

Reaction mechanisms and Kinetics of the Hydrogen Abstraction Reactions of C₄-C₆ Alkenes with Hydroxyl Radical: A Theoretical Exploration

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Table S1

Full list of the studied abstraction reactions and the computed rate coefficients by employing the corrected reaction barriers (A : cm³ mol⁻¹ s⁻¹; E_a : cal mol⁻¹)

	Reaction	Abstraction reaction site	Rate coefficients		
			A	n	E_a
1-butene	R1- <i>cis</i>	CH ₂ =CHCH ₂ CH ₃ → •HC=CHCH ₂ CH ₃	1.04E4	2.70	954
	R1- <i>trans</i>	CH ₂ =CHCH ₂ CH ₃ → •HC=CHCH ₂ CH ₃	1.10E4	2.65	1558
	R2	CH ₂ =CHCH ₂ CH ₃ → CH ₂ =C•CH ₂ CH ₃	1.60E4	2.58	76
	R3	CH ₂ =CHCH ₂ CH ₃ → CH ₂ =CHCH•CH ₃	4.14E4	2.55	-1742
	R4	CH ₂ =CHCH ₂ CH ₃ → CH ₂ =CHCH ₂ CH ₂ •	2.51E5	2.28	-1209
2-butene	R5	CH ₃ CH=CHCH ₃ → CH ₃ CH=CHCH ₂ •	5.23E4	2.44	-944
	R6	CH ₃ CH=CHCH ₃ → CH ₃ C=C•CH ₃	2.10E4	2.55	136
isobutene	R7	H ₂ C=C(CH ₃) ₂ → •HC=C(CH ₃) ₂	9.01E3	2.69	851
	R8	H ₂ C=C(CH ₃) ₂ → H ₂ C=C(CH ₃)CH ₂ •	3.33E4	2.50	-1819
1-pentene	R9- <i>cis</i>	CH ₂ =CHCH ₂ CH ₂ CH ₃ → •CH=CHCH ₂ CH ₂ CH ₃	7.46E3	2.69	956
	R9- <i>trans</i>	CH ₂ =CHCH ₂ CH ₂ CH ₃ → •CH=CHCH ₂ CH ₂ CH ₃	1.01E4	2.65	1812
	R10	CH ₂ =CHCH ₂ CH ₂ CH ₃ → CH ₂ =C•CH ₂ CH ₂ CH ₃	2.72E4	2.62	-287
	R11	CH ₂ =CHCH ₂ CH ₂ CH ₃ → CH ₂ =CHCH•CH ₂ CH ₃	2.72E5	2.37	-1929
	R12	CH ₂ =CHCH ₂ CH ₂ CH ₃ → CH=CHCH ₂ CH•CH ₃	5.21E3	2.70	-3523
2-pentene	R13	CH ₂ =CHCH ₂ CH ₂ CH ₃ → CH=CHCH ₂ CH ₂ CH ₂ •	1.41E4	2.62	-915
	R14	CH ₃ CH=CHCH ₂ CH ₃ → •CH ₂ CH=CHCH ₂ CH ₃	5.31E3	2.76	-1305
	R15	CH ₃ CH=CHCH ₂ CH ₃ → CH ₃ C=C•CHCH ₂ CH ₃	1.64E4	2.56	191
	R16	CH ₃ CH=CHCH ₂ CH ₃ → CH ₃ CH=C•CH ₂ CH ₃	2.12E4	2.55	-136
	R17	CH ₃ CH=CHCH ₂ CH ₃ → CH ₃ CH=CHCH•CH ₃	2.30E4	2.56	-2204
	R18	CH ₃ CH=CHCH ₂ CH ₃ → CH ₃ CH=CHCH ₂ CH ₂ •	1.32E4	2.57	-1917
2-methyl-1-butene	R19- <i>cis</i>	H ₂ C=C(CH ₃)CH ₂ CH ₃ → •HC=C(CH ₃)CH ₂ CH ₃	1.46E4	2.66	1575
	R19- <i>trans</i>	H ₂ C=C(CH ₃)CH ₂ CH ₃ → •HC=C(CH ₃)CH ₂ CH ₃	1.01E4	2.65	1812
	R20	H ₂ C=C(CH ₃)CH ₂ CH ₃ → H ₂ C=C(CH ₃)CH ₂ •	2.12E3	2.79	-1295
	R21	H ₂ C=C(CH ₃)CH ₂ CH ₃ → H ₂ C=C(CH ₃)CH•CH ₃	2.19E4	2.47	-2397
	R22	H ₂ C=C(CH ₃)CH ₂ CH ₃ → H ₂ C=C(CH ₃)CH ₂ CH ₂ •	7.00E3	2.62	-2058
2-methyl-2-butene	R23	HC(CH ₃)=C(CH ₃) ₂ → •C(CH ₃)=C(CH ₃) ₂	5.08E4	2.53	-772
	R24	HC(CH ₃)=C(CH ₃) ₂ → HC(CH ₂ •)=C(CH ₃) ₂	8.39E3	2.75	-2075
	R25- <i>cis</i>	HC(CH ₃)=C(CH ₃) ₂ → HC(CH ₃)=C(CH ₂ •)CH ₃	5.30E3	2.90	-2122
	R25- <i>trans</i>	HC(CH ₃)=C(CH ₃) ₂ → HC(CH ₃)=C(CH ₂ •)CH ₃	8.03E3	2.74	-2211
2-methyl-3-butene	R26- <i>cis</i>	H ₂ C=CHCH(CH ₃) ₂ → •HC=CHCH(CH ₃) ₂	1.64E4	2.70	657

1-hexene	R26- <i>trans</i>	$\text{H}_2\text{C}=\text{CHCH}(\text{CH}_3)_2 \rightarrow \bullet\text{HC}=\text{CHCH}(\text{CH}_3)_2$	1.54E4	2.67	1169
	R27	$\text{H}_2\text{C}=\text{CHCH}(\text{CH}_3)_2 \rightarrow \text{H}_2\text{C}=\text{C}\bullet\text{CH}(\text{CH}_3)_2$	2.41E4	2.56	-425
	R28	$\text{H}_2\text{C}=\text{CHCH}(\text{CH}_3)_2 \rightarrow \text{H}_2\text{C}=\text{CHC}\bullet(\text{CH}_3)_2$	7.28E4	2.41	-2655
	R29	$\text{H}_2\text{C}=\text{CHCH}(\text{CH}_3)_2 \rightarrow \text{H}_2\text{C}=\text{CHCH}(\text{CH}_2\bullet)(\text{CH}_3)$	2.41E4	2.55	-1565
	R30- <i>cis</i>	$\text{CH}_2=\text{CHCH}_2\text{CH}_2\text{CH}_2\text{CH}_3 \rightarrow \bullet\text{CH}=\text{CHCH}_2\text{CH}_2\text{CH}_2\text{CH}_3$	8.67E3	2.65	1537
	R30- <i>trans</i>	$\text{CH}_2=\text{CHCH}_2\text{CH}_2\text{CH}_2\text{CH}_3 \rightarrow \bullet\text{CH}=\text{CHCH}_2\text{CH}_2\text{CH}_2\text{CH}_3$	1.78E4	2.63	1781
	R31	$\text{CH}_2=\text{CHCH}_2\text{CH}_2\text{CH}_2\text{CH}_3 \rightarrow \text{CH}_2=\text{C}\bullet\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_3$	1.75E4	2.59	91
	R32	$\text{CH}_2=\text{CHCH}_2\text{CH}_2\text{CH}_2\text{CH}_3 \rightarrow \text{CH}_2=\text{CHCH}\bullet\text{CH}_2\text{CH}_2\text{CH}_3$	2.82E5	2.33	-1532
	R33	$\text{CH}_2=\text{CHCH}_2\text{CH}_2\text{CH}_2\text{CH}_3 \rightarrow \text{CH}_2=\text{CHCH}_2\text{CH}\bullet\text{CH}_2\text{CH}_3$	1.60E4	2.43	-2847
	R34	$\text{CH}_2=\text{CHCH}_2\text{CH}_2\text{CH}_2\text{CH}_3 \rightarrow \text{CH}_2=\text{CHCH}_2\text{CH}_2\text{CH}\bullet\text{CH}_3$	4.69E4	2.59	-989
2-hexene	R35	$\text{CH}_2=\text{CHCH}_2\text{CH}_2\text{CH}_2\text{CH}_3 \rightarrow \text{CH}_2=\text{CHCH}_2\text{CH}_2\text{CH}_2\text{CH}\bullet$	7.44E3	2.57	-377
	R36	$\text{CH}_3\text{CH}=\text{CHCH}_2\text{CH}_2\text{CH}_3 \rightarrow \bullet\text{CH}_2\text{CH}=\text{CHCH}_2\text{CH}_2\text{CH}_3$	6.25E3	2.76	-1448
	R37	$\text{CH}_3\text{CH}=\text{CHCH}_2\text{CH}_2\text{CH}_3 \rightarrow \text{CH}_3\text{C}\bullet=\text{CHCH}_2\text{CH}_2\text{CH}_3$	3.00E4	2.61	-153
	R38	$\text{CH}_3\text{CH}=\text{CHCH}_2\text{CH}_2\text{CH}_3 \rightarrow \text{CH}_3\text{CH}=\text{C}\bullet\text{CH}_2\text{CH}_2\text{CH}_3$	2.74E4	2.60	-662
	R39	$\text{CH}_3\text{CH}=\text{CHCH}_2\text{CH}_2\text{CH}_3 \rightarrow \text{CH}_3\text{CH}=\text{CHCH}\bullet\text{CH}_2\text{CH}_3$	4.65E4	2.58	-2467
3-hexene	R40	$\text{CH}_3\text{CH}=\text{CHCH}_2\text{CH}_2\text{CH}_3 \rightarrow \text{CH}_3\text{CH}=\text{CHCH}_2\text{CH}\bullet\text{CH}_3$	5.41E3	2.72	-3748
	R41	$\text{CH}_3\text{CH}=\text{CHCH}_2\text{CH}_2\text{CH}_3 \rightarrow \text{CH}_3\text{CH}=\text{CHCH}_2\text{CH}_2\text{CH}_2\bullet$	1.34E4	2.62	-944
	R42	$\text{CH}_3\text{CH}_2\text{CH}=\text{CHCH}_2\text{CH}_3 \rightarrow \bullet\text{CH}_2\text{CH}_2\text{CH}=\text{CHCH}_2\text{CH}_3$	6.59E4	2.43	-1730
	R43	$\text{CH}_3\text{CH}_2\text{CH}=\text{CHCH}_2\text{CH}_3 \rightarrow \text{CH}_3\text{CH}\bullet\text{CH}=\text{CHCH}_2\text{CH}_3$	2.67E6	2.01	-970
	R44	$\text{CH}_3\text{CH}_2\text{CH}=\text{CHCH}_2\text{CH}_3 \rightarrow \text{CH}_3\text{CH}_2\text{C}\bullet=\text{CHCH}_2\text{CH}_3$	1.18E5	2.38	351
1-4-pentadiene	R45- <i>cis</i>	$\text{CH}_2=\text{CHCH}_2\text{CH}=\text{CH}_2 \rightarrow \bullet\text{CH}=\text{CHCH}_2\text{CH}=\text{CH}_2$	1.35E5	2.33	1902
	R45- <i>trans</i>	$\text{CH}_2=\text{CHCH}_2\text{CH}=\text{CH}_2 \rightarrow \bullet\text{CH}=\text{CHCH}_2\text{CH}=\text{CH}_2$	2.37E5	2.33	2170
	R46	$\text{CH}_2=\text{CHCH}_2\text{CH}=\text{CH}_2 \rightarrow \text{CH}_2=\text{C}\bullet\text{CH}_2\text{CH}=\text{CH}_2$	9.20E4	2.27	-232
	R47	$\text{CH}_2=\text{CHCH}_2\text{CH}=\text{CH}_2 \rightarrow \text{CH}_2=\text{CHCH}\bullet\text{CH}=\text{CH}_2$	1.67E4	2.68	-1585

Table S2

Classification of the studied reactions into 10 RCs and the selected prototype reaction of each RC

RCs	Prototype Reaction	Reactions
RC1- <i>cis</i>	R1	R7, R9, R19, R26, R30, R45
RC1- <i>trans</i>	R1	R7, R9, R19, R26, R30, R45
RC2	R2	R6, R10, R15, R16, R23, R27, R31, R37, R38, R44, R46
RC3	R3	R11, R17, R21, R32, R39, R43
RC4	R4	R18, R22, R29, R42
RC5	R5	R8, R14, R20, R24, R25, R36
RC6	R12	R33, R40
RC7	R13	R35, R41
RC8	R28	—
RC9	R34	—
RC10	R47	—

Table S3

List of the T1 diagnostics during CCSD(T) calculations.

Species	CCSD(T)	
	cc-pvdz	cc-pvtz
OH	0.006	0.007
H ₂ O	0.006	0.007
1-butene	0.009	0.010
2-butene	0.008	0.010

1-pentene	0.008	0.009
2-methyl-3-butene	0.008	0.009
1-hexene	0.008	0.009
1,4-pentadiene	0.010	0.010
RC1- <i>cis</i> -TS	0.023	0.024
RC1- <i>trans</i> -TS	0.023	0.024
RC2-TS	0.022	0.023
RC3-TS	0.017	0.018
RC4-TS	0.015	0.017
RC5-TS	0.019	0.021
RC6-TS	0.014	0.016
RC7-TS	0.014	0.016
RC8-TS	0.016	0.018
RC9-TS	0.013	0.015
RC10-TS	0.021	0.022

Table S4

Comparisons of the computed reaction barriers for abstraction reactions of ethylene and propene with OH (kcal/mol).

Reaction	ΔE	Theoretical level	Reference
$\text{CH}_2=\text{CH}_2 + \text{OH} \rightarrow \text{C}_2\text{H}_3 + \text{H}_2\text{O}$	5.49	CCSD(T)-MP2/CBS//M06-2X/6-311+g(d,p)	This work
	5.6	QCISD(T)/6-311+G(2df,2p)//QCISD/6-31G(d,p)	Liu <i>et al.</i> ^a
	5.4	G2//QCISD/6-31G(d,p)	Liu <i>et al.</i> ^a
$\text{CH}_2=\text{CHCH}_3 \rightarrow \bullet\text{HC}=\text{CHCH}_3$	4.56 (<i>cis</i>)	CCSD(T)-MP2/CBS//M06-2X/6-311+g(d,p)	This work
	5.04 (<i>trans</i>)	CCSD(T)-MP2/CBS//M06-2X/6-311+g(d,p)	This work
	4.2 (<i>cis</i>)	RQCISD(T)/cc-pV ∞ Z//B3LYP/6-311++G(d,p)	Zador <i>et al.</i> ^b
	4.7 (<i>trans</i>)	RQCISD(T)/cc-pV ∞ Z//B3LYP/6-311++G(d,p)	Zador <i>et al.</i> ^b
$\text{CH}_2=\text{CHCH}_3 \rightarrow \text{CH}_2=\text{C}\bullet\text{CH}_3$	3.31	CCSD(T)-MP2/CBS//M06-2X/6-311+g(d,p)	This work
	3.3	RQCISD(T)/cc-pV ∞ Z//B3LYP/6-311++G(d,p)	Zador <i>et al.</i> ^b
$\text{CH}_2=\text{CHCH}_3 \rightarrow \text{CH}_2=\text{CHCH}_2\bullet$	1.73	CCSD(T)-MP2/CBS//M06-2X/6-311+g(d,p)	This work
	2.9	RQCISD(T)/cc-pV ∞ Z//B3LYP/6-311++G(d,p)	Zador <i>et al.</i> ^b
	0.66	UCCSD(T)/CBS//[5,5]-CASPT2/cc-pVTZ	Szori <i>et al.</i> ^c
	1.10	[5,5]-CASPT2/CBS//[5,5]-CASPT2/cc-pVTZ	Szori <i>et al.</i> ^c
	1.14	UCCSD(T)/CBS(Extrapolation of cc-pVXZ Basis)	Szori <i>et al.</i> ^c
	1.6	CCSD(T)/cc-pVDZ//B3LYP/cc-pVTZ	Huyhn <i>et al.</i> ^d
	2.6	PMP2/aug-cc-PVQZ//MP2/cc-pVTZ	Zhou <i>et al.</i> ^e

^aLiu *et al.*, Theoretical study on mechanisms of the high-temperature reactions $\text{C}_2\text{H}_3+\text{H}_2\text{O}$ and $\text{C}_2\text{H}_4+\text{OH}$, Phys. Chem. Chem. Phys., 2002, 4, 1021–1027.

^bZador *et al.*, The reaction between propene and hydroxyl, Phys. Chem. Chem. Phys., 2009, 11, 11040-11053.

^cSzori *et al.*, High Accuracy ab Initio Calculations on Reactions of OH with 1-Alkenes. The Case of Propene, J. Chem. Theory Comput., 2009, 5, 2313-2321.

^dHuyhn *et al.*, Kinetics of Enol Formation from Reaction of OH with Propene, J. Phys. Chem. A, 2009, 113, 3177-3185.

^eZhou *et al.*, Kinetics and Mechanism for Formation of Enols in Reaction of Hydroxide Radical with Propene, J. Phys. Chem. A, 2009, 113, 2372-2382.

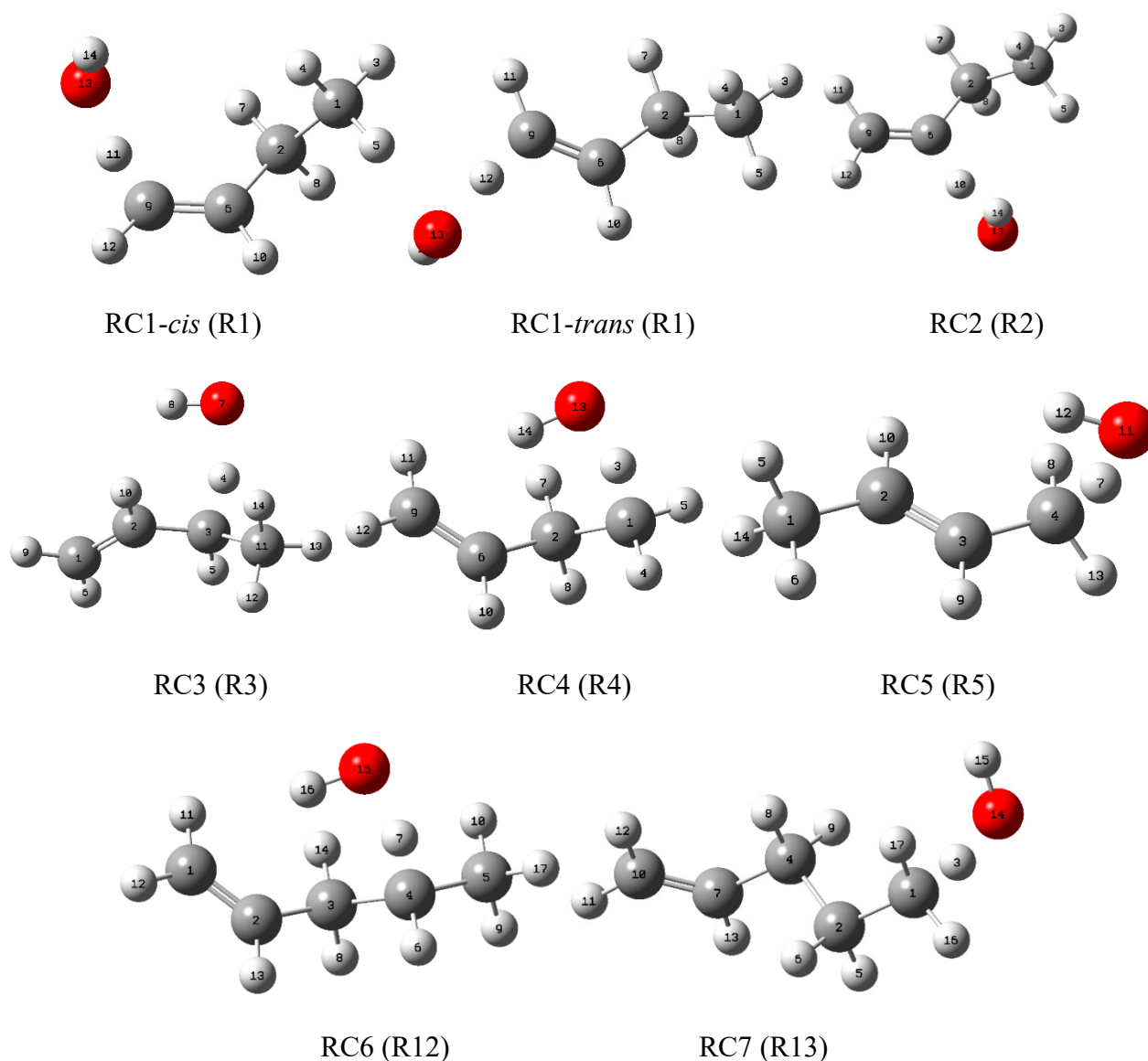


Figure S1 Optimized geometry of TS structure of prototype reactions

Additional remarks to Figure S1: Conservation of the Reaction Centers Reactions in the same reaction class should have the same reactive moiety and share similarities in the shape of the potential energy surfaces along the reaction path. Thus, the reaction centers from the optimized transition state structures for the reactions in the same class should be identical. Figure S1 displays the optimized TS structure of prototype reactions, and the labeling of atoms involved in the reaction centers are given. Table S3 to S10 lists key parameters including bond lengths and bond angles at the reaction centers in the optimized TS structures. The computed rate coefficients and energy information are also provided in these tables. It can be seen that the differences of the bond lengths and bond angles of the reaction centers at TSs are nearly identical. Thus, the reactive moiety and potential energy surfaces

along the reaction path are very well conserved among the reactions.

Table S5

Optimized geometric parameters of reaction centers at transition states, computed barriers and rate coefficients for RC1-*cis*.

RC1- <i>cis</i>	d_{C9-H11}	$d_{H11-O13}$	$\angle C9-H11-O13$	M06-2X barrier (kcal mol ⁻¹)	Corrected Barrier (kcal mol ⁻¹)	Rate coefficients		
						A	n	E_a
R1- <i>cis</i>	1.21	1.31	162	3.59	4.34	1.04E4	2.70	954
R7	1.21	1.31	162	3.45	4.19	9.01E3	2.69	851
R9- <i>cis</i>	1.20	1.31	163	3.58	4.33	7.46E3	2.69	956
R19- <i>cis</i>	1.21	1.31	162	3.92	4.71	1.46E4	2.66	1575
R26- <i>cis</i>	1.20	1.31	162	3.35	4.08	1.64E4	2.70	657
R30- <i>cis</i>	1.20	1.31	163	3.83	4.61	8.67E3	2.65	1537
R45- <i>cis</i>	1.21	1.31	163	3.83	4.61	1.35E5	2.33	1902
Averaged value	1.21	1.31	162	3.65	4.41			
SE of Mean				0.08	0.09			
Standard Deviation				0.21	0.23			

d and $\angle$ represent the bond length and the bond angle with units of Å and degree, respectively.

Table S6

Optimized geometric parameters of reaction centers at transition states, computed barriers and rate coefficients for RC1-*trans*.

