

SupplementaryMaterial:

Understanding the Reactivity of Unsaturated Alcohols: Experimental and Kinetic Modeling Study of the oxidation of 3-methyl-2-butenol and 3-methyl-3-butenol

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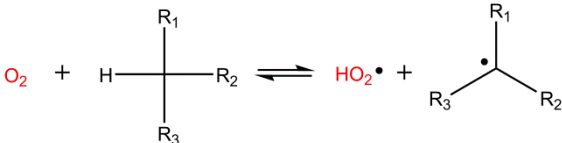

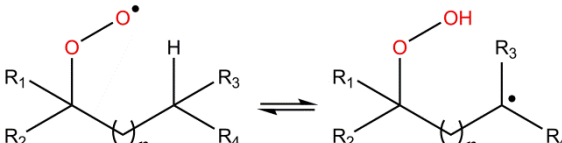
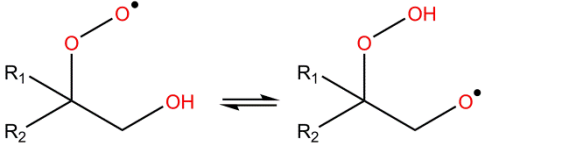
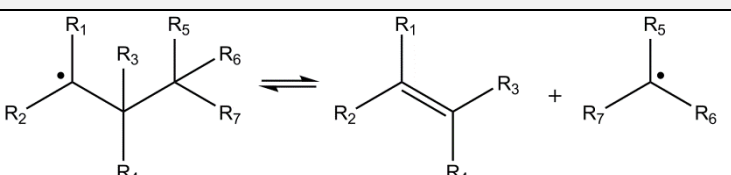
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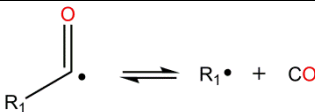
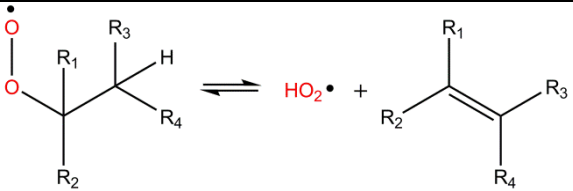
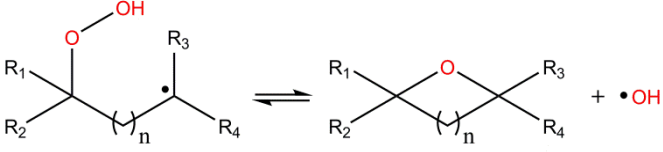
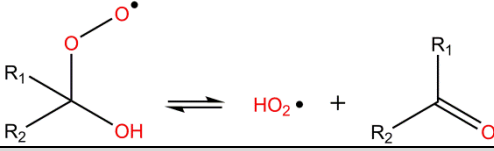
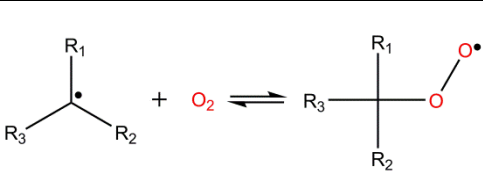
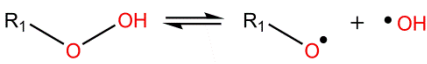
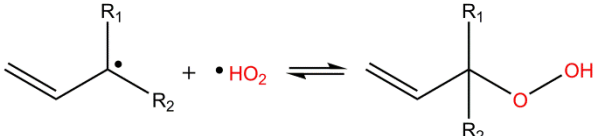
Reaction families in Genesys

Table S 1k [bimolecular - $\text{m}^3 \text{mol}^{-1} \text{s}^{-1}$; unimolecular - s^{-1}] = $A T^n \exp(-E_a/RT)$ where $R = 8.314 \cdot 10^{-3} \text{ kJ K}^{-1} \text{ mol}^{-1}$

Reaction family	Comment	Kinetic parameters			Ref	
		<i>A</i>	<i>n</i>	<i>E_a</i>		
Hydrogen abstraction						
<i>Intermolecular</i>						
by C• from C-H			Group additivity		[1, 2]	
		H abstr from C(=O)-H by CH ₃	2.5e-6	3.6	18.1	[3]
by H• from C-H			Group additivity		[4]	
		H abstr from C(=O)-H	7.15e-1	2.4	6.6	[3]
by •OH from C-H		R ₁ , R ₂ , R ₃ alkyl chains or H atoms	Rate rules for alkanes		[5, 6]	
		R ₁ , R ₂ H atoms R ₃ C=C	7.80e-1	2.3	-5.7	[7]
		R ₁ H atom R ₂ alkyl chain R ₃ C=C	7.50e-2	2.4	-3.9	[7]
		R ₁ H atom R ₂ OH R ₃ alkyl chain	1.15e-2	2.6	-8.7	[7]
		R ₁ H atom R ₂ OH R ₃ C=C	2.55e-2	2.6	-13.3	[7]
		H abstr from C(=O)-H	6.13e-2	2.7	-19.2	[3]
by HO ₂ • from C-H		R ₁ , R ₂ , R ₃ alkyl chains or H atoms	Rate rules for alkanes		[8]	

		R ₁ , R ₂ or R ₃ OH	1.23e-11	5.26	31.3	[9]
		R ₁ , R ₂ or R ₃ C=C	7.68e-2	4.4	56.7	[10]
		H abstr from C(=O)-H	1.18e-10	4.9	15.4	[3]
by O ₂ from C-H			1.00e7	0.0	ΔH _r	[11, 12]
Intramolecular						
by C• from C-H			Group additivity + rate rule A = function of # hindered rotors in TS E _a = ring strain in TS + activation energy analogous bimolecular reaction			[1, 2, 13]
by R-O-O• from C-H		Formation of alkyl radical	Rate rules for alkanes			[14]
		Formation of allylic radical	2.24e6	1.29	59.6	[15]
by R-O-O• from O-H		Analogy with 2-peroxy-2-methylpropan-1-ol	2.91e12	-0.23	93.3	[16]
β-scission/ radical addition						
Carbon-centered radicals						
•C-C-C ⇌ C=C + •C			Group additivity			[17]

$\bullet\text{C-C-H} \rightleftharpoons \text{C=C} + \bullet\text{H}$			Group additivity			[18]
$\bullet\text{C-C-OH} \rightleftharpoons \text{C=C} + \bullet\text{OH}$		Analogy with 2-hydroxy-ethyl to ethene plus OH	3.00e13	0.0	112.1	^a
$\bullet\text{C-O-H} \rightleftharpoons \text{C=O} + \bullet\text{H}$		Analogy with acetaldehyde plus H to 1-hydroxy-ethyl	1.10e8	0.0	44.7	^a
$\bullet\text{C-O-OH} \rightleftharpoons \text{C=O} + \bullet\text{OH}$			9.00e14	0.0	6.28	
$\bullet\text{C-C-O-O-H} \rightleftharpoons \text{C=C} + \text{HO}_2\bullet$			Rate rules for alkanes			[14]
<i>Oxygen-centered radicals</i>						
$\bullet\text{O-C-C} \rightleftharpoons \text{C=O} + \bullet\text{C}$		R ₁ alkyl Analogy with 2-oxy-propane	6.00e13	0.22	59.0	^a
		R ₁ C=C Analogy with allyloxy	2.70e14	0.00	100.0	[19]
$\bullet\text{O-C-H} \rightleftharpoons \text{C=O} + \bullet\text{H}$		R ₁ or R ₂ C=C. Analogy with allyloxy	1.17e10	1.00	77.6	[19]
α-scission						

$C-C(=O)\cdot \rightleftharpoons C\cdot + CO$		Analogy with acetyl radical	3.30e12	0.62	72.4	^a
Concerted reactions						
$\cdot O-O-C-C-H \rightleftharpoons HO_2\cdot + C=C$			Rate rules for alkanes			[14]
Formation of cyclic ethers from hydroperoxy-alkyl radicals			Rate rules for alkanes			[14]
$\cdot O-O-C-OH \rightleftharpoons HO_2\cdot + C=O$		Analogy with alpha-hydroxy-ethylperoxy	2.60e8	1.128	44.5	[20]
Oxygen addition on carbon-centered radicals						
$C\cdot + O_2 \rightleftharpoons C-O-O\cdot$		R_1, R_2, R_3 alkyl chains or H atoms	Rate rules for alkanes			[14]
		R_1 C=C	5.78e1	1.59	4.5	[21]
		R_1 OH	4.05e7	-0.31	-1.4	[9]
Recombination / scission						
$C-O-O-H \rightleftharpoons CO\cdot + \cdot OH$		Analogy with allylhydroperoxide	3.35e10	0.60	-8.8	[19]
$C\cdot + HO_2\cdot \rightleftharpoons C-O-O-H$		Analogy with allylhydroperoxide	1.59e20	-1.50	179.3	[19]

^a CBS-QB3 calculations

Model performance isoprenol oxidation and pyrolysis

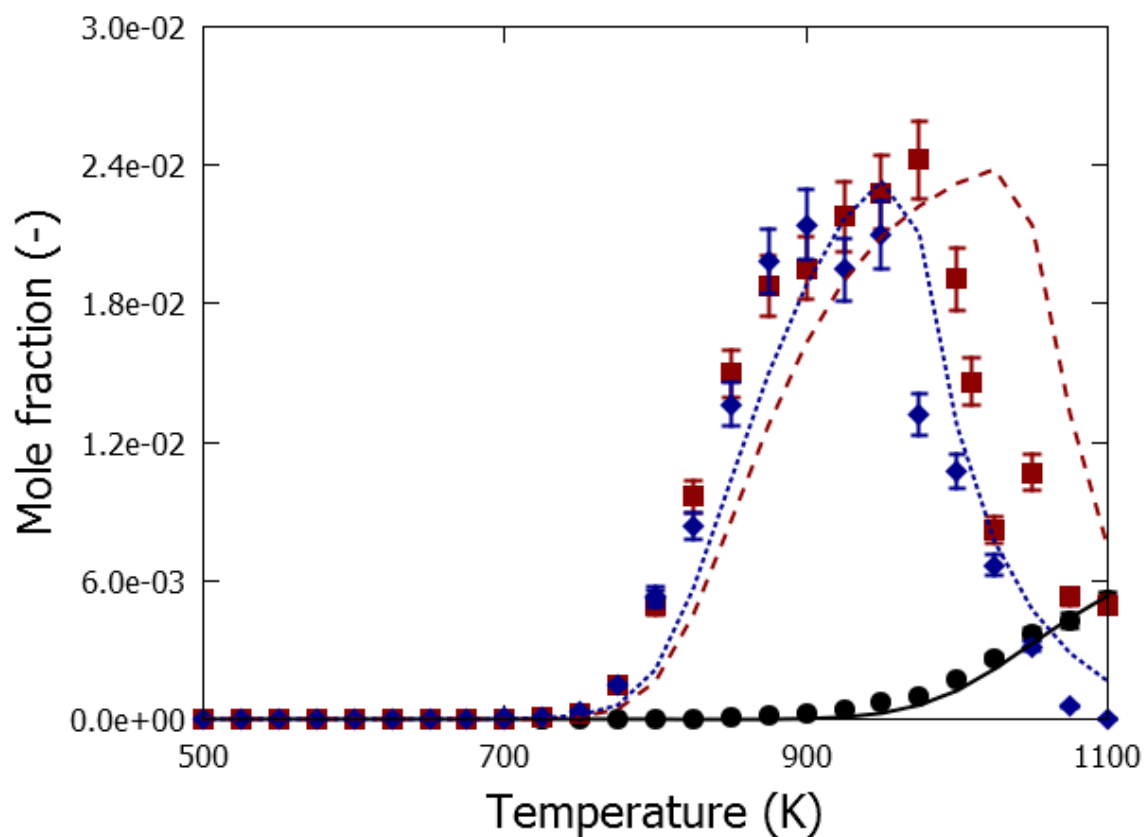


Fig. S 1CO mole fractions as a function of temperature for isoprenol oxidation and pyrolysis in a jet-stirred reactor, $P=0.107$ MPa, $F_V=4.06 \cdot 10^{-5} \text{ m}^3 \text{ s}^{-1}$, $x_{\text{isoprenol},0}=0.008$, $\varphi=0.5$ (blue), $\varphi=1.0$ (red) and $\varphi=\infty$ (black): symbols, experimental mole fraction profile; lines, mole fraction profiles calculated with CHEMKIN using the perfectly stirred reactor model and the developed kinetic model

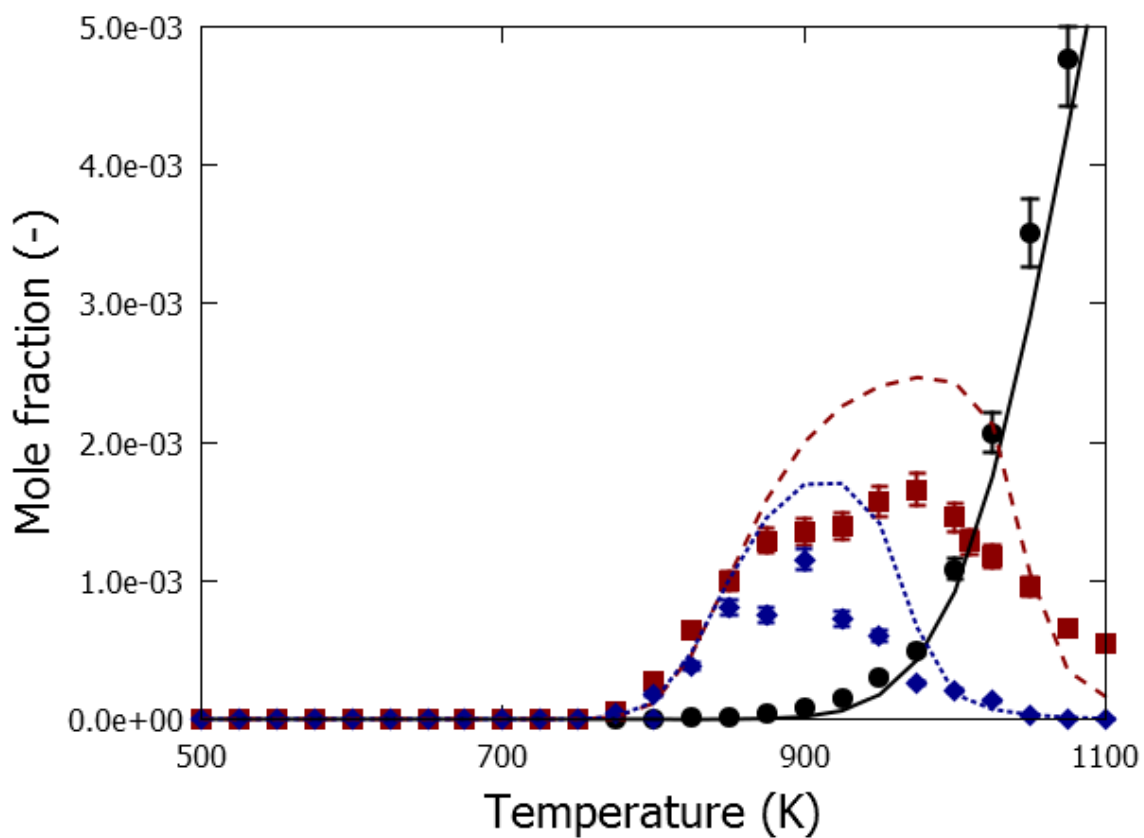


Fig. S 2 CH_4 mole fractions as a function of temperature for isoprenol oxidation and pyrolysis in a jet-stirred reactor, $P=0.107$ MPa, $F_V=4.06 \cdot 10^{-5} \text{ m}^3 \text{ s}^{-1}$, $x_{\text{isoprenol},0}=0.008$, $\phi=0.5$ (blue), $\phi=1.0$ (red) and $\phi=\infty$ (black): symbols, experimental mole fraction profile; lines, mole fraction profiles calculated with CHEMKIN using the perfectly stirred reactor model and the developed kinetic model

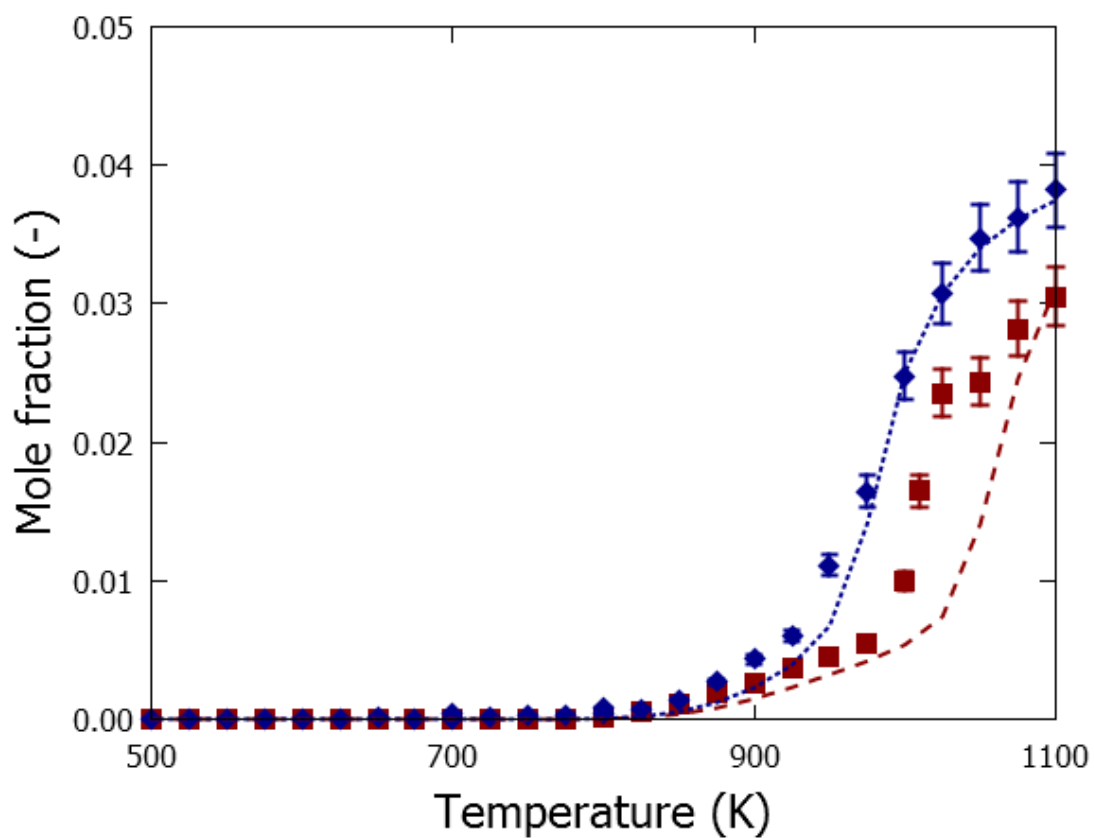


Fig. S 3CO₂ mole fractions as a function of temperature for isoprenol oxidation and pyrolysis in a jet-stirred reactor, $P=0.107$ MPa, $F_V=4.06 \cdot 10^{-5} \text{ m}^3 \text{ s}^{-1}$, $x_{\text{isoprenol},0}=0.008$, $\varphi=0.5$ (blue), $\varphi=1.0$ (red) and $\varphi=\infty$ (black): symbols, experimental mole fraction profile; lines, mole fraction profiles calculated with CHEMKIN using the perfectly stirred reactor model and the developed kinetic model

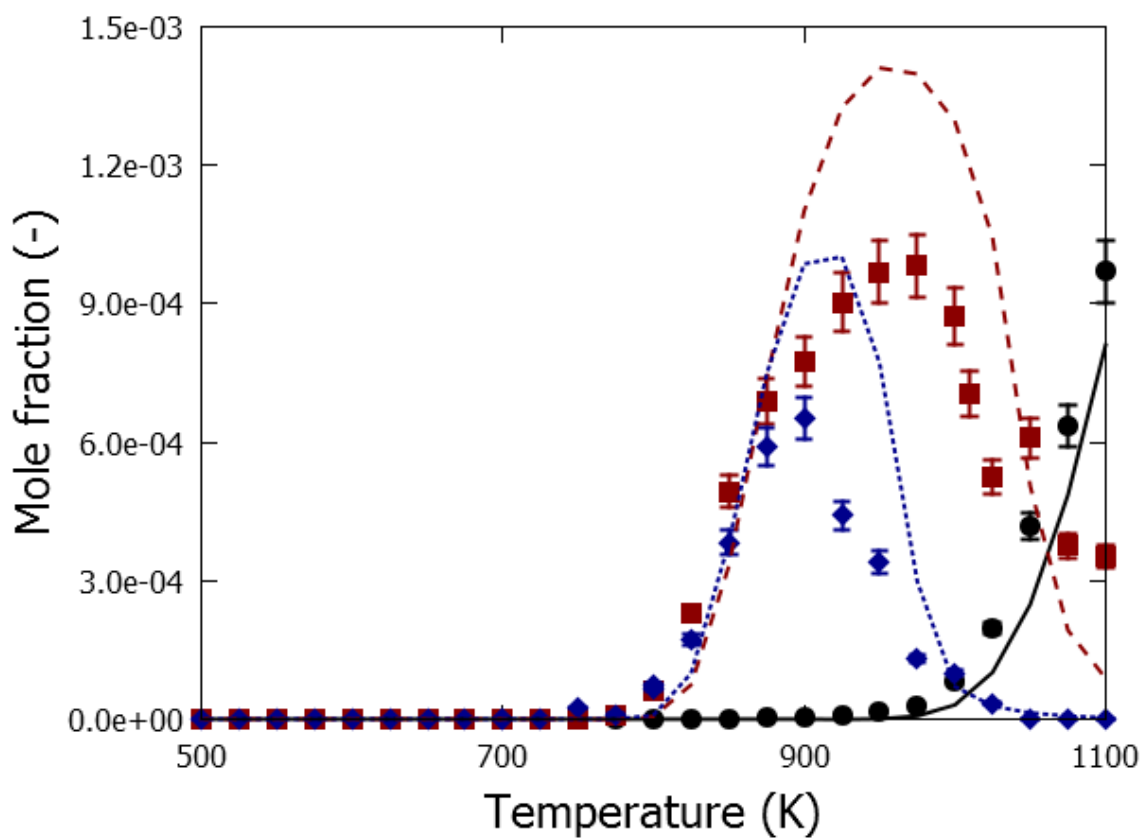


Fig. 8 $4C_2H_4$ mole fractions as a function of temperature for isoprenol oxidation and pyrolysis in a jet-stirred reactor, $P=0.107$ MPa, $F_V=4.06 \cdot 10^{-5} \text{ m}^3 \text{ s}^{-1}$, $x_{\text{isoprenol},0}=0.008$, $\phi=0.5$ (blue), $\phi=1.0$ (red) and $\phi=\infty$ (black): symbols, experimental mole fraction profile; lines, mole fraction profiles calculated with CHEMKIN using the perfectly stirred reactor model and the developed kinetic model

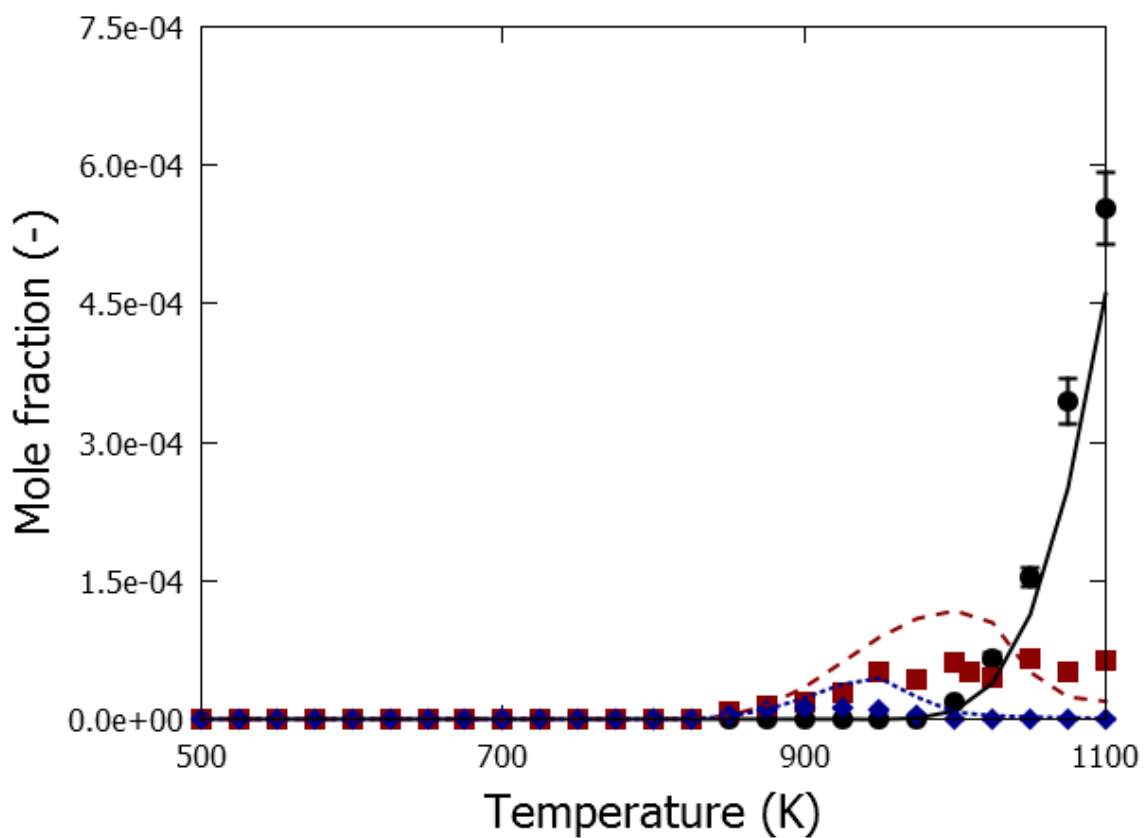


Fig. 8 $5C_2H_2$ mole fractions as a function of temperature for isoprenol oxidation and pyrolysis in a jet-stirred reactor, $P=0.107$ MPa, $F_V=4.06 \cdot 10^{-5} \text{ m}^3 \text{ s}^{-1}$, $x_{\text{isoprenol},0}=0.008$, $\phi=0.5$ (blue), $\phi=1.0$ (red) and $\phi=\infty$ (black): symbols, experimental mole fraction profile; lines, mole fraction profiles calculated with CHEMKIN using the perfectly stirred reactor model and the developed kinetic model

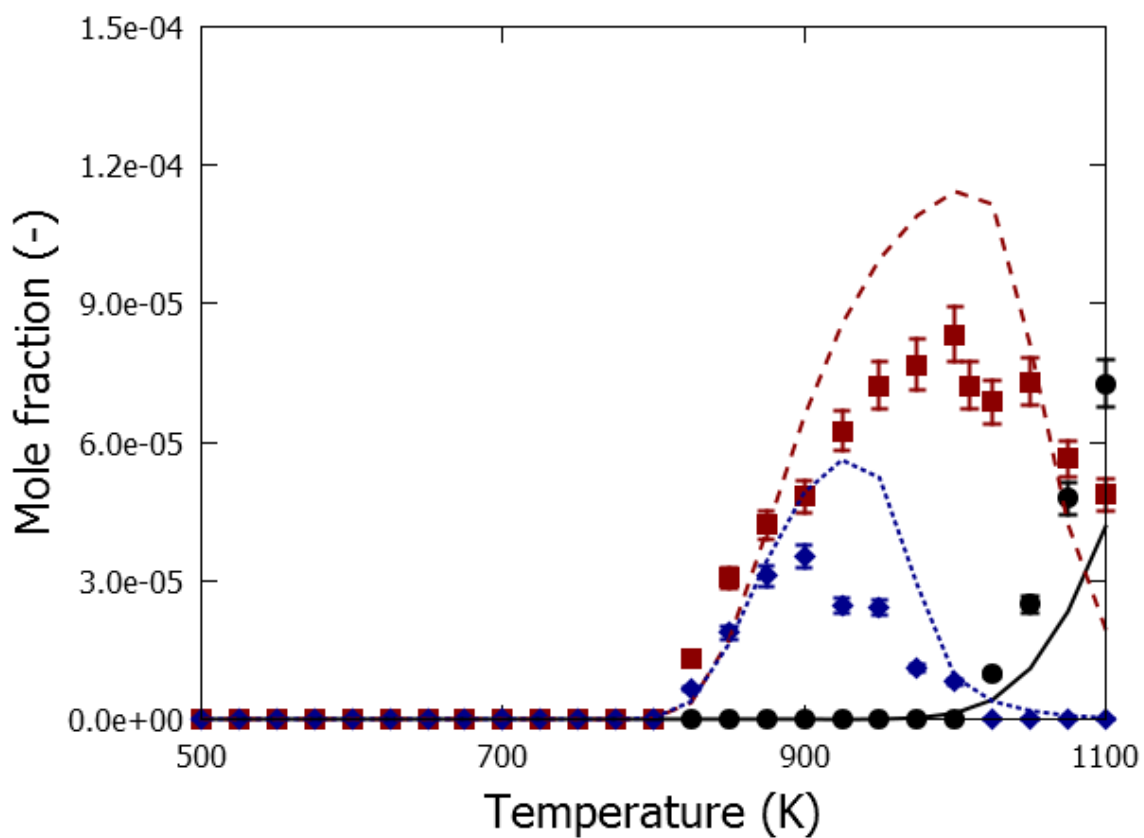


Fig. 8 $6C_2H_6$ mole fractions as a function of temperature for isoprenol oxidation and pyrolysis in a jet-stirred reactor, $P=0.107$ MPa, $F_V=4.06 \cdot 10^{-5} \text{ m}^3 \text{ s}^{-1}$, $x_{\text{isoprenol},0}=0.008$, $\phi=0.5$ (blue), $\phi=1.0$ (red) and $\phi=\infty$ (black): symbols, experimental mole fraction profile; lines, mole fraction profiles calculated with CHEMKIN using the perfectly stirred reactor model and the developed kinetic model

