427  2.571822  0.000000
 H -1.362128  1.987515  0.000000
 H  1.747413  2.216124  0.000000
 H  0.591673  3.654879  0.000000
 C -0.304163 -1.487589  1.284170
 C -0.304163 -1.487589 -1.284170
 H  0.102118 -0.982897  2.164632
 H  0.102118 -0.982897 -2.164632
 H -0.068749 -2.555626  1.376008
 H -0.068749 -2.555626 -1.376008
 H -1.394479 -1.392093  1.315008
 H -1.394479 -1.392093 -1.315008
ImagFreq  1378i
Internal rotation:
```

```
cos   0.21   0.21   0.28 F
barrier   0.52
symmetry     1
Im,red  40.83
freq   8.8  (from HO analysis)

55  allyl/buta-1,3-dien-2-yl
 C  0.607250  1.899843  0.042735
 C  1.052404  0.653344  0.014459
 C  2.391912  0.120838 -0.041727
 C  2.713227 -1.176353 -0.095484
 C -1.051086 -1.103877  0.072887
 C -2.250273 -0.341969  0.451040
 C -3.183434  0.104328 -0.399906
 H  1.289013  2.752054  0.020876
 H -0.453672  2.127588  0.084854
 H -0.062865 -0.333335  0.059654
 H -1.078467 -1.511221 -0.938830
 H -0.752094 -1.860644  0.800073
 H -2.356076 -0.104756  1.508073
 H -4.033845  0.682391 -0.057520
 H -3.127108 -0.103493 -1.464104
 H  3.194417  0.863428 -0.039114
 H  3.746538 -1.498594 -0.136960
 H  1.954156 -1.950339 -0.101025
ImagFreq  1332i
Internal rotation:
cos   0.48   3.21   0.64
barrier   3.96
symmetry     1
Im,red  120.39
freq  27.7  (from HO analysis)
```

Validation set reactions of Tables 7-8

```
8  methyl/prop-1-en-1-yl
 C -2.293088 -0.085606  0.000000
 C -0.802760 -0.315330  0.000000
 C  0.121399  0.627112  0.000000
 H -2.536599  0.978797  0.000000
 H -2.756672 -0.544344  0.880235
 H -2.756642 -0.544642 -0.880135
 H -0.487901 -1.359756  0.000000
 H  1.437069  0.240874  0.000000
 H -0.024657  1.703629  0.000000
 C  2.682232 -0.172465  0.000000
 H  3.125200  0.231082 -0.908203
 H  3.125122  0.231467  0.908152
 H  2.628382 -1.259371  0.000000
ImagFreq  1573i
Internal rotation:
cos  -0.00  -0.00   0.21 F
barrier   0.21
symmetry     3
Im,red   9.29
freq  24.0  (from HO analysis)

9  methyl/prop-1-yl
 C  2.280005 -0.469461 -0.085640
 C  0.085857  1.070183  0.301033
 C -1.091405  0.438627 -0.413461
 C -1.510590 -0.913240  0.173839
 H -0.018070  1.120224  1.387119
 H  0.403113  2.030717 -0.107931
 H  1.154250  0.304585  0.124602
 H -0.853385  0.320768 -1.477367
 H -1.948376  1.126590 -0.377559
 H -2.370660 -1.328784 -0.358095
 H -0.696333 -1.640774  0.112673
 H -1.787055 -0.813691  1.228150
 H  3.111806  0.225409  0.004812
 H  2.259373 -1.224948  0.696350
 H  2.162140 -0.876742 -1.087379
ImagFreq  1634i
Internal rotation:
cos   0.00   0.00   0.27
sin   0.00   0.00   0.07 F
barrier   0.31
symmetry     3
Im,red  11.00
freq  43.6  (from HO analysis)