RC1- <i>trans</i>	d_{C9-H12}	$d_{H12-O13}$	$\angle C9-H12-O13$	M06-2X barrier (kcal mol ⁻¹)	Corrected Barrier (kcal mol ⁻¹)	Rate coefficients		
						A	n	E_a
R1- <i>trans</i>	1.20	1.30	1.62	4.16	4.97	1.10E4	2.65	1558
R7	1.21	1.31	162	3.45	4.19	9.01E3	2.69	851
R9- <i>trans</i>	1.20	1.30	1.62	4.28	5.10	1.01E4	2.65	1812
R19- <i>trans</i>	1.20	1.31	1.62	3.47	4.21	1.10E4	2.66	1080
R26- <i>trans</i>	1.20	1.31	1.62	3.90	4.68	1.54E4	2.67	1169
R30- <i>trans</i>	1.20	1.30	1.62	4.23	5.04	1.78E4	2.63	1781
R45- <i>trans</i>	1.21	1.30	1.62	4.30	5.12	2.37E5	2.33	2170
Averaged value	1.20	1.30	1.62	3.97	4.76			
SE of Mean				0.14	0.15			
Standard Deviation				0.37	0.41			

d and $\angle$ represent the bond length and the bond angle with units of Å and degree, respectively.

Table S7

Optimized geometric parameters of reaction centers at transition states, computed barriers and rate coefficients for RC2.

RC2	d_{C6-H10}	$d_{H10-O13}$	$\angle C6-H10-O13$	M06-2X barrier (kcal mol ⁻¹)	Corrected Barrier (kcal mol ⁻¹)	Rate coefficients		
						A	n	E_a
R2	1.18	1.37	161	2.24	2.87	1.60E4	2.58	76
R6	1.18	1.37	161	2.22	2.85	2.10E4	2.55	136
R10	1.18	1.36	160	1.99	2.59	2.72E4	2.62	-287

R15	1.18	1.37	161	2.19	2.81	1.64E4	2.56	191
R16	1.18	1.38	161	1.82	2.41	2.12E4	2.55	-136
R23	1.18	1.38	162	1.39	1.94	5.08E4	2.53	-772
R27	1.18	1.37	161	1.74	2.32	2.41E4	2.56	-425
R31	1.18	1.37	161	2.17	2.79	1.75E4	2.59	91
R37	1.18	1.37	160	1.97	2.57	3.00E4	2.61	-153
R38	1.18	1.37	160	1.46	2.01	2.74E4	2.60	-662
R44	1.18	1.38	161	1.83	2.42	1.18E5	2.38	351
R46	1.19	1.33	162	1.74	2.32	9.20E4	2.27	-232
Averaged value	1.18	1.37	161	1.90	2.49			
SE of Mean				0.08	0.09			
Standard Deviation				0.29	0.31			

d and A represent the bond length and the bond angle with units of Å and degree, respectively.

Table S8

Optimized geometric parameters of reaction centers at transition states, computed barriers and rate coefficients for RC3.

RC3	d_{C3-H14}	d_{H4-O7}	$A_{C3-H4-O7}$	M06-2X barrier (kcal mol ⁻¹)	Corrected Barrier (kcal mol ⁻¹)	Rate coefficients		
						A	n	E_a
R3	1.15	1.51	164	0.03	0.45	4.14E4	2.55	-1742
R11	1.15	1.53	166	-0.39	-0.01	2.72E5	2.37	-1929
R17	1.15	1.52	163	-0.35	0.03	2.30E4	2.56	-2204
R21	1.16	1.50	157	-0.47	-0.10	2.19E4	2.47	-2397
R32	1.15	1.53	166	-0.21	0.19	2.82E5	2.33	-1532
R39	1.14	1.55	165	-0.73	-0.38	4.65E4	2.58	-2467
R43	1.15	1.52	163	-0.26	0.13	2.67E6	2.01	-970
Averaged value	1.15	1.52	163	-0.34	0.04			
SE of Mean				0.09	0.10			
Standard Deviation				0.24	0.25			

d and A represent the bond length and the bond angle with units of Å and degree, respectively.

Table S9

Optimized geometric parameters of reaction centers at transition states, computed barriers and rate coefficients for RC4.

RC4	d_{C1-H3}	d_{H3-O13}	d_{C6-H14}	$A_{C1-H3-O13}$	M06-2X barrier (kcal mol ⁻¹)	Corrected Barrier (kcal mol ⁻¹)	Rate coefficients		
							A	n	E_a
R4	1.18	1.38	2.64	163	0.72	1.20	2.51E5	2.28	-1209
R18	1.18	1.38	2.60	162	0.55	1.02	1.32E4	2.57	-1917
R22	1.19	1.38	2.55	163	0.55	1.02	7.00E3	2.62	-2058
R29	1.18	1.37	2.63	163	0.60	1.07	2.41E4	2.55	-1565
R42	1.18	1.38	2.61	162	0.52	0.99	6.59E4	2.43	-1730
Averaged value	1.18	1.38	2.61	163	0.59	1.06			
SE of Mean					0.04	0.04			
Standard Deviation					0.08	0.08			

d and A represent the bond length and the bond angle with units of Å and degree, respectively.

Table S10

Optimized geometric parameters of reaction centers at transition states, computed barriers and rate coefficients for RC5.

RC5	d_{C4-H7}	d_{H7-O11}	$A_{C4-H7-O11}$	M06-2X barrier (kcal mol ⁻¹)	Corrected Barrier (kcal mol ⁻¹)	Rate coefficients		
						A	n	E_a
R5	1.16	1.48	161	0.95	1.46	5.23E4	2.44	-944
R8	1.16	1.46	161	0.52	0.99	3.33E4	2.50	-1819
R14	1.16	1.48	161	0.87	1.37	5.31E3	2.76	-1305
R20	1.16	1.46	161	0.82	1.31	2.12E3	2.79	-1295
R24	1.16	1.48	160	0.09	0.52	8.39E3	2.75	-2075
R25- <i>cis</i>	1.16	1.48	160	0.03	0.45	5.30E3	2.90	-2122
R25- <i>trans</i>	1.16	1.48	160	0.08	0.50	8.03E3	2.74	-2211
R36	1.16	1.48	161	0.77	1.26	6.25E3	2.76	-1448
Averaged value	1.16	1.48	161	0.52	0.98			
SE of Mean				0.14	0.15			
Standard Deviation				0.39	0.43			

d and A represent the bond length and the bond angle with units of Å and degree, respectively.

Table S11

Optimized geometric parameters of reaction centers at transition states, computed barriers and rate coefficients for RC6.

RC6	d_{C4-H7}	d_{H7-O15}	d_{C2-H16}	$A_{C4-H7-O15}$	M06-2X barrier (kcal mol ⁻¹)	Corrected Barrier (kcal mol ⁻¹)	Rate coefficients		
							A	n	E_a
R12	1.16	1.44	2.65	164	-1.22	-0.92	5.21E3	2.70	-3523
R33	1.16	1.45	2.68	164	-1.11	-0.80	1.60E4	2.43	-2847
R40	1.16	1.44	2.62	163	-1.44	-1.16	5.41E3	2.72	-3748
Averaged value	1.16	1.44	2.65	164	-1.26	-0.96			
SE of Mean					0.10	0.11			
Standard Deviation					0.17	0.18			

d and A represent the bond length and the bond angle with units of Å and degree, respectively.

Table S12

Optimized geometric parameters of reaction centers at transition states, computed barriers and rate coefficients for RC7.

RC7	d_{C1-H3}	d_{H3-O14}	$A_{C1-H3-O14}$	M06-2X barrier (kcal mol ⁻¹)	Corrected Barrier (kcal mol ⁻¹)	Rate coefficients		
						A	n	E_a
R13	1.17	1.42	169	1.68	2.25	1.41E4	2.62	-915
R35	1.17	1.42	169	1.99	2.59	7.44E3	2.57	-377
R41	1.17	1.42	169	1.66	2.23	1.34E4	2.62	-944
Averaged value	1.17	1.42	169	1.78	2.36			
SE of Mean				0.11	0.12			
Standard Deviation				0.19	0.20			

d and A represent the bond length and the bond angle with units of Å and degree, respectively.

Table S13Theoretical predicted potential energies in kcal mol⁻¹ at CCSD(T)-MP2/CBS level.

Reaction Class	Reaction	RC	TS (ΔE)	PC	Products ($\Delta_f H_{0K}^0$)
RC1-cis	CH ₂ =CHCH ₂ CH ₃ → •HC=CHCH ₂ CH ₃	-1.05	4.53	-9.01	-7.58
RC1-trans	CH ₂ =CHCH ₂ CH ₃ → •HC=CHCH ₂ CH ₃	-1.32	4.98	-7.74	-7.10
RC2	CH ₂ =CHCH ₂ CH ₃ → CH ₂ =C•CH ₂ CH ₃	-1.12	2.96	-11.51	-10.99
RC3	CH ₂ =CHCH ₂ CH ₃ → CH ₂ =CHCH•CH ₃	-2.20	0.27	-36.02	-34.08
RC4	CH ₂ =CHCH ₂ CH ₃ → CH ₂ =CHCH ₂ CH ₂ •	-1.78	1.43	-19.27	-17.57
RC5	CH ₃ CH=CHCH ₃ → CH ₃ CH=CHCH ₂ •	-1.37	1.40	-32.71	-31.33
RC6	CH ₂ =CHCH ₂ CH ₂ CH ₃ → CH=CHCH ₂ CH•CH ₃	-2.06	-0.71	-21.96	-20.52
RC7	CH ₂ =CHCH ₂ CH ₂ CH ₃ → CH=CHCH ₂ CH ₂ CH ₂ •	-0.26	1.98	-19.42	-17.98
RC8	H ₂ C=CHCH(CH ₃) ₂ → H ₂ C=CHC•(CH ₃) ₂	-1.91	-0.59	-37.81	-35.59
RC9	CH ₂ =CHCH ₂ CH ₂ CH ₂ CH ₃ → CH ₂ =CHCH ₂ CH ₂ CH•CH ₃	0.05	0.68	-21.92	-20.45
RC10	CH ₂ =CHCH ₂ CH=CH ₂ → CH ₂ =CHCH•CH=CH ₂	-1.47	0.19	-43.45	-42.10

Table S14Fitted Arrhenius rate coefficients (A : cm³ mol⁻¹ s⁻¹, E_a : cal mol⁻¹) for the prototype reactions at CCSD(T)-MP2/CBS//M06-2X/6-311+G(d,p) level.

Reaction Class	Reaction	A	n	E_a
RC1-cis	CH ₂ =CHCH ₂ CH ₃ → •HC=CHCH ₂ CH ₃	1.04×10 ⁴	2.70	1071
RC1-trans	CH ₂ =CHCH ₂ CH ₃ → •HC=CHCH ₂ CH ₃	1.10×10 ⁴	2.65	1508
RC2	CH ₂ =CHCH ₂ CH ₃ → CH ₂ =C•CH ₂ CH ₃	1.61×10 ⁴	2.58	105
RC3	CH ₂ =CHCH ₂ CH ₃ → CH ₂ =CHCH•CH ₃	4.14×10 ⁴	2.55	-1965
RC4	CH ₂ =CHCH ₂ CH ₃ → CH ₂ =CHCH ₂ CH ₂ •	7.65×10 ⁴	2.41	-1171
RC5	CH ₃ CH=CHCH ₃ → CH ₃ CH=CHCH ₂ •	1.39×10 ⁵	2.34	-746
RC6	CH ₂ =CHCH ₂ CH ₂ CH ₃ → CH=CHCH ₂ CH•CH ₃	5.21×10 ³	2.70	-3368
RC7	CH ₂ =CHCH ₂ CH ₂ CH ₃ → CH=CHCH ₂ CH ₂ CH ₂ •	1.41×10 ⁴	2.62	-1250
RC8	H ₂ C=CHCH(CH ₃) ₂ → H ₂ C=CHC•(CH ₃) ₂	7.28×10 ⁴	2.41	-2610
RC9	CH ₂ =CHCH ₂ CH ₂ CH ₂ CH ₃ → CH ₂ =CHCH ₂ CH ₂ CH•CH ₃	8.94×10 ⁴	2.45	-1582
RC10	CH ₂ =CHCH ₂ CH=CH ₂ → CH ₂ =CHCH•CH=CH ₂	1.67×10 ⁴	2.68	-1836

Table S15Comparisons of computed overall rate constants with experimental results (cm³ mol⁻¹ s⁻¹).

T(K)	1-butene, this work	T(K)	1-butene ^a	T(K)	1-butene ^b	T(K)	1-butene ^c
500	3.54E+12	946	1.04E+13	650	3.97E+12	880	1.02E+13
600	4.33E+12	954	1.06E+13	691	4.55E+12	894	1.05E+13
700	5.37E+12	980	1.09E+13	732	4.95E+12	951	1.13E+13
800	6.65E+12	1008	1.14E+13	778	5.37E+12	1000	1.24E+13
900	8.18E+12	1057	1.22E+13	833	5.82E+12	980	1.21E+13

1000	9.96E+12	1162	1.6E+13	1057	1.32E+13
1100	1.2E+13	1222	1.53E+13	1095	1.4E+13
1200	1.43E+13	1256	1.72E+13	1097	1.4E+13
1300	1.7E+13			1223	1.8E+13
1400	1.99E+13			1250	1.88E+13
1500	2.31E+13			1329	2.3E+13
1600	2.67E+13			1337	2.41E+13
1700	3.06E+13			1341	2.36E+13
1800	3.49E+13				
1900	3.95E+13				
2000	4.45E+13				
2100	4.99E+13				
2200	5.57E+13				
2300	6.19E+13				
2400	6.86E+13				
2500	7.56E+13				

^a F. Khaled, J. Badra, A. Farooq, A shock tube study of C4-C6 straight chain alkenes + OH reactions, Proc. Combust. Inst. 36 (2017) 289-298.

^b F.P. Tully, Hydrogen-atom abstraction from alkenes by OH, ethene and 1-butene, Chem. Phys. Lett. 143 (1988) 510-514.

^c S.S. Vasu, L.K. Huynh, D.F. Davidson, R.K. Hanson, D.M. Golden, Reactions of OH with butene isomers: measurements of the overall rates and a theoretical study, J. Phys. Chem. A 115 (2011) 2549-2556.

Table S16

Comparisons of computed overall rate constants with experimental results ($\text{cm}^3 \text{mol}^{-1} \text{s}^{-1}$).

T(K)	1-hexene, this work	2-hexene, this work	1-pentene, this work	T(K)	1-hexene^a	T(K)	2-hexene^a	T(K)	1-pentene^a
500	5.69E+12	1.24E+13	5.34E+12	836	1.11E+13	881	1.72E+13	875	1.1E+13
600	6.7E+12	1.29E+13	5.7E+12	920	1.3E+13	958	1.95E+13	910	1.2E+13
700	8.06E+12	1.44E+13	6.57E+12	945	1.34E+13	1068	2.3E+13	944	1.25E+13
800	9.75E+12	1.66E+13	7.81E+12	1000	1.4E+13	1133	2.5E+13	1004	1.35E+13

900	1.17E+13	1.93E+13	9.38E+12	1058	1.56E+13	1183	2.7E+13	1107	1.6E+13
1000	1.41E+13	2.26E+13	1.13E+13	1087	1.68E+13	1200	2.75E+13	1160	1.7E+13
1100	1.67E+13	2.64E+13	1.35E+13	1117	1.83E+13	1214	2.82E+13	1128	1.7E+13
1200	1.97E+13	3.08E+13	1.61E+13	1270	2.5E+13	1293	3.1E+13	1140	1.75E+13
1300	2.31E+13	3.57E+13	1.9E+13	1387	3.35E+13	1304	3.15E+13	1180	1.92E+13
1400	2.68E+13	4.11E+13	2.23E+13			1377	3.5E+13	1247	2.04E+13
1500	3.09E+13	4.71E+13	2.59E+13					1337	2.6E+13
1600	3.53E+13	5.36E+13	3E+13					1379	2.9E+13
1700	4.02E+13	6.08E+13	3.44E+13						
1800	4.55E+13	6.86E+13	3.93E+13						
1900	5.12E+13	7.7E+13	4.46E+13						
2000	5.74E+13	8.61E+13	5.04E+13						
2100	6.4E+13	9.58E+13	5.67E+13						
2200	7.11E+13	1.06E+14	6.34E+13						
2300	7.86E+13	1.17E+14	7.06E+13						
2400	8.67E+13	1.29E+14	7.84E+13						
2500	9.52E+13	1.42E+14	8.66E+13						

^a Experimental results from F. Khaled, J. Badra, A. Farooq, A shock tube study of C4-C6 straight chain alkenes + OH reactions, Proc. Combust. Inst. 36 (2017) 289-298.

Table S17

Calculated single-point energies and zero-point energies (ZPE) in hartree for the studied reaction systems.

Species	E(UM062X/6-311+G(d,p))	ZPE
OH	-75.72657462	0.008577
H2O	-76.42088886	0.021623
React1	-157.1747494	0.108773
React2	-157.1789881	0.108241
React3	-157.180765	0.108608
React4	-196.4783619	0.137668
React5	-196.4820913	0.137081
React6	-196.4839572	0.137149

React7	-196.4853743	0.136898
React8	-196.4802844	0.13713
React9	-235.7817448	0.165844
React10	-235.7856962	0.165913
React11	-235.7851736	0.165821
React12	-195.248625	0.113824
R1-cis-prod	-156.4908635	0.094925
R1-trans-prod	-156.4904558	0.095245
R2-prod	-156.4964971	0.094799
R3-prod	-156.5312636	0.094626
R4-prod	-156.5043393	0.093932
R5-prod	-156.5312636	0.094624
R6-prod	-156.5001361	0.094702
R7-prod	-156.4956739	0.094494
R8-prod	-156.5292475	0.094167
R9-cis-prod	-195.7944445	0.123301
R9-trans-prod	-195.7940756	0.123993
R10-prod	-195.8001845	0.12384
R11-prod	-195.8343491	0.123348
R12-prod	-195.8127452	0.122319
R13-prod	-195.8081817	0.122382
R14-prod	-195.8343491	0.123348
R15-prod	-195.8034566	0.123773
R16-prod	-195.8030861	0.12335
R17-prod	-195.8387806	0.123414
R18-prod	-195.8118086	0.121976
R19-cis-prod	-195.8000031	0.123642
R19-trans-prod	-195.799347	0.122925
R20-prod	-195.8317518	0.123598
R21-prod	-195.8367075	0.122713
R22-prod	-195.8134742	0.122255
R23-prod	-195.8072641	0.123455
R24-prod	-195.8397595	0.123223
R25-cis-prod	-195.8367075	0.122713
R25-trans-prod	-195.8367586	0.12297
R26-cis-prod	-195.7965741	0.123255
R26-trans-prod	-195.796184	0.123375
R27-prod	-195.8018374	0.123224
R28-prod	-195.8397595	0.123223
R29-prod	-195.8097519	0.122054
R30-cis-prod	-235.0979469	0.15239
R30-trans-prod	-235.0974611	0.152178
R31-prod	-235.1036272	0.152273

R32-prod	-235.1377692	0.152835
R33-prod	-235.1159294	0.151317
R34-prod	-235.116533	0.150975
R35-prod	-235.1117189	0.150802
R36-prod	-235.1380037	0.152228
R37-prod	-235.1070252	0.151935
R38-prod	-235.1067638	0.152128
R39-prod	-235.1418761	0.151782
R40-prod	-235.1201731	0.150802
R41-prod	-235.1155668	0.150814
R42-prod	-235.1148737	0.150787
R43-prod	-235.1418761	0.151783
R44-prod	-235.1063925	0.15256
R45-cis-prod	-194.5646391	0.100053
R45-trans-prod	-194.564219	0.100375
R46-prod	-194.5690103	0.100053
R47-prod	-194.6195102	0.100314
R1-cis-TS	-232.8928435	0.114506
R1-trans-TS	-232.892011	0.114588
R2-TS	-232.8956683	0.115203
R3-TS	-232.900016	0.116044
R4-TS	-232.8985995	0.115732
R5-TS	-232.9028875	0.115624
R6-TS	-232.9000027	0.114738
R7-TS	-232.8989887	0.114243
R8-TS	-232.9046999	0.115316
R9-cis-TS	-272.1965187	0.143452
R9-trans-TS	-272.19562	0.143678
R10-TS	-272.1993037	0.1437
R11-TS	-272.2041943	0.144832
R12-TS	-272.2050689	0.144377
R13-TS	-272.1999908	0.143912
R14-TS	-272.2059772	0.144322
R15-TS	-272.2031665	0.143593
R16-TS	-272.2038356	0.143673
R17-TS	-272.207943	0.144333
R18-TS	-272.2063438	0.144166
R19-cis-TS	-272.2017279	0.143087
R19-trans-TS	-272.2023742	0.143025
R20-TS	-272.2080453	0.144511
R21-TS	-272.2102109	0.144616
R22-TS	-272.2081633	0.144191
R23-TS	-272.2072585	0.142917

R24-TS	-272.2102344	0.143852
R25-cis-TS	-272.2101275	0.143653
R25-trans-TS	-272.2102344	0.143835
R26-cis-TS	-272.1984973	0.142587
R26-trans-TS	-272.1976117	0.142573
R27-TS	-272.2017963	0.143354
R28-TS	-272.2072913	0.144494
R29-TS	-272.2040864	0.143842
R30-cis-TS	-311.4999488	0.172084
R30-trans-TS	-311.4990494	0.171807
R31-TS	-311.5027856	0.172275
R32-TS	-311.507597	0.173333
R33-TS	-311.5090093	0.173304
R34-TS	-311.506101	0.172994
R35-TS	-311.5035813	0.172806
R36-TS	-311.509613	0.173009
R37-TS	-311.5068329	0.172126
R38-TS	-311.5076696	0.172141
R39-TS	-311.5121256	0.173133
R40-TS	-311.5127183	0.172593
R41-TS	-311.5063414	0.172303
R42-TS	-311.5059916	0.172462
R43-TS	-311.5110196	0.173217
R44-TS	-311.5069453	0.172455
R45-cis-TS	-270.9665658	0.119806
R45-trans-TS	-270.9654879	0.119461
R46-TS	-270.9701806	0.120092
R47-TS	-270.9741293	0.121192
C2H4	-78.56360706	0.051316
TS-C2H4	-154.2803275	0.057202
C3H6	-117.8717307	0.079989
TS-C3H6-RC1-cis	-193.5897354	0.085659
TS-C3H6-RC1-trans	-193.5887223	0.085589
TS-C3H6-RC2	-193.5917086	0.086159
TS-C3H6-RC5	-193.5948234	0.087137

Table S18

Calculated single-point energies in hartree for selected reaction systems.

