Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplementary information

Ab-initio derived group additivity model for intramolecular hydrogen abstraction reactions

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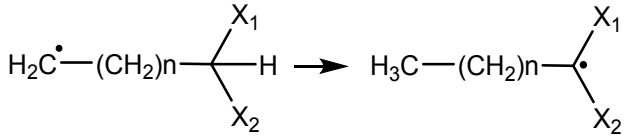
Submitted to Physical Chemistry Chemical Physics

Contents

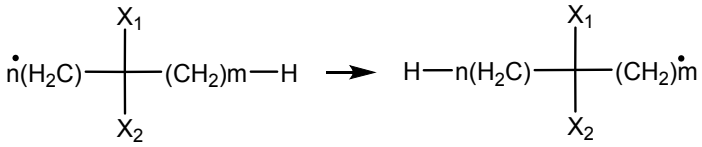
Training reactions

Table S-1: Arrhenius parameters for the reactions used to deduce primary ΔGAV°'s at 1000K regressed from the rate coefficients between 800 and 1200K. Per reaction, the first line corresponds to the forward direction, the second line to the reverse. The pre-exponential factors are expressed in s^{-1} and E_a is expressed in kJ mol^{-1}. All pre-exponential factors include tunneling and the number of single events. The letter n corresponds to the number of CH_2 groups between the radical site and the attacked carbon atom. For a 1-2 shift, n is 0, for a 1-3 shift, n is 1, and so on.



		1-2	(n=0)	1-3	(n=1)	1-4	(n=2)	1-5	(n=3)	1-6	(n=4)	1-7	(n=5)
X_1	X_2	logA	Ea	logA	Ea	logA	Ea	logA	Ea	logA	Ea	logA	Ea
H	H	13.4	177.3	12.7	176.2	11.4	106.0	10.5	73.1	10.0	69.3	8.8	76.0
		13.4	177.3	12.7	176.2	11.4	106.0	10.5	73.1	10.0	69.3	8.8	76.0
H	CH_3	13.6	167.4	13.0	166.4	11.7	93.7	10.8	62.8	9.8	57.1	8.6	63.5
		13.9	183.6	13.1	181.8	11.8	110.7	10.8	78.8	10.1	74.1	9.0	80.3
H	C_2H_3	13.4	135.6	12.9	144.0	11.1	74.9	10.3	46.6	9.7	44.4	8.3	49.4
		14.3	211.0	13.9	217.4	12.4	148.5	11.5	120.1	10.8	117.8	9.2	123.0
H	C_2H	13.5	144.7	13.0	150.9	11.6	77.2	10.7	49.0	9.3	44.5	8.6	51.8
		13.8	206.6	13.2	207.0	11.9	134.0	11.0	104.7	9.5	102.5	8.9	107.0
CH_3	CH_3	13.3	157.2	12.7	157.5	11.5	84.7	10.4	52.1	9.2	47.8	8.3	56.3
		14.1	183.8	13.0	182.5	11.8	111.1	10.6	78.5	9.7	75.0	8.4	81.9
CH_3	C_2H_3	12.9	127.6	12.6	137.8	11.1	66.8	10.0	38.7	8.7	37.2	7.3	44.6
		14.2	215.2	13.8	221.2	12.4	152.1	11.3	123.3	10.5	127.2	9.1	130.6
CH_3	C_2H	13.2	136.0	12.7	143.2	11.3	68.8	10.4	40.5	9.2	34.2	7.9	43.9
		14.0	211.7	12.9	213.2	11.6	140.6	10.8	111.2	9.7	104.9	8.9	117.2
C_2H_3	C_2H_3	12.7	115.0	12.5	126.2	11.1	56.7	10.2	35.1	9.2	33.3	7.5	38.6
		13.9	233.7	13.6	241.3	12.1	175.4	10.8	151.2	10.7	154.6	9.0	155.2
C_2H_3	C_2H	13.0	114.6	12.6	129.0	11.2	56.0	10.2	29.5	9.0	25.3	7.7	32.1
		14.3	234.8	13.8	239.3	12.4	168.5	11.5	140.0	10.4	136.6	9.3	143.4
C_2H	C_2H	13.1	115.3	12.7	130.1	11.3	55.3	10.3	30.8	9.0	26.3	8.2	32.9
		13.8	233.7	12.8	235.3	11.7	161.9	10.7	133.6	9.9	129.9	8.6	136.4

Table S-2: Arrhenius parameters for the reactions used to deduce secondary ΔGAV°'s at 1000K regressed from the rate coefficients between 800 and 1200K. The pre-exponential factors are expressed in s^{-1} and E_a is expressed in kJ mol^{-1}. All pre-exponential factors include tunneling and the number of single events. The two substituents X_1 and X_2 are bonded to a carbon atom located at a distance of n CH_2 groups of the radical site and m CH_2 groups of the attacked carbon atom.



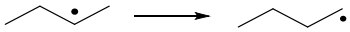
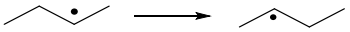
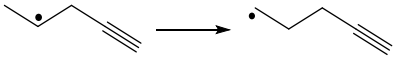
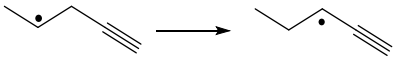
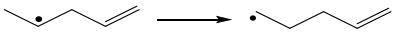
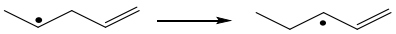
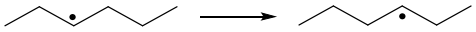
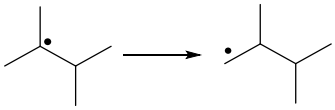
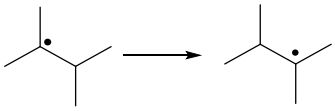
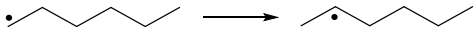
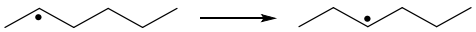
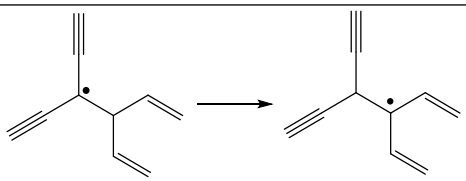
		1-3		1-4				1-5					
		n=1, m=1		n=1, m=2		n=2, m=1		n=1, m=3		n=2, m=2		n=1, m=3	
X_1	X_2	logA	E_a	logA	E_a	logA	E_a	logA	E_a	logA	E_a	logA	E_a
H	CH_3	13.1	174.5	11.7	100.5	12.1	103.9	10.7	67.7	11.1	71.0	10.6	67.3
H	C_2H_3	12.7	172.9	11.7	99.3	11.7	101.7	10.9	68.0	10.9	70.4	10.7	68.9
H	C_2H	12.6	170.5	11.6	97.9	11.8	103.4	10.8	67.2	11.0	73.8	10.6	71.3
CH_3	CH_3	13.3	171.5	11.7	98.0	12.2	102.7	11.1	66.0	11.6	70.1	10.7	66.7
CH_3	C_2H_3	13.0	169.9	11.7	95.3	11.9	100.6	11.0	63.9	11.3	67.6	10.7	65.3
CH_3	C_2H	13.0	169.5	11.7	96.9	12.1	102.7	10.9	63.0	11.3	68.3	10.6	64.2
C_2H_3	C_2H_3	12.9	167.4	11.7	95.2	11.7	104.0	11.0	61.6	11.0	68.2	11.2	62.4
C_2H_3	C_2H	12.9	168.0	11.8	93.9	11.8	101.3	11.0	62.1	11.0	69.4	10.6	68.3
C_2H	C_2H	12.7	167.3	11.7	94.4	11.7	103.2	10.9	64.4	10.8	72.6	10.8	69.2

		1-6								1-7									
		n=1, m=4		n=2, m=3		n=3, m=2		n=4, m=1		n=1, m=5		n=2, m=4		n=3, m=3		n=4, m=2		n=5, m=1	
X_1	X_2	logA	E_a	logA	E_a	logA	E_a	logA	E_a	logA	E_a	logA	E_a	logA	E_a	logA	E_a	logA	E_a
H	CH_3	10.0	65.3	10.0	66.3	10.0	65.9	10.3	68.0	8.8	72.1	8.9	73.7	9.1	72.3	8.7	74.4	8.9	74.1
H	C_2H_3	9.8	64.8	10.3	68.5	10.1	68.2	9.9	67.4	8.8	71.3	8.8	74.7	9.3	74.0	8.9	74.3	8.4	73.6
H	C_2H	9.7	62.8	10.1	67.5	9.9	67.6	9.9	69.0	8.7	71.5	8.9	72.6	9.2	79.2	8.9	74.0	8.8	78.1
CH_3	CH_3	9.8	63.2	10.1	66.7	10.1	65.5	10.4	68.5	9.0	69.2	9.5	74.7	9.3	80.1	8.9	70.4	9.1	76.3
CH_3	C_2H_3	9.9	61.2	10.3	66.5	10.4	65.5	10.3	66.2	9.1	72.5	9.2	69.6	10.0	75.7	9.3	69.1	9.1	76.8
CH_3	C_2H	9.9	61.9	10.2	62.8	10.2	63.8	10.3	67.7	8.9	73.3	9.1	70.8	9.6	77.4	9.0	72.1	9.5	79.9
C_2H_3	C_2H_3	9.9	58.7	10.4	63.3	10.6	64.5	9.8	65.2	9.0	69.9	9.2	65.8	9.9	71.4	9.2	66.3	9.5	74.9
C_2H_3	C_2H	9.9	57.7	10.3	67.0	10.3	65.9	10.0	65.9	8.9	70.3	9.0	75.0	9.8	78.1	9.1	75.1	8.5	78.4
C_2H	C_2H	9.8	60.4	10.1	65.3	10.2	68.3	10.0	72.0	9.1	73.0	9.0	69.7	9.7	77.6	9.1	74.4	9.2	83.5

Test reactions

Table S-3 to Table S-8 report the reactions belonging to the test set. The Arrhenius parameters were regressed between 800 and 1200K. The tables also show the comparison of the initial group additive model to the ab initio rate coefficients at 1000K. For thermo-neutral reactions, i.e. when the reactant and product are identical, the forward and rate coefficients are the same, and is only tabulated once. All pre-exponential factors include tunneling and the number of single events.

Table S-3: Arrhenius parameters for the test reactions for 1-2 H-shifts regressed between 800 and 1200K0and the comparison of the initial group additive model to the *ab initio* rate coefficients at 1000K. The pre-exponential factors are expressed in s^{-1} and E_a is expressed in kJ mol^{-1}. For thermo-neutral reactions, i.e. when the reactant and product are identical, the forward and rate coefficients are the same, and is only tabulated once. In the other case, the first line corresponds to the forward rate coefficient, the second line to the reverse rate coefficient. All pre-exponential factors include tunneling and the number of single events.

Reaction	logA	Ea	k_{GA}/k_{AI}
	13.6	183.1	0.95
	13.6	168.0	1.04
	13.0	173.7	0.74
	13.7	181.9	0.62
	13.8	170.5	0.95
	13.1	149.3	0.83
	13.3	194.1	0.82
	13.7	183.1	0.74
	13.5	168.0	1.24
	13.0	141.7	0.94
	13.8	199.9	1.06
	12.9	173.6	0.87
	13.9	183.8	1.08
	13.3	156.5	0.94
	13.4	180.4	2.30
	13.5	166.4	1.06
	13.6	183.4	0.96
	13.3	173.6	0.82
	13.2	173.0	0.93
	13.0	170.3	0.56
	13.6	171.2	1.02

(Table S-3 continued)

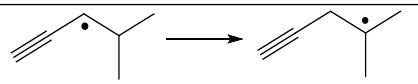
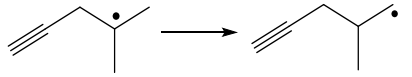
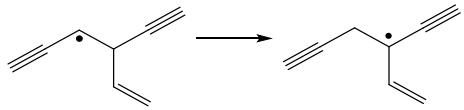
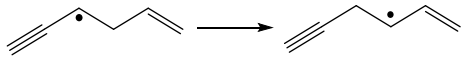
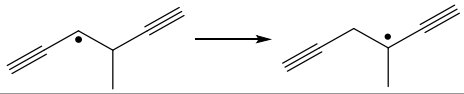
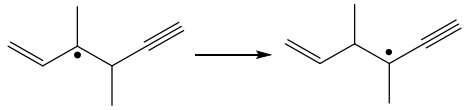
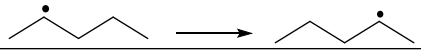
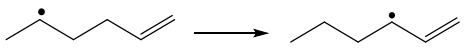
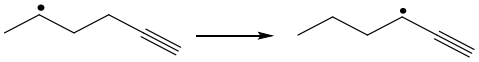
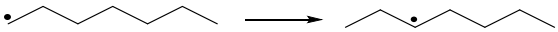
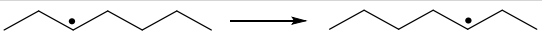
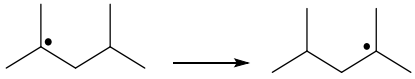
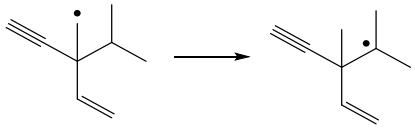
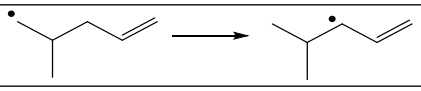
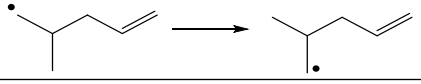
	13.4	185.5	0.77
	13.5	153.0	1.12
	13.9	185.6	1.44
	13.4	160.2	1.12
	13.3	137.9	0.28
	14.1	194.8	0.39
	13.4	159.7	0.64
	13.6	175.3	2.02
	13.4	161.8	0.49
	13.5	173.4	0.41
	13.6	173.7	1.22
	12.8	163.2	1.53

Table S-4: Arrhenius parameters for the test reactions for 1-3 H-shifts regressed between 800 and 1200K0and the comparison of the initial group additive model to the *ab initio* rate coefficients at 1000K. The pre-exponential factors are expressed in s^{-1} and E_a is expressed in kJ mol^{-1}. For thermo-neutral reactions, i.e. when the reactant and product are identical, the forward and rate coefficients are the same, and is only tabulated once. In the other case, the first line corresponds to the forward rate coefficient, the second line to the reverse rate coefficient. All pre-exponential factors include tunneling and the number of single events.

Reaction	logA	Ea	k_{GA}/k_{AI}
	12.5	172.6	1.00
	12.6	146.9	0.94
	13.6	206.1	0.94
	12.8	153.8	0.68
	13.0	195.2	0.61
	12.8	163.9	1.11
	13.0	180.8	1.03
	12.6	170.1	0.54
	13.4	173.5	0.32
	13.0	135.0	0.84
	12.7	207.7	0.97
	12.3	140.4	2.26
	13.4	214.2	3.31
	13.2	171.5	0.55

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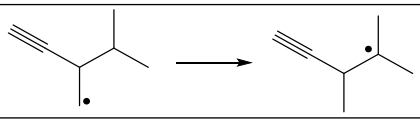
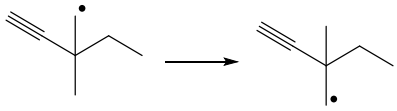
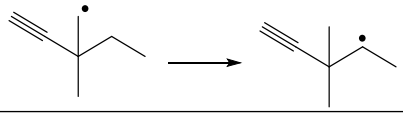
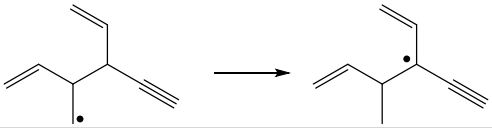
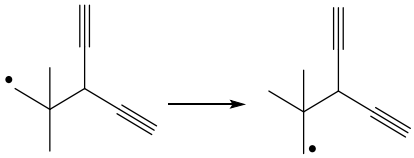
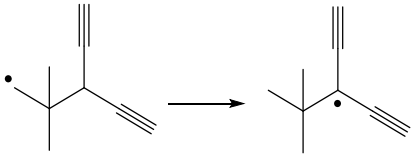
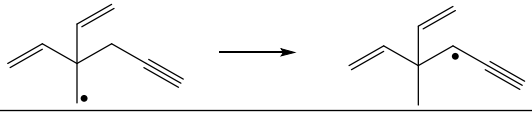
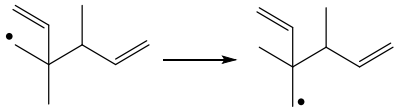
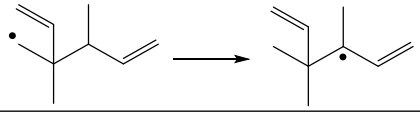
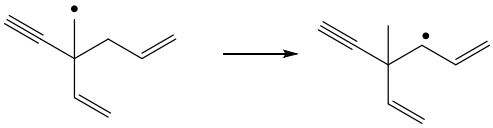
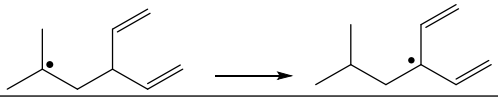
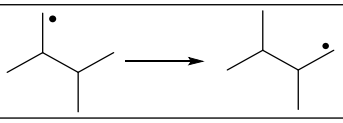
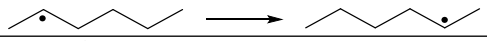
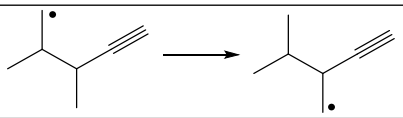
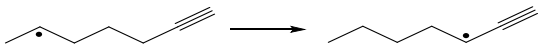
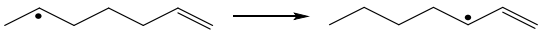
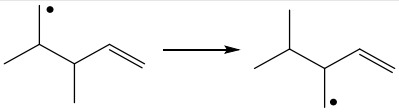
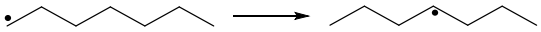
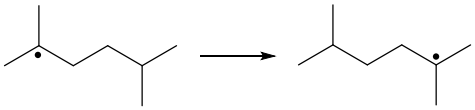
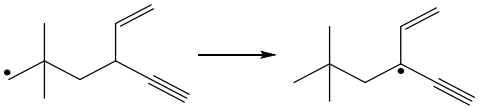
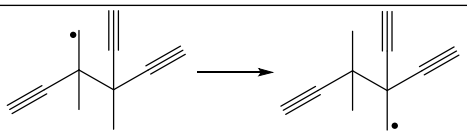
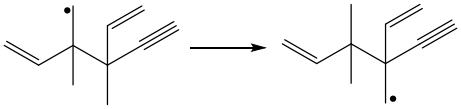
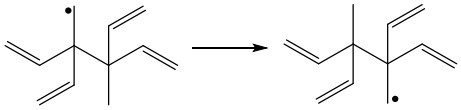
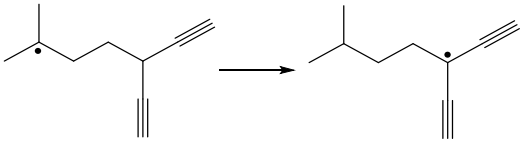
	12.6	150.2	0.87
	12.9	178.4	1.22
	13.0	166.1	0.75
	12.7	155.8	0.61
	13.0	173.1	0.96
	12.6	127.8	1.19
	13.2	237.2	2.42
	13.6	169.0	0.53
	13.4	126.9	0.73
	14.3	231.8	0.64
	13.2	138.5	0.64
	13.4	201.4	1.36
	13.1	164.4	0.38
	12.3	134.9	2.57
	13.7	219.3	2.40
	12.9	137.1	1.39
	13.7	214.0	3.28
	11.8	128.3	3.06
	13.4	222.6	1.65

Table S-5: Arrhenius parameters for the test reactions for 1-4 H-shifts regressed between 800 and 1200K0and the comparison of the initial group additive model to the *ab initio* rate coefficients at 1000K. The pre-exponential factors are expressed in s^{-1} and E_a is expressed in kJ mol^{-1}. For thermo-neutral reactions, i.e. when the reactant and product are identical, the forward and rate coefficients are the same, and is only tabulated once. In the other case, the first line corresponds to the forward rate coefficient, the second line to the reverse rate coefficient. All pre-exponential factors include tunneling and the number of single events.

Reaction	logA	Ea	k_{GA}/k_{AI}
	11.4	97.3	0.93
	11.3	99.4	0.86
	11.9	96.7	0.78
	11.8	94.9	0.66
	11.3	79.2	0.79
	11.5	120.6	0.95
	10.9	77.1	0.67
	12.1	135.1	0.93
	11.8	92.4	0.57
	11.8	92.1	0.48
	11.4	92.2	1.47
	11.9	110.0	1.48
	10.7	92.8	4.81
	11.0	49.2	1.66
	12.5	170.5	4.75
	11.8	91.2	0.60
	12.1	89.6	0.80
	11.7	87.6	0.84
	11.8	87.5	0.71
	11.8	92.7	0.60
	11.4	54.6	0.52
	11.3	132.0	0.97

(Table S-5 continued)

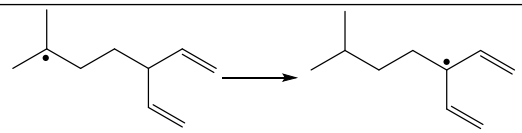
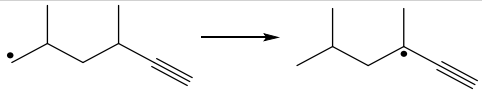
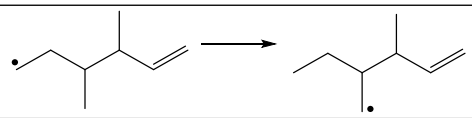
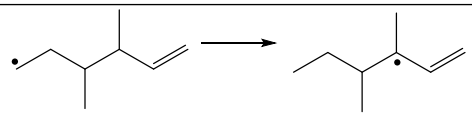
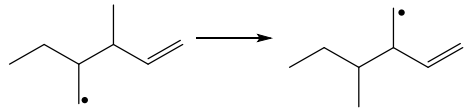
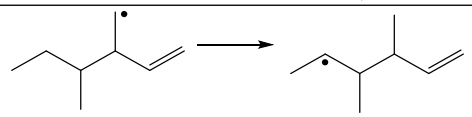
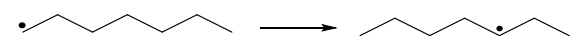
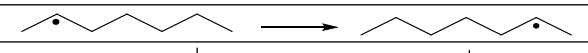
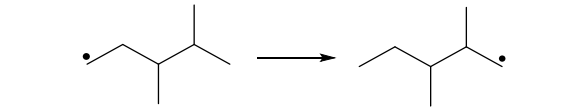
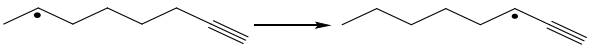
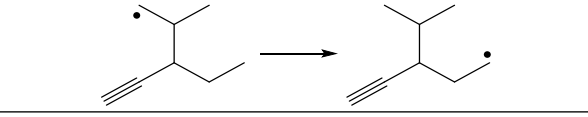
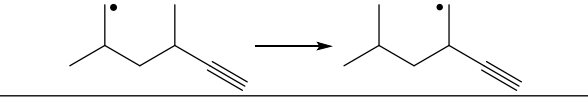
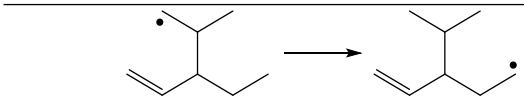
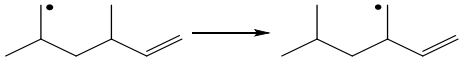
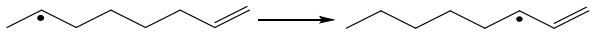
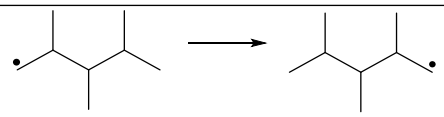
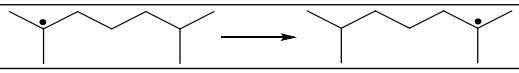
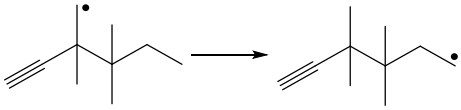
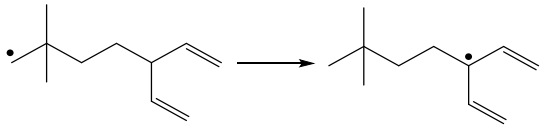
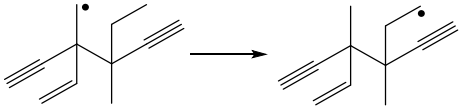
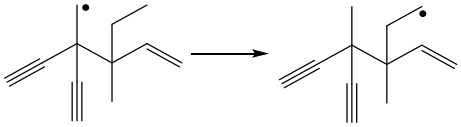
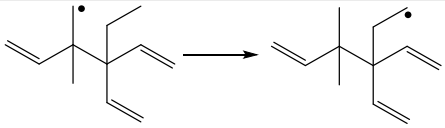
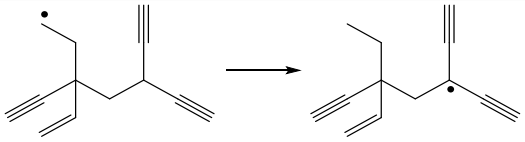
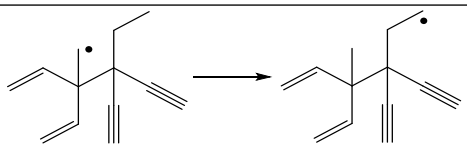
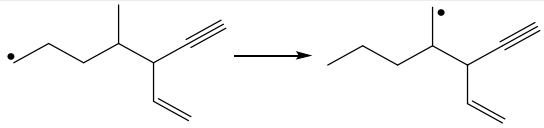
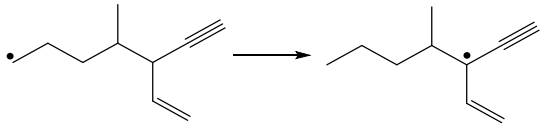
	11.1	55.3	0.45
	11.6	146.9	1.31
	11.4	63.7	0.78
	12.1	139.4	0.75
	12.0	98.9	0.32
	11.9	96.4	0.36
	11.1	59.6	0.49
	12.3	147.0	1.40
	11.8	91.2	0.47
	11.9	90.0	0.29
	12.0	76.8	0.21
	11.9	98.3	0.59

Table S-6: Arrhenius parameters for the test reactions for 1-5 H-shifts regressed between 800 and 1200K0and the comparison of the initial group additive model to the *ab initio* rate coefficients at 1000K. The pre-exponential factors are expressed in s^{-1} and E_a is expressed in kJ mol^{-1}. For thermo-neutral reactions, i.e. when the reactant and product are identical, the forward and rate coefficients are the same, and is only tabulated once. In the other case, the first line corresponds to the forward rate coefficient, the second line to the reverse rate coefficient. All pre-exponential factors include tunneling and the number of single events.

Reaction	logA	Ea	k_{GA}/k_{AI}
	10.7	60.7	1.16
	10.8	77.6	0.77
	10.5	68.0	0.96
	10.9	64.3	1.11
	10.8	65.2	1.36
	10.5	63.4	0.68
	10.2	50.3	0.71
	10.4	89.8	1.04
	10.8	66.6	1.25
	10.8	69.5	1.24
	10.9	67.4	0.59
	10.8	63.7	0.76

(Table S-6 continued)

	11.0	64.0	0.84
	11.1	67.2	0.85
	10.7	64.3	1.19
	10.8	64.1	1.02
	10.2	50.0	0.43
	11.2	106.6	0.66
	10.9	66.9	0.86
	10.2	57.0	1.69
	10.9	57.5	0.79
	11.3	62.8	0.80
	9.8	28.0	2.16
	11.3	149.0	1.19
	11.6	57.1	0.43
	11.6	62.4	0.33
	11.2	52.3	0.36
	11.3	62.6	0.44
	10.9	49.5	1.69
	11.4	66.3	5.82
	10.2	27.0	1.68
	11.4	132.8	0.73
	11.0	59.7	1.31
	10.8	58.0	0.75
	10.9	67.9	0.52
	10.9	67.0	0.68
	10.3	23.1	0.56
	11.5	135.0	0.91

(Table S-6 continued)

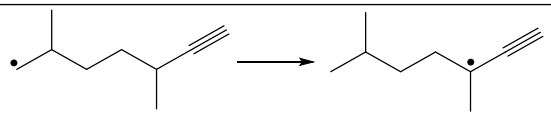
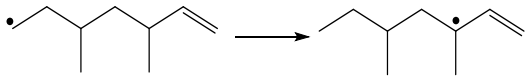
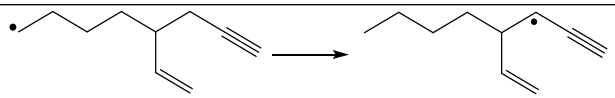
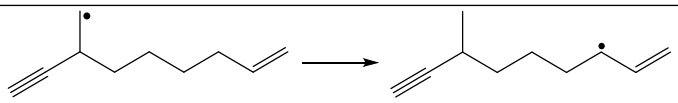
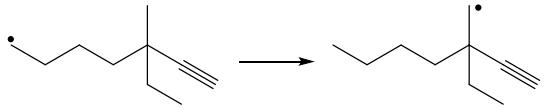
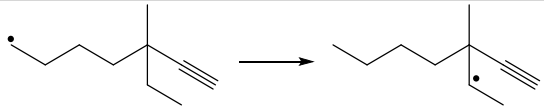
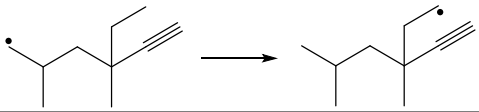
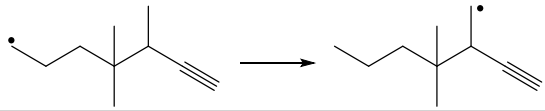
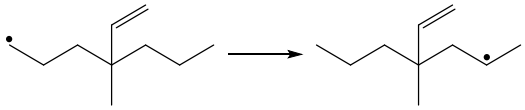
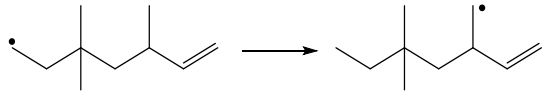
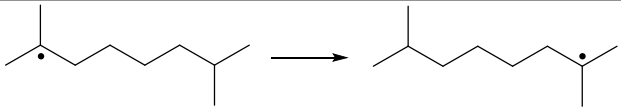
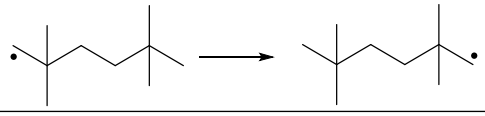
	10.2	36.3	1.52
	11.3	108.7	0.62
	10.0	31.4	1.11
	11.4	119.1	1.07

Table S-7: Arrhenius parameters for the test reactions for 1-6 H-shifts regressed between 800 and 1200K0and the comparison of the initial group additive model to the *ab initio* rate coefficients at 1000K. The pre-exponential factors are expressed in s^{-1} and E_a is expressed in kJ mol^{-1}. For thermo-neutral reactions, i.e. when the reactant and product are identical, the forward and rate coefficients are the same, and is only tabulated once. In the other case, the first line corresponds to the forward rate coefficient, the second line to the reverse rate coefficient. All pre-exponential factors include tunneling and the number of single events.

Reaction	logA	Ea	k_{GA}/k_{AI}
	9.9	42.2	0.20
	9.8	97.3	0.33
	9.5	38.3	0.99
	10.5	118.6	1.63
	10.1	66.3	0.77
	9.9	58.7	0.70
	10.1	59.0	0.83
	10.1	68.3	0.87
	10.1	52.3	0.45
	10.5	58.7	0.79
	10.1	68.0	1.01
	10.3	64.6	0.54
	10.4	52.2	0.47
	10.6	67.6	0.33
	10.0	60.3	0.52
	10.0	55.5	0.44
	8.9	51.8	0.78
	10.6	64.3	0.49

(Table S-7 continued)

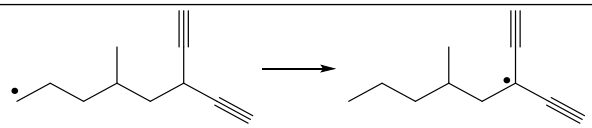
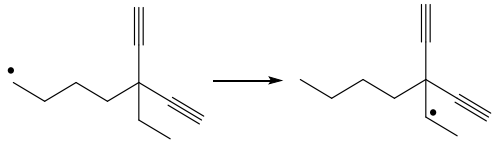
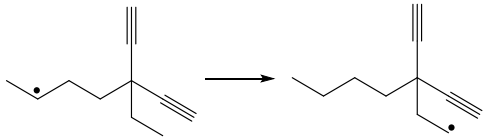
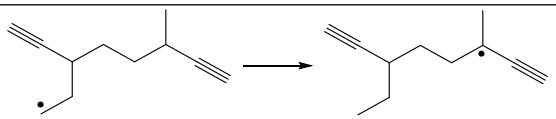
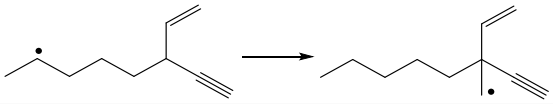
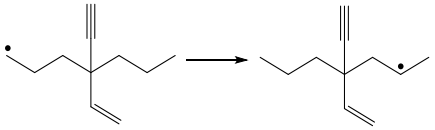
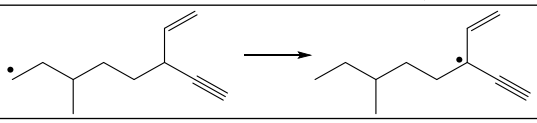
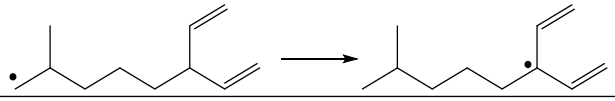
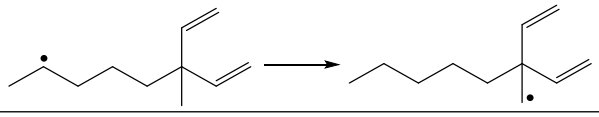
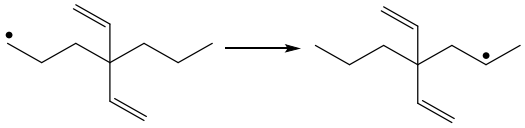
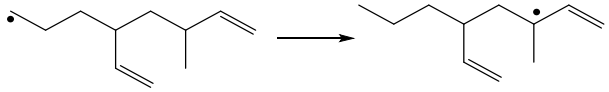
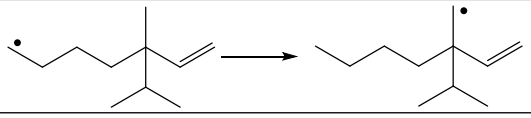
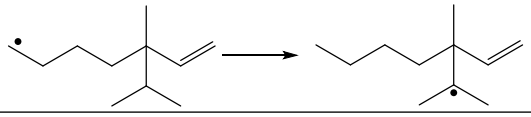
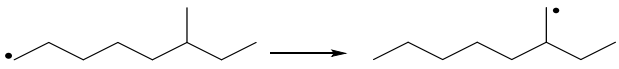
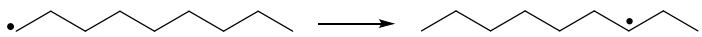
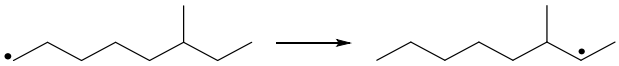
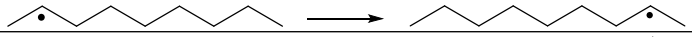
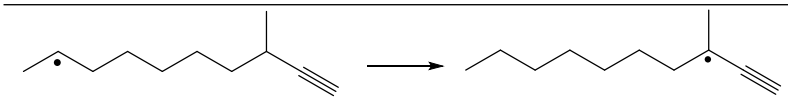
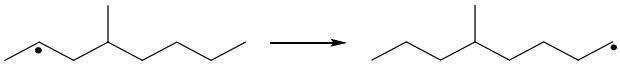
	9.5	19.4	0.21
	10.1	127.3	0.64
	10.0	59.8	0.69
	9.9	66.5	1.01
	10.3	72.9	0.92
	10.1	53.2	0.72
	9.4	38.1	1.41
	10.0	110.8	0.95
	9.9	71.7	1.51
	9.9	47.5	0.88
	10.5	51.8	0.34
	10.3	66.3	0.49
	9.4	23.5	0.43
	10.6	135.0	0.82
	8.6	25.3	2.15
	10.4	144.9	1.16
	9.8	68.3	1.04
	9.7	45.8	1.09
	10.7	50.5	0.38
	10.4	67.3	1.01
	9.3	36.2	0.37
	10.8	121.7	0.43
	10.1	64.3	0.59
	10.0	62.7	0.88
	9.0	47.0	1.99
	9.3	74.0	4.90

Table S-8: Arrhenius parameters for the test reactions for 1-7 H-shifts regressed between 800 and 1200K0and the comparison of the initial group additive model to the *ab initio* rate coefficients at 1000K. The pre-exponential factors are expressed in s^{-1} and E_a is expressed in kJ mol^{-1}. For thermo-neutral reactions, i.e. when the reactant and product are identical, the forward and rate coefficients are the same, and is only tabulated once. In the other case, the first line corresponds to the forward rate coefficient, the second line to the reverse rate coefficient. All pre-exponential factors include tunneling and the number of single events.

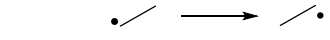
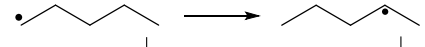
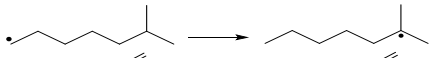
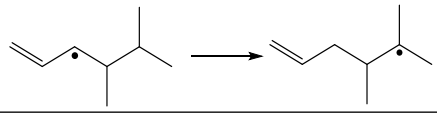
Reaction	logA	Ea	k_{GA}/k_{AI}
	8.9	72.6	0.37
	9.2	70.6	0.34
	8.6	62.5	1.00
	8.4	78.7	3.00
	8.9	74.5	1.19
	8.7	61.8	0.53
	9.3	71.6	0.56
	8.0	42.7	0.72
	7.8	97.1	3.81
	9.4	79.5	0.58
	9.2	65.7	0.30
	7.9	47.0	0.33
	8.4	116.9	3.43

Number of single events

The total rotational symmetry number and number of optical isomers were used to obtain the number of single events. A few typical symmetrical contributions have been tabulated in Table S-9. The six reference reactions all have 6 as number of single events. The reactants have a two-fold and three fold internal symmetry contribution, without any external symmetry, and the transition state has an external symmetry number of 2. The latter assumes that flipping ring structures into another conformer has a very low energy barrier. The reactants and transition states do not exhibit any optical isomerism. However, the reference reactions are all identity reactions, which implies that the number of single events needs to be increased by a factor 2, from the indistinguishability of the forward versus the reverse reaction. This leads to a number of single events of $2 \cdot \frac{6/1}{2/1} = 6$. This is illustrated by the 1-2 H-shift of ethyl (R1) in Table S-9. The value of 6 can be intuitively explained by the three indistinguishable hydrogen atoms of the methyl group and the 2 sides of the planar radical structure that can approach the abstracted hydrogen atom.

When one of the four hydrogen atoms neighboring the reactive atoms is substituted by a larger group, e.g. a methyl group, the two-fold external symmetry of the transition state disappears. Instead, a three-fold internal symmetry arises as a result of the methyl rotation. Furthermore, in the transition state, the reactive atom bonded to the methyl group is chiral. Its four neighbors are different in nature since the hydrogen atom participating in the reaction is further away from the carbon atom compared to the other hydrogen atom. This chiral center leads to a number of optical isomers of 2. R2 in Table S-9 illustrates this for the 1-4 H-shift in 1-pentyl. The value of four comes from two indistinguishable hydrogen atoms that can be abstracted by 2 possible sides of the CH_2 radical group.

Table S-9 : Numbers of single events of selected reactions.

		Reactant		TS		
	Reaction	**σ**	**n_{opt}**	**σ**	**n_{opt}**	**n_e**
R1		6	1	2	1	6
R2		6	1	3	2	4
R3		18	1	9	1	2
R4		18	2	3	2	6
R5		18	2	18	4	2

If another methyl group is added to a reactive atom, the chirality of the transition state disappears again. The transition state still does not contain any external rotational symmetry and the methyl rotor is the only contribution of the transition state to the number of single events. However,

because these methyl rotors are also present in the reactant, this contribution cancels out. Again, the resulting value of 2 can be explained by the number of hydrogen atoms, i.e. one, and the number of ways the planar CH_2 radical group can face the abstracted hydrogen atom, i.e. two.

Substituents on the carbon chain between the two reactive atoms have also an influence on the symmetry numbers and numbers of optical isomers, such as R4 in Table S-9. The optical isomers in the reactant are preserved throughout the reaction leading to a cancelation of its contribution to the number of single events. Since the internal symmetry due to the methyl substituent also cancels out, the only final contribution comes from the terminal methyl group and the radical center, leading to number of single events of 6. This values originates from the three indistinguishable hydrogen atoms than can be abstracted, and the two ways the planar CH_2 radical group can face the abstracted hydrogen atom.

R5 shows another example in which the reactant has one chiral center, leading to a number of optical isomers of 2. The transition state, however, contains two chiral centers, and 4 isomers of this transition state exist: two pairs of diastereomers. In principle, the energy of these two diastereomers is different and the rate coefficient depends thus on the specific diastereomer. However, this difference is neglected in this work, and the lowest energy diastereomer is always taken. In this case, the number of optical isomers amounts to 4, yielding a total number of single events of two. This number represents the two ways the planar radical group can face the abstracted hydrogen atom. If the diastereomers would be made distinguishable, two rate coefficients would be calculated, each with a number of single events of 1. In this case, the dihedral angle around the bond between the two chiral centers in the transition state is fixed per diastereomer, and the planar radical structure can only approach the abstracted hydrogen atom with one direction. The total rate coefficient used in this work will slightly overestimate the real total rate coefficient because the highest rate coefficient is multiplied by 2 instead of using the sum of the highest and lowest value.

The above examples give an overview of the different types of contributions. However, many other combinations are encountered in this study, but a complete analysis of all the number of single events falls outside the scope of this work.

Ab initio tunneling coefficients

Tunneling plays a crucial role in hydrogen abstractions, whether they are intramolecular or intermolecular. At low temperatures, the tunneling coefficient can amount up to 2 10^5 for 1-3 H-shifts. However, at these temperatures, the total rate coefficient is insignificant for practical purposes such as combustion, oxidation or pyrolysis reactions. At higher temperatures, tunneling is still important, where the coefficients amount up to 1.52 for 1-3 H-shifts at 1000K. The average and extreme values of 1-2 to 1-7 H-shifts are given in Table S-10. In general, 1-3 H-shifts have the highest tunneling coefficients, followed by 1-2 and 1-4 H-shifts. 1-5, 1-6 and 1-7 H-shifts have comparable values for tunneling coefficients.

Figure S-1 shows the tunneling coefficients at 1000K as a function of the imaginary frequency. The imaginary frequency is, besides the electronic energy of activation, the second parameter to calculate Eckart tunneling corrections. From Figure S-1, the range in imaginary frequencies can also be observed. 1-3 H-shifts have the highest imaginary frequencies, which range from 1945 to 2100cm^{-1}, this is also reflected in the high tunneling coefficients for these reactions. In 1-2 H-shifts, although the reaction proceeds through a three-membered ring, there are no small C-C-C bond angles. In 1-3 H-shifts, however, the four-membered ring has a small C-C-C angle, leading to a higher ring strain for these reactions. The imaginary frequencies in 1-2 H-shifts vary between 1723 and 1982cm^{-1}. From 1-4 to 1-6 H-shifts, there is a downward trend in the imaginary frequencies with averages of 1780cm^{-1} for 1-4, 1611cm^{-1} for 1-5, and 1545cm^{-1} for 1-6 H-shifts. The imaginary frequencies for 1-7 H-shifts increase again and lie in a range of 1393 to 1693cm^{-1}. For each H-shift, most of the reactions show an imaginary frequency that is relatively close to the maximum value for the family. Only a few reactions show imaginary frequencies that are closer to the minimum value. These reactions all include the formation or destruction of a strong resonantly stabilized radical, e.g. a hydrogen is abstracted between two vinyl groups.

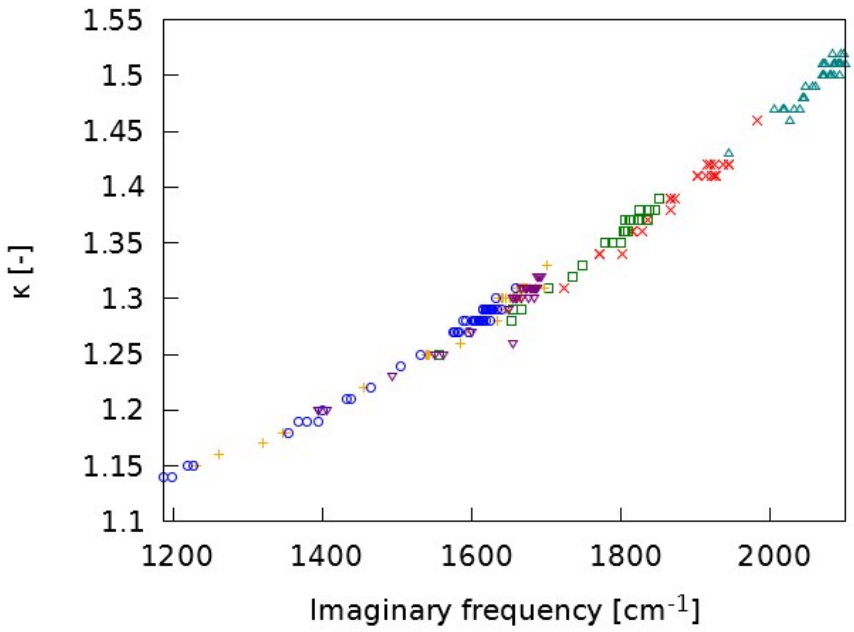


Figure S-1: Tunneling coefficients, calculated by the Eckart[27] procedure, at 1000K as a function of the imaginary frequency of the saddle point on the PES. The points correspond to 1-2 (), 1-3 (), 1-4 (), 1-5 (), 1-6 (), and 1-7 () H-shifts.

Table S-10: Average and extreme values for tunneling coefficients of 1-2 to 1-7 H-shifts at temperatures ranging from 300 to 1800K.