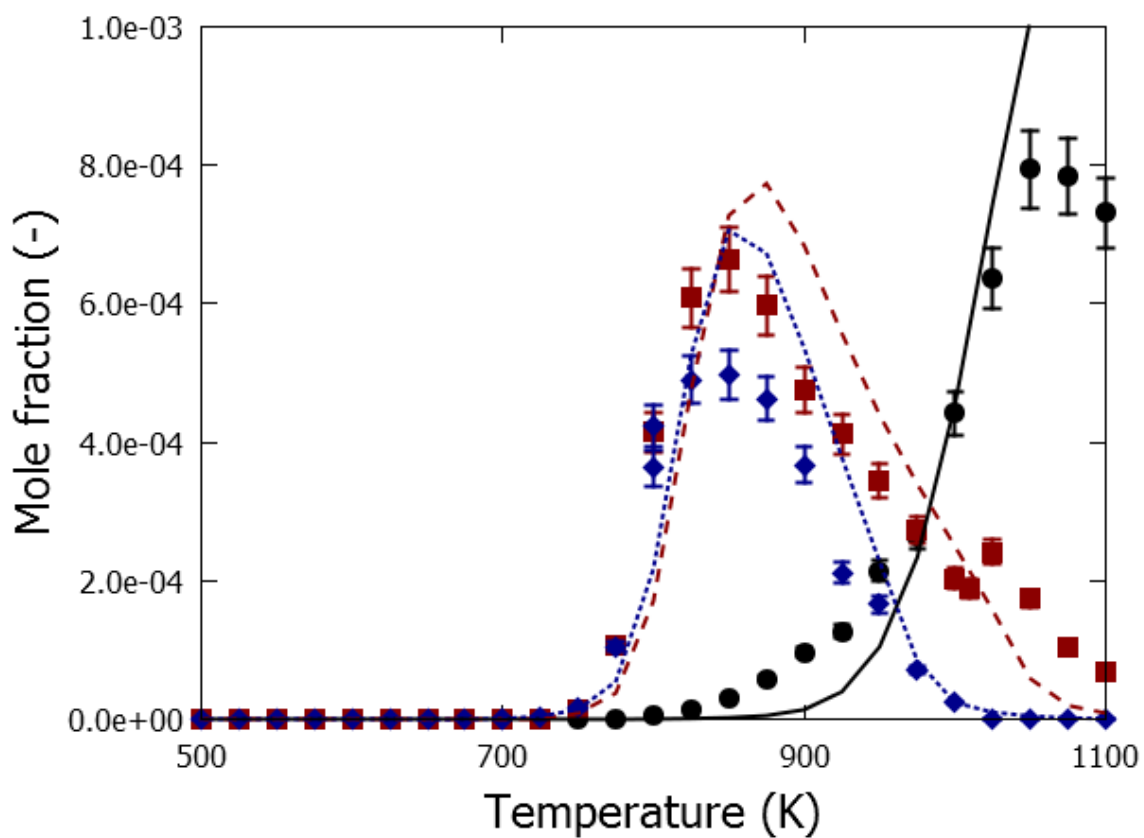


Fig. S $7C_3H_6$ mole fractions as a function of temperature for isoprenol oxidation and pyrolysis in a jet-stirred reactor, $P=0.107$ MPa, $F_V=4.06 \cdot 10^{-5} \text{ m}^3 \text{ s}^{-1}$, $x_{\text{isoprenol},0}=0.008$, $\phi=0.5$ (blue), $\phi=1.0$ (red) and $\phi=\infty$ (black): symbols, experimental mole fraction profile; lines, mole fraction profiles calculated with CHEMKIN using the perfectly stirred reactor model and the developed kinetic model

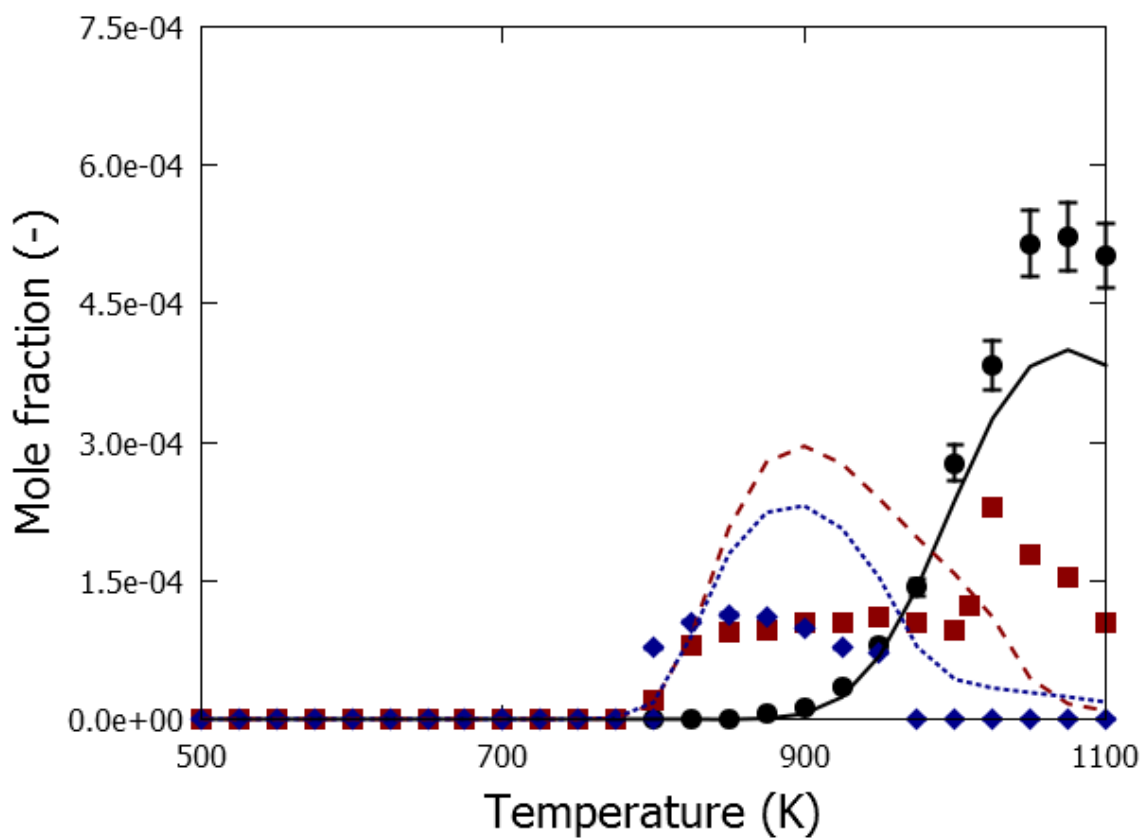


Fig. S 8 Allene mole fractions as a function of temperature for isoprenol oxidation and pyrolysis in a jet-stirred reactor, $P=0.107$ MPa, $F_V=4.06 \cdot 10^{-5} \text{ m}^3 \text{ s}^{-1}$, $x_{\text{isoprenol},0}=0.008$, $\phi=0.5$ (blue), $\phi=1.0$ (red) and $\phi=\infty$ (black): symbols, experimental mole fraction profile; lines, mole fraction profiles calculated with CHEMKIN using the perfectly stirred reactor model and the developed kinetic model

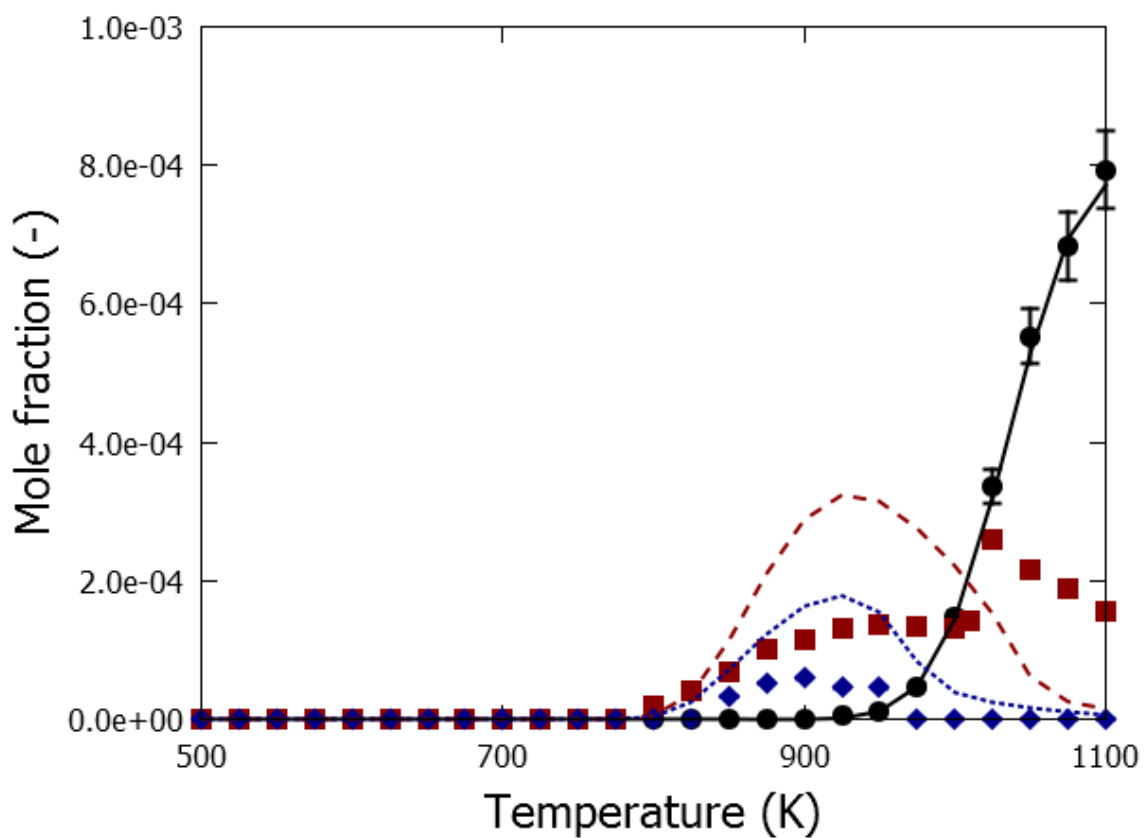


Fig. S 9 Propyne mole fractions as a function of temperature for isoprenol oxidation and pyrolysis in a jet-stirred reactor, $P=0.107$ MPa, $F_V = 4.06 \cdot 10^{-5} \text{ m}^3 \text{ s}^{-1}$, $x_{\text{isoprenol},0}=0.008$, $\phi=0.5$ (blue), $\phi=1.0$ (red) and $\phi=\infty$ (black): symbols, experimental mole fraction profile; lines, mole fraction profiles calculated with CHEMKIN using the perfectly stirred reactor model and the developed kinetic model

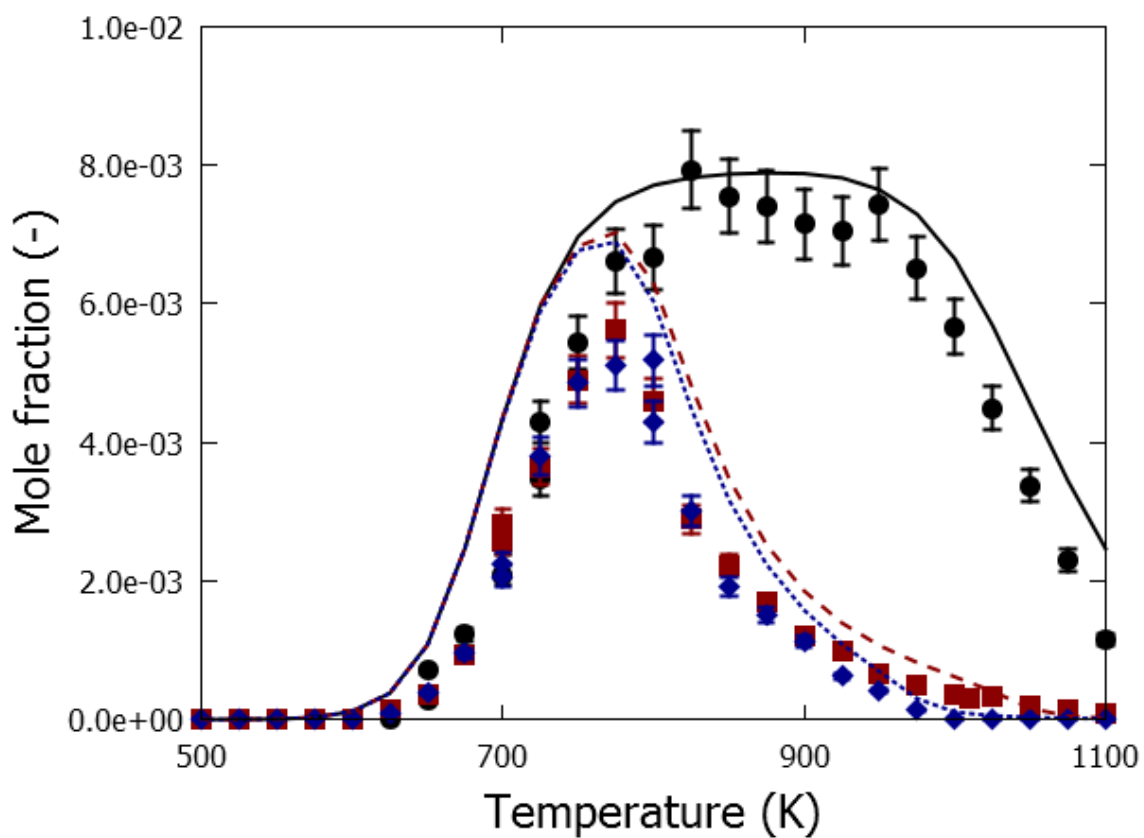


Fig. S $10\text{CH}_2\text{O}$ mole fractions as a function of temperature for isoprenol oxidation and pyrolysis in a jet-stirred reactor, $P=0.107$ MPa, $F_V=4.06 \cdot 10^{-5} \text{ m}^3 \text{ s}^{-1}$, $x_{\text{isoprenol},0}=0.008$, $\phi=0.5$ (blue), $\phi=1.0$ (red) and $\phi=\infty$ (black): symbols, experimental mole fraction profile; lines, mole fraction profiles calculated with CHEMKIN using the perfectly stirred reactor model and the developed kinetic model

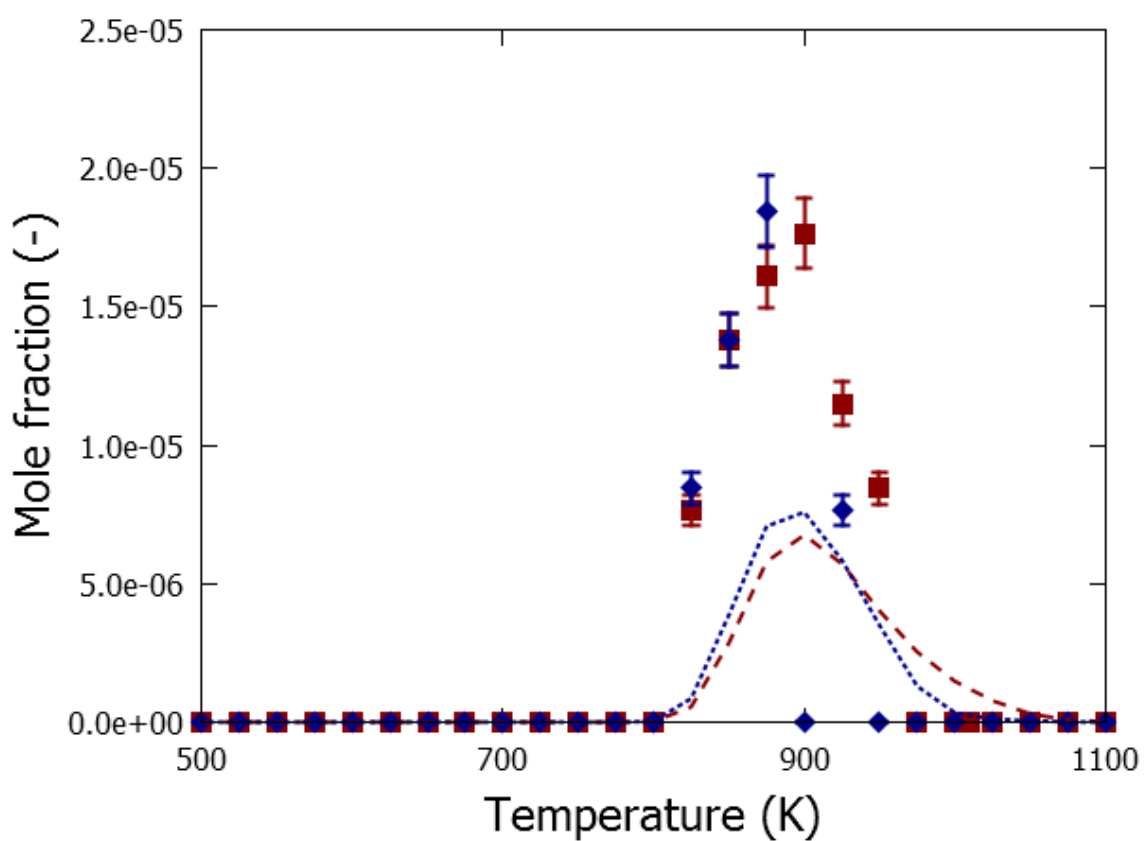


Fig. S 11 Oxiran mole fractions as a function of temperature for isoprenol oxidation and pyrolysis in a jet-stirred reactor, $P=0.107$ MPa, $F_V=4.06 \cdot 10^{-5} \text{ m}^3 \text{ s}^{-1}$, $x_{\text{isoprenol},0}=0.008$, $\phi=0.5$ (blue), $\phi=1.0$ (red) and $\phi=\infty$ (black): symbols, experimental mole fraction profile; lines, mole fraction profiles calculated with CHEMKIN using the perfectly stirred reactor model and the developed kinetic model

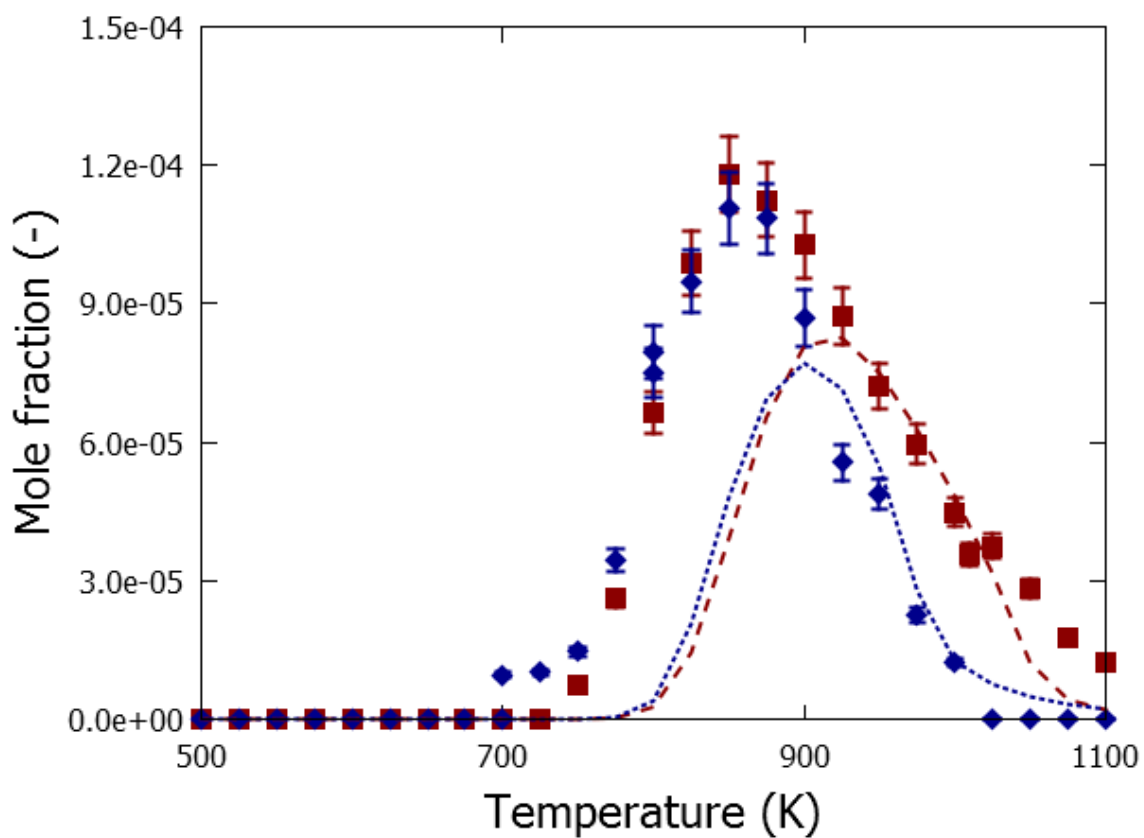


Fig. S 12 Acetaldehyde mole fractions as a function of temperature for isoprenol oxidation and pyrolysis in a jet-stirred reactor, $P=0.107$ MPa, $F_v = 4.06 \cdot 10^{-5} \text{ m}^3 \text{ s}^{-1}$, $x_{\text{isoprenol},0}=0.008$, $\phi=0.5$ (blue), $\phi=1.0$ (red) and $\phi=\infty$ (black): symbols, experimental mole fraction profile; lines, mole fraction profiles calculated with CHEMKIN using the perfectly stirred reactor model and the developed kinetic model

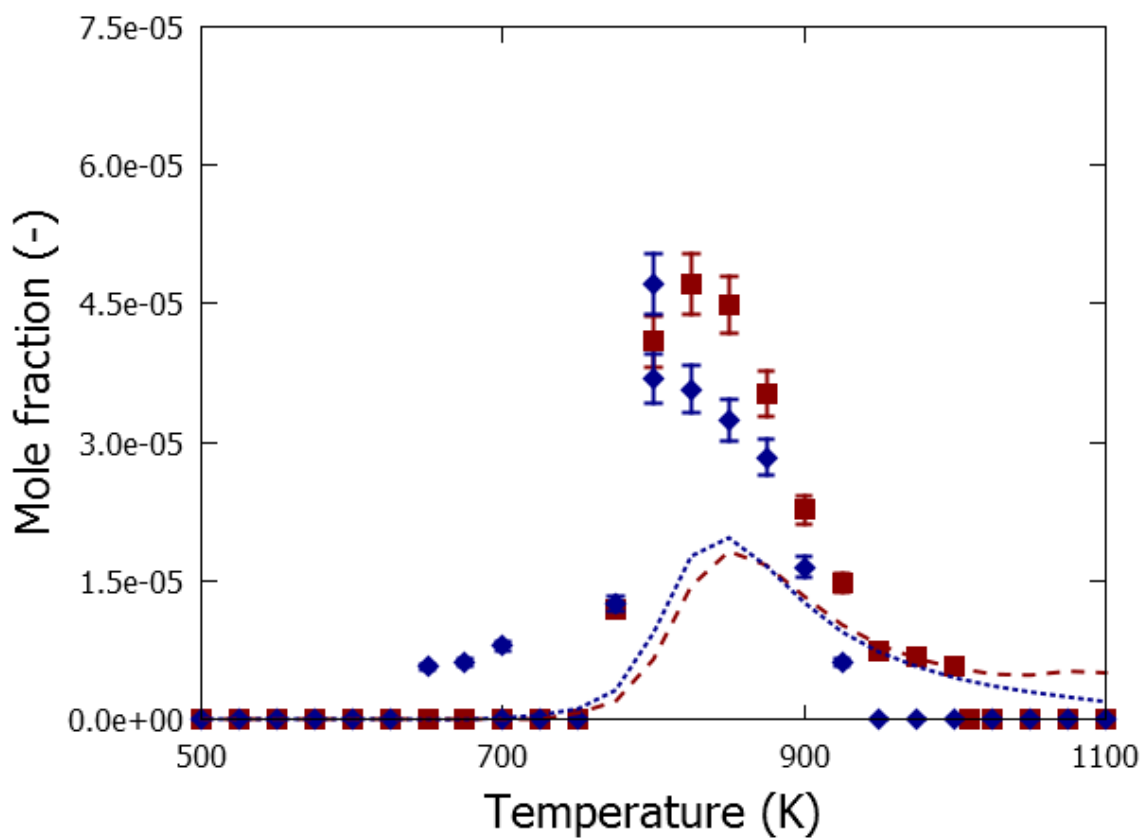


Fig. S 13Methanol mole fractions as a function of temperature for isoprenol oxidation and pyrolysis in a jet-stirred reactor, $P=0.107$ MPa, $F_V = 4.06 \cdot 10^{-5} \text{ m}^3 \text{ s}^{-1}$, $x_{\text{isoprenol},0}=0.008$, $\phi=0.5$ (blue), $\phi=1.0$ (red) and $\phi=\infty$ (black): symbols, experimental mole fraction profile; lines, mole fraction profiles calculated with CHEMKIN using the perfectly stirred reactor model and the developed kinetic model

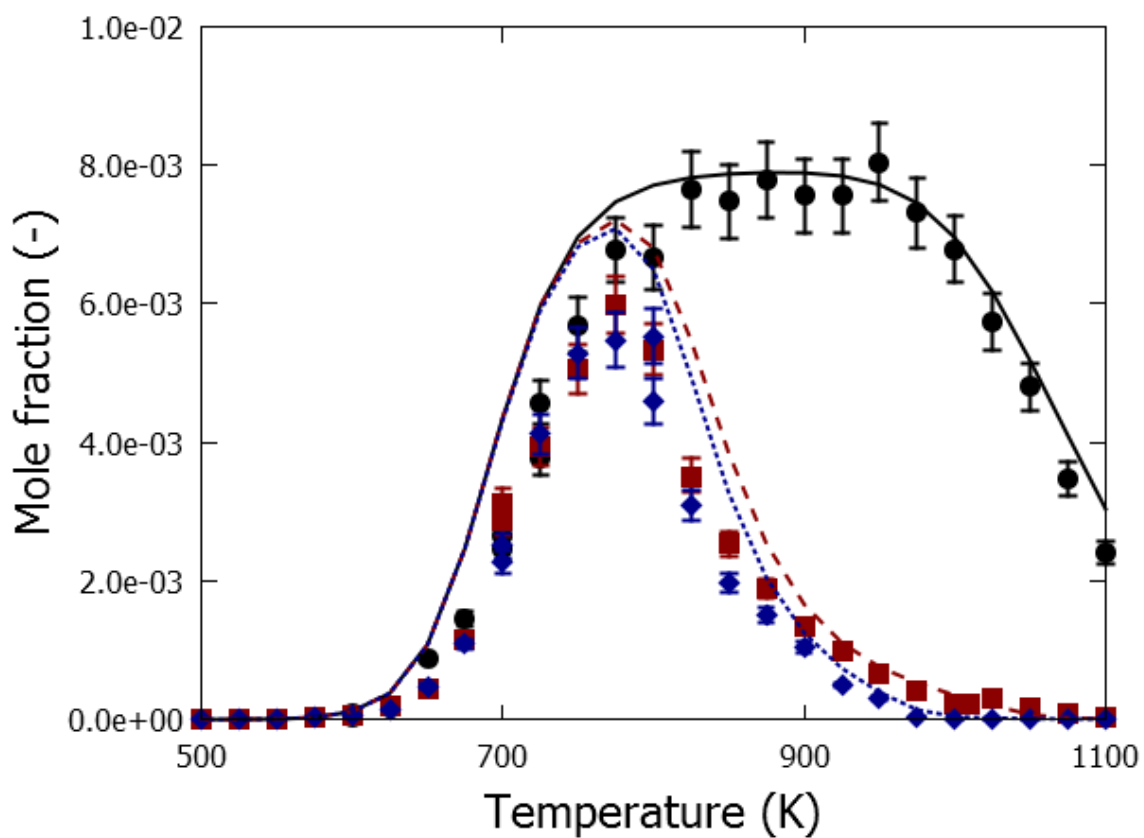


Fig. S 14 Isobutene mole fractions as a function of temperature for isoprenol oxidation and pyrolysis in a jet-stirred reactor, $P=0.107$ MPa, $F_V=4.06 \cdot 10^{-5} \text{ m}^3 \text{ s}^{-1}$, $x_{\text{isoprenol},0}=0.008$, $\phi=0.5$ (blue), $\phi=1.0$ (red) and $\phi=\infty$ (black): symbols, experimental mole fraction profile; lines, mole fraction profiles calculated with CHEMKIN using the perfectly stirred reactor model and the developed kinetic model

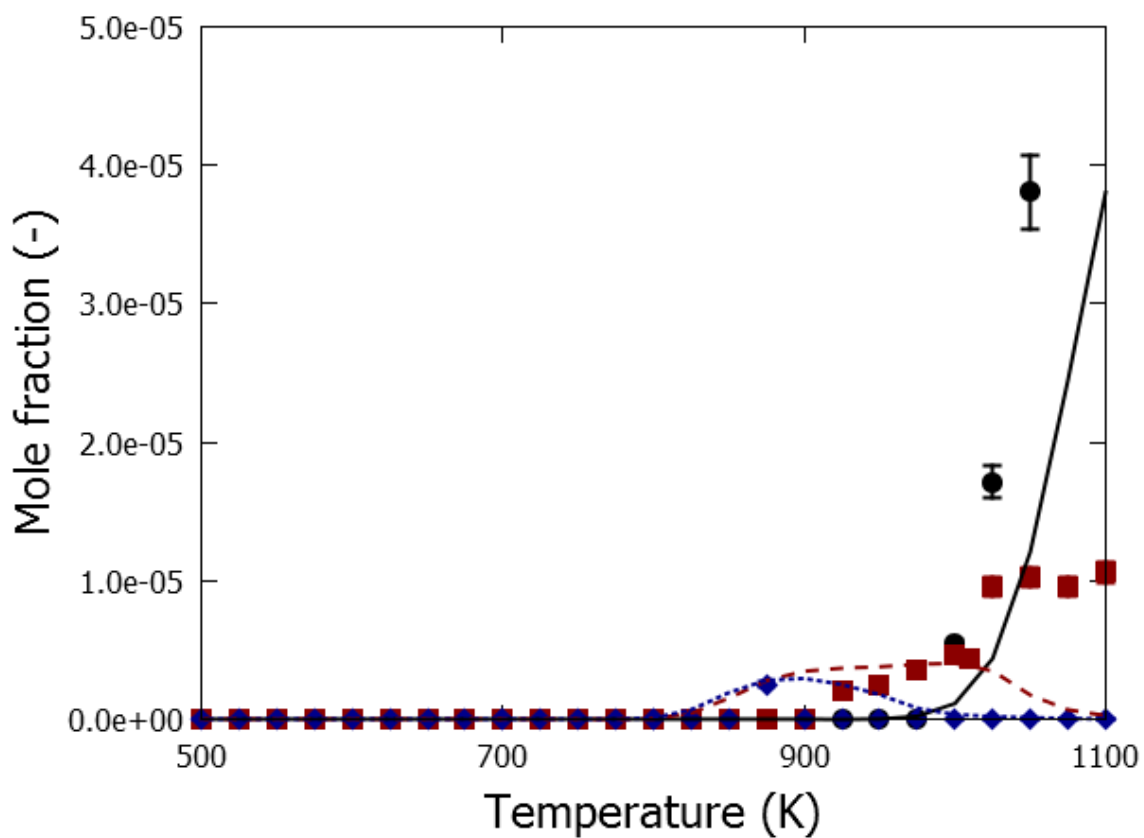


Fig. S 151,3-butadiene mole fractions as a function of temperature for isoprenol oxidation and pyrolysis in a jet-stirred reactor, $P=0.107$ MPa, $F_v = 4.06 \cdot 10^{-5} \text{ m}^3 \text{ s}^{-1}$, $x_{\text{isoprenol},0}=0.008$, $\phi=0.5$ (blue), $\phi=1.0$ (red) and $\phi=\infty$ (black): symbols, experimental mole fraction profile; lines, mole fraction profiles calculated with CHEMKIN using the perfectly stirred reactor model and the developed kinetic model