10  methyl/cis-but-2-en-1-yl
 C -2.928698 -0.818077 -0.009519
 C -0.922702  1.050486 -0.068383
 C  0.350485  0.481789  0.395730
 C  1.344170  0.055559 -0.397053
 H  1.232410  0.164087 -1.475549
 C  2.624839 -0.561535  0.078775
 H  0.468413  0.370024  1.473425
 H -0.924346  1.353002 -1.116850
 H -1.326619  1.838904  0.569116
 H -1.832771  0.173728 -0.016152
 H -3.768682 -0.292394 -0.454345
 H -3.042890 -1.051791  1.045180
 H -2.519108 -1.622701 -0.613178
 H  2.658335 -0.625854  1.169141
 H  2.752241 -1.573411 -0.324064
 H  3.494453  0.017075 -0.254034
ImagFreq  1466i
Internal rotation:
cos  -0.00  -0.00   0.27 F
barrier   0.27
symmetry     3
Im,red  11.59
freq  36.2  (from HO analysis)

11  methyl/trans-but-2-en-1-yl
 C -2.624836 -0.561536  0.078777
 C -1.344167  0.055555 -0.397054
 C -0.350485  0.481796  0.395728
 C  0.922703  1.050489 -0.068386
 H -0.468416  0.370042  1.473424
 H -1.232404  0.164070 -1.475551
 H  0.924349  1.353002 -1.116854
 H -2.658332 -0.625848  1.169143
 H  1.832769  0.173729 -0.016152
 H -2.752239 -1.573414 -0.324056
 H  1.326620  1.838908  0.569111
 H -3.494450  0.017073 -0.254035
 C  2.928693 -0.818081 -0.009515
 H  3.768702 -0.292377 -0.454269
 H  3.042827 -1.051852  1.045177
 H  2.519132 -1.622671 -0.613239
ImagFreq  1466i
Internal rotation:
cos  -0.00  -0.00   0.28 F
```

```
barrier   0.29
symmetry     3
Im,red  11.30
freq  36.2  (from HO analysis)

12  methyl/2-methylprop-2-en-1-
yl
 C  1.187607  1.340853 -0.065576
 C  0.836345 -0.115963  0.114994
 C -0.347778 -0.405039  0.946987
 C  1.536202 -1.089046 -0.488691
 H  1.406983  1.812001  0.898887
 H  0.347267  1.892438 -0.502099
 H  2.054970  1.470781 -0.715035
 H -0.467635  0.251287  1.811281
 H -0.462885 -1.452889  1.223780
 H -1.399800 -0.155472  0.274923
 H  2.387758 -0.867218 -1.122345
 H  1.279540 -2.134991 -0.359309
 C -2.642251  0.076328 -0.462815
 H -2.763367  1.155777 -0.448533
 H -3.387724 -0.470461  0.107496
 H -2.415863 -0.344055 -1.438442
ImagFreq  1498i
Internal rotation:
cos   0.01   0.01   0.24
sin  -0.00   0.00   0.04 F
barrier   0.26
symmetry     3
Im,red  11.37
freq  38.3  (from HO analysis)

13  methyl/but-1-yl
 C  0.068702 -1.257633  0.000000
 C  0.000000  0.255161  0.000000
 C  1.381975  0.933986  0.000000
 C  1.297777  2.463577  0.000000
 H -0.561951  0.598888  0.877314
 H -0.561951  0.598888 -0.877314
 H -1.166790 -1.734447  0.000000
 H  0.509120 -1.691829 -0.899824
 H  0.509120 -1.691829  0.899824
 H  1.947596  0.596555  0.876328
 H  1.947596  0.596555 -0.876328
 H  2.292409  2.917927  0.000000
 H  0.764901  2.830097 -0.882996
 H  0.764901  2.830097  0.882996
 C -2.460728 -2.214072  0.000000
 H -2.355965 -3.296576  0.000000
 H -2.907667 -1.820218  0.909969
 H -2.907667 -1.820218 -0.909969
ImagFreq  1627i
Internal rotation:
cos  -0.01  -0.01   0.26 F
barrier   0.27
symmetry     3
Im,red  11.15
freq  37.7  (from HO analysis)