	1-2			1-3			1-4		
T/K	**Average**	**Maximum**	**Minimum**	**Average**	**Maximum**	**Minimum**	**Average**	**Maximum**	**Minimum**
300	10860.65	59138.61	290.02	98656.95	213897.87	8151.39	270.59	585.33	26.95
400	22.97	46.40	9.09	63.85	85.07	28.43	10.35	14.10	4.84
500	4.88	6.52	3.39	7.59	8.59	5.58	3.74	4.39	2.55
600	2.72	3.20	2.22	3.49	3.74	2.96	2.38	2.63	1.88
700	2.02	2.25	1.76	2.38	2.49	2.14	1.86	2.00	1.58
800	1.69	1.83	1.53	1.91	1.97	1.76	1.60	1.69	1.42
900	1.51	1.60	1.40	1.65	1.69	1.56	1.45	1.51	1.32
1000	1.39	1.46	1.31	1.49	1.52	1.43	1.35	1.39	1.25
1100	1.31	1.36	1.25	1.39	1.41	1.34	1.28	1.32	1.20
1200	1.26	1.30	1.21	1.32	1.34	1.28	1.23	1.26	1.17
1300	1.21	1.25	1.17	1.27	1.28	1.23	1.20	1.22	1.14
1400	1.18	1.21	1.15	1.23	1.24	1.20	1.17	1.19	1.12
1500	1.16	1.18	1.13	1.19	1.20	1.17	1.15	1.16	1.11
1600	1.14	1.16	1.11	1.17	1.18	1.15	1.13	1.14	1.09
1700	1.12	1.14	1.10	1.15	1.16	1.13	1.11	1.13	1.08
1800	1.11	1.12	1.09	1.13	1.14	1.12	1.10	1.11	1.07
	1-5			**1-6**			**1-7**		
T/K	**Average**	**Maximum**	**Minimum**	**Average**	**Maximum**	**Minimum**	**Average**	**Maximum**	**Minimum**
300	40.64	66.41	4.95	30.04	49.12	4.37	64.99	102.65	9.48
400	5.60	6.91	2.36	4.88	6.00	2.23	6.39	7.56	3.17
500	2.79	3.13	1.72	2.58	2.94	1.66	2.96	3.22	2.04
600	2.00	2.16	1.46	1.90	2.10	1.42	2.06	2.18	1.63
700	1.65	1.76	1.32	1.59	1.72	1.30	1.69	1.75	1.43
800	1.47	1.54	1.24	1.43	1.52	1.22	1.49	1.53	1.32
900	1.36	1.41	1.19	1.33	1.40	1.17	1.37	1.40	1.25
1000	1.28	1.33	1.15	1.26	1.31	1.14	1.29	1.32	1.20
1100	1.23	1.26	1.12	1.21	1.26	1.12	1.24	1.26	1.16
1200	1.19	1.22	1.10	1.18	1.22	1.10	1.20	1.21	1.13
1300	1.16	1.19	1.09	1.15	1.18	1.08	1.17	1.18	1.11
1400	1.14	1.16	1.08	1.13	1.16	1.07	1.14	1.15	1.10
1500	1.12	1.14	1.07	1.11	1.14	1.06	1.12	1.13	1.09
1600	1.11	1.13	1.06	1.10	1.12	1.06	1.11	1.12	1.08
1700	1.10	1.11	1.05	1.09	1.11	1.05	1.10	1.11	1.07
1800	1.09	1.10	1.05	1.08	1.10	1.04	1.09	1.09	1.06

Initial group additive values

Table S-11: Primary group additive values ΔGAV° for 1-2 to 1-7 intramolecular hydrogen abstractions deduced from the training set at 1000K. The index i depends on the H-shift. For 1-2 H-shifts, i equals 2, for 1-3 H-shifts 3, etc. The units for $\Delta GAV°_{Ea}$ values are kJ mol^{-1}. For the reference reaction, the single-event pre-exponential factors are expressed in s^{-1} and Ea is expressed in kJ mol^{-1}. The reference reaction pre-exponential factor does not include tunneling nor the number of single events.

	1-2		1-3		1-4		1-5		1-6		1-7	
	logÃ	Ea	logÃ	Ea	logÃ	Ea	logÃ	Ea	logÃ	Ea	logÃ	Ea
Reference	12.78	177.3	12.04	176.2	10.82	106.0	9.94	73.1	9.12	69.3	7.89	76.0
C_1-(C)$(H)_2$	0.00	0.0	0.00	0.0	0.00	0.0	0.00	0.0	0.00	0.0	0.00	0.0
C_1-$(C)_2$(H)	-0.09	6.3	0.08	5.6	0.03	4.6	-0.04	5.7	0.06	4.8	0.22	4.3
C_1-(C_d)(C)(H)	0.61	33.7	0.95	41.3	0.69	42.5	0.71	47.0	0.85	48.5	0.45	47.0
C_1-(C_t)(C)(H)	0.08	29.3	0.17	30.9	0.19	28.0	0.13	31.5	-0.50	33.2	0.14	31.0
C_1-$(C)_3$	-0.06	6.5	-0.03	6.3	0.04	5.1	-0.27	5.4	-0.28	5.7	-0.35	5.9
C_1-$(C_d)(C)_2$	0.55	37.9	0.85	45.0	0.68	46.1	0.47	50.2	0.50	57.9	0.36	54.6
C_1-(C_t)(C)	-0.04	34.4	-0.11	37.1	-0.10	34.5	-0.03	38.1	-0.28	35.6	0.17	41.2
C_1-$(C_d)_2$(C)	0.49	56.4	0.96	65.1	0.68	69.4	0.36	78.1	0.69	85.3	0.24	79.2
C_1-$(C_d)(C_t)$(C)	0.58	57.5	0.81	63.1	0.71	62.5	0.71	66.9	0.47	67.3	0.59	67.4
C_1-$(C_t)_2$(C)	0.13	56.4	0.13	59.2	0.24	55.9	0.21	60.4	-0.06	60.6	0.11	60.4
C_i-(C)$(H)_3$	0.00	0.0	0.00	0.0	0.00	0.0	0.00	0.0	0.00	0.0	0.00	0.0
C_i-$(C)_2(H)_2$	0.05	-9.9	0.18	-9.8	0.13	-12.4	0.17	-10.3	-0.02	-12.3	0.00	-12.5
C_i-(C_d)(C)$(H)_2$	-0.15	-41.7	0.12	-32.2	-0.42	-31.1	-0.31	-26.5	-0.07	-24.9	-0.30	-26.6
C_i-(C_t)(C)$(H)_2$	-0.02	-32.6	0.19	-25.3	0.03	-28.8	0.01	-24.1	-0.48	-24.8	-0.03	-24.2
C_i-$(C)_3$(H)	0.05	-20.1	0.19	-18.7	0.21	-21.3	0.03	-21.0	-0.35	-21.5	0.01	-19.7
C_i-$(C_d)(C)_2$(H)	-0.28	-49.7	0.05	-38.4	-0.17	-39.2	-0.32	-34.4	-0.76	-32.1	-0.97	-31.4
C_i-(C_t)(C) (H)	-0.04	-41.3	0.18	-33.0	0.04	-37.3	0.05	-32.6	-0.29	-35.1	-0.38	-32.1
C_i-$(C_d)_2$(C)(H)	-0.54	-62.3	-0.01	-50.0	-0.15	-49.4	-0.15	-38.0	-0.30	-36.0	-0.80	-37.4
C_i-$(C_d)(C_t)$(C) (H)	-0.24	-62.7	0.10	-47.2	-0.02	-50.0	-0.07	-43.6	-0.50	-44.0	-0.53	-43.9
C_i-$(C_t)_2$(C)(H)	-0.07	-62.0	0.17	-46.1	0.10	-50.7	-0.01	-42.3	-0.51	-43.0	-0.04	-43.1

Table S-12: Secondary group additive values ΔGAV° for 1-2 to 1-7 intramolecular hydrogen abstractions deduced from the training set at 1000K. The units for $\Delta GAV°_{Ea}$ values are kJ mol^{-1}. For the reference reaction, the single-event pre-exponential factors are expressed in s^{-1} and Ea is expressed in kJ mol^{-1}.

	1-3		1-4				1-5					
	i=2		i=2		i=3		i=2		i=3		i=4	
	logÃ	E_a	logÃ	E_a	logA	E_a	logÃ	E_a	logÃ	E_a	logÃ	E_a
C_i-$(C)_2(H)_2$	0.00	0.0	0.00	0.0	0.00	0.0	0.00	0.0	0.00	0.0	0.00	0.0
C_i-$(C)_3(H)$	0.10	-1.7	-0.02	-5.6	0.02	-2.2	-0.09	-5.4	0.08	-5.8	-0.01	-2.2
C_i-$(C_d)(C)_2(H)$	-0.01	-3.3	-0.02	-6.7	0.01	-4.4	0.05	-5.1	0.18	-4.2	0.07	-2.8
C_i-$(C_t)(C)_2(H)$	-0.07	-5.7	-0.11	-8.2	0.09	-2.6	-0.07	-5.9	0.07	-1.9	-0.05	-0.5
C_i-$(C)_4$	0.17	-4.7	-0.03	-8.1	-0.02	-3.4	-0.01	-7.2	-0.09	-6.4	0.00	-3.0
C_i-$(C_d)(C)_3$	0.00	-6.3	-0.02	-10.7	-0.10	-5.4	0.12	-9.3	0.13	-7.9	0.15	-5.5
C_i-$(C_t)(C)_3$	0.01	-6.7	0.00	-9.1	0.06	-3.3	0.02	-10.1	0.06	-9.0	0.14	-4.8
C_i-$(C_d)_2(C)_2$	0.20	-8.8	-0.08	-10.8	-0.03	-2.1	0.17	-11.5	0.34	-10.7	0.18	-4.9
C_i-$(C_d)(C_t)(C)_2$	0.20	-8.2	0.02	-12.2	0.05	-4.8	0.13	-11.0	0.10	-4.8	0.15	-3.8
C_i-$(C_t)_2(C)_2$	-0.01	-8.9	0.00	-11.6	-0.02	-2.8	0.03	-8.7	-0.03	-4.0	0.17	0.7

	1-6								1-7									
	i=2		i=3		i=4		i=5		i=2		i=3		i=4		i=5		i=6	
	logÃ	E_a	logÃ	E_a	logÃ	E_a	logÃ	E_a	logÃ	E_a	logÃ	E_a	logÃ	E_a	logÃ	E_a	logÃ	E_a
C_i-$(C)_2(H)_2$	0.00	0.0	0.00	0.0	0.00	0.0	0.00	0.0	0.00	0.0	0.00	0.0	0.00	0.0	0.00	0.0	0.00	0.0
C_i-$(C)_3(H)$	-0.06	-4.0	-0.04	-3.0	0.02	-3.4	-0.03	-1.3	0.04	-3.9	0.10	-2.3	0.35	-3.7	-0.13	-1.6	-0.20	-1.9
C_i-$(C_d)(C)_2(H)$	-0.17	-4.5	0.24	-0.8	0.11	-1.1	-0.09	-1.9	0.03	-4.7	0.03	-1.3	0.53	-2.0	0.10	-1.7	-0.40	-2.4
C_i-$(C_t)(C)_2(H)$	-0.28	-6.5	0.08	-1.8	-0.13	-1.7	-0.13	-0.3	-0.07	-4.5	0.12	-3.4	0.46	3.2	0.08	-2.0	0.06	2.1
C_i-$(C)_4$	-0.21	-6.1	0.05	-2.6	0.12	-3.8	-0.06	-0.9	0.19	-6.8	0.73	-1.3	0.06	4.1	0.15	-5.6	0.31	0.3
C_i-$(C_d)(C)_3$	-0.12	-8.1	0.30	-2.8	0.36	-3.8	-0.03	-3.1	0.36	-3.5	0.44	-6.4	1.25	-0.3	0.55	-6.9	0.05	0.8
C_i-$(C_t)(C)_3$	-0.15	-7.4	0.23	-6.6	0.19	-5.5	0.02	-1.6	0.15	-2.7	0.30	-5.2	0.84	1.5	0.22	-3.9	0.43	3.9
C_i-$(C_d)_2(C)_2$	-0.07	-10.6	0.38	-6.0	0.59	-4.8	-0.17	-4.1	0.24	-6.1	0.43	-10.2	1.08	-4.6	0.43	-9.7	0.67	-1.1
C_i-$(C_d)(C_t)(C)_2$	-0.12	-11.6	0.26	-2.3	0.34	-3.4	-0.05	-3.4	0.13	-5.7	0.22	-1.0	1.01	2.1	0.30	-0.9	-0.26	2.4
C_i-$(C_t)_2(C)_2$	-0.19	-8.9	0.13	-4.1	0.17	-1.0	-0.02	2.7	0.28	-3.0	0.24	-6.3	0.96	1.6	0.34	-1.6	0.41	7.5

Group additive values at 300K

Table S-13: Primary group additive values ΔGAV° for 1-2 to 1-7 intramolecular hydrogen abstractions deduced from the combined training set and test set at 300K. See main text for the reference reactions. The index i depends on the H-shift. For 1-2 H-shifts, i equals 2, for 1-3 H-shifts 3, etc. The units for $\Delta GAV°_{Ea}$ values are kJ mol^{-1}. For the reference reaction, the single-event pre-exponential factors are expressed in s^{-1} and Ea is expressed in kJ mol^{-1}. The reference reaction pre-exponential factor does not include tunneling nor the number of single events.

	1-2		1-3		1-4		1-5		1-6		1-7	
	logÃ	Ea	logÃ	Ea	logÃ	Ea	logÃ	Ea	logÃ	Ea	logÃ	Ea
Reference												
C_1-(C)$(H)_2$	0.000	0.00	0.000	0.00	0.000	0.00	0.000	0.00	0.000	0.00	0.000	0.00
C_1-$(C)_2$(H)	-0.211	5.22	-0.095	3.50	-0.181	2.41	-0.171	2.91	-0.043	3.02	-0.009	1.80
C_1-(C_d)(C)(H)	0.373	32.95	0.710	41.39	0.539	40.84	0.671	45.15	0.813	48.89	0.430	46.96
C_1-(C_t)(C)(H)	0.128	25.39	0.125	30.85	0.084	26.88	0.001	29.44	-0.407	33.07	0.000	29.62
C_1-$(C)_3$	-0.283	7.19	-0.360	3.66	-0.396	0.85	-0.768	0.98	-0.793	2.26	-0.820	0.96
C_1-$(C_d)(C)_2$	0.415	34.48	0.523	44.73	0.458	45.32	0.383	49.12	0.587	57.02	-0.089	52.39
C_1-(C_t)(C)	-0.070	30.62	-0.266	35.82	-0.262	34.12	-0.211	35.77	-0.270	36.87	-0.519	35.31
C_1-$(C_d)_2$(C)	0.587	57.72	0.920	67.15	1.056	72.43	0.894	85.33	1.304	91.86	0.830	86.54
C_1-$(C_d)(C_t)$(C)	0.398	52.65	0.537	61.79	0.446	63.19	0.674	66.77	0.393	67.75	0.500	66.61
C_1-$(C_t)_2$(C)	0.229	56.56	0.044	58.41	0.091	51.42	0.313	61.46	-0.101	59.71	-0.049	58.72
C_i-(C)$(H)_3$	0.000	0.00	0.000	0.00	0.000	0.00	0.000	0.00	0.000	0.00	0.000	0.00
C_i-$(C)_2(H)_2$	0.210	-8.93	0.325	-10.11	0.317	-11.09	0.234	-9.99	0.336	-9.93	0.094	-11.36
C_i-$(C_d)(C)(H)_2$	-0.249	-43.06	0.058	-32.68	-0.329	-31.85	-0.249	-27.73	-0.218	-26.61	-0.414	-27.89
C_i-$(C_t)(C)(H)_2$	-0.023	-34.50	0.339	-25.88	0.266	-27.40	0.036	-24.60	-0.072	-22.33	-0.054	-24.11
C_i-$(C)_3$(H)	0.359	-14.02	0.495	-15.75	0.163	-19.89	0.099	-19.25	-0.165	-19.17	0.117	-18.16
C_i-$(C_d)(C)_2$(H)	-0.164	-44.98	0.056	-35.48	0.051	-38.19	-0.010	-32.01	-0.206	-27.74	-0.573	-30.13
C_i-(C_t)(C) (H)	0.146	-36.90	0.378	-31.00	0.530	-31.69	0.071	-30.69	-0.013	-30.62	-0.298	-32.90
C_i-$(C_d)_2$(C)(H)	-0.734	-65.74	-0.609	-55.18	0.259	-48.52	-0.267	-37.80	-0.443	-35.99	-0.633	-35.33
C_i-$(C_d)(C_t)$(C) (H)	-0.103	-63.69	0.183	-46.28	0.086	-47.90	0.076	-43.47	-0.319	-42.90	-0.523	-43.52
C_i-$(C_t)_2$(C)(H)	0.083	-60.14	0.315	-43.85	0.529	-48.93	0.005	-40.95	-0.060	-41.59	-0.063	-42.96

Table S-14: Secondary group additive values ΔGAV° for 1-2 to 1-7 intramolecular hydrogen abstractions deduced from the combined training set and test set at 300K. See main text for the reference reactions. The units for $\Delta GAV°_{Ea}$ values are kJ mol^{-1}. For the reference reaction, the single-event pre-exponential factors are expressed in s^{-1} and Ea is expressed in kJ mol^{-1}.

	1-3		1-4			
	i=2		i=2		i=3	
	logÃ	E_a	logÃ	E_a	logA	E_a
C_i-$(C)_2(H)_2$	0.000	0.00	0.000	0.00	0.000	0.00
C_i-$(C)_3(H)$	0.001	-2.72	0.083	-5.86	0.141	-4.13
C_i-$(C_d)(C)_2(H)$	0.015	-1.54	0.230	-7.78	0.075	-5.87
C_i-$(C_t)(C)_2(H)$	-0.117	-6.16	-0.027	-6.69	0.143	-2.18
C_i-$(C)_4$	0.322	-4.70	-0.091	-7.67	-0.101	-0.86
C_i-$(C_d)(C)_3$	0.031	-6.35	0.243	-8.97	-0.001	-4.92
C_i-$(C_t)(C)_3$	-0.027	-8.50	0.169	-8.52	0.132	-3.03
C_i-$(C_d)_2(C)_2$	0.573	-4.76	0.016	-10.57	0.046	-1.91
C_i-$(C_d)(C_t)(C)_2$	0.537	-4.51	0.400	-9.12	0.123	-4.56
C_i-$(C_t)_2(C)_2$	-0.035	-6.71	0.183	-10.15	0.069	-2.98

	1-5					
	i=2		i=3		i=4	
	logÃ	E_a	logÃ	E_a	logÃ	E_a
C_i-$(C)_2(H)_2$	0.000	0.00	0.000	0.00	0.000	0.00
C_i-$(C)_3(H)$	0.140	-3.19	0.142	-3.39	0.150	-1.72
C_i-$(C_d)(C)_2(H)$	0.309	-2.05	0.329	-2.24	0.339	0.55
C_i-$(C_t)(C)_2(H)$	0.124	-4.14	0.019	-0.94	0.339	2.78
C_i-$(C)_4$	0.075	-5.06	-0.048	-6.08	0.045	-1.93
C_i-$(C_d)(C)_3$	0.234	-9.58	0.645	-5.10	0.063	-1.64
C_i-$(C_t)(C)_3$	0.228	-8.06	0.313	-7.68	0.252	-3.76
C_i-$(C_d)_2(C)_2$	0.754	-3.83	0.419	-6.19	0.084	-7.59
C_i-$(C_d)(C_t)(C)_2$	0.683	-5.20	0.392	-0.37	0.618	0.07
C_i-$(C_t)_2(C)_2$	0.336	-7.15	0.059	-3.50	0.506	3.31

(Table S-14 continued)

	1-6							
	i=2		i=3		i=4		i=5	
	logÃ	E_a	logÃ	E_a	logÃ	E_a	logÃ	E_a
C_i-$(C)_2(H)_2$	0.000	0.00	0.000	0.00	0.000	0.00	0.000	0.00
C_i-$(C)_3(H)$	-0.030	-4.91	0.202	-1.68	0.275	-2.87	-0.279	-4.98
C_i-$(C_d)(C)_2(H)$	0.155	-4.14	0.607	1.25	0.847	5.57	0.157	-2.24
C_i-$(C_t)(C)_2(H)$	0.059	-2.86	0.320	2.13	0.360	4.68	0.105	3.90
C_i-$(C)_4$	0.030	-4.30	0.388	0.49	0.234	-3.44	0.043	-0.13
C_i-$(C_d)(C)_3$	0.131	-2.31	1.071	2.65	0.905	0.84	0.121	-0.91
C_i-$(C_t)(C)_3$	0.194	-4.53	0.449	-4.38	0.410	-5.76	0.200	0.83
C_i-$(C_d)_2(C)_2$	0.160	-7.44	1.156	3.14	1.385	2.58	-0.209	-3.94
C_i-$(C_d)(C_t)(C)_2$	0.155	-7.79	0.791	1.32	1.030	2.36	0.206	1.24
C_i-$(C_t)_2(C)_2$	0.081	-5.26	0.505	0.28	0.521	3.04	0.230	5.54

	1-7									
	i=2		i=3		i=4		i=5		i=6	
	logÃ	E_a	logÃ	E_a	logÃ	E_a	logÃ	E_a	logÃ	E_a
C_i-$(C)_2(H)_2$	0.000	0.00	0.000	0.00	0.000	0.00	0.000	0.00	0.00	0.00
C_i-$(C)_3(H)$	0.276	-3.29	0.384	0.06	0.350	-3.54	0.096	-0.79	-0.03	-2.61
C_i-$(C_d)(C)_2(H)$	0.150	-3.30	0.360	2.38	1.050	3.93	0.450	2.56	-0.26	-0.80
C_i-$(C_t)(C)_2(H)$	-0.020	-3.85	0.270	-1.70	0.790	6.97	0.220	-0.35	0.09	2.64
C_i-$(C)_4$	0.350	-4.29	0.950	1.57	0.123	5.08	0.360	-3.00	0.40	1.33
C_i-$(C_d)(C)_3$	0.520	-1.77	0.870	-1.43	1.640	4.29	0.870	-3.05	0.18	2.58
C_i-$(C_t)(C)_3$	0.260	-1.44	0.520	-2.50	1.050	4.08	0.310	-2.15	0.52	5.23
C_i-$(C_d)_2(C)_2$	0.480	-3.51	1.040	-3.14	1.730	3.21	0.900	-3.56	0.82	0.70
C_i-$(C_d)(C_t)(C)_2$	0.410	-2.50	0.620	3.66	1.720	10.12	0.780	4.75	0.05	5.92
C_i-$(C_t)_2(C)_2$	0.440	-1.14	0.580	-2.41	1.380	6.27	0.580	1.24	0.59	9.66

Group additive values at 600K

Table S-15: Primary group additive values ΔGAV° for 1-2 to 1-7 intramolecular hydrogen abstractions deduced from the combined training set and test set at 600K. See main text for the reference reactions. The index i depends on the H-shift. For 1-2 H-shifts, i equals 2, for 1-3 H-shifts 3, etc. The units for $\Delta GAV°_{Ea}$ values are kJ mol^{-1}. For the reference reaction, the single-event pre-exponential factors are expressed in s^{-1} and Ea is expressed in kJ mol^{-1}. The reference reaction pre-exponential factor does not include tunneling nor the number of single events.

	1-2		1-3		1-4		1-5		1-6		1-7	
	logÃ	Ea	logÃ	Ea	logÃ	Ea	logÃ	Ea	logÃ	Ea	logÃ	Ea
Reference												
C_1-(C)$(H)_2$	0.000	0.00	0.000	0.00	0.000	0.00	0.000	0.00	0.000	0.00	0.000	0.00
C_1-$(C)_2$(H)	-0.090	6.20	0.023	4.48	-0.036	3.59	-0.047	3.91	0.051	3.79	0.133	2.91
C_1-(C_d)(C)(H)	0.380	33.03	0.725	41.52	0.628	41.53	0.731	45.61	0.805	48.87	0.450	47.04
C_1-(C_t)(C)(H)	0.119	25.32	0.183	31.30	0.148	27.38	0.036	29.72	-0.363	33.40	0.100	30.34
C_1-$(C)_3$	-0.091	8.79	-0.060	6.11	-0.158	2.75	-0.504	3.05	-0.515	4.54	-0.520	3.39
C_1-$(C_d)(C)_2$	0.461	34.86	0.679	46.04	0.553	46.13	0.475	49.83	0.580	56.90	0.007	53.12
C_1-(C_t)(C)	-0.047	30.81	-0.160	36.74	-0.118	35.25	-0.053	37.04	-0.173	37.60	-0.403	36.24
C_1-$(C_d)_2$(C)	0.563	57.52	0.938	67.21	0.888	71.06	0.731	83.90	0.940	88.82	0.620	84.70
C_1-$(C_d)(C_t)$(C)	0.520	53.66	0.628	62.56	0.553	64.04	0.724	67.11	0.469	68.35	0.580	67.15
C_1-$(C_t)_2$(C)	0.223	56.54	0.151	59.29	0.143	51.84	0.350	61.73	-0.074	59.93	0.041	59.41
C_i-(C)$(H)_3$	0.000	0.00	0.000	0.00	0.000	0.00	0.000	0.00	0.000	0.00	0.000	0.00
C_i-$(C)_2(H)_2$	0.137	-9.53	0.270	-10.52	0.199	-12.02	0.144	-10.74	0.230	-10.77	0.052	-11.72
C_i-$(C_d)(C)(H)_2$	-0.284	-43.30	-0.021	-33.33	-0.411	-32.52	-0.256	-27.79	-0.203	-26.45	-0.374	-27.60
C_i-$(C_t)(C)(H)_2$	-0.045	-34.68	0.256	-26.53	0.119	-28.58	-0.006	-24.97	-0.121	-22.79	-0.014	-23.88
C_i-$(C)_3$(H)	0.269	-14.77	0.491	-15.79	0.031	-21.00	0.043	-19.72	-0.257	-19.96	0.097	-18.36
C_i-$(C_d)(C)_2$(H)	-0.318	-46.17	-0.054	-36.34	-0.126	-39.60	-0.238	-33.93	-0.463	-29.85	-0.700	-31.22
C_i-(C_t)(C) (H)	0.051	-37.71	0.299	-31.61	0.285	-33.67	0.036	-31.02	-0.146	-31.71	-0.360	-33.43
C_i-$(C_d)_2$(C)(H)	-0.620	-64.83	-0.514	-54.41	0.035	-50.33	-0.233	-37.59	-0.488	-36.35	-0.723	-36.06
C_i-$(C_d)(C_t)$(C) (H)	-0.188	-64.39	0.160	-46.45	-0.010	-48.67	0.010	-44.07	-0.332	-43.01	-0.513	-43.51
C_i-$(C_t)_2$(C)(H)	0.009	-60.72	0.281	-44.10	0.295	-50.84	-0.044	-41.38	-0.239	-43.08	-0.013	-42.56

Table S-16: Secondary group additive values ΔGAV° for 1-2 to 1-7 intramolecular hydrogen abstractions deduced from the combined training set and test set at 600K. See main text for the reference reactions. The units for $\Delta GAV°_{Ea}$ values are kJ mol^{-1}. For the reference reaction, the single-event pre-exponential factors are expressed in s^{-1} and Ea is expressed in kJ mol^{-1}.

	1-3		1-4			
	i=2		i=2		i=3	
	logÃ	E_a	logÃ	E_a	logA	E_a
C_i-$(C)_2(H)_2$	0.000	0.00	0.000	0.00	0.000	0.00
C_i-$(C)_3(H)$	-0.043	-3.02	0.051	-6.13	0.133	-4.20
C_i-$(C_d)(C)_2(H)$	-0.047	-2.01	0.108	-8.76	0.065	-5.94
C_i-$(C_t)(C)_2(H)$	-0.165	-6.56	-0.058	-6.95	0.128	-2.29
C_i-$(C)_4$	0.319	-4.71	-0.067	-7.47	-0.094	-0.82
C_i-$(C_d)(C)_3$	-0.001	-6.63	0.033	-10.65	-0.028	-5.12
C_i-$(C_t)(C)_3$	-0.023	-8.49	0.083	-9.25	0.108	-3.23
C_i-$(C_d)_2(C)_2$	0.325	-6.74	0.009	-10.59	0.079	-1.70
C_i-$(C_d)(C_t)(C)_2$	0.384	-5.77	0.163	-11.00	0.093	-4.77
C_i-$(C_t)_2(C)_2$	-0.003	-6.45	0.089	-10.88	0.053	-3.06

	1-5					
	i=2		i=3		i=4	
	logÃ	E_a	logÃ	E_a	logÃ	E_a
C_i-$(C)_2(H)_2$	0.000	0.00	0.000	0.00	0.000	0.00
C_i-$(C)_3(H)$	0.050	-3.95	0.109	-3.67	0.093	-2.22
C_i-$(C_d)(C)_2(H)$	0.102	-3.71	0.278	-2.69	0.129	-1.19
C_i-$(C_t)(C)_2(H)$	-0.003	-5.15	0.012	-1.03	0.169	1.35
C_i-$(C)_4$	-0.051	-6.12	-0.001	-5.78	0.032	-2.07
C_i-$(C_d)(C)_3$	0.049	-11.06	0.435	-6.86	0.118	-1.20
C_i-$(C_t)(C)_3$	0.124	-8.90	0.360	-7.33	0.213	-4.04
C_i-$(C_d)_2(C)_2$	0.420	-6.57	0.319	-7.06	0.105	-7.46
C_i-$(C_d)(C_t)(C)_2$	0.454	-7.12	0.310	-1.12	0.454	-1.36
C_i-$(C_t)_2(C)_2$	0.216	-8.17	-0.013	-4.13	0.346	1.96

(Table S-16 continued)

	1-6							
	i=2		i=3		i=4		i=5	
	logÃ	E_a	logÃ	E_a	logÃ	E_a	logÃ	E_a
C_i-$(C)_2(H)_2$	0.000	0.00	0.000	0.00	0.000	0.00	0.000	0.00
C_i-$(C)_3(H)$	-0.120	-5.67	0.158	-2.05	0.232	-3.24	-0.171	-4.19
C_i-$(C_d)(C)_2(H)$	0.036	-5.13	0.430	-0.22	0.540	2.99	0.113	-2.62
C_i-$(C_t)(C)_2(H)$	-0.033	-3.62	0.207	1.21	0.167	3.14	-0.010	2.91
C_i-$(C)_4$	-0.020	-4.68	0.276	-0.47	0.215	-3.62	0.123	0.45
C_i-$(C_d)(C)_3$	-0.022	-3.59	0.705	-0.36	0.613	-1.53	0.058	-1.44
C_i-$(C_t)(C)_3$	0.006	-6.10	0.390	-4.90	0.335	-6.40	0.165	0.50
C_i-$(C_d)_2(C)_2$	-0.067	-9.30	0.740	-0.34	1.053	-0.17	-0.170	-3.73
C_i-$(C_d)(C_t)(C)_2$	-0.012	-9.14	0.525	-0.92	0.748	-0.03	0.050	-0.13
C_i-$(C_t)_2(C)_2$	-0.060	-6.43	0.308	-1.40	0.320	1.38	0.108	4.50

	1-7									
	i=2		i=3		i=4		i=5		i=6	
	logÃ	E_a	logÃ	E_a	logÃ	E_a	logÃ	E_a	logÃ	E_a
C_i-$(C)_2(H)_2$	0.000	0.00	0.000	0.00	0.000	0.00	0.000	0.00	0.00	0.00
C_i-$(C)_3(H)$	0.166	-4.19	0.328	-0.43	0.370	-3.42	0.232	0.25	0.02	-2.27
C_i-$(C_d)(C)_2(H)$	0.090	-3.87	0.180	0.80	0.790	1.72	0.300	1.28	-0.32	-1.34
C_i-$(C_t)(C)_2(H)$	-0.030	-4.01	0.200	-2.31	0.610	5.48	0.150	-0.98	0.10	2.62
C_i-$(C)_4$	0.350	-4.44	0.880	0.90	0.133	5.09	0.280	-3.68	0.35	0.89
C_i-$(C_d)(C)_3$	0.430	-2.49	0.650	-3.32	1.450	2.65	0.730	-4.27	0.14	2.18
C_i-$(C_t)(C)_3$	0.200	-1.97	0.440	-3.28	0.970	3.31	0.350	-1.93	0.50	5.02
C_i-$(C_d)_2(C)_2$	0.330	-4.73	0.740	-5.71	1.450	0.84	0.750	-4.92	0.76	0.14
C_i-$(C_d)(C_t)(C)_2$	0.270	-3.69	0.430	1.96	1.340	7.00	0.560	2.92	-0.11	4.62
C_i-$(C_t)_2(C)_2$	0.360	-1.84	0.410	-3.87	1.140	4.25	0.470	0.30	0.52	9.02

Group additive values at 800K

Table S-17: Primary group additive values ΔGAV° for 1-2 to 1-7 intramolecular hydrogen abstractions deduced from the combined training set and test set at 800K. See main text for the reference reactions. The index i depends on the H-shift. For 1-2 H-shifts, i equals 2, for 1-3 H-shifts 3, etc. The units for $\Delta GAV°_{Ea}$ values are kJ mol^{-1}. For the reference reaction, the single-event pre-exponential factors are expressed in s^{-1} and Ea is expressed in kJ mol^{-1}. The reference reaction pre-exponential factor does not include tunneling nor the number of single events.

	1-2		1-3		1-4		1-5		1-6		1-7	
	logÃ	Ea	logÃ	Ea	logÃ	Ea	logÃ	Ea	logÃ	Ea	logÃ	Ea
Reference												
C_1-(C)$(H)_2$	0.000	0.00	0.000	0.00	0.000	0.00	0.000	0.00	0.000	0.00	0.000	0.00
C_1-$(C)_2$(H)	-0.050	6.71	0.064	5.01	0.009	4.16	-0.005	4.44	0.076	4.13	0.178	3.57
C_1-(C_d)(C)(H)	0.394	33.15	0.744	41.76	0.661	41.98	0.751	45.90	0.780	48.56	0.450	47.11
C_1-(C_t)(C)(H)	0.120	25.32	0.194	31.50	0.171	27.66	0.046	29.88	-0.344	33.68	0.120	30.79
C_1-$(C)_3$	-0.016	9.71	0.060	7.63	-0.072	3.83	-0.404	4.38	-0.410	5.90	-0.410	4.91
C_1-$(C_d)(C)_2$	0.485	35.20	0.752	46.95	0.598	46.61	0.494	50.06	0.557	56.67	0.036	53.58
C_1-(C_t)(C)	-0.028	31.00	-0.103	37.46	-0.071	35.86	0.004	37.80	-0.160	37.88	-0.359	36.81
C_1-$(C_d)_2$(C)	0.523	56.98	0.832	65.89	0.722	68.89	0.521	81.18	0.687	85.59	0.400	82.01
C_1-$(C_d)(C_t)$(C)	0.584	54.45	0.668	63.08	0.576	64.29	0.714	67.03	0.473	68.48	0.590	67.33
C_1-$(C_t)_2$(C)	0.203	56.30	0.184	59.69	0.167	52.10	0.352	61.75	-0.050	60.21	0.071	59.90
C_i-(C)$(H)_3$	0.000	0.00	0.000	0.00	0.000	0.00	0.000	0.00	0.000	0.00	0.000	0.00
C_i-$(C)_2(H)_2$	0.090	-10.15	0.240	-10.93	0.154	-12.65	0.103	-11.28	0.178	-11.47	0.025	-12.01
C_i-$(C_d)(C)(H)_2$	-0.260	-42.95	-0.020	-33.30	-0.409	-32.53	-0.237	-27.55	-0.169	-26.04	-0.334	-27.08
C_i-$(C_t)(C)(H)_2$	-0.064	-34.88	0.217	-27.04	0.051	-29.47	-0.037	-25.45	-0.179	-23.46	-0.034	-24.02
C_i-$(C)_3$(H)	0.196	-15.73	0.451	-16.28	-0.048	-22.03	-0.017	-20.51	-0.335	-20.89	0.037	-19.03
C_i-$(C_d)(C)_2$(H)	-0.328	-46.29	-0.066	-36.53	-0.169	-40.27	-0.344	-35.29	-0.570	-31.21	-0.747	-31.81
C_i-(C_t)(C) (H)	-0.013	-38.49	0.230	-32.51	0.155	-35.33	-0.013	-31.67	-0.216	-32.58	-0.417	-34.11
C_i-$(C_d)_2$(C)(H)	-0.540	-63.78	-0.469	-53.80	-0.058	-51.56	-0.253	-37.75	-0.500	-36.47	-0.783	-36.78
C_i-$(C_d)(C_t)$(C) (H)	-0.179	-64.21	0.150	-46.54	-0.054	-49.25	-0.048	-44.78	-0.353	-43.31	-0.533	-43.68
C_i-$(C_t)_2$(C)(H)	-0.051	-61.50	0.245	-44.62	0.182	-52.33	-0.091	-41.98	-0.320	-44.02	-0.033	-42.79

Table S-18: Secondary group additive values ΔGAV° for 1-2 to 1-7 intramolecular hydrogen abstractions deduced from the combined training set and test set at 800K. See main text for the reference reactions. The units for $\Delta GAV°_{Ea}$ values are kJ mol^{-1}. For the reference reaction, the single-event pre-exponential factors are expressed in s^{-1} and Ea is expressed in kJ mol^{-1}.

	1-3		1-4			
	i=2		i=2		i=3	
	logÃ	E_a	logÃ	E_a	logA	E_a
C_i-$(C)_2(H)_2$	0.000	0.00	0.000	0.00	0.000	0.00
C_i-$(C)_3(H)$	-0.055	-3.20	0.032	-6.40	0.119	-4.37
C_i-$(C_d)(C)_2(H)$	-0.067	-2.31	0.062	-9.38	0.055	-6.12
C_i-$(C_t)(C)_2(H)$	-0.192	-6.89	-0.076	-7.20	0.113	-2.50
C_i-$(C)_4$	0.302	-4.91	-0.071	-7.55	-0.121	-1.19
C_i-$(C_d)(C)_3$	-0.016	-6.74	-0.021	-11.37	-0.045	-5.43
C_i-$(C_t)(C)_3$	-0.033	-8.55	0.049	-9.75	0.088	-3.51
C_i-$(C_d)_2(C)_2$	0.241	-7.82	0.003	-10.74	0.063	-1.89
C_i-$(C_d)(C_t)(C)_2$	0.302	-6.81	0.086	-11.94	0.059	-5.28
C_i-$(C_t)_2(C)_2$	0.003	-6.36	0.039	-11.56	0.029	-3.40

	1-5					
	i=2		i=3		i=4	
	logÃ	E_a	logÃ	E_a	logÃ	E_a
C_i-$(C)_2(H)_2$	0.000	0.00	0.000	0.00	0.000	0.00
C_i-$(C)_3(H)$	0.009	-4.47	0.099	-3.77	0.059	-2.65
C_i-$(C_d)(C)_2(H)$	0.015	-4.84	0.230	-3.31	0.024	-2.49
C_i-$(C_t)(C)_2(H)$	-0.045	-5.80	-0.003	-1.21	0.079	0.14
C_i-$(C)_4$	-0.101	-6.79	-0.006	-5.81	0.002	-2.47
C_i-$(C_d)(C)_3$	0.004	-11.61	0.308	-8.48	0.113	-1.24
C_i-$(C_t)(C)_3$	0.082	-9.49	0.360	-7.29	0.191	-4.32
C_i-$(C_d)_2(C)_2$	0.269	-8.58	0.229	-8.20	0.109	-7.46
C_i-$(C_d)(C_t)(C)_2$	0.334	-8.65	0.205	-2.46	0.354	-2.57
C_i-$(C_t)_2(C)_2$	0.135	-9.17	-0.061	-4.66	0.260	0.81

(Table S-18 continued)

	1-6							
	i=2		i=3		i=4		i=5	
	logÃ	E_a	logÃ	E_a	logÃ	E_a	logÃ	E_a
C_i-$(C)_2(H)_2$	0.000	0.00	0.000	0.00	0.000	0.00	0.000	0.00
C_i-$(C)_3(H)$	-0.175	-6.36	0.130	-2.37	0.205	-3.62	-0.166	-4.06
C_i-$(C_d)(C)_2(H)$	-0.032	-5.93	0.327	-1.47	0.353	0.61	0.061	-3.24
C_i-$(C_t)(C)_2(H)$	-0.079	-4.19	0.157	0.55	0.060	1.78	-0.080	2.01
C_i-$(C)_4$	-0.053	-5.08	0.183	-1.65	0.171	-4.12	0.100	0.20
C_i-$(C_d)(C)_3$	-0.117	-4.68	0.522	-2.66	0.484	-3.17	-0.003	-2.20
C_i-$(C_t)(C)_3$	-0.079	-7.07	0.317	-5.72	0.272	-7.13	0.099	-0.27
C_i-$(C_d)_2(C)_2$	-0.156	-10.33	0.487	-3.52	0.829	-3.07	-0.213	-4.15
C_i-$(C_d)(C_t)(C)_2$	-0.086	-10.01	0.352	-3.10	0.554	-2.46	-0.063	-1.53
C_i-$(C_t)_2(C)_2$	-0.133	-7.33	0.189	-2.89	0.222	0.14	0.029	3.49

	1-7									
	i=2		i=3		i=4		i=5		i=6	
	logÃ	E_a	logÃ	E_a	logÃ	E_a	logÃ	E_a	logÃ	E_a
C_i-$(C)_2(H)_2$	0.000	0.00	0.000	0.00	0.000	0.00	0.000	0.00	0.00	0.00
C_i-$(C)_3(H)$	0.127	-4.66	0.286	-0.91	0.360	-3.56	0.236	0.35	0.01	-2.29
C_i-$(C_d)(C)_2(H)$	0.040	-4.34	0.070	-0.46	0.620	-0.41	0.180	-0.31	-0.38	-1.95
C_i-$(C_t)(C)_2(H)$	-0.060	-4.29	0.150	-2.91	0.510	4.15	0.100	-1.53	0.07	2.35
C_i-$(C)_4$	0.250	-5.66	0.790	-0.29	0.083	4.56	0.200	-4.72	0.32	0.54
C_i-$(C_d)(C)_3$	0.380	-3.05	0.510	-5.01	1.320	1.07	0.620	-5.65	0.08	1.47
C_i-$(C_t)(C)_3$	0.160	-2.41	0.350	-4.32	0.890	2.30	0.280	-2.83	0.45	4.43
C_i-$(C_d)_2(C)_2$	0.270	-5.52	0.540	-8.17	1.230	-2.05	0.560	-7.32	0.70	-0.53
C_i-$(C_d)(C_t)(C)_2$	0.180	-4.79	0.290	0.31	1.130	4.23	0.400	0.84	-0.21	3.34
C_i-$(C_t)_2(C)_2$	0.310	-2.50	0.300	-5.22	1.020	2.73	0.390	-0.71	0.45	8.21

Group additive values at 1500K

Table S-19: Primary group additive values ΔGAV° for 1-2 to 1-7 intramolecular hydrogen abstractions deduced from the combined training set and test set at 1500K. See main text for the reference reactions. The index i depends on the H-shift. For 1-2 H-shifts, i equals 2, for 1-3 H-shifts 3, etc. The units for $\Delta GAV°_{Ea}$ values are kJ mol^{-1}. For the reference reaction, the single-event pre-exponential factors are expressed in s^{-1} and Ea is expressed in kJ mol^{-1}. The reference reaction pre-exponential factor does not include tunneling nor the number of single events.

	1-2		1-3		1-4		1-5		1-6		1-7	
	logÃ	Ea	logÃ	Ea	logÃ	Ea	logÃ	Ea	logÃ	Ea	logÃ	Ea
Reference												
C_1-(C)$(H)_2$	0.000	0.00	0.000	0.00	0.000	0.00	0.000	0.00	0.000	0.00	0.000	0.00
C_1-$(C)_2$(H)	-0.020	7.37	0.104	5.73	0.044	4.84	0.028	5.16	0.085	4.27	0.220	4.42
C_1-(C_d)(C)(H)	0.415	33.66	0.761	42.04	0.691	42.53	0.754	45.89	0.732	47.53	0.420	46.48
C_1-(C_t)(C)(H)	0.121	25.37	0.205	31.65	0.186	28.04	0.049	30.04	-0.336	33.90	0.150	31.32
C_1-$(C)_3$	0.056	11.17	0.226	10.92	0.024	5.91	-0.304	6.58	-0.308	8.05	-0.300	7.18
C_1-$(C_d)(C)_2$	0.528	36.08	0.797	47.71	0.600	46.61	0.450	49.16	0.503	55.60	0.079	54.55
C_1-(C_t)(C)	-0.009	31.49	-0.027	38.91	-0.032	36.61	0.079	39.39	-0.097	39.28	-0.266	38.86
C_1-$(C_d)_2$(C)	0.373	53.81	0.520	59.20	0.353	61.04	0.091	72.31	0.236	76.25	-0.040	72.80
C_1-$(C_d)(C_t)$(C)	0.630	55.41	0.668	62.90	0.549	63.85	0.660	65.94	0.471	68.53	0.600	67.70
C_1-$(C_t)_2$(C)	0.179	55.73	0.209	60.26	0.208	53.00	0.385	62.56	0.033	62.09	0.171	62.13
C_i-(C)$(H)_3$	0.000	0.00	0.000	0.00	0.000	0.00	0.000	0.00	0.000	0.00	0.000	0.00
C_i-$(C)_2(H)_2$	0.033	-11.29	0.198	-11.79	0.094	-13.82	0.048	-12.32	0.111	-12.83	-0.002	-12.57
C_i-$(C_d)(C)(H)_2$	-0.136	-40.33	0.042	-32.00	-0.356	-31.32	-0.183	-26.33	-0.114	-24.89	-0.274	-25.70
C_i-$(C_t)(C)(H)_2$	-0.075	-35.15	0.173	-27.94	-0.021	-30.91	-0.088	-26.47	-0.252	-24.91	-0.054	-24.46
C_i-$(C)_3$(H)	0.107	-17.50	0.426	-16.79	-0.130	-23.55	-0.097	-22.19	-0.437	-22.95	-0.053	-20.91
C_i-$(C_d)(C)_2$(H)	-0.228	-44.17	-0.041	-35.99	-0.195	-40.68	-0.438	-36.96	-0.650	-32.68	-0.783	-32.37
C_i-(C_t)(C) (H)	-0.076	-39.81	0.131	-34.53	0.027	-37.94	-0.093	-33.22	-0.276	-33.68	-0.473	-35.26
C_i-$(C_d)_2$(C)(H)	-0.384	-60.37	-0.402	-52.46	-0.136	-52.97	-0.270	-38.09	-0.499	-36.31	-0.833	-37.71
C_i-$(C_d)(C_t)$(C) (H)	-0.090	-62.37	0.160	-46.38	-0.077	-49.65	-0.109	-46.04	-0.380	-43.68	-0.543	-43.82
C_i-$(C_t)_2$(C)(H)	-0.121	-62.92	0.180	-45.96	0.079	-54.35	-0.139	-42.84	-0.347	-44.46	-0.083	-43.73

Table S-20: Secondary group additive values ΔGAV° for 1-2 to 1-7 intramolecular hydrogen abstractions deduced from the combined training set and test set at 1500K. See main text for the reference reactions. The units for $\Delta GAV°_{Ea}$ values are kJ mol^{-1}. For the reference reaction, the single-event pre-exponential factors are expressed in s^{-1} and Ea is expressed in kJ mol^{-1}.

