

Supporting Information

The kinetic model of cyclohexene-air combustion over a wide temperature range

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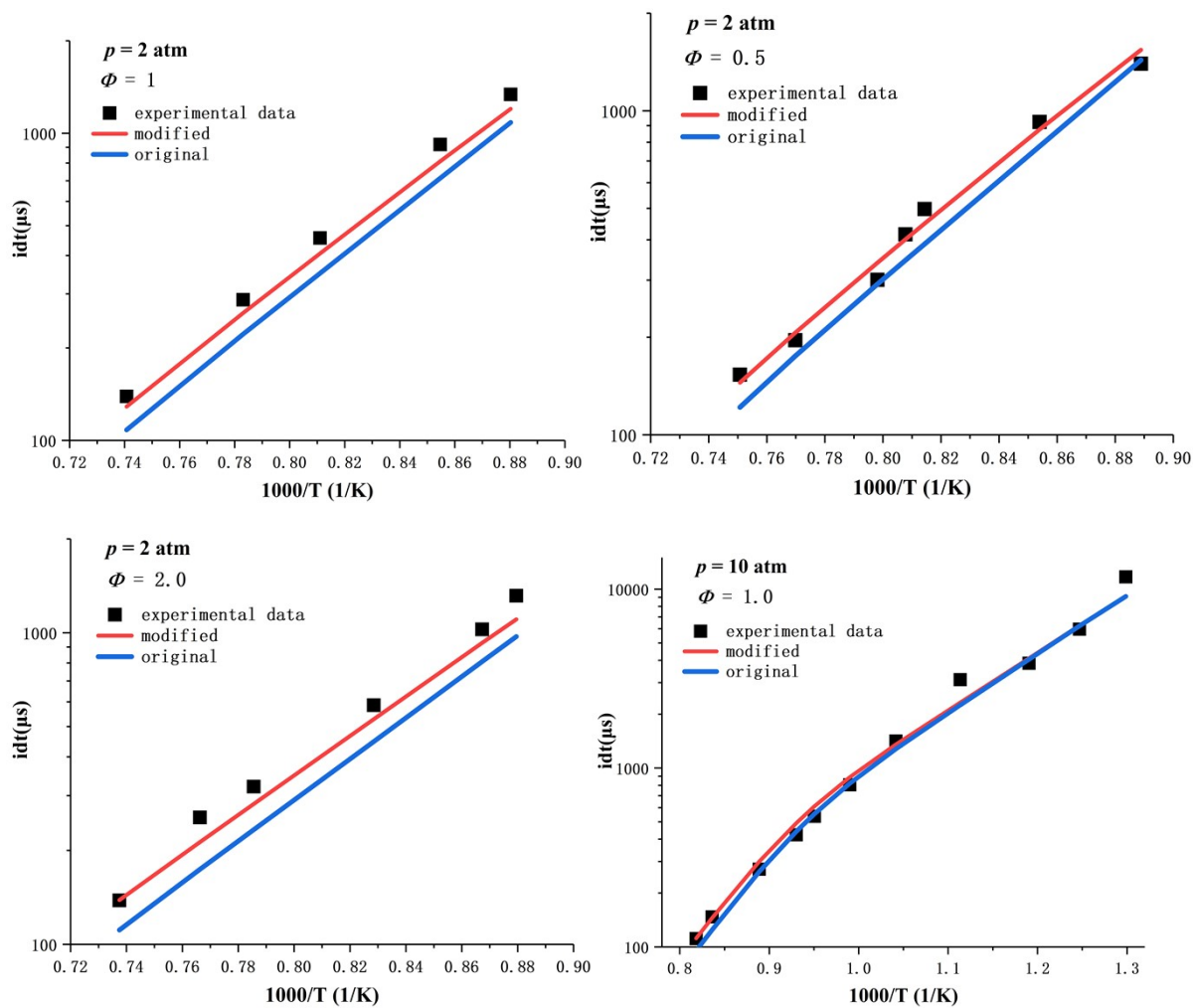


Fig. S1 The comparison of ignition delay time simulated by original and modified rate constant of reaction R5.