Species	CCSD(T)/cc-pvdz	CCSD(T)/cc-pvtz	MP2/cc-pvdz	MP2/cc-pvtz	MP2/cc-pvqz	CCSD(T)/cc-pvqz
OH	-75.559305643	-75.637722322	-75.542840711555	-75.618886250836	-75.643530916793	-75.661627517
H2O	-76.240987437	-76.332156682	-76.228376530062	-76.318593069633	-76.347601616945	-76.359766067

C2H4	-78.354406774	-78.438663344	-78.314541209632	-78.399221021288	-78.425201638543	
TS-C2H4	-153.89880519	-154.06409455	-153.83596285509	-153.99845799984	-154.04940409695	
C3H6	-117.55644854	-117.6823487	-117.49947835275	-117.62578290783	-117.66482084849	
TS-C3H6-RC1-cis	-193.10334628	-193.30953293	-193.02363710599	-193.22711543254	-193.29086647547	
TS-C3H6-RC1-trans	-193.10131127	-193.30825211	-193.02179798771	-193.2259612903	-193.28995796668	
TS-C3H6-RC2	-193.10501752	-193.31168414	-193.02633900651	-193.23018147423	-193.29408411561	
TS-C3H6	-193.10828489	-193.31512207	-193.03043029753	-193.23445693297	-193.29838363529	
React1	-156.754405	-156.92169085	-156.6799613855	-156.84767046814	-156.89964732668	-156.9679079
React2	-156.75817436	-156.92546812	-156.68401674594	-156.85173711848	-156.90377090088	
React3	-156.75959016	-156.92722006	-156.68571536365	-156.85384283473	-156.90598139371	
React4	-195.95286387	-196.16158008	-195.86076498682	-196.0699017581	-196.13489122578	
React6	-195.95719403	-196.16643644	-195.86580864165	-196.07556982444	-196.14069163016	
React8	-195.95492241	-196.16352003	-195.86342891908	-196.0725599101	-196.13752487872	
React9	-235.15121027	-235.40133034	-235.04139799826	-235.29194935638	-235.36994261597	
React12	-194.72840448	-194.92927915	-194.64257500356	-194.84356849027	-194.9069371323	
R1-cis-prod	-156.07354212	-156.2345848	-155.99231539331	-156.15270862336	-156.20276029325	-156.27954803
R1-trans-prod	-156.07326093	-156.23419362	-155.99190072867	-156.1521901796	-156.20221199413	-156.27913407
R2-prod	-156.0784711	-156.23975211	-155.99766602456	-156.15840096359	-156.20856713414	-156.28482868
R3-prod	-156.11391431	-156.27586664	-156.03287521222	-156.19403474453	-156.24443607906	-156.32119853
R4-prod	-156.08714132	-156.24902354	-156.01350939216	-156.1751634022	-156.22564074991	-156.29413738
R5-prod	-156.11392008	-156.27586769	-156.03287915037	-156.19403405471	-156.24443477381	
R8-prod	-156.1122394	-156.27461279	-156.03144213312	-156.19311862229	-156.24354051056	
R12-prod	-195.28967798	-195.49297589	-195.19754941825	-195.40064979324	-195.4642303335	
R13-prod	-195.28567994	-195.48911969	-195.19473493959	-195.39788452264	-195.46136432928	
R21-prod	-195.31301195	-195.51712331	-195.21439151954	-195.41783984933	-195.48136358389	
R28-prod	-195.31590788	-195.5199986	-195.21761637252	-195.42100050573	-195.48458204341	
R34-prod	-234.48819798	-234.73306631	-234.37910160859	-234.62368149741	-234.70024622377	
R47-prod	-194.10156324	-194.2970814	-194.00121683501	-194.19521919507	-194.25676370491	
R1-cis-TS	-232.30150839	-232.54907238	-232.20438987819	-232.44926240044	-232.52589551838	-232.61957967
R1-trans-TS	-232.29954329	-232.54792615	-232.20261187774	-232.44822196253	-232.52512963427	-232.61875138
R2-TS	-232.30482422	-232.55237629	-232.20855282129	-232.45333094693	-232.52986539775	-232.62280589
R3-TS	-232.30894392	-232.55701712	-232.21448019258	-232.45981940625	-232.53663563845	-232.62772329
R4-TS	-232.3059674	-232.55474626	-232.21331210511	-232.4592028878	-232.53605099674	-232.62550215
R5-TS	-232.31077036	-232.55898006	-232.21617808914	-232.46148227503	-232.53838365843	
R8-TS	-232.31325895	-232.56120463	-232.21900807621	-232.46426317798	-232.54099587441	
R12-TS	-271.50797628	-271.79793493	-271.39758147532	-271.68462490094	-271.77440470698	
R13-TS	-271.50455683	-271.79359192	-271.39382665185	-271.68005697055	-271.76963063341	
R21-TS	-271.51356951	-271.80285377	-271.40269456789	-271.6892983027	-271.77891147956	
R28-TS	-271.51089481	-271.80037969	-271.40020353281	-271.6870237498	-271.77678165169	
R34-TS	-310.70611669	-311.03639975	-310.57768009138	-310.90516973259	-311.00768790088	
R47-TS	-270.28313837	-270.56465065	-270.17428813775	-270.45291662222	-270.54120357874	

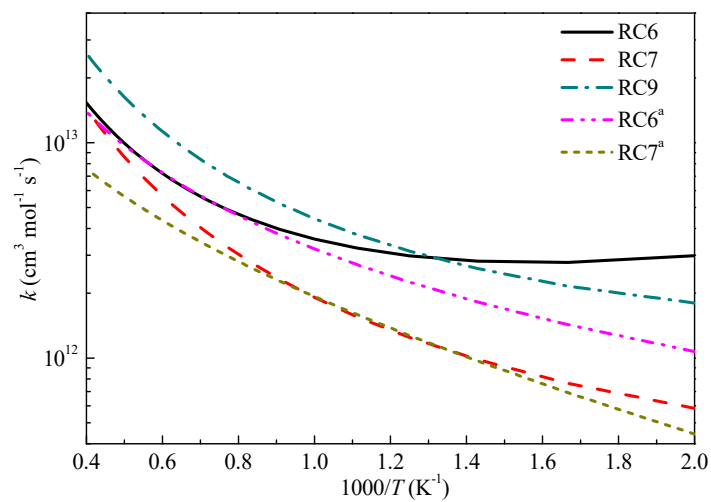


Figure S2 Comparisons of computed rate constants for prototype reactions of RC6, RC7 and RC9 with literature data (^aZhang *et al.*, Combust. Flame, 2016, 172, 116-135).

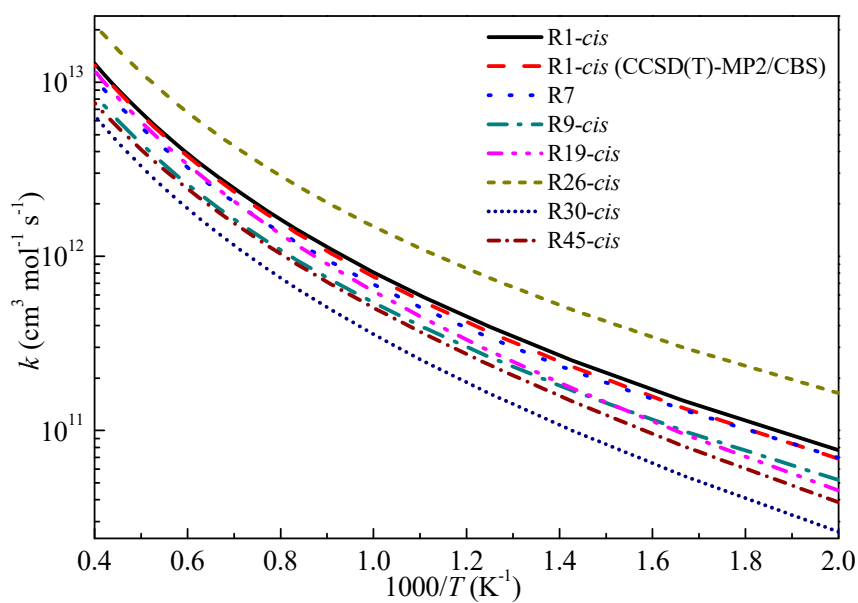


Figure S3 Predicted rate constants for RC1-*cis* in this work.

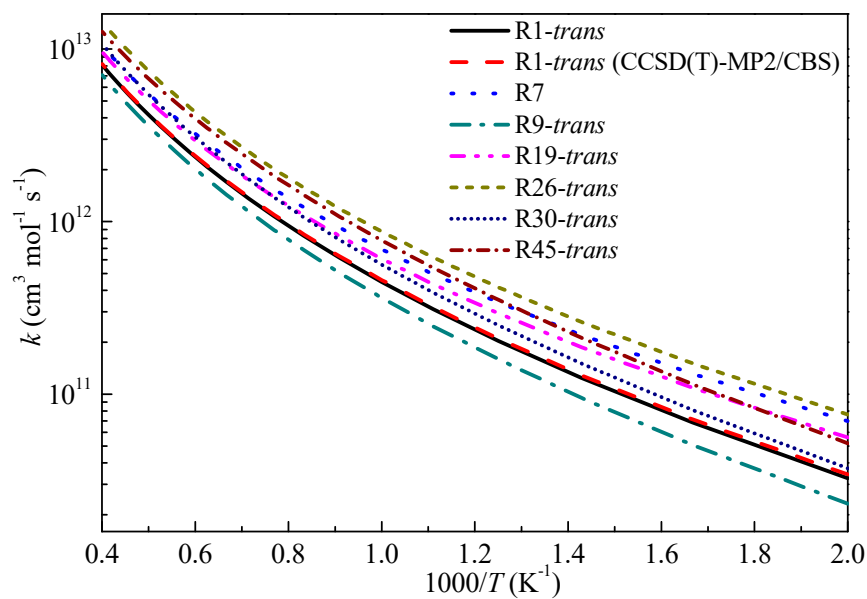


Figure S4 Predicted rate constants for RC1-*trans* in this work.

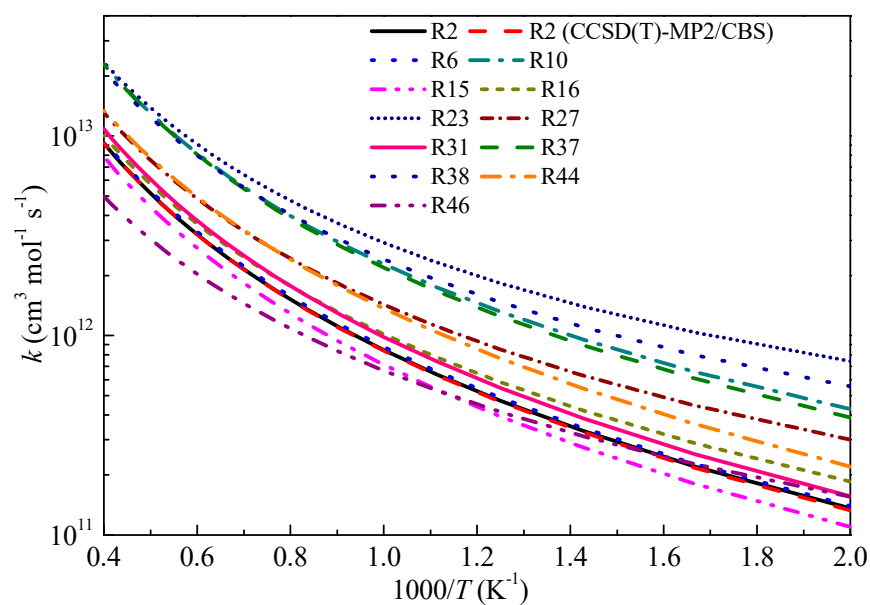


Figure S5 Predicted rate constants for RC2 in this work.

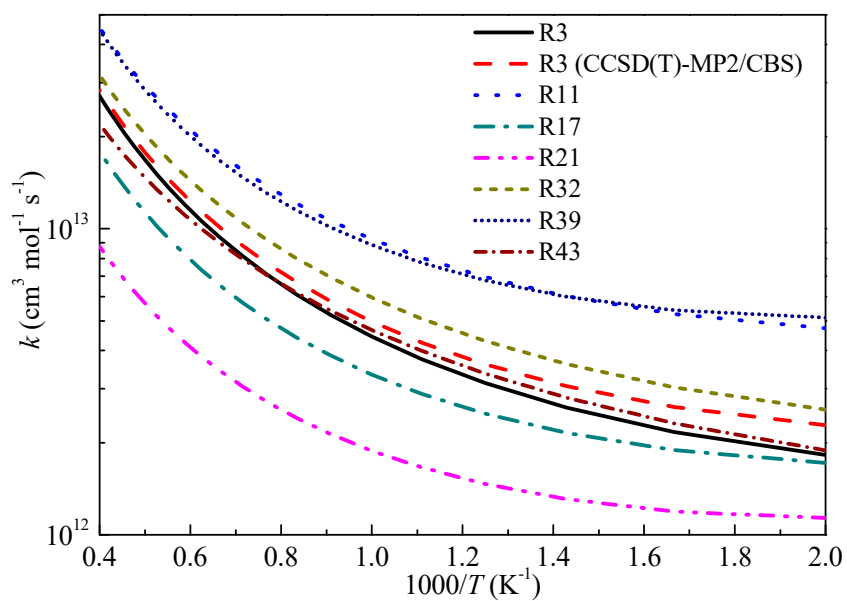


Figure S6 Predicted rate constants for RC3 in this work.

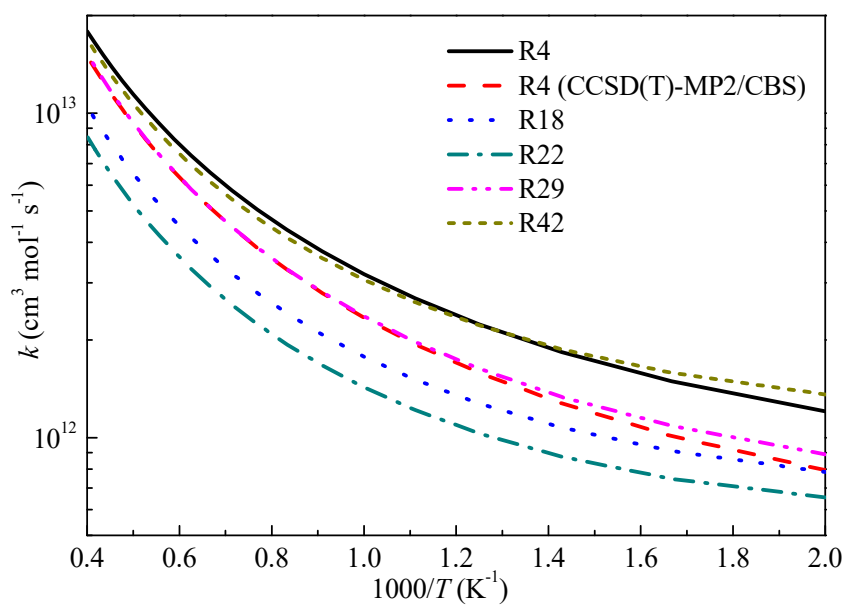


Figure S7 Predicted rate constants for RC4 in this work.

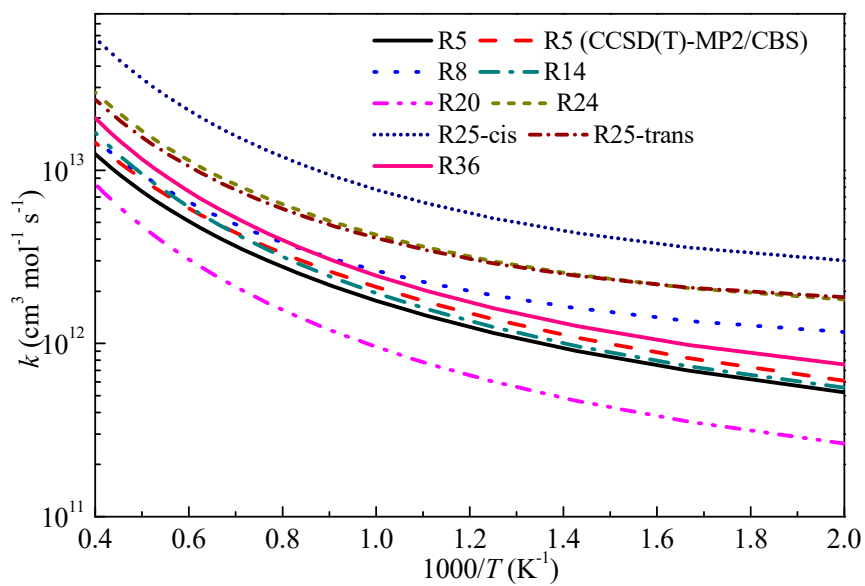


Figure S8 Predicted rate constants for RC5 in this work.

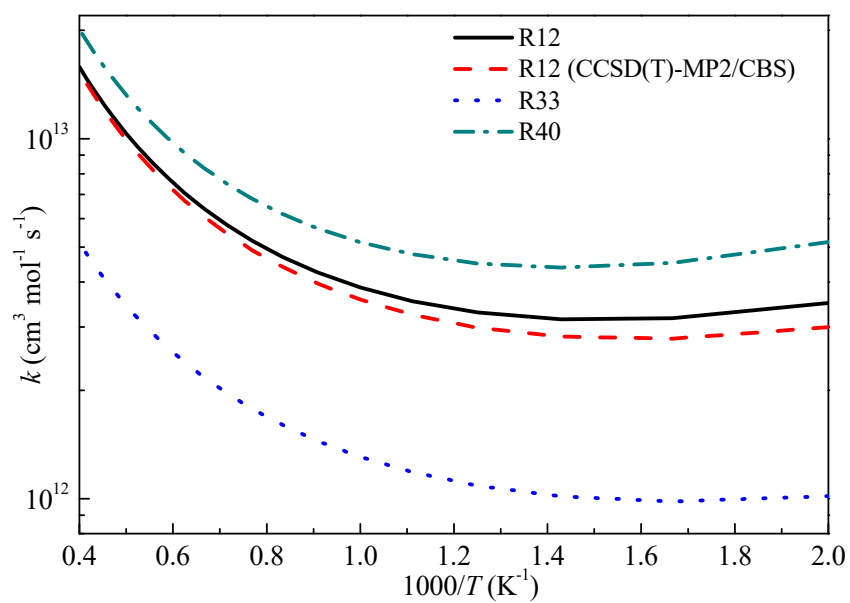


Figure S9 Predicted rate constants for RC6 in this work.