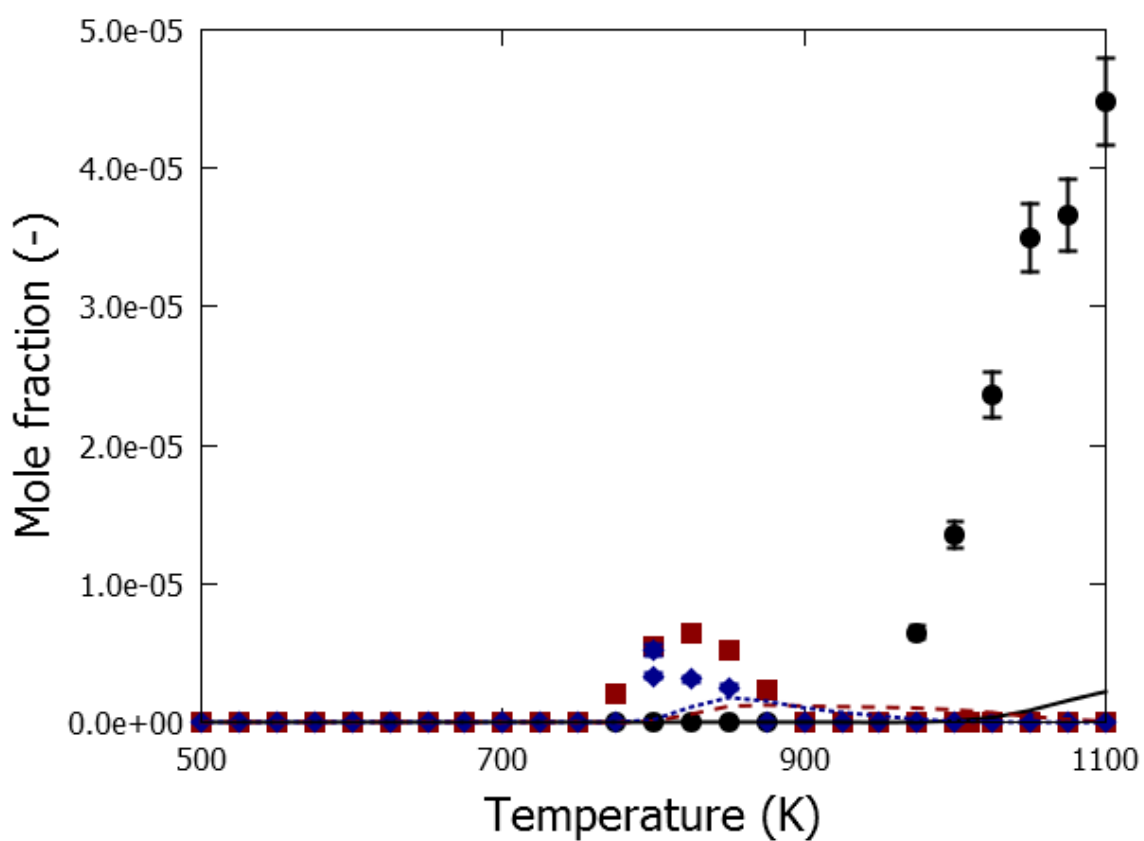


Fig. S 162-butene mole fractions as a function of temperature for isoprenol oxidation and pyrolysis in a jet-stirred reactor, $P=0.107$ MPa, $F_V = 4.06 \cdot 10^{-5} \text{ m}^3 \text{ s}^{-1}$, $x_{\text{isoprenol},0}=0.008$, $\phi=0.5$ (blue), $\phi=1.0$ (red) and $\phi=\infty$ (black): symbols, experimental mole fraction profile; lines, mole fraction profiles calculated with CHEMKIN using the perfectly stirred reactor model and the developed kinetic model

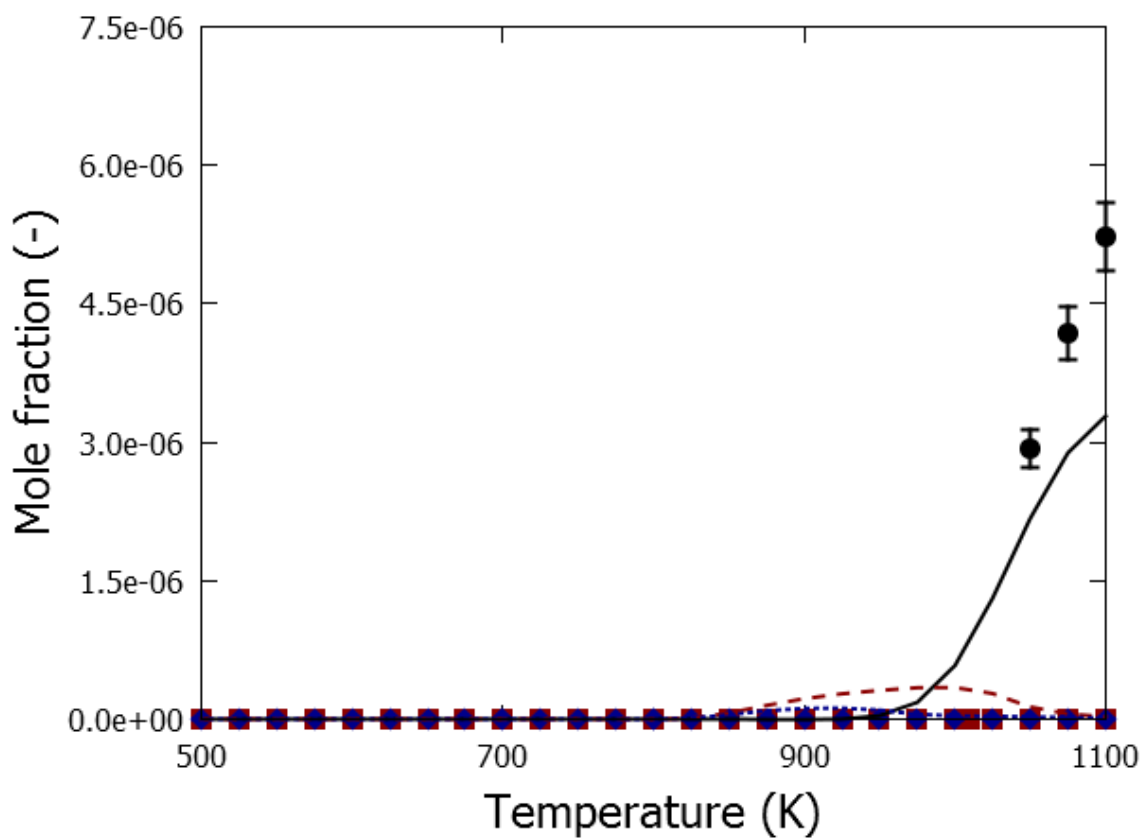


Fig. S 171,2-butadiene mole fractions as a function of temperature for isoprenol oxidation and pyrolysis in a jet-stirred reactor, $P=0.107$ MPa, $F_v = 4.06 \cdot 10^{-5} \text{ m}^3 \text{ s}^{-1}$, $x_{\text{isoprenol},0}=0.008$, $\phi=0.5$ (blue), $\phi=1.0$ (red) and $\phi=\infty$ (black): symbols, experimental mole fraction profile; lines, mole fraction profiles calculated with CHEMKIN using the perfectly stirred reactor model and the developed kinetic model

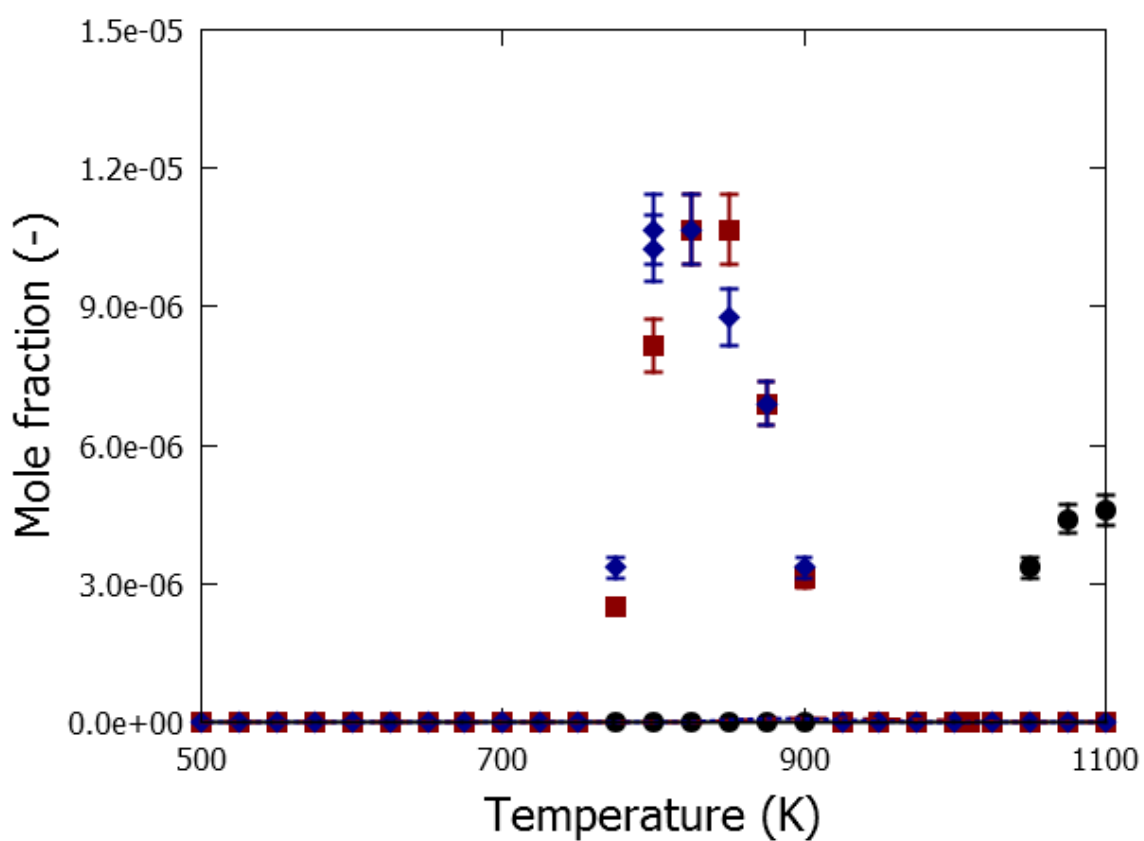


Fig. S 18furan mole fractions as a function of temperature for isoprenol oxidation and pyrolysis in a jet-stirred reactor, $P=0.107$ MPa, $F_V = 4.06 \cdot 10^{-5} \text{ m}^3 \text{ s}^{-1}$, $x_{\text{isoprenol},0}=0.008$, $\phi=0.5$ (blue), $\phi=1.0$ (red) and $\phi=\infty$ (black): symbols, experimental mole fraction profile; lines, mole fraction profiles calculated with CHEMKIN using the perfectly stirred reactor model and the developed kinetic model

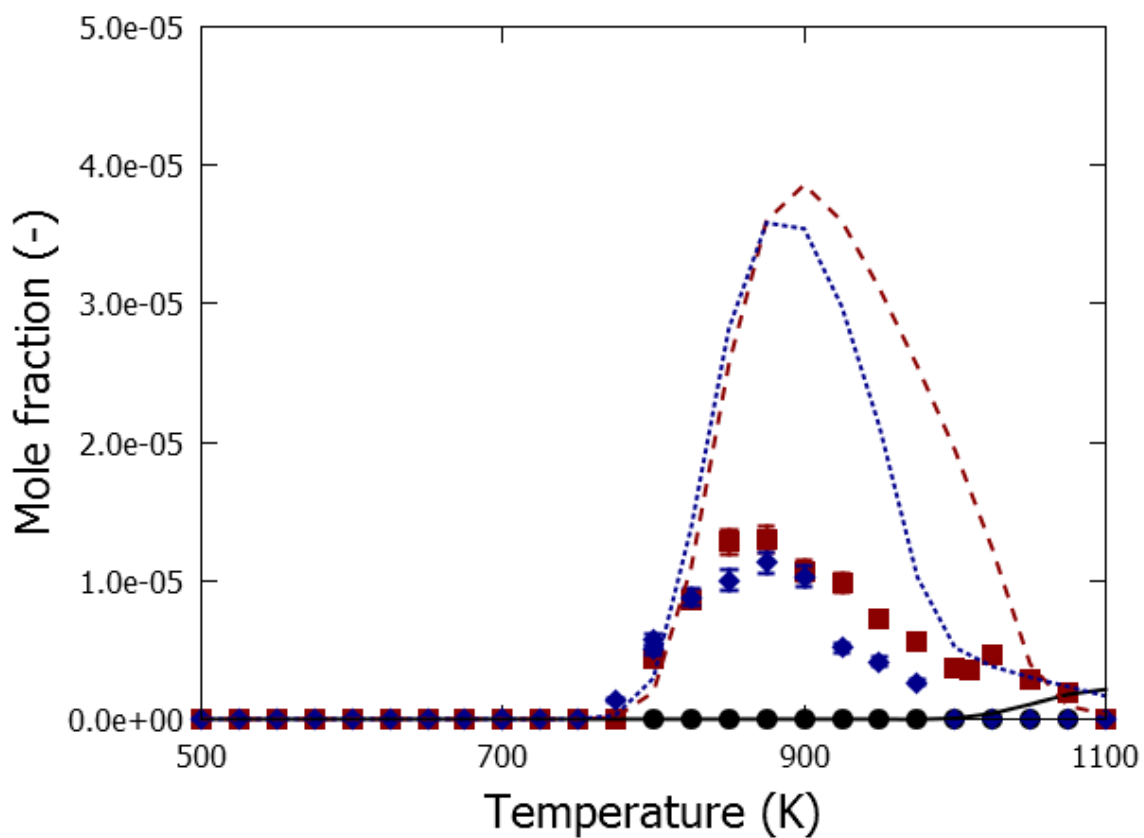


Fig. S 19acrolein mole fractions as a function of temperature for isoprenol oxidation and pyrolysis in a jet-stirred reactor, $P=0.107$ MPa, $F_V=4.06 \cdot 10^{-5} \text{ m}^3 \text{ s}^{-1}$, $x_{\text{isoprenol},0}=0.008$, $\phi=0.5$ (blue), $\phi=1.0$ (red) and $\phi=\infty$ (black): symbols, experimental mole fraction profile; lines, mole fraction profiles calculated with CHEMKIN using the perfectly stirred reactor model and the developed kinetic model

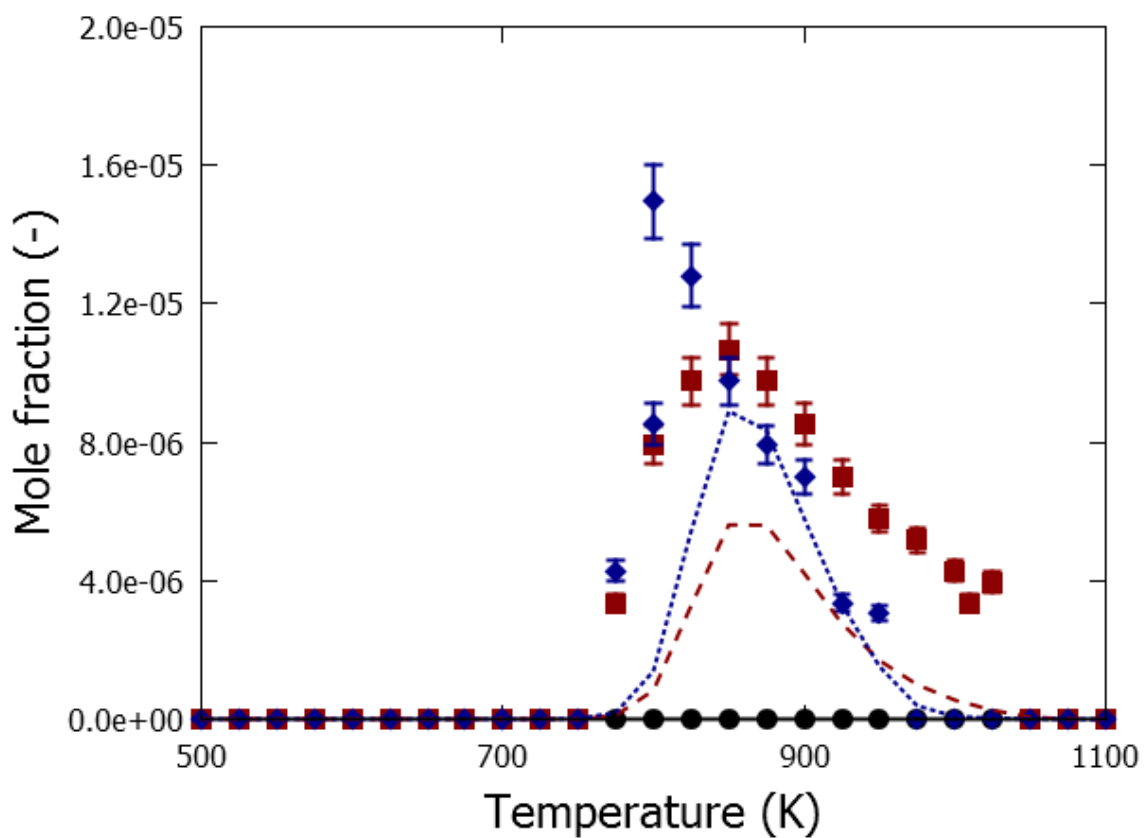


Fig. S 20 Propanal mole fractions as a function of temperature for isoprenol oxidation and pyrolysis in a jet-stirred reactor, $P=0.107$ MPa, $F_V = 4.06 \cdot 10^{-5} \text{ m}^3 \text{ s}^{-1}$, $x_{\text{isoprenol},0}=0.008$, $\phi=0.5$ (blue), $\phi=1.0$ (red) and $\phi=\infty$ (black): symbols, experimental mole fraction profile; lines, mole fraction profiles calculated with CHEMKIN using the perfectly stirred reactor model and the developed kinetic model

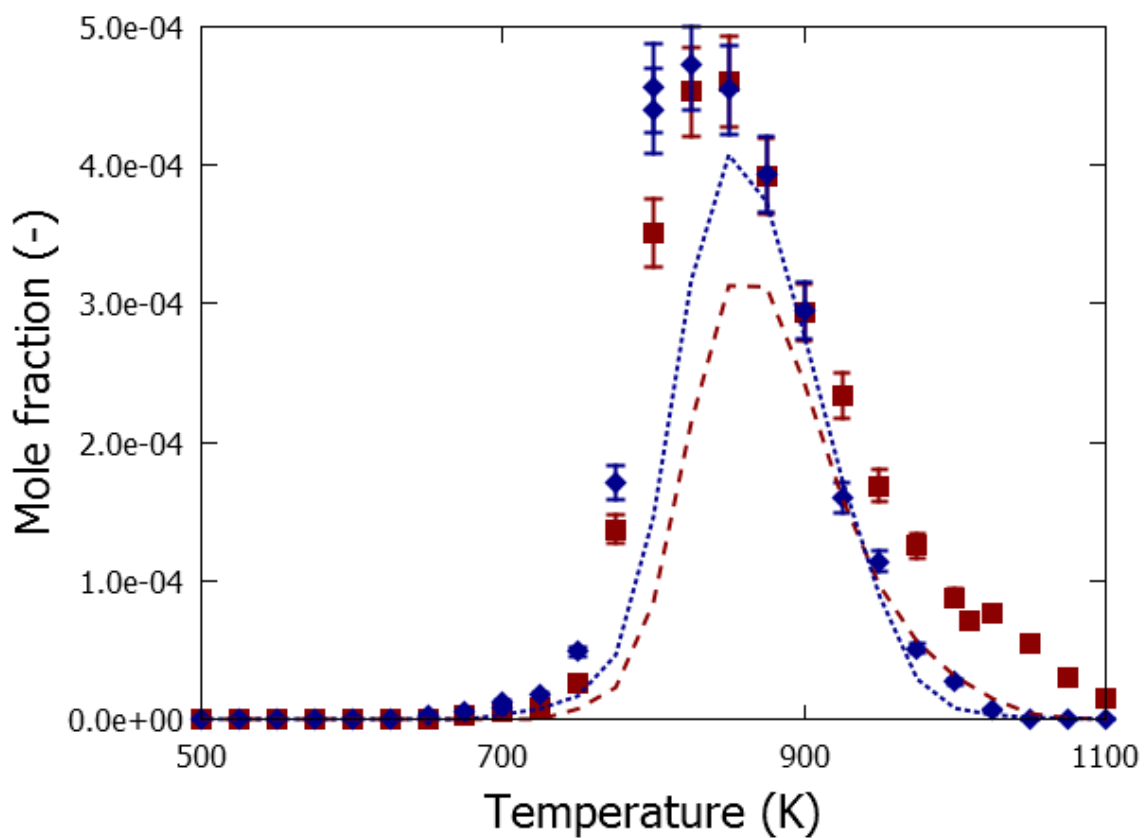


Fig. S 21 Acetone mole fractions as a function of temperature for isoprenol oxidation and pyrolysis in a jet-stirred reactor, $P=0.107$ MPa, $F_V = 4.06 \cdot 10^{-5} \text{ m}^3 \text{ s}^{-1}$, $x_{\text{isoprenol},0}=0.008$, $\phi=0.5$ (blue), $\phi=1.0$ (red) and $\phi=\infty$ (black): symbols, experimental mole fraction profile; lines, mole fraction profiles calculated with CHEMKIN using the perfectly stirred reactor model and the developed kinetic model

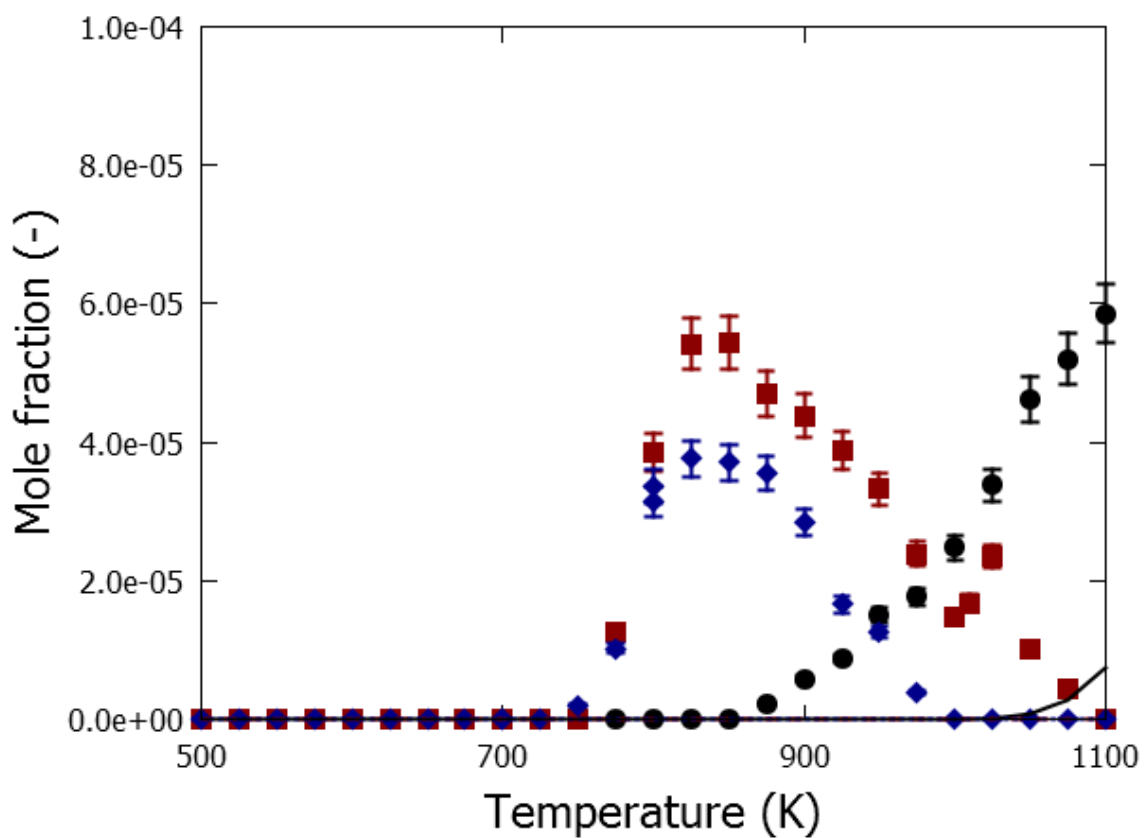


Fig. S 22CPD mole fractions as a function of temperature for isoprenol oxidation and pyrolysis in a jet-stirred reactor, $P=0.107$ MPa, $F_V=4.06 \cdot 10^{-5} \text{ m}^3 \text{ s}^{-1}$, $x_{\text{isoprenol},0}=0.008$, $\phi=0.5$ (blue), $\phi=1.0$ (red) and $\phi=\infty$ (black): symbols, experimental mole fraction profile; lines, mole fraction profiles calculated with CHEMKIN using the perfectly stirred reactor model and the developed kinetic model

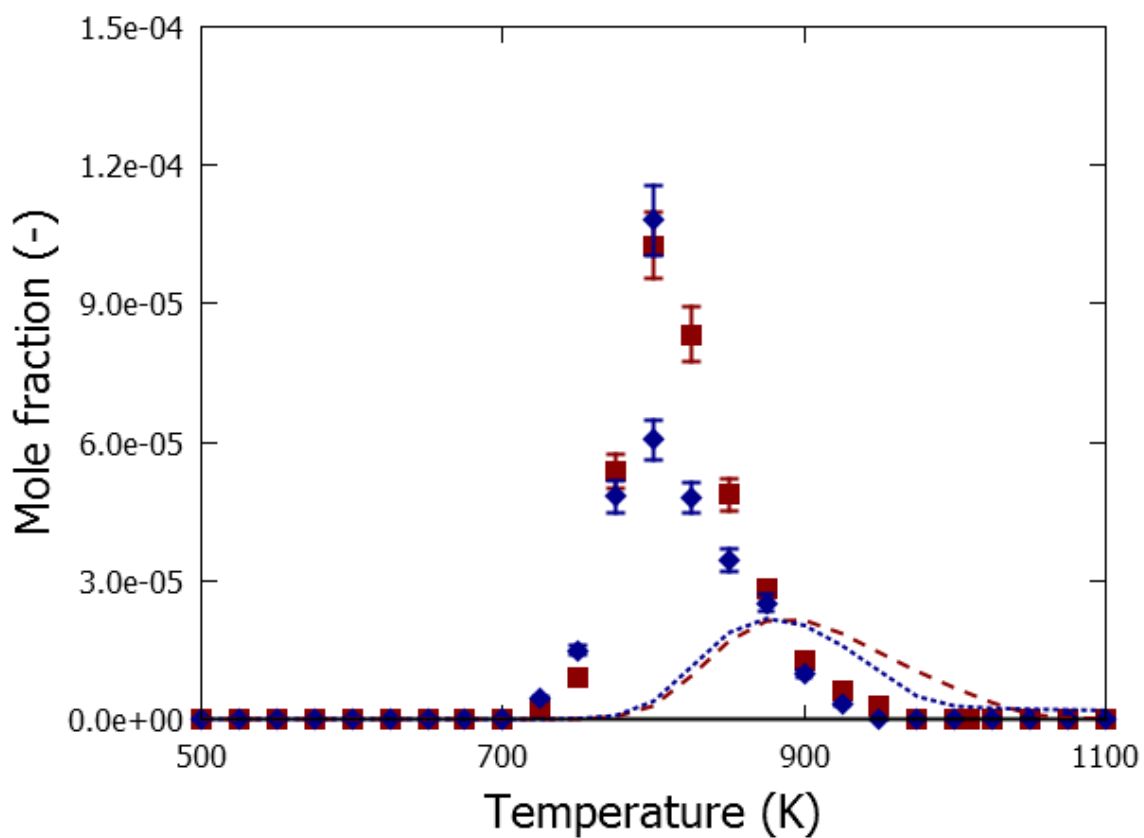


Fig. S 23 Propenol mole fractions as a function of temperature for isoprenol oxidation and pyrolysis in a jet-stirred reactor, $P=0.107$ MPa, $F_V = 4.06 \cdot 10^{-5} \text{ m}^3 \text{ s}^{-1}$, $x_{\text{isoprenol},0}=0.008$, $\phi=0.5$ (blue), $\phi=1.0$ (red) and $\phi=\infty$ (black): symbols, experimental mole fraction profile; lines, mole fraction profiles calculated with CHEMKIN using the perfectly stirred reactor model and the developed kinetic model

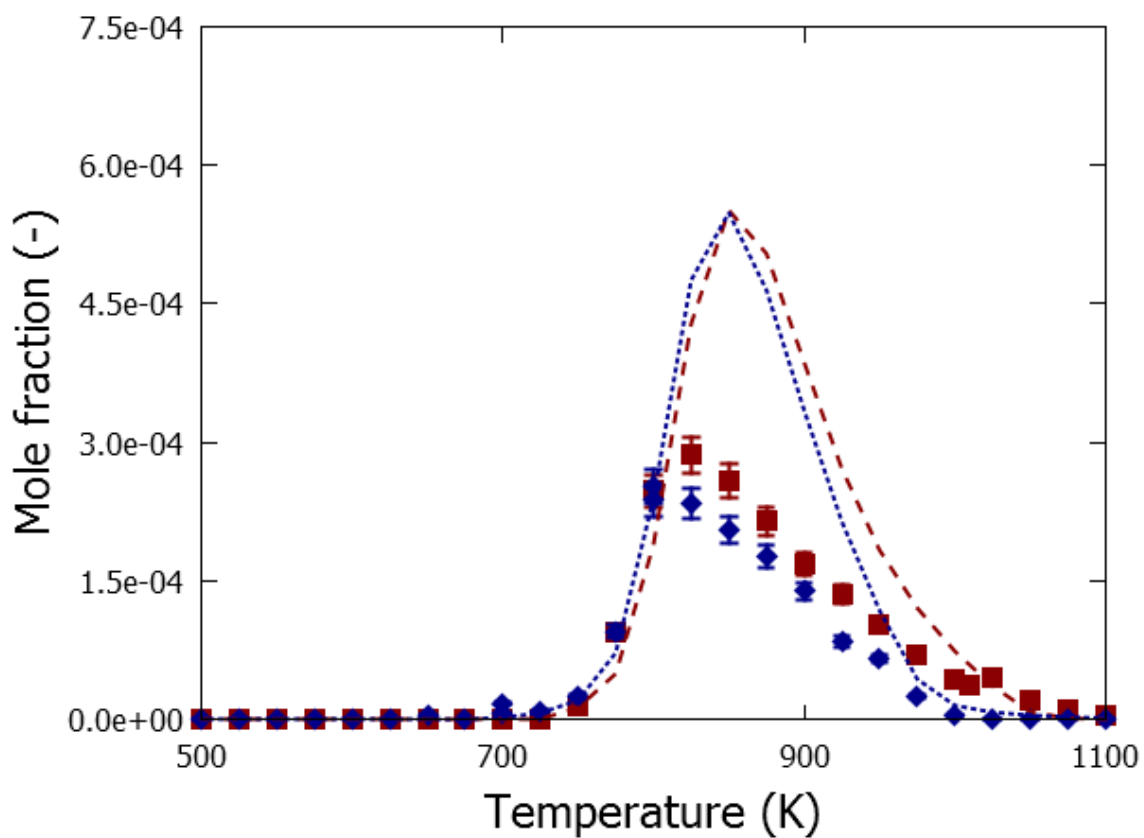


Fig. S 24Methacrolein mole fractions as a function of temperature for isoprenol oxidation and pyrolysis in a jet-stirred reactor, $P=0.107$ MPa, $F_v = 4.06 \cdot 10^{-5} \text{ m}^3 \text{ s}^{-1}$, $x_{\text{isoprenol},0}=0.008$, $\phi=0.5$ (blue), $\phi=1.0$ (red) and $\phi=\infty$ (black): symbols, experimental mole fraction profile; lines, mole fraction profiles calculated with CHEMKIN using the perfectly stirred reactor model and the developed kinetic model