14  methyl/but-2-yl
 C  2.055223  0.563215 -0.121276
 C  1.073014 -0.507745  0.363141
 C -0.241407 -0.526919 -0.396506
 C -1.234553 -1.589117  0.031376
 H  0.870284 -0.367268  1.432627
 H  1.547704 -1.497169  0.280521
 H  2.991398  0.527140  0.442291
 H  2.298507  0.423633 -1.179124
 H  1.636152  1.566766 -0.007364
 H -0.823643  0.622160 -0.176291
 H -0.092388 -0.506137 -1.480897
 H -2.175760 -1.506000 -0.518963
 H -0.839379 -2.598094 -0.144200
 H -1.462792 -1.511882  1.099521
 C -1.495816  1.833230  0.092676
 H -2.547643  1.596228 -0.048445
 H -1.236159  2.076025  1.120455
 H -1.105049  2.538608 -0.636599
ImagFreq  1576i
Internal rotation:
cos  -0.01  -0.01   0.24 F
barrier   0.29
symmetry     3
Im,red  11.45
freq  37.8  (from HO analysis)

15  methyl/isobutyl
 C -2.825874 -0.016231 -0.178807
 C -0.329326 -0.873752  0.420186
 C  0.690013 -0.011472 -0.303622
 C  0.638922  1.446001  0.175180
 C  2.109827 -0.589433 -0.148766
 H  0.445800 -0.025880 -1.374404
 H  2.839506  0.010965 -0.701815
 H  2.413041 -0.599731  0.903347
 H  2.164836 -1.615446 -0.522897
 H -1.550727 -0.436933  0.135377
 H -0.357093 -1.913665  0.089060
 H -0.277936 -0.809637  1.510083
 H -0.354687  1.878858  0.033197
 H  0.882850  1.511845  1.241257
 H  1.357198  2.066197 -0.368854
 H -2.760598  0.356522 -1.198651
 H -3.441001 -0.907980 -0.082116
 H -3.062561  0.754204  0.551386
ImagFreq  1635i
Internal rotation:
cos   0.00   0.00   0.34
sin  -0.00   0.00   0.07 F
barrier   0.37
symmetry     3
Im,red  11.10
freq  46.2  (from HO analysis)

16  methyl/neopentyl
 C  2.938884  0.000000  0.015102
 C  0.443768 -0.000498  1.071773
 C -0.646295  0.000000  0.005255
 C -0.527822 -1.259233 -0.873729
 C -0.527769  1.260018 -0.872624
 C -2.025623 -0.000303  0.704344
 H -2.147442 -0.885199  1.335813
 H -2.147415  0.884107  1.336586
 H -2.834004  0.000000 -0.034996
 H -0.605971 -2.168632 -0.269860
 H -1.323769 -1.286761 -1.624209
 H  0.430408 -1.286168 -1.399347
 H  0.430470  1.287380 -1.398203
```

```
 H -1.323703  1.288234 -1.623092
 H -0.605896  2.168889 -0.267957
 H  0.462238 -0.900868  1.689999
 H  1.652698 -0.000249  0.510410
 H  0.462270  0.899368  1.690788
 H  3.025616  0.910185 -0.573859
 H  3.568226 -0.000749  0.902387
 H  3.025423 -0.909410 -0.575187
ImagFreq  1648i
Internal rotation:
cos  -0.00  -0.00   0.21 F
barrier   0.22
symmetry     3
Im,red  11.33
freq  10.2  (from HO analysis)

17  methyl/2,3-dimethylbut-2-en-
1-yl
 C -0.034274  1.997205  0.040533
 C -0.082681  0.514656  0.347258
 C  1.146116  0.024898  1.011300
 C -1.119267 -0.289594  0.009034
 C -1.130943 -1.780240  0.253710
 C -2.391785  0.190682 -0.646504
 H -0.848842  2.346317 -0.590853
 H -0.046421  2.586374  0.965047
 H  0.903608  2.240540 -0.471282
 H -2.478797  1.273598 -0.707893
 H -2.482909 -0.212670 -1.663348
 H -3.262825 -0.178667 -0.092064
 H  1.059847 -0.907543  1.564446
 H  2.036409 -0.224636  0.146626
 H  1.634445  0.784028  1.625627
 H -0.182447 -2.176845  0.610192
 H -1.381627 -2.311053 -0.672486
 H -1.906844 -2.049813  0.981554
 C  3.120571 -0.549534 -0.810078
 H  3.905629 -0.967158 -0.186065
 H  2.642683 -1.259414 -1.479099
 H  3.361660  0.408501 -1.261916
ImagFreq  1457i
Internal rotation:
cos   0.00   0.00   0.19 F
barrier   0.19
symmetry     3
Im,red  11.89
freq  27.8  (from HO analysis)