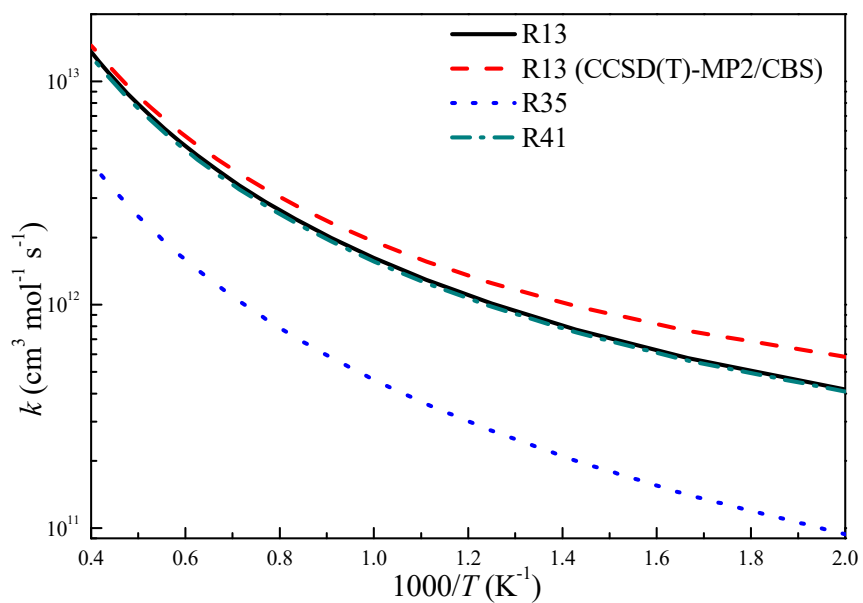
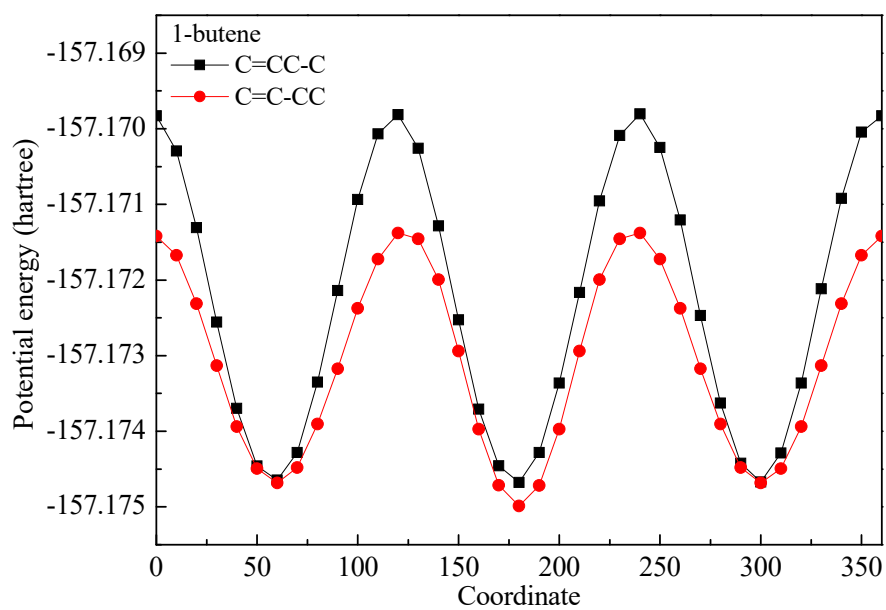
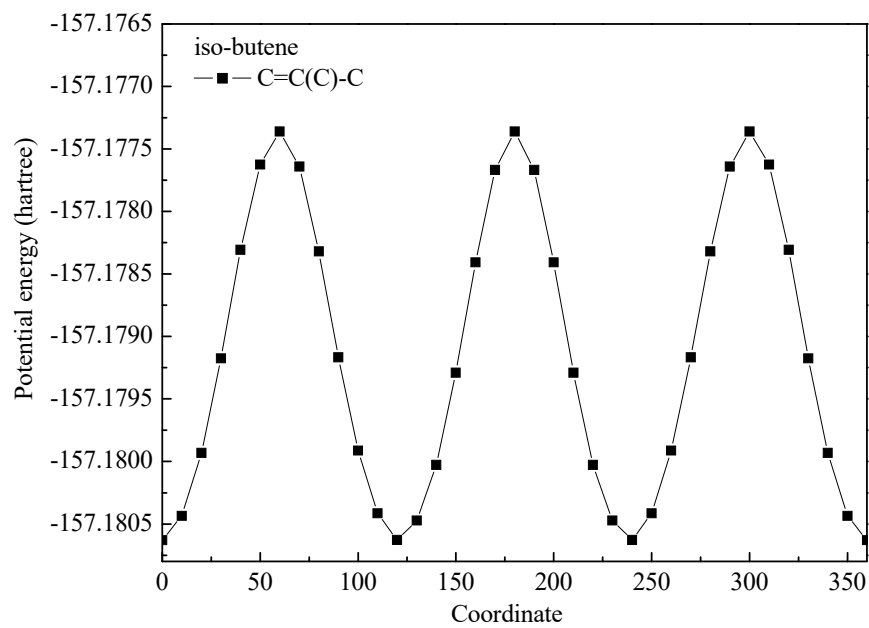
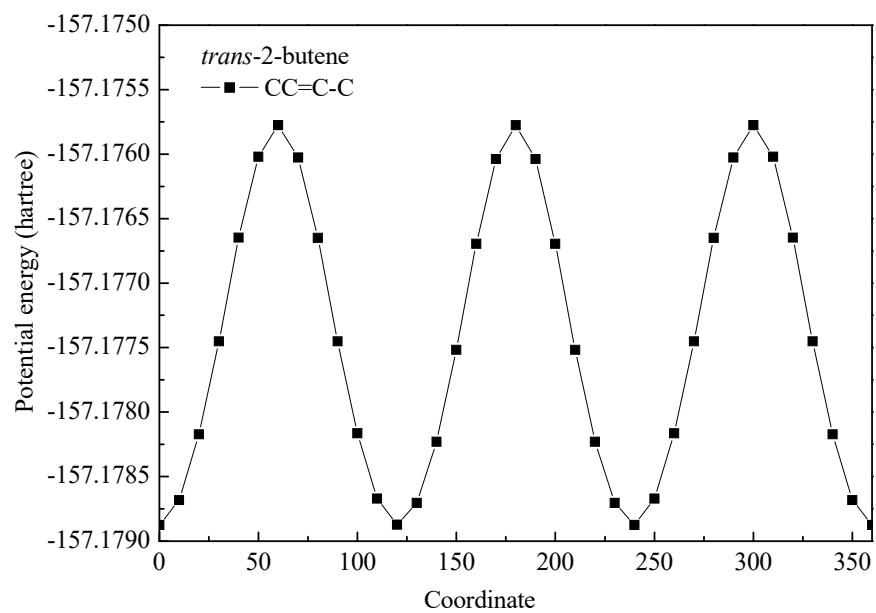
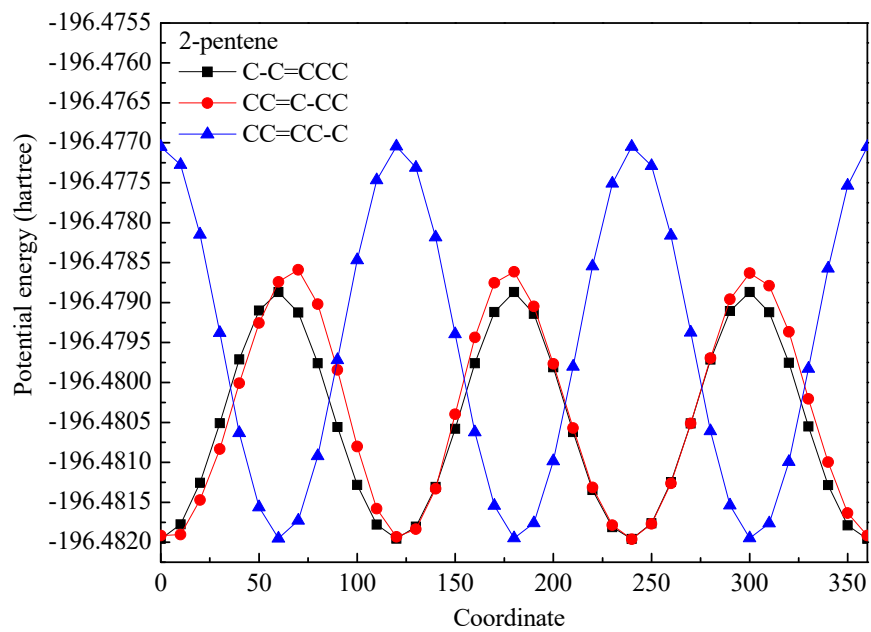
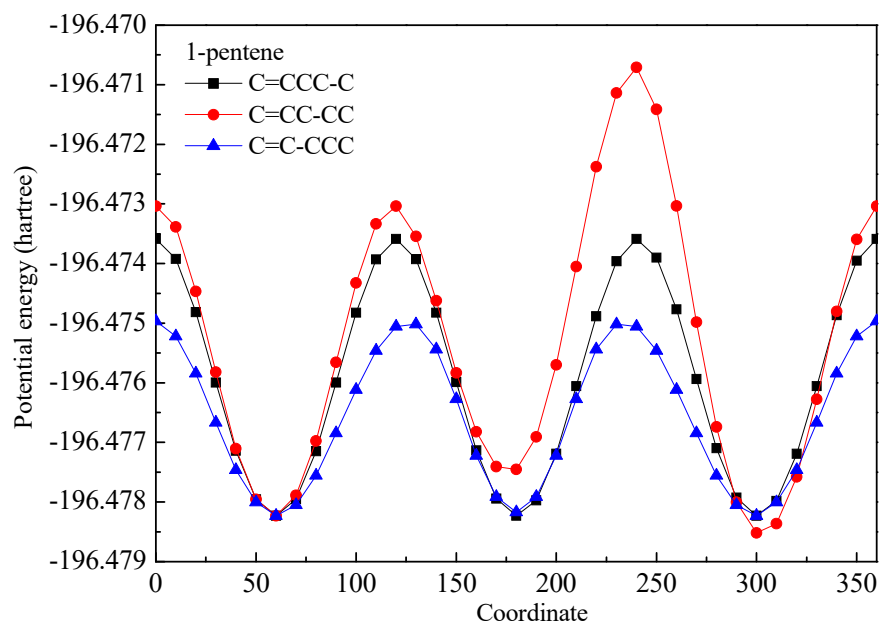
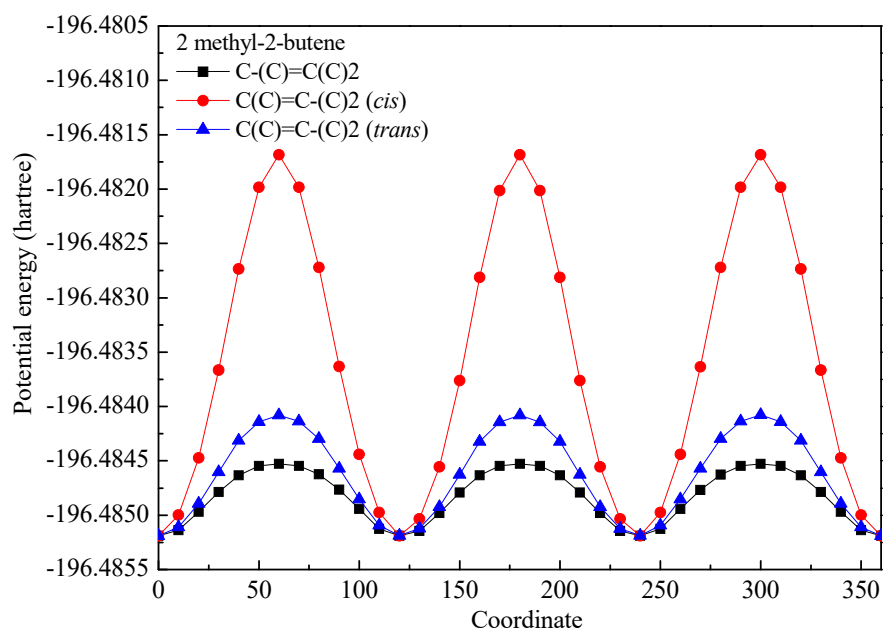
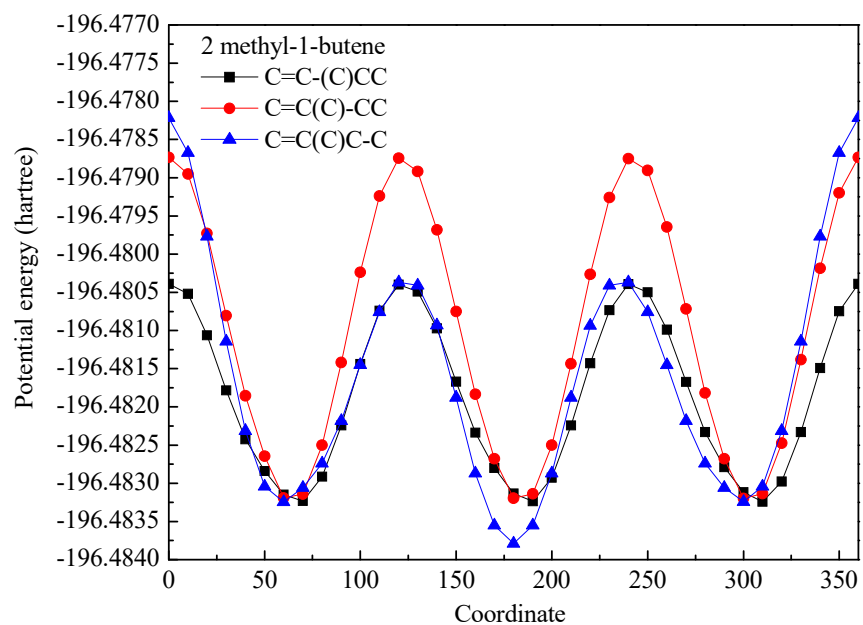


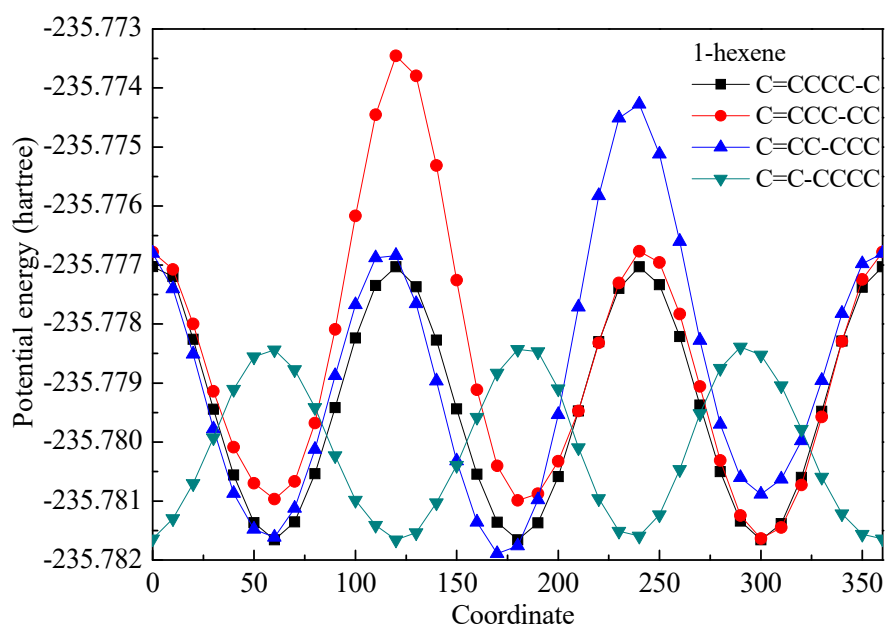
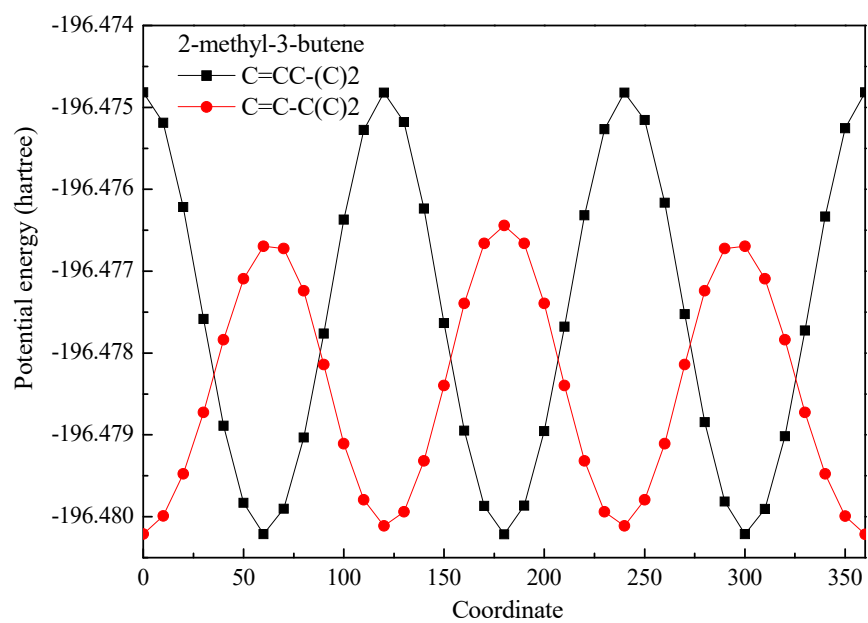
Figure S10 Predicted rate constants for RC7 in this work.

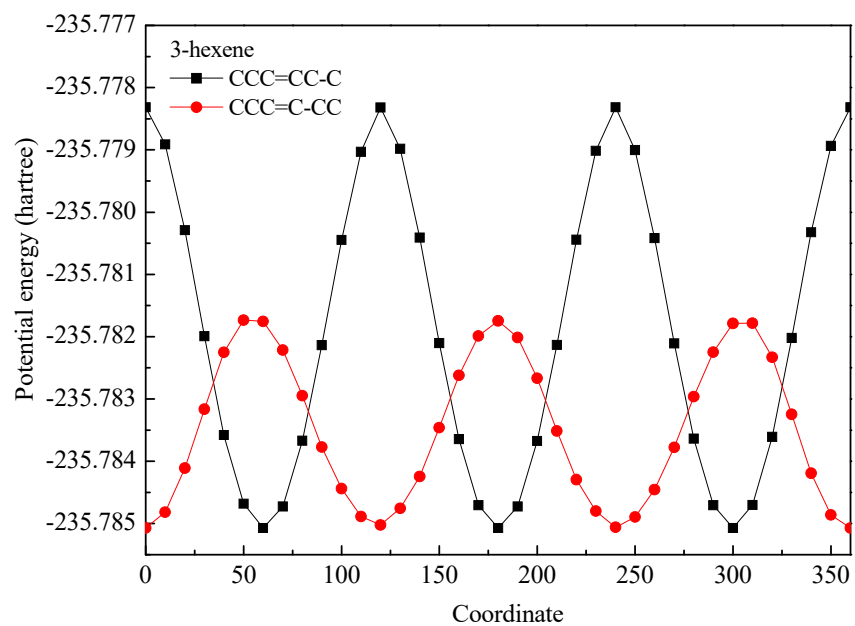
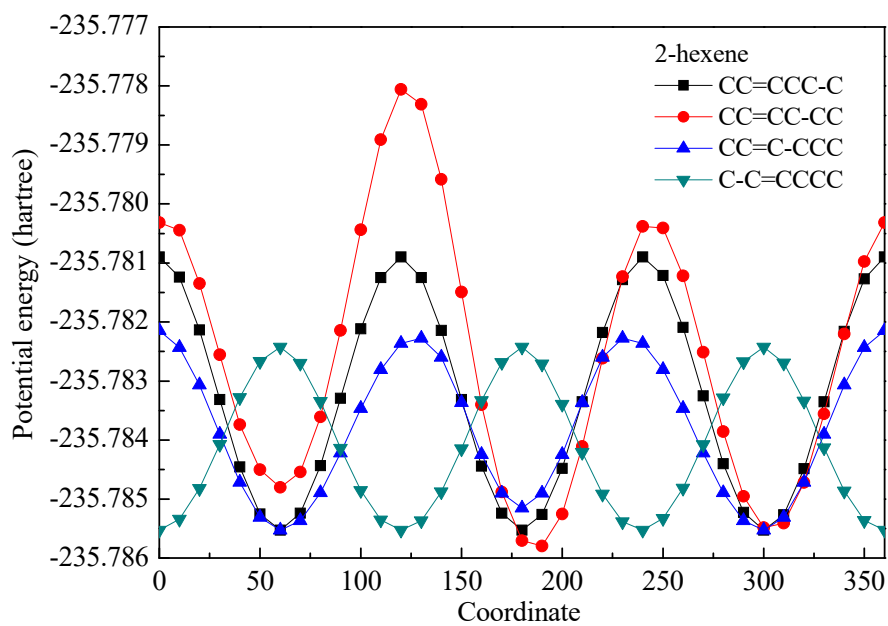












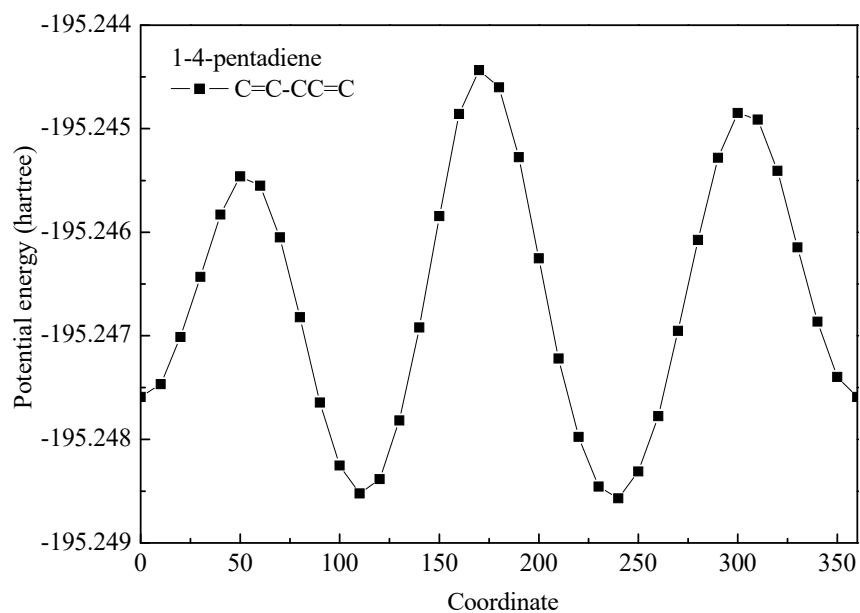
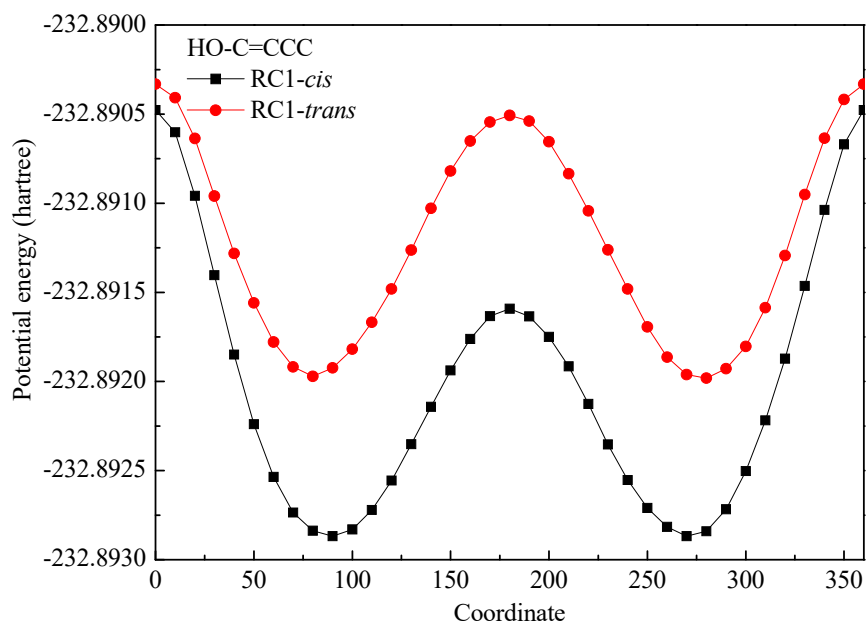
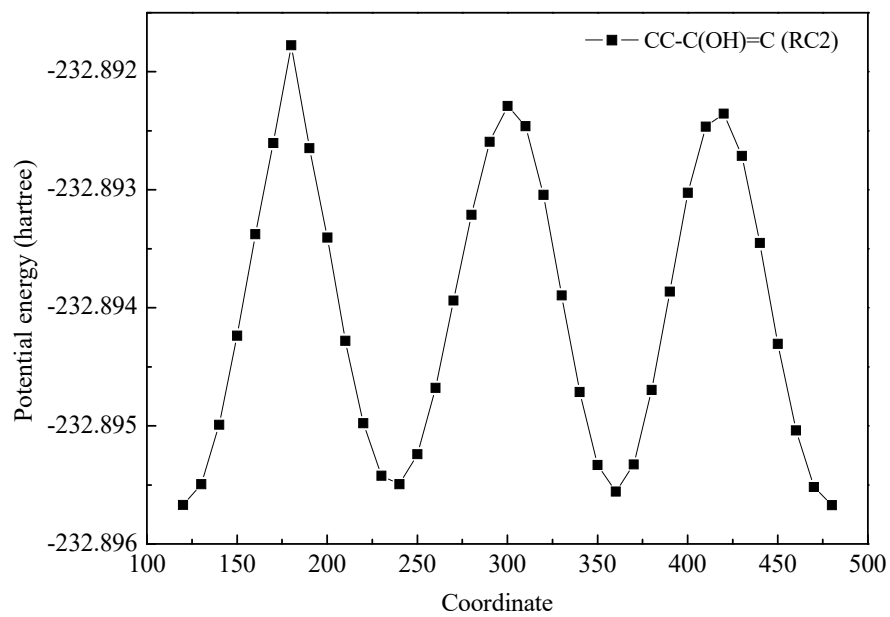
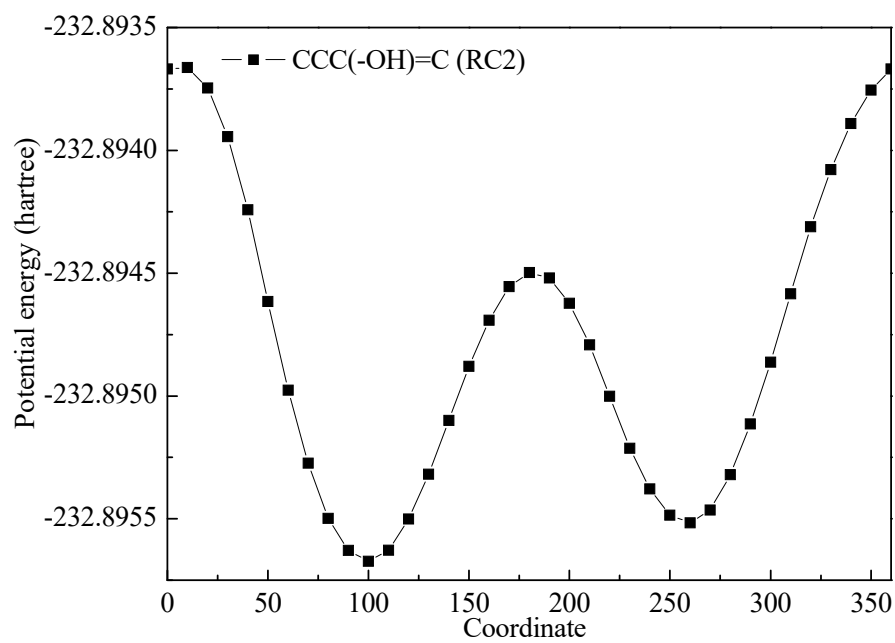
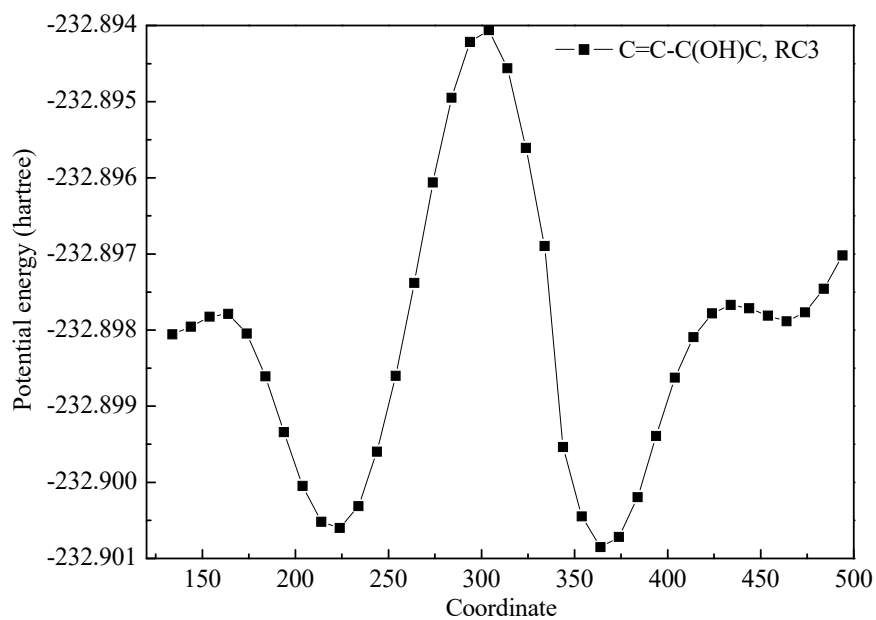
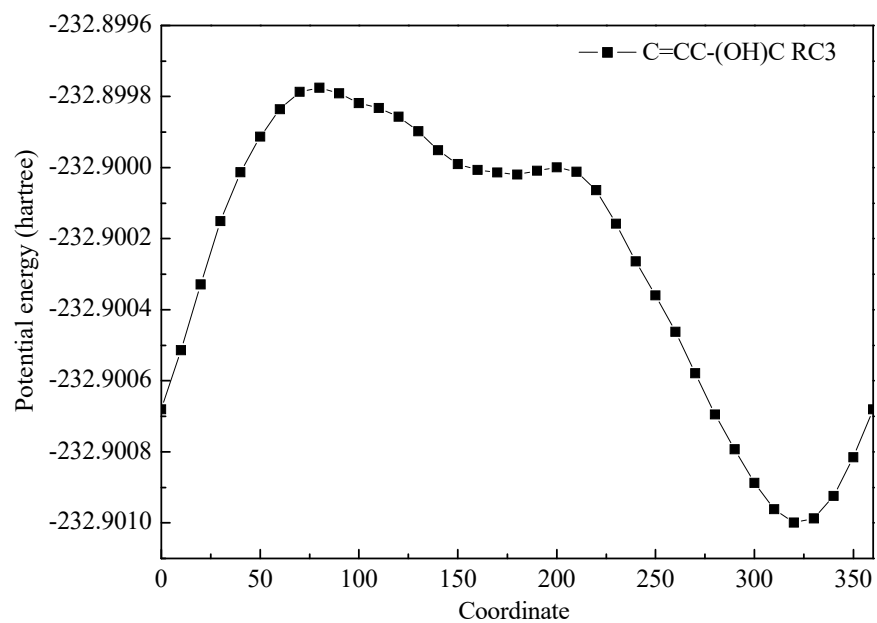
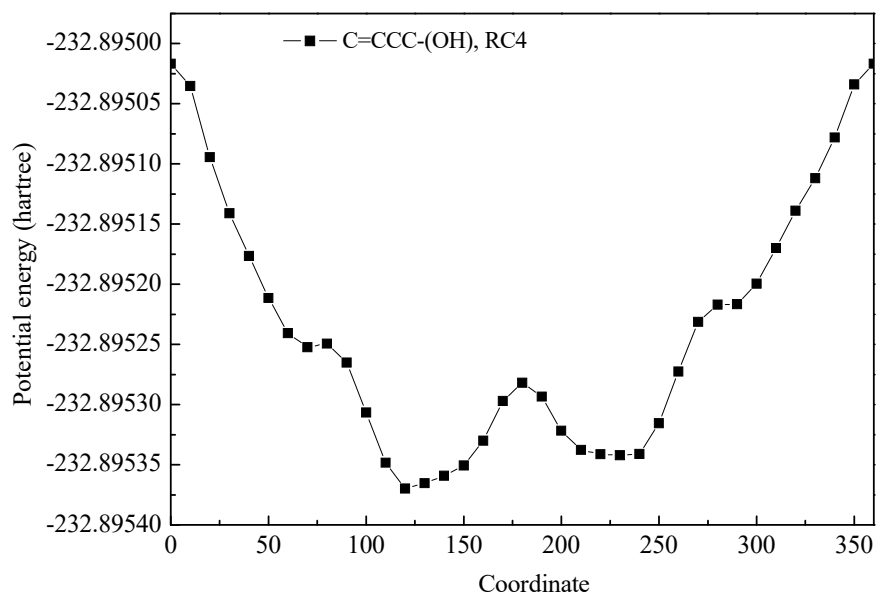
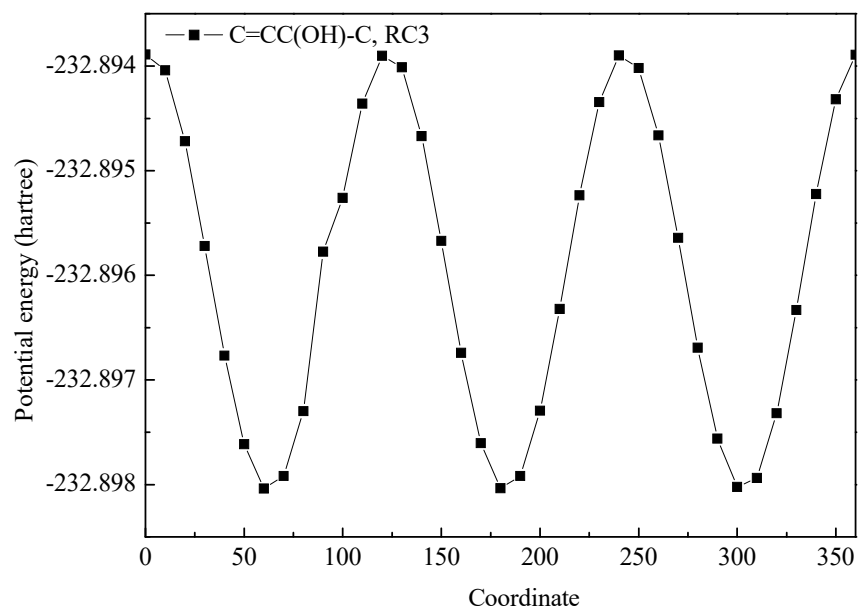