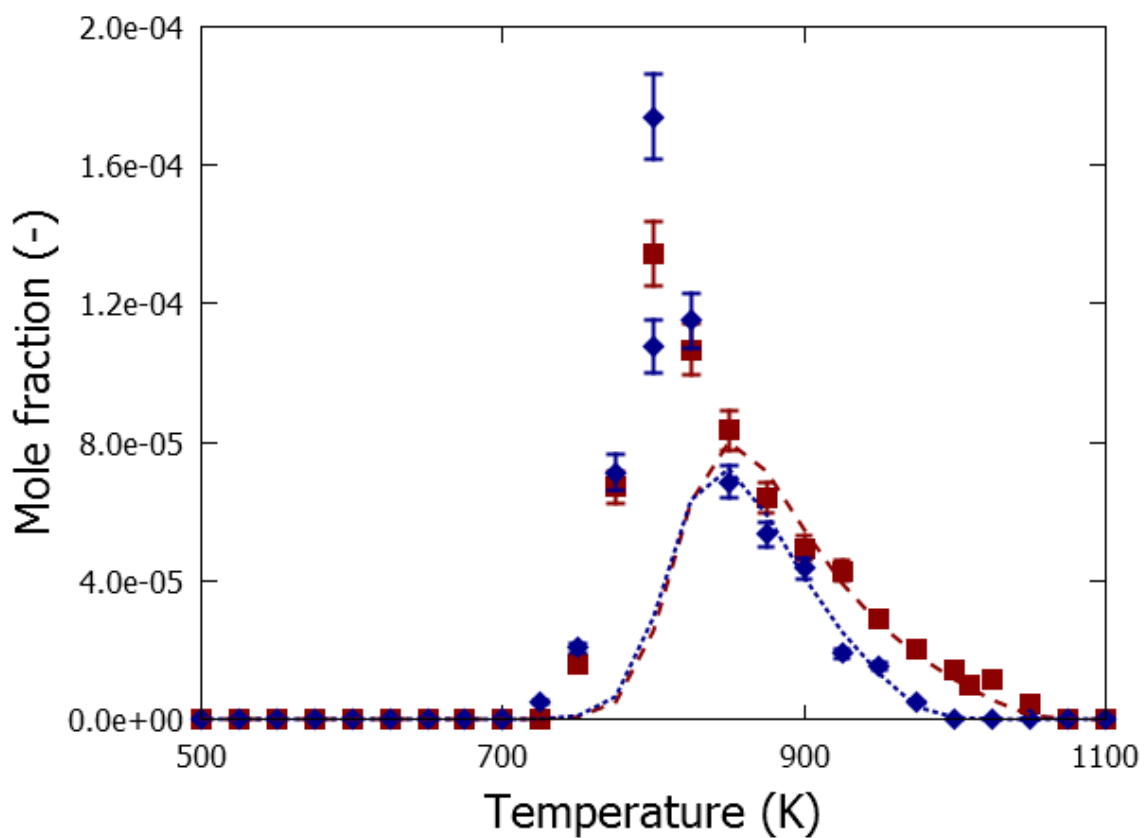


Fig. S 252-methyl-propanal mole fractions as a function of temperature for isoprenol oxidation and pyrolysis in a jet-stirred reactor, $P=0.107$ MPa, $F_v = 4.06 \cdot 10^{-5} \text{ m}^3 \text{ s}^{-1}$, $x_{\text{isoprenol},0}=0.008$, $\phi=0.5$ (blue), $\phi=1.0$ (red) and $\phi=\infty$ (black): symbols, experimental mole fraction profile; lines, mole fraction profiles calculated with CHEMKIN using the perfectly stirred reactor model and the developed kinetic model

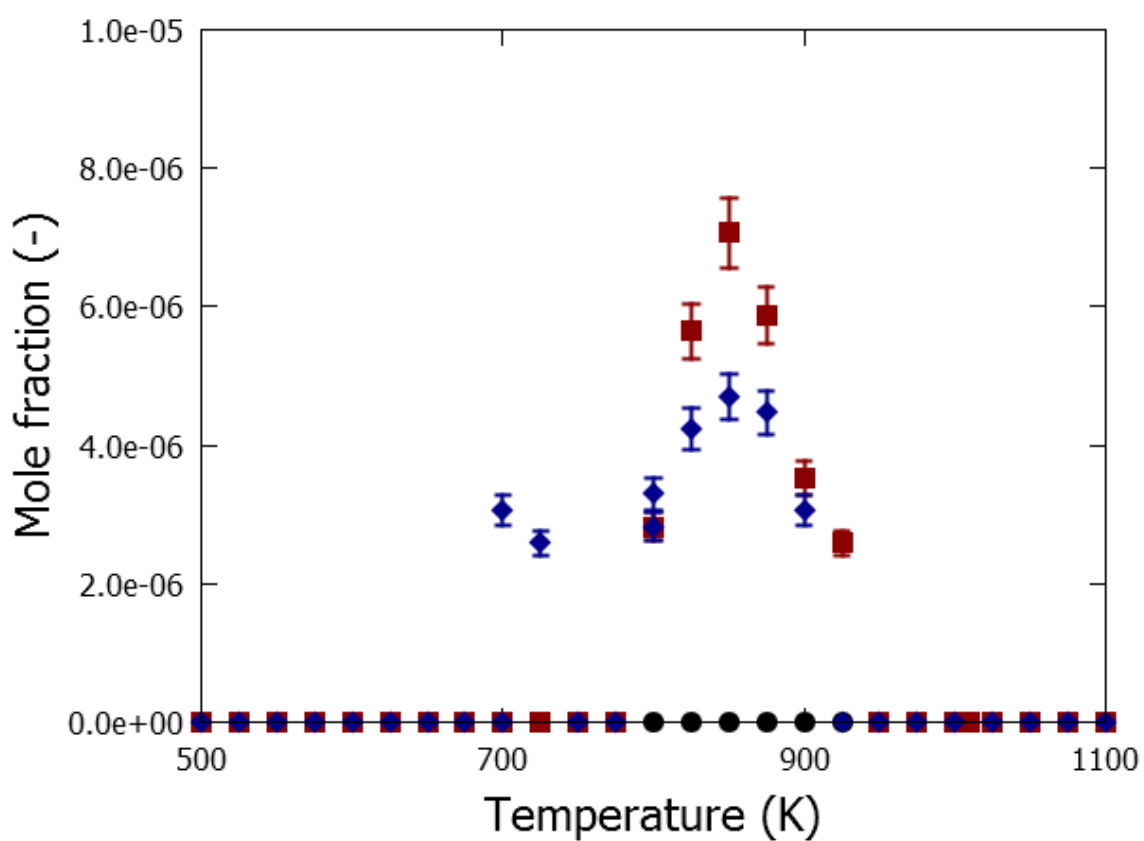


Fig. S 263-methyl-furan mole fractions as a function of temperature for isoprenol oxidation and pyrolysis in a jet-stirred reactor, $P=0.107$ MPa, $F_v = 4.06 \cdot 10^{-5} \text{ m}^3 \text{ s}^{-1}$, $x_{\text{isoprenol},0}=0.008$, $\phi=0.5$ (blue), $\phi=1.0$ (red) and $\phi=\infty$ (black): symbols, experimental mole fraction profile; lines, mole fraction profiles calculated with CHEMKIN using the perfectly stirred reactor model and the developed kinetic model

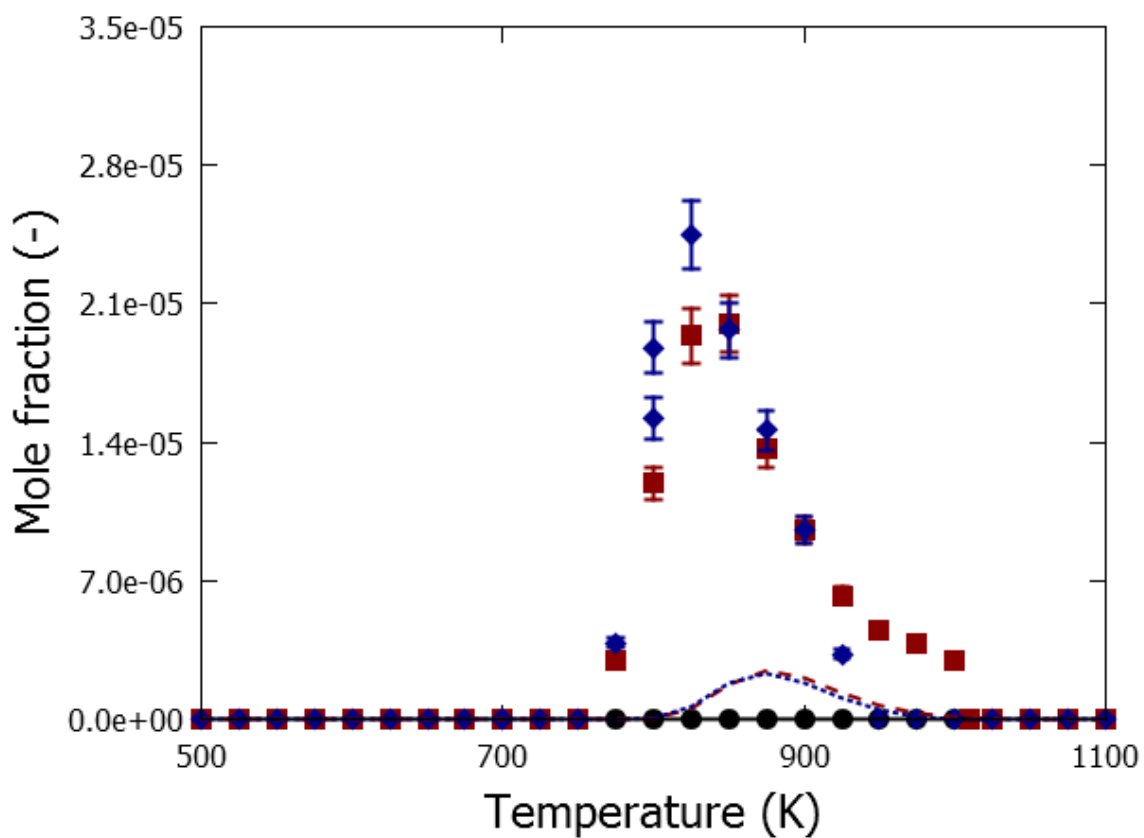


Fig. S 27butanone mole fractions as a function of temperature for isoprenol oxidation and pyrolysis in a jet-stirred reactor, $P=0.107$ MPa, $F_V = 4.06 \cdot 10^{-5} \text{ m}^3 \text{ s}^{-1}$, $x_{\text{isoprenol},0}=0.008$, $\phi=0.5$ (blue), $\phi=1.0$ (red) and $\phi=\infty$ (black): symbols, experimental mole fraction profile; lines, mole fraction profiles calculated with CHEMKIN using the perfectly stirred reactor model and the developed kinetic model

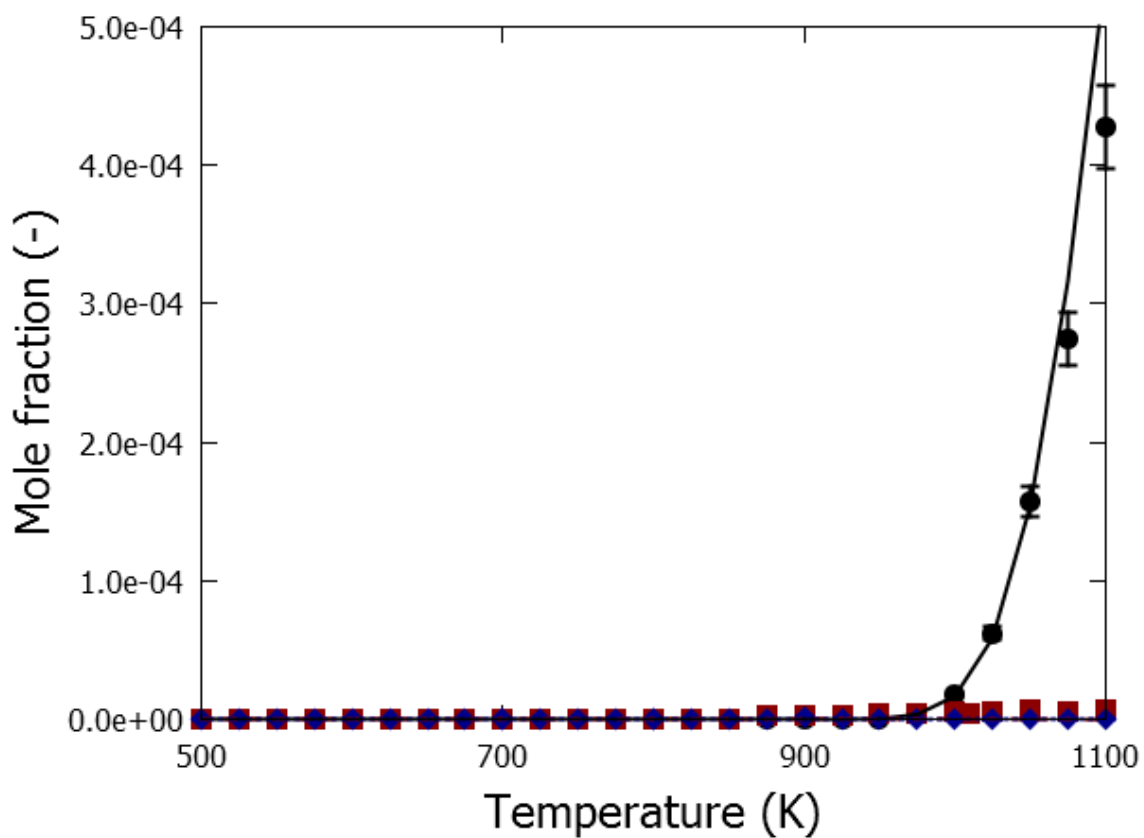


Fig. S 28benzene mole fractions as a function of temperature for isoprenol oxidation and pyrolysis in a jet-stirred reactor, $P=0.107$ MPa, $F_V=4.06 \cdot 10^{-5} \text{ m}^3 \text{ s}^{-1}$, $x_{\text{isoprenol},0}=0.008$, $\phi=0.5$ (blue), $\phi=1.0$ (red) and $\phi=\infty$ (black): symbols, experimental mole fraction profile; lines, mole fraction profiles calculated with CHEMKIN using the perfectly stirred reactor model and the developed kinetic model

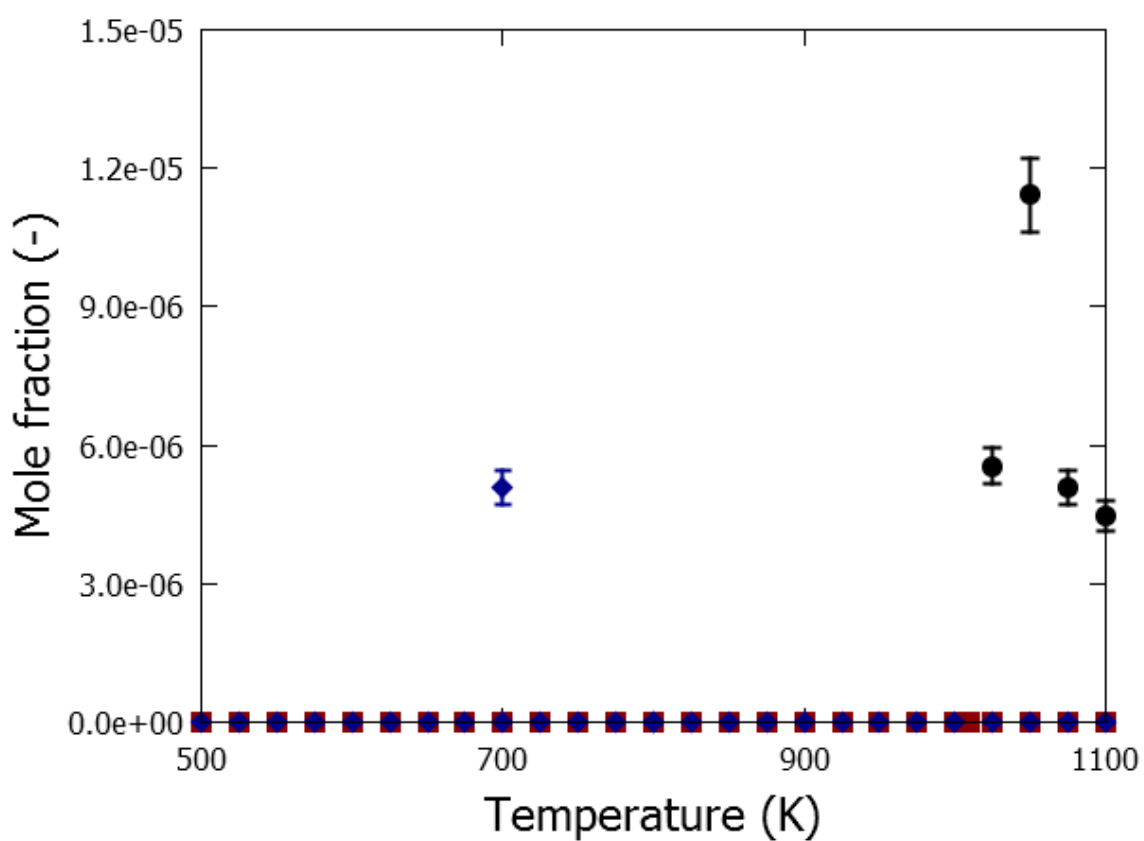


Fig. S 29cyclohexadiene mole fractions as a function of temperature for isoprenol oxidation and pyrolysis in a jet-stirred reactor, $P=0.107$ MPa, $F_v = 4.06 \cdot 10^{-5} \text{ m}^3 \text{ s}^{-1}$, $x_{\text{isoprenol},0}=0.008$, $\phi=0.5$ (blue), $\phi=1.0$ (red) and $\phi=\infty$ (black): symbols, experimental mole fraction profile; lines, mole fraction profiles calculated with CHEMKIN using the perfectly stirred reactor model and the developed kinetic model

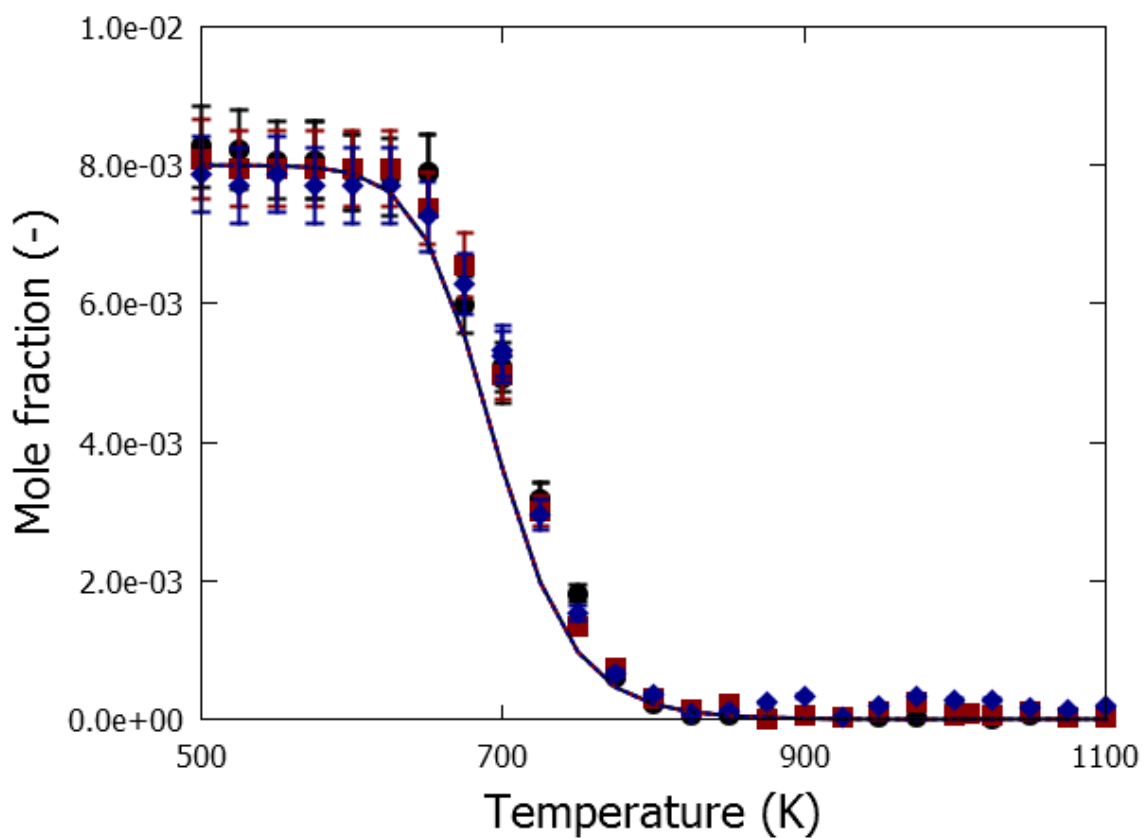


Fig. S 30isoprenol mole fractions as a function of temperature for isoprenol oxidation and pyrolysis in a jet-stirred reactor, $P=0.107$ MPa, $F_V=4.06 \cdot 10^{-5} \text{ m}^3 \text{ s}^{-1}$, $x_{\text{isoprenol},0}=0.008$, $\phi=0.5$ (blue), $\phi=1.0$ (red) and $\phi=\infty$ (black): symbols, experimental mole fraction profile; lines, mole fraction profiles calculated with CHEMKIN using the perfectly stirred reactor model and the developed kinetic model

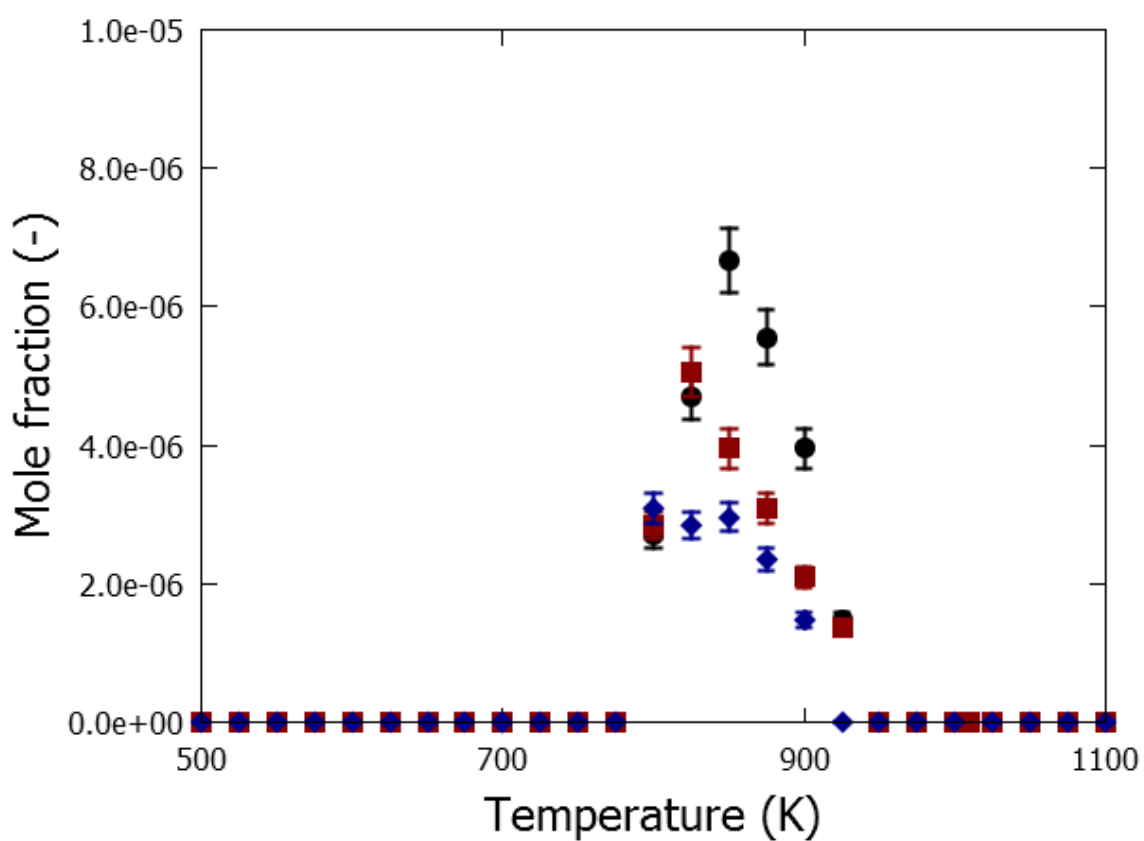


Fig. S 312-methyl-1,5-hexadiene mole fractions as a function of temperature for isoprenol oxidation and pyrolysis in a jet-stirred reactor, $P=0.107$ MPa, $F_V=4.06 \cdot 10^{-5} \text{ m}^3 \text{ s}^{-1}$, $x_{\text{isoprenol},0}=0.008$, $\phi=0.5$ (blue), $\phi=1.0$ (red) and $\phi=\infty$ (black): symbols, experimental mole fraction profile; lines, mole fraction profiles calculated with CHEMKIN using the perfectly stirred reactor model and the developed kinetic model

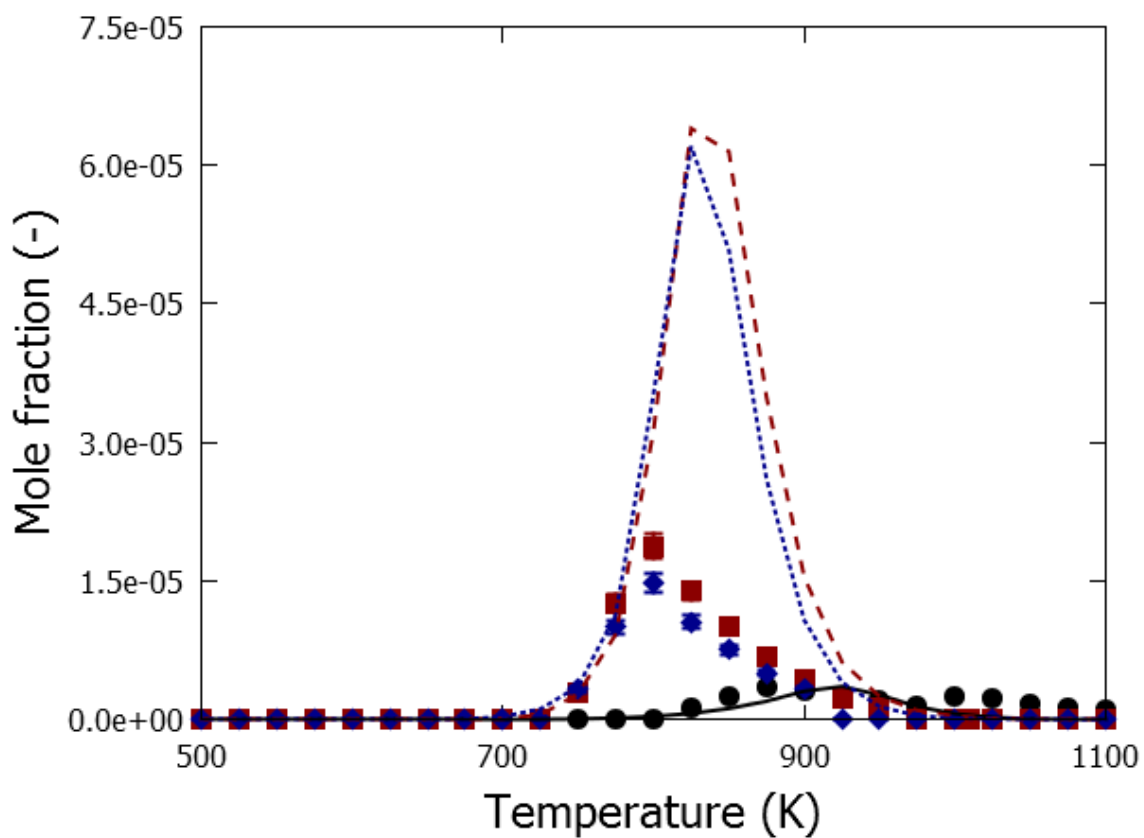


Fig. S 322,5-dimethyl-1,5-hexadiene mole fractions as a function of temperature for isoprenol oxidation and pyrolysis in a jet-stirred reactor, $P=0.107$ MPa, $F_V=4.06 \cdot 10^{-5} \text{ m}^3 \text{ s}^{-1}$, $x_{\text{isoprenol},0}=0.008$, $\phi=0.5$ (blue), $\phi=1.0$ (red) and $\phi=\infty$ (black): symbols, experimental mole fraction profile; lines, mole fraction profiles calculated with CHEMKIN using the perfectly stirred reactor model and the developed kinetic model

Model performance prenoI oxidation and pyrolysis

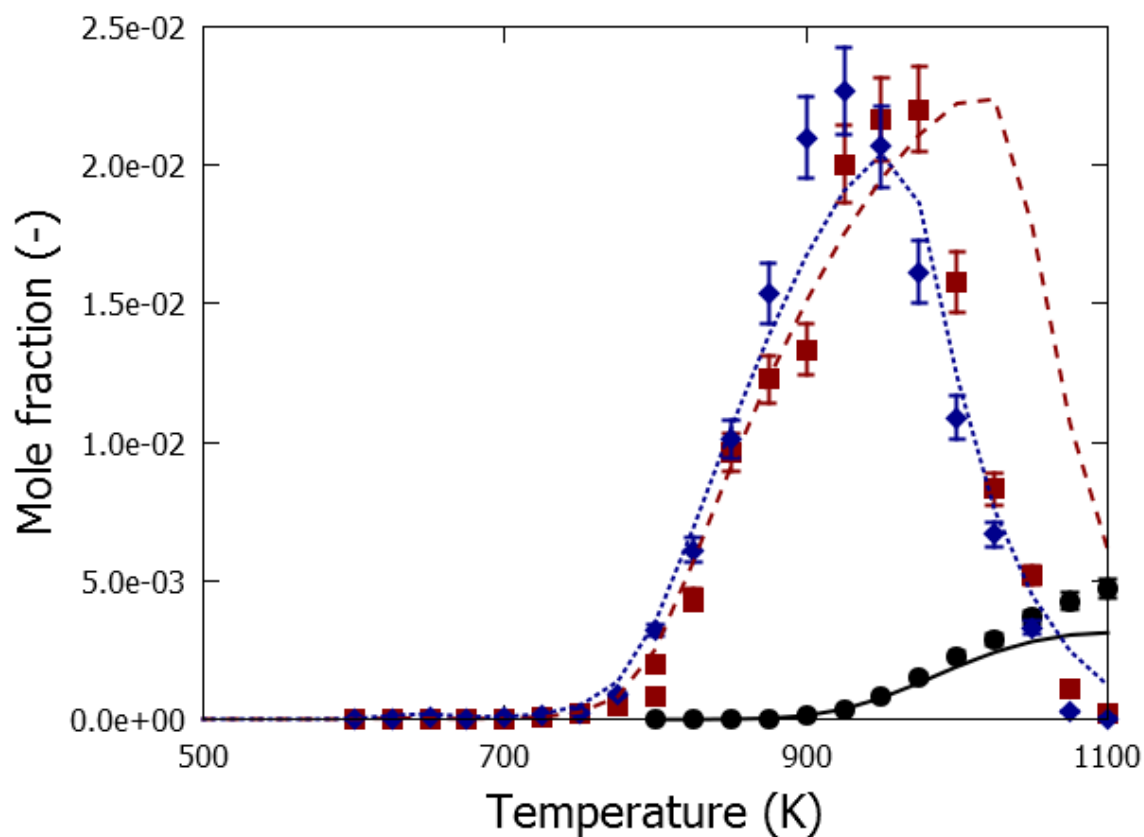


Fig. S 33CO mole fractions as a function of temperature for prenoI oxidation and pyrolysis in a jet-stirred reactor, $P=0.107$ MPa, $F_V=4.06 \cdot 10^{-5} \text{ m}^3 \text{ s}^{-1}$, $x_{\text{prenoI},0}=0.008$, $\phi=0.5$ (blue), $\phi=1.0$ (red) and $\phi=\infty$ (black): symbols, experimental mole fraction profile; lines, mole fraction profiles calculated with CHEMKIN using the perfectly stirred reactor model and the developed kinetic model