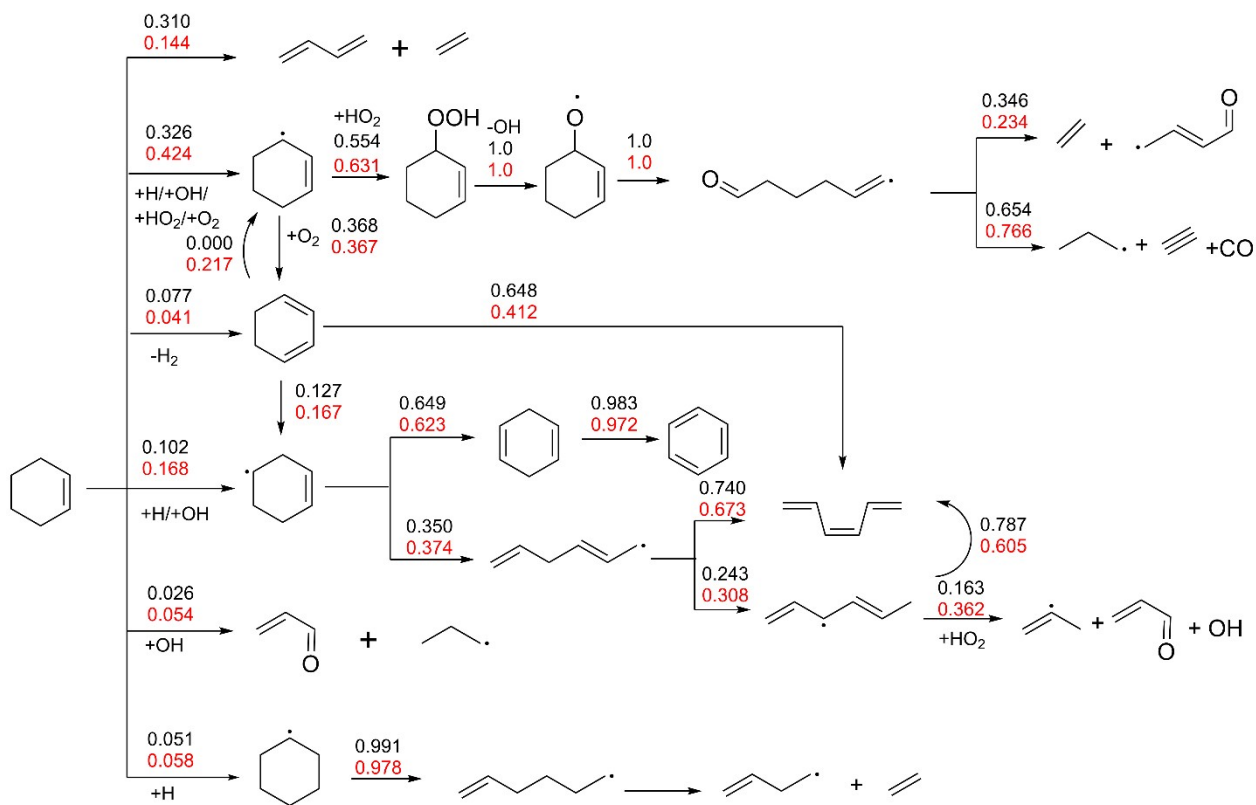


Fig. S2 The flux analysis of 80% cyclohexene consumption under $p = 2$ atm, $\Phi = 1.0$, and high temperature of 1200 K (red number) and 1350 K (black number).