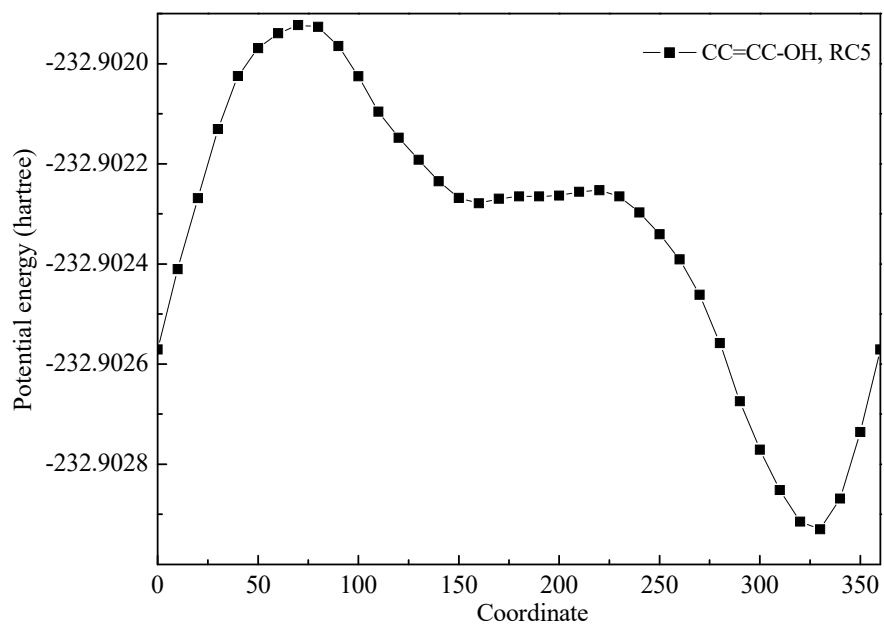
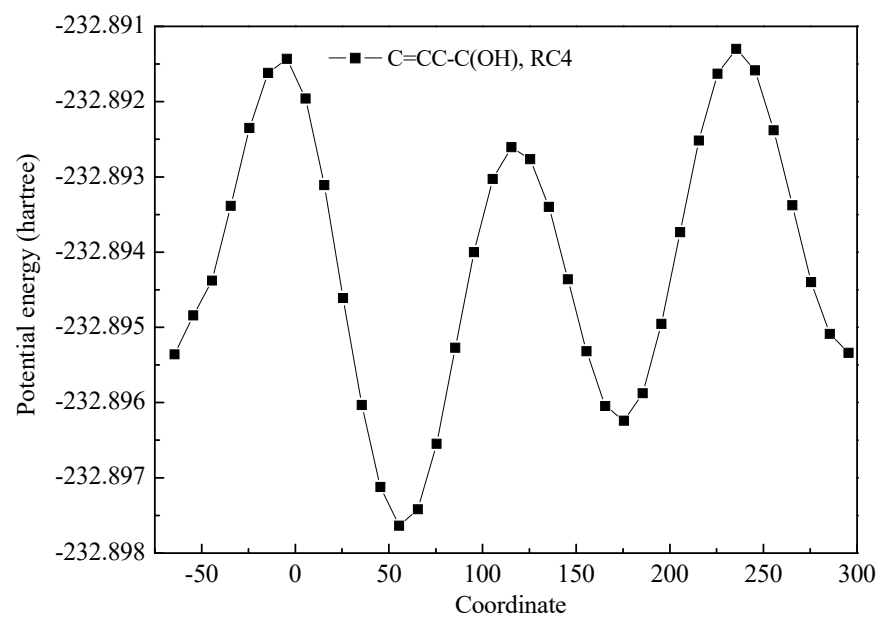
Figure S11 Hindrance potential analysis of reactants at M06-2X/6-311+G(d,p) level. The explicitly shown single C-C bond is the scanned internal rotors.

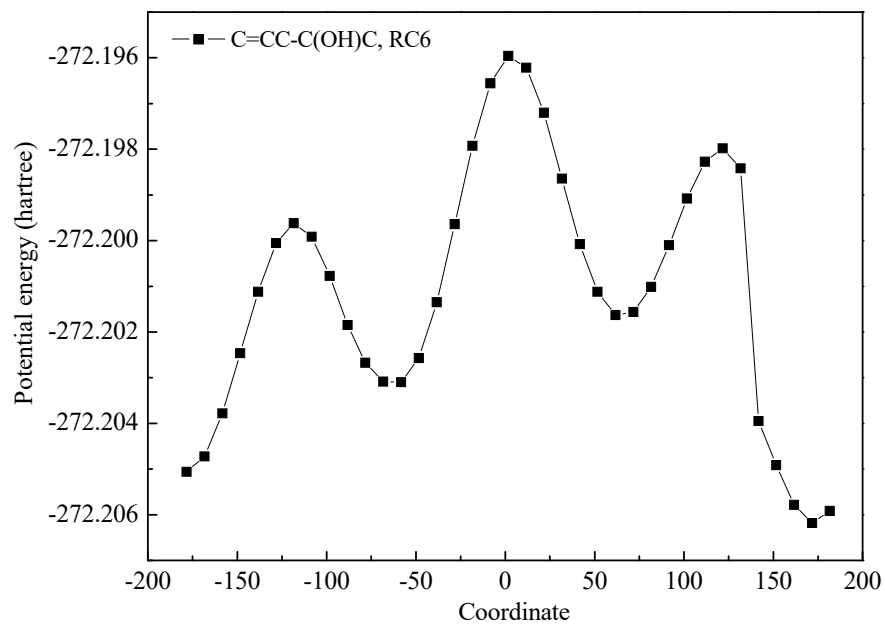
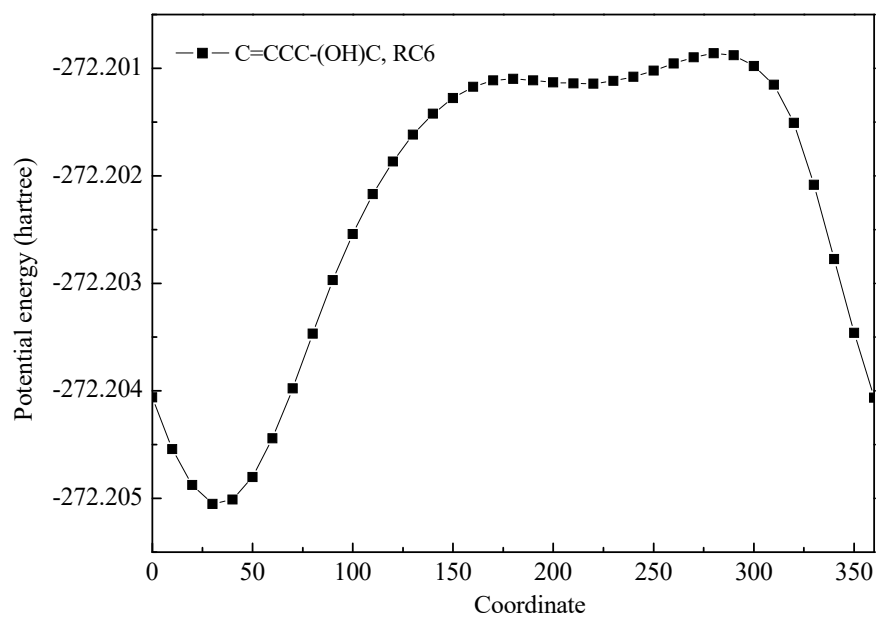


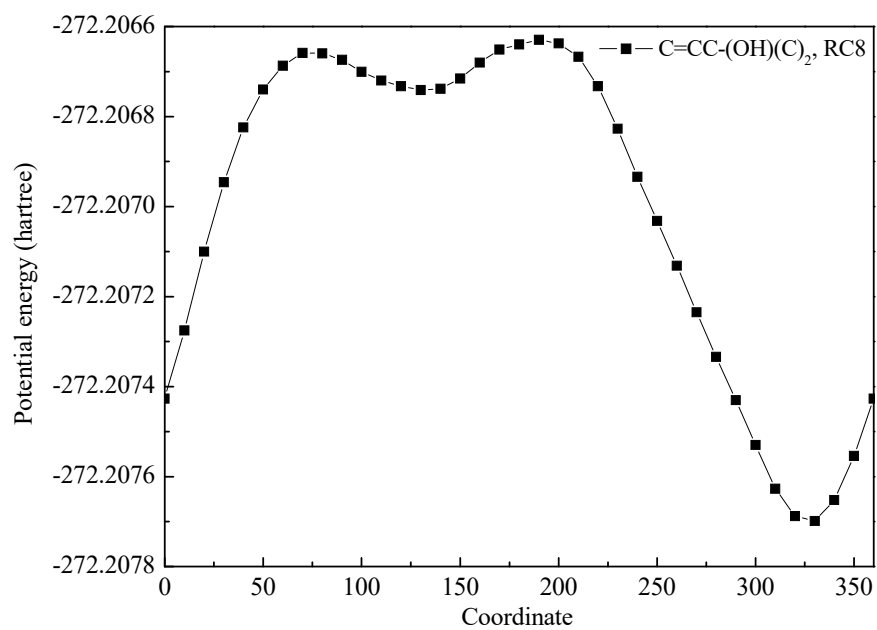
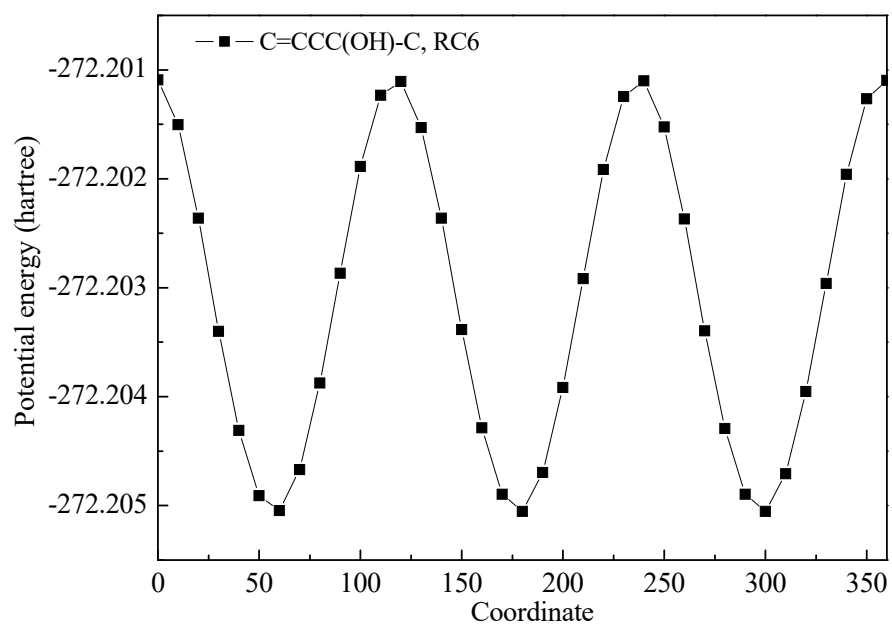


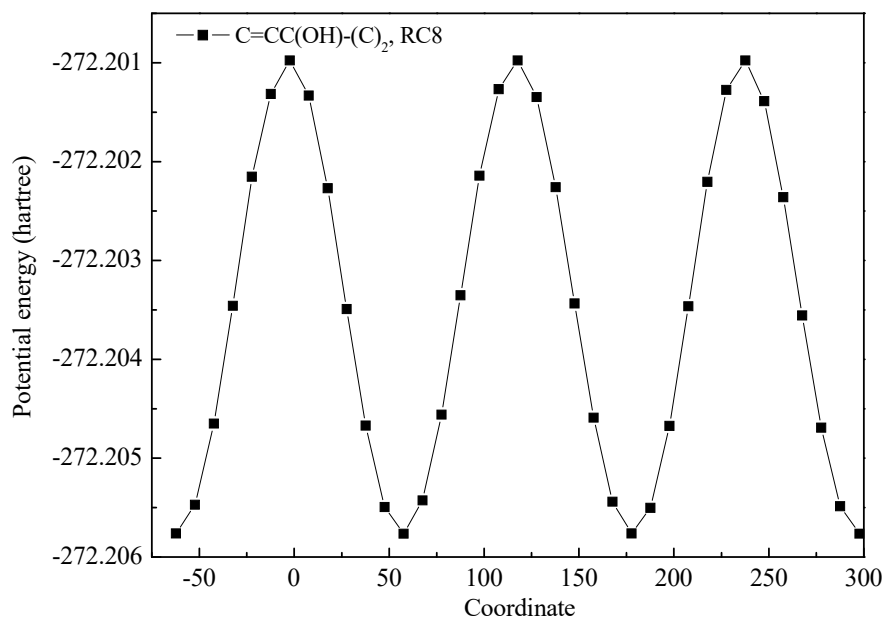
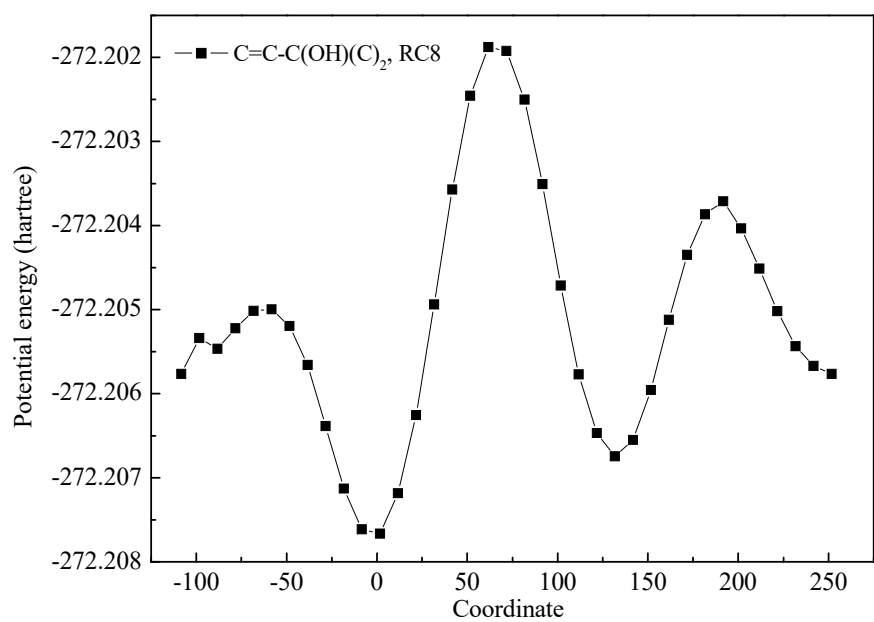












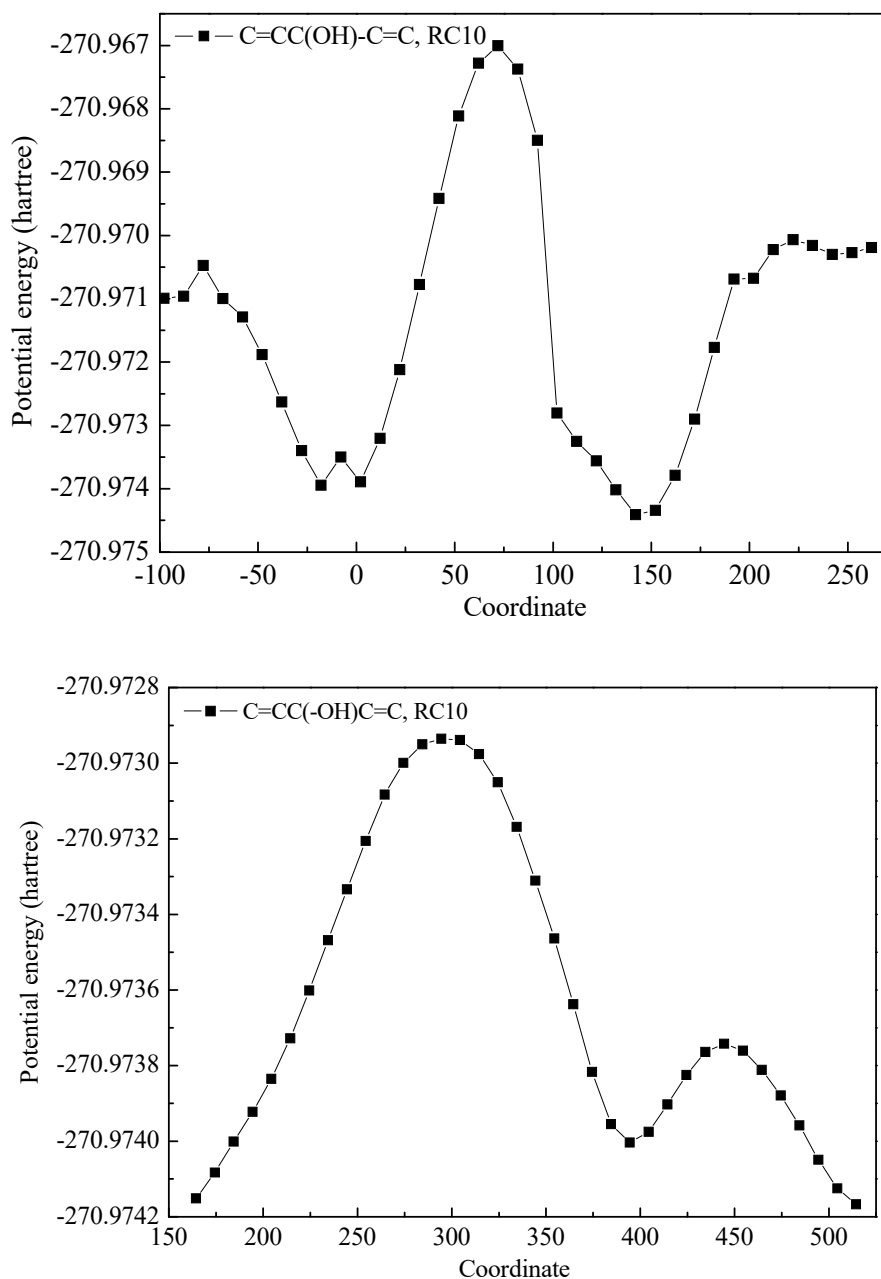


Figure S12 Hindrance potential analysis of TSs of prototype reactions at M06-2X/6-311+G(d,p) level. The explicitly shown single C-C/C-O bond is the scanned internal rotors. And the scanned results for prototype reactions were adopted for reactions within the same reaction classes since the relative potential energies are hardly affected.