	1-3		1-4			
	i=2		i=2		i=3	
	logÃ	E_a	logÃ	E_a	logA	E_a
C_i-$(C)_2(H)_2$	0.000	0.00	0.000	0.00	0.000	0.00
C_i-$(C)_3(H)$	-0.068	-3.48	0.008	-6.88	0.101	-4.72
C_i-$(C_d)(C)_2(H)$	-0.077	-2.55	0.011	-10.38	0.027	-6.61
C_i-$(C_t)(C)_2(H)$	-0.246	-7.98	-0.097	-7.71	0.085	-2.99
C_i-$(C)_4$	0.292	-5.17	-0.074	-7.66	-0.168	-2.02
C_i-$(C_d)(C)_3$	-0.026	-6.98	-0.057	-11.97	-0.085	-6.20
C_i-$(C_t)(C)_3$	-0.030	-8.53	0.003	-10.53	0.048	-4.25
C_i-$(C_d)_2(C)_2$	0.162	-9.42	-0.031	-11.40	0.009	-2.90
C_i-$(C_d)(C_t)(C)_2$	0.229	-8.29	0.026	-13.09	-0.007	-6.50
C_i-$(C_t)_2(C)_2$	-0.003	-6.58	-0.031	-12.99	-0.017	-4.46

	1-5					
	i=2		i=3		i=4	
	logÃ	E_a	logÃ	E_a	logÃ	E_a
C_i-$(C)_2(H)_2$	0.000	0.00	0.000	0.00	0.000	0.00
C_i-$(C)_3(H)$	-0.032	-5.20	0.097	-3.76	0.030	-3.20
C_i-$(C_d)(C)_2(H)$	-0.076	-6.61	0.163	-4.54	-0.080	-4.51
C_i-$(C_t)(C)_2(H)$	-0.096	-6.61	-0.033	-1.77	-0.015	-1.60
C_i-$(C)_4$	-0.128	-7.16	-0.026	-6.17	-0.018	-2.66
C_i-$(C_d)(C)_3$	-0.008	-11.80	0.155	-11.50	0.061	-2.27
C_i-$(C_t)(C)_3$	0.022	-10.58	0.315	-8.21	0.151	-5.02
C_i-$(C_d)_2(C)_2$	0.103	-11.75	0.094	-10.89	0.098	-7.60
C_i-$(C_d)(C_t)(C)_2$	0.186	-11.56	0.090	-4.73	0.226	-5.15
C_i-$(C_t)_2(C)_2$	0.046	-10.90	-0.088	-5.19	0.146	-1.31

(Table S-20 continued)

	1-6							
	i=2		i=3		i=4		i=5	
	logÃ	E_a	logÃ	E_a	logÃ	E_a	logÃ	E_a
C_i-$(C)_2(H)_2$	0.000	0.00	0.000	0.00	0.000	0.00	0.000	0.00
C_i-$(C)_3(H)$	-0.228	-7.35	0.115	-2.68	0.188	-3.76	-0.164	-3.90
C_i-$(C_d)(C)_2(H)$	-0.098	-7.22	0.223	-3.61	0.153	-3.33	-0.003	-4.53
C_i-$(C_t)(C)_2(H)$	-0.139	-5.37	0.117	-0.16	-0.037	-0.07	-0.154	0.67
C_i-$(C)_4$	-0.103	-6.11	0.067	-3.94	0.121	-5.15	0.040	-1.05
C_i-$(C_d)(C)_3$	-0.231	-7.01	0.292	-7.28	0.308	-6.62	-0.109	-4.38
C_i-$(C_t)(C)_3$	-0.165	-8.82	0.201	-8.10	0.179	-9.01	-0.005	-2.38
C_i-$(C_d)_2(C)_2$	-0.247	-12.12	0.142	-10.44	0.418	-11.47	-0.288	-5.73
C_i-$(C_d)(C_t)(C)_2$	-0.172	-11.75	0.132	-7.55	0.293	-7.73	-0.213	-4.45
C_i-$(C_t)_2(C)_2$	-0.223	-9.06	0.033	-6.05	0.092	-2.45	-0.097	1.03

	1-7									
	i=2		i=3		i=4		i=5		i=6	
	logÃ	E_a	logÃ	E_a	logÃ	E_a	logÃ	E_a	logÃ	E_a
C_i-$(C)_2(H)_2$	0.000	0.00	0.000	0.00	0.000	0.00	0.000	0.00	0.00	0.00
C_i-$(C)_3(H)$	0.093	-5.27	0.225	-2.15	0.330	-4.07	0.199	-0.32	0.00	-2.55
C_i-$(C_d)(C)_2(H)$	0.000	-5.19	-0.030	-2.59	0.420	-4.39	0.000	-3.85	-0.42	-2.81
C_i-$(C_t)(C)_2(H)$	-0.090	-4.88	0.080	-4.12	0.390	1.92	0.040	-2.78	0.03	1.69
C_i-$(C)_4$	0.090	-8.79	0.660	-2.86	0.033	3.51	0.080	-7.01	0.29	-0.12
C_i-$(C_d)(C)_3$	0.320	-4.31	0.330	-8.62	1.140	-2.63	0.450	-8.97	0.01	0.19
C_i-$(C_t)(C)_3$	0.120	-3.22	0.230	-6.85	0.770	-0.06	0.130	-5.74	0.38	3.10
C_i-$(C_d)_2(C)_2$	0.190	-6.95	0.270	-13.60	0.880	-9.09	0.230	-13.92	0.62	-2.19
C_i-$(C_d)(C_t)(C)_2$	0.070	-6.94	0.130	-3.00	0.850	-1.29	0.170	-3.80	-0.30	1.69
C_i-$(C_t)_2(C)_2$	0.240	-3.77	0.160	-8.09	0.880	-0.09	0.260	-3.15	0.36	6.47

Transition state geometries

Below the CBS-QB3 optimized geometries of all the transition states are given in Cartesian coordinates. Before each transition state, the reactant and the product are given in SMILES notation.

1-2 H-shifts

Training set

```
Reactant: [CH2]C
Product: [CH2]C
C  0.756674  0.000121 -0.053345
C -0.750777 -0.000004 -0.026365
H  1.275459 -0.932211 -0.234704
H  1.275228  0.932574 -0.234755
H  0.022438  0.000308  1.038932
H -1.275682  0.932210 -0.189858
H -1.275475 -0.932453 -0.189188

Reactant: [CH2]CC
Product: C[CH]C
C  1.319659 -0.254107 -0.100456
C -1.284552 -0.187356 -0.011540
C  0.039071  0.530335  0.052532
H  2.211795  0.255288 -0.441703
H  1.256971 -1.330919 -0.198952
H  0.846342  0.215000  1.043030
H  0.081087  1.585803 -0.195063
H -1.242444 -1.137456  0.536806
H -2.091351  0.415616  0.418681
H -1.554805 -0.425615 -1.053095

Reactant: C#CC[CH2]
Product: C#C[CH]C
C -1.964757 -0.200133  0.002145
C  1.683343 -0.449884 -0.080781
C -0.798664  0.134837 -0.026392
C  0.548401  0.545483 -0.039820
H  2.659976 -0.099619 -0.384306
H  1.449573 -1.504681 -0.072047
H  1.208426  0.227821  1.014648
H  0.781915  1.565437 -0.328010
H -2.981008 -0.503925  0.035616

Reactant: C=CC[CH2]
Product: C=C[CH]C
C -1.897230 -0.002543  0.258930
C  0.707097  1.453386  1.065153
C -0.676011 -0.343364 -0.207900
C  0.582333  0.273206  0.152603
H -0.182148  1.954901  1.418375
H  1.664377  1.665207  1.520393
H  0.779497  1.442546 -0.321194
H  1.493817 -0.291282 -0.016533
H -0.604018 -1.138564 -0.946726
H -2.793007 -0.497623 -0.097896
H -2.035506  0.762333  1.015782

Reactant: [CH2]C(C)C
Product: C[C](C)C
C  0.001494  1.502385 -0.160740
C -1.298820 -0.726931 -0.001105
C  1.297377 -0.729513 -0.001211
C  0.000034  0.025610  0.162895
H  0.936405  1.975760 -0.434133
H -0.932489  1.977630 -0.434065
H  0.001015  0.985116  1.065761
H -1.467971 -0.974025 -1.062540
H -2.152443 -0.127202  0.337349
H -1.290118 -1.663592  0.568112
H  1.466039 -0.976783 -1.062682
H  1.286794 -1.666243  0.567862
H  2.152207 -0.131565  0.337348

Reactant: C#CC([CH2])C
Product: C#C[C](C)C
C -2.265251 -0.007967 -0.015598
C  1.110661  1.324784  0.169306
C  1.112602 -1.273472  0.056624
C -1.052657  0.029353 -0.042573
C  0.360127  0.039475 -0.099888
H  2.164405  1.257234  0.403298
H  0.550202  2.223866  0.382031
H  0.806297  0.773712 -1.056385
H  1.152741 -1.556286  1.116844
H  2.141178 -1.174553 -0.308986
H  0.617745 -2.072556 -0.501908
H -3.326048 -0.030775  0.001267
```

```
Reactant: C=CC([CH2])C
Product: C=C[C](C)C
C -2.073402 -0.171169  0.112514
C  0.481318  1.519491  0.084010
C  1.689594 -0.748558  0.157010
C -0.848252 -0.684619 -0.127967
C  0.414213  0.034141 -0.110940
H  1.421716  1.964933  0.378108
H -0.427780  2.102192  0.116531
H  0.573930  0.811822 -1.112161
H  1.815808 -0.902162  1.237280
H  2.571782 -0.213116 -0.212730
H  1.654240 -1.730106 -0.327863
H -0.765454 -1.738764 -0.387966
H -2.964118 -0.784140  0.034465
H -2.221676  0.862068  0.407512

Reactant: C#CC([CH2])C#C
Product: C#C[C](C)C#C
C -2.276061 -0.966494 -0.048428
C  2.276022 -0.966537 -0.048548
C  0.000010  1.850358 -0.177108
C -1.227372 -0.366586  0.008655
C  1.227350 -0.366606  0.008595
C -0.000003  0.355262  0.089559
H  0.947251  2.329771 -0.374737
H -0.947239  2.329805 -0.374612
H  0.000063  1.165590  1.063023
H -3.192742 -1.499391 -0.096201
H  3.192690 -1.499452 -0.096372

Reactant: C#CC([CH2])C=C
Product: C#C[C](C)C=C
C  0.676514  1.883726  2.431227
C -1.800174 -1.130076 -0.406718
C  1.152447 -0.308738 -0.398671
C  0.402752  1.193953  1.475217
C -1.358517 -0.039390  0.239190
C  0.046903  0.382894  0.355450
H  0.896964 -1.038503 -1.151896
H  2.171900 -0.172529 -0.070528
H  0.499216  0.921022 -0.696063
H -2.067962  0.629309  0.718185
H -2.859727 -1.350074 -0.470265
H -1.129302 -1.844187 -0.871521
H  0.924256  2.493676  3.263724

Reactant: C=CC([CH2])C=C
Product: C=C[C](C)C=C
C -2.229681 -0.702662  0.413269
C  1.783433  0.832321 -1.952797
C  0.817842 -0.719382  0.487269
C -1.478421  0.226513 -0.198918
C  0.567849  1.006398 -1.410153
C -0.009972  0.255669 -0.284357
H  1.872660 -0.811921  0.278280
H  0.342946 -1.388943  1.188037
H  0.489818  0.640909  0.805802
H -1.971817  1.064098 -0.688184
H -3.310506 -0.621005  0.436625
H -1.802575 -1.578371  0.889597
H -0.083607  1.779048 -1.813885
H  2.467084  0.059777 -1.618404
H  2.124415  1.455297 -2.771946
```

Test set

```
Reactant: C[CH]CC
Product: [CH2]CCC
C -1.561251  1.497964  0.810484
C  1.701450 -0.526246  0.020407
C -0.639746  0.345369  0.492521
C  0.664033  0.593271 -0.224350
H -0.782085  0.884549  1.685915
H -2.616488  1.304719  0.955039
H -1.238988  2.500957  0.558842
H -1.091102 -0.640093  0.425752
H  1.081471  1.556282  0.101554
H  0.477893  0.687009 -1.307865
H  1.303650 -1.494029 -0.306657
H  2.626642 -0.331988 -0.533038
H  1.938932 -0.597752  1.087166

Reactant: C[CH]CC
Product: C[CH]CC
C  1.969691  0.100744  0.156344
C -1.969379 -0.100265  0.154616
C  0.602427 -0.457607 -0.145991
C -0.601751  0.456328 -0.149355
H  2.104642  0.260844  1.238581
H  2.114240  1.072285 -0.334277
H  2.764036 -0.570392 -0.187809
H  0.407167 -1.510417  0.033654
H  0.000962 -0.003792 -1.233555
```

H -0.406714 1.510163 0.024436
H -2.105596 -0.254140 1.237597
H -2.113431 -1.074596 -0.330589
H -2.763303 0.568916 -0.194288

Reactant: C#CC[CH]C
Product: C#CCC[CH2]
C -2.591913 -0.286256 -0.083051
C 0.880027 -1.618595 -0.651099
C -1.472371 0.151115 0.020103
C 0.957904 -0.400678 0.229912
C -0.105565 0.680968 0.137895
H 0.593350 -1.597735 0.640274
H 1.791540 -2.150715 -0.890075
H 0.000819 -1.751496 -1.267162
H 1.939110 -0.108696 0.587496
H -0.049433 1.329713 1.022200
H 0.093014 1.316669 -0.743699
H -3.578104 -0.669425 -0.169104

Reactant: C#CC[CH]C
Product: C#C[CH]CC
C -2.211101 -0.559228 -0.050495
C 1.581156 -0.972089 -0.005710
C -1.233370 0.161794 -0.063708
C 1.304432 0.502805 -0.004487
C -0.118847 1.021075 -0.058643
H 2.581321 -1.190538 0.382134
H 0.843722 -1.509687 0.601113
H 1.511122 -1.379833 -1.027263
H 2.069184 1.210164 -0.302722
H 0.565522 1.015311 1.033259
H -0.248360 2.045848 -0.392321
H -3.060885 -1.194477 -0.031333

Reactant: C=CC[CH]C
Product: C=CCC[CH2]
C 2.488022 0.057662 -0.279110
C -1.177896 -0.561027 2.397185
C 1.328311 0.228119 0.353920
C -0.339438 -1.299834 1.383495
C 0.078392 -0.599376 0.107076
H -1.624761 -1.499988 1.579219
H -1.142093 -0.864337 3.435563
H -1.536415 0.430526 2.148728
H 0.276965 -2.112359 1.752859
H 0.272819 -1.325165 -0.691353
H -0.738995 0.056161 -0.229284
H 1.235933 0.978985 1.136668
H 3.362908 0.656372 -0.046290
H 2.606910 -0.690080 -1.058957

Reactant: C=CC[CH]C
Product: C=C[CH]CC
C -2.561236 -0.080673 -0.224192
C 1.450193 -1.014254 -2.123344
C -1.363958 0.281846 0.288664
C 0.165683 -1.058770 -1.342160
C -0.061956 -0.106798 -0.206817
H 2.303295 -0.789448 -1.469861
H 1.650343 -1.966274 -2.626093
H 1.416297 -0.225423 -2.892377
H -0.699856 -1.565446 -1.750248
H 0.277053 -1.322818 0.015268
H 0.793439 0.505982 0.063609
H -1.348926 0.905448 1.180192
H -3.488909 0.231960 0.241135
H -2.648947 -0.680431 -1.124026

Reactant: CC[CH]CCC
Product: CC[CH]CCC
C 3.196236 0.204680 0.263572
C -3.203594 -0.182563 0.270540
C 1.922998 -0.470644 -0.295752
C -1.928509 0.444135 -0.338911
C 0.674255 0.334766 -0.033842
C -0.680455 -0.335382 -0.005332
H 3.117681 0.322002 1.349668
H 4.088085 -0.390246 0.038003
H 3.327247 1.199294 -0.178590
H -3.128318 -0.209150 1.362857
H -3.333384 -1.210421 -0.087952
H -4.094626 0.391516 -0.006417
H 1.814219 -1.468566 0.152091
H 2.043171 -0.629894 -1.381134
H -1.822028 1.476317 0.023606
H -2.044340 0.511093 -1.434328
H 0.683704 1.398796 -0.254509
H -0.003814 0.046958 1.065518
H -0.689464 -1.414618 -0.132449

Reactant: CC(C)[C](C)C
Product: [CH2]C(C)C(C)C
C 1.140436 -1.101876 -0.903398

```
C  1.685411  0.801498  0.698095
C -1.835823 -0.849500  0.493441
C -1.062309  1.266997 -0.756112
C  0.692881 -0.337785  0.373090
C -0.737341  0.153434  0.213555
H -1.469155  0.134100  1.309571
H -1.563231 -1.831637  0.860435
H -2.807019 -0.706027  0.036014
H -1.003136  0.907714 -1.796308
H -0.379048  2.115199 -0.647115
H -2.083694  1.634021 -0.597242
H  0.707363 -1.049428  1.211504
H  1.188414 -0.416520 -1.757115
H  0.429706 -1.901833 -1.137279
H  2.133819 -1.543813 -0.761230
H  1.373058  1.342693  1.598006
H  2.689823  0.395545  0.864442
H  1.741376  1.512810 -0.133285
```

Reactant: CC(C)[C](C)C
Product: CC(C)[C](C)C

```
C  1.508640 -1.288002  0.089277
C  1.516809  1.278369  0.087772
C -1.514810 -1.278224  0.071691
C -1.506362  1.288156  0.071257
C  0.767756 -0.002619 -0.218265
C -0.762172  0.002446 -0.226857
H -2.547909 -1.202287 -0.287553
H -1.551651 -1.470333  1.157317
H -1.060576 -2.153097 -0.402670
H -1.045334  2.160078 -0.401992
H -2.539499  1.219539 -0.289361
H -1.543293  1.479954  1.156945
H  0.008921 -0.000518 -1.314159
H  1.053669 -2.160244 -0.389212
H  2.546032 -1.219234 -0.258883
H  1.532521 -1.479426  1.175391
H  1.540862  1.471661  1.173542
H  1.068179  2.152711 -0.392874
H  2.554060  1.202123 -0.259232
```

Reactant: [CH2]CCCCC
Product: C[CH]CCCC

```
C -3.287430 -0.130460  0.184389
C  3.156224  0.262675  0.137867
C -1.943127  0.449906 -0.183877
C  1.849478 -0.538185 -0.046915
C -0.715982 -0.426451 -0.190275
C  0.598900  0.366048 -0.001343
H -4.186531  0.357615 -0.169370
H -3.335444 -1.169261  0.486990
H -2.545779  0.628500  0.973701
H -1.947115  1.346086 -0.797111
H -0.798758 -1.179314  0.607247
H -0.662722 -0.985756 -1.140953
H  0.562403  0.894661  0.960222
H  0.676482  1.128761 -0.788777
H  1.770874 -1.300050  0.740284
H  1.875303 -1.068121 -1.008480
H  3.260770  1.015319 -0.652548
H  4.031756 -0.395139  0.102509
H  3.155840  0.781496  1.103701
```

Reactant: C[CH]CCCC
Product: CC[CH]CCC

```
C  0.142412 -1.856403 -3.030123
C -0.110699  0.362961  3.061942
C  0.305772 -1.937684 -1.533613
C  0.358029  0.431662  1.593459
C  0.232155 -0.680086 -0.697547
C -0.190750 -0.743013  0.748901
H -0.917719 -1.744421 -3.310742
H  0.530495 -2.752454 -3.526492
H  0.677697 -0.988255 -3.436549
H  0.286395  1.202688  3.642901
H -1.205258  0.393551  3.119350
H  0.228699 -0.568390  3.530761
H  0.076473 -2.868710 -1.024458
H  0.028333  1.378392  1.145307
H  1.454055  0.416327  1.548660
H  1.349853 -1.314932 -1.014667
H  0.108098  0.254220 -1.238576
H -1.292906 -0.747782  0.819173
H  0.151539 -1.689979  1.191621
```

Reactant: C#CC(C)[C](C)C=C
Product: C#C[C](C)C(C)C=C

```
C  3.076534  0.129205  0.247489
C -2.943449  1.142537 -0.004198
C  0.161537 -1.905900 -0.231625
C -0.079902  2.057328  0.113974
C  1.903871 -0.107033  0.029599
C -1.910439  0.282064 -0.174664
C  0.563413 -0.438895 -0.239406
```

C -0.513805 0.641161 -0.202544
H 0.967161 2.214722 -0.156179
H -0.696850 2.786942 -0.419722
H -0.180291 2.239964 1.192436
H -2.145856 -0.771008 -0.300174
H -2.799172 2.206272 0.144302
H -3.966992 0.786137 -0.000935
H 0.086625 0.210128 -1.314603
H 4.099779 0.342662 0.430742
H -0.266700 -2.176414 0.743363
H -0.583420 -2.129554 -1.003931
H 1.039481 -2.528852 -0.417494

Reactant: C#C[C](C#C)C(C=C)C=C
Product: C#CC(C#C)[C](C=C)C=C
C -2.279598 2.283768 -0.165893
C -2.370332 -2.232851 -0.116515
C 2.470817 1.570953 0.236605
C 2.455057 -1.588458 -0.303918
C -1.687984 1.233316 -0.045581
C -1.736684 -1.203934 -0.028291
C 1.221073 1.260048 -0.150968
C 1.192529 -1.318671 0.076151
C -1.000226 0.001019 0.089500
C 0.544427 -0.013825 0.090301
H -2.809294 3.198932 -0.258846
H -2.935887 -3.127531 -0.196620
H -0.233321 0.040460 1.187664
H 0.626313 2.009407 -0.667708
H 2.900454 2.537477 -0.002699
H 3.086474 0.889615 0.811890
H 0.550787 -2.146053 0.369562
H 3.128984 -0.822312 -0.666161
H 2.825707 -2.607171 -0.292081

Reactant: C#C[CH]C(C)C
Product: C#CC[C](C)C
C 2.780136 -0.100318 -0.149599
C -0.727556 -1.513276 0.030804
C -2.204371 0.619651 -0.195750
C 1.648576 0.331116 -0.048299
C 0.350093 0.853443 0.093533
C -0.889481 -0.023803 0.162926
H 0.178310 1.900457 -0.137288
H 3.766462 -0.482952 -0.231398
H -0.232870 0.568003 1.213208
H -0.663420 -1.794569 -1.033647
H -1.579481 -2.041908 0.472677
H 0.194008 -1.857553 0.511313
H -2.244823 1.664440 0.135898
H -2.351082 0.613287 -1.288614
H -3.043139 0.082071 0.260545

Reactant: C#CC[C](C)C
Product: C#CCC([CH2])C
C 0.696525 1.355428 3.099669
C -1.456875 -1.165959 -0.577818
C -1.224530 1.390614 -0.228786
C 0.554438 0.624019 2.150931
C 0.378771 -0.262440 0.993029
C -0.913967 -0.011652 0.230740
H 1.233845 -0.133459 0.304808
H 0.819634 1.996534 3.936590
H 0.404579 -1.307792 1.333157
H -1.938554 -0.757407 0.592237
H -0.959119 -2.126608 -0.526776
H -2.104023 -0.949593 -1.418221
H -0.581353 1.665275 -1.081312
H -2.266362 1.475613 -0.559519
H -1.054709 2.110687 0.577542

Reactant: C#C[CH]C(C#C)C=C
Product: C#CC[C](C#C)C=C
C -3.302484 -0.053881 -0.186468
C 2.643620 1.429221 -0.141553
C 1.356307 -2.098533 -0.040305
C -2.191711 0.430604 -0.081203
C 1.583388 0.858601 -0.014704
C 0.287526 -1.288308 0.036718
C -0.926305 1.004157 0.050058
C 0.349742 0.169346 0.123792
H -0.781510 2.069709 -0.076366
H -4.272338 -0.476685 -0.272176
H -0.265691 0.613378 1.189553
H -0.716800 -1.702507 0.032919
H 2.367488 -1.706396 -0.052138
H 1.238564 -3.173772 -0.107094
H 3.570003 1.937569 -0.243186

Reactant: C#C[CH]CC=C
Product: C#CC[CH]C=C
C -3.099530 -0.228480 0.187471
C 2.246591 1.550492 -0.174982
C -1.970799 0.133185 -0.077986

```
C  1.878195  0.254052 -0.046781
C -0.676007  0.561693 -0.402985
C  0.537613 -0.267164 -0.085181
H -0.511973  1.586841 -0.713667
H -4.082811 -0.555328  0.416951
H -0.041156 -0.242367 -1.273495
H  0.334513 -1.249355  0.325874
H  2.655735 -0.495615  0.080534
H  1.524335  2.354524 -0.268642
H  3.291310  1.838212 -0.169517
```

```
Reactant: C#C[CH]C(C)C#C
Product: C#CC[C](C)C#C
C  3.094444 -0.190918 -0.203390
C -3.024655 -0.606880 -0.133355
C -0.202481  1.660125 -0.025455
C  1.919774 -0.475476 -0.071500
C -1.871188 -0.248600 -0.009444
C  0.576884 -0.835368  0.094426
C -0.543793  0.193416  0.145015
H  0.268038 -1.865974 -0.037929
H  4.119489  0.062411 -0.310722
H  0.020745 -0.365985  1.214920
H -4.032777 -0.924154 -0.230706
H -0.133247  1.899464 -1.095118
H  0.767099  1.884944  0.429518
H -0.971606  2.289426  0.429631
```

```
Reactant: C#CC(C)[C](C)C=C
Product: C#C[C](C)C(C)C=C
C  3.076534  0.129205  0.247489
C -2.943449  1.142537 -0.004198
C  0.161537 -1.905900 -0.231625
C -0.079902  2.057328  0.113974
C  1.903871 -0.107033  0.029599
C -1.910439  0.282064 -0.174664
C  0.563413 -0.438895 -0.239406
C -0.513805  0.641161 -0.202544
H  0.967161  2.214722 -0.156179
H -0.696850  2.786942 -0.419722
H -0.180291  2.239964  1.192436
H -2.145856 -0.771008 -0.300174
H -2.799172  2.206272  0.144302
H -3.966992  0.786137 -0.000935
H  0.086625  0.210128 -1.314603
H  4.099779  0.342662  0.430742
H -0.266700 -2.176414  0.743363
H -0.583420 -2.129554 -1.003931
H  1.039481 -2.528852 -0.417494
```

1-3 H-shifts

Training set

Primary contributions

```
Reactant: [CH2]CC
Product: [CH2]CC
C -1.122448 -0.332707 -0.000070
C  1.114598 -0.343134  0.000041
C  0.001106  0.735801  0.000025
H -1.680255 -0.470368 -0.923926
H -1.680430 -0.470377  0.923679
H  0.004061  1.365678 -0.891479
H  0.003970  1.365593  0.891589
H -0.008096 -1.224854 -0.000005
H  1.671312 -0.485852 -0.923711
H  1.671252 -0.485878  0.923826
```

```
Reactant: [CH2]CCC
Product: C[CH]CC
C -1.580391 -0.536431 -0.078151
C  1.722032 -0.235514 -0.213994
C -0.718225  0.744512 -0.201381
C  0.470442  0.105097  0.569599
H -1.707917 -1.139904 -0.974403
H -2.428622 -0.507280  0.602277
H -0.465611  1.005719 -1.232214
H -1.150390  1.613384  0.299499
H -0.421244 -0.999232  0.630846
H  0.611521  0.463552  1.589942
H  2.266900  0.676979 -0.502154
H  1.466642 -0.771834 -1.136408
H  2.402167 -0.863609  0.371259
```

```
Reactant: [CH2]CC(C)C
Product: CC[C](C)C
C -1.860213  0.000038 -0.469405
C  1.154113 -1.293100 -0.097007
C  1.154173  1.293148 -0.096913
C -0.940454  0.000018  0.775384
C  0.357540  0.000043 -0.088606
H -2.388605  0.921892 -0.702563
H -2.388660 -0.921778 -0.702590
H -1.042505  0.892608  1.397952
```

```
H -1.042491 -0.892601  1.397913
H -0.586295  0.000051 -1.143739
H  0.497839 -2.158489 -0.247311
H  1.675955 -1.429815  0.863756
H  1.907226 -1.286819 -0.893096
H  1.907270  1.286896 -0.893018
H  1.676042  1.429760  0.863849
H  0.497939  2.158582 -0.247133

Reactant: C#CCC[CH2]
Product: C#C[CH]CC
C -2.417239 -0.310702  0.163223
C  1.875667 -0.674407 -0.078239
C -1.310404  0.076348 -0.146951
C  1.120038  0.504184  0.571167
C -0.002976  0.482001 -0.515127
H  1.795624 -1.644866  0.404665
H  2.799729 -0.464676 -0.611167
H  0.734088  0.285773  1.567260
H  1.680532  1.440502  0.584436
H  0.734982 -0.580771 -1.013626
H  0.082070  1.249783 -1.283769
H -3.383518 -0.653009  0.438003

Reactant: C=CCC[CH2]
Product: C=C[CH]CC
C  2.372990  0.149143 -0.047061
C -0.713563  1.507545 -1.939142
C  1.111618 -0.005451  0.396536
C -0.077354  0.102435 -1.955689
C -0.105533 -0.018527 -0.408955
H -1.747867  1.613595 -2.255590
H -0.055702  2.355306 -2.112168
H  0.929504  0.084483 -2.374527
H -0.688938 -0.653379 -2.451989
H -0.660352  1.240398 -0.468908
H -0.933854 -0.613464 -0.023312
H  0.948958 -0.086101  1.470471
H  3.210087  0.183211  0.641318
H  2.611715  0.239993 -1.101105

Reactant: C=CC(C)C[CH2]
Product: C=C[C](C)CC
C  2.135991 -1.022625 -0.483449
C  0.078609  2.162728 -1.132723
C -1.138406  0.112681  1.031513
C  1.247750 -0.530446  0.397965
C -0.286620  0.681094 -1.352374
C  0.067711  0.290656  0.111817
H  1.015333  2.516438 -1.555184
H -0.725616  2.888647 -1.047333
H  0.332189  0.186382 -2.102170
H -1.340665  0.512991 -1.585723
H  0.410190  1.614040  0.219633
H -0.827051  0.049286  2.080172
H -1.675177 -0.811134  0.775638
H -1.834804  0.952616  0.927681
H  1.420268 -0.709340  1.459462
H  2.032763 -0.884877 -1.554132
H  2.999520 -1.589062 -0.152393

Reactant: C#CC(C)C[CH2]
Product: C#C[C](C)CC
C -2.439579 -0.758855 -0.043899
C  1.829895 -0.932060 -0.475117
C  0.103133  1.805936 -0.130058
C -1.329806 -0.270274 -0.029994
C  1.082174 -0.446764  0.783871
C -0.018833  0.284685 -0.055424
H  1.743962 -1.983718 -0.735383
H  2.757929 -0.435339 -0.746871
H  1.654715  0.241045  1.410364
H  0.674211 -1.255007  1.391978
H  0.692489 -0.236813 -1.119894
H -0.168807  2.251362  0.835936
H -0.558751  2.211167 -0.900585
H  1.134659  2.092106 -0.364494
H -3.409626 -1.189183 -0.055206

Reactant: C=CC(C=C)C[CH2]
Product: C=C[C](C=C)CC
C -1.695260 -0.000151 -2.139277
C  2.182459 -0.592736  0.775924
C -0.764216  1.719001  1.054970
C -1.010986 -0.642651 -1.183510
C  0.977520 -0.946747  0.309821
C  0.131074  1.480697 -0.171967
C -0.101917 -0.054997 -0.172766
H -1.759750  2.122991  0.896448
H -0.289429  1.911977  2.012464
H -0.226559  1.966387 -1.080305
H  1.175188  1.752175 -0.013732
H -0.874147  0.187822  0.902694
H -1.141893 -1.720275 -1.087079
```

```
H -1.621551  1.070033 -2.297408
H -2.356672 -0.538647 -2.809107
H  0.713698 -2.004100  0.303176
H  2.885046 -1.339281  1.129676
H  2.517172  0.437716  0.817705

Reactant: C#CC(C#C)C[CH2]
Product: C#C[C](C#C)CC
C  2.288937  1.357787 -0.078798
C -2.288258  1.358629 -0.078920
C -0.000719 -2.177231 -0.497914
C  1.227321  0.779268 -0.048497
C -1.226863  0.779709 -0.048572
C -0.000199 -1.312543  0.774335
C  0.000098  0.039109 -0.036886
H  0.927565 -2.659290 -0.791345
H -0.929627 -2.658127 -0.791286
H  0.896248 -1.413989  1.386475
H -0.896390 -1.413431  1.386941
H -0.000090 -0.796502 -1.114872
H  3.213826  1.877922 -0.103091
H -3.212954  1.879106 -0.103251

Reactant: C#CC(C=C)C[CH2]
Product: C#C[C](C=C)CC
C  2.003906  0.208949 -1.887979
C -2.006324 -1.374766  0.261662
C  0.289721  1.160243  1.846635
C  1.133397  0.087762 -1.055952
C -0.733066 -1.264431 -0.137937
C -0.464276  1.283528  0.511740
C  0.119201 -0.054578 -0.051914
H -0.266237  0.837787  2.722613
H  1.157965  1.792206  2.008542
H -0.161255  2.140224 -0.090785
H -1.550349  1.267858  0.609156
H  0.768221 -0.102919  1.137360
H -0.221249 -2.138347 -0.533877
H -2.533290 -2.319474  0.186838
H -2.569968 -0.541374  0.665977
H  2.768942  0.317670 -2.615536
```

Secondary contributions

```
Reactant: [CH2]C(C)C
Product: [CH2]C(C)C
C  0.827893  1.119765 -0.115903
C  0.829769 -1.114442 -0.119156
C -1.506656  0.000667 -0.114483
C -0.083426  0.001050  0.458806
H  1.463903  1.660603  0.582132
H  0.427724  1.696040 -0.949143
H -0.106959 -0.000569  1.551844
H  1.551762  0.003996 -0.621838
H  1.466477 -1.656592  0.577222
H  0.430579 -1.688604 -0.954327
H -1.470370  0.002306 -1.210896
H -2.058895 -0.889285  0.208900
H -2.060424  0.888713  0.211513

Reactant: [CH2]C(C)(C)C
Product: [CH2]C(C)(C)C
C -1.012698 -0.000169  1.119015
C -1.013646 -0.000291 -1.115714
C  0.937604 -1.269456  0.000879
C  0.936774  1.270006  0.000750
C  0.071149 -0.000013  0.001191
H -1.147578 -0.925149  1.678265
H -1.147220  0.924340  1.679132
H -1.887747  0.000145  0.002023
H -1.148685  0.924258 -1.675641
H -1.148908 -0.925221 -1.674962
H  1.578425 -1.296245  0.890404
H  0.308165 -2.167228  0.001198
H  1.577648 -1.296333 -0.889202
H  0.306738  2.167359  0.000990
H  1.576788  1.297217 -0.889341
H  1.577581  1.297296  0.890268

Reactant: C#CC([CH2])C
Product: C#CC([CH2])C
C  2.256901 -0.001577 -0.135592
C -1.167103  1.122460 -0.190959
C -1.170656 -1.114383 -0.197995
C  1.082218 -0.000613  0.141718
C -0.330160  0.000484  0.497754
H -1.826489  1.709114  0.445205
H -0.675885  1.646612 -1.006749
H -0.455178 -0.002734  1.584648
H  3.285218 -0.002399 -0.398291
H -1.861705  0.006851 -0.726849
H -0.681005 -1.635316 -1.016788
H -1.832052 -1.702734  0.434511

Reactant: C=CC([CH2])C
```

```
Product: C=CC([CH2])C
C  2.048861 -0.006410 -0.307516
C -0.802878 -0.221466  2.020473
C -1.526596 -0.853878  0.007576
C  1.022854 -0.639118  0.259740
C -0.318990 -0.033590  0.551575
H -1.174579  0.657819  2.543097
H -0.244917 -0.937841  2.621636
H -0.349622  1.011810  0.234185
H  1.125703 -1.684969  0.551624
H  1.978727  1.034947 -0.609536
H  2.996863 -0.501081 -0.492026
H -1.869845 -0.909776  1.384489
H -1.306348 -1.865606 -0.329800
H -2.287581 -0.315277 -0.553910

Reactant: C=CC([CH2])(C)C
Product: C=CC([CH2])(C)C
C  2.198806 -0.376098  0.073436
C -1.369646 -0.347916  1.008733
C -0.954210  1.536545 -0.107522
C -0.385876 -0.642319 -1.349132
C  1.091723  0.169777  0.575090
C -0.293557  0.123492 -0.020982
H -2.044601 -1.142851  0.693827
H -1.063781 -0.363838  2.053831
H  1.148529  0.717423  1.516598
H  2.201262 -0.931435 -0.858375
H  3.153250 -0.286755  0.582034
H -1.913964  0.933100  0.742859
H -1.391290  1.822030 -1.063562
H -0.468992  2.332781  0.455224
H  0.253877 -0.178498 -2.108090
H -1.419066 -0.630864 -1.714224
H -0.077784 -1.685406 -1.217020

Reactant: C#CC([CH2])(C)C
Product: C#CC([CH2])(C)C
C -2.407060 -0.087602 -0.000459
C  0.930963 -0.791723 -1.115715
C  0.929141 -0.790219  1.121119
C  0.728260  1.537882  0.000977
C -1.201206 -0.028791  0.000464
C  0.257133  0.067488  0.001576
H  1.678881 -0.293425 -1.730994
H  0.291739 -1.517782 -1.611866
H -3.466453 -0.151458 -0.001255
H  1.528147 -1.423029  0.003615
H  1.676053 -0.291098  1.736952
H  0.289112 -1.515617  1.617198
H  0.356061  2.054519  0.891086
H  1.823633  1.574083  0.001809
H  0.357448  2.053353 -0.890385

Reactant: C=CC([CH2])(C)C=C
Product: C=CC([CH2])(C)C=C
C  0.303332  0.776784  2.454907
C -1.084813  2.354998 -0.607961
C -0.693400 -1.117567  0.283004
C  1.176823 -0.606006 -0.821419
C  0.691593  0.908004  1.188287
C -0.683768  1.122021 -0.910068
C  0.104174  0.192583 -0.005690
H -0.564693 -1.553729  1.271188
H -1.681599 -1.206057 -0.163662
H  1.495876  1.599013  0.938571
H -0.506654  0.113951  2.742484
H  0.781459  1.331764  3.255753
H -0.935671  0.691059 -1.879151
H -0.861912  2.804387  0.353884
H -1.658369  2.952011 -1.309404
H  0.297112 -1.680720 -0.552368
H  2.112447 -0.807681 -0.302704
H  1.243891 -0.407577 -1.889996

Reactant: C#CC([CH2])(C)C#C
Product: C#CC([CH2])(C)C#C
C  2.228232 -1.231974 -0.000653
C -2.227853 -1.232822 -0.000673
C -0.000545  1.340143  1.122950
C -0.000541  1.342824 -1.118015
C  1.214785 -0.578714  0.000151
C -1.214681 -0.579141  0.000132
C -0.000084  0.240887  0.001122
H -0.930275  1.445032  1.676404
H  0.930155  1.447478  1.674303
H  3.117472 -1.811545 -0.001366
H -3.116874 -1.812729 -0.001381
H -0.002182  2.203996  0.003538
H  0.930135  1.451377 -1.669180
H -0.930227  1.448908 -1.671320

Reactant: C#CC([CH2])(C)C=C
Product: C#CC([CH2])(C)C=C
```

```
C -0.432910  1.079649  2.469488
C -2.174770 -0.938808 -0.009469
C  0.532142  1.391453 -0.961190
C  1.487142 -0.450957 -0.131044
C -0.198662  0.697278  1.348887
C -1.030691 -0.612666 -0.603799
C  0.079473  0.231150 -0.006806
H  0.087492  1.393304 -1.954966
H  0.693386  2.359286 -0.492796
H -0.817027 -0.955937 -1.615120
H -2.918437 -1.549107 -0.510710
H -2.402700 -0.604982  0.997223
H -0.623978  1.423749  3.455311
H  1.740252  0.656998 -0.972264
H  1.521923 -1.373701 -0.707874
H  2.122220 -0.397195  0.749749
```

Test reactions

```
Reactant: C[CH]CCC
Product: C[CH]CCC
C -2.322944 -0.292664 -0.158834
C  2.321454 -0.296913  0.155601
C -0.987217 -0.143615  0.541504
C  0.985843 -0.137420 -0.542612
C -0.000179  0.929151  0.006530
H -2.186571 -0.341821 -1.246505
H -2.843956 -1.201141  0.162334
H -2.979258  0.566250  0.052632
H -0.984155 -0.283194  1.623129
H -0.438473  1.565517 -0.766999
H  0.438757  1.554759  0.788443
H -0.001109 -1.020353 -0.006336
H  0.982561 -0.262748 -1.625982
H  2.841397 -1.201780 -0.177266
H  2.185062 -0.359881  1.242546
H  2.978723  0.563904 -0.044870

Reactant: C=CCC[CH]C
Product: C=C[CH]CCC
C -2.872202 -0.251508 -0.668134
C  1.370418 -2.722768  1.424446
C -1.873636  0.284779  0.059531
C  0.015209 -2.348814  0.870131
C -0.533617 -0.258055  0.245855
C -0.056744 -1.555631 -0.455190
H  2.050302 -1.861355  1.407957
H  1.296829 -3.082798  2.456090
H  1.837531 -3.518822  0.821976
H -0.810719 -3.036150  1.050359
H -0.777016 -1.957110 -1.169914
H  0.914608 -1.444544 -0.943894
H -0.469461 -1.038012  1.384990
H  0.259852  0.467856  0.425900
H -2.077051  1.198983  0.615838
H -2.747338 -1.160535 -1.246437
H -3.850255  0.214865 -0.708879

Reactant: C#CCC[CH]C
Product: C#C[CH]CCC
C -0.469768  0.255532  2.592473
C  0.079678  1.483420 -1.596363
C -0.022612 -0.328553  1.627098
C  0.589229  0.061766 -1.517445
C  0.515303 -0.970297  0.483731
C -0.325052 -0.981195 -0.831906
H -0.314190  1.801651 -0.623129
H  0.871599  2.178043 -1.894935
H -0.739596  1.566049 -2.328026
H  1.221229 -0.296816 -2.329581
H -0.326022 -1.957439 -1.321021
H -1.350082 -0.637043 -0.682398
H  1.309051 -0.089070 -0.246391
H  1.140023 -1.846721  0.652179
H -0.862813  0.769364  3.433729

Reactant: [CH2]CCCCCC
Product: CC[CH]CCCC
C  1.241194  3.222820  3.108732
C -3.180225 -0.728390 -0.213671
C  1.542018  3.375024  1.596899
C -2.482850  0.648871 -0.236098
C  0.886674  2.008106  1.255216
C -1.146268  0.639223  0.536355
C -0.438478  2.012984  0.518200
H  2.081524  3.024828  3.770603
H  0.442174  3.835114  3.521514
H  1.030210  4.221090  1.131099
H  2.608008  3.421204  1.364426
H  0.686346  1.976696  2.662742
H  1.579078  1.203090  1.001900
H -1.100945  2.768014  0.965697
H -0.276112  2.318041 -0.530039
H -1.327679  0.345666  1.578781
H -0.480242 -0.116497  0.096935
```

H -3.147042 1.404537 0.204292
H -2.295417 0.949377 -1.275739
H -3.395020 -1.033774 0.817132
H -4.125356 -0.702370 -0.767393
H -2.537588 -1.491769 -0.667977

Reactant: CC[CH]CCCC
Product: CC[CH]CCCC
C 0.340144 -1.329239 -4.464921
C -3.319257 0.611905 0.036314
C 0.816741 -1.426138 -2.998961
C -2.339867 -0.552024 0.304060
C -0.309303 -1.770725 -2.043439
C -1.020819 -0.379146 -0.424301
C -0.063632 -1.597191 -0.520570
H -0.422207 -0.548949 -4.564088
H -0.099665 -2.279845 -4.788788
H 1.173403 -1.090653 -5.134907
H -4.258672 0.469720 0.581638
H -2.878542 1.564315 0.353492
H -3.543076 0.678874 -1.033853
H 1.269117 -0.471918 -2.694937
H 1.610853 -2.187934 -2.923624
H -2.801381 -1.500304 -0.004708
H -2.155887 -0.630912 1.388759
H -0.938646 -2.616725 -2.326494
H -1.162694 -0.645536 -1.821674
H -0.536769 0.593669 -0.318393
H -0.393513 -2.449837 0.079278
H 0.976297 -1.361513 -0.278227

Reactant: CC(C)C[C](C)C
Product: CC(C)C[C](C)C
C 1.922004 1.288628 -0.211982
C 1.921847 -1.288877 -0.212034
C -1.929376 1.288919 -0.203695
C -1.929574 -1.288628 -0.203759
C -0.001153 -0.000030 1.000581
C 1.128916 -0.000080 -0.070343
C -1.135900 0.000081 -0.065586
H -1.266142 2.161138 -0.232694
H -2.532809 1.283185 -1.118770
H -2.612896 1.416441 0.651949
H -2.533018 -1.282750 -1.118825
H -2.613103 -1.416096 0.651886
H -1.266474 -2.160947 -0.232818
H 0.000244 0.893306 1.633013
H 0.000117 -0.893404 1.632959
H -0.005271 0.000015 -0.942170
H 2.608944 1.416327 0.640892
H 2.521779 1.282532 -1.129450
H 1.258776 2.160930 -0.238590
H 2.521613 -1.282823 -1.129509
H 1.258516 -2.161099 -0.238662
H 2.608783 -1.416687 0.640827

Reactant:
C#CC(C)C([CH2])(C#C)C=C
Product: C#C[C](C)C(C)(C#C)C=C
C -2.985333 0.823042 -0.593613
C 2.544062 -1.123073 -0.766748
C 1.323631 2.262524 -0.585392
C -0.853484 -2.057864 -0.432113
C 0.378833 -0.219195 1.935430
C -2.020144 0.160503 -0.278103
C 1.603158 -0.584811 -0.235332
C 0.433744 1.577688 0.126817
C -0.924878 -0.644777 0.144181
C 0.479668 0.086758 0.407595
H 1.002032 -1.024151 2.315556
H 0.209251 0.632713 2.589965
H -0.418794 2.079096 0.576864
H 2.175355 1.776877 -1.049230
H 1.224972 3.333310 -0.728256
H 3.368700 -1.608611 -1.226352
H -0.916970 -0.760402 1.501960
H -0.130132 -2.664155 0.120776
H -0.534914 -2.017853 -1.480169
H -1.837680 -2.531412 -0.375231
H -3.826892 1.404205 -0.877657