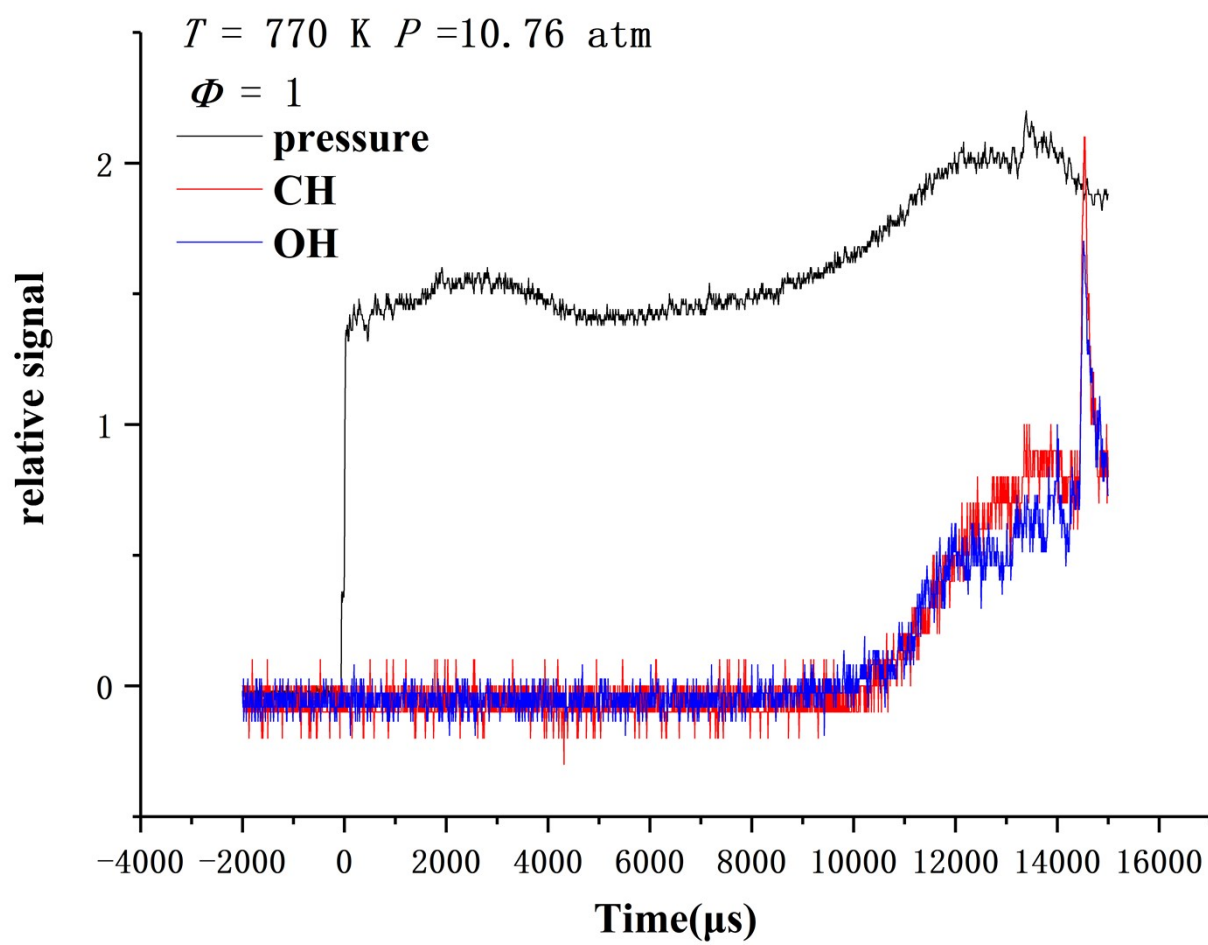


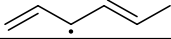
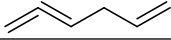

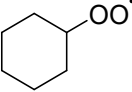
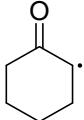


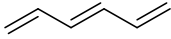
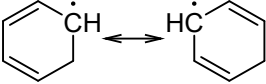

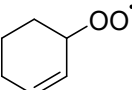
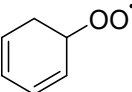
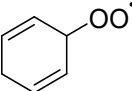
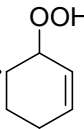
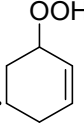
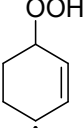
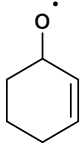
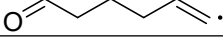
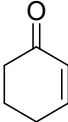
Fig. S3 The data of pressure history and CH* trace at $P = 10.76 \text{ atm}$, $T = 770 \text{ K}$, $\Phi = 1$.

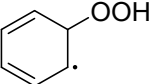
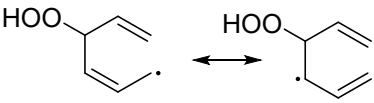

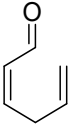
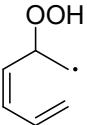


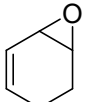
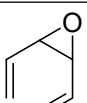


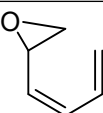
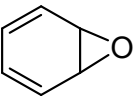
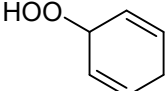
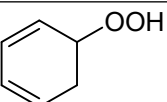
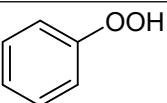
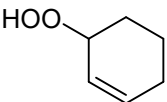
Table S1 The ignition delay time of cyclohexene-air mixture measured in this work.