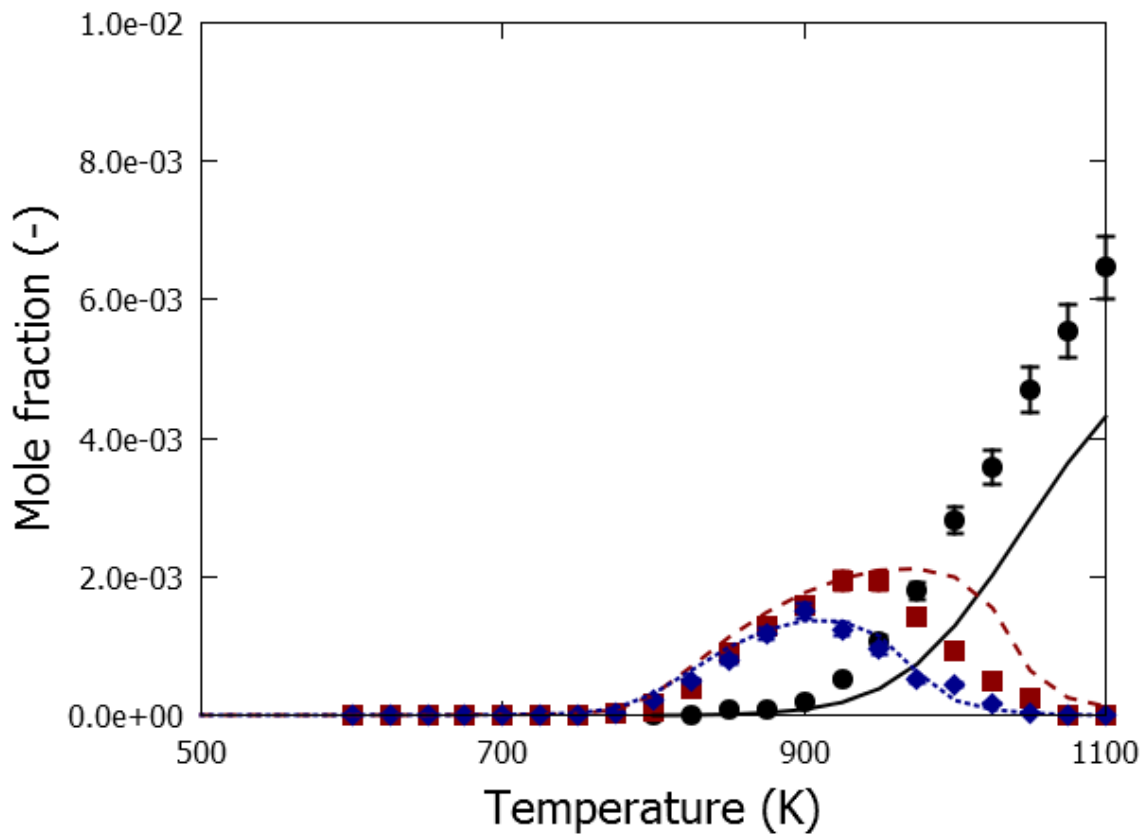


Fig. S 34 CH₄ mole fractions as a function of temperature for pre-nol oxidation and pyrolysis in a jet-stirred reactor, $P=0.107$ MPa, $F_V=4.06 \cdot 10^{-5} \text{ m}^3 \text{ s}^{-1}$, $x_{\text{prenol},0}=0.008$, $\phi=0.5$ (blue), $\phi=1.0$ (red) and $\phi=\infty$ (black): symbols, experimental mole fraction profile; lines, mole fraction profiles calculated with CHEMKIN using the perfectly stirred reactor model and the developed kinetic model

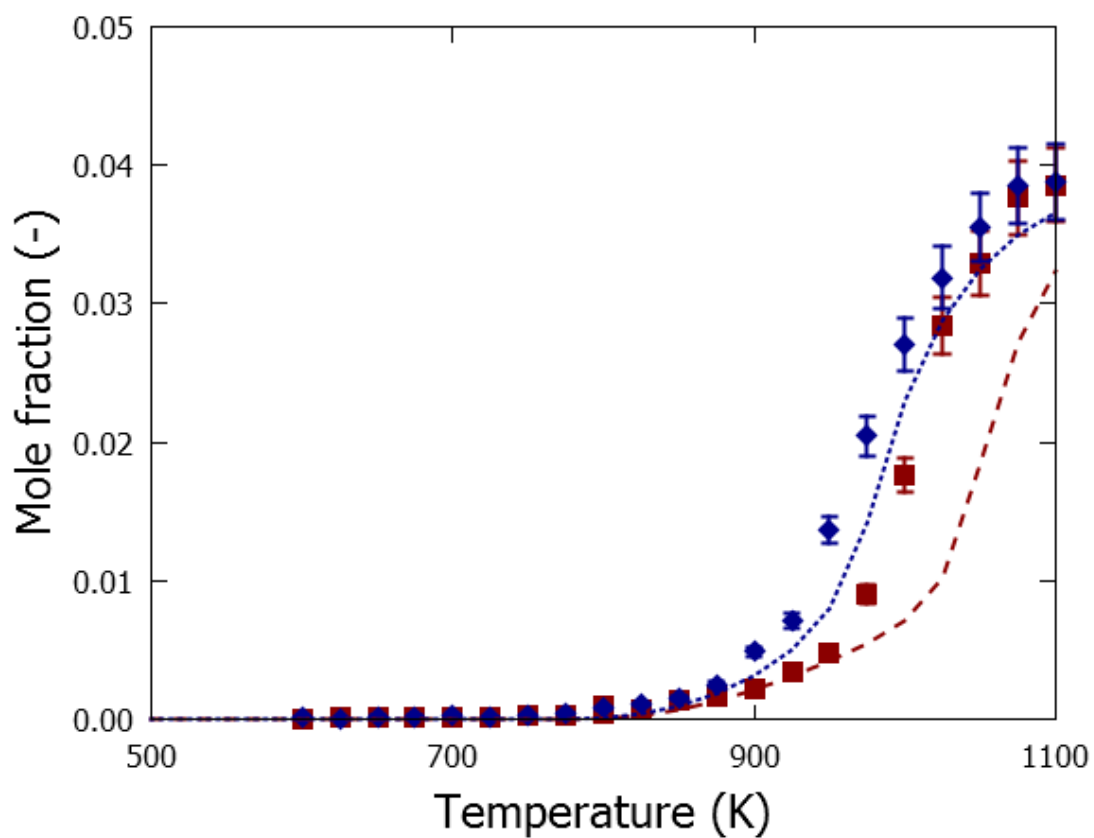


Fig. S 35 CO₂ mole fractions as a function of temperature for prenil oxidation and pyrolysis in a jet-stirred reactor, $P=0.107$ MPa, $F_V=4.06 \cdot 10^{-5} \text{ m}^3 \text{ s}^{-1}$, $x_{\text{prenil},0}=0.008$, $\phi=0.5$ (blue), $\phi=1.0$ (red) and $\phi=\infty$ (black): symbols, experimental mole fraction profile; lines, mole fraction profiles calculated with CHEMKIN using the perfectly stirred reactor model and the developed kinetic model

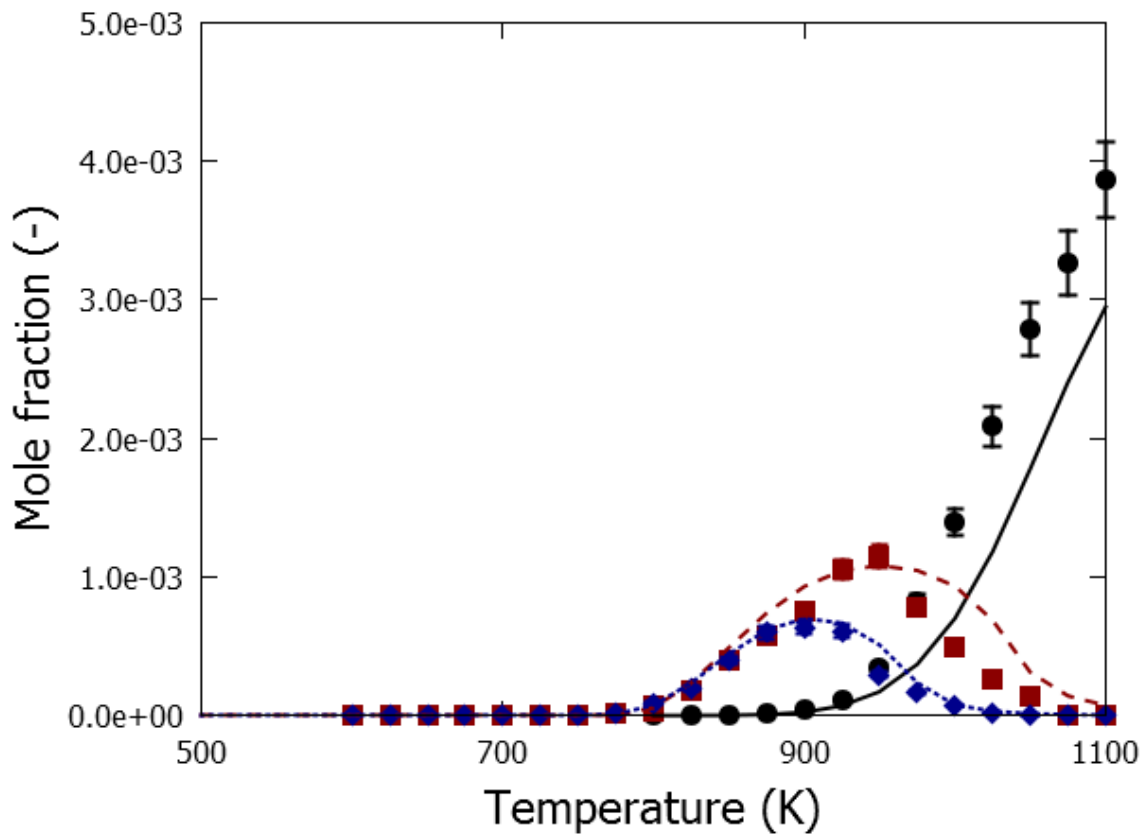


Fig. S 36 C_2H_4 mole fractions as a function of temperature for pre-nol oxidation and pyrolysis in a jet-stirred reactor, $P=0.107$ MPa, $F_V = 4.06 \cdot 10^{-5} \text{ m}^3 \text{ s}^{-1}$, $x_{\text{prenol},0}=0.008$, $\phi=0.5$ (blue), $\phi=1.0$ (red) and $\phi=\infty$ (black): symbols, experimental mole fraction profile; lines, mole fraction profiles calculated with CHEMKIN using the perfectly stirred reactor model and the developed kinetic model

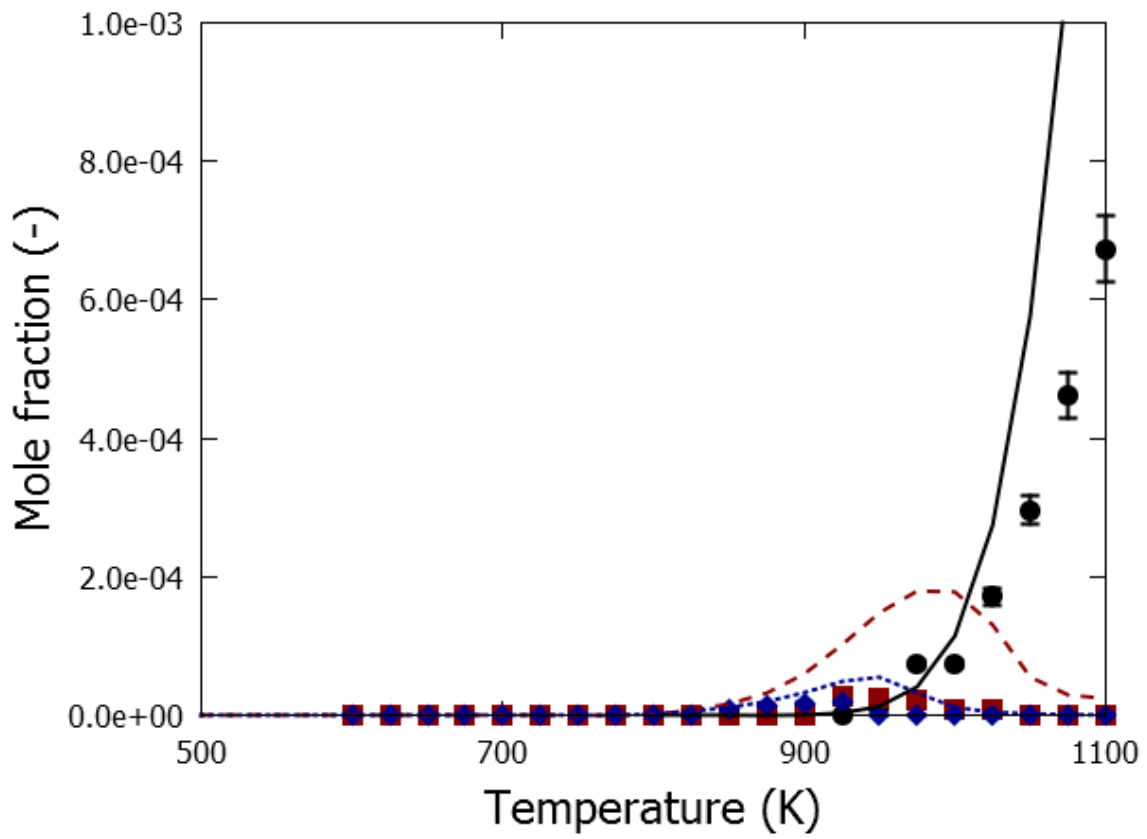


Fig. S 37 C_2H_2 mole fractions as a function of temperature for preneol oxidation and pyrolysis in a jet-stirred reactor, $P=0.107$ MPa, $F_V=4.06 \cdot 10^{-5} \text{ m}^3 \text{ s}^{-1}$, $x_{\text{preneol},0}=0.008$, $\phi=0.5$ (blue), $\phi=1.0$ (red) and $\phi=\infty$ (black): symbols, experimental mole fraction profile; lines, mole fraction profiles calculated with CHEMKIN using the perfectly stirred reactor model and the developed kinetic model

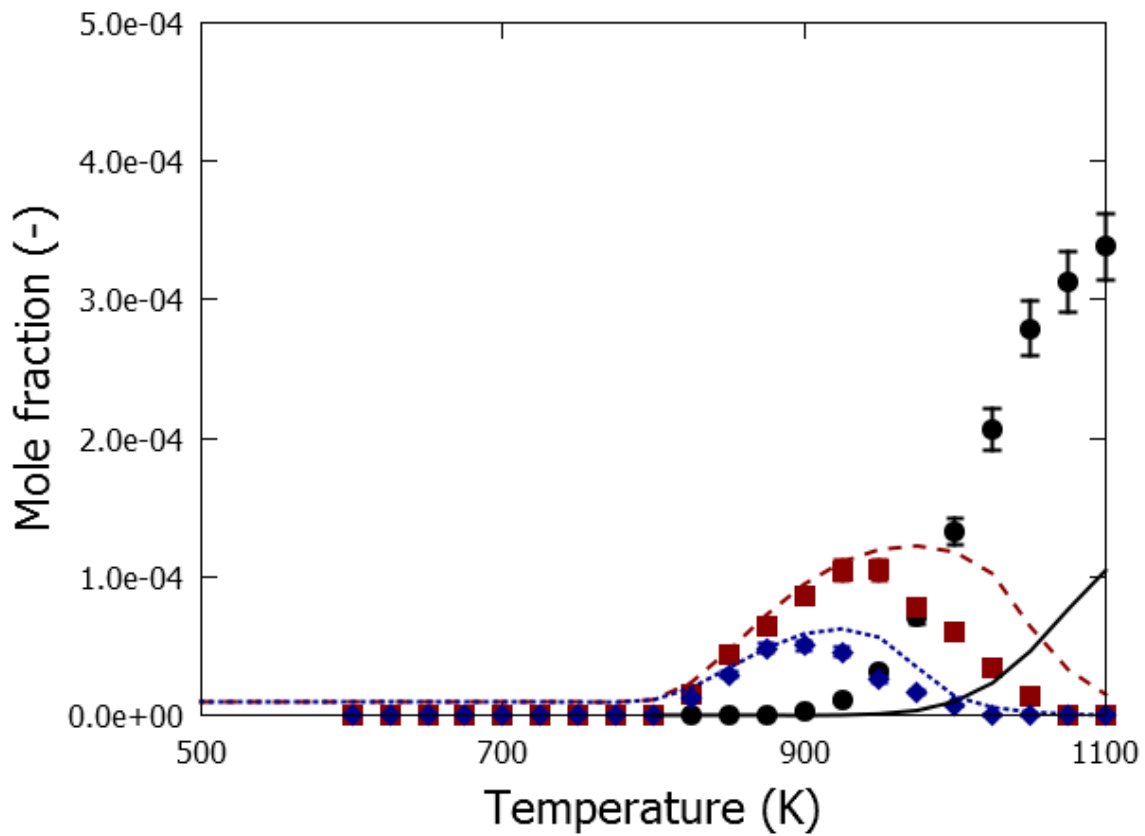


Fig. S $38C_2H_6$ mole fractions as a function of temperature for preneol oxidation and pyrolysis in a jet-stirred reactor, $P=0.107$ MPa, $F_V=4.06 \cdot 10^{-5} \text{ m}^3 \text{ s}^{-1}$, $x_{\text{preneol},0}=0.008$, $\phi=0.5$ (blue), $\phi=1.0$ (red) and $\phi=\infty$ (black): symbols, experimental mole fraction profile; lines, mole fraction profiles calculated with CHEMKIN using the perfectly stirred reactor model and the developed kinetic model

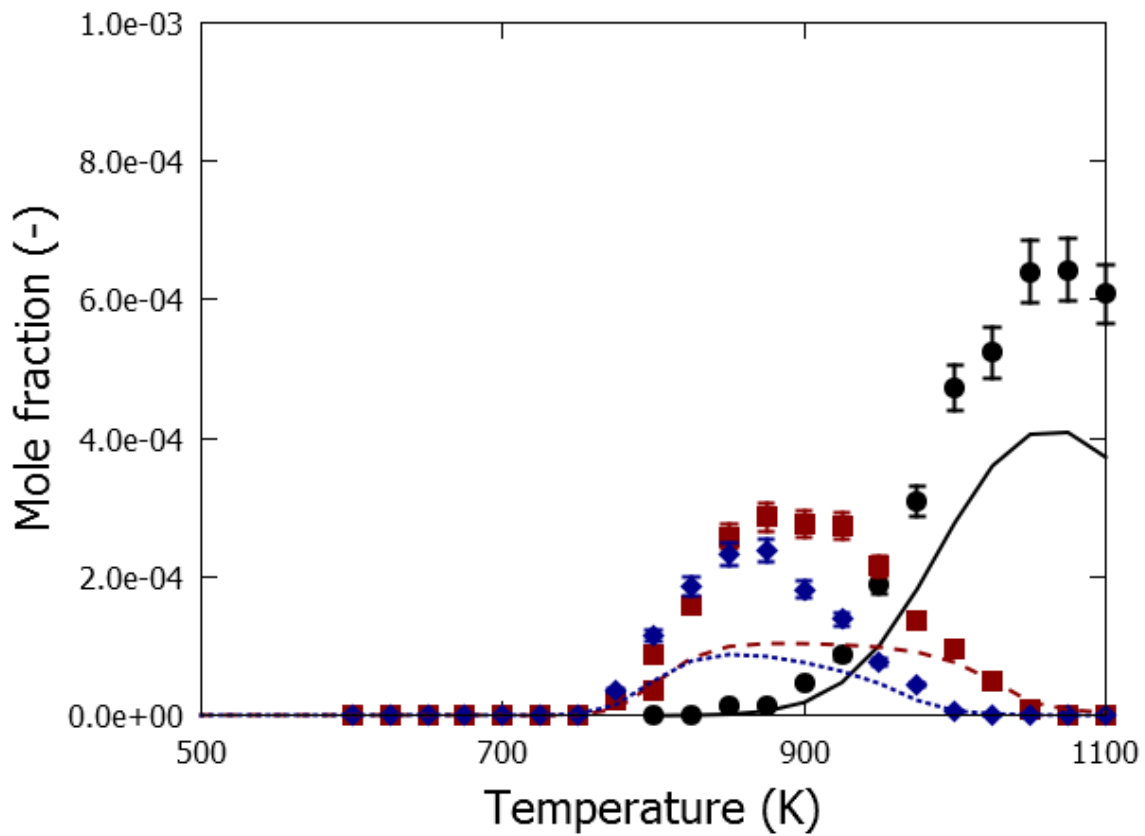


Fig. S 39 C_3H_6 mole fractions as a function of temperature for pre-nol oxidation and pyrolysis in a jet-stirred reactor, $P=0.107$ MPa, $F_V = 4.06 \cdot 10^{-5} \text{ m}^3 \text{ s}^{-1}$, $x_{\text{pre-nol},0}=0.008$, $\phi=0.5$ (blue), $\phi=1.0$ (red) and $\phi=\infty$ (black): symbols, experimental mole fraction profile; lines, mole fraction profiles calculated with CHEMKIN using the perfectly stirred reactor model and the developed kinetic model

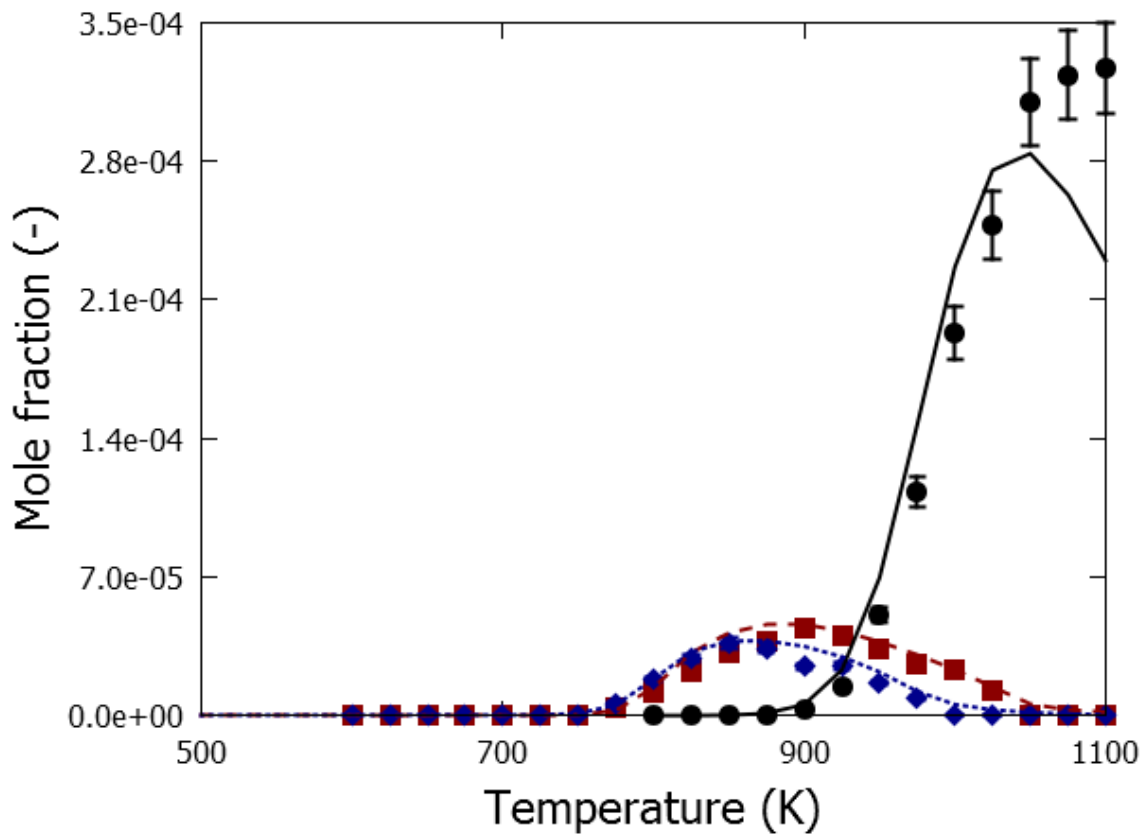


Fig. S 40 Allene mole fractions as a function of temperature for prenenol oxidation and pyrolysis in a jet-stirred reactor, $P=0.107$ MPa, $F_V=4.06 \cdot 10^{-5} \text{ m}^3 \text{ s}^{-1}$, $x_{\text{prenol},0}=0.008$, $\varphi=0.5$ (blue), $\varphi=1.0$ (red) and $\varphi=\infty$ (black): symbols, experimental mole fraction profile; lines, mole fraction profiles calculated with CHEMKIN using the perfectly stirred reactor model and the developed kinetic model

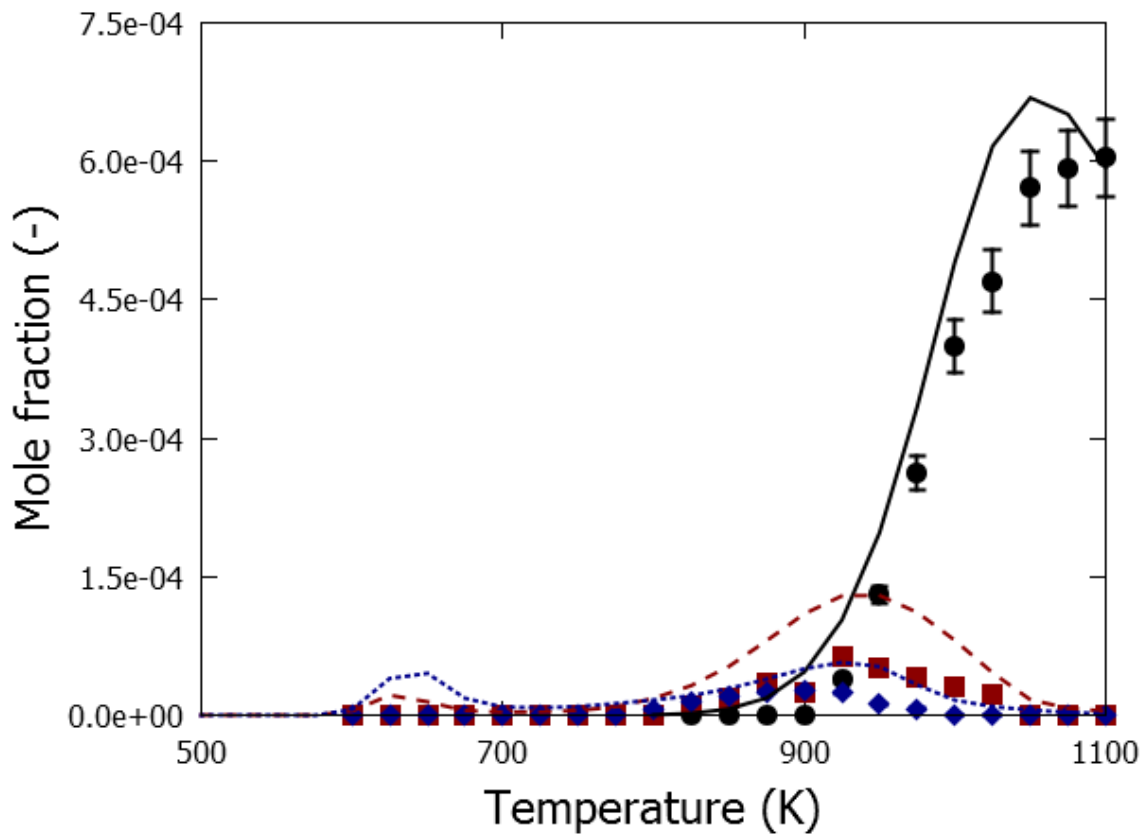


Fig. S 41 Propyne mole fractions as a function of temperature for pre-nol oxidation and pyrolysis in a jet-stirred reactor, $P=0.107$ MPa, $F_v = 4.06 \cdot 10^{-5} \text{ m}^3 \text{ s}^{-1}$, $x_{\text{pre-nol},0}=0.008$, $\phi=0.5$ (blue), $\phi=1.0$ (red) and $\phi=\infty$ (black): symbols, experimental mole fraction profile; lines, mole fraction profiles calculated with CHEMKIN using the perfectly stirred reactor model and the developed kinetic model

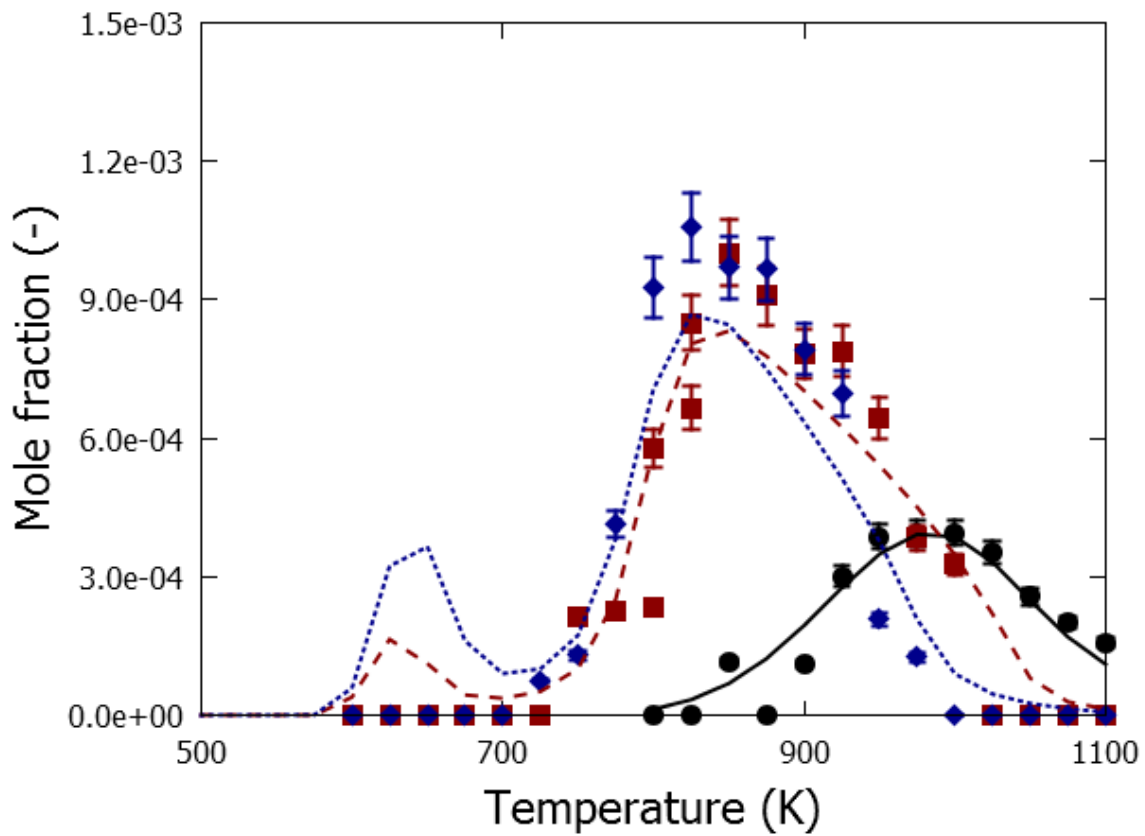


Fig. S 42 Formaldehyde mole fractions as a function of temperature for pre-nol oxidation and pyrolysis in a jet-stirred reactor, $P=0.107$ MPa, $F_v = 4.06 \cdot 10^{-5} \text{ m}^3 \text{ s}^{-1}$, $x_{\text{pre-nol},0}=0.008$, $\phi=0.5$ (blue), $\phi=1.0$ (red) and $\phi=\infty$ (black): symbols, experimental mole fraction profile; lines, mole fraction profiles calculated with CHEMKIN using the perfectly stirred reactor model and the developed kinetic model