Reactant: C=CCC([CH2])C
Product: C=C[CH]C(C)C
C 2.312251 -0.164397 -0.688429
C -1.165846 1.396446 -0.240438
C -1.935425 -1.061980 -0.025274
C 1.710746 -0.066287 0.512141
C 0.277032 0.010203 0.771724
C -0.788527 -0.097184 -0.354793
H -2.135670 1.645929 0.185348
H -0.763170 2.078383 -0.985382
H -0.347052 -0.346118 -1.322585
H -2.377345 -0.807860 0.946106
H -1.574896 -2.095877 0.020805

```
H -2.723630 -1.003127 -0.784729
H -0.134218  1.317416  0.834626
H -0.062331 -0.387491  1.730074
H  2.340052  0.011037  1.397910
H  3.393039 -0.177849 -0.775297
H  1.753239 -0.239465 -1.614851
```

```
Reactant: C=CCC([CH2])C
Product: C=CCC([CH2])C
C  2.301111  0.171245 -1.544718
C -1.132108  1.228405 -0.406311
C -2.113024 -0.622339  0.372837
C  1.706122 -0.162972 -0.400789
C  0.377483 -0.873936 -0.294462
C -0.687866 -0.009014  0.414247
H -0.731596  1.316047 -1.414767
H -1.275371  2.161893  0.134492
H -0.358884  0.242944  1.426410
H -2.373554  0.530570 -0.419276
H -2.710682 -0.567245  1.280530
H -2.244780 -1.516723 -0.235206
H  0.013926 -1.135409 -1.296954
H  0.500112 -1.809628  0.270069
H  2.175539  0.096842  0.547704
H  1.860576 -0.073866 -2.507550
H  3.251332  0.695143 -1.567233
```

```
Reactant: C#CC([CH2])C(C)C
Product: C#CC(C)[C](C)C
C  2.611935 -0.696946  0.405570
C -2.151549 -0.031248  0.777180
C -0.701001 -1.415227 -0.853527
C  0.208870  1.734467 -0.763009
C  1.576519 -0.076120  0.378039
C -0.942789 -0.098715 -0.139912
C  0.331479  0.677401  0.372864
H  0.916685  1.632276 -1.581584
H -0.055770  2.749254 -0.474126
H  0.149249  1.113992  1.360955
H  3.521958 -1.243030  0.412683
H -0.955143  0.955013 -1.069135
H -2.328811  0.992699  1.127081
H -3.051985 -0.380390  0.259876
H -1.997301 -0.669421  1.661296
H -1.616106 -1.750497 -1.353788
H  0.096081 -1.323991 -1.598251
H -0.393715 -2.189799 -0.135278
```

```
Reactant: C#CC([CH2])(C)CC
Product: C#CC([CH2])(C)CC
C  2.662858 -0.781452  0.004655
C -0.716600 -1.809858  1.426115
C -0.127000  1.114830 -1.186693
C -0.065979  1.308799  1.040118
C  1.535951 -0.347441  0.009259
C -0.872013 -0.992156  0.129304
C  0.163412  0.154919  0.012032
H -1.049966  0.936976 -1.737272
H  0.734643  1.439560 -1.764620
H -0.345168  2.041204 -0.137977
H -0.961210  1.238491  1.656127
H  0.821711  1.724920  1.509772
H  3.658745 -1.148311 -0.003734
H -1.872836 -0.542392  0.086615
H -0.762777 -1.645517 -0.744408
H  0.277609 -2.265344  1.469087
H -1.468486 -2.605146  1.474265
H -0.838139 -1.166668  2.304838
```

```
Reactant: C#CC([CH2])(C)CC
Product: C#CC(C)(C)[CH]C
C  1.447370  1.974599  0.010050
C -2.004578  0.890942 -0.179996
C  0.096491 -1.053055  1.407028
C  1.043481 -1.383235 -0.972090
C  0.916012  0.890121  0.010109
C -1.254182 -0.420163 -0.271342
C  0.296692 -0.432412 -0.009631
H  0.151857 -0.359445  2.242650
H  0.506700 -2.048253  1.572044
H  0.562750 -2.368190 -0.962621
H  2.086353 -1.496038 -0.659649
H  1.018722 -0.986555 -1.991935
H  1.911073  2.929224  0.018885
H -1.259819 -1.091887  0.967818
H -1.571432 -1.113790 -1.052421
H -1.736420  1.554359 -1.014836
H -1.758865  1.421744  0.746249
H -3.085948  0.720129 -0.208718
```

```
Reactant: C=CC([CH2])C(C#C)C=C
Product: C=CC(C)[C](C#C)C=C
C -2.802450  0.164095 -1.223314
C  1.040687  2.372191  0.478161
```

```
C  2.808666 -0.636682 -0.848602
C -0.961562 -1.069162  1.677073
C -1.901723  0.340041 -0.257634
C  0.833842  1.184669  0.366681
C  1.606795 -1.055564 -0.436597
C -0.907833 -0.695499  0.176879
C  0.601031 -0.224859  0.271135
H -1.381291 -0.320561  2.345612
H -1.089606 -2.111301  1.958849
H -0.970763 -1.580098 -0.463069
H -1.856728  1.281513  0.285237
H -3.512582  0.939751 -1.490422
H -2.863992 -0.763212 -1.786382
H  0.497924 -0.683638  1.541515
H  1.217521  3.414491  0.573750
H  1.313764 -2.092919 -0.584532
H  3.123490  0.393159 -0.718304
H  3.504415 -1.311712 -1.334629
```

Reactant: C#CC(C#C)C([CH2])(C)C
Product: C#CC(C#C)C([CH2])(C)C

```
C -1.931206  2.089984  0.398952
C -0.547013 -0.038272 -3.267764
C  1.708694 -1.246944 -0.363675
C  1.013719 -0.184624  1.476311
C  1.697112  1.340348 -0.503587
C -1.294562  1.178533 -0.067484
C -0.540561  0.019987 -2.063531
C -0.513834  0.041677 -0.589387
C  0.956291  0.076450 -0.054020
H  1.132949 -2.059060 -0.805397
H  2.737532 -1.151478 -0.706087
H  1.690706 -1.357576  1.051386
H  0.083382 -0.455176  1.973702
H  1.696435  0.439408  2.050204
H  1.185507  2.232730 -0.128787
H  2.721215  1.331413 -0.113863
H  1.737192  1.387772 -1.596606
H -0.974164 -0.889832 -0.222693
H -2.490784  2.901207  0.793332
H -0.557654 -0.071762 -4.328662
```

Reactant: C#CC(C#C)C([CH2])(C)C
Product: C#C[C](C#C)C(C)(C)C

```
C  1.857290 -2.257715 -0.126192
C  1.857094  2.257822 -0.126766
C -1.358007 -0.000728  1.509481
C -1.518720 -1.266253 -0.724803
C -1.519053  1.266504 -0.723659
C  1.264315 -1.216067  0.038237
C  1.264207  1.216162  0.037910
C  0.542859  0.000053  0.278795
C -1.036685 -0.000141 -0.002761
H -1.699959 -0.930914  1.957912
H -1.701382  0.928682  1.958428
H -1.140741 -1.289645 -1.752506
H -2.614666 -1.271516 -0.752290
H -1.174985 -2.169135 -0.212201
H -1.141007  1.290984 -1.751308
H -1.175643  2.169020 -0.210190
H -2.615000  1.271449 -0.751210
H  0.144163  0.000054  1.566944
H  2.389380 -3.163693 -0.276515
H  2.389111  3.163808 -0.277309
```

Reactant: C#CCC([CH2])(C=C)C=C
Product: C#C[CH]C(C)(C=C)C=C

```
C -2.798435 -1.346846 -0.403945
C  0.391214  1.889144 -1.757872
C  3.053032  0.106831  0.126883
C  0.491477  0.780315  1.614578
C -1.670697 -1.196711  0.018001
C -0.194474  1.184874 -0.791987
C  1.860676 -0.205643 -0.376261
C -0.378830 -1.002209  0.564380
C  0.520219  0.242039  0.156490
H -0.066369  1.695745  1.793722
H  1.365356  0.601083  2.235728
H -1.264068  1.276077 -0.618220
H  1.456263  1.816183 -1.952031
H -0.177249  2.568384 -2.384656
H  1.793925 -0.829901 -1.265980
H  3.163045  0.743279  0.999028
H  3.970562 -0.260093 -0.321573
H -0.404026 -0.367794  1.777358
H  0.213077 -1.896178  0.763638
H -3.782558 -1.480107 -0.778566
```

Reactant: C=CC(C)C([CH2])(C)C=C
Product: C=CC(C)C([CH2])(C)C=C

```
C -2.934027 -0.509296 -0.535037
C  2.311940  1.054593 -1.011170
C -0.576519  1.724563  0.952280
C  0.419847 -1.950596 -0.076952
```

```
C  1.488541 -0.638070  1.378028
C -1.786231  0.164818 -0.595345
C  1.235394  0.270702 -1.050197
C -0.774678  0.250259  0.526275
C  0.588266 -0.414981  0.129127
H  1.053158 -2.401470 -0.839361
H -0.581734 -2.362932  0.029387
H  1.153755 -1.988444  1.134864
H  2.562365 -0.545319  1.232681
H  1.101868 -0.317226  2.343907
H  0.745996  0.085810 -2.005556
H  2.716226  1.511344 -1.909027
H  2.831561  1.269558 -0.082641
H -1.160674 -0.320284  1.382854
H -1.527183  2.151489  1.287979
H -0.200231  2.313052  0.109912
H  0.149305  1.795447  1.769914
H -1.536601  0.725823 -1.494743
H -3.634464 -0.527784 -1.364068
H -3.222032 -1.065470  0.353370
```

Reactant: C=CC(C)C([CH2])(C)C=C
Product: C=C[C](C)C(C)(C)C=C

```
C -2.883832  0.823042  1.279774
C  2.964203  0.447874 -0.037263
C -0.447669  1.954506 -0.028194
C  0.514220 -0.585141 -1.501318
C  0.426074 -1.820571  0.716651
C -1.880349  0.028214  0.864607
C  1.818506  0.235565  0.607244
C -0.712614  0.454067  0.083932
C  0.594122 -0.441655  0.036807
H  1.045637  0.148010 -2.102931
H  0.416496 -1.583700 -1.921077
H  1.324465 -2.418241  0.530130
H  0.295966 -1.713393  1.799066
H -0.436339 -2.359254  0.309008
H  1.726534  0.525819  1.653852
H  3.097520  0.158812 -1.075322
H  3.815518  0.912374  0.449945
H -0.809236  0.040404 -1.214301
H -1.334740  2.481475 -0.393924
H  0.380315  2.151756 -0.714018
H -0.181756  2.369977  0.952598
H -1.945999 -1.032372  1.089617
H -2.894862  1.892286  1.100455
H -3.732141  0.416282  1.819953
```

Reactant: C=CCC([CH2])(C#C)C#C
Product: C=C[CH]C(C)(C#C)C#C

```
C  2.454157 -1.444961 -1.717535
C -3.016790 -0.218456 -0.799450
C  0.326304  2.514729  0.247486
C -0.461503 -0.631525  1.697265
C  1.686198 -0.633933 -0.967282
C -1.916902 -0.100133 -0.319272
C -0.084110  1.380796  0.247010
C  0.441350 -1.044528 -0.331521
C -0.579676  0.001299  0.270937
H -1.261770 -1.310736  1.978413
H -0.024232 -0.008193  2.471893
H -3.984865 -0.315050 -1.223941
H  0.679757  3.515741  0.246986
H  0.580818 -1.409016  0.973453
H -0.079797 -1.901914 -0.757229
H  2.006079  0.386550 -0.774449
H  3.393187 -1.103669 -2.138933
H  2.165887 -2.469457 -1.934397
```

Reactant: C=CC(C=C)C[C](C)C
Product: C=C[C](C=C)CC(C)C

```
C  1.045216  2.560700  0.011404
C  1.564007 -2.131389  1.168331
C -2.086812 -1.643797  0.051928
C -2.364890  0.859726 -0.573515
C  1.370933  1.296578 -0.298036
C  1.639092 -1.113536  0.297704
C -0.505374  0.142347  1.111350
C -1.504916 -0.247901 -0.004435
C  0.734152  0.050787  0.181608
H -2.575275 -1.906346 -0.892982
H -2.841632 -1.715424  0.853664
H -1.306216 -2.383682  0.260434
H -1.765195  1.754489 -0.773247
H -2.846964  0.545288 -1.505780
H -3.159135  1.138702  0.139988
H -0.476584 -0.569280  1.938677
H -0.670550  1.144637  1.511130
H -0.176926 -0.286197 -0.761468
H  2.184255  1.131852 -1.004940
H  0.258101  2.808838  0.714610
H  1.578234  3.397098 -0.427247
H  2.437370 -1.126938 -0.444406
H  0.807653 -2.185731  1.942918
```

```
H  2.280272 -2.945086  1.138317
```

1-4 H-shifts

Training set

Primary contributions

```
Reactant: [CH2]CCC
Product: [CH2]CCC
C -1.263259 -0.678090 -0.147174
C  1.244321 -0.700158  0.146191
C -0.752322  0.728012  0.208178
C  0.757933  0.715155 -0.207028
H -1.498452 -0.832326 -1.201909
H -1.972828 -1.148745  0.531629
H -0.825511  0.881807  1.291113
H -1.310752  1.527705 -0.290677
H  0.833686  0.869300 -1.289730
H  1.330162  1.504296  0.292997
H -0.014380 -1.246678 -0.000957
H  1.945715 -1.181992 -0.533260
H  1.476582 -0.860046  1.200727

Reactant: [CH2]CCCC
Product: C[CH]CCC
C -1.405284  1.085193 -0.160829
C  2.154040  0.262924 -0.145562
C -1.578094 -0.429689  0.028307
C  0.798069  0.018922  0.491742
C -0.138876 -1.018143 -0.156544
H -1.984750  1.749008  0.478682
H -1.341649  1.419053 -1.198117
H -1.924055 -0.636532  1.047782
H -2.294442 -0.872682 -0.672608
H  0.087992 -1.082690 -1.228556
H -0.037655 -2.019659  0.276901
H -0.073584  1.043880  0.259743
H  0.818044 -0.041593  1.584129
H  2.668488  1.109272  0.323948
H  2.806440 -0.618961 -0.046582
H  2.045445  0.474777 -1.216065

Reactant: C=CCCC[CH2]
Product: C=C[CH]CCC
C -2.851329  0.188241  0.201081
C  1.748652  1.210756 -0.277705
C -1.656204 -0.106022 -0.342592
C  2.076329 -0.220945  0.148511
C -0.372499 -0.054960  0.356742
C  0.752782 -1.024775 -0.068557
H  2.129804  2.036243  0.319200
H  1.728791  1.398209 -1.351840
H  2.341374 -0.239980  1.211889
H  2.908292 -0.654397 -0.418728
H  0.732969 -1.967184  0.488314
H  0.639543 -1.252001 -1.136352
H  0.315759  1.006750  0.025231
H -0.459168  0.053665  1.442680
H -1.608895 -0.377770 -1.397211
H -3.765814  0.164588 -0.381538
H -2.946521  0.461188  1.248198

Reactant: [CH2]CCC(C)C
Product: CCC[C](C)C
C  1.651678 -0.224965 -1.053555
C -1.712515 -1.176775 -0.094252
C -1.237657  1.336430 -0.214313
C  1.739389  0.280623  0.393490
C  0.402902 -0.186352  1.065530
C -0.670812 -0.069278 -0.040742
H  1.907223 -1.276242 -1.196628
H  2.015953  0.426921 -1.845812
H  2.615114 -0.102714  0.929630
H  1.790446  1.375114  0.402366
H  0.500028 -1.237601  1.364194
H  0.154009  0.403213  1.956306
H  0.243377 -0.223569 -1.025012
H -2.387216 -1.120023  0.775239
H -1.237825 -2.164791 -0.086279
H -2.328047 -1.093570 -0.998171
H -1.879526  1.596910  0.641655
H -1.844369  1.406951 -1.124639
H -0.437270  2.082579 -0.274521

Reactant: C#CCCC[CH2]
Product: C#C[CH]CCC
C -2.896785 -0.215522 -0.190309
C  1.655433 -1.162457 -0.163206
C -1.756558 -0.056951  0.191790
C  1.931360  0.342021 -0.107210
C -0.406790  0.097789  0.615234
C  0.526694  1.018886 -0.214254
H  1.445717 -1.572288 -1.151715
H  2.222242 -1.822405  0.489854
```

```
H  2.600797  0.681066 -0.905911
H  2.388111  0.600251  0.855135
H  0.522012  2.052068  0.145771
H  0.191011  1.007652 -1.256372
H  0.317139 -0.979706  0.375983
H -0.287616  0.225553  1.695906
H -3.894671 -0.352137 -0.524841
```

```
Reactant: [CH2]CCC(C)C#C
Product: CCC[C](C)C#C
C  1.728000 -0.707897 -1.036330
C -2.761402 -0.920462 -0.025357
C -0.433140  1.774271 -0.294580
C  1.996839 -0.200235  0.381893
C -1.680845 -0.370287 -0.013598
C  0.597885 -0.170843  1.083137
C -0.398128  0.261213 -0.030793
H  2.244449 -0.233858 -1.868127
H  1.591754 -1.784511 -1.141389
H  2.414435  0.811610  0.344963
H  2.699311 -0.836760  0.932420
H  0.335841 -1.179562  1.418329
H  0.565422  0.505586  1.943963
H  0.344635 -0.237248 -0.986580
H -0.870251  2.293816  0.567521
H -1.036097  1.999371 -1.179194
H  0.580599  2.156999 -0.453524
H -3.708554 -1.399124 -0.033533
```

```
Reactant: [CH2]CCC(C)C=C
Product: CCC[C](C)C=C
C -1.847440 -0.683352  1.087630
C  2.766823 -0.469090 -0.008323
C  0.591764  1.532659  0.423404
C -2.162461  0.058256 -0.211425
C  1.484803 -0.753216 -0.294860
C -0.848240 -0.011172 -1.059181
C  0.312785  0.099679 -0.034302
H -1.883567 -1.772075  1.041607
H -2.185032 -0.258480  2.030236
H -3.007041 -0.381707 -0.754978
H -2.408812  1.103359  0.004324
H -0.793201 -0.987008 -1.557282
H -0.796602  0.769990 -1.825782
H -0.395277 -0.420898  0.923209
H  1.082780  2.097518 -0.380349
H  1.242508  1.549301  1.303967
H -0.342038  2.042573  0.681563
H  1.256366 -1.718362 -0.747524
H  3.066808  0.473712  0.436174
H  3.560812 -1.178491 -0.215877
```

```
Reactant: [CH2]CCC(C#C)C=C
Product: CCC[C](C#C)C=C
C  2.088266  1.671030 -0.496879
C -0.897225  0.305188  2.187585
C  0.203452 -2.656529  0.267340
C  0.705106  2.123118 -0.956972
C -0.342112  0.080010  1.136584
C  0.505297 -1.597823 -0.494252
C -0.085631  0.811422 -1.251139
C  0.336140 -0.171017 -0.112998
H  2.770167  1.318430 -1.270886
H  2.560960  2.178989  0.339786
H  0.744492  2.771458 -1.840691
H  0.205908  2.667761 -0.149029
H -1.168471  0.955990 -1.285581
H  0.247465  0.390539 -2.207739
H  1.495624  0.373677  0.015791
H  0.939239 -1.749183 -1.481046
H  0.381711 -3.669539 -0.076329
H -0.234690 -2.535158  1.252320
H -1.386521  0.509120  3.107174
```

```
Reactant: [CH2]CCC(C=C)C=C
Product: CCC[C](C=C)C=C
C  2.388704 -1.502199  0.106832
C -1.002829 -0.335483 -2.076097
C  0.220386  0.903714  2.458372
C  2.635493 -0.001068  0.189869
C -0.958122 -0.528830 -0.752156
C -0.305771  0.049243  1.574134
C  1.324660  0.677331 -0.330878
C  0.162058 -0.211314  0.179541
H  2.718696 -2.143378  0.919961
H  2.412551 -1.951071 -0.885639
H  2.810606  0.285895  1.230954
H  3.503792  0.314090 -0.402867
H  1.221538  1.715910 -0.002517
H  1.337048  0.665151 -1.424443
H  0.869186 -1.258094  0.266760
H -1.817660 -0.997132 -0.272155
H -1.869733 -0.635292 -2.655155
H -0.195595  0.129857 -2.630723
```

```
H -1.161147 -0.553474  1.880042
H  1.065806  1.541142  2.223726
H -0.192206  1.001764  3.456894

Reactant: [CH2]CCC(C#C)C#C
Product: CCC[C](C#C)C#C
C  1.939795 -0.298558 -1.116498
C -1.158327  2.430737 -0.099824
C -2.222832 -1.965636 -0.091639
C  2.083423  0.157526  0.333434
C -0.815335  1.273087 -0.042549
C -1.390569 -1.089557 -0.035862
C  0.792282 -0.335346  1.055415
C -0.350044 -0.095269  0.011003
H  2.100616 -1.358481 -1.312904
H  2.240724  0.373554 -1.915979
H  2.983104 -0.244645  0.814280
H  2.125169  1.250656  0.375999
H  0.592566  0.182045  1.996561
H  0.856670 -1.412629  1.239963
H  0.442409 -0.240223 -0.996542
H -1.473881  3.443069 -0.146225
H -2.967176 -2.720868 -0.137211
```

Secondary contributions

```
Reactant: [CH2]CC(C)C
Product: CCC([CH2])C
C -1.931312 -0.132016 -0.014201
C  0.057852  1.408993 -0.169390
C  1.905358 -0.388716 -0.055615
C -0.627545 -0.937626 -0.113547
C  0.492954  0.039356  0.382003
H -2.668269 -0.257800 -0.806023
H -2.367330 -0.074042  0.984666
H -0.428592 -1.191495 -1.162526
H -0.644134 -1.866596  0.467836
H  0.446719  0.077409  1.478574
H -1.281349  1.073238 -0.167620
H  0.286282  1.561088 -1.227281
H  0.239080  2.288181  0.447847
H  2.144031 -1.389980  0.324209
H  2.662935  0.309433  0.317936
H  1.966753 -0.411335 -1.150420

Reactant: C=CC(C)C[CH2]
Product: C=CC([CH2])CC
C -2.610221 -0.123179  0.302466
C  2.276381 -0.544819  0.009665
C  0.674506  1.396573  0.101194
C -1.462616  0.100843 -0.337406
C  0.857730 -1.005837 -0.348363
C -0.095099  0.072986  0.290927
H  3.048902 -0.645682 -0.750950
H  2.613262 -0.807858  1.013710
H  0.722969 -0.988328 -1.436757
H  0.618294 -2.011467  0.011786
H -0.184771 -0.136532  1.364074
H -1.470016  0.323657 -1.404773
H -2.633578 -0.346809  1.365549
H -3.568123 -0.091067 -0.206550
H  1.906602  0.774094  0.112593
H  0.606062  1.815558 -0.905625
H  0.593681  2.142193  0.890683

Reactant: [CH2]CC(C)(C)C
Product: CCC([CH2])(C)C
C  2.030343 -0.218360 -0.158243
C  0.149229  0.256867  1.449650
C -1.593672  1.027951 -0.267148
C -0.884752 -1.396212 -0.152328
C  0.811433  0.350978 -0.899683
C -0.424503  0.068013  0.030700
H  2.942484  0.376715 -0.162290
H  2.209279 -1.286394 -0.285885
H  0.665129 -0.083253 -1.895733
H  0.924379  1.436436 -1.011751
H  1.427391 -0.099611  1.070554
H  0.255752  1.297554  1.765290
H -0.226544 -0.401778  2.233127
H -1.281836  2.069055 -0.122425
H -2.441844  0.823629  0.396973
H -1.932451  0.908401 -1.304442
H -1.708291 -1.624966  0.534750
H -1.232650 -1.560821 -1.179079
H -0.063418 -2.091933  0.052122

Reactant: C#CC(C)C[CH2]
Product: C#CC([CH2])CC
C -2.706211 -0.269685 -0.030192
C  2.205364 -0.354803 -0.143256
C  0.429489  1.434488 -0.215992
C -1.537857 -0.070628  0.200826
C  0.813190 -0.992489 -0.063803
C -0.120798  0.163247  0.470063
```

```
H  2.824353 -0.606354 -1.002547
H  2.755928 -0.312298  0.797898
H  0.467580 -1.275503 -1.062943
H  0.766496 -1.871678  0.585789
H  0.036117  0.254841  1.553285
H -3.732339 -0.440766 -0.240568
H  1.707997  0.911536 -0.306517
H  0.416222  2.357227  0.361083
H  0.113255  1.550224 -1.253160
```

Reactant: C#CC(C)(C)C[CH2]
Product: C#CC([CH2])(C)CC

```
C -2.675187 -0.680976 -0.104214
C  2.211365 -0.497394 -0.217429
C  0.424050  0.029256  1.479524
C -0.077847  1.679059 -0.381515
C -1.536127 -0.285937 -0.030211
C  0.821831 -0.678475 -0.841454
C -0.152549  0.191673  0.053007
H  2.771327  0.380787 -0.539226
H  2.826484 -1.389340 -0.110626
H  0.511250 -1.725499 -0.771436
H  0.764169 -0.366011 -1.888989
H -3.676439 -1.027687 -0.164747
H  1.709216 -0.176950  1.013498
H  0.168254 -0.913028  1.965515
H  0.363513  0.899294  2.132309
H -0.430086  1.788757 -1.411885
H -0.702674  2.294643  0.273375
H  0.956118  2.034706 -0.318476
```

Reactant: C=CC(C)(C)C[CH2]
Product: C=CC([CH2])(C)CC

```
C -2.169154 -1.106314  0.382181
C  1.804540  1.841169  0.380275
C -0.183236  1.522071 -1.131032
C  0.568604 -0.844125 -0.677706
C -1.550259  0.074340  0.403215
C  0.729230  0.997740  1.077884
C -0.151433  0.383758 -0.084408
H  2.030382  2.816583  0.808446
H  2.688483  1.301444  0.039995
H  0.094812  1.644324  1.695765
H  1.135559  0.205440  1.715472
H -2.073619  0.940063  0.810936
H -1.700125 -2.001974 -0.010698
H -3.180179 -1.220814  0.759885
H  1.041295  2.025540 -0.742728
H -0.189652  1.226496 -2.179995
H -0.875568  2.335409 -0.901002
H  1.570442 -0.562981 -1.018830
H  0.666897 -1.634432  0.074548
H  0.012426 -1.240130 -1.534731
```

Reactant: C#CC(C)(C=C)C[CH2]
Product: C#CC([CH2])(C=C)CC

```
C  0.137659 -0.894468  2.391697
C -2.602913 -0.273885  0.102134
C  2.068195  1.308626 -0.168192
C  0.820863 -0.693060 -1.046467
C  0.032254 -0.445111  1.276396
C -1.529414  0.131962 -0.571447
C  0.558784  1.555972 -0.098663
C -0.091701  0.108197 -0.079294
H  2.541163  1.067731  0.783754
H  2.657293  1.967717 -0.803522
H  0.237434  2.133699  0.771811
H  0.216269  2.064888 -1.007335
H -1.631711  0.530930 -1.579617
H -2.520348 -0.675040  1.106597
H -3.596385 -0.219386 -0.330352
H  0.242111 -1.288438  3.371808
H  1.924305  0.098823 -0.781408
H  0.610359 -0.508231 -2.102202
H  0.995629 -1.737652 -0.799794
```

Reactant: C=CC(C)(C=C)C[CH2]
Product: C=CC([CH2])(C=C)CC

```
C  1.257932  0.742621 -2.159324
C -1.887487  1.558186 -0.013874
C -0.965974 -1.479735  1.693380
C  0.554829  0.481207  1.285105
C  1.200252 -0.040834 -1.082600
C -1.182777  0.585735 -0.589183
C -0.310497 -1.578710  0.312533
C  0.074290 -0.085846 -0.065410
H -0.735049 -2.260116  2.416467
H -2.009872 -1.167659  1.690227
H  0.613302 -2.166521  0.375731
H -0.954734 -2.026161 -0.451452
H  2.031099 -0.708775 -0.855179
H  2.113996  0.729037 -2.826089
H  0.458411  1.434019 -2.404931
H -1.529862  0.168358 -1.534190
```

```
H -1.600076  2.012318  0.927755
H -2.795049  1.939846 -0.471026
H -0.281321 -0.339029  2.021408
H  1.550722  0.135560  1.570838
H  0.399633  1.542532  1.468816

Reactant: C#CC(C)(C#C)C[CH2]
Product: C#CC([CH2])(C#C)CC
C -2.000355  1.997822 -0.192487
C -1.057803 -2.343198 -0.151940
C  2.285403 -0.354052 -0.309341
C  0.625643  0.277081  1.479005
C -1.160251  1.142559 -0.057649
C -0.639699 -1.218293 -0.034543
C  1.081533  0.347282 -0.942576
C -0.094373  0.144912  0.108751
H  2.314390 -1.435711 -0.439231
H  3.253706  0.133333 -0.406182
H  1.263112  1.423201 -1.028289
H  0.791380 -0.047351 -1.919091
H -2.751018  2.739083 -0.309061
H -1.433829 -3.330301 -0.256003
H  1.828842 -0.180995  0.961159
H  0.827093  1.310337  1.763786
H  0.256692 -0.356968  2.281205
```

Test set

```
Reactant: [CH2]C(C)C(C)C
Product: [CH2]C(C)C(C)C
C  1.262223  1.339971  0.137503
C  1.632313 -1.196256 -0.100109
C -1.238245  1.357251 -0.134868
C -1.643460 -1.173655  0.100951
C  0.694247 -0.070133  0.372026
C -0.689699 -0.060314 -0.370399
H  1.727991  1.481630 -0.840836
H  1.809854  1.808984  0.954298
H  0.489185 -0.190472  1.445263
H  1.850558 -1.077580 -1.168407
H  1.174451 -2.181046  0.052279
H  2.580323 -1.173901  0.449265
H -0.486361 -0.182702 -1.443736
H  0.015785  1.907378  0.001619
H -1.779205  1.834369 -0.951422
H -1.702273  1.504515  0.843472
H -2.591420 -1.136983 -0.447744
H -1.859298 -1.053077  1.169539
H -1.200051 -2.164871 -0.052858

Reactant: C[CH]CCCC
Product: C[CH]CCCC
C -2.412966 -0.861817 -0.118703
C  2.403803 -0.873443  0.118467
C -1.178591 -0.216066  0.483237
C  1.172332 -0.220592 -0.481781
C -0.781816  1.192057  0.003741
C  0.782258  1.188424  0.000586
H -2.513283 -1.905476  0.201138
H -2.365243 -0.839386 -1.214275
H -3.330800 -0.332449  0.183151
H -1.080944 -0.346968  1.565250
H -1.144604  1.335899 -1.022259
H -1.194385  1.992555  0.628719
H  1.145750  1.328549  1.026852
H  1.198542  1.988230 -0.622813
H -0.004345 -0.764732  0.000283
H  1.073677 -0.348871 -1.564017
H  2.498897 -1.916984 -0.203358
H  3.324086 -0.347994 -0.182766
H  2.356616 -0.852832  1.214101

Reactant: C#CC(C)C([CH2])C
Product: C#CC([CH2])C(C)C
C -2.701871 -0.753282 -0.047940
C  1.965249  0.735442 -0.309466
C  1.233845 -1.702585  0.138230
C -0.251427  1.846234  0.136323
C -1.628857 -0.254443  0.194356
C  0.841733 -0.308474 -0.375582
C -0.323793  0.341085  0.472156
H  2.555877  0.711028  0.609402
H  2.558515  0.893165 -1.208878
H  0.481070 -0.381108 -1.408531
H  0.363548 -2.369189  0.130127
H  1.610800 -1.633677  1.165920
H  2.016446 -2.145642 -0.487423
H -0.074961  0.202666  1.534016
H -3.647191 -1.183138 -0.267192
H  1.102789  1.786010 -0.133513
H -0.459687  2.546398  0.943320
H -0.709048  2.112144 -0.816987

Reactant: C#CCCC[CH]C
Product: C#C[CH]CCCC
```

```
C -3.207510 -0.772595 -0.159684
C  2.535938 -1.160362  0.111597
C -2.126040 -0.363270  0.207894
C  1.406316 -0.358868 -0.499248
C -0.839732  0.093375  0.605833
C  1.263073  1.125513 -0.137609
C -0.274990  1.381745 -0.046219
H  3.512062 -0.841042 -0.288260
H  2.566493 -1.023538  1.199279
H  2.426565 -2.229662 -0.101158
H  1.189709 -0.583218 -1.547000
H  1.743143  1.789317 -0.866019
H  1.721325  1.303833  0.843693
H -0.521838  2.282032  0.524755
H -0.695356  1.478070 -1.052625
H  0.140924 -0.662881  0.111030
H -0.654123  0.038180  1.683254
H -4.154253 -1.128519 -0.480936
```

Reactant: C=CCCC[CH]C
Product: C=C[CH]CCCC

```
C -3.101696 -0.790815 -0.200730
C  2.485855 -1.368444 -0.041602
C -2.083082 -0.068741  0.303073
C  1.547574 -0.326676  0.528906
C -0.798960  0.159344 -0.354766
C  1.480620  1.060315 -0.120589
C -0.027361  1.466725 -0.071488
H  3.539814 -1.108356  0.150522
H  2.361332 -1.449740 -1.128196
H  2.304468 -2.353749  0.402784
H  1.475746 -0.313129  1.619779
H  1.802676  0.983882 -1.166940
H  2.119318  1.797346  0.380704
H -0.271374  2.264847 -0.780214
H -0.277022  1.815233  0.938798
H  0.156529 -0.589950  0.163424
H -0.776052 -0.135382 -1.408995
H -2.187875  0.365688  1.297523
H -4.017745 -0.953213  0.356674
H -3.045169 -1.239467 -1.188464
```

Reactant: C=CC(C)C([CH2])C
Product: C=CC([CH2])C(C)C

```
C  1.957307 -1.834696  0.634347
C -1.861863  1.121406 -0.160763
C -1.825188 -1.456040  0.000151
C  0.597524  1.515160  0.193970
C  1.365948 -0.887766 -0.095149
C -1.080753 -0.176145 -0.414062
C  0.266965  0.022025  0.382292
H -2.440342  1.535274 -0.985747
H -2.379634  1.157848  0.800676
H -0.823548 -0.230220 -1.480915
H -1.175972 -2.330533 -0.125300
H -2.728035 -1.601725 -0.603282
H -2.121079 -1.392731  1.054433
H  0.059144 -0.169660  1.443438
H  1.668617 -0.732919 -1.131321
H  2.741962 -2.465913  0.229764
H  1.679622 -2.010111  1.670039
H -0.726170  1.867594  0.040081
H  1.052161  2.038467  1.033834
H  1.048677  1.759315 -0.770638
```

Reactant: [CH2]CCCCCC
Product: CCC[CH]CCC

```
C  2.810820 -0.489659 -0.252649
C -2.136275 -3.140214 -1.272937
C  2.365431  0.874820  0.294743
C -1.007581 -2.588263 -0.376595
C  0.822374  0.924108  0.033066
C -0.770107 -1.076421 -0.600120
C  0.333671 -0.515786  0.279418
H  2.937966 -0.536719 -1.335745
H  3.569945 -1.038848  0.301935
H  2.548896  0.915527  1.374791
H  2.886809  1.717655 -0.172742
H  0.316150  1.664168  0.663092
H  0.644300  1.186821 -1.017646
H  1.549396 -1.052161 -0.038405
H  0.223554 -0.762161  1.340869
H -0.519256 -0.900495 -1.655860
H -1.715033 -0.539479 -0.406658
H -0.073706 -3.127443 -0.580023
H -1.257688 -2.758795  0.678890
H -2.290326 -4.211047 -1.099784
H -3.079635 -2.620324 -1.067809
H -1.891460 -2.996146 -2.331962
```

Reactant: CC(C)CC[C](C)C
Product: CC(C)CC[C](C)C

```
C -2.081471  1.177403 -0.753463
C -1.861656 -1.337841 -0.333833
```

```
C  2.090930 -1.173946 -0.747038
C  1.870909  1.339345 -0.315995
C -0.721819  0.303225  1.293677
C  0.720147 -0.308987  1.296498
C -1.270855  0.053094 -0.127492
C  1.277632 -0.052069 -0.120194
H  2.297938 -0.964993 -1.803773
H  1.561026 -2.131234 -0.680526
H  3.060594 -1.289954 -0.235050
H  1.195577  2.116769  0.059537
H  2.069346  1.537922 -1.375841
H  2.824176  1.430365  0.228951
H  0.658295 -1.389205  1.474970
H  1.350555  0.129742  2.080110
H -0.661058  1.382597  1.477563
H -1.356825 -0.139180  2.071491
H  0.004969  0.002313 -0.654713
H -3.054490  1.289571 -0.247012
H -1.553128  2.134927 -0.678510
H -2.281595  0.973851 -1.812580
H -1.187885 -2.116469  0.041991
H -2.818154 -1.432486  0.204801
H -2.053409 -1.531356 -1.395838
```

Reactant: C#CC(C=C)CC([CH2])(C)C
Product: C#C[C](C=C)CC(C)(C)C

```
C  1.816998  2.299384 -0.097214
C  3.236217 -1.065543  0.000624
C -1.210361 -0.516239  1.466938
C -1.966017  1.390069 -0.001793
C -2.879203 -0.931712 -0.411904
C  1.378671  1.172031 -0.056011
C  1.911970 -1.249630 -0.025082
C -0.402872 -0.449300 -0.850073
C  0.873299 -0.177602  0.010344
C -1.645355 -0.121979  0.052159
H -1.483339  0.132287  2.297178
H -1.207469 -1.583720  1.694116
H -2.807026  1.620903  0.663135
H -1.099994  1.983253  0.305151
H -2.240480  1.680580 -1.022749
H -3.127643 -0.681670 -1.451153
H -2.680277 -2.008203 -0.351028
H -3.748267 -0.701510  0.214698
H -0.401744  0.127183 -1.779629
H -0.419923 -1.517066 -1.102319
H  0.243767 -0.289605  1.116910
H  1.508338 -2.260275 -0.050965
H  3.923048 -1.904852 -0.004489
H  3.667123 -0.070268  0.021867
H  2.191675  3.291669 -0.138292
```

Reactant:
C#CC([CH2])(C)C(C)(C#C)C#C
Product:
C#CC(C)(C)C([CH2])(C#C)C#C

```
C -2.990372  0.301635  0.147439
C  0.159912  2.772832 -0.624564
C  3.004265 -0.571111 -0.332893
C -0.370776 -1.911763  0.814905
C -0.354048 -1.141114 -1.661468
C  0.417889  0.233231  1.871868
C -1.882846 -0.156068  0.007836
C  0.348387  1.659649 -0.200287
C  1.903064 -0.168829 -0.049514
C -0.551868 -0.749283 -0.181237
C  0.560559  0.309019  0.331176
H -1.272687 -2.443159  1.108872
H  0.491908 -2.545170  0.605784
H -1.134227 -1.845617 -1.964578
H -0.416737 -0.247422 -2.290870
H  0.626370 -1.605797 -1.794017
H -3.962167  0.710181  0.270961
H -0.000815  3.753230 -0.997971
H  3.977946 -0.911333 -0.584034
H  0.039288 -1.090431  1.827917
H -0.459232  0.757266  2.249424
H  1.330754  0.373506  2.445006
```

Reactant:
C=CC([CH2])(C)C(C)(C#C)C=C
Product:
C=CC(C)(C)C([CH2])(C#C)C=C

```
C  2.954123  0.076466  0.197668
C -2.981589  0.814468  0.273257
C -1.485578 -2.446402  0.574204
C  0.666313  1.935266  0.022074
C -0.095297  0.324243 -1.826433
C  0.023661  0.564126  2.023839
C  1.800707 -0.308370 -0.348221
C -1.864687  0.399985  0.470630
C -0.475948 -1.617474  0.835094
C  0.498736  0.475900 -0.409415
C -0.508329 -0.102044  0.730895
```

```
H -0.193727  2.562867 -0.214184
H  1.626383  2.409075 -0.172444
H -1.025923  0.890715 -1.911660
H  0.619237  0.692269 -2.570602
H -0.307474 -0.731792 -2.033587
H  1.743688 -1.288864 -0.818798
H  3.080535  1.037808  0.683421
H  3.828636 -0.566257  0.173519
H  0.484164 -2.009306  1.160394
H -1.374579 -3.520798  0.678011
H -2.455811 -2.077201  0.259436
H -3.961924  1.186715  0.108087
H  0.498774  1.665782  1.351418
H  0.917423  0.090042  2.430176
H -0.722293  0.842426  2.764544
```

```
Reactant:
C=CC([CH2])(C=C)C(C)(C=C)C=C
Product:
C=CC([CH2])(C=C)C(C)(C=C)C=C
C  2.171667  2.273245  0.336455
C  2.877404 -1.198581 -0.669175
C -1.691031 -0.254726 -2.331889
C -2.242774  1.564793  1.021427
C  0.851165  0.091469  1.927622
C -1.127710 -1.163596  1.005617
C  1.505378  1.293661 -0.271214
C  1.720932 -1.182115 -0.008282
C -0.788586 -0.665976 -1.440053
C -1.320986  1.214111  0.125959
C  0.927441  0.060604  0.389059
C -0.636119 -0.134783 -0.026385
H  0.481137  1.027871  2.344872
H  1.681118 -0.356288  2.471292
H  1.355255  1.328038 -1.350558
H  2.562551  3.121893 -0.216279
H  2.350847  2.267651  1.406728
H  1.295389 -2.122371  0.337168
H  3.355638 -0.286397 -1.008522
H  3.394168 -2.129969 -0.878305
H -0.097088 -1.464580 -1.699189
H -2.404710  0.530594 -2.104619
H -1.754969 -0.702116 -3.318680
H -0.976786  1.958266 -0.587986
H -2.648077  2.571700  1.039132
H -2.630328  0.883535  1.770436
H -0.246192 -0.733872  1.968710
H -0.834668 -2.192580  0.796144
H -2.162761 -1.078212  1.329300
```

```
Reactant: C#CC(C#C)CC[C](C)C
Product: C#C[C](C#C)CCC(C)C
C  1.909685 -2.365700  0.282668
C  2.448610  2.124872  0.627613
C -2.129437  1.401816  0.375671
C -2.219461 -1.084574  1.041910
C  1.501607 -1.242176  0.098162
C  1.792468  1.168125  0.282795
C -1.198173 -0.382011 -1.252654
C  0.213917  0.234774 -1.495830
C -1.589250 -0.004781  0.186441
C  0.951870  0.075119 -0.125719
H -3.150997  1.475872 -0.032171
H -1.509206  2.143252 -0.140367
H -2.173035  1.667115  1.437844
H -2.298527 -0.762839  2.086663
H -3.237252 -1.318240  0.686470
H -1.630168 -2.007501  1.001779
H -1.927434 -0.016684 -1.986382
H -1.132977 -1.472274 -1.338437
H  0.761255 -0.253135 -2.305837
H  0.130299  1.303632 -1.714187
H -0.167453  0.099859  0.544542
H  2.285646 -3.344806  0.445083
H  3.040332  2.951497  0.932287
```

```
Reactant: C=CC(C=C)CC[C](C)C
Product: C=C[C](C=C)CCC(C)C
C -1.696240 -2.495344 -0.441593
C -1.669651  2.097046  1.173702
C  2.154691 -1.078808 -0.628986
C  2.109966  1.498927 -0.598577
C -1.718475 -1.166467 -0.612481
C -1.695446  1.183826  0.194532
C  1.143943  0.148526  1.411436
C -0.259242 -0.546553  1.466800
C  1.552590  0.195272 -0.067270
C -0.989431 -0.129459  0.166714
H  3.174254 -1.228906 -0.235483
H  1.557639 -1.955747 -0.355422
H  2.221370 -1.036034 -1.722083
H  1.473740  2.341434 -0.304604
H  3.122092  1.685759 -0.200068
H  2.184827  1.479491 -1.692292
```

H 1.064277 1.169567 1.798348
H 1.880221 -0.392599 2.020377
H -0.120112 -1.630705 1.477977
H -0.828244 -0.270787 2.359918
H 0.092083 0.112247 -0.465427
H -2.316211 -0.766219 -1.432081
H -1.142960 -2.977488 0.356731
H -2.253394 -3.152274 -1.100852
H -2.267221 1.405969 -0.706748
H -2.206834 3.034882 1.080618
H -1.129945 1.942189 2.101567

Reactant: C#CC(C)CC([CH2])C
Product: C#C[C](C)CC(C)C
C 2.961700 1.396520 0.110134
C -1.176297 -0.074580 1.432624
C -2.837038 0.525945 -0.434913
C 1.287724 -1.743918 -0.195435
C 2.024179 0.630687 0.042329
C -0.310879 0.199719 -0.842726
C -1.570799 -0.260270 -0.036080
C 0.910801 -0.266706 -0.003764
H -1.217524 0.953373 1.797660
H -1.482716 -0.825962 2.157760
H -1.737268 -1.327869 -0.225987
H -3.709542 0.177976 0.128792
H -2.693961 1.593198 -0.228264
H -3.047958 0.405899 -1.504729
H -0.306863 1.294242 -0.898494
H -0.290345 -0.204915 -1.860770
H 0.245462 -0.218197 1.121551
H 3.783332 2.065913 0.165849
H 2.055175 -2.044255 0.524018
H 1.678453 -1.900819 -1.208833
H 0.408856 -2.382959 -0.059168

Reactant: C=CC(C)C(C)C[CH2]
Product: C=CC(C)C([CH2])CC
C -2.455372 -1.511072 0.259088
C 2.735840 -0.913916 -0.078662
C -1.411356 1.862446 -0.112996
C 1.593460 1.287749 0.353879
C -1.752767 -0.598350 -0.409650
C 1.217344 -1.109593 0.036040
C -0.859723 0.451496 0.217160
C 0.600728 0.296707 -0.282410
H 3.370427 -1.427462 0.642137
H 3.130704 -0.924716 -1.096149
H 0.954121 -1.377944 1.066996
H 0.825326 -1.887696 -0.625925
H 0.612491 0.439603 -1.372523
H 2.659853 0.422554 0.233653
H 1.801373 2.217717 -0.173179
H 1.479719 1.410437 1.434008
H -0.858019 0.312454 1.307585
H -1.807609 -0.560956 -1.498491
H -3.090240 -2.232280 -0.245914
H -2.424564 -1.570008 1.343773
H -1.426460 2.015745 -1.199103
H -0.781670 2.637344 0.336872
H -2.432939 1.972551 0.265441

Reactant: C=CC(C)C(C)C[CH2]
Product: C=C[C](C)C(C)CC
C 2.910296 0.130965 -0.366686
C -1.331400 -1.971588 0.180228
C 0.644183 0.333497 1.556033
C -1.167486 1.832085 -0.423575
C 1.645879 -0.120499 -0.747838
C -1.978741 -0.596077 0.035235
C 0.451646 -0.140569 0.113265
C -0.870246 0.330779 -0.566426
H -1.498310 -2.537045 1.094275
H -1.273906 -2.576651 -0.724752
H -2.866898 -0.607689 -0.608612
H -2.278762 -0.211307 1.017020
H -0.781806 0.084409 -1.634309
H -0.357470 2.432285 -0.852838
H -1.279310 2.103224 0.631756
H -2.098779 2.089649 -0.942628
H 0.019747 -1.360260 0.237657
H 1.457676 -0.357256 -1.795433
H 3.168818 0.378933 0.657055
H 3.730066 0.097279 -1.076362
H 1.427141 -0.249172 2.053185
H 0.936999 1.390751 1.582649
H -0.280639 0.216261 2.129532