18  methyl/2,2,3,3-
tetramethylbut-1-yl
 C -1.146067 -0.931292 -0.285814
 C -0.240808  0.265768  0.003186
 C -0.638851  0.852934  1.377102
 C  1.299141 -0.176649 -0.004964
 C  1.640797 -0.986084 -1.274867
 C -0.512067  1.345586 -1.068566
 C  2.235694  1.050684  0.035909
 C  1.630681 -1.060913  1.216874
 H -2.421658 -0.586365 -0.142194
 H -1.122830 -1.287972 -1.315774
 H -1.058020 -1.760111  0.417798
 H  3.272826  0.717192  0.138754
 H  2.174847  1.643937 -0.878839
 H  2.021581  1.707923  0.882025
 H  0.028085  1.660647  1.687923
 H -1.648975  1.266613  1.324732
 H -0.638623  0.093218  2.161640
 H  0.001118  2.282264 -0.841105
 H -0.203836  1.024749 -2.066715
 H -1.582111  1.562965 -1.112429
 H  2.655133 -1.435891  1.133065
 H  1.564037 -0.506487  2.155479
 H  0.971501 -1.929496  1.288597
 H  2.714942 -1.192644 -1.302852
 H  1.121756 -1.946712 -1.296832
 H  1.389946 -0.445364 -2.190740
 C -3.779168 -0.350791 -0.012440
 H -4.244792 -1.158879 -0.572266
 H -3.974809 -0.396201  1.056388
 H -3.956229  0.631152 -0.445179
ImagFreq  1656i
Internal rotation:
cos   0.04   0.04   0.40
sin  -0.00   0.00   0.07 F
barrier   0.46
symmetry     3
Im,red  11.56
freq  33.1  (from HO analysis)

19  ethyl/iso-propyl
 C  1.520735 -0.596627  0.483185
 C -0.958245  0.060121 -0.415301
 C -1.302749  1.388560  0.225631
 C -1.858635 -1.101573 -0.049443
 H  1.459206 -0.372726  1.548765
 H  1.568320 -1.671350  0.304287
 H  0.260966 -0.265162  0.021421
 C  2.531503  0.223524 -0.285294
 H -0.795795  0.142997 -1.493464
 H -2.294664  1.740674 -0.088914
 H -1.321563  1.308637  1.317854
 H -0.581804  2.166403 -0.041280
 H -2.890451 -0.931087 -0.385287
 H -1.517638 -2.035984 -0.504119
 H -1.893565 -1.249639  1.035275
 H  3.560091 -0.003539  0.024245
 H  2.470842  0.030618 -1.360713
 H  2.380406  1.296128 -0.130733
ImagFreq  1668i
Internal rotation:
cos   0.52   0.02   0.26
sin  -0.23  -0.12   0.22 F
barrier   0.94
symmetry     1
Im,red  60.58
freq  25.3  (from HO analysis)

20  ethyl/but-1-en-3-yl
 C -1.824237 -0.650996 -0.325807
 C  0.773858 -0.466620  0.489699
 C  1.250957  0.832882  0.121683
 C  1.616660  1.929795 -0.224523
 C  1.484763 -1.653127 -0.154374
 H  1.953228  2.893838 -0.516356
 H -0.457358 -0.543270  0.102712
 H  0.672387 -0.573498  1.572982
 H  1.486526 -1.562131 -1.243009
 H  2.526095 -1.717429  0.176223
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 H  0.986516 -2.588866  0.112210
 C -2.508483  0.607881  0.138587
 H -1.695993 -0.754847 -1.402643
 H -2.147339 -1.577534  0.147795
 H -3.555280  0.640850 -0.193107
 H -2.514876  0.684699  1.229647
 H -2.015010  1.499292 -0.258046
ImagFreq  1578i
Internal rotation:
cos   1.81  -0.33   0.63
sin   0.48   0.15  -0.10
barrier   2.47
symmetry     1
Im,red  67.57
freq  19.9  (from HO analysis)