Full list of the optimized geometries and frequencies for the studied abstraction reactions

Reactant		Geometry in Cartesian Coordinate (Å)			Frequency (cm ⁻¹)	Moment of inertia in au
1-butene	6	-1.711012	-0.245072	-0.296471	101.6424	80.93145
	6	-0.540230	0.529766	0.316392	227.2872	430.13440
	1	-2.624123	0.353299	-0.292611	319.5593	439.84766
	1	-1.487404	-0.525163	-1.327944	433.8483	

	1	-1.907607	-1.162454	0.264059	660.5609	
	6	0.714850	-0.292210	0.353730	794.0495	
	1	-0.356337	1.446356	-0.250968	869.5205	
	1	-0.804358	0.831417	1.335799	963.2479	
	6	1.838704	0.008656	-0.286944	984.1441	
	1	0.668321	-1.209004	0.940219	1033.4658	
	1	1.919411	0.911963	-0.884066	1046.6822	
	1	2.711978	-0.630847	-0.237202	1100.8308	
					1202.5711	
					1291.3676	
					1320.3301	
					1346.4855	
					1410.5137	
					1452.7314	
					1487.2332	
					1504.9515	
					1510.1560	
					1729.8315	
					3042.4602	
					3050.9200	
					3084.9277	
					3123.2699	
					3137.1327	
					3137.4992	
					3147.5322	
					3231.2601	
2-butene	6	-0.533497	-0.396441	-0.000019	162.9416	51.80555
	6	0.533497	0.396440	-0.000040	225.4364	482.69824
	6	1.955506	-0.078810	0.000014	241.8250	512.26120
	6	-1.955506	0.078810	0.000021	284.7486	
	1	-0.380851	-1.475004	-0.000059	505.7261	
	1	0.380850	1.475004	-0.000037	768.5711	
	1	2.005742	-1.168997	-0.001074	881.1894	
	1	2.492757	0.289516	-0.878319	984.8878	
	1	2.492066	0.287689	0.879548	1008.7412	
	1	-2.492372	-0.288409	-0.879019	1067.1266	
	1	-2.492450	-0.288795	0.878849	1076.9949	
	1	-2.005741	1.168998	0.000256	1096.4268	
					1171.6691	
					1328.9043	
					1338.7991	
					1414.6285	
					1416.0058	
					1483.9310	
					1484.4683	
					1495.0740	
					1503.0686	
					1772.7685	
					3038.3084	
					3038.5042	
					3097.0847	
					3097.5869	
					3122.2472	

					3123.1865	
					3137.3311	
					3144.0129	
isobutene	6	0.000000	1.456194	0.000000	190.8355	196.83213
	6	0.000000	0.125300	0.000000	235.4964	213.96331
	1	-0.925421	2.021469	-0.000115	383.6814	388.54983
	1	0.925421	2.021469	0.000115	436.3662	
	6	1.271161	-0.678280	0.000111	445.7548	
	6	-1.271161	-0.678280	-0.000110	712.7483	
	1	1.312700	-1.328853	-0.878994	832.9388	
	1	2.153713	-0.038247	0.000384	949.1420	
	1	1.312379	-1.329168	0.878993	971.0626	
	1	-1.312700	-1.328853	0.878994	993.8611	
	1	-2.153713	-0.038247	-0.000384	1019.2202	
	1	-1.312379	-1.329168	-0.878993	1087.7813	
					1107.7637	
					1308.4744	
					1411.2472	
					1418.2021	
					1447.5005	
					1481.9870	
					1489.9064	
					1501.4455	
					1508.2582	
					1741.9696	
					3046.3116	
					3049.9602	
					3102.9779	
					3105.1260	
					3150.1568	
					3150.4314	
					3153.2184	
					3239.4356	
1-pentene	6	0.000000	1.456194	0.000000	95.8605	99.71765
	6	0.000000	0.125300	0.000000	115.9711	844.71141
	1	-0.925421	2.021469	-0.000115	235.4737	857.04442
	1	0.925421	2.021469	0.000115	262.5383	
	6	1.271161	-0.678280	0.000111	388.2875	
	6	-1.271161	-0.678280	-0.000110	444.4945	
	1	1.312700	-1.328853	-0.878994	652.9062	
	1	2.153713	-0.038247	0.000384	750.6083	
	1	1.312379	-1.329168	0.878993	876.8940	
	1	-1.312700	-1.328853	0.878994	900.4082	
	1	-2.153713	-0.038247	-0.000384	963.7817	
	1	-1.312379	-1.329168	-0.878993	968.8264	
					1032.4109	
					1043.7560	
					1073.6858	
					1124.7205	
					1200.6362	
					1270.9678	
					1296.1836	
					1323.9922	

					1335.5089	
					1386.0016	
					1414.5793	
					1454.9052	
					1485.2019	
					1497.1503	
					1507.1816	
					1512.2986	
					1731.4924	
					3034.0260	
					3049.3694	
					3052.7794	
					3074.3662	
					3095.2432	
					3123.2240	
					3135.3214	
					3136.9355	
					3146.5680	
					3234.5744	
2-pentene	6	-1.299962	0.569201	-0.211710	74.5455	105.87031
	6	0.063014	-0.026704	-0.413513	171.2032	856.51535
	1	-1.234014	1.389067	0.509158	198.2118	881.28673
	1	-1.651424	1.002243	-1.154798	210.0986	
	6	1.160538	0.336928	0.243473	303.8810	
	6	2.517424	-0.272332	0.051919	411.9276	
	1	2.898149	-0.686111	0.989846	493.1431	
	1	2.486329	-1.073516	-0.688577	767.9028	
	1	3.239914	0.476914	-0.283958	815.1629	
	6	-2.315323	-0.472691	0.268177	893.6703	
	1	-2.006285	-0.895902	1.226263	961.3922	
	1	-3.307152	-0.032350	0.389670	1000.5908	
	1	-2.397367	-1.293625	-0.448753	1038.0231	
	1	1.085439	1.139191	0.976712	1073.9285	
	1	0.132270	-0.832326	-1.145639	1093.8346	
					1113.5782	
					1183.9341	
					1276.3768	
					1319.4154	
					1338.7921	
					1372.4157	
					1413.2358	
					1417.8432	
					1486.1796	
					1488.5230	
					1500.8908	
					1504.6566	
					1511.4029	
					1764.5446	
					3043.5279	
					3046.2726	
					3050.6010	
					3086.0919	
					3106.6752	

					3119.1723	
					3120.9669	
					3124.9024	
					3135.2804	
					3138.7771	
2-methyl-1-butene	6	0.687663	-0.762222	-0.000051	86.2380	209.24117
	6	2.029684	-0.041072	0.000116	175.9396	507.07759
	6	-0.536607	0.120838	-0.000048	253.7693	683.01359
	6	-1.845088	-0.623299	0.000043	288.1101	
	6	-0.485141	1.451310	-0.000098	408.3976	
	1	0.624303	-1.425597	-0.871539	435.2483	
	1	0.624181	-1.425782	0.871286	501.4490	
	1	2.135639	0.591950	0.883887	692.8510	
	1	2.851159	-0.759270	0.000150	796.3949	
	1	2.135815	0.592051	-0.883562	806.9664	
	1	-1.918401	-1.270543	0.879533	948.5755	
	1	-2.696415	0.057704	-0.000221	970.2056	
	1	-1.918259	-1.271070	-0.879066	1008.7212	
	1	-1.393590	2.043461	-0.000119	1038.0909	
	1	0.452500	1.993769	-0.000117	1042.1294	
					1108.4813	
					1123.7528	
					1264.5395	
					1299.8068	
					1391.7990	
					1411.1785	
					1414.1981	
					1454.7837	
					1476.1701	
					1488.0342	
					1498.6320	
					1500.8205	
					1514.9249	
					1738.5454	
					3031.1726	
					3040.8059	
					3045.1109	
					3058.1288	
					3097.3233	
					3119.4747	
					3123.4938	
					3139.8294	
					3161.5850	
					3245.6399	
2-methyl-2-butene	6	0.731745	-0.675012	-0.000004	113.2688	223.05408
	6	-0.444689	-0.043657	-0.000001	144.9992	512.39902
	1	0.708050	-1.763305	0.000005	205.0914	702.11935
	6	-1.738408	-0.815613	0.000016	279.9923	
	6	-0.624334	1.450729	-0.000002	306.7965	
	6	2.106856	-0.074425	-0.000013	394.0819	
	1	-2.339414	-0.561079	-0.879039	460.4714	
	1	-1.566261	-1.892401	0.000036	525.8014	
	1	-2.339413	-0.561045	0.879062	783.5712	

	1	-1.200079	1.759623	0.878377	841.8968	
	1	0.314568	2.000525	-0.000086	970.0405	
	1	-1.200230	1.759606	-0.878287	981.2769	
	1	2.096838	1.014369	-0.000165	1022.4455	
	1	2.669417	-0.404093	0.878288	1066.3268	
	1	2.669503	-0.404335	-0.878168	1075.6915	
					1110.3829	
					1144.0809	
					1247.2966	
					1370.8023	
					1418.2400	
					1426.1320	
					1429.8802	
					1478.8725	
					1488.8306	
					1489.9332	
					1500.6236	
					1505.7009	
					1506.2924	
					1769.1931	
					3046.5751	
					3047.7940	
					3052.4463	
					3099.6186	
					3102.1633	
					3104.5585	
					3129.2266	
					3137.6835	
					3147.7173	
					3165.3874	
2-methyl-3-butene	6	2.141611	-0.000005	-0.159675	91.6369	238.31384
	6	0.943760	-0.000018	0.413808	235.6090	506.54901
	6	-0.369717	0.000000	-0.317444	259.0470	654.74316
	6	-1.171094	-1.259468	0.029240	323.3383	
	6	-1.171060	1.259486	0.029253	327.4648	
	1	3.053039	-0.000017	0.426421	350.3100	
	1	2.248056	0.000015	-1.240227	509.0346	
	1	0.872674	-0.000041	1.502231	706.7902	
	1	-0.160832	0.000004	-1.392833	817.1788	
	1	-2.127528	-1.268211	-0.499325	933.2219	
	1	-0.619229	-2.162940	-0.236928	951.9346	
	1	-1.380275	-1.293784	1.102887	969.4605	
	1	-2.127498	1.268256	-0.499304	971.4549	
	1	-1.380231	1.293801	1.102903	1004.4944	
	1	-0.619173	2.162945	-0.236915	1041.8324	
					1137.8643	
					1190.5855	
					1227.9769	
					1314.7478	
					1337.6837	
					1345.6298	
					1398.0691	
					1417.8399	

					1458.9901	
					1491.3448	
					1493.0385	
					1505.2902	
					1516.8128	
					1724.8307	
					3039.4377	
					3041.4840	
					3052.6275	
					3108.8774	
					3114.0611	
					3126.5941	
					3132.0161	
					3133.5912	
					3150.5687	
					3240.5087	
1-hexene	6	3.067003	-0.187521	-0.432351	74.4295	133.56733
	6	2.027925	-0.197497	0.394883	85.5322	1438.25541
	6	0.769828	0.597336	0.207638	116.4740	1466.31773
	6	-0.469622	-0.294979	0.084584	180.8014	
	6	-1.765704	0.503290	-0.032339	237.3156	
	1	-0.528420	-0.955742	0.957933	359.0686	
	1	-0.356611	-0.947079	-0.788831	363.0811	
	1	0.861676	1.229641	-0.681392	461.8950	
	1	0.634820	1.268653	1.064764	655.5718	
	1	3.945574	-0.794376	-0.248247	728.6945	
	1	3.071381	0.433964	-1.322763	789.4191	
	1	2.059362	-0.836430	1.276537	911.6834	
	6	-2.994626	-0.393004	-0.160190	923.2000	
	1	-1.868804	1.149657	0.846227	948.4827	
	1	-1.702370	1.169409	-0.899681	967.4608	
	1	-3.082663	-1.056836	0.703885	1034.7129	
	1	-3.913643	0.192493	-0.227928	1045.8867	
	1	-2.929131	-1.019105	-1.053849	1058.9032	
					1086.0752	
					1132.8550	
					1199.3182	
					1245.4374	
					1264.8855	
					1309.0883	
					1323.6991	
					1334.7300	
					1351.3859	
					1399.8944	
					1411.8751	
					1455.1785	
					1482.4313	
					1488.8675	
					1499.5659	
					1504.1671	
					1511.6602	
					1731.8863	
					3020.0154	

					3028.7583	
					3038.3031	
					3044.1172	
					3057.6257	
					3072.0173	
					3088.4408	
					3115.8559	
					3123.0094	
					3143.0175	
					3156.6638	
					3233.8083	
2-hexene	6	-0.646202	-0.487057	0.369316	75.5212	121.88199
	6	-1.666723	0.527976	-0.157896	103.8980	1485.35428
	6	0.739569	0.081461	0.454747	135.8650	1502.96770
	6	1.789306	-0.358061	-0.233400	210.9211	
	6	3.169602	0.223313	-0.159445	263.5092	
	1	-0.968410	-0.822323	1.362980	291.3763	
	1	-0.641820	-1.371624	-0.276367	315.5287	
	1	3.201400	1.073586	0.524081	391.5071	
	1	3.506906	0.561149	-1.143205	539.0921	
	1	3.890814	-0.522167	0.187405	750.1988	
	1	1.653745	-1.206135	-0.903688	791.0000	
	1	0.870147	0.932263	1.124479	881.8973	
	6	-3.081420	-0.043093	-0.200515	912.6899	
	1	-1.645853	1.421240	0.475573	933.9131	
	1	-1.359792	0.850079	-1.157619	1001.6436	
	1	-3.410818	-0.342552	0.797918	1046.4043	
	1	-3.796804	0.686114	-0.585690	1068.3702	
	1	-3.124314	-0.926860	-0.842715	1074.1607	
					1109.9041	
					1124.2449	
					1185.0524	
					1255.9426	
					1292.8943	
					1320.6423	
					1337.7595	
					1345.1622	
					1395.2368	
					1417.8169	
					1419.3610	
					1483.2157	
					1484.6984	
					1497.9649	
					1501.8359	
					1508.0125	
					1512.9686	
					1762.8275	
					3030.0446	
					3044.8470	
					3049.8462	
					3053.7817	
					3076.8489	
					3095.1640	

					3104.1888	
					3115.1674	
					3119.5345	
					3122.0710	
					3136.2986	
					3136.5492	
3-hexene	6	-0.545633	0.038156	-0.378243	45.8147	136.58613
	6	0.545637	-0.038155	0.378260	119.7802	1425.11175
	6	1.849538	0.646658	0.087853	131.9793	1466.41664
	6	-1.849535	-0.646657	-0.087838	193.0609	
	6	2.989978	-0.356997	-0.111131	235.8848	
	6	-2.989984	0.356995	0.111104	329.1493	
	1	-0.520263	0.660457	-1.273904	331.0643	
	1	0.520266	-0.660455	1.273921	475.5302	
	1	1.741795	1.273651	-0.801712	489.8937	
	1	2.102105	1.313921	0.919265	757.4784	
	1	-2.102084	-1.313942	-0.919236	789.3272	
	1	-1.741800	-1.273628	0.801744	856.3357	
	1	3.939144	0.151841	-0.290865	909.2576	
	1	3.108819	-0.988790	0.772819	920.3738	
	1	2.781745	-1.009330	-0.961760	1013.3512	
	1	-3.939149	-0.151845	0.290840	1029.1063	
	1	-2.781767	1.009354	0.961717	1052.4287	
	1	-3.108819	0.988761	-0.772866	1096.3308	
					1098.2396	
					1127.5627	
					1189.5654	
					1261.6309	
					1282.4783	
					1324.0007	
					1334.3096	
					1348.6780	
					1386.8304	
					1405.6256	
					1405.7128	
					1484.0414	
					1484.9001	
					1500.0232	
					1500.4135	
					1510.2778	
					1510.7054	
					1765.4055	
					3037.7852	
					3038.5750	
					3042.8586	
					3042.9894	
					3079.2534	
					3080.1548	
					3116.3265	
					3116.4941	
					3128.7798	
					3128.8103	
					3136.6914	

					3141.6972	
1-4-pentadiene	6	-1.161245	-0.170178	-0.440714	78.4819	92.36139
	6	0.000001	0.681093	0.000053	103.8898	758.27482
	6	1.161242	-0.170259	0.440684	310.0265	764.66957
	6	-2.350292	-0.189684	0.150024	376.0552	
	6	2.350293	-0.189659	-0.150051	464.1876	
	1	-0.972180	-0.820398	-1.292367	624.0432	
	1	-0.321628	1.326979	0.823540	692.7247	
	1	0.321637	1.327109	-0.823329	902.0598	
	1	0.972174	-0.820624	1.292225	921.6550	
	1	-3.147666	-0.833484	-0.201465	969.8678	
	1	-2.565055	0.442938	1.005948	973.3578	
	1	3.147669	-0.833514	0.201332	978.9659	
	1	2.565060	0.443121	-1.005858	1036.2356	
					1043.4624	
					1092.6578	
					1177.4663	
					1268.1571	
					1299.8277	
					1316.7438	
					1330.2337	
					1444.0087	
					1450.1203	
					1482.1004	
					1715.5980	
					1729.2376	
					3042.5977	
					3089.1151	
					3140.1551	
					3140.3073	
					3151.3658	
					3151.4038	
					3233.4708	
					3233.5011	

Reaction	TS Geometry in Cartesian Coordinate (Å)				Frequency(cm ⁻¹)	Moment of inertia in au
R1-cis	6	2.054844	-0.627238	-0.385781	1211.5088i	276.01942
	6	0.995137	-0.155067	0.614448	46.5608	710.97445
	1	2.599342	-1.489209	0.003505	127.3655	893.16927
	1	1.591134	-0.914216	-1.331974	177.3043	
	1	2.779199	0.164159	-0.593715	179.0615	
	6	0.263480	1.056425	0.111692	228.8173	
	1	0.274683	-0.950810	0.815254	325.2427	
	1	1.480813	0.096398	1.562893	457.3392	
	6	-1.028903	1.119139	-0.150889	564.2299	
	1	0.865715	1.952025	-0.056772	717.6837	
	1	-1.704524	0.144849	0.064515	794.6701	
	1	-1.582967	1.964631	-0.541782	831.2832	
	8	-2.236048	-1.048590	-0.036478	886.2411	
	1	-2.036386	-1.228482	-0.968035	946.1188	
					971.3622	
					1042.5263	

					1094.4423	
					1177.4391	
					1241.0423	
					1279.3512	
					1290.6602	
					1320.1767	
					1377.1448	
					1408.2057	
					1491.4144	
					1501.1677	
					1508.1471	
					1711.8519	
					3041.7602	
					3049.1099	
					3098.1221	
					3112.3423	
					3123.5423	
					3126.6618	
					3194.1528	
					3819.9039	
R1-trans	6	-2.497394	-0.521346	-0.286053	1231.0048i	116.04582
	6	-1.519348	0.460643	0.364448	87.5902	1150.86449
	1	-3.525981	-0.169825	-0.188113	100.4571	1188.84023
	1	-2.273815	-0.640565	-1.347849	119.4635	
	1	-2.430049	-1.505726	0.183225	190.4102	
	6	-0.100156	-0.034199	0.278630	243.4918	
	1	-1.595201	1.443007	-0.108256	348.2205	
	1	-1.780634	0.589691	1.420265	367.8080	
	6	0.878521	0.596581	-0.343399	559.4728	
	1	0.105255	-0.997903	0.743677	751.4940	
	1	0.828199	1.560842	-0.839573	803.3339	
	1	1.958655	0.066752	-0.392141	858.6854	
	8	3.116342	-0.420519	-0.046338	876.0110	
	1	3.213098	0.007805	0.817720	961.7954	
					979.4901	
					1041.8441	
					1096.0492	
					1174.0997	
					1241.6547	
					1286.3287	
					1299.9070	
					1315.0833	
					1359.9507	
					1412.6561	
					1483.9486	
					1503.3797	
					1509.2953	
					1722.5503	
					3042.8533	
					3051.2675	
					3095.8405	
					3128.5967	
					3132.9535	

					3144.7677	
					3176.7923	
					3830.6197	
R2	6	1.778147	-0.577511	0.371283	907.4206i	401.65432
	6	1.077774	0.478493	-0.487989	69.6300	511.93184
	1	2.840489	-0.635108	0.128846	95.5269	829.82339
	1	1.680582	-0.336836	1.432102	162.9524	
	1	1.334920	-1.560850	0.200547	216.7142	
	6	-0.382259	0.563632	-0.184681	251.3279	
	1	1.523825	1.465805	-0.326197	344.7047	
	1	1.208674	0.232207	-1.546255	406.9292	
	6	-1.100320	1.584116	0.250747	601.4363	
	1	-0.955979	-0.456886	-0.352747	726.0417	
	1	-0.645713	2.559826	0.405651	792.2218	
	1	-2.160987	1.489206	0.451365	841.5005	
	8	-1.524685	-1.673556	-0.107203	898.7235	
	1	-1.467878	-1.666515	0.861267	952.1813	
					980.1547	
					1042.2652	
					1097.6834	
					1176.8421	
					1218.2947	
					1280.6469	
					1328.4198	
					1404.1037	
					1420.7574	
					1435.6329	
					1475.9178	
					1503.3314	
					1514.7488	
					1731.5122	
					3039.0828	
					3050.3822	
					3082.3690	
					3127.1664	
					3128.0931	
					3134.1926	
					3226.7424	
					3810.1106	
R3	6	-2.090201	-0.634772	0.118972	665.5269i	398.97317
	6	-0.982691	-0.110659	-0.400086	53.7932	570.40165
	6	0.146470	0.445729	0.396964	84.4409	884.84747
	1	1.033376	-0.279943	0.294394	124.7187	
	1	-0.090102	0.453021	1.464002	191.6347	
	1	-2.243085	-0.677263	1.192919	218.8023	
	8	1.903430	-1.462815	-0.041436	309.0207	
	1	1.167917	-2.094598	-0.098514	444.4220	
	1	-2.879813	-1.028628	-0.509559	592.1244	
	1	-0.862551	-0.078210	-1.482037	688.2907	
	6	0.648235	1.797517	-0.093948	801.8506	
	1	-0.135674	2.553056	0.007193	876.8633	
	1	1.517287	2.124357	0.478271	972.0328	
	1	0.934331	1.743836	-1.146601	987.6710	