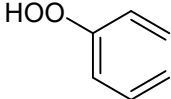
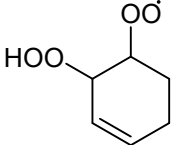
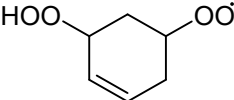
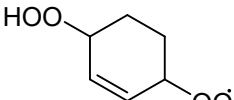
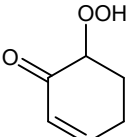
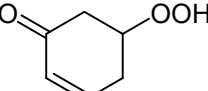
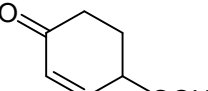
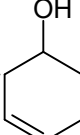
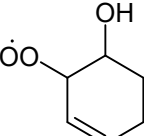
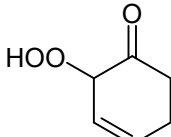
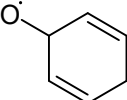
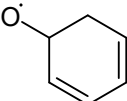
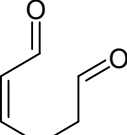
$\Phi=0.5$			$\Phi=1.0$			$\Phi=2.0$		
T (K)	p (atm)	τ_{ign} (μs)	T (K)	p (atm)	τ_{ign} (μs)	T (K)	p (atm)	τ_{ign} (μs)
1332	2.16	142	1350	2.14	130	1356	2.25	123
1299	2.2	178	1277	2.05	280	1305	2.22	230
1253	2.11	285	1233	2.23	409	1273	2.22	289
1238	2.09	398	1170	2.12	867	1207	2.23	525
1228	2.04	488	1136	2.13	1257	1153	2.14	958
1171	2.11	876	1222	9.76	114	1137	2.16	1217
			1196	10.58	139			
			1125	10.1	269			
			1075	10	423			
			1052	10.03	535			
			1010	10.05	802			
			960	9.9	1429			
			898	10.88	2864			
			840	10.2	3775			
			802	10.43	5719			
			770	10.76	10885			

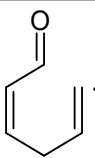
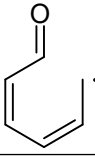
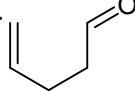
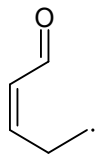
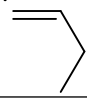
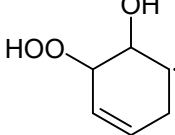
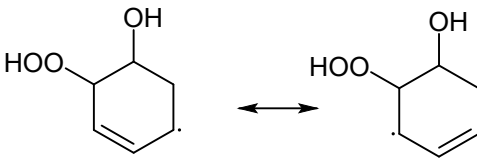
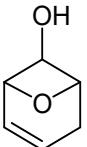
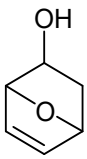
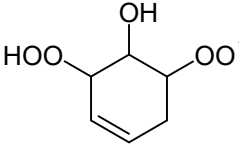
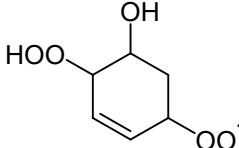
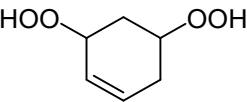
Table S2 Names and the corresponding molecular structures to the species involved in the kinetic model of cyclohexene.

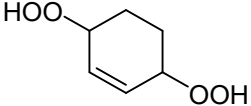
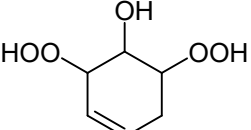
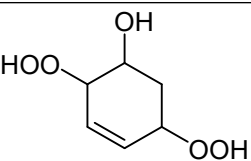
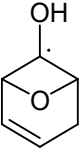
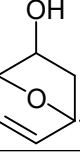



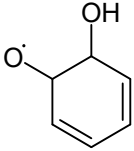
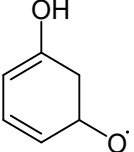