Reactant: C=CC(C)C([CH2])CC
Product: C=CC([CH2])C(C)CC
C 2.370308 -0.999829 0.241645
C -2.824571 -1.356494 -0.504887
C 0.654691 2.204459 0.129570
C -1.784125 1.591545 0.116821

```
C  1.586283 -0.104833 -0.360799
C -1.493838 -0.980448  0.181668
C  0.491248  0.682593  0.305877
C -0.938341  0.375972 -0.291166
H -3.592331 -0.602618 -0.298485
H -3.189889 -2.326176 -0.148349
H -1.638068 -0.937170  1.270142
H -0.742287 -1.755211 -0.019101
H -0.841273  0.362886 -1.386371
H -2.690772 -1.419827 -1.591427
H -2.504991  1.979543 -0.601320
H -2.159094  1.557998  1.142659
H  0.463103  0.445947  1.377957
H  1.712348  0.098191 -1.424805
H  3.142573 -1.541606 -0.294918
H  2.270353 -1.220025  1.300926
H -0.702896  2.432737  0.182214
H  0.934014  2.514369 -0.880121
H  1.178937  2.747609  0.914505
```

```
Reactant: C=CC([CH2])C(C)CC
Product: C=CC(C)C(C)[CH]C
C  3.144222  0.315212 -0.004106
C -2.965613 -0.294528 -0.462558
C  0.224901 -1.813806  0.438758
C -0.343937  1.963123  0.028865
C  2.002905 -0.225453 -0.432218
C -1.713996 -0.197888  0.391639
C  0.743274 -0.364744  0.380033
C -0.462202  0.451625 -0.224116
H -2.743551 -0.779564 -1.420550
H -3.374643  0.704184 -0.682793
H -1.103504 -1.401963  0.551015
H -1.893915  0.128742  1.421338
H -0.476031  0.260230 -1.307337
H -3.750753 -0.868814  0.042326
H -1.166707  2.510209 -0.445610
H  0.602957  2.343583 -0.371789
H  0.917773 -0.000926  1.401449
H  1.931418 -0.604892 -1.452103
H  3.247192  0.698190  1.007445
H  4.018979  0.391248 -0.642011
H -0.369598  2.166410  1.106449
H  0.526772 -2.421528  1.290273
H  0.258750 -2.345807 -0.514895
```

1-5 H-shift

Training set

Primary contributions

```
Reactant: [CH2]CCCC
Product: [CH2]CCCC
C  1.331735 -1.001738 -0.061264
C -1.305478 -1.026131 -0.062903
C  1.274897  0.494712  0.246480
C -1.276422  0.471108  0.245144
C -0.006466  1.136030 -0.355519
H  1.607412 -1.241553 -1.090728
H  1.843632 -1.626009  0.672120
H  1.263778  0.651453  1.332816
H  2.161794  1.011295 -0.149593
H -0.004651  1.000806 -1.445719
H -0.016540  2.213137 -0.150926
H -2.172306  0.971381 -0.151620
H -1.269150  0.627747  1.331532
H  0.015975 -1.310644 -0.006010
H -1.806672 -1.659812  0.669810
H -1.575527 -1.270748 -1.092733
```

```
Reactant: [CH2]CCCCC
Product: C[CH]CCCC
C -1.072705  1.474154  0.132887
C  2.396272  0.416071 -0.251595
C -1.775586  0.226697 -0.401720
C  1.112450  0.024349  0.467740
C -1.174390 -1.063091  0.226319
C  0.338668 -1.168392 -0.103221
H -1.003851  2.321859 -0.549671
H -1.364571  1.762691  1.145068
H -2.855636  0.262200 -0.194959
H -1.654155  0.169248 -1.491096
H -1.703701 -1.944311 -0.155046
H -1.310071 -1.035797  1.316044
H  0.740684 -2.115793  0.286866
H  0.458512 -1.188222 -1.195615
H  0.197306  0.980430  0.299718
H  1.216146 -0.024020  1.556768
H  2.841301  1.314846  0.189941
H  2.199147  0.614636 -1.312246
H  3.145380 -0.389207 -0.198444
```

```
Reactant: C#CCCCC[CH2]
```

Product: C#C[CH]CCCC
C 3.161680 -0.295868 -0.362634
C -1.223213 -1.558705 0.188958
C 2.064478 -0.069937 0.098854
C -1.988379 -0.440444 -0.504653
C 0.750624 0.166249 0.617753
C -1.611502 0.950372 0.083656
C -0.100791 1.232666 -0.107555
H -0.947911 -2.426266 -0.408986
H -1.549952 -1.798841 1.201771
H -3.074329 -0.590217 -0.403721
H -1.757075 -0.438984 -1.577088
H -2.198121 1.732615 -0.411623
H -1.860239 0.973429 1.153574
H 0.137906 1.208981 -1.177120
H 0.149279 2.232724 0.269720
H 0.021317 -0.866579 0.430485
H 0.730207 0.283254 1.706921
H 4.123466 -0.491600 -0.766207

Reactant: C=CCCCC[CH2]
Product: C=C[CH]CCCC
C -2.521058 0.825922 -0.819062
C 0.158542 -2.760581 0.293847
C -2.151546 0.066797 0.223778
C 0.448972 -2.776000 1.786843
C -0.762890 -0.272679 0.582945
C 0.771198 -1.347376 2.313585
C -0.428522 -0.395499 2.080917
H -0.569793 -3.475018 -0.087084
H 1.020902 -2.609397 -0.356554
H 1.295992 -3.441691 2.014990
H -0.422046 -3.159825 2.333153
H 1.656048 -0.958635 1.791468
H 1.008463 -1.393348 3.382895
H -0.209196 0.594981 2.502160
H -1.303280 -0.792320 2.614638
H -0.514517 -1.456438 0.209087
H -0.019426 0.316529 0.034945
H -2.922089 -0.375070 0.856092
H -3.564565 1.009307 -1.051779
H -1.787453 1.289460 -1.472726

Reactant: [CH2]CCCC(C)C
Product: CCCC[C](C)C
C -1.290031 1.405815 0.430690
C 1.937537 0.670221 -1.007375
C 1.549708 -0.278549 1.331923
C -2.073381 0.255608 -0.198412
C -1.343932 -1.098676 0.028705
C 0.068093 -1.068248 -0.615761
C 0.940753 0.055898 -0.028905
H -1.353352 1.460815 1.519639
H -1.376499 2.378143 -0.054910
H -2.171677 0.419601 -1.279499
H -3.091041 0.194219 0.216019
H -1.256893 -1.288813 1.106425
H -1.931848 -1.916349 -0.405292
H 0.564120 -2.041829 -0.478334
H -0.050512 -0.910218 -1.696476
H 0.002322 0.949214 0.210332
H 1.434137 1.010494 -1.919950
H 2.452998 1.525806 -0.555147
H 2.702271 -0.067544 -1.297824
H 0.788381 -0.640642 2.031974
H 2.314309 -1.064090 1.227206
H 2.029963 0.603032 1.772760

Reactant: [CH2]CCCC(C)C#C
Product: CCCC[C](C)C#C
C 1.439251 0.107856 1.485371
C -2.326660 1.617551 0.202763
C -1.373236 -1.822894 0.239779
C 2.256901 0.207847 0.204424
C -1.590349 0.661564 0.099132
C 1.372340 0.625382 -1.006860
C 0.241139 -0.407474 -1.229041
C -0.695363 -0.464889 0.002003
H 1.147804 1.056969 1.937090
H 1.718523 -0.662875 2.202450
H 3.071409 0.939559 0.320046
H 2.719563 -0.761473 -0.020849
H 0.927329 1.610408 -0.817892
H 1.993401 0.700863 -1.907008
H 0.687813 -1.400090 -1.374770
H -0.337290 -0.160799 -2.128132
H 0.170000 -0.300159 0.921184
H -2.045103 -2.066043 -0.593683
H -0.616327 -2.611742 0.316098
H -1.960667 -1.805602 1.162683
H -2.976381 2.452022 0.290973

Reactant: [CH2]CCCC(C)C=C
Product: CCCC[C](C)C=C

```
C -0.940497 -3.039671  0.381108
C -2.441732  1.288420 -0.332288
C -0.074234 -0.212934 -1.329731
C  0.139619 -3.011051  1.450439
C -1.742353  0.479909  0.476531
C  1.184157 -1.893387  1.165822
C  0.506673 -0.499634  1.160793
C -0.609899 -0.398904  0.093767
H -1.945665 -3.329683  0.682806
H -0.636342 -3.416737 -0.595961
H -0.312248 -2.824753  2.433234
H  0.659568 -3.980243  1.510349
H  1.662405 -2.081900  0.196103
H  1.969052 -1.918443  1.931049
H  0.073625 -0.321725  2.154438
H  1.256647  0.284442  0.983809
H -1.031965 -1.581659  0.130802
H  0.344005  0.795320 -1.450340
H -0.868907 -0.347607 -2.071477
H  0.715290 -0.940884 -1.542709
H -2.026970  0.422507  1.527616
H -3.276111  1.873411  0.040174
H -2.209203  1.398447 -1.386021
```

Reactant: [CH2]CCCC(C#C)C#C
Product: CCCC[C](C#C)C#C

```
C -1.539846 -0.355343  1.511674
C  1.406399  2.452120  0.355729
C  2.522857 -1.914696  0.066472
C -2.373006 -0.439964  0.245487
C  1.081719  1.303594  0.167587
C  1.683211 -1.047302  0.010943
C -1.729327  0.359019 -0.926742
C -0.331705 -0.205653 -1.268080
C  0.625319 -0.059406 -0.045777
H -1.490509 -1.229527  2.157585
H -1.531005  0.604629  2.027682
H -2.481208 -1.487155 -0.062681
H -3.385557 -0.045437  0.426108
H -2.376174  0.298055 -1.809377
H -1.637241  1.416144 -0.647491
H -0.416232 -1.271450 -1.508949
H  0.103215  0.310784 -2.130456
H -0.172426 -0.290839  0.874896
H  1.712073  3.455360  0.518644
H  3.274075 -2.662835  0.114456
```

Reactant: [CH2]CCCC(C#C)C=C
Product: CCCC[C](C#C)C=C

```
C -1.594449  0.510569  1.539351
C  1.472377 -2.224483  0.531890
C  2.803228  1.176455 -0.007763
C -2.510930  0.365845  0.337886
C  1.041133 -1.136568  0.226536
C  1.495092  1.263376 -0.262225
C -1.878607 -0.531180 -0.767427
C -0.551708  0.079015 -1.272328
C  0.494262  0.158846 -0.123610
H -1.475966 -0.370173  2.170144
H -1.581707  1.461788  2.067795
H -2.724511  1.352489 -0.092410
H -3.475392 -0.073389  0.639154
H -1.684928 -1.532669 -0.363670
H -2.582224 -0.632671 -1.601793
H -0.140167 -0.510915 -2.099163
H -0.741182  1.095426 -1.642218
H -0.261175  0.457455  0.813086
H  1.068106  2.212022 -0.583495
H  3.255397  0.242378  0.308494
H  3.458040  2.034855 -0.111913
H  1.851033 -3.180063  0.796626
```

Reactant: [CH2]CCCC(C=C)C=C
Product: CCCC[C](C=C)C=C

```
C -2.701301 -2.286720 -0.059857
C  0.555252 -0.706491 -2.304500
C  1.088856  0.031777  1.633062
C -3.599584 -1.203029 -0.626472
C  0.371922 -1.021682 -1.018427
C -0.187337 -0.084079  1.253413
C -2.801367 -0.217062 -1.528824
C -1.700155  0.502230 -0.709057
C -0.682448 -0.494196 -0.100028
H -2.330950 -3.028403 -0.767473
H -2.915306 -2.666899  0.937181
H -4.415250 -1.645803 -1.220566
H -4.064605 -0.635206  0.189486
H -2.346450 -0.773198 -2.356631
H -3.487261  0.524603 -1.955534
H -1.172307  1.238949 -1.327895
H -2.182814  1.054100  0.108060
H -1.439421 -1.453323  0.104204
H  1.029009 -1.761603 -0.562837
H -0.056787  0.026390 -2.819202
```

```
H  1.340091 -1.172239 -2.891653
H -0.975849  0.137244  1.972750
H  1.910536 -0.144361  0.947062
H  1.353167  0.324471  2.643991
```

Secondary contributions

```
Reactant: [CH2]CCC(C)C
Product: CCCC([CH2])C
C  2.069368  0.581944 -0.139428
C -0.419780  1.436033 -0.017872
C -2.325019 -0.250512 -0.075023
C  1.558369 -0.813814  0.220525
C  0.101732 -1.018665 -0.280101
C -0.861869  0.020732  0.358276
H  2.794039  1.022183  0.546577
H  2.347823  0.705825 -1.188471
H  2.204675 -1.591793 -0.211717
H  1.573558 -0.945752  1.310062
H  0.069415 -0.909333 -1.373502
H -0.237621 -2.032637 -0.034560
H -0.794902 -0.092321  1.449529
H  0.927469  1.290758 -0.029934
H -0.656786  1.712126 -1.049187
H -0.662544  2.221761  0.699291
H -2.637691 -1.259204  0.221729
H -3.006426  0.474573  0.383669
H -2.414251 -0.166245 -1.164784

Reactant: [CH2]CC(C)CC
Product: [CH2]CC(C)CC
C  1.488799 -1.316350 -0.066201
C  1.479546  1.318061 -0.071028
C -2.198649 -0.012014 -0.053649
C -0.004221 -1.273279  0.254042
C -0.013138  1.265634  0.249360
C -0.684849 -0.007279 -0.342741
H  1.724703 -1.600457 -1.094155
H  2.124939 -1.811953  0.668124
H -0.156118 -1.257004  1.341849
H -0.515432 -2.167700 -0.133901
H -0.525665 -0.008746 -1.431165
H -2.374971 -0.010754  1.029268
H -2.675783 -0.903072 -0.478102
H -2.681916  0.874262 -0.481161
H -0.164932  1.252287  1.337213
H -0.530654  2.155009 -0.141834
H  1.782253  0.002116 -0.023206
H  1.713471  1.600245 -1.099963
H  2.112028  1.820921  0.661533

Reactant: C#CC(C[CH2])CC
Product: C#CC(C[CH2])CC
C -3.010666  0.001097 -0.034510
C  1.782061  1.322633  0.042804
C  1.784272 -1.312679  0.039059
C -1.819466  0.001830  0.160303
C  0.283067  1.282820 -0.241473
C  0.285159 -1.274662 -0.244846
C -0.370830  0.002737  0.381215
H  2.396842  1.811754 -0.713123
H  2.045191  1.614029  1.061911
H -0.225204  2.167958  0.164386
H  0.095911  1.258843 -1.321114
H -0.171629  0.001475  1.463372
H -4.057421  0.000459 -0.210047
H -0.221560 -2.161680  0.158843
H  0.097774 -1.248254 -1.324391
H  2.078195  0.005298 -0.004272
H  2.399783 -1.798521 -0.718385
H  2.048127 -1.606481  1.057285

Reactant: [CH2]CCC(C)C#C
Product: CCCC([CH2])C#C
C  1.936440 -0.019191  0.904562
C -2.481838 -0.636034  0.736947
C  0.107075  1.686769  0.078517
C  1.233811 -1.108521  0.094676
C -1.613888 -0.104041  0.088304
C  0.519658 -0.504314 -1.141999
C -0.560826  0.544530 -0.706767
H  2.867803  0.345640  0.465040
H  2.012800 -0.193744  1.978276
H  1.949347 -1.872224 -0.243400
H  0.481419 -1.608708  0.714088
H  1.251439  0.004068 -1.783602
H  0.038810 -1.294223 -1.728472
H -1.024950  0.946309 -1.622221
H -3.242888 -1.102546  1.311175
H  1.082650  0.998226  0.728637
H -0.516004  2.169014  0.830268
H  0.655380  2.389613 -0.552209

Reactant: [CH2]CCC(C)C=C
Product: CCCC([CH2])C=C
```

```
C  2.514005  0.444831  0.023183
C -2.991518 -0.234377  0.314907
C  0.103289  1.500807 -0.028847
C  1.862310 -0.918936  0.255704
C -1.878921  0.005760 -0.376679
C  0.452501 -0.979395 -0.394130
C -0.487224  0.105276  0.217257
H  3.207969  0.785428  0.792562
H  2.893335  0.597800 -0.989692
H  1.756788 -1.102365  1.332651
H  2.485598 -1.727477 -0.153797
H  0.536322 -0.810472 -1.476863
H  0.007607 -1.969097 -0.240983
H -0.550080 -0.073984  1.298827
H -1.926938  0.154826 -1.455504
H -2.971442 -0.383011  1.391162
H -3.964465 -0.290523 -0.162924
H  1.428247  1.241344  0.076362
H -0.157314  2.260772  0.708438
H -0.007998  1.850717 -1.058541
```

Reactant: C=CC(C[CH2])CC
Product: C=CC(C[CH2])CC

```
C -2.604296 -0.494760  0.315527
C  1.726295 -0.267084 -1.940696
C  1.911335  1.362391  0.119036
C -1.784022  0.289473 -0.381691
C  0.209101 -0.106661 -1.877891
C  0.388424  1.472156  0.115077
C -0.280386  0.163961 -0.418009
H  2.203488  0.051017 -2.868346
H  2.096606 -1.228929 -1.579492
H -0.107283  0.738863 -2.503091
H -0.301703 -1.003822 -2.255522
H  0.030188 -0.675505  0.219590
H -2.192130  1.099372 -0.987636
H -2.228038 -1.309705  0.928145
H -3.680738 -0.356451  0.303510
H  0.071092  2.302182 -0.529991
H  0.001909  1.673995  1.124218
H  2.104558  0.604890 -0.982176
H  2.320646  0.754145  0.928510
H  2.459437  2.292949 -0.032734
```

Reactant: [CH2]CCC(C)(C)C
Product: CCCC([CH2])(C)C

```
C -2.241800  0.561907 -0.111155
C  0.221425  1.489794 -0.135852
C  1.026177 -0.546910 -1.389551
C  2.085868  0.068586  0.812924
C -1.677853 -0.845557  0.090793
C -0.287940 -0.798712  0.785680
C  0.758115  0.061063  0.007750
H -2.862497  0.710897 -0.995549
H -2.671128  1.010903  0.787392
H -2.357512 -1.453924  0.705618
H -1.580426 -1.352312 -0.875524
H  0.104440 -1.817275  0.901332
H -0.405650 -0.372081  1.792090
H -1.104047  1.256488 -0.289583
H  0.570550  2.040392 -1.011579
H  0.266234  2.079183  0.783848
H  1.351562 -1.590333 -1.297782
H  0.129374 -0.515050 -2.017060
H  1.816820  0.018193 -1.897294
H  2.474252 -0.952296  0.918736
H  2.839131  0.677788  0.300216
H  1.923121  0.485419  1.813770
```

Reactant: [CH2]CC(C)(C)CC
Product: [CH2]CC(C)(C)CC

```
C  1.594503  1.317501 -0.011817
C  1.587943 -1.318093 -0.008094
C -2.039350  0.007871 -0.620588
C -0.744841  0.007768  1.536132
C  0.146169  1.272800 -0.496005
C  0.139809 -1.267609 -0.492302
C -0.623345  0.005233 -0.003893
H  2.306317  1.786330 -0.692485
H  1.731413  1.634432  1.023364
H  0.125106  1.271539 -1.593856
H -0.409891  2.161996 -0.160217
H -2.595122  0.898738 -0.303574
H -2.599450 -0.879441 -0.301237
H -1.981889  0.006290 -1.715916
H -1.295271 -0.879290  1.873117
H -1.290847  0.898527  1.870535
H  0.237696  0.006022  2.017687
H  0.118636 -1.269491 -1.590152
H -0.420669 -2.153010 -0.153841
H  1.883618 -0.000973 -0.000091
H  2.297401 -1.792300 -0.687492
H  1.723407 -1.632744  1.027972
```

Reactant: [CH2]CCC(C)(C)C#C
Product: CCCC([CH2])(C)C#C

C	2.337680	0.248023	0.567948
C	-1.695083	1.992109	0.217174
C	0.071729	-0.831708	1.359498
C	-1.676117	-1.459284	-0.381056
C	1.664713	0.599658	-0.759140
C	-1.182476	0.902407	0.130170
C	0.533866	-0.408332	-1.092098
C	-0.571250	-0.434833	0.018743
H	3.032027	-0.594088	0.518108
H	2.728454	1.086811	1.144867
H	1.226174	1.601630	-0.701674
H	2.393901	0.601208	-1.582302
H	0.950528	-1.421597	-1.173418
H	0.066000	-0.152315	-2.049202
H	-2.147876	2.948843	0.295560
H	1.292849	-0.243571	1.243028
H	0.303116	-1.897760	1.426104
H	-0.415183	-0.434104	2.249207
H	-2.132137	-1.169848	-1.333772
H	-1.229551	-2.454456	-0.486067
H	-2.452420	-1.496604	0.388962

Reactant: C#CC(C)(C[CH2])CC
Product: C#CC(C)(C[CH2])CC

C	1.603096	-1.972969	-0.002465
C	-1.599589	-0.429072	-1.314948
C	-1.593561	-0.423092	1.316865
C	1.530372	1.530353	-0.010561
C	1.068541	-0.890001	-0.003868
C	-0.470418	0.594652	-1.277911
C	-0.464759	0.600595	1.270054
C	0.431119	0.436994	-0.005583
H	-2.513203	-0.109390	-1.816986
H	-1.286467	-1.438202	-1.584796
H	0.173946	0.514688	-2.164962
H	-0.881776	1.612069	-1.255085
H	2.075578	-2.923371	-0.001232
H	2.158914	1.433736	-0.901558
H	2.162858	1.437960	0.878088
H	1.062775	2.522029	-0.011880
H	-0.876344	1.617857	1.244263
H	0.183580	0.524863	2.154578
H	-1.879615	-0.529245	0.001792
H	-2.505040	-0.101291	1.821415
H	-1.279007	-1.430914	1.589889

Reactant: C=CC(C)(C[CH2])CC
Product: C=CC(C)(C[CH2])CC

C	1.523107	-1.366241	-1.240791
C	1.103320	-1.227329	2.072396
C	2.332489	1.071047	1.728642
C	-0.890869	0.986084	-0.475901
C	1.295927	-0.100747	-0.893260
C	-0.052272	-0.693394	1.224865
C	1.093637	1.560701	0.986772
C	0.378286	0.408507	0.207517
H	1.734166	-1.972386	1.587997
H	0.849331	-1.487202	3.100853
H	-0.552213	-1.503888	0.673658
H	-0.807478	-0.242023	1.880891
H	1.763590	0.696500	-1.473554
H	1.081182	-2.203706	-0.711511
H	2.165938	-1.615404	-2.079230
H	-0.618596	1.762938	-1.199959
H	-1.428996	0.192560	-1.005172
H	-1.556294	1.428269	0.275795
H	0.372204	1.982428	1.698690
H	1.346844	2.356441	0.268313
H	1.894681	-0.138131	2.131666
H	3.184722	0.834786	1.089378
H	2.606756	1.632472	2.622533

Reactant: [CH2]CCC(C)(C)C=C
Product: CCCC([CH2])(C)C=C

C	2.203307	0.668744	0.574441
C	-1.406599	1.901132	-0.207692
C	-0.116435	-0.143546	1.509344
C	-1.541650	-1.707463	0.126317
C	1.746870	0.240166	-0.820747
C	-1.250744	0.648381	-0.632477
C	0.706099	-0.909036	-0.739262
C	-0.559301	-0.497969	0.090062
H	2.475541	1.718741	0.688253
H	2.918050	-0.008831	1.047588
H	1.284484	1.089981	-1.333444
H	2.600918	-0.093836	-1.428006
H	0.392435	-1.203663	-1.748801
H	1.160579	-1.787008	-0.259404
H	-1.639395	0.370241	-1.613321
H	-1.918829	2.642983	-0.812377
H	-1.030897	2.240083	0.751577
H	1.074034	0.468165	1.272121

```
H -0.765936  0.536329  2.061110
H  0.175041 -1.017584  2.097001
H -2.431837 -1.454986  0.711849
H -1.853883 -1.978543 -0.890034
H -1.050829 -2.574242  0.583653
```

Reactant: [CH2]CCC(C)(C#C)C#C
Product: CCCC([CH2])(C#C)C#C

```
C  2.531913 -0.438934  0.458612
C -2.877480 -1.200693 -0.263762
C -0.607853  2.584828  0.074731
C  0.107051 -0.563185  1.475538
C  1.920117 -0.005679 -0.875027
C -1.804948 -0.674966 -0.095205
C -0.558999  1.379924  0.088730
C  0.491001 -0.578777 -1.044476
C -0.461017 -0.094307  0.115136
H  3.239809  0.257449  0.909068
H  2.877876 -1.474829  0.485376
H  1.863933  1.086879 -0.922889
H  2.536942 -0.345019 -1.719672
H  0.057227 -0.266864 -1.998839
H  0.513333 -1.674679 -1.013127
H -3.828470 -1.648700 -0.410079
H -0.667513  3.644521  0.062118
H  1.446067 -0.453861  1.232554
H -0.045559 -1.628963  1.651499
H -0.152809  0.069763  2.322030
```

Reactant: C#CC(C#C)(C[CH2])CC
Product: C#CC(C#C)(C[CH2])CC

```
C  0.055991  2.585985  0.007953
C  2.953927 -0.761026  0.000084
C -1.812416 -0.410389  1.319138
C -1.813050 -0.404599 -1.315241
C  0.212981  1.389926  0.005332
C  1.795811 -0.424731  0.001040
C -0.315744 -0.693444  1.285888
C -0.316349 -0.687783 -1.284057
C  0.363518 -0.077717  0.002105
H -2.422617 -1.174331  1.801041
H -2.077942  0.606565  1.608598
H -0.126205 -1.772164  1.254446
H  0.198760 -0.283888  2.163964
H -0.064877  3.640528  0.010247
H  3.977822 -1.040681 -0.000744
H  0.197697 -0.274344 -2.160581
H -0.126758 -1.766621 -1.257431
H -2.102241 -0.452504  0.001970
H -2.078767  0.613612 -1.600064
H -2.423558 -1.166456 -1.800039
```

Reactant: [CH2]CCC(C)(C#C)C=C
Product: CCCC([CH2])(C#C)C=C

```
C  2.678616 -0.138539  0.431015
C -0.906581  2.369072  0.176414
C -2.842340 -0.643510 -0.251691
C  0.311219 -0.669480  1.448522
C  1.993103  0.249863 -0.879588
C -0.658509  1.188036  0.147362
C -1.599366 -1.094645 -0.112345
C  0.664507 -0.527707 -1.063461
C -0.342683 -0.248815  0.113462
H  3.278168  0.637895  0.907260
H  3.177711 -1.110275  0.412742
H  1.768526  1.321600 -0.880734
H  2.645589  0.044975 -1.740971
H  0.180436 -0.250214 -2.005032
H  0.863989 -1.607630 -1.083461
H -1.392622 -2.162952 -0.151261
H -3.066656  0.417074 -0.215162
H -3.675440 -1.321412 -0.405968
H -1.121554  3.408198  0.205384
H  1.610913 -0.348896  1.209504
H  0.334967 -1.752420  1.592597
H -0.034296 -0.121187  2.323503
```

Reactant: C#CC(C=C)(C[CH2])CC
Product: C#CC(C=C)(C[CH2])CC

```
C -0.169330 -1.516814  1.960081
C  2.792955 -0.337832  0.263595
C -1.903598 -0.561894 -1.244875
C -1.791991  1.500758  0.386152
C  0.053457 -0.787037  1.024181
C  1.799969  0.247535 -0.399383
C -0.390819 -0.470314 -1.404896
C -0.281256  1.532889  0.185545
C  0.309400  0.103636 -0.115707
H -2.483188 -0.436921 -2.159945
H -2.244799 -1.391053 -0.624482
H -0.137017  0.202695 -2.233652
H  0.057004 -1.449576 -1.618827
H  2.015718  0.906568 -1.239573
H  2.600389 -0.997690  1.102771
```

```
H  3.829933 -0.175980 -0.011598
H -0.368171 -2.157609  2.782683
H -0.025930  2.171429 -0.669713
H  0.239340  1.929144  1.067122
H -2.134688  0.524370 -0.478561
H -2.112809  1.111686  1.352839
H -2.327458  2.400220  0.080917
```

```
Reactant: C=CC(C=C)(C[CH2])CC
Product: C=CC(C=C)(C[CH2])CC
C -0.578286 -1.063211 -2.070145
C  2.247267 -1.754084  0.095830
C -0.694742  2.038605 -0.849882
C -1.948949  0.773516  1.081231
C -0.441560 -1.134021 -0.747131
C  1.598702 -0.723497  0.634063
C  0.564721  1.238330 -0.516270
C -0.625513  0.103842  1.432100
C  0.266508 -0.144810  0.162448
H -1.200987  1.750652 -1.770842
H -0.607725  3.119159 -0.729320
H  1.186645  1.808567  0.184945
H  1.178707  1.055629 -1.408832
H -0.838828 -2.002188 -0.220250
H -0.192700 -0.232851 -2.651584
H -1.088786 -1.842529 -2.627359
H  2.035650 -0.192421  1.480255
H  3.204971 -2.085880  0.483991
H  1.846905 -2.295590 -0.754572
H -0.783102 -0.863635  1.932348
H -0.055563  0.739574  2.121997
H -1.531770  1.611503  0.113648
H -2.395235  1.383363  1.867511
H -2.668106  0.129656  0.572795
```

```
Reactant: [CH2]CCC(C)(C=C)C=C
Product: CCCC([CH2])(C=C)C=C
C  2.609351  0.104306  0.568926
C -0.577665  2.278241 -0.131517
C -2.859329 -0.802697 -0.012336
C  0.160387 -0.093596  1.500102
C  2.055849 -0.138889 -0.836063
C -0.714886  1.045828 -0.617043
C -1.589915 -1.181411  0.125935
C  0.748794 -0.974421 -0.784705
C -0.365207 -0.264449  0.068483
H  3.155838  1.036796  0.714448
H  3.111697 -0.757366  1.014860
H  1.835413  0.820151 -1.315843
H  2.790665 -0.665852 -1.462383
H  0.366131 -1.143255 -1.798425
H  0.953527 -1.955250 -0.333801
H -1.102026  0.912398 -1.627272
H -0.193637  2.474654  0.863447
H -0.845153  3.148826 -0.722303
H -1.353121 -2.224144  0.336609
H -3.127932  0.231193 -0.202906
H -3.675727 -1.512958  0.071398
H  1.465398  0.193465  1.269525
H  0.212535 -1.036705  2.049316
H -0.303945  0.702371  2.081829
```

Test set

```
Reactant: [CH2]CCCCCC
Product: CC[CH]CCCC
C  1.242851  1.462273  0.479292
C -2.694075  0.850223  1.548905
C  1.953551  0.530482 -0.502206
C -2.050797 -0.077967  0.494913
C  1.689513 -0.960139 -0.144310
C -0.598635 -0.405780  0.819219
C  0.168047 -1.263867 -0.192019
H  1.727783  1.551976  1.453798
H  0.905659  2.419732  0.080474
H  3.037896  0.716550 -0.509218
H  1.585328  0.710885 -1.520469
H  2.224064 -1.611510 -0.845862
H  2.072906 -1.167020  0.864081
H -0.198572 -1.045324 -1.204906
H -0.004240 -2.334478 -0.004816
H  0.123993  0.715031  0.751189
H -0.449989 -0.734019  1.854279
H -2.100198  0.396443 -0.494872
H -2.637449 -1.009386  0.427294
H -3.737142  1.070917  1.296751
H -2.672039  0.379133  2.538579
H -2.144000  1.795951  1.608793
```

```
Reactant: C[CH]CCCCC
Product: C[CH]CCCCC
C  2.075845 -1.246172 -0.500517
C -2.408105 -1.093013  0.280541
C  1.185741 -0.643348  0.580351
C -1.251338 -0.399297 -0.424439
```

```
C  1.237435  0.884323  0.707329
C -1.126041  1.113935 -0.224998
C  0.349532  1.573947 -0.367553
H  3.140614 -1.103821 -0.260013
H  1.889995 -0.770685 -1.471165
H  1.897033 -2.322024 -0.608920
H  1.231282 -1.176889  1.533114
H  2.274083  1.243422  0.611935
H  0.875001  1.188258  1.697857
H  0.415906  2.663101 -0.259716
H  0.716004  1.317091 -1.370113
H -1.757710  1.657614 -0.944195
H -1.478951  1.376184  0.782393
H -0.085299 -0.784246  0.141110
H -1.124457 -0.702599 -1.468963
H -2.380183 -0.890456  1.358397
H -3.379832 -0.738352 -0.097753
H -2.370290 -2.178370  0.133600
```

Reactant: CCC(C)C([CH2])C
Product: [CH2]CC(C)C(C)C

```
C -2.260782 -0.537221  0.142875
C  0.009904 -1.837514 -0.046060
C  2.215104 -0.614824  0.058488
C  0.681844  2.025898  0.044562
C -1.486868  0.738376 -0.178197
C  0.725064 -0.520889 -0.364658
C -0.010649  0.674734  0.321039
H  0.091339 -2.617743 -0.804645
H  0.198775 -2.207439  0.965468
H  0.680300 -0.345104 -1.449438
H  2.287773 -0.714097  1.148588
H  2.681398 -1.495641 -0.396995
H  2.779800  0.270163 -0.251777
H -0.016688  0.489141  1.406055
H  0.106052  2.846143  0.489372
H  1.692555  2.056994  0.462157
H  0.746868  2.202026 -1.036786
H -1.971665  1.616127  0.275172
H -1.467860  0.903229 -1.264106
H -1.283541 -1.443275 -0.003297
H -2.557356 -0.637366  1.189332
H -3.058210 -0.803706 -0.551979
```

Reactant: [CH2]C(C)CC(C)C
Product: [CH2]C(C)CC(C)C

```
C -1.323605  1.368047  0.100580
C -2.551362 -0.861284  0.107277
C  1.307396  1.377481  0.101384
C  2.550952 -0.843179  0.108070
C -0.000451 -0.780968  0.164070
C -1.290757 -0.090875 -0.359978
C  1.285105 -0.081564 -0.359410
H -1.849386  2.066420 -0.552432
H -1.585311  1.492137  1.155164
H -1.255984 -0.113523 -1.458302
H -2.525755 -1.898942 -0.247487
H -3.461490 -0.384874 -0.273713
H -2.599227 -0.870433  1.202805
H -0.000774 -0.756083  1.263962
H  0.003446 -1.833969 -0.146244
H  1.250857 -0.104200 -1.457752
H -0.009215  1.676713  0.064260
H  1.828484  2.079667 -0.551301
H  1.567735  1.503297  1.156101
H  2.532914 -1.880772 -0.247333
H  3.457856 -0.360053 -0.272143
H  2.598286 -0.852670  1.203617
```

Reactant: C#CCCCC[CH]C
Product: C#C[CH]CCCCC

```
C  2.662498  1.024619 -0.586088
C -1.225478  1.940785 -0.187131
C  1.908078  0.358564  0.090097
C -1.422449  0.680738  0.638506
C  0.987670 -0.412503  0.872769
C -1.864842 -0.574087 -0.116185
C  0.417123 -1.671777  0.182125
C -0.676456 -1.271464 -0.838876
H -0.521162  1.766359 -1.008204
H -0.833079  2.759378  0.425714
H -2.179636  2.273491 -0.626080
H -1.908989  0.839263  1.603048
H -2.311532 -1.292042  0.583394
H -2.635424 -0.314420 -0.859346
H -0.241464 -0.594778 -1.584279
H -1.040213 -2.161317 -1.365739
H  1.219341 -2.228709 -0.317077
H -0.026731 -2.325884  0.943350
H -0.106364  0.281562  0.964470
H  1.317006 -0.570401  1.903450
H  3.326631  1.605603 -1.175705
```

Reactant: C#CC(CC)C([CH2])C

Product: C#CC(C[CH2])C(C)C
C -0.069922 2.479026 0.698810
C -2.031696 -0.782170 0.481597
C 0.476084 -1.263562 1.118905
C 2.350050 -0.308678 -0.323514
C -0.081434 1.481823 0.017496
C -1.550553 -0.322295 -0.891790
C 0.889053 -0.817786 -0.281266
C -0.103713 0.273869 -0.816732
H 0.699896 -0.534962 1.900318
H 0.749210 -2.284975 1.387432
H 0.795280 -1.670847 -0.967461
H 2.452825 0.574787 0.314838
H 3.034909 -1.084209 0.036142
H 2.637038 -0.036607 -1.346757
H 0.211800 0.547628 -1.833663
H -0.064240 3.353959 1.299721
H -1.521034 -1.171295 -1.585937
H -2.221302 0.435727 -1.318425
H -0.871883 -1.213572 1.014117
H -2.330378 0.027129 1.148952
H -2.725158 -1.623526 0.484647

Reactant: C#CC(C)CC([CH2])C
Product: C#CC([CH2])CC(C)C
C -3.379049 -0.788878 -0.211016
C 1.783003 1.214495 -0.202302
C 2.667125 -1.171292 -0.125344
C -0.812153 1.633432 -0.099713
C -2.299551 -0.342051 0.093335
C 0.160758 -0.715682 -0.096485
C 1.556350 -0.198104 0.343709
C -0.981186 0.204771 0.447624
H 2.440329 1.856342 0.386257
H 2.007813 1.240743 -1.272128
H 1.567475 -0.158990 1.442109
H 2.665684 -1.240722 -1.219636
H 3.652651 -0.817477 0.196727
H 2.504294 -2.174231 0.287140
H 0.104358 -0.737235 -1.192538
H 0.005524 -1.735697 0.272287
H -0.894258 0.229952 1.543333
H -4.328004 -1.178123 -0.483786
H 0.540605 1.721825 -0.132023
H -1.109970 1.735558 -1.144300
H -1.191051 2.430507 0.539839

Reactant: C=CC(CC)C([CH2])C
Product: C=CC(C[CH2])C(C)C
C -2.441952 -0.965063 1.393545
C 2.157239 -1.397104 -0.113572
C 1.687964 1.184300 -0.187781
C -0.625602 2.073890 0.333015
C -1.632799 -0.755647 0.356016
C 0.650743 -1.620460 -0.211741
C 0.187130 0.901075 -0.271618
C -0.156614 -0.450129 0.444549
H 2.111939 1.749212 -1.019351
H 2.012144 1.555822 0.788019
H -0.096871 0.783882 -1.327511
H -0.358392 2.205048 1.388657
H -0.404160 3.006433 -0.197615
H -1.700297 1.874955 0.273187
H 0.136753 -0.365577 1.501002
H -2.025435 -0.824317 -0.659610
H -3.493075 -1.203020 1.264431
H -2.080949 -0.906694 2.416738
H 0.348045 -1.690216 -1.265000
H 0.354991 -2.559195 0.277087
H 2.205397 -0.062439 -0.242669
H 2.580683 -1.582400 0.875914
H 2.757729 -1.820636 -0.919487

Reactant: C=CC(C)CC([CH2])C
Product: C=CC([CH2])CC(C)C
C -3.075795 -1.089009 -1.225438
C 1.707970 1.315763 0.228724
C 2.809801 -0.977664 0.254452
C -0.898275 1.483539 -0.074440
C -2.226848 -0.628623 -0.308242
C 0.278103 -0.755983 0.029115
C 1.652542 -0.115377 -0.310011
C -0.900796 0.043290 -0.606373
H 1.844580 1.373859 1.312195
H 2.347498 2.010360 -0.318201
H 1.743230 -0.084586 -1.404872
H 3.780365 -0.533620 0.006786
H 2.774913 -1.993052 -0.158648
H 2.728919 -1.043686 1.346055
H 0.250200 -1.789584 -0.335821
H 0.150458 -0.780173 1.121264
H -0.749308 0.060561 -1.693819
H -2.467085 -0.714800 0.751567
H -2.861867 -1.012111 -2.288065

```
H -4.016269 -1.558110 -0.954246
H  0.427381  1.705789  0.052223
H -1.312327  2.236118 -0.746202
H -1.271884  1.575755  0.948876

Reactant: C=CCCCC[CH]C
Product: C=C[CH]CCCCC
C -3.204925  0.590008  0.140861
C  1.359329  2.236321 -0.265075
C -2.078435  0.088091 -0.391022
C  1.340528  0.912955  0.474472
C -0.943938 -0.459112  0.369696
C  2.020495 -0.285056 -0.179486
C -0.153236 -1.619562 -0.262154
C  1.322961 -1.617952  0.211289
H  2.383911  2.633677 -0.352766
H  0.966253  2.116804 -1.282448
H  0.754243  2.989791  0.251032
H  1.503987  0.983169  1.553066
H  1.979101 -0.175297 -1.272158
H  3.084366 -0.331190  0.102459
H  1.858490 -2.462519 -0.237815
H  1.359732 -1.742325  1.302189
H -0.171897 -1.514234 -1.355822
H -0.625139 -2.580843 -0.017727
H -0.021218  0.419483  0.424513
H -1.172922 -0.631502  1.426994
H -1.952545  0.107365 -1.474072
H -3.377525  0.587160  1.213507
H -3.988201  1.016317 -0.476661

Reactant: [CH2]C(C)C(C)C(C)C
Product: [CH2]C(C)C(C)C(C)C
C  1.319686 -1.659690 -0.007018
C  2.595171  0.505264 -0.164655
C -1.291264 -1.675189 -0.009838
C -2.592185  0.474669 -0.166626
C -0.007908  2.025096  0.022506
C  1.287692 -0.167435  0.333626
C -1.277218 -0.182970  0.332139
C  0.001430  0.506348 -0.256853
H  1.596511 -1.867762 -1.044367
H  1.843854 -2.296920  0.707297
H  1.234270 -0.054143  1.426337
H  2.623160  0.501777 -1.261251
H  3.464814 -0.052209  0.201114
H  2.682172  1.538447  0.185656
H  0.003047  0.342221 -1.346234
H -0.009913  2.209794  1.104648
H  0.871712  2.511384 -0.408383
H -0.892618  2.500822 -0.409804
H -1.225882 -0.070181  1.425013
H  0.015871 -1.969823  0.044961
H -1.809771 -2.318956  0.702744
H -1.563306 -1.885392 -1.048021
H -3.455527 -0.093479  0.197679
H -2.619096  0.472004 -1.263249
H -2.692024  1.506370  0.184650

Reactant: CC(C)CCC[C](C)C
Product: CC(C)CCC[C](C)C
C  1.955268  1.361033 -0.863739
C  1.809613  0.321716  1.463015
C -1.827796  0.293724  1.458816
C -1.984651  1.330562 -0.868361
C  0.009521 -1.898824 -0.162510
C  1.278994 -1.118027 -0.600456
C -1.270694 -1.137639 -0.603566
C  1.321265  0.289659  0.016992
C -1.335966  0.269225  0.013819
H -1.291905 -0.434119  2.078159
H -2.901057  0.046555  1.503177
H -1.694092  1.287168  1.903302
H -1.901121  2.324345 -0.412275
H -3.056693  1.117979 -1.012700
H -1.513930  1.362549 -1.858230
H -1.259878 -1.054722 -1.699045
H -2.165796 -1.717094 -0.327032
H  0.017806 -2.900455 -0.609109
H  0.009161 -2.026640  0.927378
H  1.269681 -1.035420 -1.695975
H  2.182117 -1.683794 -0.321629
H -0.009296  0.528646  0.060872
H  1.487347  1.384554 -1.855167
H  3.031172  1.166271 -1.004370
H  1.853664  2.353584 -0.408624
H  1.660385  1.313217  1.906886
H  1.283195 -0.413751  2.081468
H  2.886301  0.090378  1.509625

Reactant:
C#CC([CH2])(C)C(C)(C)CC
Product: C#CC(C)(C)C(C)(C)C[CH2]
C -2.496729 -1.107306 -0.943656
```

```
C  1.613893 -1.846387  0.141057
C -0.226294 -0.788427  1.686981
C -1.303823  1.426062  1.124937
C  0.226532  1.379502 -1.572002
C  1.725205  1.217583  0.438587
C -1.648849 -0.547148 -0.290870
C  1.212106 -0.850431 -0.944990
C -0.634671  0.145525  0.531065
C  0.630748  0.487478 -0.376168
H  0.301126 -0.285325  2.499362
H -1.014962 -1.455817  2.032980
H -0.594655  1.963172  1.761579
H -2.162719  1.129447  1.734658
H -1.654152  2.090368  0.330405
H -3.245089 -1.602301 -1.510663
H -0.590630  0.919324 -2.136041
H -0.088765  2.374023 -1.239701
H  1.087078  1.504949 -2.239838
H  2.065218  0.624872  1.292352
H  2.588581  1.403300 -0.211713
H  1.367187  2.185374  0.804356
H  0.450015 -1.298064 -1.591487
H  2.074172 -0.590635 -1.577489
H  0.715873 -1.555793  1.077345
H  1.469398 -2.898017 -0.109313
H  2.577301 -1.656066  0.617756
```

Reactant:
C=CC(C=C)CCC([CH2])(C)C
Product: C=C[C](C=C)CCC(C)(C)C

```
C -1.881048  2.067081 -0.199073
C -3.026702 -1.819705 -0.088438
C  1.327859 -0.376969 -1.407729
C  3.372577  0.702972 -0.418361
C  2.487525 -1.448735  0.555033
C -1.802256  0.803385 -0.626921
C -1.719438 -1.611147  0.094865
C -0.147680  0.047200  1.219071
C  1.188417  0.738057  0.846318
C -0.994979 -0.305221 -0.030402
C  2.082723 -0.113381 -0.112971
H  1.517770 -1.315765 -1.927008
H  1.166478  0.486607 -2.054381
H  4.025735  0.144221 -1.097963
H  3.921471  0.904118  0.510340
H  3.115934  1.659816 -0.887365
H  1.614966 -2.085308  0.734528
H  2.986056 -1.260910  1.513338
H  3.180420 -1.996966 -0.094140
H  0.977423  1.696314  0.355428
H  1.759923  0.948682  1.759788
H -0.730715  0.691557  1.889318
H  0.064843 -0.873470  1.773172
H -0.088717 -0.503840 -0.838486
H -2.349475  0.521001 -1.525602
H -1.366546  2.416327  0.689774
H -2.477304  2.803821 -0.727633
H -1.082809 -2.453137  0.367288
H -3.709370 -1.011836 -0.329701
H -3.460552 -2.809139  0.013106
```

Reactant:
C#CC([CH2])(C=C)C(C)(C#C)CC
Product:
C#CC(C)(C=C)C(C)(C#C)C[CH2]

```
C  2.308322 -1.862416  0.418732
C  2.544174  1.677903 -0.161392
C -2.435520  1.885594 -0.262619
C -1.790243 -1.771529 -0.855892
C  0.147384 -0.292816 -1.831048
C -0.243450  0.390683  2.024397
C  1.538495 -1.003516  0.061884
C  1.262377  1.416596 -0.403297
C -1.634298  1.059529  0.104626
C -1.357013 -1.362483  0.548471
C  0.602139  0.035575 -0.393327
C -0.674890  0.048945  0.576991
H  0.913781 -0.756443 -2.449986
H -0.378089  0.530817 -2.315627
H  0.570549  2.213614 -0.663776
H  2.932675  2.689412 -0.220285
H  3.245646  0.893224  0.100720
H  2.986408 -2.620250  0.723617
H  0.463824 -0.364060  2.381477
H  0.240872  1.369974  2.054907
H -1.120651  0.402825  2.678658
H -3.145265  2.609630 -0.577091
H -0.629928 -2.078738  0.944057
H -2.212050 -1.328782  1.237717
H -0.828884 -1.200976 -1.586685
H -2.699949 -1.285613 -1.210652
H -1.759229 -2.840880 -1.065804
```