21  ethyl/cyclohex-1-en-3-yl
 C -1.377915  1.429505 -0.023776
 C -2.181387  0.377687 -0.744442
 C -1.479627 -0.989364 -0.746734
 C -0.892333 -1.321998  0.632398
 C  0.082939 -0.240868  1.084657
 C -0.361342  1.135559  0.804022
 C  2.422270 -0.732551 -0.273074
 C  3.064869  0.610120 -0.501581
 H -1.661172  2.467212 -0.177423
 H  0.175804  1.945697  1.290624
 H -2.378412  0.700005 -1.773586
 H  0.430697 -0.375967  2.112249
 H -3.171039  0.292882 -0.271960
 H  1.170559 -0.450408  0.444278
 H -2.175633 -1.771254 -1.065300
 H -0.395811 -2.297853  0.610509
 H -0.667597 -0.970954 -1.482483
 H -1.707905 -1.404575  1.363796
 H  2.935360 -1.400771  0.417280
 H  2.062172 -1.247023 -1.162937
 H  3.998841  0.522722 -1.073723
 H  2.405512  1.278603 -1.063152
 H  3.313785  1.103142  0.443011
ImagFreq  1531i
Internal rotation:
cos   1.91   0.46  -0.01
sin   0.41  -0.44   0.09
barrier   2.66
symmetry     1
Im,red  81.56
freq  68.5  (from HO analysis)

22  isobutyl/allyl
 C  0.886169 -1.067284  0.427073
 C  1.601309  0.058589 -0.287599
 C  1.132563  1.434521  0.206248
 C  3.130845 -0.084515 -0.143750
 C -1.730775 -1.153968 -0.359327
 C -2.592114 -0.190304  0.331212
 C -3.025420  0.971975 -0.177565
 H -2.787470  1.270848 -1.194059
 H -3.638896  1.651937  0.401804
 H -2.867760 -0.438866  1.354871
 H -1.638556 -0.992679 -1.434383
 H -1.939221 -2.199505 -0.128320
 H -0.510341 -1.048055  0.056180
 H  1.165039 -2.074389  0.115241
 H  0.822807 -0.971633  1.512577
 H  1.369495 -0.017389 -1.358961
 H  3.648689  0.708208 -0.693705
 H  3.430447 -0.015278  0.906969
 H  3.479658 -1.046314 -0.529594
 H  1.629576  2.239716 -0.342613
 H  0.053546  1.557157  0.087548
 H  1.367525  1.562158  1.268688
ImagFreq  1615i
Internal rotation:
cos   0.87   0.26   0.61
sin   0.45   0.02  -0.28
barrier   1.77
symmetry     1
Im,red  113.74
freq  19.4  (from HO analysis)

23  penta-1,4-dien-3-yl/allyl
 C -1.230612 -1.074677  0.839947
 C  0.972091  0.205416 -0.178120
 C  2.136060 -0.603043  0.216478
 C  2.658010 -1.608275 -0.496373
 C  0.897275  1.592854  0.303530
 C  0.246531  2.589754 -0.308475
 H -0.067054 -0.378397  0.362771
 H  0.690939  0.090284 -1.227447
 H -0.986661 -1.036952  1.899197
 C -2.391541 -0.347856  0.399811
 H -1.040611 -2.041393  0.377074
 H  1.383297  1.794169  1.257352
 H  2.573268 -0.368299  1.186106
 H -0.253332  2.443230 -1.260526
 H  2.263980 -1.878907 -1.471134
 H  0.202916  3.583712  0.120850
 H  3.500248 -2.183958 -0.131511
 C -3.088294 -0.602929 -0.730396
 H -2.697948  0.498237  1.011151
 H -3.935918  0.004759 -1.022791
 H -2.830245 -1.433951 -1.379504
ImagFreq  1679i
Internal rotation:
cos  -0.11   1.51   0.62
barrier   1.99
symmetry     1
Im,red  169.78
freq  31.4  (from HO analysis)