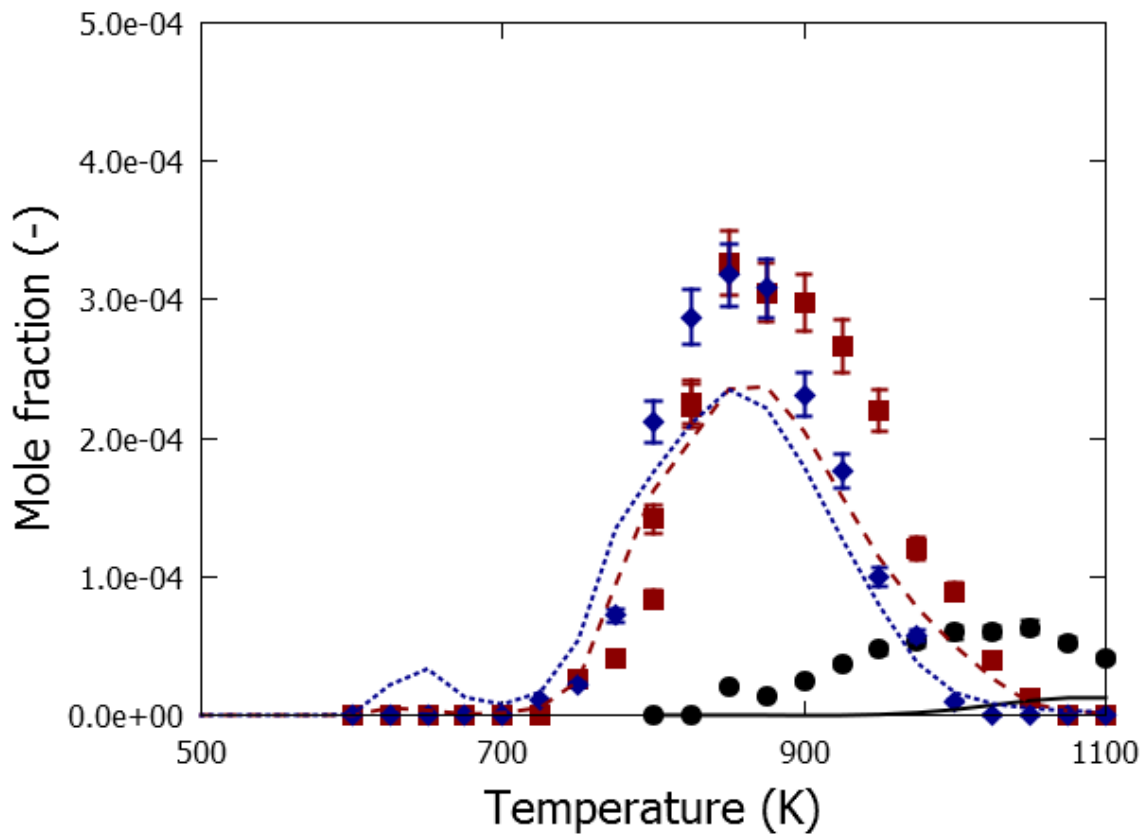


Fig. S 43 Acetaldehyde mole fractions as a function of temperature for prenoI oxidation and pyrolysis in a jet-stirred reactor, $P=0.107$ MPa, $F_v = 4.06 \cdot 10^{-5} \text{ m}^3 \text{ s}^{-1}$, $x_{\text{prenoI},0}=0.008$, $\phi=0.5$ (blue), $\phi=1.0$ (red) and $\phi=\infty$ (black): symbols, experimental mole fraction profile; lines, mole fraction profiles calculated with CHEMKIN using the perfectly stirred reactor model and the developed kinetic model

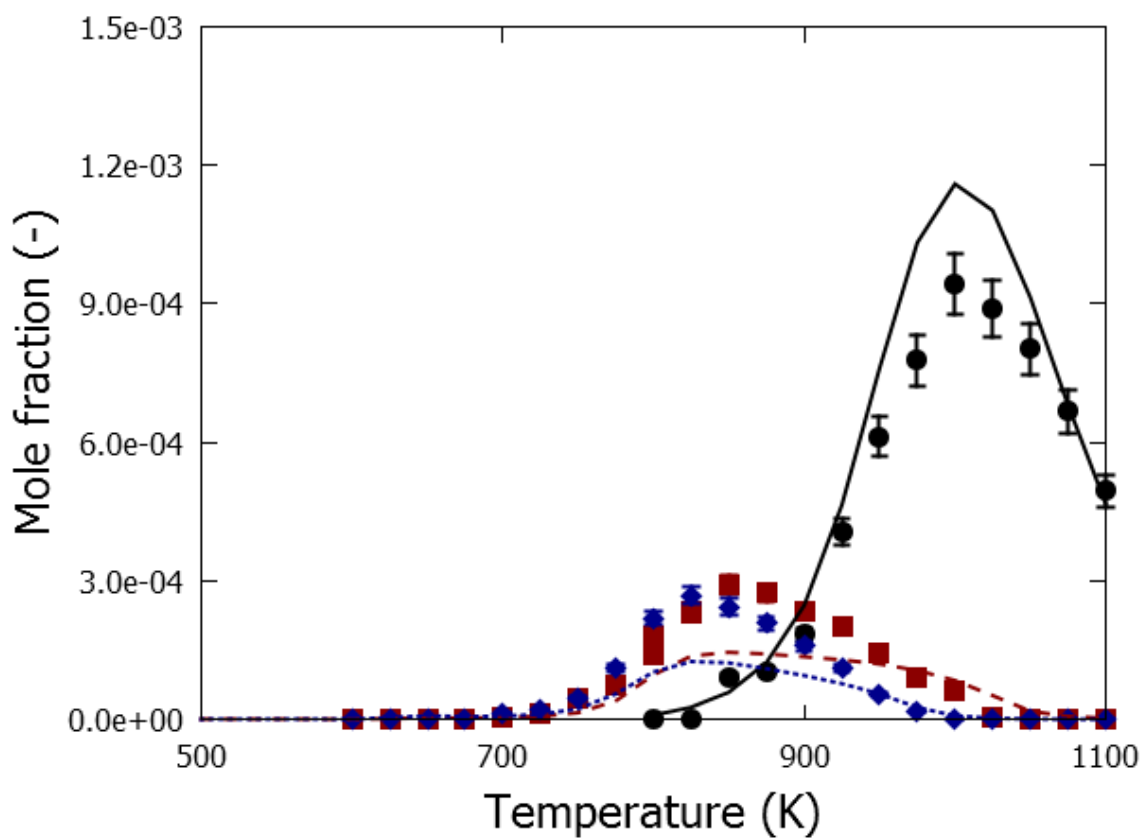


Fig. S 44 isobutene mole fractions as a function of temperature for preneol oxidation and pyrolysis in a jet-stirred reactor, $P=0.107$ MPa, $F_v = 4.06 \cdot 10^{-5} \text{ m}^3 \text{ s}^{-1}$, $x_{\text{preneol},0}=0.008$, $\varphi=0.5$ (blue), $\varphi=1.0$ (red) and $\varphi=\infty$ (black): symbols, experimental mole fraction profile; lines, mole fraction profiles calculated with CHEMKIN using the perfectly stirred reactor model and the developed kinetic model

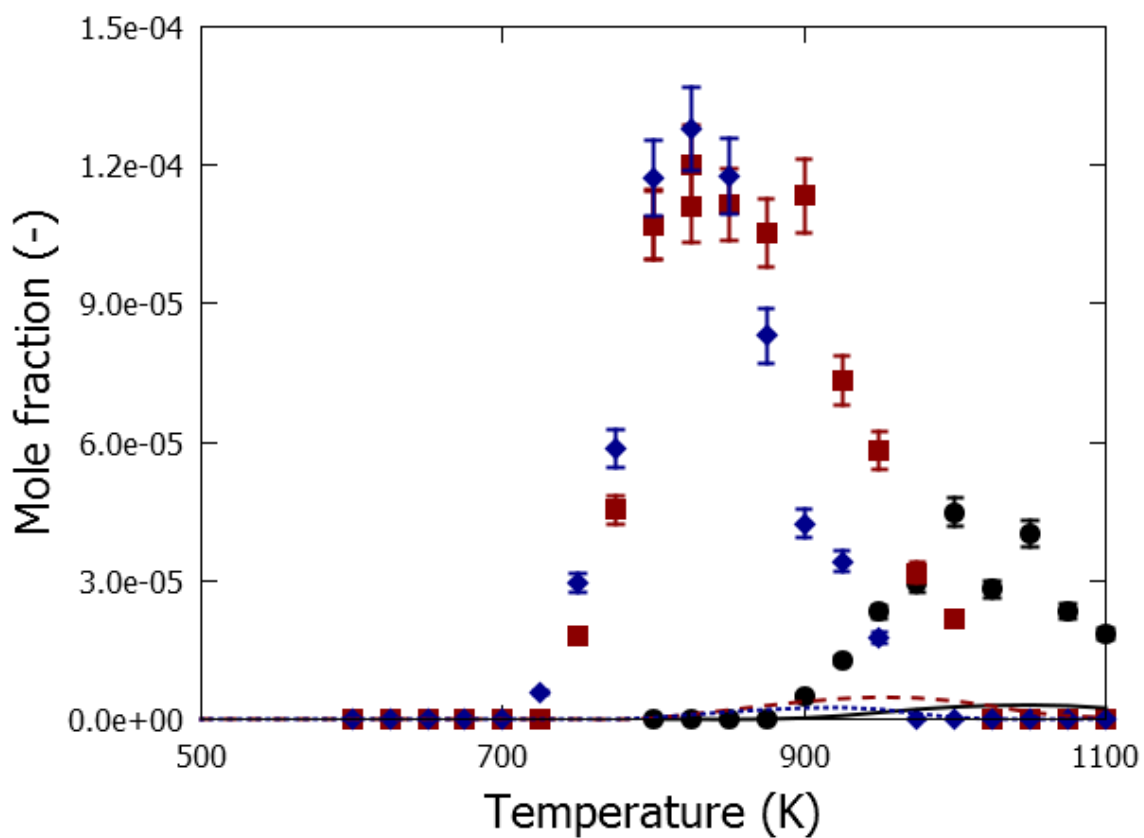


Fig. S 45 2-butene mole fractions as a function of temperature for pre-nol oxidation and pyrolysis in a jet-stirred reactor, $P=0.107$ MPa, $F_v = 4.06 \cdot 10^{-5} \text{ m}^3 \text{ s}^{-1}$, $x_{\text{prenol},0}=0.008$, $\phi=0.5$ (blue), $\phi=1.0$ (red) and $\phi=\infty$ (black): symbols, experimental mole fraction profile; lines, mole fraction profiles calculated with CHEMKIN using the perfectly stirred reactor model and the developed kinetic model

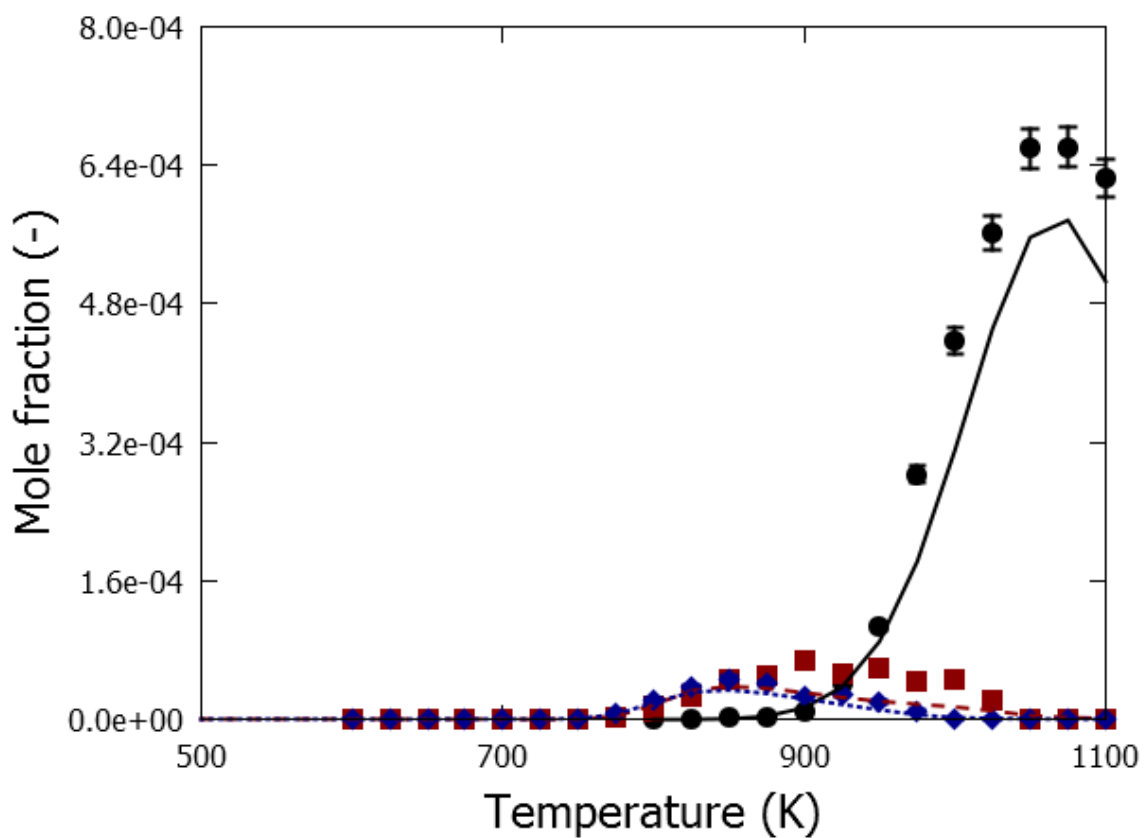


Fig. S 46 1,3-butadiene mole fractions as a function of temperature for preneol oxidation and pyrolysis in a jet-stirred reactor, $P=0.107$ MPa, $F_v = 4.06 \cdot 10^{-5} \text{ m}^3 \text{ s}^{-1}$, $x_{\text{preneol},0}=0.008$, $\phi=0.5$ (blue), $\phi=1.0$ (red) and $\phi=\infty$ (black): symbols, experimental mole fraction profile; lines, mole fraction profiles calculated with CHEMKIN using the perfectly stirred reactor model and the developed kinetic model

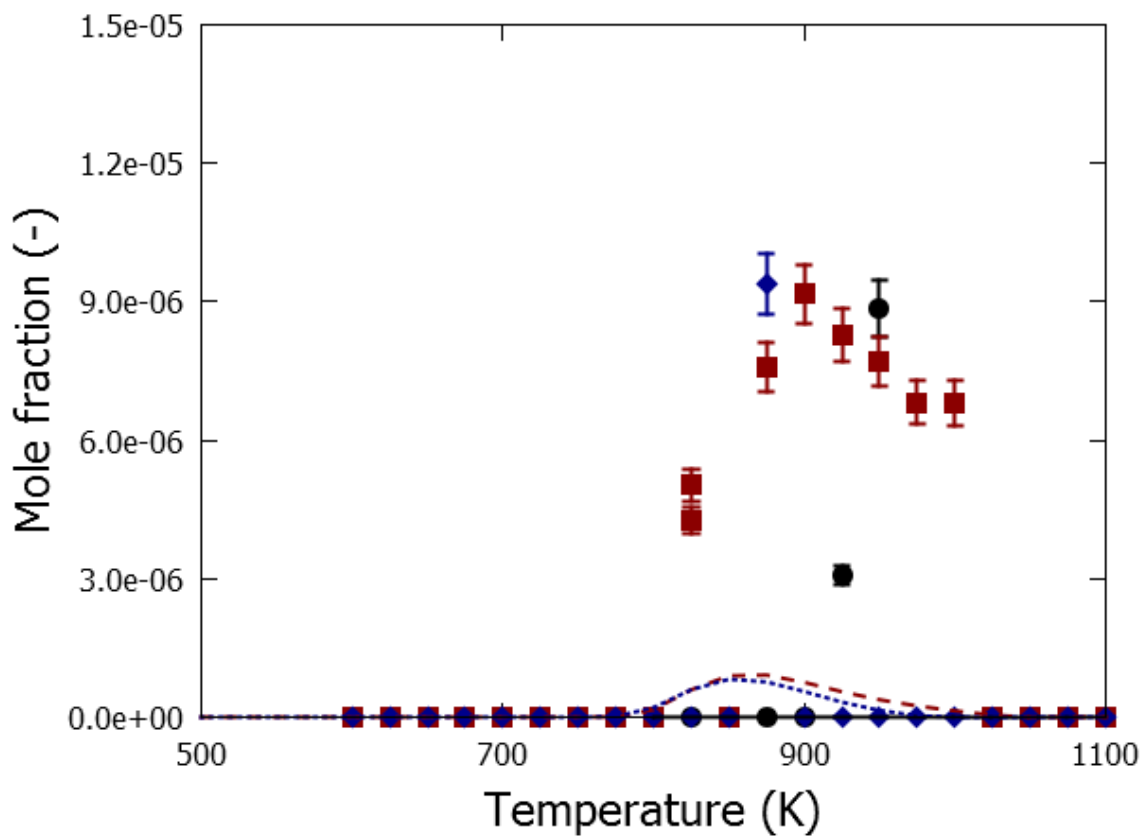


Fig. S 47furan mole fractions as a function of temperature for prenil oxidation and pyrolysis in a jet-stirred reactor, $P=0.107$ MPa, $F_V=4.06 \cdot 10^{-5} \text{ m}^3 \text{ s}^{-1}$, $x_{\text{prenil},0}=0.008$, $\phi=0.5$ (blue), $\phi=1.0$ (red) and $\phi=\infty$ (black): symbols, experimental mole fraction profile; lines, mole fraction profiles calculated with CHEMKIN using the perfectly stirred reactor model and the developed kinetic model

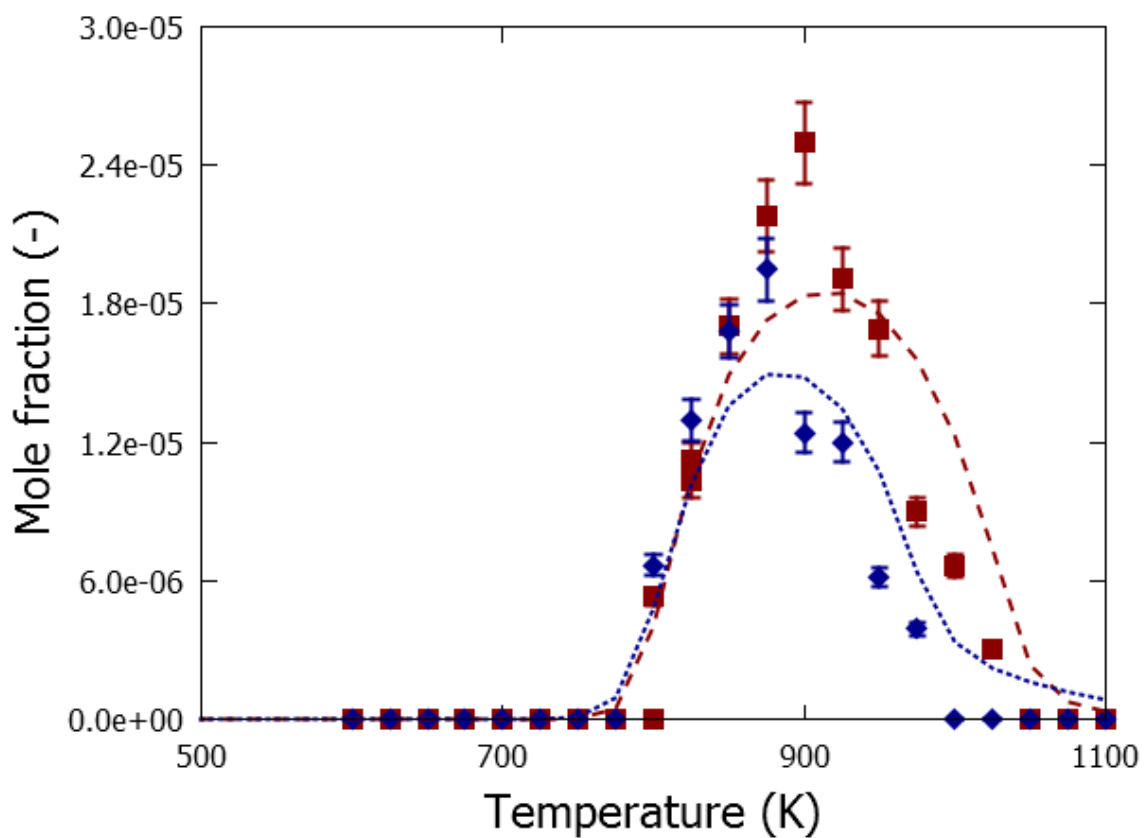


Fig. S 48 acrolein mole fractions as a function of temperature for pre-nol oxidation and pyrolysis in a jet-stirred reactor, $P=0.107$ MPa, $F_v = 4.06 \cdot 10^{-5} \text{ m}^3 \text{ s}^{-1}$, $x_{\text{prenol},0}=0.008$, $\phi=0.5$ (blue), $\phi=1.0$ (red) and $\phi=\infty$ (black): symbols, experimental mole fraction profile; lines, mole fraction profiles calculated with CHEMKIN using the perfectly stirred reactor model and the developed kinetic model

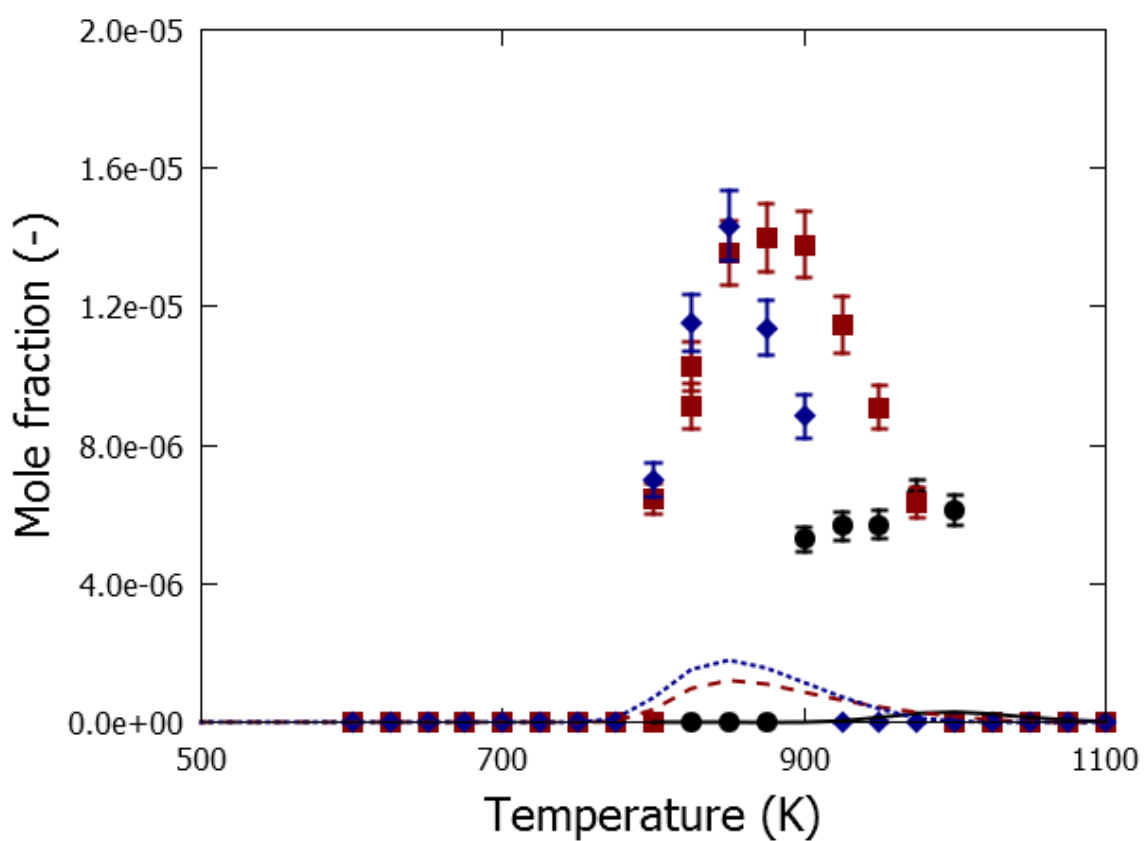


Fig. S 49 Propanal mole fractions as a function of temperature for pre-nol oxidation and pyrolysis in a jet-stirred reactor, $P=0.107$ MPa, $F_v = 4.06 \cdot 10^{-5} \text{ m}^3 \text{ s}^{-1}$, $x_{\text{pre-nol},0}=0.008$, $\phi=0.5$ (blue), $\phi=1.0$ (red) and $\phi=\infty$ (black): symbols, experimental mole fraction profile; lines, mole fraction profiles calculated with CHEMKIN using the perfectly stirred reactor model and the developed kinetic model

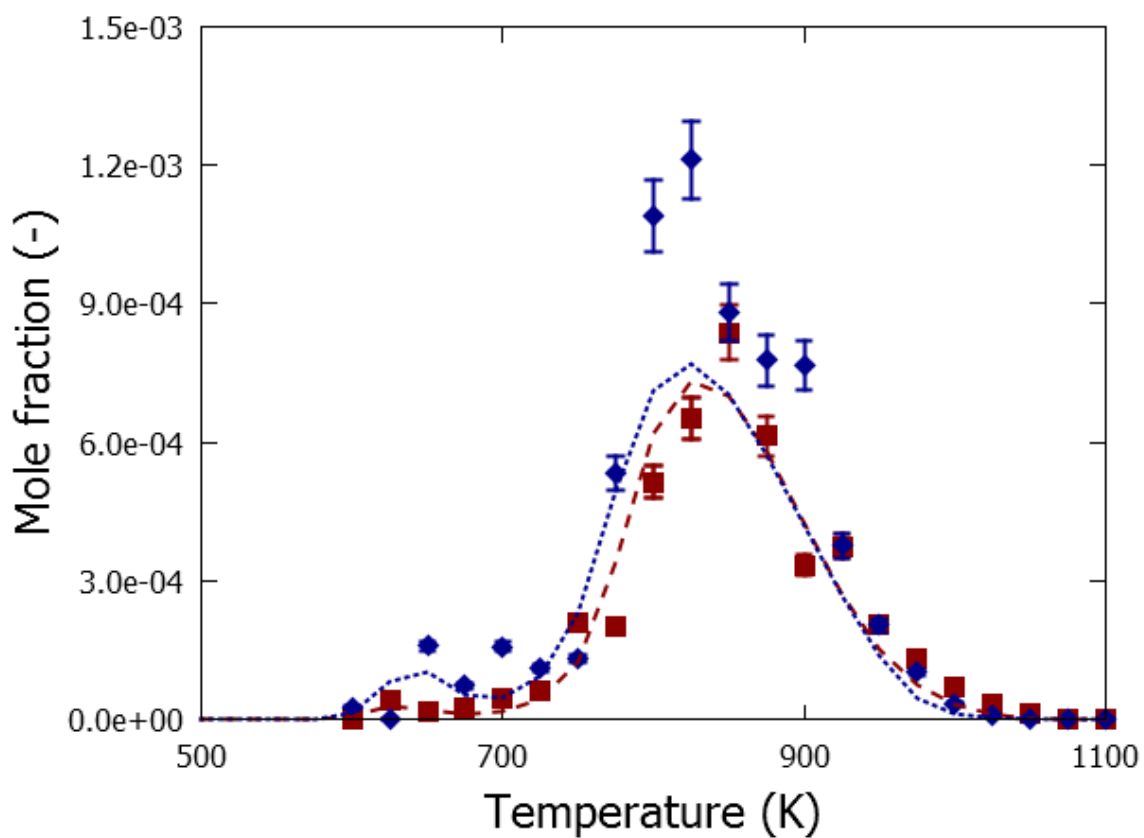


Fig. S 50 acetone mole fractions as a function of temperature for prenil oxidation and pyrolysis in a jet-stirred reactor, $P=0.107$ MPa, $F_v = 4.06 \cdot 10^{-5} \text{ m}^3 \text{ s}^{-1}$, $x_{\text{prenil},0}=0.008$, $\phi=0.5$ (blue), $\phi=1.0$ (red) and $\phi=\infty$ (black): symbols, experimental mole fraction profile; lines, mole fraction profiles calculated with CHEMKIN using the perfectly stirred reactor model and the developed kinetic model

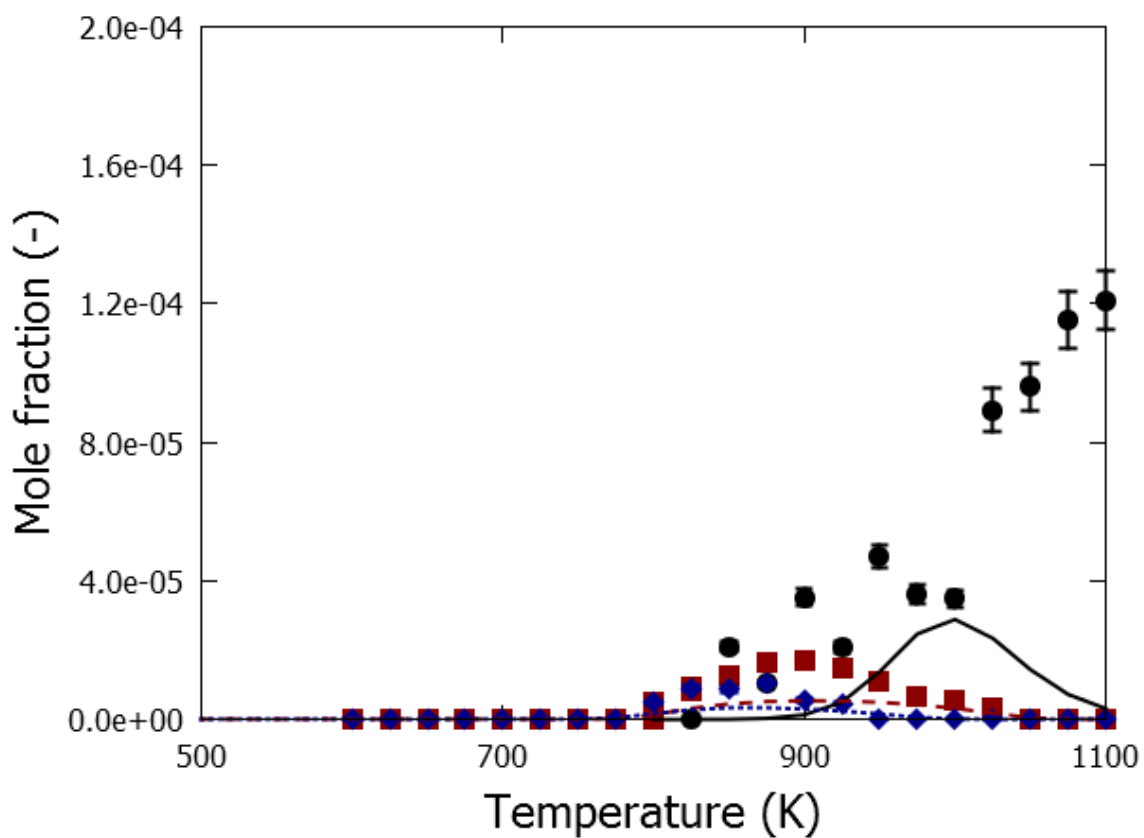


Fig. S 51 2-methyl-1-butene mole fractions as a function of temperature for preno oxidation and pyrolysis in a jet-stirred reactor, $P=0.107$ MPa, $F_V=4.06 \cdot 10^{-5} \text{ m}^3 \text{ s}^{-1}$, $x_{\text{preno},0}=0.008$, $\varphi=0.5$ (blue), $\varphi=1.0$ (red) and $\varphi=\infty$ (black): symbols, experimental mole fraction profile; lines, mole fraction profiles calculated with CHEMKIN using the perfectly stirred reactor model and the developed kinetic model