Reactant:
C#CC([CH2])(C#C)C(C)(C=C)CC
Product:
C#CC(C)(C#C)C(C)(C=C)C[CH2]

C	2.538958	1.657353	-0.780966
C	1.908768	-2.507983	0.464440
C	-2.812361	-0.948198	0.328203
C	-1.345543	1.987211	0.808483
C	0.509400	0.408733	1.779063
C	-0.256524	-0.581823	-1.949344
C	1.766226	0.871867	-0.289993
C	1.426887	-1.404145	0.383894
C	-1.503915	-1.097728	0.129456
C	-1.131503	1.353895	-0.568136
C	0.806641	-0.060741	0.337568
C	-0.556116	-0.093979	-0.508795
H	1.361113	0.846743	2.296211
H	-0.046120	-0.326012	2.361258
H	3.232672	2.337531	-1.208615
H	2.351149	-3.470401	0.534106
H	0.475904	0.077551	-2.426170
H	-1.182792	-0.576128	-2.532740
H	0.143175	-1.600223	-1.934886
H	-1.033400	-2.047508	0.378838
H	-3.412582	-1.753682	0.739590
H	-3.342673	-0.033040	0.087926
H	-2.069016	1.319817	-1.140961
H	-0.422914	1.958812	-1.142482
H	-0.400599	1.386106	1.516077
H	-2.263617	1.696698	1.318652
H	-1.143160	3.057219	0.865563

Reactant:
C=CC([CH2])(C)C(C=C)(C=C)CC
Product:
C=CC(C)(C)C(C=C)(C=C)C[CH2]

C	-2.311436	0.329642	2.105303
C	2.439119	1.191612	1.391012
C	1.621708	-2.327508	0.797264
C	0.752314	-0.016612	-2.559738
C	-1.530816	-0.213324	-1.274230
C	-0.986854	1.879494	-0.006494
C	-1.559601	-0.289541	1.195387
C	1.316727	0.480525	1.289593
C	0.813996	-1.606933	0.020028
C	1.418860	0.449010	-1.266187
C	-0.857442	0.340865	-0.005003
C	0.694860	-0.082493	0.022221
H	-2.361210	0.393559	-1.638359
H	-1.771465	-1.277772	-1.251094
H	-0.560012	2.296881	-0.922908
H	-0.469106	2.316867	0.851636
H	-2.044107	2.162983	0.028772
H	-1.418223	-1.366727	1.266434
H	-2.790524	-0.223956	2.906992
H	-2.484202	1.400131	2.093121
H	0.749234	0.250000	2.189385
H	3.050218	1.451240	0.533578
H	2.793625	1.544704	2.354627
H	0.207311	-2.114750	-0.725583
H	1.678657	-3.407736	0.705246
H	2.259788	-1.864598	1.542350
H	2.458635	0.098223	-1.219958
H	1.436747	1.542475	-1.227410
H	-0.526906	-0.107472	-2.166995
H	0.777731	0.697082	-3.384023
H	1.005971	-1.030924	-2.872142

Reactant:
C#CC(C#C)CC(C#C)(C=C)C[CH2]
Product:
C#C[C](C#C)CC(C#C)(C=C)CC

C	2.442945	2.198123	-0.860320
C	3.151348	-2.110744	0.082652
C	-1.429976	2.648652	-0.206526
C	-3.433278	-0.107479	-1.329505
C	-0.021742	0.165969	2.202008
C	1.973593	1.143172	-0.507293
C	2.375547	-1.188459	-0.002943
C	-1.327402	1.447567	-0.151555
C	-2.411039	-0.704888	-0.725141
C	-1.184138	-0.444433	1.453351
C	0.076610	-0.525876	-0.784374
C	1.399121	-0.113987	-0.060970
C	-1.219417	-0.014004	-0.064622
H	-0.041814	1.244530	2.342748
H	0.429264	-0.412838	3.004875
H	-1.128121	-1.539514	1.484908
H	-2.146083	-0.144515	1.893569
H	-1.499973	3.706566	-0.258956
H	-2.367941	-1.791400	-0.662412
H	-4.241829	-0.680649	-1.770771
H	-3.493632	0.973058	-1.402031
H	0.083367	-0.161628	-1.814971

```
H  0.029149 -1.619867 -0.801640
H  0.996982  0.059328  1.087757
H  2.861189  3.120300 -1.177832
H  3.847666 -2.909163  0.146451

Reactant:
C=CC([CH2])(C=C)C(C#C)(C#C)CC
Product:
C=CC(C)(C=C)C(C#C)(C#C)C[CH2]
C  2.224935 -1.649380  0.921054
C  2.414833  1.394341 -1.289421
C -2.595952  0.902172 -1.547248
C -0.437219  2.333729  1.994824
C -1.520061 -2.195666  0.299255
C  0.337166 -1.296323 -1.327270
C  1.593439 -0.490223  0.743439
C  1.134564  1.045902 -1.178408
C -1.774466  0.633529 -0.704935
C -0.596095  1.418895  1.224982
C -1.330499 -0.954635  1.164198
C  0.613815 -0.139929 -0.364611
C -0.783380  0.266875  0.325043
H -0.237858 -0.999527 -2.204484
H  1.205898 -1.905379 -1.572096
H  1.768159  0.328436  1.438067
H  2.913132 -1.789177  1.748908
H  2.088969 -2.500903  0.263927
H  0.365890  1.579428 -1.732410
H  2.720951  2.221815 -1.921314
H  3.200215  0.865942 -0.758922
H -3.325320  1.152229 -2.276906
H -0.307087  3.150459  2.660165
H -0.597496 -1.145526  1.952208
H -2.269072 -0.633423  1.631750
H -0.544198 -2.027759 -0.609195
H -1.324782 -3.144751  0.798308
H -2.428930 -2.198941 -0.303123

Reactant: [CH2]CCC(C)C(C#C)C=C
Product: CCCC([CH2])C(C#C)C=C
C  2.649984  1.662855  1.746235
C -2.671373  1.662649  0.701804
C -2.383902 -1.962632  0.721656
C  0.595235  0.015091  1.770091
C  2.517521  1.729098  0.224227
C -1.894078  0.853106  0.256890
C -1.346698 -1.565424 -0.009005
C  1.039915  1.526010 -0.211460
C  0.516391  0.139055  0.252044
C -0.944317 -0.122310 -0.290402
H  3.602487  1.297659  2.132025
H  2.290678  2.551337  2.270150
H  2.878385  2.694160 -0.160342
H  3.131163  0.944777 -0.237582
H  0.959451  1.601879 -1.303300
H  0.411090  2.309651  0.228921
H  1.154736 -0.629222 -0.206954
H  1.718210  0.734023  2.023086
H  0.750573 -0.989781  2.161809
H -0.187900  0.565869  2.294326
H -0.906469  0.014074 -1.383742
H -0.681853 -2.298974 -0.462151
H -3.059054 -1.247266  1.179134
H -2.592933 -3.014864  0.883613
H -3.354531  2.375616  1.091576

Reactant: [CH2]CCC(C)C(C#C)C=C
Product: CCCC(C)[C](C#C)C=C
C -1.500314  1.929929 -0.509923
C  1.413130 -0.528724 -2.259765
C  2.843357  0.735259  0.895504
C -0.121258 -2.176786  0.746209
C -2.480103  0.890293  0.003671
C  1.005259 -0.193303 -1.171288
C  1.527399  0.653986  1.110089
C -1.912736 -0.555447 -0.115124
C -0.604339 -0.712780  0.695346
C  0.491665  0.233743  0.114553
H -1.356652  1.973545 -1.589321
H -1.449580  2.889289  0.001178
H -3.426786  0.943526 -0.557122
H -2.715917  1.086212  1.057246
H -1.710638 -0.791898 -1.167739
H -2.658661 -1.269345  0.254801
H -0.800318 -0.369762  1.721855
H  0.067643 -2.545433 -0.267000
H  0.809391 -2.248940  1.319254
H -0.878002 -2.813318  1.219152
H -0.210904  1.224313 -0.138221
H  1.121034  0.927493  2.082749
H  3.522910  1.071310  1.671312
H  3.276954  0.466443 -0.061927
H  1.772156 -0.823857 -3.214054
```

```
Reactant: C#CC(C)CCC([CH2])C
Product: C#C[C](C)CCC(C)C
C  2.448520  1.928971  0.141385
C -1.056521 -0.135481  1.401007
C -3.177291  0.510735  0.167321
C  2.098528 -1.616273  0.376320
C  1.891739  0.855244  0.079811
C -0.982209  0.225856 -1.101574
C  0.325446 -0.592035 -1.229174
C -1.838517 -0.271368  0.099280
C  1.207726 -0.413363  0.030969
H -0.958813  0.885059  1.777258
H -1.231816 -0.883636  2.173474
H -2.063718 -1.333299 -0.071376
H -2.977620  1.577542  0.322273
H -3.739786  0.393695 -0.767015
H -3.796870  0.150544  0.995715
H -0.734679  1.285656 -0.955288
H -1.569199  0.139654 -2.024196
H  0.072249 -1.655865 -1.330578
H  0.885216 -0.290918 -2.123292
H  0.292653 -0.348948  0.907905
H  2.941751  2.867231  0.192784
H  2.642356 -1.439608  1.309205
H  1.485015 -2.517250  0.489410
H  2.830070 -1.792414 -0.422983

Reactant: C=CC(C)CC(C)C[CH2]
Product: C=C[C](C)CC(C)CC
C -3.356267 -0.178634 -0.560777
C  0.610532  2.047308  0.323546
C -1.306389 -0.497147  1.570861
C  2.865294 -1.070874 -0.347917
C -2.047955 -0.092257 -0.839679
C  1.757479  1.222342 -0.234063
C  0.329883 -0.875560 -0.378261
C -0.926724 -0.132464  0.131735
C  1.650811 -0.277377  0.174340
H  0.253311  2.886762 -0.270716
H  0.628637  2.230631  1.398343
H  1.763588  1.277028 -1.331075
H  2.728032  1.610393  0.115695
H  1.636125 -0.334250  1.271769
H  2.801444 -2.124332 -0.051638
H  2.903972 -1.024246 -1.443427
H  3.800886 -0.657571  0.046696
H  0.367751 -0.818714 -1.475454
H  0.263976 -1.939421 -0.106684
H -0.459110  1.028784  0.201947
H -1.744969  0.045401 -1.878072
H -4.104744 -0.110378 -1.343263
H -3.726990 -0.321885  0.448485
H -2.062610  0.189653  1.966265
H -0.429365 -0.449254  2.224476
H -1.711554 -1.517072  1.610710
```

1-6 H-shift

Training set

Primary contributions

```
Reactant: [CH2]CCCCC
Product: [CH2]CCCCC
C  1.304926  1.282816  0.259337
C -1.311238  1.279001 -0.259793
C  1.643449 -0.098757 -0.289441
C -1.645393 -0.103538  0.289248
C  0.728554 -1.221248  0.269501
C -0.726974 -1.223236 -0.269545
H  1.366668  1.359326  1.348376
H  1.792148  2.118749 -0.247510
H  2.688498 -0.348812 -0.046798
H  1.567250 -0.092453 -1.385308
H  1.182957 -2.188299  0.014981
H  0.706991 -1.157530  1.366704
H -1.178605 -2.191618 -0.015164
H -0.705399 -1.159300 -1.366734
H -2.689633 -0.357025  0.046701
H -1.569173 -0.096706  1.385107
H -0.003328  1.423875 -0.000451
H -1.373773  1.355288 -1.348806
H -1.800598  2.113560  0.247252

Reactant: [CH2]CCCCCC
Product: C[CH]CCCCC
C -0.651706  1.724103  0.199018
C  2.672810  0.532825  0.106362
C -1.826427  0.855508 -0.233410
C  1.333791  0.060855 -0.448797
C -1.779678 -0.578203  0.360183
C  0.761127 -1.202586  0.190038
C -0.696472 -1.512531 -0.241921
H -0.553197  1.843712  1.281353
H -0.538139  2.665380 -0.342779
```

```
H -2.773235  1.327638  0.074574
H -1.852345  0.784373 -1.329414
H -2.759086 -1.047221  0.194703
H -1.635964 -0.514041  1.447996
H -0.763727 -1.482937 -1.338731
H -0.931328 -2.541017  0.063660
H  0.795541 -1.103206  1.284670
H  1.398649 -2.063496 -0.069558
H  0.440034  0.979801 -0.144923
H  1.302701  0.027524 -1.543740
H  2.603965  0.696456  1.188951
H  2.990304  1.470154 -0.364145
H  3.461288 -0.215425 -0.067413
```

Reactant: C#CCCCCC[CH2]
Product: C#C[CH]CCCCC

```
C  2.738030  0.587248 -1.010565
C -1.086824  1.596999  0.705781
C  1.982630  0.305098 -0.106348
C -1.642945  0.977848 -0.563783
C  1.054496 -0.005317  0.946519
C -1.861047 -0.555981 -0.457107
C  0.301570 -1.343814  0.794802
C -0.568570 -1.413033 -0.484527
H -1.649738  1.389571  1.618202
H -0.724685  2.623037  0.630646
H -0.966535  1.185512 -1.403353
H -2.608808  1.449726 -0.810020
H -2.425697 -0.778130  0.459584
H -2.488460 -0.868946 -1.302266
H -0.862152 -2.460309 -0.636189
H  0.045006 -1.121956 -1.346662
H  1.031599 -2.164017  0.778846
H -0.336014 -1.487635  1.676892
H  0.120408  0.850071  0.891703
H  1.484845  0.131924  1.944434
H  3.405683  0.831645 -1.798505
```

Reactant: C=CCCCCC[CH2]
Product: C=C[CH]CCCCC

```
C -3.293718  0.580193  1.284711
C  0.777319  1.732730 -0.079306
C -2.376368  0.168120  0.398677
C  2.060419  0.952130  0.132853
C -0.971671 -0.167429  0.714868
C  2.053399 -0.444093 -0.546130
C -0.365593 -1.343629 -0.066408
C  1.161306 -1.510223  0.143408
H  0.489284  1.893233 -1.120264
H  0.614248  2.598220  0.563411
H  2.247565  0.823996  1.207640
H  2.913477  1.525825 -0.267364
H  1.742814 -0.334963 -1.594757
H  3.084555 -0.821919 -0.555753
H  1.380979 -1.520969  1.220498
H  1.449757 -2.494715 -0.248704
H -0.566946 -1.207446 -1.138493
H -0.868721 -2.272602  0.238278
H -0.259244  0.800793  0.361971
H -0.784226 -0.244433  1.792363
H -2.652101  0.093675 -0.653754
H -4.302435  0.843532  0.984427
H -3.063320  0.665084  2.343130
```

Reactant: [CH2]CCCCC(C)C
Product: CCCCC[C](C)C

```
C -0.871483 -1.745726  0.168646
C  1.575085  0.040301 -1.489183
C  2.327512 -0.547027  0.872453
C -1.995938 -0.851579 -0.334662
C -2.032106  0.536873  0.359682
C -0.902053  1.514129 -0.060933
C  0.496753  1.208727  0.538013
C  1.187232 -0.045974 -0.013389
H -0.654672 -2.624805 -0.441522
H -0.915901 -1.970131  1.237623
H -2.967897 -1.345568 -0.171958
H -1.898380 -0.702669 -1.418703
H -2.994102  1.011274  0.122959
H -2.003988  0.397472  1.449766
H -1.189598  2.522902  0.265482
H -0.842813  1.544429 -1.156685
H  1.153613  2.077553  0.364485
H  0.388837  1.105163  1.627036
H  0.256221 -0.950423  0.061873
H  1.975843 -0.917984 -1.840152
H  2.352501  0.806301 -1.636431
H  0.718642  0.304375 -2.118417
H  3.147951  0.187041  0.901365
H  2.734328 -1.490643  0.489828
H  1.982842 -0.708397  1.900818
```

Reactant: [CH2]CCCCC(C)C#C
Product: CCCCC[C](C)C#C

```
C -1.119773  1.465046 -0.959210
C  2.102198 -1.341116 -1.449559
C  1.953151  1.443335  0.770749
C -1.977933  0.215826 -1.035703
C  1.607221 -0.576849 -0.650656
C -2.192268 -0.469966  0.340927
C -0.962151 -1.230784  0.901663
C  0.197118 -0.337003  1.404527
C  0.994548  0.348323  0.272812
H -1.442345  2.218359 -0.237691
H -0.766320  1.875259 -1.905803
H -2.966483  0.472622 -1.452371
H -1.521341 -0.504174 -1.727434
H -3.013463 -1.191640  0.236933
H -2.519432  0.282972  1.072219
H -0.577419 -1.916945  0.136557
H -1.302854 -1.846700  1.744763
H  0.891836 -0.941903  2.003908
H -0.207308  0.446233  2.060009
H  0.096300  0.944597 -0.367301
H  2.450732  1.934105 -0.071212
H  2.721389  1.009701  1.423719
H  1.396917  2.196049  1.340997
H  2.544763 -2.009599 -2.144966
```

Reactant: [CH2]CCCCC(C)C=C
Product: CCCCC[C](C)C=C

```
C -0.867275  1.552918  0.867528
C  3.411936  0.366315  0.456595
C  1.112180 -1.221521  1.459205
C -2.135983  0.741572  0.693136
C  2.243490  0.353716 -0.197561
C -2.188653 -0.043814 -0.645984
C -1.260000 -1.284776 -0.713971
C  0.241309 -0.981739 -0.955738
C  0.985695 -0.321231  0.226444
H -0.619797  1.877424  1.878462
H -0.680112  2.307594  0.101124
H -2.246839  0.032351  1.524265
H -3.012235  1.410876  0.734296
H -1.949519  0.636131 -1.475563
H -3.221565 -0.384311 -0.798344
H -1.603474 -1.918788 -1.542705
H -1.382703 -1.875510  0.202764
H  0.758852 -1.919380 -1.208639
H  0.322668 -0.326528 -1.834436
H  0.211453  0.593201  0.562078
H  1.515996 -0.663802  2.311058
H  1.784320 -2.064716  1.249121
H  0.137371 -1.624256  1.750532
H  2.166977  0.904469 -1.135877
H  3.561363 -0.164692  1.390363
H  4.267295  0.911961  0.071719
```

Reactant: [CH2]CCCCC(C#C)C#C
Product: CCCCC[C](C#C)C#C

```
C  1.099348 -1.068312  1.500099
C -1.299027  2.433293  0.809757
C -3.006996 -1.645622 -0.061913
C  2.203537 -0.165462  0.996576
C -1.139293  1.304923  0.407407
C -2.061572 -0.893503 -0.058186
C  2.373482 -0.188332 -0.547350
C  1.287422  0.581735 -1.343200
C -0.099551 -0.098917 -1.408199
C -0.880194 -0.047424 -0.061711
H  1.116639 -2.103341  1.156489
H  0.761478 -0.929745  2.526509
H  2.019640  0.866012  1.324297
H  3.160326 -0.474330  1.452487
H  3.345838  0.261562 -0.787038
H  2.409352 -1.231138 -0.892304
H  1.174738  1.590495 -0.926242
H  1.644600  0.699132 -2.374943
H  0.016948 -1.153132 -1.686403
H -0.715824  0.384963 -2.174874
H -0.092150 -0.539614  0.735061
H -1.462842  3.421356  1.161063
H -3.848968 -2.291714 -0.062685
```

Reactant: [CH2]CCCCC(C#C)C=C
Product: CCCCC[C](C#C)C=C

```
C -1.038786  0.561783 -1.708294
C  1.263060 -2.672275 -0.051460
C  3.349176  0.334859 -0.461709
C -2.168063 -0.146239 -0.992472
C  1.117730 -1.473771  0.026502
C  2.138268  0.790868 -0.135883
C -2.348548  0.305631  0.482696
C -1.288853 -0.237442  1.477003
C  0.118749  0.395059  1.364964
C  0.910720 -0.040908  0.101434
H -1.042974  1.651969 -1.667274
H -0.695984  0.139734 -2.652302
```

```
H -3.115080  0.040978 -1.528085
H -2.002358 -1.231138 -1.019143
H -2.360254  1.404012  0.525668
H -3.334210 -0.037421  0.824100
H -1.656517 -0.051480  2.495072
H -1.202557 -1.325029  1.360670
H  0.025052  1.489344  1.347410
H  0.712607  0.128584  2.248282
H  0.135679  0.234254 -0.803785
H  1.971902  1.862374 -0.034906
H  3.543397 -0.727664 -0.563663
H  4.181080  1.009824 -0.632393
H  1.394514 -3.723534 -0.116397
```

```
Reactant: [CH2]CCCCC(C=C)C=C
Product: CCCCC[C](C=C)C=C
C  1.248082  1.732431 -0.572973
C -2.939070  0.751467  0.486752
C -1.013378 -0.529744 -2.190664
C  2.424836  0.809719 -0.819985
C -1.697334  0.586256  0.958071
C -0.975335 -0.936509 -0.921423
C  2.739157 -0.125125  0.378474
C  1.722621 -1.276251  0.598635
C  0.370319 -0.855488  1.226585
C -0.567293 -0.096163  0.258812
H  1.313885  2.358173  0.319508
H  0.830445  2.244453 -1.440341
H -3.692495  1.286366  1.055354
H -3.234731  0.358605 -0.479871
H -0.725679  0.477764 -2.474410
H -1.335548 -1.187113 -2.992174
H  3.325861  1.409636 -1.034752
H  2.235309  0.196213 -1.710179
H -1.441682  0.999459  1.934082
H -1.273270 -1.958496 -0.677047
H  3.726701 -0.574205  0.207519
H  2.815106  0.474164  1.296883
H  1.536130 -1.779587 -0.358796
H  2.187425 -2.014051  1.266343
H -0.155004 -1.754341  1.583288
H  0.562380 -0.225397  2.105760
H  0.169986  0.811375 -0.176816
```

Secondary contributions

```
Reactant: CCCCC([CH2])C
Product: [CH2]CCCC(C)C
C  1.920988 -1.150824  0.246359
C -0.687976 -1.423530 -0.237581
C -2.696100  0.086118  0.002059
C  2.099894  0.261130 -0.299976
C  1.068414  1.270741  0.270396
C -0.384068  1.109914 -0.252926
C -1.186422 -0.091921  0.317572
H -1.078299 -2.309823  0.268842
H -0.758402 -1.498055 -1.327142
H -1.062822 -0.094247  1.410219
H -2.849935  0.121432 -1.083277
H -3.279116 -0.749276  0.405647
H -3.076279  1.018752  0.437227
H -0.371339  1.038180 -1.350332
H -0.933451  2.027633 -0.000100
H  1.406736  2.283623  0.013611
H  1.065875  1.203842  1.367522
H  3.112027  0.626288 -0.064172
H  2.015665  0.248795 -1.395113
H  0.634101 -1.425005  0.007066
H  2.010242 -1.224543  1.333744
H  2.485220 -1.928303 -0.273568
```

```
Reactant: CCCC(C)C[CH2]
Product: [CH2]CCC(C)CC
C -2.256741 -0.083911 -0.274631
C -0.582028  1.911243  0.273249
C  2.452765 -0.526919 -0.032039
C -1.417035 -1.219247  0.298846
C  0.698382  1.278013 -0.259045
C  0.039824 -1.242651 -0.237591
C  0.992237 -0.140509  0.306631
H -0.894467  2.824056 -0.238824
H -0.616070  2.009036  1.361739
H  1.556089  1.926241 -0.016350
H  0.654987  1.211303 -1.355329
H  0.887227 -0.104420  1.401250
H  2.587758 -0.572336 -1.120152
H  2.704694 -1.508007  0.386340
H  3.155087  0.212304  0.369998
H  0.026017 -1.185947 -1.335846
H  0.477974 -2.215428  0.025499
H -1.390905 -1.144532  1.394546
H -1.887406 -2.186305  0.060262
H -1.533760  1.009091 -0.003946
H -3.220630  0.076693  0.213430
H -2.334030 -0.089706 -1.365269
```

Reactant: CCCCC([CH2])C#C
Product: [CH2]CCCC(C)C#C
C -1.592657 0.960543 -0.994688
C 2.462200 -0.249259 -1.307198
C 0.290798 1.601653 0.777328
C -2.084745 -0.329153 -0.346483
C 1.799260 -0.028751 -0.322625
C -0.936994 -1.324514 -0.031729
C -0.017447 -0.925662 1.148841
C 0.991798 0.241457 0.877249
H 0.914761 2.410860 0.396382
H -0.263815 1.870762 1.679661
H 1.682027 0.265844 1.738060
H 3.045480 -0.440671 -2.173087
H -0.631750 -0.644513 2.014854
H 0.572631 -1.804532 1.436687
H -0.322802 -1.469995 -0.928772
H -1.384730 -2.296388 0.215163
H -2.624315 -0.097295 0.582113
H -2.804135 -0.828604 -1.014145
H -0.667647 1.406147 -0.158724
H -2.332996 1.760994 -1.062640
H -1.046108 0.810273 -1.928899

Reactant: CCCC(C#C)C[CH2]
Product: [CH2]CCC(C#C)CC
C 2.139949 0.205747 0.691020
C -2.457500 0.737041 0.957579
C 0.347883 -1.766899 0.710031
C 1.223835 1.324566 0.208333
C -1.675833 0.375762 0.110872
C -0.258401 -1.536088 -0.666532
C 0.446705 0.963756 -1.082236
C -0.722695 -0.063488 -0.918334
H 0.843425 -2.731820 0.834522
H -0.319184 -1.518755 1.537407
H -1.131524 -2.189644 -0.811308
H 0.470327 -1.791247 -1.447143
H -1.259149 -0.069376 -1.879516
H -3.147864 1.054342 1.698796
H 1.143037 0.565047 -1.832334
H 0.011637 1.882429 -1.494789
H 0.501404 1.582291 0.991907
H 1.815479 2.231191 0.006792
H 1.325708 -0.851347 0.794906
H 2.557702 0.345747 1.690287
H 2.892684 -0.106802 -0.038263

Reactant: CCCCC([CH2])C=C
Product: [CH2]CCCC(C)C=C
C 2.289852 1.108044 0.387682
C -3.338570 -0.034668 0.441900
C -0.254897 1.442322 -0.332367
C 2.494333 -0.293504 -0.175120
C -2.264035 -0.011136 -0.346024
C 1.398084 -1.296850 0.271974
C 0.005384 -1.103898 -0.386078
C -0.829102 0.102489 0.137123
H -0.686339 2.317609 0.157361
H -0.217726 1.545405 -1.420950
H -0.827558 0.073720 1.235440
H -2.379635 -0.059369 -1.428999
H -4.344659 -0.104251 0.040512
H -3.251440 0.015625 1.523975
H 0.125303 -1.007561 -1.474843
H -0.583566 -2.012771 -0.206091
H 1.290267 -1.251736 1.364846
H 1.743502 -2.310190 0.027371
H 2.514045 -0.254565 -1.272687
H 3.473428 -0.682906 0.145791
H 1.033756 1.412047 0.037157
H 2.911413 1.887569 -0.058223
H 2.276781 1.154804 1.480076

Reactant: CCCC(C=C)C[CH2]
Product: [CH2]CCC(C=C)CC
C -2.604713 -0.358620 0.100103
C 3.163340 -0.288985 -0.383540
C -1.168121 1.837238 -0.352721
C -1.556782 -1.382705 -0.319566
C 2.085226 -0.133906 0.382521
C 0.122056 1.413943 0.339858
C -0.182182 -1.182185 0.373707
C 0.665839 0.028488 -0.127113
H -1.094967 1.896171 -1.442008
H -1.658719 2.711258 0.081327
H -0.030129 1.377697 1.427508
H 0.907281 2.162569 0.152981
H 0.684620 0.011187 -1.226305
H 2.188389 -0.119541 1.468293
H 3.092997 -0.307835 -1.467891
H 4.157088 -0.402751 0.038126
H -0.329616 -1.085858 1.458971

```
H  0.416917 -2.086799  0.208853
H -1.414329 -1.344077 -1.408052
H -1.912914 -2.397865 -0.083925
H -2.010471  0.815953 -0.137742
H -3.516007 -0.349591 -0.501888
H -2.810375 -0.341564  1.173831

Reactant: CCCCC([CH2])(C)C
Product: [CH2]CCCC(C)(C)C
C  2.069200  1.124240 -0.265270
C -0.474713  1.414560  0.485265
C -1.243532  0.082457 -1.512806
C -2.472436 -0.087112  0.675986
C  2.288154 -0.266893  0.318571
C  1.218902 -1.292162 -0.142923
C -0.189445 -1.118856  0.488065
C -1.070069  0.083603  0.024327
H -0.385789  1.508206  1.571944
H -0.926563  2.297598  0.025301
H -0.292485  0.268868 -2.020581
H -1.948399  0.868382 -1.809452
H -1.639199 -0.882302 -1.852967
H -2.385849 -0.117318  1.768509
H -2.939162 -1.020609  0.336176
H -3.125649  0.749164  0.401274
H -0.761950 -2.033667  0.276694
H -0.078790 -1.060109  1.580768
H  1.572216 -2.296132  0.129348
H  1.145406 -1.272392 -1.237581
H  2.278458 -0.213696  1.415923
H  3.281670 -0.643000  0.027747
H  0.806463  1.401925  0.069025
H  2.081267  1.159189 -1.357972
H  2.668110  1.919698  0.184071

Reactant: CCCC(C)(C)C[CH2]
Product: [CH2]CCC(C)(C)CC
C -2.424468 -0.183981  0.286095
C -0.817334  1.890138 -0.167182
C  2.265482 -0.367772  0.682200
C  1.102441 -0.118072 -1.525576
C -1.483847 -1.289402 -0.178082
C  0.451379  1.338972  0.473618
C -0.074229 -1.212715  0.469782
C  0.897315 -0.081392  0.005943
H -1.220387  2.779464  0.322840
H -0.779136  1.999630 -1.252811
H  1.290714  2.026050  0.275264
H  0.322679  1.308198  1.564701
H  3.001949  0.391801  0.393780
H  2.645102 -1.351075  0.380384
H  2.164540 -0.355168  1.774574
H  1.474097 -1.103422 -1.832619
H  0.173447  0.081512 -2.067404
H  1.842056  0.635275 -1.823552
H -0.191903 -1.135620  1.560621
H  0.436395 -2.166262  0.273075
H -1.913729 -2.271708  0.074822
H -1.390100 -1.265357 -1.270458
H -1.737110  0.937700  0.043934
H -3.351587 -0.088888 -0.283550
H -2.591345 -0.162577  1.366565

Reactant: CCCCC([CH2])(C)C#C
Product: [CH2]CCCC(C)(C)C#C
C  2.084021 -0.401077  1.146297
C -1.598701 -2.188670  0.139311
C -0.273313  0.815897  1.400510
C -2.233211  1.240536 -0.128649
C  2.416439  0.064230 -0.266979
C -1.291400 -1.021222  0.110595
C  1.275286 -0.217408 -1.278499
C  0.023466  0.685120 -1.139734
C -0.928228  0.407695  0.074093
H -0.017716  1.878484  1.440234
H -0.799956  0.465800  2.289643
H -1.981544  2.305629 -0.185250
H -2.731880  0.940860 -1.056822
H -2.917893  1.080593  0.709721
H -1.875056 -3.213081  0.166450
H  0.333030  1.738046 -1.082325
H -0.580637  0.571432 -2.049052
H  1.671645 -0.070728 -2.292176
H  0.967469 -1.267185 -1.200393
H  3.327471 -0.443451 -0.620804
H  2.635900  1.140812 -0.263298
H  0.927360  0.187361  1.406617
H  2.768834 -0.056943  1.924803
H  1.856491 -1.466848  1.224542

Reactant: CCCC(C)(C#C)C[CH2]
Product: [CH2]CCC(C)(C#C)CC
C -2.532519 -0.147023  0.053432
C  1.566950 -1.104463 -1.886110
```

```
C -0.843537  1.622637 -0.993009
C  2.004555  0.234326  1.312175
C -1.518821 -1.257708  0.297847
C  1.203638 -0.562232 -0.869666
C  0.250514  1.542556  0.061769
C -0.285831 -0.794167  1.114194
C  0.768978  0.097561  0.373617
H -1.315344  2.603412 -1.082304
H -0.566003  1.192729 -1.957059
H -0.106006  1.970678  1.008462
H  1.121094  2.137366 -0.254278
H  2.418952 -0.752144  1.541894
H  1.702874  0.719697  2.248068
H  2.779685  0.840152  0.832505
H  1.896020 -1.580954 -2.775649
H -0.619000 -0.241211  2.003396
H  0.249747 -1.685223  1.465359
H -1.995190 -2.084971  0.847062
H -1.172636 -1.667417 -0.658568
H -1.805454  0.808371 -0.535719
H -3.324047 -0.388052 -0.659353
H -2.914587  0.324284  0.963296
```

Reactant: CCCCC([CH2])(C)C=C
Product: [CH2]CCCC(C)(C)C=C

```
C -2.160011 -0.540330  0.879235
C  0.921656 -2.288615 -0.294159
C  0.377066  0.000876  1.503361
C  2.381944  0.916195  0.310375
C -2.375436  0.608272 -0.100050
C  1.212566 -1.042876 -0.665464
C -1.279245  0.678395 -1.196238
C  0.099700  1.208752 -0.723894
C  0.987267  0.236832  0.125117
H  0.838412 -0.803503  2.080218
H  0.271848  0.920956  2.085178
H  2.858725  1.084376 -0.663528
H  3.035521  0.278580  0.914640
H  2.264365  1.882977  0.813519
H  1.680361 -0.875427 -1.636908
H  1.144082 -3.135959 -0.935240
H  0.449642 -2.514952  0.655730
H -0.044439  2.132327 -0.145399
H  0.682527  1.478181 -1.616290
H -1.150266 -0.315666 -1.641600
H -1.633821  1.347804 -1.991520
H -3.354458  0.497980 -0.592388
H -2.400659  1.562750  0.443454
H -0.905900 -0.367483  1.289367
H -2.151182 -1.527888  0.412208
H -2.772388 -0.505738  1.783299
```

Reactant: CCCC(C)(C=C)C[CH2]
Product: [CH2]CCC(C)(C=C)CC

```
C -2.487961 -0.642464  0.170387
C  1.707319 -1.347277 -1.297955
C -1.291127  1.381360 -1.056139
C  1.817038  0.871256  1.264675
C -1.230832 -1.489715  0.321385
C  1.385368 -0.097952 -0.964274
C -0.199772  1.616372 -0.020370
C -0.077155 -0.755240  1.059144
C  0.689628  0.373832  0.305604
H -1.967935  2.225637 -1.204586
H -0.942793  0.946853 -1.995784
H  0.475268  2.417290 -0.365743
H -0.649557  1.968741  0.917873
H  2.477687  0.040705  1.533394
H  1.377190  1.288588  2.179151
H  2.417208  1.649908  0.780259
H  1.698684  0.716240 -1.619634
H  1.441894 -2.202057 -0.684899
H  2.261737 -1.564186 -2.205719
H  0.667250 -1.503281  1.363590
H -0.476300 -0.319039  1.985970
H -0.886030 -1.810100 -0.667627
H -1.463577 -2.403012  0.891876
H -2.041597  0.416482 -0.509076
H -2.874525 -0.230695  1.106714
H -3.270864 -1.079517 -0.453341
```

Reactant: CCCCC([CH2])(C#C)C#C
Product: [CH2]CCCC(C)(C#C)C#C

```
C  2.367156 -0.112029  1.093884
C -3.245006  1.134713 -0.069821
C -0.839928 -2.575731  0.009342
C -0.184778  0.554377  1.470871
C  2.556177  0.508661 -0.285984
C -2.146059  0.642304  0.008051
C -0.828057 -1.370430  0.053341
C  1.476495  0.057895 -1.303873
C  0.067031  0.664673 -1.096403
C -0.769238  0.105208  0.116236
H -0.166222  1.640692  1.579182
```

H -0.610183 0.034839 2.329074
H -4.218316 1.552670 -0.136274
H -0.871637 -3.636007 -0.029148
H -0.529679 0.479003 -1.996065
H 0.140452 1.751304 -0.964193
H 1.805796 0.354231 -2.308584
H 1.401099 -1.036137 -1.298685
H 3.544643 0.230961 -0.683548
H 2.542585 1.604302 -0.207684
H 1.125139 0.195255 1.410610
H 2.983231 0.316913 1.887449
H 2.373452 -1.204661 1.097634

Reactant: CCCC(C#C)(C#C)C[CH2]
Product: [CH2]CCC(C#C)(C#C)CC
C 2.630187 -0.645985 0.214467
C -3.108950 -1.099810 0.046707
C -0.670079 2.539435 0.584976
C 1.229521 0.393639 -1.795802
C 1.638820 -0.339599 1.330100
C -2.007848 -0.608767 0.019035
C -0.672798 1.364528 0.310422
C -0.112314 -0.261104 -1.508780
C 0.208932 -0.861898 1.045288
C -0.628836 -0.071733 -0.031956
H 1.252759 1.469608 -1.616619
H 1.668037 0.109463 -2.754320
H -0.889142 0.145427 -2.170573
H -0.059984 -1.341330 -1.690353
H -4.084969 -1.515736 0.076121
H -0.692363 3.572300 0.828863
H 0.248199 -1.908687 0.719205
H -0.372509 -0.825032 1.972639
H 1.977412 -0.802756 2.269870
H 1.592781 0.741419 1.506910
H 2.055632 -0.113990 -0.867931
H 3.596433 -0.144870 0.301935
H 2.727198 -1.708352 -0.025260

Reactant: CCCCC([CH2])(C#C)C=C
Product: [CH2]CCCC(C)(C#C)C=C
C 2.435396 -0.159945 1.055709
C -0.536819 2.719168 0.343487
C -3.295712 0.398852 0.264295
C -0.155405 -0.562095 1.524302
C 2.482439 -0.678234 -0.377028
C -0.646062 1.517607 0.299246
C -2.226220 -0.389018 0.186751
C 1.411208 -0.029830 -1.292276
C -0.046794 -0.491629 -1.045711
C -0.759334 0.051490 0.246670
H -0.248991 -1.651030 1.558794
H -0.477447 -0.073077 2.443980
H -2.342787 -1.467012 0.085867
H -3.199764 1.474541 0.365453
H -4.301080 -0.007719 0.227318
H -0.442306 3.775677 0.384579
H -0.084468 -1.589053 -1.005917
H -0.661309 -0.172628 -1.896065
H 1.656142 -0.276008 -2.334144
H 1.460716 1.061570 -1.198125
H 2.349099 -1.768701 -0.384289
H 3.474839 -0.478143 -0.810621
H 1.174819 -0.350416 1.418943
H 2.568769 0.920714 1.146260
H 3.033679 -0.721933 1.776432

Reactant: CCCC(C#C)(C=C)C[CH2]
Product: [CH2]CCC(C#C)(C=C)CC
C -2.556546 1.011470 0.034871
C 0.124211 -2.674347 0.691758
C 3.016645 -0.535104 0.831278
C -1.088395 -0.204251 -1.822412
C -1.781665 0.521242 1.251553
C 0.340550 -1.508302 0.463214
C 2.049778 0.280076 0.421471
C 0.291880 0.213102 -1.336305
C -0.260460 0.804669 1.168008
C 0.582000 -0.086189 0.180598
H -1.308478 -1.264802 -1.690083
H -1.344397 0.163736 -2.818201
H 0.433319 1.291799 -1.486037
H 1.072808 -0.300591 -1.915214
H 2.266227 1.328664 0.220532
H 2.824801 -1.582692 1.037133
H 4.032233 -0.180510 0.973916
H -0.060941 -3.699996 0.893530
H 0.179392 0.659129 2.161484
H -0.096792 1.853908 0.886044
H -1.932924 -0.556390 1.384508
H -2.162161 1.012476 2.160768
H -1.937803 0.414121 -0.988274
H -2.448836 2.080356 -0.169274
H -3.594316 0.675938 -0.021033

```
Reactant: CCCCC([CH2])(C=C)C=C
Product: [CH2]CCCC(C)(C=C)C=C
C  2.360706  0.521399  1.116831
C -3.350794  0.163890  0.155191
C -0.619558 -1.539921  2.103734
C -0.217569  1.194932  1.023128
C  2.553372  0.257052 -0.372160
C -2.174576  0.576261 -0.316600
C -0.928173 -1.254209  0.839957
C  1.493350 -0.713761 -0.957875
C  0.077678 -0.111091 -1.152591
C -0.794365  0.086083  0.138338
H -0.174838  2.162225  0.514947
H -0.673932  1.268850  2.011619
H -2.137226  1.362168 -1.070879
H -4.284547  0.587774 -0.200434
H -3.420032 -0.603490  0.919132
H -1.329956 -2.039029  0.198867
H -0.755607 -2.539245  2.505385
H -0.218249 -0.798475  2.785743
H  0.162898  0.860671 -1.659140
H -0.490423 -0.773035 -1.820664
H  1.844290 -1.048907 -1.943061
H  1.424371 -1.601824 -0.317995
H  3.552169 -0.173486 -0.545563
H  2.516693  1.204221 -0.927421
H  1.081162  0.892696  1.203990
H  2.415798 -0.373285  1.741159
H  2.935623  1.357011  1.522281

Reactant: CCCC(C=C)(C=C)C[CH2]
Product: [CH2]CCC(C=C)(C=C)CC
C  2.492106 -1.139332 -0.411124
C  0.067954  2.629335 -0.115014
C -2.943828  0.880812 -0.673319
C  1.047043 -0.798090  1.785813
C  1.841458 -0.007447 -1.196114
C -0.406104  1.558879  0.521921
C -2.026103 -0.060597 -0.467363
C -0.322754 -0.879372  1.127257
C  0.296064 -0.133502 -1.304794
C -0.568830  0.151534 -0.029513
H  1.329824  0.197810  2.133128
H  1.240473 -1.576854  2.526778
H -1.114164 -0.714760  1.876497
H -0.478504 -1.888635  0.722159
H -0.777770  1.676580  1.540195
H  0.432908  2.587111 -1.135542
H  0.104678  3.601484  0.366980
H -2.280224 -1.107539 -0.636365
H -2.723967  1.932305 -0.524549
H -3.946545  0.628815 -1.003990
H -0.057989  0.551284 -2.085237
H  0.050060 -1.148403 -1.647240
H  2.098278  0.951545 -0.733782
H  2.242763  0.013218 -2.221902
H  1.894432 -1.047116  0.778256
H  2.247633 -2.142679 -0.770476
H  3.558202 -1.011613 -0.210915
```

Test set

```
Reactant: [CH2]CCCC(C=C)CC#C
Product: CCCCC(C=C)[CH]C#C
C  2.313664 -0.189232 -1.167444
C -0.347841 -2.850786  0.868141
C -3.164895  1.221745 -0.475312
C  2.542556  0.335510  0.237827
C -0.336770 -1.924474  0.086927
C -2.210242  0.480163  0.084189
C  1.549362  1.456989  0.644956
C -0.274184 -0.821555 -0.833058
C  0.102257  0.990552  0.954260
C -0.740304  0.550040 -0.276637
H  2.292389  0.564561 -1.957178
H  2.840486 -1.104480 -1.439935
H  3.567477  0.734620  0.318398
H  2.467272 -0.490436  0.957062
H  1.939216  1.945118  1.547937
H  1.524106  2.220992 -0.144942
H  0.125483  0.165511  1.677527
H -0.427550  1.826260  1.429176
H -0.607886  1.293020 -1.074697
H -2.457706 -0.247973  0.854816
H -2.941620  1.949034 -1.251666
H -4.206163  1.133214 -0.182043
H  0.951174 -0.621947 -1.088902
H -0.729996 -1.049229 -1.802135
H -0.362611 -3.665849  1.547809

Reactant: C=CCCCCC([CH2])C#C
Product: C=C[CH]CCCC(C)C#C
C -3.531821 -1.191557  0.426708
C  2.523647 -1.565928  1.264427
```

```
C  0.464834 -0.847245 -1.515403
C -2.735034 -0.238452 -0.074578
C  2.161254 -0.961636  0.284309
C -1.330026 -0.002079  0.326917
C -0.886206  1.468419  0.387137
C  0.636207  1.644188  0.612380
C  1.539504  1.299032 -0.597198
C  1.720316 -0.225620 -0.911162
H  0.110040 -0.365734 -2.428042
H  0.419376 -1.934894 -1.524860
H  2.535515 -0.293995 -1.654349
H  2.842122 -2.099794  2.124813
H  2.538546  1.710579 -0.407801
H  1.150317  1.785816 -1.501599
H  0.951828  1.043023  1.473928
H  0.821615  2.695644  0.869118
H -1.176336  1.973390 -0.545510
H -1.423947  1.971289  1.203537
H -0.597737 -0.477563 -0.551656
H -1.042978 -0.558628  1.225973
H -3.116355  0.413067 -0.861489
H -3.192079 -1.859542  1.213313
H -4.546768 -1.335503  0.071366
```

Reactant: [CH2]CCCC(C)(C#C)CC
Product: CCCCC([CH2])(C#C)CC

```
C -2.343527 -0.205257  1.328575
C  0.892358  2.391737  0.567503
C  3.139358 -0.655289  0.291875
C  0.179197 -1.020828  1.050746
C -2.779779 -0.321363 -0.127139
C  0.760811  1.235577  0.243337
C  1.979515 -0.691783 -0.721556
C -1.816325  0.402889 -1.103107
C -0.443469 -0.283607 -1.315511
C  0.607838 -0.175443 -0.155277
H -2.260064  0.822294  1.690530
H -2.868681 -0.859086  2.028666
H -2.850133 -1.380134 -0.412070
H -3.786740  0.107542 -0.249838
H -1.652981  1.431876 -0.760338
H -2.305005  0.462880 -2.084830
H  0.021903  0.159113 -2.205768
H -0.595402 -1.351983 -1.523115
H  1.010157  3.407524  0.851914
H -1.090329 -0.634951  1.314801
H  0.732976 -0.826624  1.969451
H  0.090808 -2.085195  0.815007
H  2.232840 -0.075493 -1.593389
H  1.820779 -1.719522 -1.073727
H  2.943823 -1.322429  1.137480
H  3.276526  0.361095  0.674551
H  4.071444 -0.974708 -0.187519
```