				1021.1896	
				1050.3812	
				1087.0430	
				1202.0628	
				1233.5468	
				1315.5046	
				1333.9727	
				1365.8899	
				1412.8087	
				1460.3242	
				1499.2983	
				1500.8068	
				1627.4905	
				1736.0638	
				3054.2278	
				3097.5406	
				3127.2787	
				3140.0530	
				3144.0991	
				3149.6288	
				3234.5925	
				3797.8052	
R4	6	-0.029058	-0.026287	-0.032885	744.3069i 111.28362
	6	0.053092	0.000538	1.485582	46.5238 1163.37530
	1	1.071100	-0.052031	-0.467386	64.3170 1188.37800
	1	-0.514869	-0.921041	-0.425633	109.1832
	1	-0.470847	0.874230	-0.460422	176.1663
	6	0.710719	-1.233019	2.033424	296.1976
	1	0.599732	0.888473	1.814289	332.2264
	1	-0.962765	0.077606	1.893059	431.4940
	6	1.842518	-1.238934	2.731188	660.0434
	1	0.218150	-2.178379	1.810423	711.2348
	1	2.358455	-0.314190	2.972811	812.4630
	1	2.281535	-2.161008	3.093482	917.5260
	8	2.428859	-0.231191	-0.598566	972.7016
	1	2.554318	-0.785389	0.190469	981.9995
				1037.0990	
				1053.5159	
				1074.3208	
				1162.2058	
				1226.6682	
				1282.3526	
				1307.2209	
				1327.8378	
				1349.4355	
				1420.3209	
				1455.2227	
				1480.9763	
				1493.5251	
				1729.0606	
				3060.2161	
				3085.4164	
				3105.6263	

					3141.0649	
					3150.9073	
					3156.2763	
					3242.2448	
					3799.9636	
R5	6	-2.493657	-0.528619	-0.071501	893.8934i	205.03753
	6	-1.224778	0.121759	0.386378	52.0692	946.71886
	6	-0.214896	0.469831	-0.412711	98.3762	1070.26374
	6	1.044930	1.098435	0.056287	182.0642	
	1	-2.633816	-1.497566	0.416217	209.8490	
	1	-2.490180	-0.684460	-1.151339	238.1202	
	1	1.909269	0.330595	-0.008441	284.7076	
	1	1.002154	1.416266	1.098253	317.8996	
	1	-0.295093	0.266958	-1.479332	507.3953	
	1	-1.138785	0.328702	1.452438	673.8621	
	8	2.637847	-0.954806	0.014150	795.1382	
	1	1.850811	-1.490408	0.205851	888.9280	
	1	1.384646	1.914984	-0.583481	960.0099	
	1	-3.361379	0.084948	0.185924	997.7318	
					1012.4956	
					1073.8811	
					1106.0394	
					1171.9062	
					1309.2667	
					1332.9318	
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					1421.7096	
					1467.9215	
					1487.5403	
					1500.0254	
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					1760.3803	
					3051.8585	
					3081.2088	
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					3127.5064	
					3137.6800	
					3144.5062	
					3159.7740	
					3795.5331	
R6	6	1.853526	-0.907085	0.004100	870.3029i	421.37249
	6	0.475044	-0.340436	-0.068610	104.8367	497.70249
	1	2.397096	-0.729970	-0.926612	131.5403	889.15797
	1	2.426291	-0.442140	0.810203	164.5792	
	1	1.811161	-1.984231	0.185317	195.1001	
	6	-0.694613	-0.948601	0.050708	226.3078	
	6	-2.035016	-0.279702	-0.024390	231.6981	
	1	-2.586998	-0.411894	0.910138	284.1463	
	1	-1.924467	0.787327	-0.221116	507.2852	
	1	-2.640845	-0.720119	-0.820365	588.2463	
	1	-0.689336	-2.029306	0.204068	832.2135	
	1	0.444646	0.823479	-0.273757	856.3115	

	8	0.367591	2.174590	-0.066513	908.5104	
	1	0.228086	2.165079	0.893383	986.2248	
					1057.6096	
					1070.7257	
					1095.9527	
					1154.0830	
					1219.2191	
					1309.5542	
					1385.8486	
					1411.2567	
					1426.9611	
					1473.4629	
					1490.8509	
					1494.5954	
					1501.6545	
					1770.6016	
					3041.9988	
					3042.9607	
					3102.3256	
					3107.9950	
					3116.2954	
					3120.3679	
					3143.5177	
					3809.2090	
R7	6	1.853526	-0.907085	0.004100	1164.0012i	212.18290
	6	0.475044	-0.340436	-0.068610	112.9768	736.07444
	1	2.397096	-0.729970	-0.926612	124.6843	916.65954
	1	2.426291	-0.442140	0.810203	162.4358	
	1	1.811161	-1.984231	0.185317	211.8433	
	6	-0.694613	-0.948601	0.050708	236.7768	
	6	-2.035016	-0.279702	-0.024390	352.9161	
	1	-2.586998	-0.411894	0.910138	398.7129	
	1	-1.924467	0.787327	-0.221116	441.0297	
	1	-2.640845	-0.720119	-0.820365	540.6105	
	1	-0.689336	-2.029306	0.204068	767.1563	
	1	0.444646	0.823479	-0.273757	821.8251	
	8	0.367591	2.174590	-0.066513	890.3660	
	1	0.228086	2.165079	0.893383	966.6047	
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					987.2593	
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					1499.5173	
					1731.9015	
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					3106.3619	
					3146.2574	
					3152.4445	
					3196.2628	
					3821.8602	
R8	6	-1.498107	-0.943794	-0.584919	911.5316i	305.34001
	6	-0.736609	-0.099758	0.114784	56.7184	651.67691
	6	0.372373	-0.585349	0.981850	95.9872	741.63388
	1	1.378604	-0.265980	0.496648	156.1454	
	1	0.404892	-1.668640	1.090787	223.2818	
	1	-1.353272	-2.016876	-0.524091	308.2742	
	8	2.373018	0.120839	-0.505113	394.8416	
	1	1.899124	-0.255995	-1.264692	430.8080	
	1	0.402569	-0.091266	1.955978	440.8268	
	6	-0.905762	1.392897	0.051167	677.4506	
	1	0.032679	1.862349	-0.258865	756.6916	
	1	-1.693820	1.680118	-0.644902	845.4157	
	1	-1.151835	1.790831	1.040150	909.4083	
	1	-2.294448	-0.585229	-1.227400	949.4472	
					974.0737	
					996.3751	
					1070.6899	
					1081.2102	
					1295.5075	
					1337.0035	
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					1413.5963	
					1440.8166	
					1468.7783	
					1486.3823	
					1500.6428	
					1541.3659	
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					3075.4130	
					3099.7314	
					3136.5019	
					3144.1005	
					3160.9468	
					3233.3425	
					3778.7423	
R9-cis	6	1.670139	-0.290635	-0.392703	1163.8539i	353.91659
	6	0.445948	-0.178326	0.523135	63.2464	1211.89074
	1	2.079550	-1.304474	-0.329339	73.3135	1467.30088
	1	1.349584	-0.145978	-1.428544	126.3211	
	6	-0.600499	-1.201490	0.190086	156.6582	
	1	0.767892	-0.319280	1.561889	242.5704	
	1	0.011618	0.822100	0.444876	255.3667	
	6	-1.825770	-0.939616	-0.226813	283.9109	
	1	-0.298779	-2.248031	0.271697	388.6183	
	1	-2.149289	0.211228	-0.369510	452.0372	

	1	-2.604400	-1.651329	-0.475455	555.8430	
	6	2.747290	0.727835	-0.030608	723.1332	
	1	3.097989	0.578132	0.993905	752.3680	
	1	3.609387	0.649440	-0.695472	846.6112	
	1	2.357367	1.746020	-0.104476	882.2162	
	8	-2.503149	1.451118	-0.128767	900.1334	
	1	-2.818377	1.346617	0.781989	949.1422	
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					3125.9404	
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					3816.7407	
R9-trans	6	1.761075	-0.587664	-0.080151	1222.4515i	150.99873
	6	0.864909	0.602137	0.281896	69.7815	1819.09632
	1	1.638906	-1.372061	0.673967	81.8378	1878.63786
	1	1.420048	-1.011476	-1.029497	109.5972	
	6	-0.576787	0.197171	0.426312	138.3181	
	1	1.210637	1.032990	1.228886	223.9193	
	1	0.957392	1.382585	-0.479421	253.3284	
	6	-1.563660	0.662549	-0.316789	264.3872	
	1	-0.799291	-0.538306	1.198558	373.5131	
	1	-1.492338	1.378540	-1.129660	408.7638	
	1	-2.681732	0.279560	-0.088261	537.6416	
	6	3.230716	-0.188579	-0.180317	752.5872	
	1	3.591856	0.211288	0.770730	781.1647	
	1	3.857146	-1.042250	-0.445328	862.8734	
	1	3.374249	0.582291	-0.941782	888.2956	
	8	-3.739385	-0.476498	0.003428	893.5919	
	1	-3.459302	-1.204862	-0.571317	949.9031	
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					1287.0709	
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					3087.1542	
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					3134.2570	
					3137.9026	
					3141.7431	
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					3827.5477	
R10	6	-1.286187	0.288278	-0.365918	926.6365i	427.36804
	6	-0.432513	-0.657701	0.486068	51.7693	1022.10328
	1	-0.950802	1.315324	-0.192387	75.1897	1353.91256
	1	-1.109011	0.069206	-1.423605	101.4397	
	6	1.024430	-0.534826	0.185573	150.4137	
	1	-0.604884	-0.436365	1.545296	185.8666	
	1	-0.739588	-1.697158	0.317458	238.1694	
	6	1.874132	-1.437163	-0.273370	270.0819	
	1	1.455889	0.550924	0.372747	376.8916	
	1	1.556913	-2.462812	-0.447419	422.6534	
	1	2.910702	-1.192847	-0.474351	588.2372	
	6	-2.772824	0.162593	-0.045966	725.0770	
	1	-2.966300	0.401789	1.002805	749.3895	
	1	-3.369978	0.839223	-0.659749	862.7774	
	1	-3.127506	-0.855368	-0.226952	872.0144	
	8	1.846437	1.836600	0.136777	903.1006	
	1	1.730840	1.848189	-0.826382	950.9974	
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					1420.8132	
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					3812.5453	
R11	6	-1.286187	0.288278	-0.365918	634.6449i	513.20123
	6	-0.432513	-0.657701	0.486068	39.5656	894.91983
	1	-0.950802	1.315324	-0.192387	78.3647	1291.41560
	1	-1.109011	0.069206	-1.423605	88.5673	
	6	1.024430	-0.534826	0.185573	119.1372	
	1	-0.604884	-0.436365	1.545296	155.4970	
	1	-0.739588	-1.697158	0.317458	224.9740	
	6	1.874132	-1.437163	-0.273370	270.2832	
	1	1.455889	0.550924	0.372747	395.9494	
	1	1.556913	-2.462812	-0.447419	435.5977	
	1	2.910702	-1.192847	-0.474351	583.4771	
	6	-2.772824	0.162593	-0.045966	668.9685	
	1	-2.966300	0.401789	1.002805	742.5152	
	1	-3.369978	0.839223	-0.659749	858.8333	
	1	-3.127506	-0.855368	-0.226952	902.3743	
	8	1.846437	1.836600	0.136777	971.8463	
	1	1.730840	1.848189	-0.826382	975.4398	
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					3138.9286	
					3144.0907	
					3148.2918	
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					3793.5956	
R12	6	-2.458621	-0.156175	-0.263522	769.0202i	442.61474
	6	-1.425829	-0.696851	0.376528	71.0499	858.89693
	6	-0.090027	-0.979980	-0.244991	101.1894	1189.98353
	6	1.038722	-0.199452	0.420004	110.0588	
	6	2.401043	-0.427724	-0.207018	137.2390	
	1	1.049593	-0.360473	1.502232	212.5807	
	1	0.791126	0.931894	0.298585	235.3064	
	1	0.131247	-2.052022	-0.158123	292.2892	
	1	2.689532	-1.480548	-0.121601	388.3250	
	1	2.386270	-0.167744	-1.267892	444.8792	
	1	-2.396720	0.095714	-1.318389	649.8280	
	1	-3.399538	0.037003	0.238068	676.4292	
	1	-1.525245	-0.940537	1.433257	743.5522	
	1	-0.118162	-0.742827	-1.313269	889.6762	
	8	0.149159	2.176876	-0.017323	910.5393	
	1	-0.762540	1.851971	0.079460	967.6596	
	1	3.169442	0.173650	0.280253	972.9993	
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R13	6	1.637067	1.090381	-0.241489	783.5928i	286.97187
	6	0.254686	0.959598	0.365479	46.1456	1353.28013
	1	2.233294	0.115181	0.001860	67.2623	1524.45712
	6	-0.532168	-0.216471	-0.223478	101.2297	
	1	0.338246	0.836893	1.449809	132.4995	
	1	-0.305466	1.887078	0.196896	151.5554	
	6	-1.891105	-0.358201	0.394673	232.9920	
	1	-0.632761	-0.087814	-1.306698	316.2666	
	1	0.046130	-1.131872	-0.052533	391.1072	
	6	-3.039528	-0.256862	-0.264701	442.8893	
	1	-3.994570	-0.360447	0.236409	653.4876	
	1	-3.059303	-0.070438	-1.334156	724.7052	
	1	-1.909245	-0.545580	1.467134	788.1901	
	8	2.769755	-1.194950	0.135787	865.3034	
	1	2.693176	-1.466205	-0.792855	898.9394	
	1	2.239294	1.888525	0.194440	966.4680	
	1	1.619449	1.183611	-1.329511	970.7643	
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					3792.7751	
R14	6	2.016977	-0.368080	0.274280	892.7173i	345.72087
	6	0.661899	-0.603135	-0.322562	37.8727	1335.29528
	1	1.951252	-0.430877	1.363919	70.2966	1578.36807
	1	2.696605	-1.163314	-0.051165	112.6467	
	6	-0.459432	-0.796301	0.374407	158.1500	

	6	-1.799141	-0.995514	-0.231785	181.5877	
	1	-2.376055	-1.788899	0.247119	222.5893	
	1	-2.446279	-0.051885	-0.056759	286.6604	
	1	-1.762661	-1.142578	-1.311290	332.8083	
	6	2.598863	0.986686	-0.142985	415.7458	
	1	1.961747	1.803077	0.203759	491.9342	
	1	3.597163	1.130856	0.274411	697.5346	
	1	2.674958	1.059317	-1.230783	780.2261	
	1	-0.408565	-0.790584	1.461875	830.2657	
	1	0.608157	-0.605326	-1.411984	894.7660	
	8	-2.834267	1.365796	0.104305	956.0168	
	1	-1.937186	1.711910	-0.031673	980.2746	
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R15	6	-1.477485	0.260075	-0.468138	864.2298i	465.85626
	6	-0.334967	-0.709243	-0.362728	61.5215	974.22264
	1	-1.119311	1.263774	-0.227281	102.0384	1333.29369
	1	-1.836904	0.279609	-1.502781	129.9965	
	6	0.898780	-0.412620	0.014506	174.2459	
	6	2.091682	-1.298434	0.151916	191.8182	
	1	1.831242	-2.327756	-0.108311	206.9709	
	1	2.901858	-0.969475	-0.503386	226.6700	
	6	-2.634289	-0.126456	0.458168	299.6947	
	1	-2.308438	-0.120323	1.500170	413.5421	
	1	-3.467096	0.571574	0.355083	495.4631	
	1	-3.003438	-1.128757	0.226515	589.1856	
	1	1.106627	0.716910	0.296101	783.3018	

	1	-0.562073	-1.754504	-0.587966	865.2013	
	1	2.473346	-1.282204	1.175189	877.5294	
	8	1.408815	2.046759	0.175793	896.2746	
	1	1.451339	2.097149	-0.792016	967.1807	
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R16	6	-1.407783	-0.595495	-0.562456	803.4283i	486.83278
	6	-0.004772	-0.242098	-0.188869	52.4103	892.98306
	1	-1.683385	-0.059079	-1.476711	83.8717	1254.95842
	1	-1.448347	-1.665359	-0.794904	141.7869	
	6	1.075018	-1.004075	-0.109078	167.0584	
	6	2.443424	-0.529549	0.281103	186.4525	
	1	3.162525	-0.712470	-0.521886	214.1071	
	1	2.432100	0.537451	0.507345	227.8755	
	6	-2.399432	-0.244050	0.549306	295.3951	
	1	-2.348488	0.822427	0.779600	405.7633	
	1	-3.422281	-0.482404	0.252070	490.8856	
	1	-2.166145	-0.797845	1.460698	635.6986	
	1	0.125788	0.892311	0.103871	777.1790	
	1	2.801129	-1.069057	1.161922	844.2904	
	1	0.962951	-2.066936	-0.331002	868.9372	
	8	0.342164	2.251901	-0.003143	908.4691	
	1	0.608111	2.277362	-0.935902	967.5711	
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R17	6	1.554339	-0.037609	0.427272	637.6091i	453.01319
	6	0.411306	-0.218176	-0.234120	53.2067	1095.02691
	6	-0.915480	-0.438197	0.406672	74.1245	1434.95096
	1	-1.544772	0.509175	0.251778	109.5418	
	1	-0.816397	-0.534632	1.491122	175.9796	
	1	1.533633	-0.060221	1.516091	200.8254	
	8	-1.977813	1.926576	-0.097978	204.7892	
	1	-1.074461	2.282129	-0.068784	229.0361	
	1	0.422011	-0.202326	-1.324352	290.6097	
	6	-1.717822	-1.582461	-0.200462	415.4030	
	1	-1.192874	-2.531232	-0.059852	483.5933	
	1	-2.702624	-1.662456	0.261702	638.2212	
	1	-1.857355	-1.428325	-1.272744	752.6376	
	6	2.889331	0.188433	-0.214212	836.3857	
	1	3.320404	1.140771	0.107350	895.0762	
	1	3.597131	-0.594087	0.072829	967.5346	
	1	2.807768	0.196663	-1.302222	1002.3618	
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R18	6	-2.056893	-0.504969	-0.305508	757.5037i	117.74480
	6	-0.863956	-1.177083	0.356585	49.2816	1925.66786
	1	-1.965891	0.662383	-0.142893	55.3488	1950.66197
	1	-2.085197	-0.642386	-1.387730	89.9898	
	1	-3.013680	-0.772442	0.144403	159.7661	
	6	0.439379	-0.747840	-0.254029	177.8787	
	1	-0.860486	-0.957390	1.427664	214.8662	
	1	-0.971712	-2.264399	0.253492	279.7454	
	6	1.416079	-0.124354	0.401729	331.9377	
	1	0.567238	-0.956494	-1.316702	406.0459	
	1	1.279976	0.079271	1.463649	498.6920	
	8	-1.439511	1.917306	0.086087	731.2567	
	1	-0.505859	1.666578	-0.019050	777.1280	
	6	2.715144	0.313843	-0.205698	813.1309	
	1	3.558123	-0.181505	0.283792	917.8283	
	1	2.751044	0.080197	-1.270976	993.0630	
	1	2.864021	1.390159	-0.082818	1003.3091	
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R19-cis	6	-1.208906	1.723647	-0.385694	1182.3625i	470.72099
	6	-0.486029	0.820465	0.619400	40.0733	837.86479
	1	-1.230512	2.753871	-0.026461	117.6161	1203.14000
	1	-0.696463	1.711540	-1.350753	126.0270	
	1	-2.241644	1.407512	-0.546177	187.9670	
	6	-0.358123	-0.602912	0.133374	211.6193	
	1	0.508997	1.216326	0.828816	239.7675	
	1	-1.043149	0.814256	1.563279	272.4574	
	6	0.816224	-1.171649	-0.093283	363.3876	
	1	1.820447	-0.542225	0.126984	411.3194	
	1	0.998639	-2.175871	-0.460726	505.6803	
	8	2.800240	0.314248	0.005243	588.7694	
	1	2.701296	0.526546	-0.935212	757.6528	
	6	-1.643524	-1.365282	-0.080673	786.1702	
	1	-2.224117	-0.914457	-0.890045	799.5128	
	1	-1.454657	-2.408423	-0.333594	883.0267	
	1	-2.258604	-1.328668	0.823202	941.6592	
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R19-trans	6	-0.495120	-0.799147	-0.146256	1142.9883i	331.38559
	6	0.152404	0.350993	-0.038874	82.0552	1072.37010
	6	-0.558678	1.677673	-0.016884	100.9074	1361.01606
	6	1.661921	0.429790	0.049757	112.9628	
	1	-1.691529	-0.771781	-0.270847	143.7280	
	1	-0.202357	2.308320	-0.836571	237.6180	
	1	-1.636882	1.552737	-0.109439	247.7571	
	1	-0.339347	2.207791	0.914729	269.9723	
	1	2.006349	1.057397	-0.780645	386.1748	
	1	-0.078906	-1.799393	-0.153104	428.9504	
	8	-2.972569	-0.687822	-0.009950	467.1989	
	1	-2.946167	-0.869676	0.941684	549.9006	
	6	2.402155	-0.901136	0.037301	740.4160	
	1	2.201656	-1.454306	-0.882772	791.9164	
	1	3.479044	-0.739210	0.103788	811.6299	
	1	2.103844	-1.526456	0.881735	883.6277	
	1	1.908763	0.988109	0.960771	956.4683	
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R20	6	-0.558580	1.529169	0.676563	929.0200i	440.67554
	6	-0.131903	0.599221	-0.181466	58.3439	928.72672
	6	1.204603	0.704506	-0.832235	65.4629	1114.23900
	1	1.895694	-0.110887	-0.376868	117.2832	
	1	1.699801	1.660938	-0.669357	228.6819	
	1	0.045376	2.402158	0.898821	280.4981	
	8	2.449529	-1.084256	0.565979	291.9956	
	1	2.043310	-0.691567	1.356017	311.4124	

	1	1.186683	0.448129	-1.894293	411.8596	
	6	-0.912410	-0.642420	-0.536336	426.8327	
	1	-0.262837	-1.504537	-0.342511	493.8255	
	1	-1.073671	-0.637810	-1.621023	662.0630	
	1	-1.519307	1.457150	1.171739	761.4259	
	6	-2.244002	-0.816436	0.182475	802.4704	
	1	-2.923869	0.009938	-0.036937	807.5429	
	1	-2.728939	-1.741516	-0.132479	907.0403	
	1	-2.104716	-0.862190	1.265063	951.3798	
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R21	6	-1.217084	1.060389	-0.925639	853.6418i	567.40719
	6	-0.831228	0.217336	0.033952	56.0501	695.58624
	6	0.528145	0.261382	0.661266	90.1948	994.61593
	1	1.044676	-0.729657	0.364382	129.9379	
	1	0.442477	0.155408	1.748630	185.1285	
	1	-0.574599	1.853070	-1.289902	235.4383	
	8	1.478236	-1.842651	-0.539304	248.6055	
	1	1.019103	-1.498748	-1.323635	292.3351	
	6	-1.726801	-0.877016	0.549306	401.5173	
	1	-1.940001	-0.725173	1.611641	409.7398	
	1	-1.230268	-1.847533	0.456529	503.6070	
	1	-2.205546	0.986883	-1.365114	637.5356	
	1	-2.672554	-0.910456	0.008244	740.3892	
	6	1.450835	1.401135	0.275708	801.4216	
	1	1.014722	2.365083	0.552109	817.0301	
	1	2.410802	1.302153	0.783386	943.1068	