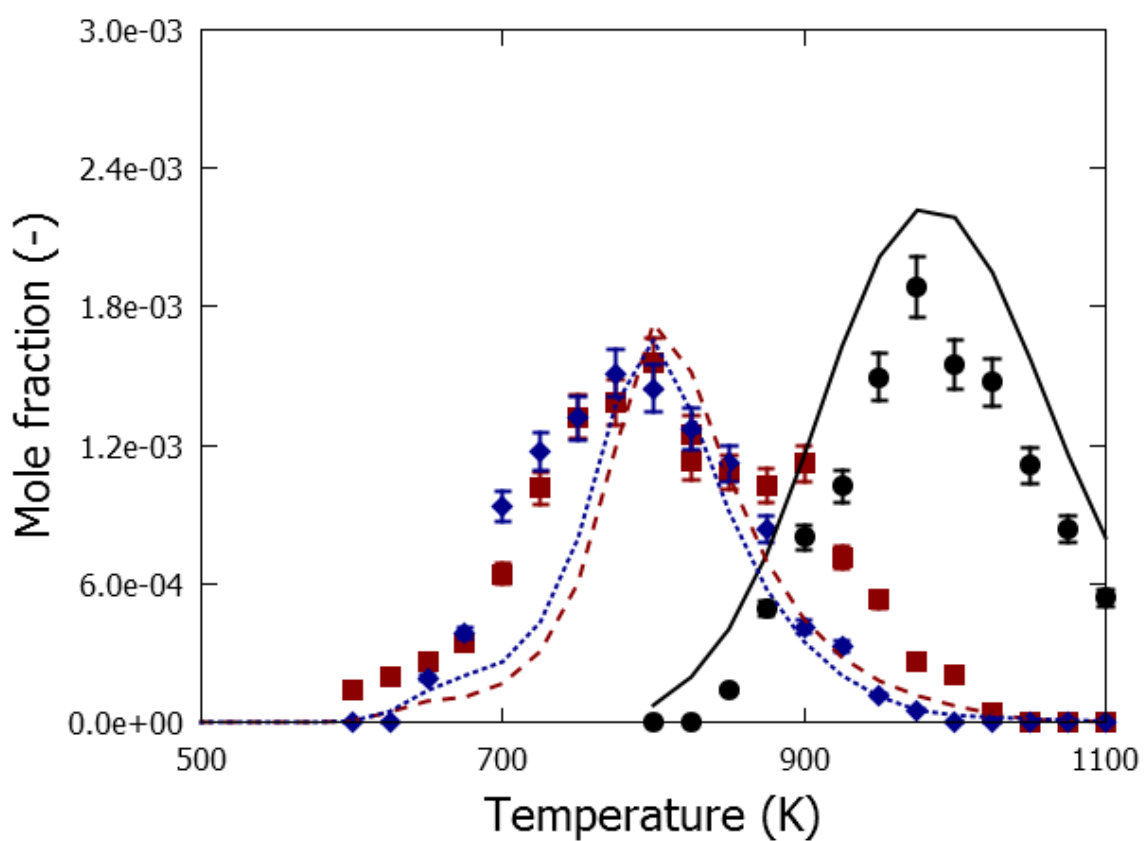


Fig. S 52 2-methyl-1,3-butadiene mole fractions as a function of temperature for pre-oxidation and pyrolysis in a jet-stirred reactor, $P=0.107$ MPa, $F_v = 4.06 \cdot 10^{-5} \text{ m}^3 \text{ s}^{-1}$, $x_{\text{pre-oxid},0}=0.008$, $\phi=0.5$ (blue), $\phi=1.0$ (red) and $\phi=\infty$ (black): symbols, experimental mole fraction profile; lines, mole fraction profiles calculated with CHEMKIN using the perfectly stirred reactor model and the developed kinetic model

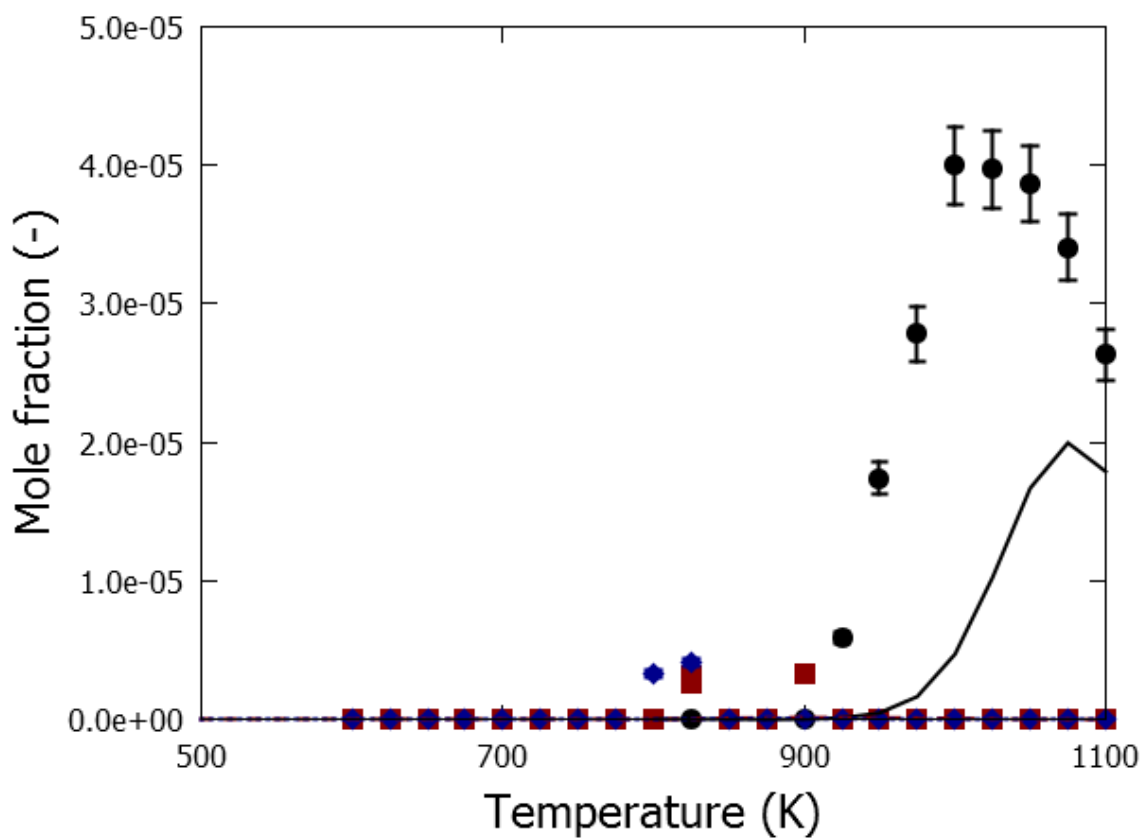


Fig. S 53 1,3-pentadiene mole fractions as a function of temperature for prenel oxidation and pyrolysis in a jet-stirred reactor, $P=0.107$ MPa, $F_v = 4.06 \cdot 10^{-5} \text{ m}^3 \text{ s}^{-1}$, $x_{\text{prenol},0}=0.008$, $\varphi=0.5$ (blue), $\varphi=1.0$ (red) and $\varphi=\infty$ (black): symbols, experimental mole fraction profile; lines, mole fraction profiles calculated with CHEMKIN using the perfectly stirred reactor model and the developed kinetic model

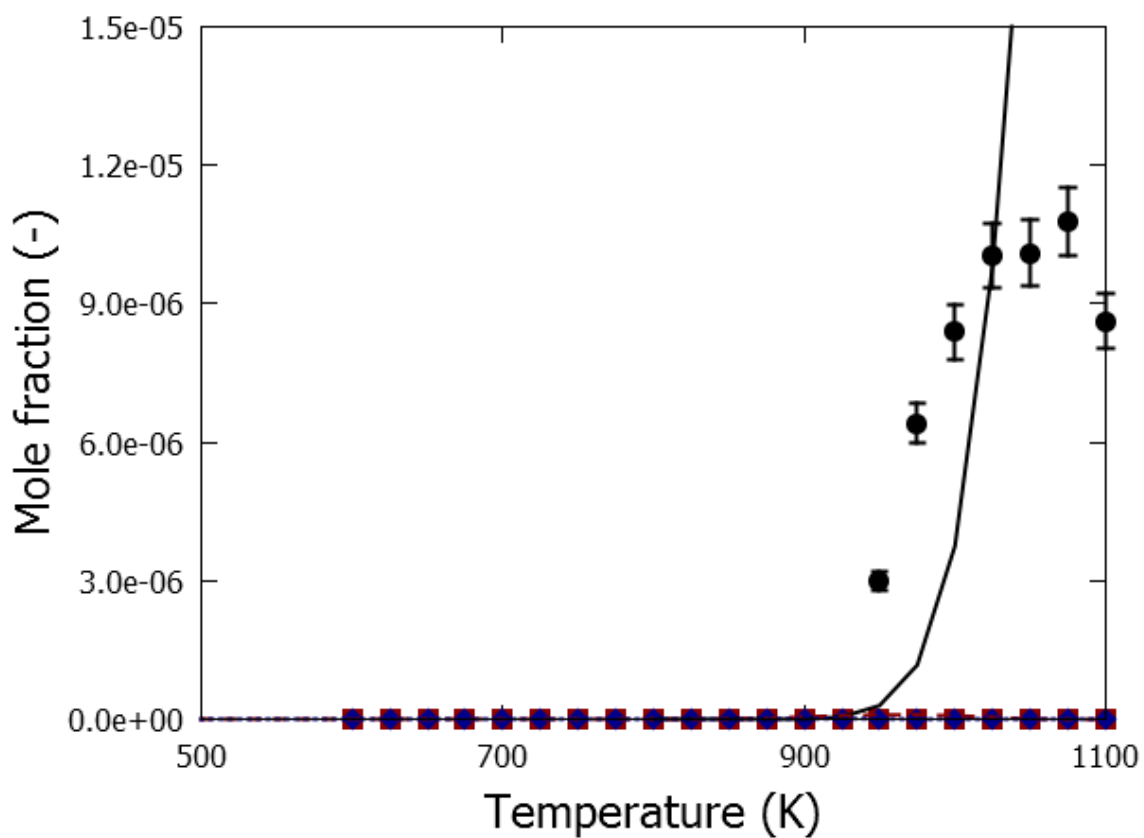


Fig. S 54 1,3-cyclopentadiene mole fractions as a function of temperature for prenoI oxidation and pyrolysis in a jet-stirred reactor, $P=0.107$ MPa, $F_V=4.06 \cdot 10^{-5} \text{ m}^3 \text{ s}^{-1}$, $x_{\text{prenoI},0}=0.008$, $\varphi=0.5$ (blue), $\varphi=1.0$ (red) and $\varphi=\infty$ (black): symbols, experimental mole fraction profile; lines, mole fraction profiles calculated with CHEMKIN using the perfectly stirred reactor model and the developed kinetic model

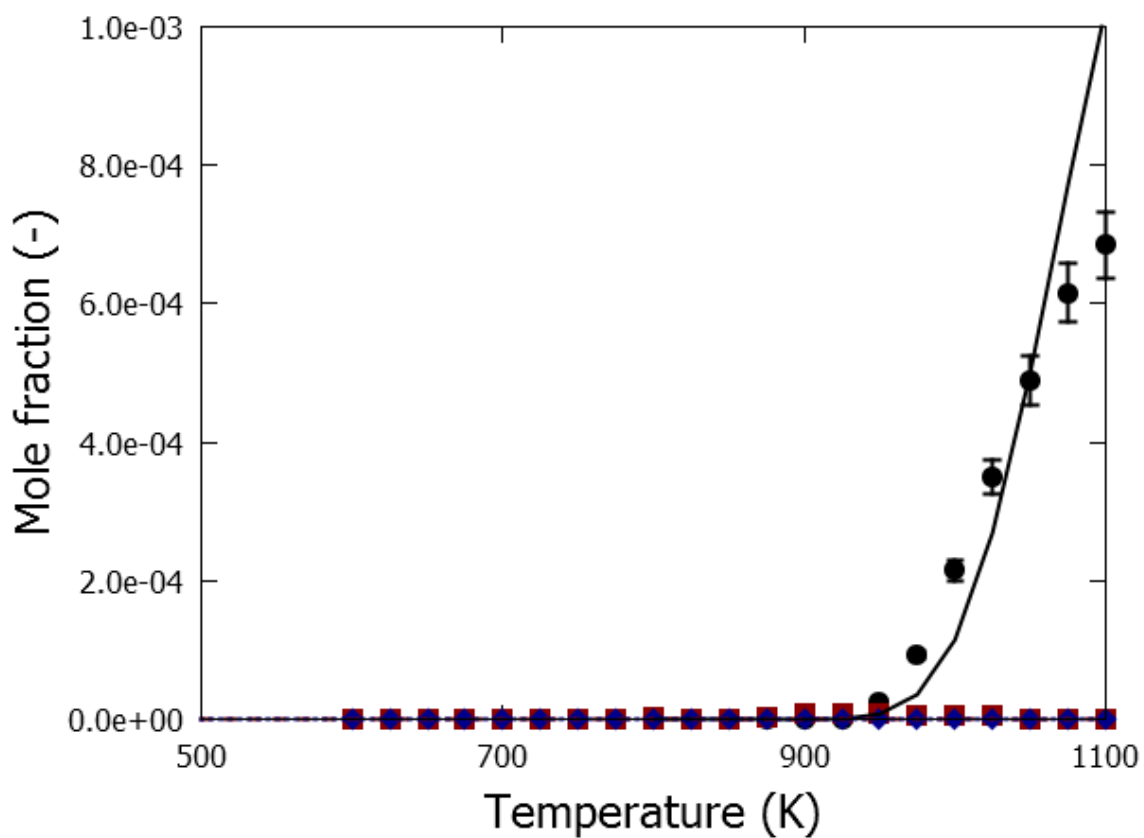


Fig. S 55 benzene mole fractions as a function of temperature for prenil oxidation and pyrolysis in a jet-stirred reactor, $P=0.107$ MPa, $F_v = 4.06 \cdot 10^{-5} \text{ m}^3 \text{ s}^{-1}$, $x_{\text{prenil},0}=0.008$, $\phi=0.5$ (blue), $\phi=1.0$ (red) and $\phi=\infty$ (black): symbols, experimental mole fraction profile; lines, mole fraction profiles calculated with CHEMKIN using the perfectly stirred reactor model and the developed kinetic model

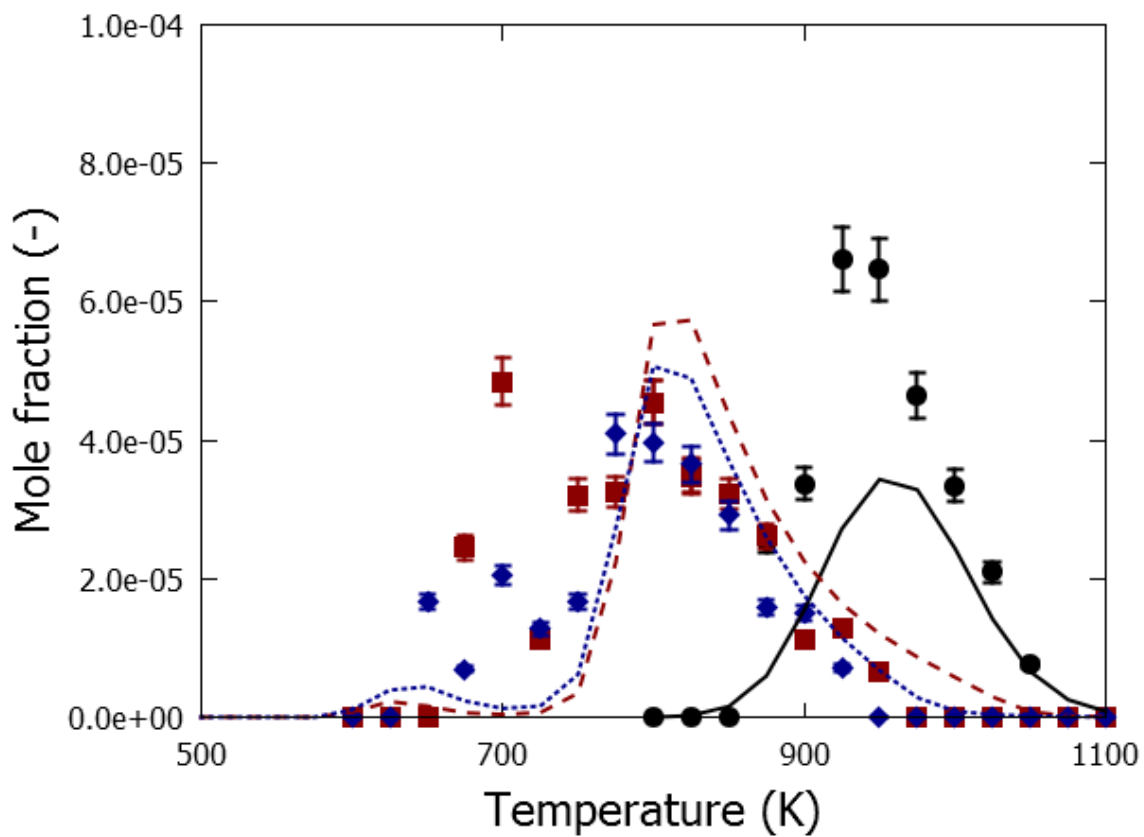


Fig. S 56 2-methyl-propanal mole fractions as a function of temperature for isoprenol oxidation and pyrolysis in a jet-stirred reactor, $P=0.107$ MPa, $F_V = 4.06 \cdot 10^{-5} \text{ m}^3 \text{ s}^{-1}$, $x_{\text{isoprenol},0}=0.008$, $\phi=0.5$ (blue), $\phi=1.0$ (red) and $\phi=\infty$ (black): symbols, experimental mole fraction profile; lines, mole fraction profiles calculated with CHEMKIN using the perfectly stirred reactor model and the developed kinetic model

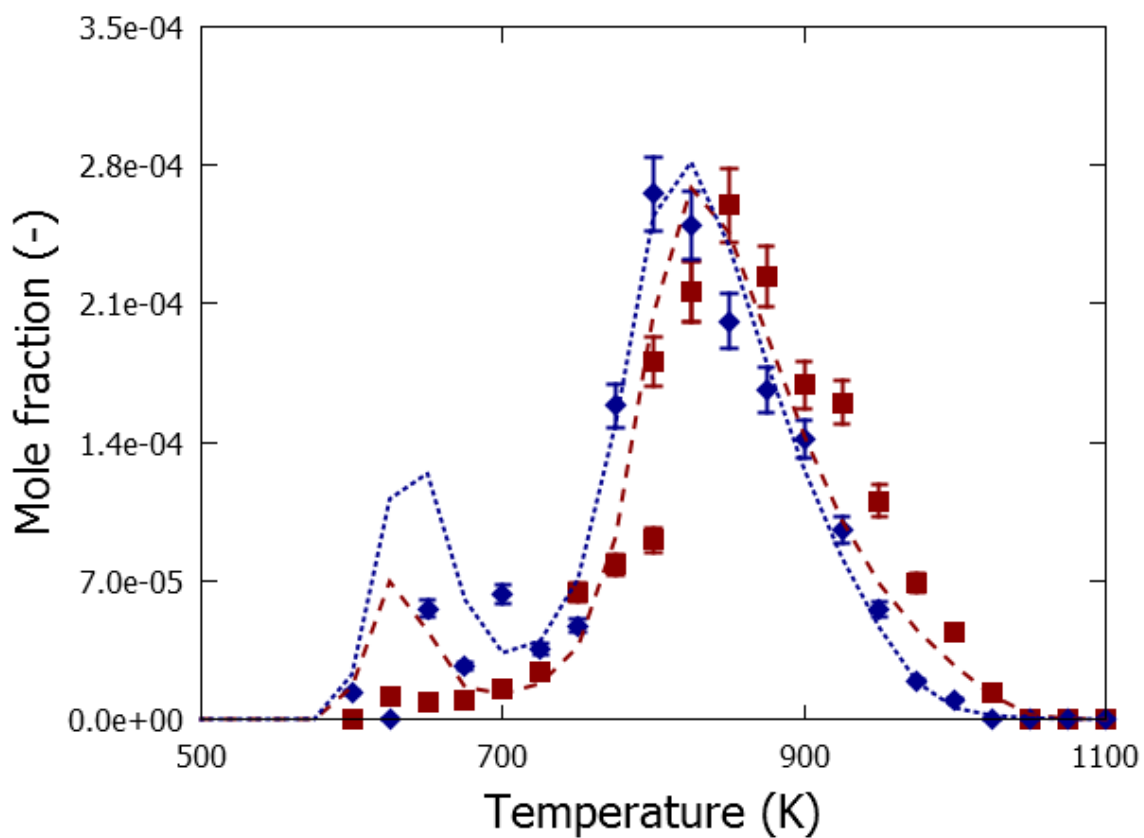


Fig. S 57 methacrolein mole fractions as a function of temperature for isoprenol oxidation and pyrolysis in a jet-stirred reactor, $P=0.107$ MPa, $F_v = 4.06 \cdot 10^{-5} \text{ m}^3 \text{ s}^{-1}$, $x_{\text{isoprenol},0}=0.008$, $\phi=0.5$ (blue), $\phi=1.0$ (red) and $\phi=\infty$ (black): symbols, experimental mole fraction profile; lines, mole fraction profiles calculated with CHEMKIN using the perfectly stirred reactor model and the developed kinetic model

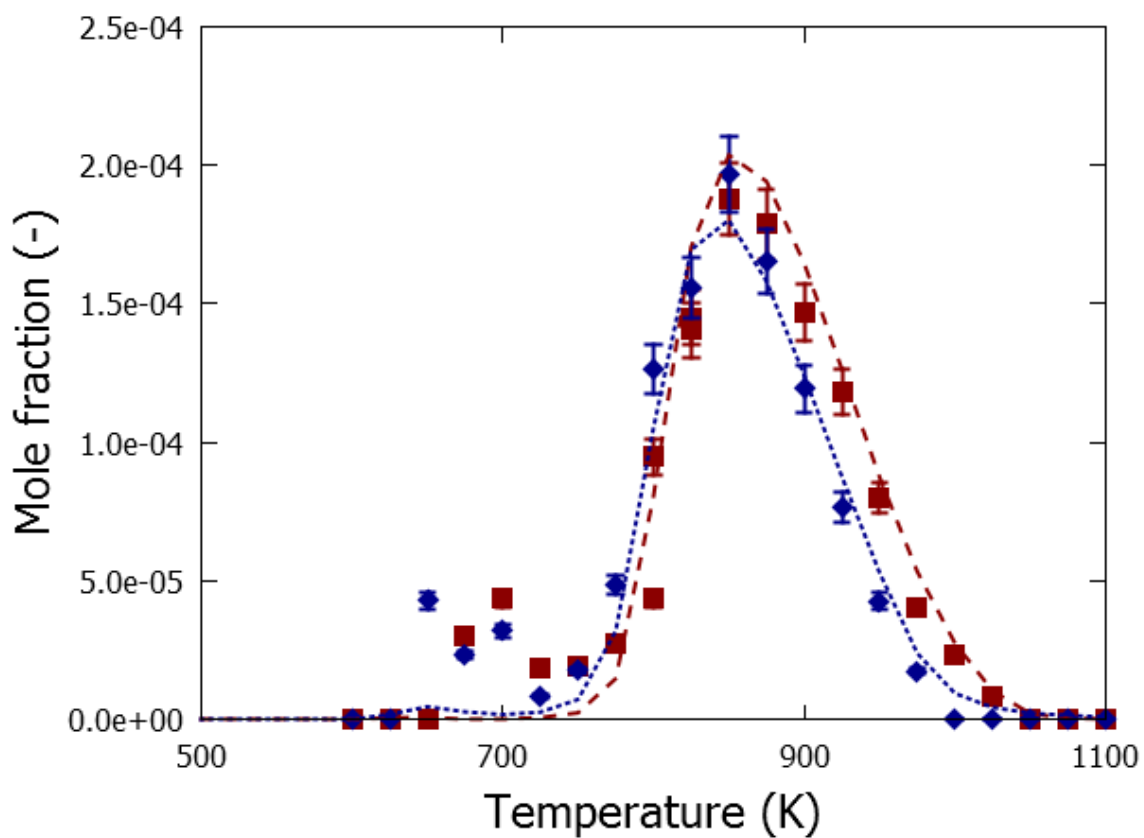


Fig. S 58 but-3-en-2-one mole fractions as a function of temperature for isoprenol oxidation and pyrolysis in a jet-stirred reactor, $P=0.107$ MPa, $F_v = 4.06 \cdot 10^{-5} \text{ m}^3 \text{ s}^{-1}$, $x_{\text{isoprenol},0}=0.008$, $\phi=0.5$ (blue), $\phi=1.0$ (red) and $\phi=\infty$ (black): symbols, experimental mole fraction profile; lines, mole fraction profiles calculated with CHEMKIN using the perfectly stirred reactor model and the developed kinetic model

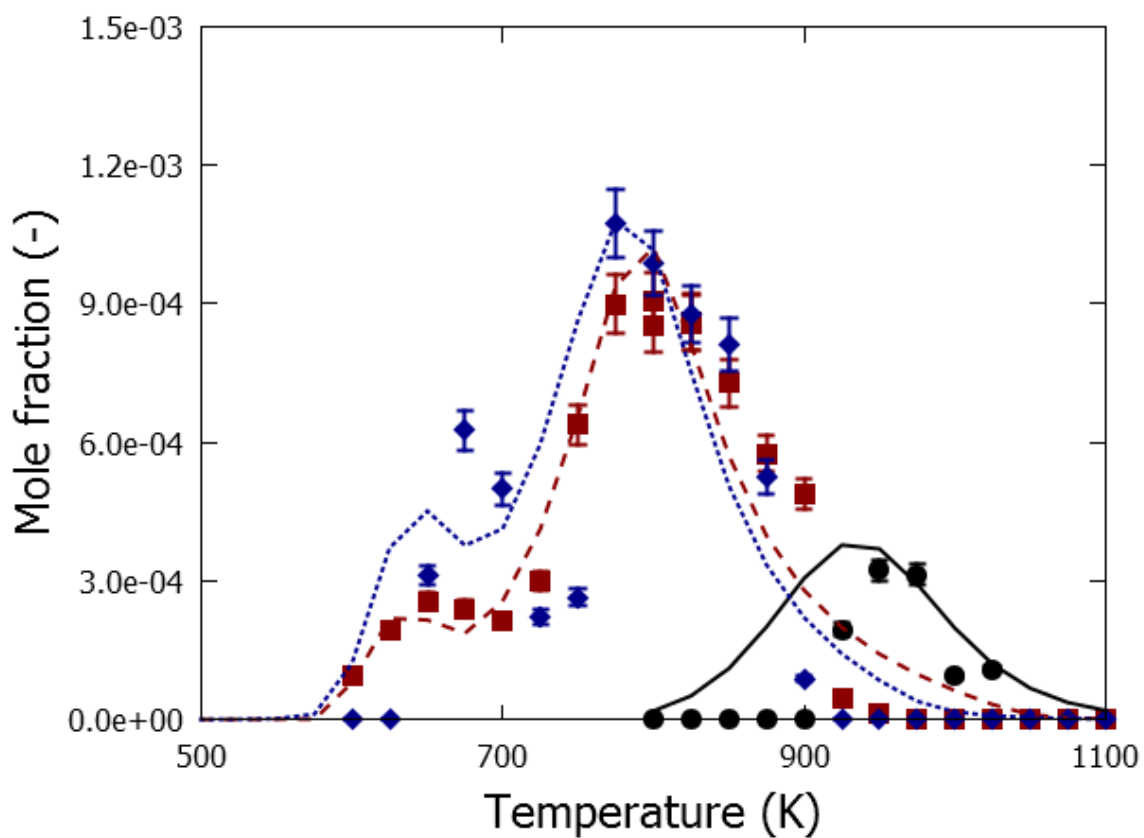
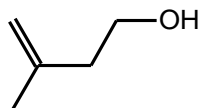


Fig. S 59 Prenal mole fractions as a function of temperature for isoprenol oxidation and pyrolysis in a jet-stirred reactor, $P=0.107$ MPa, $F_V=4.06 \cdot 10^{-5} \text{ m}^3 \text{ s}^{-1}$, $x_{\text{isoprenol},0}=0.008$, $\phi=0.5$ (blue), $\phi=1.0$ (red) and $\phi=\infty$ (black): symbols, experimental mole fraction profile; lines, mole fraction profiles calculated with CHEMKIN using the perfectly stirred reactor model and the developed kinetic model

Species and transition state information from CBS-QB3 calculations

The species and transition state are organized based on their appearance in Table 1 of the main text. The radical site notated in the main text with a ‘•’ is represented by ‘J’ in the following list. If a distinction is made between cis and trans transition states, rate coefficients for each isomer are calculated that the overall rate expression is the sum of both (assuming that both are approximately of equal importance, hence of similar energy).