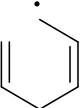
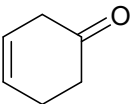
Name in the mechanism	Molecular structure	Molecular formula
C2H4		C ₂ H ₄
C4H6		C ₄ H ₆
C2H3CHOZ		C ₃ H ₄ O
R19C3H7		C ₃ H ₇
C5H10Z		C ₅ H ₁₀
C3H5Y		C ₃ H ₅
R10C2H3V		C ₂ H ₃
iC4H5		C ₄ H ₅
R13CH2CHO		C ₂ H ₃ O
R7CH3O		CH ₃ O
cC6H10O		C ₆ H ₁₀ O
cC6H11		C ₆ H ₁₁
cC6H10OH		C ₆ H ₁₁ O
CH3cC6H10		C ₇ H ₁₃
CH3cC6H9		C ₇ H ₁₂
C6H11-16		C ₆ H ₁₁
cC6H10O2H-2		C ₆ H ₁₁ O ₂
SOOcC6O2H		C ₆ H ₁₁ O ₄
SOOcC6O		C ₆ H ₁₀ O ₃
C6H9-5		C ₆ H ₉
C6H9-6		C ₆ H ₉
C6H9-7		C ₆ H ₉
C6H9-8		C ₆ H ₉
C6H9-9		C ₆ H ₉

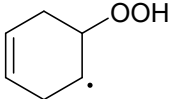
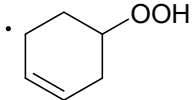
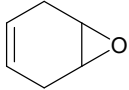
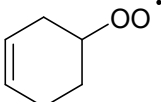
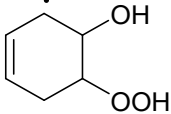
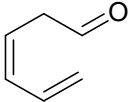
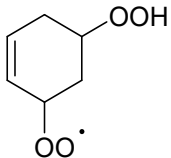
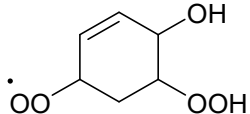
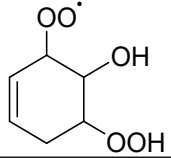
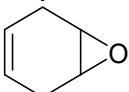
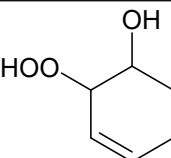
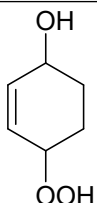
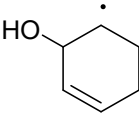
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C6H8-125		C ₆ H ₈
C6H8T		C ₆ H ₈
cC6H11O2		C ₆ H ₁₁ O ₂
RC6H9OK		C ₆ H ₉ O
CYHEXDN13		C ₆ H ₈
bicyclohexene		C ₆ H ₈
HXT_trans		C ₆ H ₈
C6H7		C ₆ H ₇
CYHEXEN-3J		C ₆ H ₉
xC6H9OO-1		C ₆ H ₉ O ₂
xC6H7OO-1		C ₆ H ₇ O ₂
xC6H7OO-2		C ₆ H ₇ O ₂
xC6H8OOH-1		C ₆ H ₉ O ₂
xC6H8OOH-2		C ₆ H ₉ O ₂
xC6H8OOH-3		C ₆ H ₉ O ₂
xC6H9O-1		C ₆ H ₉ O
C6H9O-1		C ₆ H ₉ O
xC5H8CO-1		C ₆ H ₈ O

xC6H6OOH-1		C ₆ H ₇ O ₂
C6H8OOH-4		C ₆ H ₉ O ₂
IC6H8		C ₆ H ₈
C5H7CHO-1		C ₆ H ₈ O
C6H8OOH-5		C ₆ H ₉ O ₂
C6H9-2		C ₆ H ₉
C6H6		C ₆ H ₆
xC6H8O-1		C ₆ H ₈ O
xC6H8O-2		C ₆ H ₈ O
xC6H8O-3		C ₆ H ₈ O
xC6H8O-4		C ₆ H ₈ O
xC6H8O-5		C ₆ H ₈ O
xC6H6O-1		C ₆ H ₆ O
xC6H7OOH-1		C ₆ H ₈ O ₂
xC6H7OOH-2		C ₆ H ₈ O ₂
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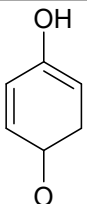
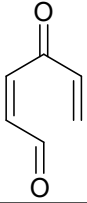
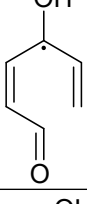
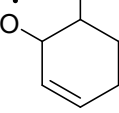
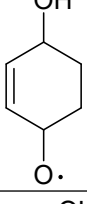
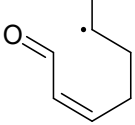
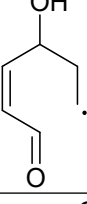