	1	1.642103	1.410822	-0.799392	970.0695	
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R22	6	-1.364302	-1.065742	0.084038	1000.4636i	502.38620
	6	-0.079760	-0.895028	0.881257	52.4166	769.11795
	1	-1.786450	0.006028	-0.194897	108.4170	886.42173
	1	-1.225355	-1.568112	-0.873622	146.8136	
	1	-2.163444	-1.540821	0.653176	187.7445	
	6	0.938278	-0.027332	0.180804	268.0842	
	1	-0.304188	-0.474594	1.864169	315.0643	
	1	0.361770	-1.886882	1.048447	363.4588	
	6	1.427417	1.071781	0.755233	407.4481	
	1	1.117154	1.375313	1.749542	436.7105	
	8	-1.892022	1.348939	-0.472969	533.4063	
	1	-0.980303	1.598908	-0.241955	694.3198	
	1	2.163420	1.690721	0.253767	727.6748	
	6	1.347716	-0.460165	-1.200882	790.0820	
	1	1.628240	-1.517991	-1.206082	880.7968	
	1	0.518694	-0.341759	-1.905106	939.5401	
	1	2.190539	0.126594	-1.566377	948.3570	
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R23	6	0.350764	0.492933	-0.112572	838.5251i	489.45835
	6	-0.759132	-0.232605	-0.026344	89.6197	763.66373
	1	1.346269	-0.116639	-0.279958	100.6833	1208.11226
	6	-0.733818	-1.737538	-0.093724	104.5836	
	6	-2.136202	0.365322	0.124410	116.2511	
	6	0.595506	1.964754	-0.047353	158.3773	
	1	-1.368610	-2.089452	-0.912645	192.6513	
	1	0.276410	-2.116203	-0.246464	246.7076	
	1	-1.138309	-2.165350	0.829159	287.2988	
	1	-2.615084	-0.028617	1.026027	380.5144	
	1	-2.128132	1.451935	0.184876	406.8425	
	1	-2.762073	0.073583	-0.724170	517.6904	
	1	-0.312529	2.519280	0.195205	580.7806	
	1	1.345664	2.193097	0.713870	760.8098	
	1	0.981539	2.334278	-1.000671	877.7102	
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R24	6	1.189024	-0.662483	-0.245575	859.9117i	388.33530
	6	0.175373	0.201166	-0.391831	46.9349	1077.45264
	6	-1.050682	-0.198496	-1.139205	89.0708	1135.93342
	1	-1.927915	-0.290493	-0.389043	107.5298	
	1	-0.964193	-1.161178	-1.642211	111.9327	
	1	1.075869	-1.640237	-0.711191	192.3402	
	8	-2.652810	-0.506915	0.888477	221.0566	
	1	-1.919924	-0.978487	1.317357	305.7892	
	1	-1.398618	0.571930	-1.832348	329.3357	
	6	0.126587	1.592762	0.178808	400.2017	
	1	-0.786463	1.712342	0.770032	443.3195	
	1	0.980789	1.832257	0.808736	524.2067	
	1	0.080936	2.328742	-0.629879	714.7804	
	6	2.487849	-0.448316	0.470810	793.4231	
	1	2.567287	0.538026	0.924853	838.0530	
	1	2.618840	-1.196344	1.258212	928.4640	
	1	3.326971	-0.569038	-0.220381	967.7108	
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R25-cis	6	-1.343635	0.260040	-0.355918	930.7670i
	6	-0.163979	0.617757	0.168787	27.9537
	6	0.605254	-0.212966	1.137377	77.7585
	1	1.461115	-0.746039	0.565036	95.4855
	8	2.217348	-1.320251	-0.569325	181.5305
	1	1.476015	-1.255152	-1.193840	235.0282
	1	1.135377	0.394895	1.873743	244.1788
	6	0.517204	1.898821	-0.236042	293.6596
	1	1.523160	1.688351	-0.612972	318.1588
	1	0.630877	2.563546	0.625645	392.4317
	1	-1.799282	0.949655	-1.064046	423.6241
	6	-2.131753	-0.985622	-0.080788	523.3443
	1	-3.092471	-0.739220	0.381061	709.6853
	1	-2.357392	-1.506410	-1.015580	797.5968
	1	-1.611406	-1.684638	0.572346	838.0437
	1	-0.041723	2.427084	-1.009084	911.8267
	1	0.038402	-0.998241	1.631789	968.4630
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				1502.4409	
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R25-trans	6	-2.488468	-0.446756	0.471839	858.8932i
	6	-1.189669	-0.662988	-0.243970	46.3865
	1	-2.567053	0.540102	0.924901	89.0131

	1	-3.327508	-0.567277	-0.219497	107.7320	
	6	-0.175618	0.199888	-0.391944	112.1212	
	6	1.050214	-0.201692	-1.138687	185.2474	
	1	1.398149	0.567202	-1.833541	220.9753	
	1	1.927678	-0.292381	-0.388751	305.7599	
	1	0.963324	-1.165391	-1.639692	329.0533	
	1	-1.076991	-1.641684	-0.707704	400.1058	
	8	2.654407	-0.504360	0.888694	443.1903	
	1	1.921635	-0.973184	1.320786	524.1566	
	1	-2.620445	-1.193922	1.259885	714.1492	
	6	-0.126387	1.592739	0.175642	793.3623	
	1	-0.082499	2.326979	-0.634727	838.2074	
	1	-0.979614	1.833229	0.806517	928.6680	
	1	0.787634	1.714063	0.764991	967.7827	
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					3158.4387	
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R26-cis	6	-1.344256	1.012729	-0.559652	1183.9132i	417.31221
	6	-0.034465	0.855005	-0.602999	28.9959	1026.96480
	6	0.756246	-0.172165	0.161905	98.2207	1082.89974
	6	1.451466	-1.129257	-0.811958	160.0385	
	6	1.781066	0.520929	1.064752	196.9936	
	1	-1.983204	0.298655	0.170139	201.4534	
	1	0.549562	1.526156	-1.239073	240.9967	
	1	0.056976	-0.739211	0.783059	322.1717	
	1	2.031316	-1.876963	-0.265757	342.3659	
	1	0.726411	-1.648273	-1.442106	356.9661	
	1	2.138465	-0.581962	-1.464959	509.2135	

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	1	2.479969	1.114832	0.467574	736.9852	
	1	1.291679	1.186528	1.777995	804.2722	
	1	-1.942163	1.728494	-1.111701	868.9479	
	8	-2.590131	-0.752954	0.666057	929.6950	
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R26-trans	6	1.253549	-0.208002	0.706709	1227.5304i	273.69668
	6	0.227090	-0.078810	-0.112829	74.5798	1386.96428
	6	-1.216982	-0.007819	0.317742	78.8959	1510.51684
	6	-1.825724	1.330517	-0.112995	97.3243	
	6	-2.000572	-1.179960	-0.280377	208.9462	
	1	2.355333	-0.297354	0.233002	215.8246	
	1	1.226010	-0.253605	1.790949	239.3703	
	1	0.406831	-0.030384	-1.187578	288.6034	
	1	-1.252907	-0.077955	1.409773	350.2313	
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R27	6	-1.326048	1.683864	0.098176	842.6320i	569.34534
	6	-0.580488	0.602350	-0.046926	51.5313	756.12682
	6	0.899198	0.422098	0.090192	86.2291	936.48858
	6	1.216187	-0.508611	1.265479	142.7408	
	6	1.487278	-0.130115	-1.212123	200.6566	
	1	-1.128952	-0.399837	-0.341759	224.9781	
	1	1.328367	1.412098	0.291058	259.2584	
	1	2.296308	-0.631171	1.375102	290.4508	
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R28	6	-2.012030	-0.868701	-0.074556	558.9104i
	6	-0.924137	-0.386762	-0.670375	55.7488
	6	0.167846	0.402869	-0.015688	64.6514
	1	1.101460	-0.262853	-0.072251	125.1204
	1	-2.207625	-0.711773	0.980370	201.5918
	8	1.972885	-1.522470	-0.026178	213.9488
	1	1.218280	-2.132335	0.025534	248.2696
	1	-2.752285	-1.429178	-0.632794	302.0153
	1	-0.783796	-0.568424	-1.734992	363.8122
	6	0.517087	1.650202	-0.825146	371.3222
	1	-0.324173	2.350455	-0.806841	530.3530
	1	1.390862	2.151805	-0.405338	595.2058
	1	0.730438	1.401053	-1.866557	705.7273
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R29	6	0.098881	-1.429299	0.243103	997.8284i	498.77916
	6	-0.662177	-0.221746	-0.285466	73.7659	732.51957
	1	1.258034	-1.266528	0.069356	100.4420	1131.28003
	1	-0.018610	-1.570583	1.320236	134.3225	
	1	-0.133273	-2.350397	-0.294646	213.7220	
	6	-0.244802	1.024879	0.444929	292.4249	
	1	-0.423452	-0.096411	-1.346956	295.2290	
	6	0.336343	2.079502	-0.118627	315.6498	
	1	-0.446480	1.032708	1.516555	334.0569	
	1	0.544306	2.103112	-1.184490	382.5628	
	8	2.490601	-0.697372	-0.143428	505.1999	
	1	2.225031	0.219076	0.043927	693.6545	
	1	0.611157	2.953669	0.459992	757.1456	
	6	-2.174907	-0.443929	-0.140004	821.8469	
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R30-cis	6	2.448940	-0.838991	-0.379828	1157.9664i	399.28297
	6	1.289356	-1.210382	0.131324	43.5062	2008.53889
	6	0.218902	-0.285182	0.632838	73.8429	2252.69085
	6	-1.085635	-0.437068	-0.156126	112.4070	
	6	-2.193170	0.475610	0.364733	124.5348	
	1	-1.422109	-1.480051	-0.112357	141.6324	
	1	-0.892507	-0.215854	-1.211441	179.6787	
	1	0.576569	0.746256	0.572653	231.6159	
	1	0.021374	-0.506127	1.688645	246.8324	
	1	3.241574	-1.479266	-0.749124	364.9203	
	1	2.685844	0.337572	-0.471775	382.2956	
	1	1.063444	-2.278362	0.167965	456.7968	
	6	-3.491702	0.324819	-0.423148	565.7033	
	1	-2.374275	0.254901	1.422396	725.2509	
	1	-1.851183	1.514940	0.319349	739.5419	
	1	-3.868188	-0.699660	-0.362159	802.8017	
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R30-trans	6	-2.204962	0.401936	0.541610	1194.8937i
	6	-1.225917	0.145551	-0.306062	44.8518
	6	0.135483	0.784440	-0.262056	62.0248
	6	1.245320	-0.246989	-0.035858	72.5265
	6	2.640032	0.373677	-0.061358	113.5795
	1	1.178895	-1.025630	-0.804889	129.5107
	1	1.079859	-0.745910	0.925246	198.3570
	1	0.164812	1.543733	0.525079	228.7218
	1	0.314841	1.298715	-1.213905	246.1525
	1	-3.227621	-0.222455	0.434395	314.8363
	1	-1.385288	-0.602422	-1.081943	382.2483
	6	3.739290	-0.658631	0.176825	428.1283
	1	2.796892	0.865456	-1.027546	554.4615
	1	2.700075	1.159387	0.699524	734.7489
	1	3.707547	-1.442350	-0.584474	760.5945
	1	4.730675	-0.202641	0.147986	808.8324
	1	3.617646	-1.137513	1.151793	864.4437
	1	-2.200599	1.122186	1.353759	911.9597
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R31	6	-2.594325	-1.166896	-0.502488	917.0561i	493.19766
	6	-1.669425	-0.453656	0.116122	47.0854	1699.83702
	6	-0.295564	-0.840606	0.553252	71.6236	2043.00735
	6	0.789683	-0.010489	-0.140012	91.4642	
	6	2.198495	-0.391183	0.308230	122.0810	
	1	0.611949	1.050357	0.068710	128.7996	
	1	0.700927	-0.140246	-1.224835	180.5541	
	1	-0.147341	-1.906758	0.343414	220.2958	
	1	-0.209652	-0.707698	1.637474	248.0232	
	1	-1.938792	0.673396	0.350665	353.9824	
	6	3.272730	0.439593	-0.388715	375.3723	
	1	2.277310	-0.262482	1.393103	428.5498	
	1	2.366570	-1.455020	0.108770	599.2488	
	1	3.138471	1.503570	-0.177945	727.1432	
	1	4.274386	0.156119	-0.060380	738.9769	
	1	3.224917	0.306556	-1.472675	796.5600	
	1	-2.427304	-2.217498	-0.728765	861.8550	
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R32	6	-2.947708	-1.091392	0.168116	633.6835i	576.36821
	6	-1.866335	-0.562753	-0.399240	44.6364	1520.60320
	6	-0.649424	-0.124994	0.338660	56.2988	1959.89606
	1	-0.601506	1.020615	0.298884	73.2472	
	1	-3.001855	-1.245080	1.241371	102.9582	
	8	-0.715652	2.491570	-0.088091	119.0580	
	1	-1.683481	2.477261	-0.170527	142.6712	
	1	-3.807093	-1.392358	-0.419261	188.5214	
	1	-1.842433	-0.426890	-1.479560	242.1387	
	6	0.666891	-0.595103	-0.268640	340.2673	
	1	0.687129	-0.323146	-1.330349	368.5990	
	1	0.709336	-1.690654	-0.223562	468.6349	
	6	1.883571	0.003735	0.432396	595.0603	
	1	1.816704	1.095305	0.380628	691.1948	
	1	1.854162	-0.261355	1.494910	733.1721	
	6	3.198021	-0.469560	-0.181688	791.3769	
	1	4.057724	-0.026689	0.324536	912.3143	
	1	3.292273	-1.556805	-0.115234	919.1470	
	1	3.253729	-0.194578	-1.238213	944.5456	
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R33	6	-2.988998	0.032337	-0.157967	731.6682i
	6	-1.978042	-0.601792	0.428777	65.5542
	6	-0.714615	-1.017998	-0.265433	81.3117
	6	0.517445	-0.338856	0.321103	104.2091
	6	1.821628	-0.663224	-0.385349	109.5913
	1	0.590844	-0.501899	1.402257	151.0338
	1	0.366543	0.808428	0.212612	174.6600
	1	-0.590565	-2.105223	-0.175244	259.8588
	6	3.000453	0.118610	0.187710	301.0037
	1	2.008630	-1.741574	-0.305516	366.2665
	1	1.711072	-0.443080	-1.451987	368.7523
	1	3.143732	-0.111895	1.246420	464.1303
	1	3.927561	-0.118638	-0.336860	657.0497
	1	2.823393	1.193020	0.099333	679.8332
	1	-2.965093	0.267889	-1.218187	722.1632
	1	-3.875252	0.321295	0.394713	803.9922
	1	-2.037726	-0.825643	1.492823	914.2943
	1	-0.785353	-0.788701	-1.333311	938.1228
	8	-0.147843	2.121996	-0.105389	955.1573
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R34	6	3.462652	-0.142649	-0.213343	546.6705i	530.59905
	6	2.338224	0.152205	0.429062	43.8225	1610.46901
	6	1.004723	0.355999	-0.226339	50.1813	1990.97026
	6	-0.035838	-0.664581	0.245577	73.0311	
	6	-1.397305	-0.454852	-0.394954	117.2833	
	1	-0.137842	-0.608335	1.335301	125.0528	
	1	0.629049	1.358844	0.007803	169.6480	
	6	-2.477294	-1.404731	0.091443	177.5377	
	1	-1.730013	0.610304	-0.111041	237.1140	
	1	-1.320481	-0.457706	-1.487310	356.9944	
	1	-2.596903	-1.332063	1.174737	363.4294	
	1	-3.440979	-1.188947	-0.372345	460.3225	
	1	-2.210293	-2.438964	-0.148329	627.4584	
	1	3.482625	-0.243591	-1.294287	659.6967	
	1	4.397838	-0.289593	0.313580	767.5890	
	1	2.355030	0.244648	1.513935	845.5636	
	1	1.117835	0.293434	-1.314002	912.1040	
	1	0.318316	-1.677425	0.015808	929.9185	
	8	-2.033680	2.039122	0.187598	953.3048	
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R35	6	-3.541071	0.338089	-0.453363	774.8461i	403.21543
	6	-2.415800	0.576323	0.210739	46.8213	2000.37993
	6	-1.374234	-0.454261	0.531735	59.1235	2258.24883
	6	-0.026965	-0.136619	-0.124677	81.9097	
	6	1.059743	-1.145100	0.239613	119.5911	
	1	0.302342	0.863034	0.179676	152.0644	
	1	-1.232437	-0.501717	1.618188	173.9464	
	6	2.380795	-0.849686	-0.442035	201.8183	
	1	1.200570	-1.155343	1.325038	317.6369	
	1	3.191324	-1.520396	-0.153879	359.0801	
	1	2.299011	-0.804163	-1.530194	366.1064	
	1	2.743710	0.203836	-0.090742	464.4236	
	1	-3.788818	-0.660307	-0.800715	656.3387	
	1	-4.252272	1.126823	-0.668035	725.8873	
	1	-2.200103	1.590955	0.542384	773.7505	
	1	-1.722143	-1.441174	0.209873	819.9416	
	1	-0.157800	-0.111718	-1.212743	885.8854	
	1	0.730843	-2.153718	-0.042166	937.2299	
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R36	6	-1.354197	-0.716096	-0.179573	878.7419i	409.34450
	6	0.045589	-0.811471	0.346574	38.1392	2108.94546
	1	-1.337117	-0.703977	-1.274127	64.4301	2395.86208
	1	-1.919309	-1.607269	0.120103	85.5010	
	6	1.148478	-0.802047	-0.404121	104.5234	
	6	2.530006	-0.858060	0.135276	164.0200	
	1	3.185704	-1.527462	-0.424673	192.9575	
	1	3.035440	0.175514	0.011578	242.6493	
	1	2.563964	-1.085422	1.200910	266.2579	
	6	-2.090264	0.524866	0.339909	312.5666	
	1	-1.538391	1.418805	0.032725	327.5179	
	1	-2.081802	0.515166	1.434893	395.4702	
	1	1.046149	-0.728092	-1.485648	534.7169	
	1	0.151015	-0.883289	1.429819	688.1923	
	8	3.223519	1.640326	-0.081975	748.8022	
	1	2.289190	1.853137	0.075839	812.0386	
	6	-3.528062	0.597830	-0.166298	882.2791	
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R37	6	-0.893614	-0.277653	-0.630231	880.4465i	499.37562
	6	-1.933588	-0.423359	0.486529	32.7480	1605.40863
	6	0.412059	-0.931025	-0.281268	66.7220	1965.10550
	6	1.564984	-0.303548	-0.109359	102.2921	
	6	2.900061	-0.849890	0.272159	120.0250	
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	1	-0.722918	0.780931	-0.846223	214.7077	
	1	2.836813	-1.930464	0.425168	228.5931	
	1	3.640712	-0.650047	-0.505512	237.2435	
	1	1.555401	0.866168	-0.285832	286.7892	
	1	0.397287	-2.015890	-0.151444	306.1687	
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	1	-3.683484	-0.241488	-0.784666	743.4387	
	1	-4.000746	0.109469	0.917121	830.1995	
	1	-3.142404	1.285230	-0.084521	869.7040	
	1	3.263341	-0.390296	1.194574	890.7711	
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R38	6	0.867958	-0.610203	-0.545013	869.6966i	488.71365
	6	1.808746	0.146416	0.398664	37.8552	1559.94474
	6	-0.568163	-0.266344	-0.321471	77.7853	1923.71968
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	1	1.142670	-0.379417	-1.580620	153.1799	
	1	0.994499	-1.691714	-0.411240	211.1124	
	1	-3.074112	0.496939	0.112642	231.6125	
	1	-3.679100	-1.089492	-0.401463	248.1916	
	1	-0.811351	0.881774	-0.475479	284.4821	
	6	3.272973	-0.210286	0.159387	301.6193	
	1	1.658192	1.221095	0.255872	372.6132	
	1	1.530674	-0.080489	1.433003	541.1298	
	1	3.567203	0.024816	-0.866779	605.8568	
	1	3.931938	0.342236	0.831545	748.9249	
	1	3.447000	-1.277358	0.320208	832.6163	
	1	-3.305455	-0.809938	1.293908	860.8688	
	1	-1.383913	-2.107740	0.154501	886.5068	
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R39	6	-2.055201	-0.244792	0.436545	606.3242i	531.43412
	6	-0.922313	-0.081413	-0.246288	43.6795	1634.45441
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	1	0.426049	2.688216	-0.034080	195.3245	
	1	-0.973795	0.111859	-1.318267	204.0087	
	6	1.432702	-1.006998	-0.433718	250.2526	
	1	1.441923	-0.676768	-1.477386	265.8587	
	1	1.075078	-2.042748	-0.432894	317.8602	
	6	2.840987	-0.927425	0.147708	396.3286	
	1	3.199751	0.104584	0.133335	530.1328	
	1	2.855028	-1.274436	1.184199	635.5287	
	1	0.407550	-0.423448	1.401974	720.3089	
	1	3.541198	-1.541081	-0.421724	793.4115	
	6	-3.429563	-0.187797	-0.157161	868.5967	
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R40	6	-0.512926	-0.992165	-0.267042	748.6961i	456.87916
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	6	0.859829	-0.737120	0.283699	70.4528	1848.64444
	6	1.879599	-0.243622	-0.416538	98.4574	
	6	3.248969	0.024034	0.132668	128.0166	
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	1	3.302055	-0.220156	1.194922	191.7403	
	1	4.001665	-0.568324	-0.394558	213.6573	
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	1	-3.015510	-0.142300	-1.190591	670.4725	
	1	3.525669	1.074347	0.006065	737.1501	
	1	1.724535	-0.023097	-1.472548	790.7001	
	1	1.007819	-0.962696	1.340210	891.7061	
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R41	6	-2.333288	1.061108	0.171002	773.5017i	305.14317
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	6	-0.111577	-0.151621	0.302943	83.9247	
	1	-0.956462	0.780968	-1.452751	135.4271	
	1	-0.407527	1.916317	-0.230356	147.0158	
	6	1.272026	-0.275361	-0.263537	162.6256	
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	6	2.396460	-0.073838	0.417017	313.7522	
	1	2.326495	0.189019	1.472048	320.0972	
	1	1.336042	-0.537979	-1.319871	392.9039	
	8	-3.379858	-1.273621	-0.169090	540.5306	
	1	-3.259434	-1.535983	0.757392	727.8042	
	1	-2.943879	1.821049	-0.318487	784.3866	
	1	-2.365201	1.194709	1.254603	795.1844	
	6	3.778080	-0.185907	-0.154759	869.1596	
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R42	6	-2.614072	-0.590672	-0.233466	983.7352i
	6	-1.346594	-1.201887	0.343866	47.0632
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	1	-3.524612	-0.918384	0.269498	128.5617
	6	-0.109562	-0.690016	-0.337197	164.3840
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	1	0.778124	0.183386	1.337199	375.0125
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	1	3.431094	0.087090	1.266343	912.3421
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R43	6	0.976942	-0.502128	0.373579	630.2338i	533.87150
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	1	0.985963	-0.495175	1.464167	80.4945	
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R47	6	-1.356262	-0.769397	0.343886	643.2651i	546.12307
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