24  penta-1,4-diyn-3-yl/tert-
butyl
 C -1.499558 -0.000014  0.047953
 C  1.142839  0.000001 -0.692993
 C  1.705401  1.225547 -0.188438
 C  2.122848  2.270176  0.242164
 C  1.705444 -1.225527 -0.188440
 C  2.122924 -2.270143  0.242160
 H  1.056420  0.000000 -1.783216
 H -0.111431 -0.000025 -0.346433
 C -1.384914  0.000022  1.554437
 C -2.026423  1.278362 -0.562191
 C -2.026432 -1.278413 -0.562132
 H  2.515633  3.182858  0.617335
 H  2.515735 -3.182813  0.617332
 H -2.382601  0.000041  2.018829
 H -0.855765 -0.885726  1.915919
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 H -0.855750  0.885777  1.915877
 H -3.086784 -1.421448 -0.304909
 H -1.959136 -1.263896 -1.654015
 H -1.481606 -2.152806 -0.196350
 H -3.086771  1.421420 -0.304967
 H -1.481585  2.152767 -0.196456
 H -1.959136  1.263790 -1.654074
ImagFreq  1504i
Internal rotation:
cos   0.04   0.04   2.18
barrier   2.22
symmetry     3
Im,red  261.16
freq  18.4  (from HO analysis)

25  tert-butyl/penta-1,4-dien-3-
yl
 C -1.489711  0.547692  0.000000
 C  1.017563 -0.625765  0.000000
 C  1.675044 -0.214092  1.257633
 C  1.675044 -0.908106  2.401068
 C  1.675044 -0.214092 -1.257633
 C  1.675044 -0.908106 -2.401068
 H -0.125760 -0.060127  0.000000
 H  0.722896 -1.678607  0.000000
 C -1.155685  2.019932  0.000000
 C -2.101985  0.024167 -1.276922
 C -2.101985  0.024167  1.276922
 H  2.176018  0.753136 -1.235828
 H  2.176018  0.753136  1.235828
 H  1.198860 -1.880877 -2.476544
 H  1.198860 -1.880877  2.476544
 H  2.157725 -0.528832 -3.294067
 H  2.157725 -0.528832  3.294067
 H -2.071683  2.630561  0.000000
 H -0.580849  2.302391  0.887177
 H -0.580849  2.302391 -0.887177
 H -3.115107  0.431805  1.420317
 H -2.193556 -1.066020  1.263254
 H -1.510942  0.305089  2.152657
 H -3.115107  0.431805 -1.420317
 H -1.510942  0.305089 -2.152657
 H -2.193556 -1.066020 -1.263254
ImagFreq  1444i
Internal rotation:
cos  -0.01  -0.01   1.13
barrier   1.13
symmetry     3
Im,red  273.43
freq  20.3  (from HO analysis)

26  but-2-yl/cis-but-2-en-2-yl
 C  1.476345 -0.358191 -0.613508
 C -1.109215 -0.260668  0.201531
 C -1.903293  0.347586 -0.665982
 C -3.396055  0.545132 -0.554947
 H -3.805760  0.122182  0.363872
 H -3.912733  0.078325 -1.400944
 H -3.649352  1.610841 -0.578242
 H -1.451682  0.758676 -1.569839
 H  0.239354 -0.296226 -0.203584
 C -1.364227 -0.927563  1.507828
 C  2.301448  0.501521  0.327745
 C  1.838259 -1.829946 -0.653567
 H  1.406006  0.078742 -1.614998
 H -2.422944 -0.899286  1.792300
 H -1.057148 -1.978704  1.479586
 H -0.792869 -0.451360  2.312116
 H  2.853670 -1.981314 -1.042798
 H  1.807264 -2.275837  0.346255
 H  1.153882 -2.393890 -1.293189
 H  3.366429  0.395208  0.070535
 C  1.921498  1.985299  0.302703
 H  2.207161  0.112013  1.349761
 H  2.533763  2.564438  0.999309
 H  2.064023  2.409461 -0.696186
 H  0.872372  2.127707  0.575234
ImagFreq  1562i
Internal rotation:
cos   0.02   3.37   0.43
barrier   3.94
symmetry     1
Im,red  198.54
freq  16.6  (from HO analysis)
```