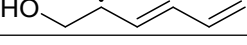
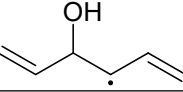
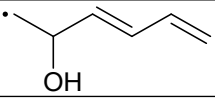
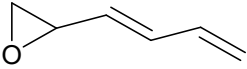
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xC6H8OOHOO-1		C ₆ H ₉ O ₄
xC6H8OOHOO-2		C ₆ H ₉ O ₄
xC6H8OOHOO-3		C ₆ H ₉ O ₄
xC5H7OOHCO-1		C ₆ H ₈ O ₃
xC5H7OOHCO-2		C ₆ H ₈ O ₃
xC5H7OOHCO-3		C ₆ H ₈ O ₃
xC6H8OH-1		C ₆ H ₉ O
xC6H8OHOO-1		C ₆ H ₉ O ₃
xC5H7OOHCO-4		C ₆ H ₈ O ₃
xC6H7O-1		C ₆ H ₇ O
xC6H7O-2		C ₆ H ₇ O
C4H6CHOCHO-1		C ₆ H ₈ O ₂

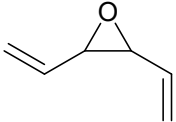
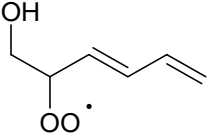
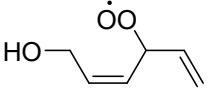
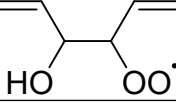
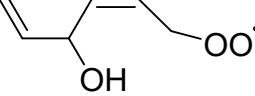
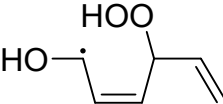
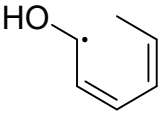
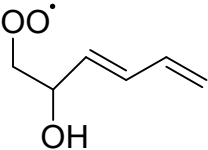
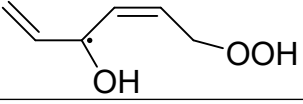
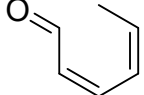
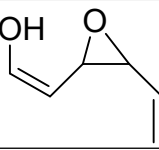
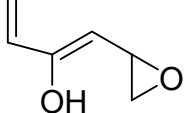
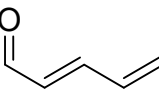
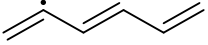
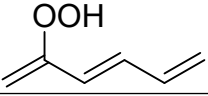
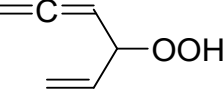
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C6H7O-4		C ₆ H ₇ O
C4H6CHO-1		C ₅ H ₇ O
C4H6CHO-2		C ₅ H ₇ O
C4H7-3		C ₄ H ₇
xC6H7OHOOH-1		C ₆ H ₉ O ₃
xC6H7OHOOH-2		C ₆ H ₉ O ₃
xC6H7OHO-1		C ₆ H ₈ O ₂
xC6H7OHO-2		C ₆ H ₈ O ₂
xC6H7OHOOHOO-1		C ₆ H ₉ O ₅
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xC6H8OOHOOH-2		C ₆ H ₁₀ O ₄

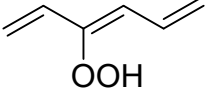
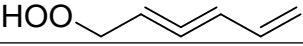
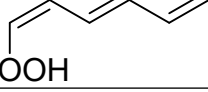
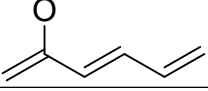
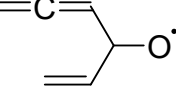
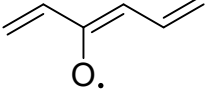
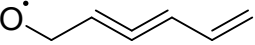
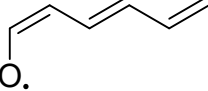
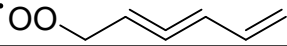
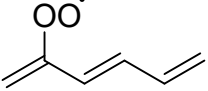
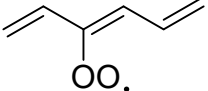
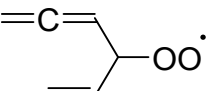
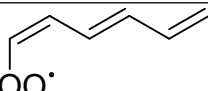
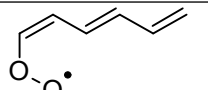
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xC6H7OHOOHOOH-1		$C_6H_{10}O_5$
xC6H7OHOOHOOH-2		$C_6H_{10}O_5$
xC6H6OHO-3		$C_6H_7O_2$
xC6H6OHO-5		$C_6H_7O_2$
CYHEXEN		C_6H_{10}
xC6H7O-7		C_6H_7O
xC6H7O-9		C_6H_7O
xC6H6OHO-7		$C_6H_7O_2$
xC6H6OHO-8		$C_6H_7O_2$
CYHEXDN14		C_6H_8
CYHEXEN-4J		C_6H_9
C6H9-4		C_6H_9
xC5H8CO-2		C_6H_8O