Reactant: [CH2]CCCC(C)(C#C)CC
Product: CCCCC(C)(C#C)[CH]C

```
C  2.484619  0.510051 -0.290757
C -3.294452 -0.555620 -0.433144
C -0.505650  1.987009 -1.516940
C -0.757909  1.052083  1.384653
C  2.495785 -0.931787  0.200294
C -2.154023 -0.293028 -0.132361
C -0.073623  0.602483 -1.050648
C  1.374968 -1.228382  1.231320
C -0.063652 -1.310049  0.653911
C -0.752477  0.030904  0.214771
H  3.107143  0.715949 -1.163978
H  2.602462  1.258413  0.497333
H  3.466706 -1.162331  0.666688
H  2.384021 -1.614986 -0.652446
H  1.417240 -0.485379  2.037042
H  1.585650 -2.202838  1.692367
H -0.065730 -1.988589 -0.209374
H -0.711787 -1.759967  1.416592
H -4.296085 -0.788259 -0.695805
H -1.378278  1.916941  1.135709
H  0.258477  1.397592  1.596165
H -1.167761  0.580757  2.284077
H  1.208927  0.668588 -0.722219
H -0.078532 -0.139588 -1.855941
H -0.275497  2.752577 -0.768189
H  0.010116  2.254193 -2.445865
H -1.587728  2.012514 -1.709506
```

Reactant: C#CC(C)(CC)CC([CH2])C
Product: C#CC(C)(C[CH2])CC(C)C

```
C -1.600695 -0.918956 -2.144782
C -0.528595  2.192291 -0.354418
C  1.931637  1.225112 -0.050944
C  2.869398 -1.116983  0.051744
C -1.957485 -1.043964  1.327865
C -1.324230 -0.619884 -1.007541
C -1.251046  1.268107  0.614564
C  0.463506 -0.710473  0.726104
```

```
C  1.606363 -0.255499 -0.219315
C -0.997911 -0.260262  0.383383
H  2.599839  1.638256 -0.810375
H  2.228186  1.501358  0.965657
H  1.280997 -0.435657 -1.251663
H  2.658650 -2.179621 -0.120778
H  3.691011 -0.814621 -0.607063
H  3.197553 -0.991180  1.090818
H  0.453546 -1.808385  0.738689
H  0.685857 -0.374551  1.748984
H -1.850560 -1.187571 -3.140779
H -1.731031 -0.793770  2.371094
H -2.998001 -0.777892  1.117029
H -1.833033 -2.121989  1.186697
H -0.950991  1.495579  1.646313
H -2.337825  1.430068  0.550423
H  0.755347  1.841395 -0.240212
H -0.564877  3.249808 -0.084266
H -0.765598  2.011456 -1.404292
```

Reactant: [CH2]CCC(C)(C)C(C)C#C
Product: CCCC(C)(C)C([CH2])C#C

```
C -2.539214 -1.257585  0.282720
C  3.318517 -0.842809 -0.058693
C  0.011836 -1.830651 -0.196104
C  0.234033  0.961993 -1.531118
C  0.969335  1.888251  0.686608
C -2.497701  0.195558 -0.171452
C  2.140573 -0.716001  0.179686
C -1.350473  1.008192  0.486948
C  0.693305 -0.612798  0.449534
C  0.119194  0.786519 -0.001905
H -2.664823 -1.385678  1.361495
H -3.193700 -1.912942 -0.296180
H -2.408584  0.244947 -1.262928
H -3.446829  0.690944  0.086608
H -1.380140  0.842072  1.574038
H -1.563505  2.074041  0.326585
H -0.112137  1.962246 -1.817299
H -0.365147  0.225178 -2.074082
H  1.278948  0.853328 -1.840359
H  2.021948  1.796928  0.405219
H  0.891777  1.806966  1.778116
H  0.607826  2.878795  0.387336
H  0.548229 -0.670361  1.539242
H  4.352308 -0.959176 -0.269184
H -1.309305 -1.675956  0.043895
H  0.100800 -1.866264 -1.282434
H  0.274227 -2.778043  0.277987
```

Reactant: [CH2]CCC(C)(C=C)CCC
Product: C[CH]CC(C)(C=C)CCC

```
C -1.915131  1.660782 -0.185275
C -2.514066 -1.823341  0.086410
C  2.127152  0.556057 -1.831840
C  2.071506 -0.161018  1.482392
C -0.500119  2.145155 -0.470539
C -1.338236 -0.929261 -0.290616
C  1.590892 -0.272674 -0.936549
C  0.554963  1.587244  0.524258
C -0.197508 -0.900484  0.722378
C  0.968494  0.088733  0.405903
H -2.659799  1.920285 -0.940613
H -2.263887  1.837630  0.835738
H -0.462128  3.245114 -0.414519
H -0.218812  1.868422 -1.492468
H  0.189635  1.746559  1.548701
H  1.471327  2.184867  0.425029
H  1.643565 -1.346965 -1.120063
H  2.601643  0.182557 -2.733938
H  2.124195  1.633344 -1.704390
H  2.427318 -1.196468  1.434690
H  1.666947  0.022999  2.485554
H  2.921946  0.507051  1.312417
H -0.602059 -0.648936  1.713444
H  0.239790 -1.910296  0.808190
H -1.772649  0.312022 -0.271889
H -0.994025 -1.065030 -1.320658
H -2.919940 -1.535277  1.064223
H -2.207029 -2.878539  0.151782
H -3.318738 -1.753211 -0.654016
```

Reactant: C=CC(C)CC(C)(C)C[CH2]
Product: C=CC([CH2])CC(C)(C)CC

```
C  3.625517 -0.722504  0.328557
C -1.401869  2.038795  0.371233
C  1.146414  1.676793 -0.300146
C -1.317562 -0.833243  1.517413
C -2.142264 -1.651256 -0.704752
C  2.624611 -0.307157 -0.447147
C -1.988520  0.814411 -0.320589
C  0.145027 -0.665533 -0.578770
C  1.280715  0.193854  0.053726
C -1.302101 -0.550343 -0.002175
```

```
H -1.749456  2.994026 -0.028805
H -1.427826  2.014500  1.462340
H -1.956447  0.962534 -1.409050
H -3.052317  0.714340 -0.047978
H -0.746985 -0.087557  2.078785
H -2.349329 -0.827043  1.889567
H -0.885228 -1.820515  1.721129
H -2.158020 -1.489824 -1.789661
H -3.175071 -1.636651 -0.336818
H -1.717721 -2.642602 -0.507712
H  0.443679 -1.718104 -0.477446
H  0.106499 -0.446477 -1.656304
H  1.256812  0.077534  1.143869
H  2.742477 -0.294309 -1.530890
H  4.571803 -1.058020 -0.083950
H  3.535713 -0.742025  1.411432
H -0.100580  1.993152  0.064332
H  1.805525  2.340748  0.262773
H  1.168484  1.874277 -1.376061
```

Reactant: CC(C)CCCC[C](C)C
Product: CC(C)CCCC[C](C)C

```
C -1.801469 -1.570080  1.010590
C -1.812556 -0.729670 -1.393395
C  1.798134 -1.571849 -1.010528
C  1.810014 -0.731352  1.393421
C -0.758883  2.045112 -0.160664
C  0.759075  2.044418  0.160543
C -1.581173  0.938223  0.551396
C  1.580319  0.936692 -0.551431
C -1.340987 -0.486136  0.038715
C  1.338708 -0.487407 -0.038707
H  1.517050 -2.568195 -0.648546
H  2.894479 -1.554039 -1.123533
H  1.356771 -1.424606 -2.003323
H  1.388801  0.001704  2.089923
H  2.908235 -0.659455  1.453300
H  1.521416 -1.733028  1.733351
H  2.653758  1.172032 -0.449085
H  1.350113  0.974622 -1.625571
H  1.170929  3.015198 -0.147219
H  0.897697  1.974336  1.247174
H -0.897573  1.975084 -1.247289
H -1.169824  3.016305  0.147020
H -1.350887  0.975971  1.625527
H -2.654384  1.174619  0.449091
H -0.001177 -0.568791  -0.000000
H -1.521465 -2.566729  0.648604
H -2.897787 -1.551115  1.123680
H -1.359877 -1.423282  2.003349
H -1.524917 -1.731628 -1.733301
H -1.390662  0.002964 -2.089929
H -2.910710 -0.656730 -1.453247
```

Reactant: [CH2]C(C)(C)CCC(C)(C)C
Product: [CH2]C(C)(C)CCC(C)(C)C

```
C -1.243433  0.483573  1.381770
C -1.996923 -1.511219  0.037228
C -3.050987  0.741607 -0.338982
C  1.244601 -0.488931  1.379368
C  3.051384 -0.740729 -0.343062
C  1.998042  1.510875  0.042119
C -0.683456  0.370786 -1.099235
C  0.683607 -0.366531 -1.100982
C -1.722342  0.010799  0.008680
C  1.723020 -0.010959  0.007897
H -1.803441  0.071296  2.225739
H -1.113647  1.567293  1.458027
H -1.108608 -2.069788  0.347525
H -2.303420 -1.864264 -0.954942
H -2.803617 -1.731869  0.746557
H -3.808562  0.541508  0.427517
H -3.435073  0.395529 -1.307304
H -2.889478  1.824638 -0.394741
H -1.163071  0.156517 -2.065574
H -0.513373  1.455010 -1.071139
H  0.513421 -1.450831 -1.076984
H  1.162823 -0.148590 -2.066694
H  0.000647 -0.002894  1.499318
H  1.805003 -0.079942  2.224677
H  1.114812 -1.572931  1.451497
H  2.889617 -1.823495 -0.403095
H  3.435362 -0.390928 -1.310093
H  3.809193 -0.543883  0.424050
H  1.110301  2.068491  0.355681
H  2.805644  1.728522  0.751342
H  2.303449  1.867760 -0.949012
```

Reactant: [CH2]CCC(C)CC(C#C)C#C
Product: CCCC(C)C[C](C#C)C#C

```
C  0.213806  2.312314  0.086088
C -1.471991 -0.825846  2.475165
C -3.288222  0.124548 -1.536531
C  2.343066 -1.861086 -0.689425
```

```
C  1.493387  1.749735  0.662340
C -1.324792 -0.494961  1.322086
C -2.307988  0.021175 -0.837974
C  2.111950  0.603431 -0.184765
C  0.038884 -0.858071 -0.766363
C  1.420387 -0.783002 -0.068325
C -1.091257 -0.064120 -0.047685
H -0.394020  2.947965  0.729018
H  0.234235  2.603385 -0.964738
H  1.314956  1.389406  1.683886
H  2.241570  2.557565  0.741150
H  3.154957  0.476525  0.135117
H  2.136149  0.902593 -1.242652
H  1.281047 -1.015167  0.995839
H  1.901612 -2.858496 -0.584608
H  2.495754 -1.662084 -1.757695
H  3.322245 -1.862556 -0.197453
H  0.126641 -0.469372 -1.788592
H -0.279438 -1.905579 -0.832309
H -0.638463  1.069657  0.023210
H -1.622837 -1.124225  3.482498
H -4.159056  0.205424 -2.137736
```

Reactant: [CH2]CCCC(C#C)(C#C)CC
Product: CCCCC(C#C)(C#C)[CH]C

```
C  2.322541 -1.115239  0.045827
C -0.702782  0.037558 -2.594160
C -3.091002  0.912756  1.026048
C -0.999952 -2.317624  0.283674
C  2.694316  0.300520  0.468596
C -0.702824  0.141391 -1.392085
C -2.010966  0.628850  0.568279
C -0.251647 -1.075859  0.740425
C  1.748584  1.375898 -0.126229
C  0.326586  1.428858  0.484866
C -0.659678  0.266764  0.079747
H  2.310933 -1.275728 -1.034673
H  2.825759 -1.916753  0.590862
H  2.683835  0.378251  1.564378
H  3.722359  0.528041  0.145267
H  1.667702  1.233853 -1.210480
H  2.202689  2.362311  0.037139
H -0.152315  2.363920  0.174690
H  0.386658  1.433855  1.580373
H -0.723231 -0.046838 -3.652097
H -4.046285  1.164342  1.414116
H  1.027569 -1.211780  0.392339
H -0.212227 -0.956681  1.827661
H -2.069198 -2.239682  0.525990
H -0.601300 -3.208468  0.781409
H -0.906523 -2.447524 -0.799143
```

Reactant: C[CH]CCC(C#C)(C#C)CC
Product: CCCCC(C#C)(C#C)C[CH2]

```
C -3.595510 -0.035433  0.138767
C  1.030251  2.564767  0.498393
C  3.538224 -1.055365  0.223729
C -0.725703  0.294038 -1.882324
C -2.218994 -0.688078  0.095852
C  1.060528  1.380159  0.271184
C  2.433220 -0.582786  0.123909
C  0.611701 -0.322234 -1.508012
C -1.277377 -0.314735  1.238052
C  0.169778 -0.828494  1.048357
C  1.051589 -0.068787 -0.015940
H -3.501574  1.056922  0.170592
H -4.190924 -0.305364 -0.740539
H -4.155258 -0.347959  1.033470
H -2.251018 -1.767526 -0.090600
H -1.257275  0.776078  1.355837
H -1.660909 -0.731443  2.183083
H  0.703137 -0.748378  2.001438
H  0.159322 -1.887402  0.761832
H  1.028356  3.606541  0.702028
H  4.517294 -1.454607  0.315830
H  1.413926  0.074766 -2.145441
H  0.588571 -1.409303 -1.651418
H -1.595508 -0.208316 -0.954189
H -1.119873 -0.036246 -2.844991
H -0.782924  1.373996 -1.738905
```

Reactant: C#CC(C)CCC(C#C)C[CH2]
Product: C#C[C](C)CCC(C#C)CC

```
C  3.107798  1.780405  0.403038
C -2.608957  2.019525 -0.105104
C -0.432319 -0.347832  1.846773
C  2.086272 -1.567039 -0.203542
C  2.338886  0.879604  0.151996
C -2.288400  0.857960 -0.182408
C -1.512471 -1.129076  1.129554
C  0.448009  0.132487 -1.289407
C -0.803080 -0.774151 -1.372713
C  1.405770 -0.188561 -0.118002
C -1.895596 -0.554527 -0.274986
```

```
H -0.647756  0.707487  2.012796
H  0.048748 -0.848297  2.687221
H -2.430899 -1.147783  1.738168
H -1.200946 -2.172258  0.989564
H -2.778907 -1.120661 -0.607520
H -2.892371  3.040272 -0.037417
H -0.513145 -1.831668 -1.351236
H -1.280778 -0.592378 -2.343529
H  0.120958  1.173909 -1.201801
H  1.010778  0.041650 -2.229428
H  0.638016 -0.245903  0.868797
H  3.783859  2.568966  0.620510
H  2.725626 -1.616219 -1.094132
H  2.708735 -1.740084  0.679548
H  1.341584 -2.367131 -0.266746
```

Reactant: C[CH]CCCC(C)(C#C)C=C
Product: CCCCCC([CH2])(C#C)C=C

```
C -2.774923  0.845829  0.789365
C  0.475643  2.617446 -0.740661
C  3.505390  0.743155 -0.248881
C  0.503982 -0.253559  1.288323
C -2.121801 -0.531573  0.863101
C  0.733015  1.471403 -0.460072
C  2.550403 -0.170231 -0.092920
C -2.052762 -1.316249 -0.450155
C -1.089586 -0.714675 -1.507905
C  0.420332 -0.884292 -1.203965
C  1.036255  0.072208 -0.119077
H -2.772215  1.332259  1.771181
H -2.244492  1.496897  0.087799
H -3.820596  0.761816  0.456220
H -2.501389 -1.135490  1.694074
H -1.743025 -2.349796 -0.243714
H -3.061919 -1.368084 -0.889773
H -1.285567 -1.217335 -2.464518
H -1.307126  0.348354 -1.657978
H  0.986080 -0.711390 -2.127261
H  0.618618 -1.916771 -0.884363
H  2.810125 -1.211279  0.092989
H  4.555949  0.476400 -0.197602
H  3.267535  1.785060 -0.433999
H  0.254628  3.626585 -0.985114
H -0.865937 -0.343081  1.162883
H  0.697544  0.521314  2.030163
H  0.782456 -1.255515  1.626402
```

Reactant: [CH2]CCC(C#C)(C=C)CCC
Product: C[CH]CC(C#C)(C=C)CCC

```
C -2.131239  1.568436 -0.310821
C -2.739090 -1.896071  0.015090
C  1.348495  0.188928  2.380946
C  3.210173 -0.772734 -0.544146
C -0.742833  2.144385 -0.068508
C -1.601527 -0.949170  0.381190
C  1.099791  0.082267  1.203874
C  2.001368 -0.499642 -1.025289
C  0.382211  1.372351 -0.803130
C -0.327835 -1.133552 -0.437018
C  0.778840 -0.037535 -0.225855
H -2.921354  1.966995  0.328648
H -2.424592  1.511921 -1.362643
H -0.704457  3.190946 -0.410346
H -0.521066  2.152872  1.005201
H  1.295370  1.978536 -0.783616
H  0.104067  1.230524 -1.856511
H  1.801017 -0.598069 -2.091570
H  4.017195 -1.096425 -1.193311
H  3.431933 -0.682639  0.513840
H  1.570673  0.280568  3.414944
H  0.131444 -2.105406 -0.202549
H -0.578023 -1.142404 -1.507349
H -1.992558  0.268481  0.066329
H -1.406284 -0.887805  1.455131
H -2.995539 -1.803021 -1.047622
H -2.458931 -2.944323  0.199742
H -3.636619 -1.680310  0.605385
```

Reactant: [CH2]CC(C)CCC(C#C)C=C
Product: CCC(C)CC[C](C#C)C=C

```
C -0.581852 -1.688109 -1.135034
C  1.709884  1.959385 -1.367113
C  3.625791 -0.670929  0.358766
C -3.571246  0.431849  0.171893
C -1.741584 -0.717178 -1.140635
C  1.474412  1.026532 -0.633678
C  2.353589 -0.883051  0.700479
C -1.182284  0.814478  0.888795
C  0.180083  0.262732  1.371608
C -2.167951 -0.215093  0.269098
C  1.163894 -0.098953  0.225399
H -0.663741 -2.542184 -0.461312
H -0.099855 -1.900946 -2.088561
H -1.501819  0.152997 -1.766484
```

```
H -2.617479 -1.205141 -1.604070
H -2.231499 -1.084487  0.940557
H -3.539074  1.303969 -0.493185
H -4.302000 -0.279646 -0.229509
H -3.916801  0.764841  1.157069
H -1.009323  1.622351  0.165905
H -1.680408  1.264513  1.758657
H  0.666351  1.005455  2.016365
H  0.014540 -0.639994  1.975051
H  0.499417 -0.867959 -0.449880
H  2.102932 -1.700457  1.375114
H  3.903670  0.139049 -0.307418
H  4.425673 -1.298364  0.737333
H  1.919837  2.779754 -2.007065
```

```
Reactant: C=CC(C=C)CCCC([CH2])C
Product: C=C[C](C=C)CCCC(C)C
C -1.019957 -2.519076 -0.334701
C -3.093734  0.094875 -1.548796
C  1.329485 -0.015097 -1.372453
C  3.745148 -0.206275 -0.696525
C -1.389789 -1.418583  0.320754
C -2.081132  0.680615 -0.898763
C  0.723567  0.326945  1.800673
C  2.028463  0.586519  1.002021
C -0.578530  0.840972  1.138086
C  2.268227 -0.336735 -0.224094
C -1.045617 -0.005751 -0.068647
H  1.267745 -0.751488 -2.175066
H  1.359681  1.019101 -1.724142
H  2.100716 -1.375181  0.092851
H  4.433279 -0.484867  0.111144
H  3.937211 -0.855902 -1.557539
H  3.954212  0.829137 -0.990642
H  2.874385  0.451421  1.690410
H  2.053384  1.634381  0.668308
H  0.628813 -0.749010  1.996006
H  0.822885  0.823542  2.775240
H -1.383861  0.851115  1.888011
H -0.430699  1.878995  0.810463
H -0.019053 -0.059477 -0.768521
H -2.008529 -1.510431  1.216168
H -1.318940 -3.508783 -0.003877
H -0.406177 -2.470208 -1.228629
H -1.951474  1.759947 -0.981933
H -3.785532  0.671832 -2.153466
H -3.257081 -0.976049 -1.496133
```

```
Reactant: C[CH]CCCC(C)(C=C)C=C
Product: CCCCCC([CH2])(C=C)C=C
C  3.284672 -1.265650  0.664508
C -3.461850  0.121741  0.949938
C -1.194041 -1.567647 -1.542470
C -0.154142 -0.695602  1.096771
C  2.187324 -0.634263 -0.184418
C -2.229297  0.606230  1.099996
C -1.456127 -0.348370 -1.074666
C  2.265992  0.881664 -0.350873
C  0.992760  1.499006 -0.986387
C -0.238376  1.587927 -0.047956
C -1.005521  0.249884  0.246550
H  3.307507 -0.813715  1.663976
H  3.129828 -2.344547  0.777820
H  4.275024 -1.113938  0.208799
H  2.013506 -1.151010 -1.133728
H  2.441268  1.347063  0.629976
H  3.134167  1.134172 -0.980898
H  0.723324  0.929911 -1.884492
H  1.232210  2.520854 -1.309522
H  0.068441  2.024654  0.913030
H -0.966107  2.278278 -0.496389
H -2.011946  1.294038  1.917016
H -3.705565 -0.578405  0.157608
H -4.267072  0.401842  1.621657
H -2.061699  0.332759 -1.672783
H -0.598610 -2.286467 -0.990463
H -1.567710 -1.893512 -2.508260
H  1.055158 -0.791973  0.456723
H -0.551352 -1.707661  1.188360
H  0.123380 -0.267690  2.063973
```

```
Reactant: [CH2]CCC(C=C)(C=C)CCC
Product: C[CH]CC(C=C)(C=C)CCC
C -1.798204  1.429303  1.134364
C -3.215225 -1.076741 -0.937662
C  1.759890  1.241184 -1.608092
C  2.863131 -1.778775 -0.148017
C -0.321626  1.765266  0.977445
C -1.872505 -0.364478 -0.820466
C  1.088765  0.105130 -1.419914
C  1.635253 -1.587616  0.328149
C  0.612746  0.528187  1.088761
C -0.726875 -1.232259 -0.309103
C  0.640899 -0.495984 -0.097118
```

```
H -2.050295  0.877437  2.043771
H -2.488486  2.250179  0.929389
H -0.160221  2.258516  0.012943
H -0.014476  2.479849  1.758075
H  1.643211  0.877085  1.229588
H  0.347313 -0.030650  1.997214
H  0.859863 -0.518784 -2.284282
H  2.038239  1.896874 -0.790135
H  2.063031  1.558756 -2.601070
H  1.258319 -2.233548  1.121833
H  3.500270 -2.569853  0.234762
H  3.274713 -1.149846 -0.929786
H -1.021261 -1.689568  0.646472
H -0.545138 -2.061072 -1.013609
H -1.991552  0.540361  0.126871
H -1.606359  0.223499 -1.703979
H -3.504087 -1.517724  0.024567
H -3.170344 -1.891345 -1.676651
H -4.005029 -0.384070 -1.249164
```

Reactant: [CH2]CCC(C=C)CC(C)C=C
Product: CCCC(C=C)C[C](C)C=C

```
C  0.627787  2.300315  0.446372
C  3.607987 -1.025635  0.491311
C -3.270355 -1.647632 -1.227398
C  1.657320 -0.262359 -1.611780
C -0.739470  2.345464 -0.204646
C  2.336308 -0.741913  0.800248
C -2.540155 -1.123837 -0.244853
C -1.667224  1.171620  0.213058
C -0.093685 -0.919173  0.163952
C  1.274648 -0.263866 -0.128456
C -1.344170 -0.208960 -0.436646
H  0.632535  2.299537  1.537966
H  1.411741  2.911608 -0.001009
H -1.247009  3.287958  0.062435
H -0.636742  2.348099 -1.297948
H -2.694357  1.431840 -0.072665
H -1.653611  1.064218  1.307026
H -1.197195 -0.060201 -1.514131
H -2.788399 -1.345022  0.793902
H -3.046717 -1.446998 -2.271839
H -4.117656 -2.297016 -1.031012
H -0.233340 -0.981518  1.252890
H -0.071563 -1.951056 -0.215909
H  1.084340  0.929016  0.166098
H  2.017559 -0.841557  1.838448
H  3.989840 -0.954757 -0.521335
H  4.314401 -1.345283  1.250392
H  1.836411 -1.288197 -1.961222
H  2.567930  0.322750 -1.779860
H  0.859068  0.172586 -2.220715
```

Reactant: [CH2]CCCC(C)(C=C)C(C)C
Product: CCCCC([CH2])(C=C)C(C)C

```
C -2.599901 -0.194280  1.308501
C  0.339147 -2.394284  0.811888
C  2.939943  0.192478  0.514933
C  1.848636  2.140549 -0.656193
C -0.021973  0.508633  1.269870
C -2.974406  0.258453 -0.097790
C  0.564740 -1.509955 -0.158845
C -1.996499 -0.271528 -1.180073
C -0.609442  0.424798 -1.206187
C  1.842327  0.602958 -0.493102
C  0.423235  0.005498 -0.098685
H -3.097857  0.338246  2.121965
H -2.606775 -1.277913  1.445121
H -2.995989  1.355871 -0.143674
H -3.990266 -0.089513 -0.342998
H -2.460131 -0.116331 -2.163633
H -1.862337 -1.351674 -1.049339
H -0.762429  1.509602 -1.153293
H -0.139988  0.212927 -2.177858
H  0.895342 -1.871695 -1.134354
H  0.004352 -2.098656  1.800114
H  0.479962 -3.458546  0.649814
H -1.307269  0.130166  1.405633
H  0.500496  0.073842  2.123337
H -0.091786  1.596517  1.336172
H  2.090349  0.158529 -1.468941
H  2.949992 -0.890728  0.665965
H  2.768907  0.676211  1.483283
H  3.923429  0.506621  0.146384
H  1.598226  2.630258  0.291067
H  1.145249  2.477918 -1.422767
H  2.851778  2.471282 -0.950331
```

Reactant: [CH2]CCCC(C)(C=C)C(C)C
Product: CCCCC(C)(C=C)[C](C)C

```
C -2.178324  0.368738 -1.147002
C  2.250958 -1.733041 -1.021446
C -0.222371  2.167628  0.920190
C  1.024093  1.810774 -1.253720
```

```
C  1.941834  0.024428  1.297569
C -2.653964 -0.456639  0.039639
C  1.105103 -1.080491 -0.829941
C -1.622801 -1.527598  0.483892
C -0.354186 -0.989310  1.201011
C  0.183293  1.154674 -0.155499
C  0.725951 -0.210315  0.362465
H -1.957309 -0.211357 -2.046441
H -2.750023  1.274924 -1.357086
H -3.597732 -0.968473 -0.209974
H -2.871319  0.204535  0.889460
H -1.333781 -2.136466 -0.381259
H -2.121331 -2.205733  1.190137
H  0.168013 -1.853160  1.633579
H -0.667875 -0.356336  2.041056
H  0.323413 -1.173132 -1.581668
H  3.077840 -1.684162 -0.321692
H  2.407294 -2.348623 -1.902062
H  2.339749 -0.931913  1.655178
H  1.637331  0.609789  2.170537
H  2.740795  0.560571  0.774974
H -0.940611  0.827965 -0.721234
H  0.661482  2.603105  1.407456
H -0.782477  2.990139  0.458686
H -0.853866  1.721282  1.694429
H  1.988327  2.156461 -0.852157
H  1.232929  1.115314 -2.071434
H  0.499787  2.684621 -1.658876
```

1-7 H-shift

Training set

Primary contributions

```
Reactant: [CH2]CCCCCC
Product: [CH2]CCCCCC
C -1.348135  1.407692  0.369147
C  1.348653  1.407233  0.369175
C -1.627249  0.299239 -0.639953
C  1.627409  0.298719 -0.639957
C -1.321727 -1.124768 -0.098983
C  1.321358 -1.125210 -0.099064
C -0.000190 -1.290354  0.691464
H -1.698325  1.205609  1.384899
H -1.622499  2.409206  0.028425
H -1.046543  0.487007 -1.550913
H -2.686166  0.324437 -0.944524
H -2.141577 -1.411597  0.574587
H -1.334180 -1.835703 -0.936170
H -0.000346 -2.304090  1.116409
H -0.000048 -0.601996  1.544218
H  1.333488 -1.836093 -0.936299
H  2.141139 -1.412399  0.574435
H  2.686348  0.323549 -0.944480
H  1.046817  0.486744 -1.550939
H  0.000266  1.459369  0.461585
H  1.623367  2.408662  0.028490
H  1.698751  1.204999  1.384927

Reactant: [CH2]CCCCCCC
Product: C[CH]CCCCCC
C  0.299690  1.853691 -0.384242
C -2.841819  0.506259 -0.000408
C  1.288161  1.319709  0.644995
C -1.523056 -0.134395 -0.423481
C  2.147936  0.138005  0.119277
C -0.907168 -1.081734  0.603979
C  1.393895 -0.956198 -0.677526
C  0.368777 -1.815328  0.104387
H  0.702089  1.978744 -1.392707
H -0.278779  2.720501 -0.055176
H  0.741496  1.014089  1.545401
H  1.974470  2.121355  0.963837
H  2.672160 -0.327960  0.964609
H  2.919561  0.551548 -0.545388
H  0.897779 -0.498901 -1.541188
H  2.150410 -1.641769 -1.084773
H  0.049451 -2.628301 -0.562718
H  0.869957 -2.285599  0.961103
H -1.648722 -1.845735  0.892100
H -0.685139 -0.515429  1.517018
H -0.648368  0.864435 -0.495317
H -1.549592 -0.550011 -1.436660
H -2.727154  1.024149  0.960145
H -3.630091 -0.251654  0.122156
H -3.186800  1.233865 -0.743701

Reactant: C#CCCCCCC[CH2]
Product: C#C[CH]CCCCCC
C -3.047256  0.287377 -1.003144
C  1.058067  1.818848 -0.244125
C -2.194501  0.451961 -0.158113
C  2.123542  0.824775  0.182852
C -1.155915  0.659043  0.812165
```

```
C  2.088861 -0.506587 -0.616723
C -0.526884 -0.609999  1.420626
C  0.687914 -1.118820 -0.863594
C -0.079511 -1.658007  0.368889
H  0.880376  1.904305 -1.317730
H  1.073777  2.780862  0.271442
H  2.024157  0.623411  1.256181
H  3.123863  1.272073  0.053877
H  2.725214 -1.244183 -0.109800
H  2.540383 -0.319332 -1.600977
H  0.820220 -1.963630 -1.554101
H  0.056263 -0.394202 -1.388290
H -0.980058 -2.160895 -0.005686
H  0.529943 -2.420020  0.873121
H  0.322390 -0.303822  2.041020
H -1.255125 -1.084477  2.093743
H -0.170595  1.242624  0.232845
H -1.442256  1.386136  1.580837
H -3.799065  0.142514 -1.738066
```

Reactant: C=CCCCCCC[CH2]
Product: C=C[CH]CCCCCC

```
C  3.013308 -0.359880 -1.395634
C -0.288794  1.816521  0.153727
C  2.540664 -0.162925 -0.156167
C -1.407936  1.351679 -0.758124
C  1.174202 -0.478901  0.320408
C -2.428121  0.411836 -0.059221
C  0.311252 -1.391511 -0.557289
C -1.825183 -0.701406  0.832439
C -1.023258 -1.816668  0.114450
H -0.574667  2.092240  1.170381
H  0.442463  2.490037 -0.296202
H -1.962673  2.222290 -1.148037
H -0.977160  0.854547 -1.635236
H -3.074315 -0.044911 -0.820671
H -3.075005  1.029592  0.579410
H -2.659204 -1.187592  1.357769
H -1.199115 -0.246090  1.608521
H -1.665077 -2.290862 -0.640133
H -0.791943 -2.586203  0.864200
H  0.108226 -0.888800 -1.509783
H  0.878856 -2.301711 -0.801280
H  0.540952  0.622739  0.325603
H  1.158967 -0.770765  1.376836
H  3.191749  0.306532  0.580598
H  2.417883 -0.822533 -2.175843
H  4.021482 -0.067098 -1.669380
```

Reactant: [CH2]CCCCCC(C)C
Product: CCCCCC[C](C)C

```
C -0.603759  1.774835  0.664167
C  2.419150  0.965149 -0.602806
C  1.910603 -0.703181  1.247492
C -1.648193  1.388900 -0.375759
C -2.383569  0.058704 -0.049363
C -1.502743 -1.093049  0.495011
C -0.483472 -1.731815 -0.481202
C  0.655217 -0.820175 -1.011957
C  1.371010  0.046305  0.030583
H -0.128148  2.744029  0.495312
H -0.904625  1.631751  1.704749
H -1.166875  1.319853 -1.359201
H -2.408538  2.181944 -0.466062
H -2.920857 -0.285038 -0.943418
H -3.142950  0.273465  0.715565
H -2.180748 -1.894810  0.821063
H -0.982811 -0.749755  1.395709
H -0.030805 -2.590750  0.032590
H -1.028327 -2.137624 -1.344716
H  0.262203 -0.160719 -1.795015
H  1.402980 -1.467126 -1.503308
H  0.432583  0.877919  0.447654
H  2.835694  1.654502  0.141086
H  1.983011  1.555133 -1.417912
H  3.249283  0.374051 -1.019420
H  1.129391 -1.277601  1.754751
H  2.346786 -0.002311  1.969244
H  2.702220 -1.406038  0.942175
```

Reactant: [CH2]CCCCCC(C)C#C
Product: CCCCCC[C](C)C#C

```
C -0.839065  1.479586  1.074505
C  2.315000  1.023513 -1.523355
C  2.015755 -0.401891  1.727324
C -1.511626  1.573299 -0.283502
C  1.787752  0.419504 -0.614650
C -2.528830  0.435131 -0.546102
C -2.023175 -0.986850 -0.196332
C -0.719096 -1.437399 -0.926215
C  0.486579 -1.605137  0.032916
C  1.136011 -0.274893  0.471300
H -0.222329  2.335578  1.355246
H -1.440477  1.085683  1.895332
```

```
H -0.735331  1.567534 -1.061057
H -2.036387  2.537248 -0.384250
H -3.432827  0.628123  0.048060
H -2.826478  0.463106 -1.602676
H -1.867316 -1.051289  0.887613
H -2.830188 -1.692005 -0.432804
H -0.898543 -2.401419 -1.417264
H -0.451333 -0.724593 -1.714793
H  0.156649 -2.145610  0.929925
H  1.261783 -2.217512 -0.449441
H  0.178071  0.502447  0.822760
H  2.854861 -1.084107  1.539892
H  2.420580  0.572874  2.016401
H  1.423430 -0.799956  2.558987
H  2.787324  1.547294 -2.316430
```

Reactant: [CH2]CCCCCC(C)C=C
Product: CCCCCC[C](C)C=C

```
C -0.807578  1.759720 -0.768395
C  3.062651 -0.449178 -1.129489
C  1.940429  1.155620  1.097700
C -2.023359  1.367936  0.050187
C  1.818862 -0.668992 -0.680116
C -2.619777 -0.011932 -0.344851
C -1.596608 -1.143822 -0.608785
C -0.800885 -1.675137  0.610344
C  0.190596 -0.687677  1.285746
C  1.087551  0.134441  0.333592
H -0.373783  2.734624 -0.540683
H -0.847040  1.537309 -1.835950
H -1.762531  1.374996  1.115521
H -2.818008  2.124717 -0.067578
H -3.327049 -0.333739  0.431026
H -3.199239  0.124075 -1.268584
H -2.153335 -1.994696 -1.026377
H -0.899974 -0.820677 -1.389856
H -1.511040 -2.022604  1.372982
H -0.242117 -2.561171  0.280858
H -0.366115  0.017072  1.913804
H  0.838298 -1.263515  1.964890
H  0.252130  0.849924 -0.283603
H  2.442260  1.846063  0.411401
H  2.706573  0.646498  1.697301
H  1.309152  1.744306  1.772677
H  1.263577 -1.504891 -1.100785
H  3.505010 -1.081805 -1.892262
H  3.683564  0.358160 -0.756788
```

Reactant: [CH2]CCCCCC(C#C)C#C
Product: CCCCCC[C](C#C)C#C

```
C -0.760853 -1.438649 -1.340170
C  1.731518  2.243162 -1.226733
C  3.059137 -1.714365  0.455053
C -1.845435 -1.566860 -0.292229
C  1.459669  1.230405 -0.625228
C  2.181877 -0.903658  0.273820
C -2.658335 -0.261097 -0.071782
C -1.835553  1.048812 -0.004165
C -0.916356  1.246664  1.227456
C  0.268066  0.262070  1.384444
C  1.074885  0.018804  0.076579
H -0.156176 -2.326080 -1.529346
H -0.993332 -0.851205 -2.228902
H -2.552849 -2.361643 -0.586642
H -1.401005 -1.903716  0.652028
H -3.364817 -0.159973 -0.907262
H -3.258359 -0.363550  0.842000
H -1.240327  1.157971 -0.917316
H -2.550262  1.883547 -0.006122
H -0.504814  2.261679  1.165528
H -1.522085  1.198337  2.142400
H  0.958293  0.654208  2.141728
H -0.079769 -0.712971  1.738211
H  0.273638 -0.593298 -0.658351
H  1.991079  3.128815 -1.750877
H  3.843433 -2.412500  0.609558
```

Reactant: [CH2]CCCCCC(C#C)C=C
Product: CCCCCC[C](C#C)C=C

```
C -1.229319 -1.345318 -1.396110
C  1.645054  2.049377 -1.510133
C  3.155957 -1.237573 -0.870821
C -2.161095 -1.426507 -0.204986
C  1.342925  1.040758 -0.913663
C  1.987103 -1.260502 -0.227889
C -2.782456 -0.059137  0.193430
C -1.817993  1.151452  0.191026
C -0.712859  1.180256  1.276663
C  0.374111  0.078627  1.200225
C  0.955241 -0.167421 -0.218285
H -0.770155 -2.279638 -1.721275
H -1.521653 -0.682938 -2.211316
H -1.626821 -1.862658  0.647981
H -2.988448 -2.123845 -0.424301
```

```
H -3.249554 -0.152850  1.182736
H -3.588097  0.163653 -0.519858
H -2.427991  2.054824  0.331679
H -1.352214  1.249520 -0.795243
H -0.210315  2.152600  1.201827
H -1.180004  1.133658  2.269841
H -0.022745 -0.875639  1.564588
H  1.201937  0.356309  1.866332
H -0.011128 -0.649650 -0.839577
H  1.702425 -2.141068  0.346630
H  3.836788 -2.081500 -0.837830
H  3.466653 -0.371591 -1.445783
H  1.912501  2.935719 -2.029232
```

```
Reactant: [CH2]CCCCCC(C=C)C=C
Product: CCCCCC[C](C=C)C=C
C  0.779394  1.023419  1.695573
C -2.644040 -1.987863  0.674341
C -2.649836  1.828923 -0.635514
C  1.744024  1.544060  0.650230
C -1.427605 -1.489821  0.430896
C -2.259266  0.872518  0.213235
C  2.621619  0.434631  0.003961
C  1.898960 -0.893659 -0.330661
C  0.869146 -0.865461 -1.487987
C -0.370922  0.049793 -1.311297
C -1.116528 -0.076794  0.036313
H  0.152121  1.769422  2.184792
H  1.142807  0.239367  2.360947
H  1.181178  2.083984 -0.120854
H  2.421463  2.289520  1.101655
H  3.094342  0.832340 -0.903747
H  3.431808  0.195256  0.706564
H  1.421706 -1.276015  0.578303
H  2.670308 -1.627575 -0.603488
H  1.385091 -0.558651 -2.408166
H  0.522669 -1.894401 -1.651467
H -0.072269  1.094940 -1.441731
H -1.081957 -0.181325 -2.117621
H -0.271899  0.334250  0.864047
H -0.567732 -2.150710  0.513606
H -3.541945 -1.386543  0.578142
H -2.782305 -3.024554  0.964623
H -2.782177  0.769229  1.163268
H -3.470231  2.496262 -0.391760
H -2.179046  1.981141 -1.600602
```

Secondary contributions

```
Reactant: [CH2]CCC(C)(C#C)CCC
Product: [CH2]CCC(C)(C#C)CCC
C -2.046627  1.679564 -0.164095
C -2.530821 -0.865209  0.591573
C  2.912918  0.838042  1.146071
C  1.554380 -1.345781 -1.226903
C -0.533763  1.869731 -0.223929
C -1.295001 -1.673838  0.208096
C  2.022598  0.320768  0.515062
C  0.181602  0.776102 -1.069807
C  0.014682 -1.061690  0.790448
C  0.928078 -0.318257 -0.242720
H -2.535448  1.730913 -1.141669
H -2.559208  2.292587  0.581557
H -0.315068  2.854981 -0.663309
H -0.106736  1.885335  0.785298
H -0.547648  0.278657 -1.720891
H  0.930859  1.239206 -1.722119
H  3.699972  1.290973  1.695479
H  2.215205 -0.834966 -1.934553
H  0.766737 -1.858033 -1.789864
H  2.137769 -2.089952 -0.675711
H -0.244088 -0.362096  1.592889
H  0.631568 -1.847471  1.241303
H -1.229563 -1.752494 -0.883475
H -1.402620 -2.702910  0.583160
H -2.294676  0.412403  0.223967
H -3.445672 -1.135505  0.058331
H -2.689800 -0.787631  1.670789
```

```
Reactant: CCCCC(C)(C#C)C[CH2]
Product: [CH2]CCCC(C)(C#C)CC
C -2.763693 -0.062973 -0.016627
C  2.597388  1.512477 -0.925786
C -0.918437 -1.954875 -0.537204
C  1.853288 -1.326412  0.980400
C -1.976197  1.191311 -0.376336
C  1.870550  0.685418 -0.429475
C  0.258485 -1.098518 -0.987840
C -0.863761  1.543712  0.648800
C  0.000382  0.371065  1.170067
C  0.979411 -0.324316  0.169994
H -0.753807 -2.548487  0.364521
H -1.362631 -2.547748 -1.340596
H -0.081310 -0.378810 -1.740078
H  1.022449 -1.720426 -1.479984
H  3.242917  2.235661 -1.357940
```

H 2.389789 -0.801490 1.776927
H 1.219232 -2.097042 1.432156
H 2.583000 -1.807621 0.321845
H 0.621624 0.760709 1.987231
H -0.642831 -0.401712 1.605382
H -0.203577 2.305306 0.217449
H -1.346278 1.993844 1.527607
H -2.655569 2.056300 -0.443910
H -1.541248 1.071906 -1.375833
H -1.896651 -1.075553 -0.216348
H -3.588980 -0.291270 -0.695670
H -3.058733 -0.137075 1.033517

Reactant: CCCCCC([CH2])(C)C#C
Product: [CH2]CCCCC(C)(C)C#C
C -2.027095 -0.610587 -1.434340
C 2.589573 1.013903 -1.336708
C 0.316299 -1.542018 -0.502113
C 2.069795 -1.238370 1.280055
C -2.700183 -0.180990 -0.134503
C 1.911267 0.339629 -0.599788
C -2.228857 1.209064 0.360395
C -0.696240 1.421133 0.315355
C 0.140798 0.408686 1.152932
C 1.099835 -0.495916 0.305147
H 0.868408 -1.964365 -1.343244
H -0.127091 -2.311449 0.138210
H 3.188946 1.605955 -1.982210
H 1.487383 -1.843510 1.984242
H 2.742503 -1.894042 0.719096
H 2.667240 -0.512227 1.841827
H -0.516047 -0.257841 1.726148
H 0.761807 0.952090 1.874075
H -0.359099 1.387323 -0.725298
H -0.485815 2.437352 0.669876
H -2.593467 1.368149 1.383881
H -2.693378 1.979244 -0.270567
H -2.498703 -0.937394 0.637110
H -3.793612 -0.154457 -0.259042
H -0.805151 -0.988442 -1.059605
H -1.886963 0.184057 -2.171051
H -2.441694 -1.518711 -1.880141

Reactant: CCCCC(C)(C=C)C[CH2]
Product: [CH2]CCCC(C)(C=C)CC
C -2.907048 -0.114206 0.308786
C 1.865942 -0.885468 -2.019608
C -1.201807 1.873868 -0.320829
C 1.741831 1.287626 0.770592
C -2.133056 -1.312339 -0.228550
C 1.736662 -0.694147 -0.707397
C -0.072238 1.088079 -0.978825
C -0.881881 -1.675187 0.616999
C 0.004095 -0.495744 1.089182
C 0.819761 0.286197 0.010945
H -0.934744 2.409709 0.592569
H -1.765262 2.503553 -1.014021
H 0.586895 1.770267 -1.539544
H -0.504410 0.404665 -1.718933
H 2.362809 -1.274517 -0.027429
H 2.574422 -1.605649 -2.416832
H 1.282718 -0.337319 -2.751483
H 2.354908 1.849781 0.058041
H 1.142755 1.993318 1.357137
H 2.408376 0.750518 1.455619
H -0.603005 0.220148 1.654328
H 0.738469 -0.906285 1.797535
H -1.226425 -2.196859 1.520933
H -0.264047 -2.382804 0.050936
H -2.785596 -2.199905 -0.260736
H -1.838684 -1.116358 -1.266214
H -2.104608 0.942794 0.062481
H -3.063632 -0.113459 1.390842
H -3.821737 0.119601 -0.241798

Reactant: CCCCCC([CH2])(C)C=C
Product: [CH2]CCCCC(C)(C)C=C
C 2.127541 1.013658 -1.113590
C -1.807248 0.142421 -2.184152
C -0.295384 1.678104 -0.159784
C -2.193794 0.950016 1.299012
C 2.693511 0.317817 0.120566
C -1.878475 -0.176470 -0.892686
C 2.234025 -1.156119 0.248919
C 0.722206 -1.385262 0.004248
C -0.236478 -0.614257 0.960419
C -1.128688 0.470810 0.260193
H -0.786000 2.347571 -0.869632
H 0.107613 2.223230 0.699504
H -2.536621 -0.989517 -0.582725
H -2.394600 -0.384165 -2.929940
H -1.162815 0.934284 -2.550787
H -2.825715 1.730662 0.862957
H -1.695058 1.352338 2.188446

```
H -2.832258  0.111880  1.605297
H -0.913358 -1.326787  1.449255
H  0.331594 -0.117124  1.757385
H  0.480400 -1.120089 -1.029553
H  0.529729 -2.461675  0.096815
H  2.507396 -1.531255  1.244204
H  2.787830 -1.757661 -0.485189
H  2.389590  0.879552  1.014985
H  3.794018  0.339327  0.103999
H  0.864236  1.290260 -0.768864
H  2.074513  0.396005 -2.013219
H  2.554110  2.000415 -1.312636
```

Reactant: [CH2]CCC(C)(C=C)CCC
Product: [CH2]CCC(C)(C=C)CCC

```
C  2.452163  1.436793  0.101383
C  2.543157 -1.202860 -0.451316
C -2.068764  0.709809 -1.939276
C -1.607781 -0.910629  1.198390
C  0.985270  1.856602  0.069423
C  1.178524 -1.772967 -0.075799
C -1.836309  0.740310 -0.627607
C  0.078734  0.949395  0.954047
C  0.006800 -1.004872 -0.761626
C -0.811192 -0.063910  0.164170
H  2.904927  1.490749  1.095951
H  3.083002  1.900394 -0.661411
H  0.903634  2.896086  0.423169
H  0.607592  1.853223 -0.959560
H  0.702221  0.394453  1.666454
H -0.601009  1.571727  1.550502
H -2.438934  1.401479 -0.002720
H -1.512141  0.073577 -2.618456
H -2.840552  1.327486 -2.387979
H -2.209017 -0.257869  1.842378
H -0.927203 -1.486359  1.835194
H -2.279986 -1.603594  0.680988
H  0.416486 -0.418369 -1.592633
H -0.700250 -1.721343 -1.197955
H  1.059261 -1.757864  1.013361
H  1.134202 -2.831575 -0.374343
H  2.507533  0.118613 -0.179866
H  3.381772 -1.579205  0.140084
H  2.751693 -1.229741 -1.524746
```