XC6H8OOH-7		$C_6H_9O_2$
XC6H8OOH-6		$C_6H_9O_2$
XC6H8O-6		C_6H_8O
xC6H9OO-2		$C_6H_9O_2$
xC6H7OHOOH-3		$C_6H_9O_3$
C5H7CHO-2		C_6H_8O
xC6H8OOHOO-4		$C_6H_9O_4$
xC6H7OHOOHOO-5		$C_6H_9O_5$
xC6H7OHOOHOO-4		$C_6H_9O_5$
xC6H7O-10		C_6H_7O
xC6H8OHOOH-1		$C_6H_{10}O_3$
xC6H8OHOOH-3		$C_6H_{10}O_3$
xC6H8OH-3		C_6H_9O

xC6H8OHOO-3		C ₆ H ₈ O ₃
xC6H8OHOO-4		C ₆ H ₉ O ₃
xC6H7OHOOH-4		C ₆ H ₉ O ₃
xC6H7OHO-3		C ₆ H ₈ O ₂
xC6H7OHO-4		C ₆ H ₈ O ₂
xC6H7OHOOHOO-6		C ₆ H ₉ O ₅
xC6H7OHOOH-5		C ₆ H ₉ O ₃
xC6H7OHOOH-6		C ₆ H ₉ O ₃
xC6H7OHO-5		C ₆ H ₈ O ₂
xC6H6OHO-6		C ₆ H ₇ O ₂

xC6H6OHO-9		C ₆ H ₇ O ₂
C4H5COCHO-1		C ₆ H ₆ O ₂
C5H5OHCHO-1		C ₆ H ₇ O ₂
xC6H8OHO-1		C ₆ H ₉ O ₂
xC6H8OHO-2		C ₆ H ₉ O ₂
C5H7OHCHO-1		C ₆ H ₉ O ₂
C5H7OHCHO-2		C ₆ H ₉ O ₂
C3H6OH-1		C ₃ H ₇ O
IC6H8OH-1		C ₆ H ₉ O
IC6H8OH-2		C ₆ H ₉ O
IC6H8OH-3		C ₆ H ₉ O
IC6H8O-2		C ₆ H ₈ O

IC6H8O-1		C_6H_8O
IC6H8OHOO-1		$C_6H_9O_3$
IC6H8OHOO-2		$C_6H_9O_3$
IC6H8OHOO-3		$C_6H_9O_3$
IC6H8OHOO-4		$C_6H_9O_3$
IC6H7OHOOH-2		$C_6H_9O_3$
IC6H8OH-4		C_6H_9O
IC6H8OHOO-5		$C_6H_9O_3$
IC6H7OHOOH-4		$C_6H_9O_3$
IC5H7CHO-1		C_6H_8O
IC6H7OHO-1		$C_6H_8O_2$
IC6H7OHO-2		$C_6H_8O_2$
IC4H5CHO-1		C_5H_6O
IC6H7-1		C_6H_7
IC6H7OOH-1		$C_6H_8O_2$
IC6H7OOH-2		$C_6H_8O_2$

IC6H7OOH-3		$C_6H_8O_2$
IC6H7OOH-4		$C_6H_8O_2$
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IC6H7O-4		C_6H_7O
IC6H7O-5		C_6H_7O
IC6H7O2-1		$C_6H_7O_2$
IC6H7O2-2		$C_6H_7O_2$
IC6H7O2-3		$C_6H_7O_2$
IC6H7O2-4		$C_6H_7O_2$
IC6H7O2-5		$C_6H_7O_2$
IC6H7O2-6		$C_6H_7O_2$