Reactant: CCCCC(C#C)(C#C)C[CH2]
Product: [CH2]CCCC(C#C)(C#C)CC

```
C  2.805656 -0.677512  0.134982
C -1.867105  2.368486 -0.878522
C -2.806621 -1.566804  0.920553
C  0.632696 -1.900045 -0.888024
C  2.414096  0.784572 -0.047790
C -1.444673  1.308273 -0.487774
C -1.956862 -0.831322  0.482587
C -0.216783 -0.698116 -1.271257
C  1.296260  1.258703  0.921616
C  0.121518  0.283037  1.161008
C -0.866047  0.026649 -0.034965
H  1.019518 -2.456362 -1.744963
H  0.186998 -2.552399 -0.134144
H  0.385071  0.032213 -1.821261
H -1.043266 -0.992427 -1.932828
H -2.260613  3.294688 -1.215989
H -3.568576 -2.200604  1.300327
H -0.491292  0.683345  1.976501
H  0.497129 -0.689836  1.490704
H  0.899531  2.220433  0.576096
H  1.754361  1.433861  1.904836
H  2.105895  0.949565 -1.087119
H  3.291277  1.431917  0.112149
H  1.747275 -1.376963 -0.322299
H  3.628476 -1.008259 -0.503585
H  2.935168 -0.995140  1.173075
```

Reactant: CCCCCC([CH2])(C#C)C#C
Product: [CH2]CCCCC(C)(C#C)C#C

```
C  2.207717  0.287324  1.473620
C -3.200489  1.614546 -0.675372
C -1.847906 -2.302996  0.843723
C -0.399462  0.878961  1.237453
C  2.704358  0.728743  0.101012
C -2.265502  0.928344 -0.341974
C -1.515831 -1.201139  0.483039
C  2.471526 -0.337564 -0.997989
C  1.058731 -0.970749 -0.997708
C -0.117888  0.029540 -1.190761
C -1.072861  0.143710  0.058019
H -0.244409  1.938654  1.020340
H -0.888721  0.707000  2.196213
H -4.033170  2.206945 -0.961963
H -2.158477 -3.268340  1.157131
H -0.741019 -0.280942 -2.034532
H  0.251067  1.038449 -1.407252
H  1.022610 -1.714663 -1.802400
```

```
H  0.910017 -1.526729 -0.066525
H  2.673227  0.109856 -1.980167
H  3.200684 -1.147107 -0.857029
H  2.199303  1.664876 -0.176002
H  3.779647  0.960230  0.139039
H  0.891569  0.443619  1.399556
H  2.377039 -0.764485  1.715612
H  2.490511  0.952098  2.293986

Reactant: [CH2]CCC(C#C)(C#C)CCC
Product: [CH2]CCC(C#C)(C#C)CCC
C  2.440093  1.168086 -0.677537
C  2.442428 -1.166952  0.676149
C -2.388828  1.914293  1.111935
C -2.388828 -1.916648 -1.108906
C  1.011504  1.704056 -0.679991
C  1.014150 -1.704053  0.678688
C -1.731972  1.041710  0.599919
C -1.731917 -1.043782 -0.597442
C -0.021204  0.642198 -1.154645
C -0.018711 -0.642783  1.154768
C -0.870240 -0.000700  0.000667
H  2.799649  0.871841 -1.667231
H  3.165895  1.788430 -0.146149
H  0.734862  2.069916  0.315497
H  0.952451  2.573675 -1.351600
H  0.491985 -0.166768 -1.685393
H -0.738848  1.086204 -1.851072
H -2.984641  2.673218  1.554202
H -2.984700 -2.675802 -1.550692
H  0.494830  0.166509  1.684701
H -0.735015 -1.087102  1.852354
H  0.955911 -2.574054  1.349885
H  0.737194 -2.069655 -0.316807
H  2.441260  0.000543 -0.000680
H  3.168528 -1.786498  0.144262
H  2.802441 -0.870681  1.665679

Reactant: CCCCC(C#C)(C=C)C[CH2]
Product: [CH2]CCCC(C#C)(C=C)CC
C  2.958644  0.502318 -0.177014
C -2.604579  1.588068 -1.057174
C -2.673154 -1.573524  0.682512
C  0.848913  1.926583  0.703382
C  2.490319 -0.915655  0.129658
C -1.788822  0.860928 -0.543732
C -1.382717 -1.251894  0.682781
C -0.061269  0.815448  1.206983
C  1.360834 -1.410721 -0.813003
C  0.208759 -0.418052 -1.109060
C -0.758808 -0.004877  0.062262
H  0.435326  2.511902 -0.120469
H  1.262069  2.555420  1.495830
H  0.509111  0.124511  1.839329
H -0.865777  1.222766  1.836000
H -0.660883 -1.906609  1.166772
H -3.414908 -0.936103  0.213160
H -3.029797 -2.484110  1.152894
H -3.322300  2.228344 -1.506205
H -0.430066 -0.871465 -1.876289
H  0.621237  0.499211 -1.540298
H  0.952879 -2.353151 -0.428519
H  1.816902 -1.643235 -1.785614
H  3.333663 -1.619276  0.039191
H  2.163996 -0.971190  1.175406
H  1.935024  1.294768  0.204383
H  3.109631  0.717111 -1.238269
H  3.794720  0.845432  0.437302

Reactant: CCCCCC([CH2])(C#C)C=C
Product: [CH2]CCCCC(C)(C#C)C=C
C -2.301657 -0.516666  1.418504
C  1.886186  1.961093  1.170619
C  3.410118 -0.808277 -0.547526
C  0.275419 -1.155019  1.009186
C -2.846804 -0.647337  0.000073
C  1.476047  0.965466  0.624940
C  2.108687 -1.067250 -0.642020
C -2.578044  0.606138 -0.869451
C -1.132748  1.152787 -0.781339
C -0.016248  0.149227 -1.195919
C  0.964033 -0.248215 -0.031695
H  0.788610 -1.187158  1.970895
H  0.065226 -2.153829  0.613795
H  1.760320 -1.943338 -1.187084
H  4.149750 -1.455148 -1.007985
H  3.776763  0.059050 -0.009296
H  2.245768  2.837284  1.649941
H -0.452842 -0.778497 -1.586681
H  0.598723  0.581551 -1.992044
H -0.939701  1.501800  0.237707
H -1.067708  2.039424 -1.423283
H -2.821825  0.376203 -1.915121
H -3.259756  1.405430 -0.547819
```

H -3.931998 -0.830511 0.021632
H -2.396895 -1.531060 -0.474213
H -0.988420 -0.713949 1.281179
H -2.413698 0.470817 1.872264
H -2.602412 -1.320303 2.095805

Reactant: [CH2]CCC(C#C)(C=C)CCC
Product: [CH2]CCC(C#C)(C=C)CCC
C -2.646864 -1.142703 -0.560608
C -2.524601 1.319139 0.535845
C 2.283307 1.619697 -1.346615
C 2.913890 -1.139450 0.880058
C -1.258060 -1.755245 -0.407206
C -1.071811 1.780880 0.479261
C 1.606270 0.850001 -0.708557
C 1.586128 -1.093836 0.819970
C -0.142299 -0.844898 -1.004006
C -0.082035 0.746587 1.091610
C 0.745482 -0.079144 0.045017
H -2.930427 -0.947370 -1.598567
H -3.440126 -1.648435 -0.004521
H -1.063347 -1.962077 0.651510
H -1.229737 -2.728911 -0.919149
H 0.548697 -1.438313 -1.611403
H -0.601903 -0.103637 -1.667221
H 0.994847 -1.824312 1.368091
H 3.530417 -0.423223 0.347532
H 3.427469 -1.897052 1.463151
H 2.880269 2.296854 -1.905048
H -0.632520 0.044248 1.729828
H 0.651035 1.252258 1.728545
H -0.975230 2.727089 1.033155
H -0.777681 2.001559 -0.552997
H -2.593581 0.092487 -0.018053
H -2.893154 1.147332 1.551558
H -3.221566 1.917684 -0.056201

Reactant: CCCCC(C=C)(C=C)C[CH2]
Product: [CH2]CCCC(C=C)(C=C)CC
C 3.054164 -0.847810 -0.014036
C -1.793984 -1.002493 2.100744
C -1.362697 1.954055 -1.490272
C 0.677054 -1.933307 -0.671941
C 2.763893 0.618811 -0.311055
C -1.707132 -0.588334 0.837495
C -1.146772 1.512653 -0.251901
C -0.105377 -0.684042 -1.057476
C 1.796541 1.284246 0.709050
C 0.592796 0.433961 1.187317
C -0.552700 0.168911 0.168786
H 0.272189 -2.472251 0.187123
H 0.906197 -2.593774 -1.511821
H -1.011818 -0.962579 -1.618809
H 0.495793 -0.065164 -1.732584
H -2.534755 -0.783229 0.155753
H -2.672283 -1.531855 2.456889
H -1.008925 -0.836018 2.829682
H -1.434898 2.136857 0.593944
H -1.811114 2.926120 -1.670072
H -1.108743 1.375084 -2.371435
H 0.142035 0.964534 2.037289
H 0.953436 -0.524524 1.574097
H 1.428363 2.227895 0.289075
H 2.379154 1.535347 1.606241
H 2.358495 0.707129 -1.325878
H 3.701723 1.197523 -0.309293
H 1.892454 -1.483045 -0.285549
H 3.269953 -1.073376 1.033601
H 3.771244 -1.314207 -0.694154

Reactant: CCCCCC([CH2])(C=C)C=C
Product: [CH2]CCCCC(C)(C=C)C=C
C 1.901976 -1.456107 0.680691
C -3.381116 1.331036 0.635765
C -1.749430 -1.482797 -1.317324
C -0.535360 -0.445973 1.173966
C 2.695018 -0.153524 0.691276
C -2.057883 1.423894 0.763207
C -1.636680 -0.171069 -1.114313
C 2.635376 0.603734 -0.659307
C 1.221614 0.712609 -1.282535
C 0.155671 1.440762 -0.410480
C -1.018521 0.520089 0.087790
H -1.236330 -1.252005 1.398343
H -0.219205 0.077022 2.081742
H -1.627037 2.172449 1.427994
H -3.840147 0.583679 -0.003159
H -4.050997 1.994027 1.174082
H -2.006775 0.520515 -1.870951
H -2.201258 -1.877362 -2.222116
H -1.394599 -2.213647 -0.598829
H -0.298717 2.255747 -0.987455
H 0.623406 1.896490 0.472070
H 1.320528 1.242290 -2.238381

```
H  0.855510 -0.289622 -1.525722
H  3.056419  1.609076 -0.525486
H  3.278228  0.078733 -1.379474
H  2.309105  0.491079  1.493682
H  3.750950 -0.347231  0.934671
H  0.630639 -1.046209  0.813881
H  2.053884 -2.087667  1.559798
H  1.947168 -2.022522 -0.252158
```

Reactant: [CH2]CCC(C=C)(C=C)CCC
Product: [CH2]CCC(C=C)(C=C)CCC

```
C -2.105151  1.797349 -0.680505
C -2.839969 -0.471977  0.583034
C  1.979397  0.960529  2.130216
C  1.502046 -1.948420 -1.497190
C -0.588205  1.917137 -0.560474
C -1.600222 -1.354003  0.705394
C  1.846437  0.596864  0.855300
C  1.361915 -1.517526 -0.244134
C  0.146016  0.604629 -0.969120
C -0.375610 -0.582389  1.283073
C  0.710291 -0.215417  0.228644
H -2.451619  1.624391 -1.703699
H -2.676679  2.583940 -0.181641
H -0.240157  2.735732 -1.209044
H -0.303367  2.193667  0.460606
H -0.540026 -0.028160 -1.544160
H  0.989647  0.841336 -1.629132
H  2.617998  0.875098  0.137863
H  2.839134  1.533303  2.463612
H  1.249626  0.707245  2.891247
H  1.754471 -2.120963  0.573910
H  1.140383 -1.389701 -2.353254
H  1.994610 -2.891014 -1.714576
H  0.113218 -1.187539  2.056246
H -0.726060  0.334834  1.770307
H -1.336882 -1.784174 -0.267523
H -1.828723 -2.204424  1.365981
H -2.472648  0.662387 -0.048556
H -3.640330 -0.883298 -0.037291
H -3.213454 -0.100206  1.541726
```

Reactant: [CH2]CCC(C)CCC
Product: [CH2]CCC(C)CCC

```
C  1.664169  1.347540 -0.634806
C  1.664439 -1.347422 -0.634617
C -2.585200 -0.000331 -0.515058
C  0.844210  1.616026  0.622639
C  0.844511 -1.615904  0.622851
C -0.669605  1.311392  0.454573
C -0.669359 -1.311590  0.454714
C -1.052837 -0.000175 -0.280625
H  1.210533  1.700475 -1.564754
H  2.717956  1.626510 -0.556409
H  0.941766  2.674112  0.915505
H  1.257704  1.034049  1.454594
H -1.150921  1.314468  1.442655
H -1.113599  2.139020 -0.117100
H -0.565285 -0.000180 -1.263095
H -3.114721 -0.000322  0.446102
H -2.894204  0.888570 -1.077016
H -2.894042 -0.889354 -1.076911
H -1.150699 -1.314662  1.442784
H -1.113170 -2.139366 -0.116887
H  0.942269 -2.673933  0.915857
H  1.257877 -1.033737  1.454738
H  1.695970  0.000053 -0.742309
H  1.210890 -1.700581 -1.564522
H  2.718280 -1.626171 -0.556162
```

Reactant: CCCCC(C)C[CH2]
Product: [CH2]CCCC(C)CC

```
C -2.341780  0.205081  0.035129
C -0.403426  2.062504  0.265529
C  2.404859 -0.562028 -0.511786
C -1.600743 -0.873194 -0.746230
C  0.751781  1.365734 -0.443752
C -0.542024 -1.634548  0.096760
C  0.359941 -0.773936  1.019316
C  1.381346  0.195765  0.362879
H -0.799142  2.933114 -0.263570
H -0.236050  2.265398  1.326731
H  1.555725  2.090443 -0.655044
H  0.413449  0.997123 -1.420450
H  1.932747  0.653613  1.198612
H  1.908025 -1.037527 -1.365112
H  2.913330 -1.340528  0.069002
H  3.163747  0.126816 -0.901716
H -0.276120 -0.205695  1.708301
H  0.940280 -1.468889  1.643786
H  0.081314 -2.239854 -0.573049
H -1.077937 -2.339729  0.747820
H -1.127793 -0.420126 -1.625850
H -2.316678 -1.615127 -1.136102
```

H -1.425162 1.177657 0.228897
H -2.664920 -0.091173 1.036635
H -3.136073 0.704990 -0.524875

Reactant: CCCCCC([CH2])C
Product: [CH2]CCCCC(C)C
C 1.702477 1.500911 0.258711
C -0.947059 1.259857 0.701304
C -2.855030 0.083600 -0.484940
C 1.899665 0.444257 -0.822476
C 1.801417 -1.012363 -0.290102
C 0.654699 -1.302928 0.710520
C -0.792801 -1.235990 0.164775
C -1.315949 0.156577 -0.286832
H -1.353114 2.242457 0.445264
H -1.113719 1.004063 1.751713
H -0.873433 0.401915 -1.260562
H -3.244526 1.036662 -0.859868
H -3.345606 -0.141002 0.469617
H -3.114868 -0.704749 -1.202597
H -0.897331 -1.938971 -0.673405
H -1.460587 -1.591943 0.963642
H 0.809189 -2.321620 1.093616
H 0.747890 -0.634715 1.574046
H 2.745675 -1.248433 0.220396
H 1.719780 -1.700113 -1.142465
H 2.888059 0.566136 -1.294340
H 1.162433 0.603261 -1.618574
H 0.390937 1.424328 0.573523
H 1.826589 2.530502 -0.086144
H 2.236145 1.310321 1.193617

Reactant: [CH2]CCC(C#C)CCC
Product: [CH2]CCC(C#C)CCC
C 1.906671 -1.259507 -0.718376
C 2.104440 1.383197 -0.199306
C -3.457622 0.107505 -0.399619
C 1.093190 -1.756324 0.472627
C 0.732841 2.008570 0.045031
C -2.257622 0.032707 -0.290396
C -0.428136 -1.510463 0.324078
C -0.248169 1.066309 0.791724
C -0.798016 -0.069860 -0.146007
H 1.454634 -1.437372 -1.697468
H 2.960971 -1.546815 -0.694121
H 1.247598 -2.836715 0.616877
H 1.461948 -1.269283 1.385614
H -0.833266 -2.212972 -0.414592
H -0.931230 -1.708548 1.277791
H -0.357784 0.074331 -1.141791
H -4.512661 0.174077 -0.493568
H -1.092473 1.650248 1.169925
H 0.256862 0.621389 1.657121
H 0.274724 2.307233 -0.906239
H 0.856384 2.928234 0.638701
H 1.963663 0.080597 -0.563953
H 2.678935 1.828650 -1.014534
H 2.702841 1.277221 0.710759

Reactant: CCCCC(C#C)C[CH2]
Product: [CH2]CCCC(C#C)CC
C -2.527937 -0.268650 -0.216127
C 3.148655 -0.489823 -0.665215
C -1.089335 1.987153 0.103403
C -1.464432 -1.198454 -0.788972
C 2.193438 -0.009661 -0.104044
C 0.268584 1.531554 -0.414641
C -0.404864 -1.649604 0.253367
C 0.136720 -0.552467 1.199616
C 1.017861 0.567627 0.563280
H -1.584577 2.721406 -0.536355
H -1.112368 2.276379 1.157456
H 0.927229 2.396518 -0.586249
H 0.150319 1.037901 -1.384591
H 1.377070 1.183874 1.402198
H 3.990326 -0.910535 -1.156258
H 0.756055 -1.044892 1.960333
H -0.694275 -0.075763 1.730149
H 0.438703 -2.117744 -0.267563
H -0.861761 -2.421280 0.888372
H -1.939065 -2.104470 -1.199157
H -0.971083 -0.707179 -1.636287
H -1.882629 0.893990 0.009569
H -2.928571 -0.569342 0.755693
H -3.316342 0.007108 -0.920930

Reactant: CCCCCC([CH2])C#C
Product: [CH2]CCCCC(C)C#C
C -1.963977 1.510183 0.184757
C 3.735898 0.026189 -0.347611
C 0.647929 1.252776 0.798773
C -2.106460 0.454556 -0.906871
C 2.531210 0.078628 -0.282178
C -2.051859 -1.003008 -0.370144

```
C -0.967534 -1.302537  0.694923
C  0.509415 -1.256901  0.235993
C  1.061883  0.145195 -0.181919
H  0.757334  0.980211  1.850605
H  1.080075  2.228145  0.567784
H  0.672331  0.398771 -1.176666
H  4.794918 -0.019254 -0.400704
H  0.659532 -1.950276 -0.600647
H  1.131404 -1.612581  1.066985
H -1.150870 -2.320020  1.067567
H -1.104179 -0.634154  1.552266
H -3.025566 -1.229859  0.085798
H -1.928134 -1.691875 -1.216252
H -1.325456  0.608089 -1.661608
H -3.065233  0.585875 -1.433399
H -0.684212  1.424911  0.583041
H -2.557572  1.325416  1.083994
H -2.056206  2.540610 -0.167218
```

Reactant: CCCCC(C=C)C[CH2]
Product: [CH2]CCCC(C=C)CC

```
C -2.605700  0.333559 -0.359317
C  3.226551 -1.056478  0.558029
C -0.636970  2.015638  0.386208
C -1.793512 -0.791645 -0.990807
C  2.011766 -0.813615  0.068968
C  0.591437  1.253294 -0.096757
C -1.023706 -1.654290  0.045647
C -0.275577 -0.884509  1.163823
C  0.943807  0.002624  0.765780
H -0.840818  2.935275 -0.168005
H -0.692698  2.165287  1.467731
H  0.444917  0.949509 -1.140881
H  1.475800  1.909684 -0.092815
H  1.366029  0.374006  1.711122
H  1.734408 -1.210855 -0.906793
H  3.537411 -0.669908  1.525136
H  3.958181 -1.647828  0.016329
H  0.102150 -1.629757  1.876588
H -0.993887 -0.263678  1.711096
H -0.324316 -2.314565 -0.481568
H -1.753608 -2.306431  0.545604
H -1.095254 -0.366501 -1.722264
H -2.458048 -1.461922 -1.559891
H -1.685633  1.219757  0.079554
H -3.175867  0.047084  0.528513
H -3.204895  0.912206 -1.066728
```

Reactant: CCCCCC([CH2])C=C
Product: [CH2]CCCCC(C)C=C

```
C  1.984238 -1.539090  0.189098
C -3.380366 -0.224851 -0.854419
C -0.535375 -1.124064  1.050090
C  2.041171 -0.565760 -0.983291
C -2.531324  0.059379  0.132263
C  2.102914  0.924230 -0.548193
C  1.149646  1.343246  0.598705
C -0.369203  1.323678  0.296828
C -1.019673 -0.071163  0.047815
H -0.509344 -0.785290  2.089580
H -1.025683 -2.093962  0.939360
H -0.770079 -0.410543 -0.964599
H -2.907574  0.407232  1.094477
H -4.454505 -0.122336 -0.736659
H -3.030868 -0.573078 -1.822763
H -0.582241  1.964152 -0.568631
H -0.880731  1.774582  1.159914
H  1.351704  0.726808  1.481702
H  1.409333  2.374229  0.877359
H  1.918115  1.561340 -1.423439
H  3.127936  1.134346 -0.211837
H  1.172239 -0.731967 -1.631247
H  2.927513 -0.774707 -1.603737
H  0.750126 -1.370030  0.712388
H  2.676651 -1.319893  1.006124
H  1.999770 -2.593885 -0.096077
```

Reactant: [CH2]CCC(C=C)CCC
Product: [CH2]CCC(C=C)CCC

```
C -1.796730 -1.346133  0.873074
C -1.797212  1.348600  0.870972
C  3.138186  0.001618  0.854278
C -1.268994 -1.617335 -0.531859
C -1.269289  1.617901 -0.534262
C  2.291129  0.000874 -0.173123
C  0.246134 -1.316134 -0.697014
C  0.245951  1.316918 -0.698670
C  0.776864  0.000832 -0.058715
H -2.843530 -1.621527  1.023648
H -1.154456 -1.701482  1.683136
H -1.426510 -2.675928 -0.794687
H -1.852156 -1.036399 -1.255703
H  0.806922 -2.138150 -0.232493
H  0.501364 -1.318450 -1.765732
```

```
H  0.518617  0.001484  1.006110
H  2.675758  0.000227 -1.193840
H  2.785403  0.002270  1.882352
H  4.214490  0.001605  0.713005
H  0.501439  1.318043 -1.767330
H  0.806409  2.139631 -0.234984
H -1.852126  1.035737 -1.257386
H -1.427069  2.676064 -0.798662
H -1.802007  0.001312  0.982826
H -1.155232  1.705417  1.680624
H -2.844144  1.623829  1.020928
```

Reactant: [CH2]CCC(C)(C)CCC
Product: [CH2]CCC(C)(C)CCC

```
C  2.197111 -1.315479 -0.228862
C  2.177176  1.350015  0.179726
C -2.089682  0.694458 -0.996622
C -2.046622 -0.741906  1.055724
C  0.784751 -1.812511  0.063654
C  0.749148  1.820426 -0.079351
C -0.301718 -1.056765 -0.762206
C -0.302714  1.046212  0.773562
C -1.155893 -0.014195  0.017158
H  2.488913 -1.407188 -1.279089
H  2.969351 -1.692239  0.446901
H  0.726452 -2.887324 -0.167961
H  0.576706 -1.720515  1.135991
H  0.185225 -0.554324 -1.608361
H -1.006247 -1.780766 -1.192983
H -1.514592  1.247871 -1.747208
H -2.711282 -0.043403 -1.518571
H -2.751624  1.398262 -0.477673
H -2.709130 -1.457980  0.554697
H -1.438840 -1.284623  1.788165
H -2.667119 -0.017102  1.596783
H  0.214097  0.554862  1.608418
H -1.010128  1.757741  1.220159
H  0.676711  2.894380  0.152216
H  0.516840  1.722459 -1.146052
H  2.200248  0.017149 -0.024210
H  2.926000  1.740082 -0.514572
H  2.492041  1.448473  1.222640
```

Reactant: CCCCC(C)(C)C[CH2]
Product: [CH2]CCCC(C)(C)CC

```
C -2.527247  0.581961  0.269752
C -0.304400  2.053478 -0.105870
C  2.316556  0.468755  0.847362
C  1.762574 -1.153796 -0.983523
C -2.122533 -0.707636 -0.435263
C  0.569219  1.068518 -0.875962
C -1.067092 -1.533535  0.347829
C  0.133505 -0.750995  0.940129
C  1.164874 -0.096525 -0.025334
H -0.642219  2.907567 -0.698611
H  0.080926  2.360423  0.869084
H  1.417993  1.599064 -1.339345
H -0.013297  0.648803 -1.706288
H  1.947987  1.233847  1.539910
H  2.778122 -0.332536  1.436687
H  3.088264  0.919471  0.211856
H  0.994672 -1.570361 -1.644705
H  2.540512 -0.698762 -1.608867
H  2.214953 -1.975091 -0.414600
H -0.246289  0.022808  1.617591
H  0.697663 -1.458345  1.565549
H -1.579656 -2.010208  1.195631
H -0.701230 -2.345976 -0.291530
H -1.747210 -0.469245 -1.437910
H -3.006523 -1.348477 -0.586103
H -1.445109  1.382830  0.157808
H -2.703608  0.483092  1.344193
H -3.319907  1.143819 -0.230552
```

Reactant: CCCCCC([CH2])(C)C
Product: [CH2]CCCCC(C)(C)C

```
C -1.714773  1.566131  0.308460
C  0.650501  1.121752 -0.893071
C  2.304293  0.780292  0.971784
C  2.290362 -0.791223 -1.001149
C -2.566570  0.417351 -0.223499
C -2.167712 -0.986371  0.296492
C -0.753968 -1.470569 -0.126057
C  0.409320 -0.852002  0.710593
C  1.400206  0.070998 -0.065436
H  1.175256  2.074163 -1.002011
H  0.270421  0.756200 -1.851253
H  2.815338  0.044157  1.604173
H  1.706013  1.435928  1.615520
H  3.063044  1.388730  0.465319
H  2.988058 -0.155358 -1.558635
H  2.870525 -1.513438 -0.412796
H  1.675394 -1.342784 -1.721372
H  1.002045 -1.655217  1.167652
```

```
H -0.017167 -0.268462  1.535199
H -0.726187 -2.561697 -0.016582
H -0.612211 -1.262769 -1.193358
H -2.908687 -1.704551 -0.080059
H -2.237748 -1.001071  1.392890
H -2.522917  0.413048 -1.321989
H -3.621717  0.591513  0.044274
H -0.491545  1.402902 -0.235080
H -1.559295  1.558491  1.390273
H -2.016817  2.551984 -0.055617
```

Test set

```
Reactant: [CH2]CCCCC(C)CC
Product: CCCCCC([CH2])CC
C -2.284090  1.352897  0.154579
C  3.222288 -0.501903  0.781050
C  0.239361  1.517721 -0.782105
C -2.155908  0.152426  1.085562
C  2.466273  0.510467 -0.108714
C -2.008039 -1.197772  0.332345
C -1.039994 -1.202339 -0.877443
C  0.467891 -1.016991 -0.571560
C  0.915006  0.371900 -0.031981
H  2.896745 -0.410353  1.824378
H  4.302091 -0.318170  0.743394
H  3.042422 -1.531020  0.454447
H  2.776005  0.393004 -1.155933
H  0.643582  0.445241  1.029848
H -1.057531  1.488938 -0.395125
H  0.223279  1.406002 -1.869971
H  0.575854  2.511416 -0.473279
H  1.016885 -1.194688 -1.508953
H  0.781764 -1.796155  0.134369
H -1.362328 -0.446390 -1.601864
H -1.150668 -2.174777 -1.377821
H -1.700312 -1.974972  1.044760
H -3.000306 -1.484594 -0.043479
H -3.041965  0.082530  1.737053
H -1.299424  0.304727  1.753044
H  2.738335  1.528551  0.199136
H -2.448493  2.306085  0.663193
H -2.964070  1.210685 -0.689608

Reactant: [CH2]CCCCCCCC
Product: CC[CH]CCCCCC
C -0.130740  1.667353 -0.714535
C  3.174981  0.060190 -1.677437
C -1.098193  1.587111  0.460748
C  2.509658 -0.537612 -0.418107
C -2.323132  0.669017  0.194415
C  1.013149 -0.777597 -0.606202
C -2.022910 -0.689019 -0.486221
C  0.282012 -1.349232  0.607042
C -1.202338 -1.716711  0.332500
H  0.705982  2.355210 -0.568330
H -0.601136  1.785789 -1.694010
H -0.557757  1.241597  1.350131
H -1.477274  2.592474  0.707617
H -2.849357  0.490646  1.141854
H -3.018361  1.215398 -0.458478
H -2.988959 -1.156395 -0.723498
H -1.524312 -0.508490 -1.445037
H -1.708864 -1.902425  1.289209
H -1.216851 -2.664032 -0.224521
H  0.347403 -0.629412  1.432312
H  0.799705 -2.259246  0.953982
H  0.475282  0.431908 -0.756169
H  0.782076 -1.302827 -1.540627
H  3.005795 -1.488075 -0.161977
H  2.662362  0.136437  0.436560
H  2.713751  1.020089 -1.934136
H  4.246623  0.223086 -1.518133
H  3.053295 -0.616491 -2.531383

Reactant: CCCCCC(C)[CH]C
Product: [CH2]CCCCC(C)CC
C -1.276613  1.811781  0.129050
C  2.123400  1.701980  0.167694
C  2.374667 -1.292816 -0.525141
C -1.909081  0.835778 -0.854614
C  1.111635  0.635873  0.582211
C -2.351446 -0.497674 -0.192480
C -1.346307 -1.122042  0.806334
C -0.008167 -1.642871  0.225718
C  1.001663 -0.593133 -0.325728
H  2.008467  2.604130  0.779835
H  1.979676  1.981500 -0.883646
H  3.157669  1.350218  0.284094
H  1.174150  0.374938  1.645052
H  0.661984 -0.252980 -1.313281
H  3.097051 -0.624316 -1.004219
H  2.779265 -1.608192  0.444315
H  2.258916 -2.182289 -1.156539
H  0.504308 -2.190652  1.030710
```

```
H -0.219408 -2.372715 -0.568216
H -1.141339 -0.405963  1.609575
H -1.847212 -1.978807  1.279078
H -2.584716 -1.229637 -0.977339
H -3.284620 -0.309267  0.356829
H -2.794178  1.291077 -1.328410
H -1.200648  0.632882 -1.666826
H -0.066212  1.236241  0.449107
H -0.989682  2.774638 -0.300702
H -1.803155  1.918473  1.080840
```

Reactant: C[CH]CCCCCCC
Product: C[CH]CCCCCCC

```
C  0.215331  2.792875 -0.014260
C -2.795789  0.536197  0.288825
C  0.592385  1.377141  0.411535
C -1.558325 -0.043133 -0.387997
C  1.692369  0.727626 -0.424681
C -1.333767 -1.539218 -0.180385
C  2.226573 -0.599246  0.168274
C  0.111837 -2.007601 -0.495655
C  1.128442 -1.596055  0.614379
H -0.630164  3.174120  0.569458
H -0.061970  2.813855 -1.076013
H  1.059413  3.486018  0.121487
H  0.737242  1.271170  1.491548
H  2.539305  1.424364 -0.537142
H  1.303647  0.552855 -1.438522
H  2.877498 -1.083673 -0.571713
H  2.850457 -0.365899  1.042141
H  1.627110 -2.493531  1.001818
H  0.578214 -1.159865  1.456654
H  0.419965 -1.597600 -1.465897
H  0.109815 -3.099370 -0.599051
H -2.040836 -2.097294 -0.817043
H -1.570015 -1.806658  0.859217
H -0.491660  0.631745  0.122529
H -1.475496  0.240388 -1.444465
H -2.872391  1.616547  0.121846
H -2.763593  0.355453  1.370347
H -3.716253  0.071511 -0.097777
```

Reactant: C[CH]CCCCCC(C)C#C
Product: CCCCCCC[C](C)C#C

```
C  1.614778  2.449308 -0.470540
C -2.786547 -0.165851 -1.598252
C -1.495931  1.823009  1.048603
C  1.351615  0.965865 -0.672973
C -2.037674  0.130524 -0.692493
C  2.175120  0.016518  0.185775
C  2.002171 -1.482766 -0.184407
C  0.555795 -1.953417 -0.478986
C -0.432406 -1.987683  0.712558
C -0.787045 -0.623597  1.354769
C -1.119970  0.501556  0.353692
H  2.624463  2.719396 -0.819690
H  0.895842  3.062717 -1.024774
H  1.553096  2.717654  0.591180
H  1.265690  0.667423 -1.721945
H  3.245306  0.270500  0.088641
H  1.924282  0.180469  1.241733
H  2.597349 -1.675623 -1.087797
H  2.430153 -2.101099  0.615963
H  0.124923 -1.343889 -1.280272
H  0.620271 -2.977166 -0.873734
H -0.034216 -2.647159  1.495614
H -1.363196 -2.441653  0.349771
H  0.038624 -0.274743  1.985289
H -1.653084 -0.766184  2.019097
H  0.020197  0.741255 -0.211782
H -3.449587 -0.423538 -2.385772
H -2.425487  1.699969  1.619514
H -1.643738  2.620538  0.314312
H -0.702536  2.123498  1.742230
```

Reactant: CCCCC(C)C[CH]C
Product: [CH2]CCCC(C)CCC

```
C  1.930326  1.258861 -0.136606
C -1.119433  2.708730 -0.063197
C -2.202736 -1.657577 -0.493677
C  2.497359 -0.153039 -0.228020
C -0.760634  1.250274 -0.336731
C  1.615512 -1.214511  0.485230
C -1.141721  0.278703  0.779463
C  0.320034 -1.554023 -0.315945
C -1.015900 -1.222607  0.398369
H -0.687939  3.039203  0.890105
H -0.745310  3.366532 -0.855838
H -2.209644  2.841388  0.001208
H -1.053934  0.918019 -1.336826
H -0.509199  0.493146  1.652950
H -2.180173  0.465435  1.099631
H -1.058774 -1.806687  1.328980
H -2.211944 -1.083612 -1.427706
```

```
H -2.127545 -2.721424 -0.748180
H -3.156449 -1.492297  0.020713
H  0.311763 -2.625407 -0.554824
H  0.338149 -1.021741 -1.275200
H  1.359148 -0.850563  1.488322
H  2.207736 -2.127546  0.620566
H  2.615601 -0.445939 -1.279243
H  3.504534 -0.170506  0.219850
H  0.563375  1.220671 -0.339103
H  2.290093  1.958361 -0.894425
H  1.972152  1.685471  0.870305

Reactant: C[CH]CCCCCC(C)C=C
Product: CCCCCCC[C](C)C=C
C -0.306393  2.541256  0.889089
C  2.722371  1.087836 -1.044374
C  2.009236 -0.294375  1.507589
C -0.988931  1.191160  0.747457
C  1.715646  0.201012 -0.978778
C -1.790134  0.983098 -0.527467
C -2.672524 -0.288998 -0.508279
C -1.948725 -1.569351 -0.023637
C -0.671489 -1.956459 -0.832552
C  0.628937 -1.853681  0.009046
C  1.147571 -0.416564  0.245370
H  0.365597  2.719953  0.041205
H -1.046332  3.357750  0.909353
H  0.280392  2.598546  1.812607
H -1.466424  0.822043  1.658881
H -1.092876  0.945798 -1.377875
H -2.440123  1.855867 -0.708685
H -3.075043 -0.459474 -1.515600
H -3.529778 -0.110263  0.155190
H -2.668334 -2.396867 -0.064118
H -1.678342 -1.445368  1.031848
H -0.767892 -2.990634 -1.184846
H -0.587949 -1.328531 -1.727664
H  1.428259 -2.430925 -0.479506
H  0.443818 -2.328567  0.981384
H  0.108689  0.293024  0.522972
H  1.241716 -0.103503 -1.911752
H  3.251729  1.433233 -0.162996
H  3.055476  1.491817 -1.994823
H  1.472161 -0.703506  2.370554
H  2.254546  0.750776  1.724132
H  2.949802 -0.849660  1.389858
```

IRC calculations

IRC calculations have been done for the reference reactions of each reaction family to assess whether the reactions proceed in a single step and to verify whether classical transition state theory is appropriate for these reactions. First, IRC calculations have been done in Gaussian with steps of 0.05 Bohr at the B3LYP/cbsb7 level of theory. These calculations have been visually examined to assess the formation of the reactants and products in a single step, which was indeed the case. Second, each of the geometries obtained in the previous steps was used for a single-point energy and frequency calculation at the CBSQB3 level of theory. From these calculations, the standard Gibbs free energy has been compared to the standard Gibbs free energy of the transition state at 300, 1000 and 2000K. The results are shown in Figure 2 to Figure 7. For all reactions at all temperatures, the standard Gibbs free energy reaches a maximum at the saddle point, indicating the use of classical transition state theory is adequate for intramolecular hydrogen abstraction reaction in hydrocarbons.

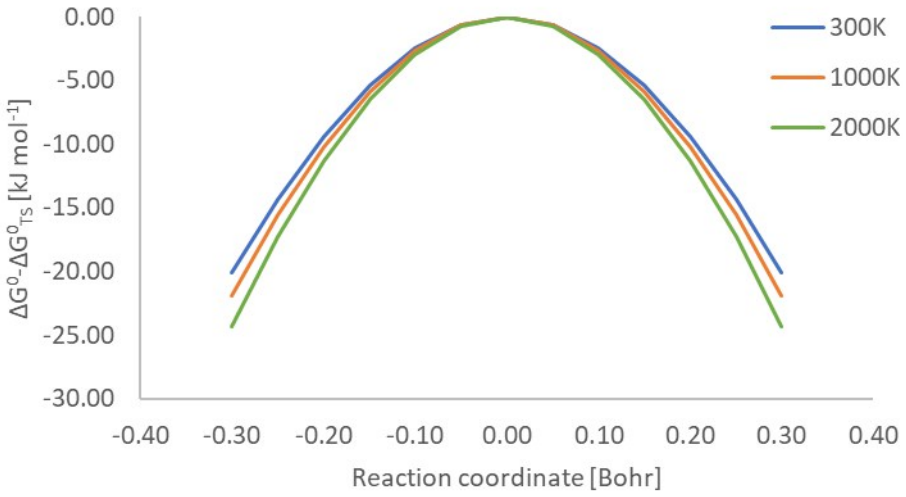


Figure 2: Standard Gibbs free energy profile for the 1-2 H-shift of the ethyl radical.

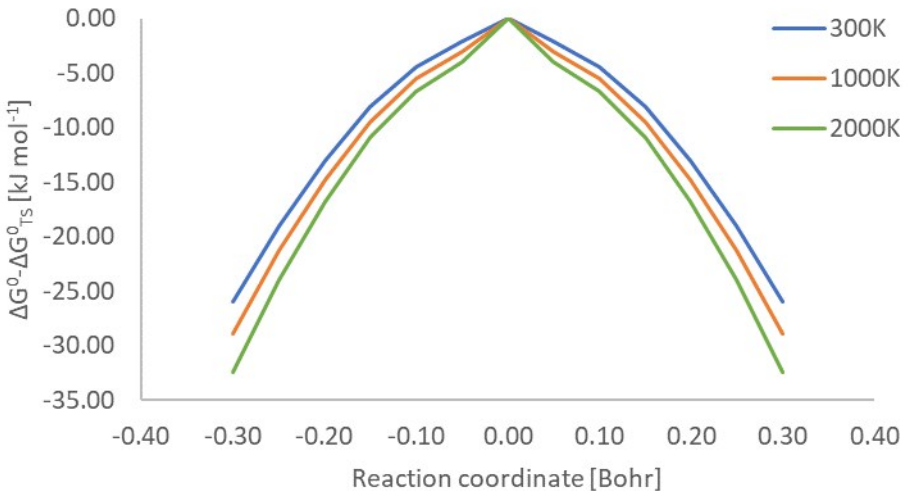


Figure 3: Standard Gibbs free energy profile for the 1-3 H-shift of the 1-propyl radical.

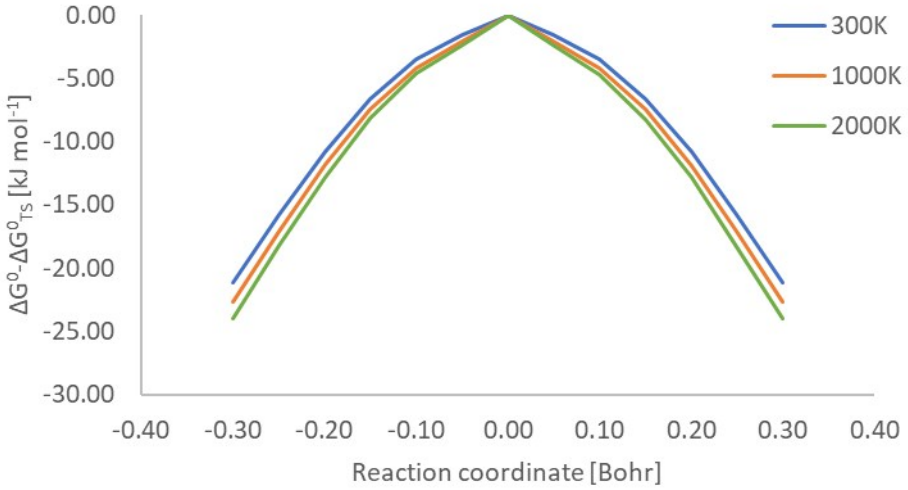


Figure 4: Standard Gibbs free energy profile for the 1-4 H-shift of the 1-butyl radical.

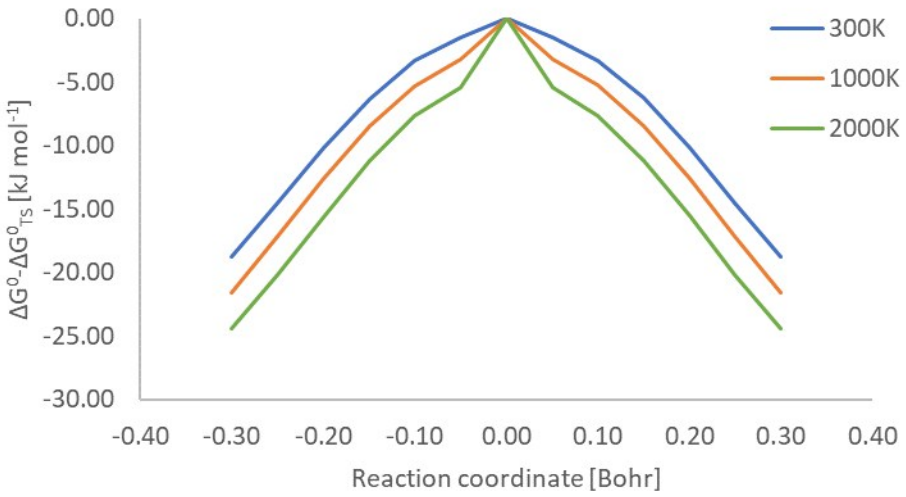


Figure 5: : Standard Gibbs free energy profile for the 1-5 H-shift of the 1-pentyl radical.

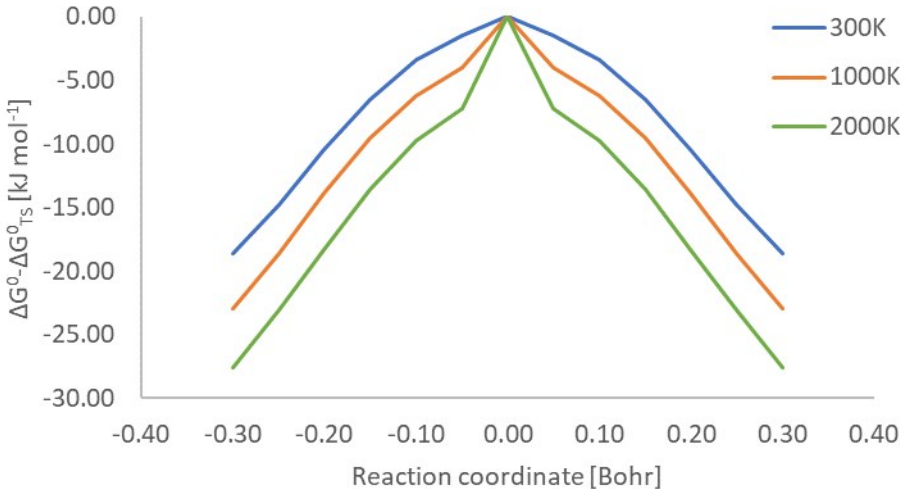


Figure 6: Standard Gibbs free energy profile for the 1-6 H-shift of the 1-hexyl radical.

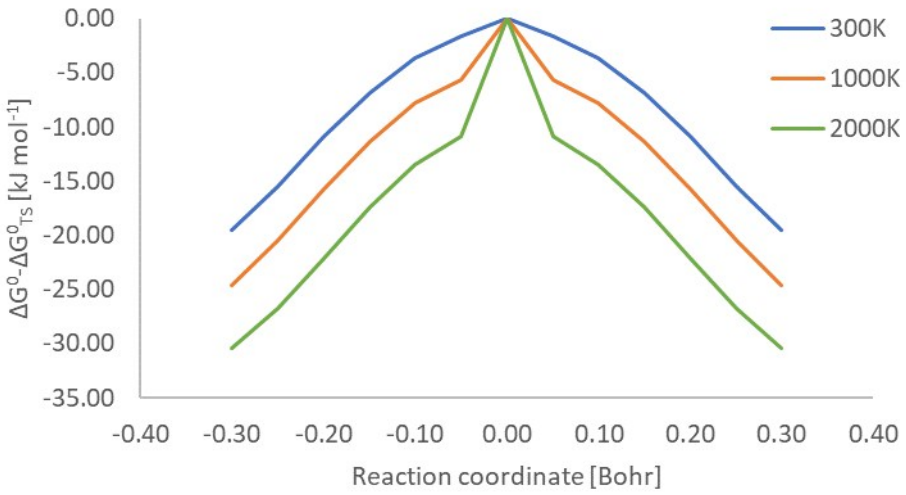


Figure 7: Standard Gibbs free energy profile for the 1-7 H-shift of the 1-heptyl radical.