Isoprenol C=C(C)CCOH



Geometry [Angstroms]

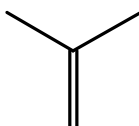
6	0.155731	-0.430050	0.091110
6	0.058706	-0.022589	1.544733
6	1.261951	0.290764	-0.679185
1	0.347703	-1.506996	0.014733
1	-0.790221	-0.234459	-0.419919
6	-0.958812	0.712664	1.994835
6	1.161796	-0.496446	2.459236
1	-1.032288	1.006831	3.036596
1	-1.756665	1.040182	1.336678
1	2.139822	-0.117056	2.144482
1	0.993294	-0.176908	3.489172
1	1.231907	-1.590161	2.446238
8	1.239108	-0.207855	-2.015239
1	1.075772	1.373520	-0.654589
1	2.238774	0.104881	-0.211728
1	1.916142	0.253676	-2.517988

Rotational Constants [GHz] = 1.599 1.840 7.131

Frequencies [cm-1]

44.1188	97.7605	176.3435
197.0601	267.7102	341.6938
403.2608	466.2012	539.0742
722.3127	809.0395	847.8323
927.6755	978.8450	998.4776
1020.1737	1050.8394	1076.1260
1101.9467	1222.9518	1242.8540
1291.1323	1318.5790	1341.4192
1412.2537	1445.3906	1453.4183
1480.1814	1491.0833	1500.9836
1529.0244	1712.1541	2973.4226
3001.3821	3013.5015	3022.8738
3057.6560	3079.7671	3102.7300
3125.8608	3205.2688	3839.9419

C2C=C



Geometry [Angstroms]

6	-0.008006	-0.152524	-0.004816
6	0.013390	0.015758	1.492959
6	1.377980	-0.006393	2.132903
6	-1.102088	0.173837	2.205392
1	0.450708	-1.104144	-0.297712

1	-1.024466	-0.126591	-0.401462			
1	0.572235	0.637816	-0.495184			
1	-1.075924	0.294135	3.283236			
1	-2.079633	0.188352	1.735185			
1	2.012689	0.790201	1.727486			
1	1.320447	0.119900	3.215458			
1	1.892084	-0.951895	1.924326			
Rotational Constants [GHz] =				4.620	8.368	9.153
Frequencies [cm-1]						
168.4944	208.1867	380.5237				
439.1494	440.9440	704.9992				
813.6941	918.5160	960.5673				
983.8539	1021.5856	1083.2653				
1105.7559	1293.1761	1409.8623				
1413.5787	1442.2336	1472.3876				
1485.6305	1490.3470	1502.7919				
1719.0052	3005.9309	3011.6887				
3049.0374	3052.1636	3101.8828				
3103.6863	3126.4939	3205.4385				

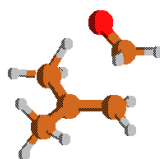
CH2O

Geometry [Angstroms]						
6	-0.000086	0.525856	0.000000			
1	0.938496	1.118323	0.000000			
8	-0.000025	-0.674081	0.000000			
1	-0.938728	1.118228	0.000000			
Rotational Constants [GHz] =				34.335	39.046	284.593
Frequencies [cm-1]						
1202.1785	1270.1422	1539.1178				
1827.0549	2869.5789	2918.8086				

Rxn1

TS C=C(C)CCOH => C2C=C+CH2O

Geometry [Angstroms]						
6	0.085237	0.013737	-0.037664			
6	0.013966	-0.020054	1.380127			
6	1.279875	-0.043237	2.191034			
6	-1.201526	-0.427453	1.947556			
6	-1.183523	-2.270278	1.387063			
8	-0.865659	-2.370561	0.141916			
1	-1.284743	-0.469308	3.029783			
1	-2.112122	-0.122972	1.441072			
1	1.046124	0.253178	-0.487820			
1	-0.762572	0.447267	-0.565194			
1	1.121359	-0.447994	3.192170			
1	2.058761	-0.627317	1.691536			
1	1.667035	0.976189	2.297441			
1	-0.493530	-2.686149	2.139894			
1	-2.238602	-2.428094	1.649495			
1	-0.195466	-1.221248	-0.171983			
Rotational Constants [GHz] =				2.311	2.679	5.074



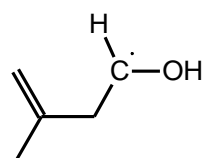
Frequencies [cm-1]

-1137.5406	76.1114	136.2534
176.0563	368.8711	405.0896
453.6654	497.6875	574.5224
596.7416	667.0401	824.2939
892.7602	937.7783	988.9911
1020.2337	1059.6075	1062.5592
1077.6581	1085.0446	1214.9930
1240.3469	1325.2452	1366.0004
1403.5094	1417.3958	1430.0083
1479.6650	1487.3527	1528.3698
1556.2013	1573.3467	1649.5830
2928.2368	2993.5930	3021.0835
3071.4861	3090.8455	3107.3157
3112.2393	3164.7395	3189.3174

C=C(C)CCJOH

Geometry [Angstroms]

6	0.020979	0.050604	-0.028553
6	-0.029061	0.016301	1.303084
6	1.211289	-0.061390	2.155557
6	-1.349343	0.050363	2.046316
6	-1.652885	-1.237431	2.738653
8	-2.640385	-1.149314	3.690611
1	-1.329863	0.842596	2.806754
1	-2.157590	0.317193	1.346429
1	0.964538	0.022726	-0.563317
1	-0.880472	0.113270	-0.629076
1	1.175651	-0.933368	2.816408
1	2.115888	-0.120157	1.547616
1	1.289255	0.818875	2.804400
1	-1.567213	-2.178946	2.198454
1	-2.834190	-2.030763	4.023314

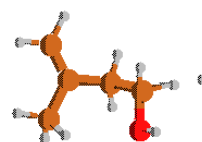
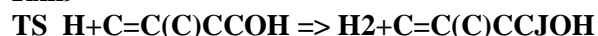


Rotational Constants [GHz] =

1.646 1.899 7.306

Frequencies [cm-1]

72.9856	82.6046	179.7092
196.8562	345.9027	368.1214
396.1781	462.0801	538.2463
599.5846	724.9664	832.2096
925.2889	936.1967	979.2075
1029.0670	1042.2557	1068.0793
1174.3070	1189.7303	1244.4667
1292.2725	1338.7604	1408.3707
1440.5272	1444.6333	1470.3212
1479.8727	1497.3625	1714.3000
2943.9617	3009.5586	3014.3174
3060.1548	3103.8784	3108.6260
3125.6938	3204.9734	3841.8872

Rxn9

Geometry [Angstroms]

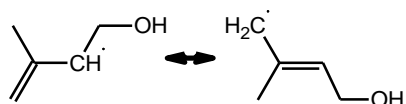
6	-0.016517	0.035602	0.008676
6	-0.002052	0.005575	1.342640
6	1.308700	0.007052	2.106636
6	1.660201	1.347392	2.730231
8	0.841999	1.629522	3.830256
6	-1.265848	-0.028863	2.162207
1	1.282941	-0.739015	2.909348
1	2.126487	-0.267415	1.434175
1	-0.947089	0.044897	-0.548852
1	0.900323	0.046163	-0.571771
1	-1.294776	0.805946	2.866908
1	-2.154542	0.004224	1.529023
1	-1.306183	-0.943707	2.764894
1	2.830926	1.250424	3.104512
1	1.682025	2.160490	1.993357
1	0.998533	2.536631	4.111127
1	3.874426	1.141460	3.416032

Rotational Constants [GHz] =

1.819 2.292 5.350

Frequencies [cm-1]

-823.7136	51.9530	123.9881
196.0791	196.5110	281.9335
340.6296	347.1141	378.1954
423.7589	447.3453	570.3415
724.8404	803.2413	885.8864
921.3110	943.0761	999.1075
1036.2770	1063.1970	1093.1907
1121.9939	1190.7153	1241.1187
1285.4913	1301.6486	1346.7985
1354.0668	1400.8756	1412.7375
1443.7656	1446.5317	1468.8071
1481.0535	1501.0791	1705.8245
3010.2029	3017.2278	3026.6782
3073.7847	3075.5068	3108.9211
3124.8962	3203.9858	3830.7339

t-C=C(C)CJOH or t-C2JC=CCOH

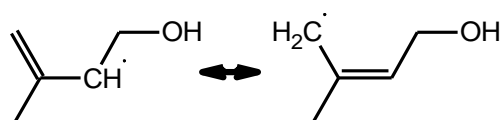
Geometry [Angstroms]

6	-0.000317	0.001936	0.002997
6	-0.002188	-0.000911	1.386675
6	1.324700	0.006545	2.124497
6	-1.208536	-0.018394	2.092039
6	-1.381564	-0.034714	3.574928
8	-2.391818	0.884499	4.008155
1	-2.135852	-0.032805	1.524592
1	0.922874	0.014962	-0.562927
1	-0.928614	-0.010222	-0.556316
1	1.453493	-0.896447	2.727796
1	2.157999	0.059596	1.422499
1	1.403630	0.862543	2.800937

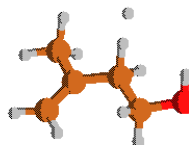
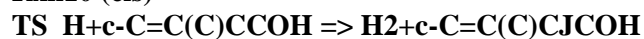
1	-1.740922	-1.014825	3.911217
1	-0.433093	0.153837	4.093140
1	-2.156733	1.749171	3.655350
Rotational Constants [GHz] =			
	1.618	1.921	7.231
Frequencies [cm-1]			
57.5540	139.9527	142.5146	
236.6491	358.2362	376.5610	
466.3723	492.4262	516.6029	
566.3114	746.7213	798.1607	
837.4494	923.4803	996.2976	
1020.7852	1034.0576	1056.3759	
1139.9290	1195.6840	1270.7084	
1349.2839	1378.9615	1407.3309	
1419.7638	1463.7841	1487.7614	
1500.0011	1503.5507	1518.1605	
2998.6238	3025.7053	3031.4343	
3080.6018	3109.2231	3135.9758	
3142.7141	3230.6775	3813.6299	

c-C=C(C)CJOH or c-C2JC=CCOH

Geometry [Angstroms]			
6	0.003418	-0.010095	0.001055
6	0.004533	-0.000366	1.384973
6	1.166746	0.002087	2.161077
6	2.580232	-0.021227	1.676736
8	3.411032	0.881580	2.414883
6	-1.328138	-0.020751	2.114572
1	1.066485	0.007016	3.243665
1	-0.927519	-0.006019	-0.552334
1	0.916078	-0.020817	-0.580040
1	-1.295432	0.594715	3.016660
1	-2.135342	0.348989	1.479425
1	-1.586285	-1.039262	2.421305
1	3.025876	-1.008608	1.843793
1	2.644472	0.182135	0.601158
1	3.015302	1.756103	2.338808



Rotational Constants [GHz] =			
	1.580	1.852	7.595
Frequencies [cm-1]			
45.9276	57.5740	136.4569	
241.3355	354.6352	379.4326	
458.2051	489.8037	514.1468	
555.1449	730.4854	790.7422	
856.2278	928.3252	1001.8546	
1026.1534	1053.5623	1058.8320	
1121.0474	1194.5865	1257.4919	
1341.7927	1355.2186	1406.2581	
1412.1947	1478.0868	1492.9022	
1494.0288	1496.6945	1533.7914	
3004.6233	3028.2878	3034.8657	
3083.8259	3106.0012	3140.3774	
3149.3054	3236.4514	3815.9084	

Rxn10 (cis)

Geometry [Angstroms]

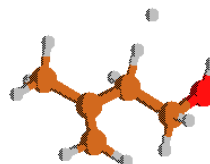
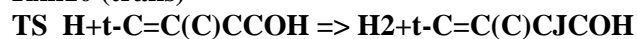
6	-0.000816	0.119627	0.015775
6	0.005133	0.012170	1.350666
6	1.245706	0.048174	2.170462
6	2.548284	0.449163	1.515917
8	3.546645	0.455654	2.532022
6	-1.267988	-0.200203	2.131309
1	1.108258	0.601962	3.103952
1	1.420358	-1.088020	2.593352
1	-0.927775	0.072738	-0.544841
1	0.903963	0.263195	-0.562604
1	-1.426469	0.609933	2.851352
1	-2.138652	-0.252352	1.475659
1	-1.215964	-1.130523	2.708315
1	2.803630	-0.256513	0.713672
1	2.437229	1.446708	1.064048
1	4.391617	0.655909	2.120166
1	1.593948	-2.108276	2.956336

Rotational Constants [GHz] =

1.503 1.781 7.057

Frequencies [cm-1]

-832.5806	78.9009	119.2387
179.3549	189.1961	247.2498
297.6072	341.8155	364.5472
434.1057	503.4662	509.6005
693.4592	846.3409	876.2566
918.0674	978.2810	1008.2308
1033.7837	1059.5908	1079.2913
1097.0568	1170.4377	1241.3351
1281.0201	1328.2679	1352.4003
1398.9282	1412.4813	1424.0000
1447.1707	1475.6506	1483.4563
1497.3044	1511.3463	1685.5758
2995.7205	3014.0569	3053.5400
3060.0647	3067.1494	3106.8135
3139.4604	3219.4890	3820.3494

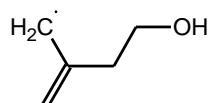
Rxn10 (trans)

Geometry [Angstroms]

6	0.001781	0.004859	0.003035
6	0.000108	0.002722	1.342011
6	1.283227	-0.007438	2.135115
6	-1.247411	0.037930	2.155787
6	-2.594115	-0.136572	1.470942
8	-3.665967	-0.136122	2.406158
1	-1.185303	-0.617609	3.030255
1	-1.292538	1.128856	2.677836
1	0.932001	-0.015488	-0.553905
1	-0.909368	0.018227	-0.582464
1	1.336578	-0.889283	2.782681

1	2.158819	-0.006317	1.483944			
1	1.341303	0.869807	2.789490			
1	-2.739535	0.634647	0.703215			
1	-2.634227	-1.108796	0.971855			
1	-3.698361	0.734611	2.815517			
1	-1.449825	2.148263	3.161147			
Rotational Constants [GHz] =				1.492	1.760	7.045
Frequencies [cm-1]						
-832.5806	78.9009	119.2387				
179.3549	189.1961	247.2498				
297.6072	341.8155	364.5472				
434.1057	503.4662	509.6005				
693.4592	846.3409	876.2566				
918.0674	978.2810	1008.2308				
1033.7837	1059.5908	1079.2913				
1097.0568	1170.4377	1241.3351				
1281.0201	1328.2679	1352.4003				
1398.9282	1412.4813	1424.0000				
1447.1707	1475.6506	1483.4563				
1497.3044	1511.3463	1685.5758				
2995.7205	3014.0569	3053.5400				
3060.0647	3067.1494	3106.8135				
3139.4604	3219.4890	3820.3494				

C=C(CJ)CCOH



Geometry [Angstroms]						
6	-0.065373	-0.174412	0.017339			
6	0.068459	-0.045629	1.392773			
6	1.314746	-0.012172	2.002663			
6	-1.180509	0.023521	2.255381			
6	-1.653778	-1.359344	2.697065			
8	-2.821531	-1.178787	3.494136			
1	-0.993525	0.622741	3.150434			
1	-1.995642	0.505234	1.708881			
1	0.804014	-0.256446	-0.624620			
1	-1.039213	-0.186030	-0.457023			
1	1.416146	0.102625	3.075071			
1	2.225472	-0.089361	1.420178			
1	-1.866742	-1.974998	1.811606			
1	-0.855488	-1.856470	3.266292			
1	-3.127237	-2.045130	3.777253			
Rotational Constants [GHz] =				1.658	1.877	7.645
Frequencies [cm-1]						
46.5519	104.3099	190.4382				
265.6180	349.0249	410.3537				
471.0588	542.2573	555.3006				
590.8330	772.2262	804.0503				
816.1638	893.1970	978.1213				
1015.1238	1045.7444	1056.3256				
1061.8882	1211.4232	1242.7898				
1308.3221	1322.3635	1356.0909				
1384.6128	1452.9115	1487.7354				
1501.1820	1528.0485	1529.1895				

2969.8284	2999.7661	3045.1868
3087.5117	3132.8982	3140.3921
3228.2668	3230.4014	3839.9685

Rxn11

TS H+C=C(C)CCOH => H2+C=C(CJ)CCOH



Geometry [Angstroms]

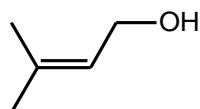
6	0.042408	-0.046598	0.016541
6	-0.014398	0.004736	1.355197
6	1.220295	0.027369	2.173295
6	-1.338348	0.020429	2.087520
6	-1.608258	-1.244111	2.901074
8	-2.881953	-1.077039	3.520310
1	-1.372920	0.872425	2.776774
1	-2.159317	0.147598	1.377884
1	0.989615	-0.056617	-0.512071
1	-0.857382	-0.069260	-0.588063
1	1.467298	-1.103014	2.615694
1	2.124348	0.268811	1.614926
1	1.147786	0.619531	3.087465
1	-1.600767	-2.116902	2.233203
1	-0.823393	-1.391171	3.654922
1	-3.067421	-1.865311	4.038379
1	1.767145	-2.048285	3.021523

Rotational Constants [GHz] = 1.566 1.819 6.358

Frequencies [cm-1]

-1162.4744	69.0698	99.3308
156.9161	187.9647	271.3428
308.4507	343.2193	408.2193
466.6709	558.4828	590.3397
706.1461	813.7107	860.1820
922.1877	984.2633	1012.2206
1022.0245	1042.3258	1067.1417
1099.7559	1224.1909	1243.7115
1280.9579	1303.9214	1319.6716
1336.7922	1338.4858	1393.7819
1444.6893	1459.5770	1471.7988
1497.8110	1529.0931	1671.4008
2976.5298	3007.3767	3024.1089
3065.7146	3082.7737	3130.2129
3139.5950	3213.3022	3840.2881

Prenol CC(C)=CCOH

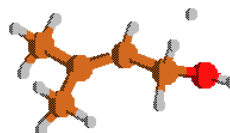
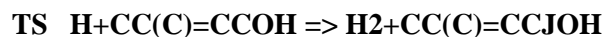


Geometry [Angstroms]

6	-0.002685	0.002717	0.001000
6	-0.003898	0.000060	1.509463
6	1.370721	-0.004807	2.131921
6	-1.101806	0.015443	2.276263
6	-2.540043	0.007644	1.849719
8	-3.277517	-1.035412	2.498216
1	-0.973408	0.016548	3.357396

1	0.593555	-0.833053	-0.382425			
1	-0.999497	-0.062706	-0.433680			
1	0.466305	0.918014	-0.378489			
1	1.945901	0.874282	1.818183			
1	1.322714	-0.009069	3.222197			
1	1.942568	-0.882773	1.809022			
1	-3.032546	0.932893	2.164037			
1	-2.645053	-0.061902	0.760823			
1	-2.816026	-1.860433	2.315725			
Rotational Constants [GHz] =				1.580	1.851	6.823
Frequencies [cm-1]						
69.1736	139.5620	152.4776				
205.9689	269.7759	360.6302				
369.2916	433.0363	501.1512				
512.9534	786.9810	868.4107				
956.3680	963.6875	1015.4524				
1028.4303	1054.1108	1101.9493				
1131.0146	1189.6023	1240.2190				
1337.0114	1381.6655	1410.5428				
1419.0396	1423.3737	1473.4189				
1484.7673	1492.9370	1495.6108				
1509.1342	1729.7607	3006.1414				
3009.7981	3015.7830	3047.8479				
3052.5449	3053.7900	3102.9519				
3120.8381	3122.3040	3817.5969				

Rxn12



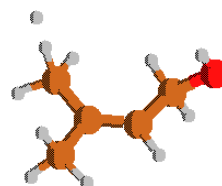
Geometry [Angstroms]						
6	-0.008956	0.025142	-0.002177			
6	-0.002580	-0.002096	1.505160			
6	1.100457	-0.022114	2.263067			
6	2.521551	-0.039879	1.814733			
8	3.284929	0.766293	2.701185			
6	-1.371053	-0.017659	2.138545			
1	0.992746	-0.052842	3.344708			
1	-0.634340	0.847494	-0.367273			
1	0.984391	0.135984	-0.436527			
1	-0.444981	-0.898609	-0.400439			
1	-1.946365	-0.890929	1.808666			
1	-1.313718	-0.039003	3.228054			
1	-1.947529	0.866378	1.841791			
1	2.905931	-1.107092	1.850860			
1	2.639527	0.283789	0.773442			
1	4.213215	0.666733	2.469184			
1	3.601245	-2.436911	1.853660			
Rotational Constants [GHz] =				1.512	1.753	6.353
Frequencies [cm-1]						
-212.5800	60.2673	129.1004				
142.0272	162.3706	190.5613				
212.3524	277.4211	312.5138				
359.0831	435.6603	488.3205				
515.3175	799.7411	855.6188				

960.6371	988.3128	1013.9152
1048.2000	1063.4613	1102.0195
1122.4301	1209.0138	1237.1227
1275.0880	1356.0585	1410.7764
1420.2162	1445.2738	1462.9572
1473.8990	1486.7144	1492.8582
1497.1589	1727.7181	2374.5461
3005.8955	3008.7439	3014.9656
3047.5195	3053.0830	3104.4746
3117.2847	3137.7871	3830.9521

Rxn13 (cis)

TS H+C2C=CCOH => H2+c-C2JC=CCOH

aka H+CC(C)=CCOH => H2+c-C=C(C)CJCOH



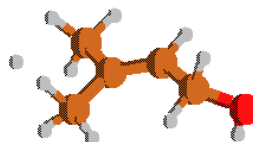
Geometry [Angstroms]

6	0.035494	0.093807	0.038238
6	0.031490	0.081819	1.517867
6	1.398256	0.103215	2.158495
6	-1.080746	0.015574	2.274175
6	-2.509149	-0.056683	1.823074
8	-3.191820	-1.163572	2.421834
1	-0.965735	-0.005938	3.356018
1	0.394136	-1.021133	-0.363285
1	-0.924563	0.249848	-0.447803
1	0.800139	0.740890	-0.395261
1	1.944782	1.013684	1.888960
1	1.336270	0.050493	3.246537
1	2.001302	-0.742252	1.807193
1	-3.057329	0.826773	2.164521
1	-2.594933	-0.092086	0.731209
1	-2.694932	-1.957446	2.197946
1	0.703645	-1.972977	-0.759278

Rotational Constants [GHz] = 1.558 1.803 6.105

Frequencies [cm-1]

-1141.3152	62.6317	114.2666
150.6073	193.0325	263.0024
277.5575	370.5097	373.2171
455.7042	497.3857	544.0728
563.0683	796.9488	870.8786
960.1698	979.3404	1021.6866
1031.0479	1056.9825	1094.2156
1130.5520	1190.6766	1245.4677
1288.5734	1327.3810	1340.2142
1369.0354	1395.1384	1414.8209
1421.4115	1472.6342	1484.5254
1495.7841	1506.0529	1687.4681
3011.3721	3014.2437	3054.7422
3055.7896	3075.6726	3106.9827
3129.8955	3155.7000	3816.4507

Rxn13 (trans)**TS H+C2C=CCOH => H2+t-C2JC=CCOH****aka H+CC(C)=CCOH => H2+t-C=C(C)CJCOH**

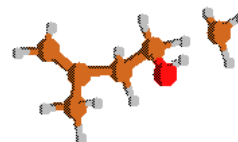
Geometry [Angstroms]

6	0.005163	-0.004805	0.000886
6	0.003524	-0.005376	1.479995
6	1.116923	-0.002410	2.237936
6	2.546313	0.047980	1.789401
8	3.282357	1.058691	2.486010
6	-1.362440	-0.075658	2.119092
1	1.003486	-0.020677	3.320060
1	-0.206254	-1.154997	-0.399264
1	-0.829651	0.542332	-0.440907
1	0.945257	0.259875	-0.478940
1	-1.891341	-0.981757	1.801290
1	-1.299708	-0.083167	3.208383
1	-1.982618	0.774591	1.814459
1	3.051774	-0.889562	2.041099
1	2.632296	0.179117	0.704270
1	2.824008	1.893021	2.341858
1	-0.390896	-2.135732	-0.807405

Rotational Constants [GHz] = 1.521 1.788 6.257

Frequencies [cm-1]

-1145.0885	66.2875	108.9368
154.7348	193.3356	264.8337
276.0446	364.5743	372.9910
470.3051	496.5683	532.5198
564.2199	800.1082	869.1586
959.8280	980.9665	1019.9458
1031.3856	1055.4670	1091.1089
1130.3292	1191.1219	1241.6637
1288.6967	1329.2642	1341.3658
1370.6785	1396.7314	1414.5265
1420.2582	1471.3662	1484.4294
1495.2407	1504.1740	1685.6786
3009.6326	3011.5518	3052.7317
3055.7778	3070.8398	3106.5913
3129.3733	3148.7158	3817.9880

Rxn14**TS CH3+C=C(C)CCOH => CH4+C=C(C)CCJOH**

Geometry [Angstroms]

6	0.035054	-0.030605	-0.028140
6	0.017065	-0.007653	1.306077
6	1.279912	0.015309	2.127662
6	-1.294471	-0.008253	2.069359
6	-1.644532	-1.338850	2.711514
8	-0.826443	-1.596919	3.824771
1	-1.270861	0.750234	2.861234
1	-2.110360	0.256874	1.390320
1	0.966891	-0.043070	-0.583677
1	-0.880550	-0.033778	-0.610765

1	1.301224	-0.822065	2.829470
1	2.169640	-0.020875	1.495878
1	1.325061	0.927392	2.734372
1	-2.857916	-1.244361	3.103500
1	-1.650344	-2.166018	1.989805
1	-0.994659	-2.494294	4.128294
6	-4.238117	-1.119471	3.561652
1	-4.457863	-2.081041	4.019395
1	-4.202909	-0.291324	4.264608
1	-4.812109	-0.916791	2.661090

Rotational Constants [GHz] = 1.034 1.252 3.903

Frequencies [cm-1]

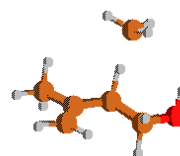
-1447.1787	26.5918	40.4756
75.9311	92.8286	172.0178
200.6977	231.7686	320.6583
335.3832	418.2033	429.1901
470.0835	522.2327	542.9154
624.5928	728.3443	814.4816
885.9209	916.5557	948.6713
996.3028	1039.0723	1064.9526
1101.8362	1110.3318	1117.3096
1191.8947	1284.0490	1311.5653
1321.8289	1375.7365	1412.2146
1416.7021	1427.3918	1444.8717
1453.7968	1465.1982	1469.7417
1480.6077	1501.0293	1704.8669
3003.1492	3015.3586	3020.0520
3056.4956	3068.4575	3073.8015
3108.1587	3123.4712	3188.8071
3194.1772	3202.0913	3833.3757

Rxn15 (cis)

TS CH₃+C=C(C)CCOH => CH₄+c-C=C(C)CJCOH

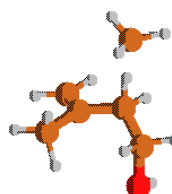
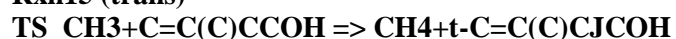
Geometry [Angstroms]

6	0.012671	0.108866	0.015879
6	0.002914	0.002356	1.353387
6	1.288594	-0.109135	2.137535
6	-1.237390	0.018335	2.166080
6	-2.576301	-0.213279	1.486997
8	-3.653147	-0.209564	2.420085
1	-1.156623	-0.604689	3.061707
1	-1.329336	1.169654	2.676268
1	0.945020	0.109615	-0.537816
1	-0.894805	0.190926	-0.569791
1	1.325701	-1.052472	2.693184
1	2.163386	-0.060418	1.486798
1	1.366775	0.695644	2.877039
1	-2.743905	0.529327	0.695312
1	-2.595240	-1.200396	1.015734
1	-3.694438	0.667436	2.813597
6	-1.551778	2.526985	3.261773
1	-0.541783	2.923852	3.299461
1	-2.199508	3.017961	2.540332



1	-1.999991	2.337948	4.233183			
Rotational Constants [GHz] =				1.186	1.518	2.768
Frequencies [cm-1]						
-1387.4681	52.4990	53.1672				
84.2558	117.9812	157.1059				
174.6032	191.7132	313.8273				
357.4158	412.6235	438.9449				
466.4753	520.4772	531.3643				
588.7755	708.8685	879.0230				
883.6291	901.8085	976.9924				
1010.5614	1034.2632	1059.7747				
1083.0890	1091.1787	1116.4427				
1196.2343	1250.0995	1329.9308				
1361.5741	1400.4993	1406.2395				
1411.7177	1425.1750	1436.3167				
1438.7737	1447.4794	1482.8260				
1496.5573	1510.3207	1668.9363				
2988.8679	3014.2119	3054.2908				
3059.2090	3061.6575	3064.0164				
3104.4607	3138.4883	3200.2925				
3205.4563	3218.1614	3829.8950				

Rxn15 (trans)

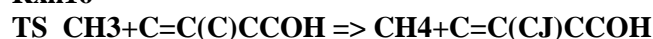


Geometry [Angstroms]

6	-0.007631	0.006680	0.000430			
6	0.006045	-0.004287	2.751007			
6	1.485863	0.002762	3.103500			
8	1.734971	0.095171	4.507747			
6	-0.832424	1.118689	3.243801			
6	-0.219549	2.497033	3.244725			
6	-2.098076	0.913347	3.636864			
1	-0.458190	-0.973850	2.957374			
1	-0.004075	0.029231	1.486544			
1	-2.731412	1.730334	3.964571			
1	-2.535821	-0.079486	3.643913			
1	0.155909	2.764594	2.250473			
1	-0.945945	3.252570	3.548166			
1	0.628935	2.535317	3.933919			
1	1.963045	-0.891469	2.680001			
1	1.984768	0.871569	2.668793			
1	1.219415	-0.591218	4.943596			
1	0.716034	0.766909	-0.278947			
1	0.280772	-1.010933	-0.246149			
1	-1.041987	0.256280	-0.216210			
Rotational Constants [GHz] =				1.303	1.929	2.092
Frequencies [cm-1]						
-1404.2079	28.7730	65.7001				
84.4571	100.2164	131.4187				
212.8106	251.5082	303.5403				
359.6564	406.4609	441.2936				
460.8418	530.5118	548.4595				
629.1119	722.8731	779.7375				

900.2161	937.3021	950.4903
1001.6168	1031.1779	1064.0181
1071.2107	1083.4899	1109.3397
1199.5969	1302.1849	1311.7627
1359.8198	1387.4705	1404.5262
1408.4235	1425.2156	1430.0240
1431.3904	1451.4874	1485.4106
1499.3420	1517.6295	1668.9624
2990.3113	3017.4880	3047.3274
3064.4031	3072.0657	3081.5359
3108.1365	3126.6013	3205.7205
3207.9790	3208.9619	3819.8491

Rxn16



Geometry [Angstroms]

6	0.027739	0.072579	0.004949
6	0.017371	0.012086	1.346385
6	1.310397	-0.027968	2.133282
6	1.575352	1.233694	2.951961
8	2.811956	1.039460	3.636143
6	-1.248066	0.010864	2.110190
1	1.297240	-0.876309	2.827656
1	2.157479	-0.177351	1.459392
1	-0.892500	0.095319	-0.569268
1	0.956113	0.089252	-0.554974
1	-1.550512	1.185473	2.486988
1	-2.121160	-0.275984	1.524033
1	-1.207897	-0.538031	3.052815
1	1.624996	2.101908	2.279746
1	0.758077	1.405029	3.665200
1	2.997850	1.831849	4.147661
6	-2.021422	2.513269	2.905786
1	-1.429922	3.177473	2.282260
1	-3.081898	2.494765	2.671929
1	-1.792099	2.555538	3.966760

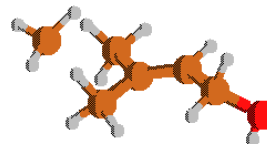
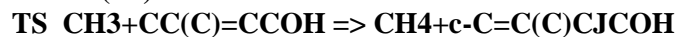
Rotational Constants [GHz] = 1.073 1.533 2.456

Frequencies [cm-1]

-1503.4293	37.5180	56.5196
67.4033	100.7492	106.6329
197.6121	269.6524	339.1519
361.7858	400.6934	445.3880
490.9932	509.7430	630.2395
695.6303	713.4717	815.3516
868.8272	906.1958	984.9835
1022.9601	1023.8509	1056.1482
1077.8604	1097.0618	1115.4707
1224.4868	1242.3851	1301.5345
1319.9495	1340.0717	1393.7087
1404.8423	1431.3748	1435.5491
1443.1523	1455.9092	1473.0175
1498.0376	1528.4709	1659.8090
2974.9902	3006.9685	3024.0254

3062.5547	3063.0332	3081.3584
3128.1431	3133.8079	3203.6675
3205.4841	3210.7996	3840.1335

Rxn17 (cis)



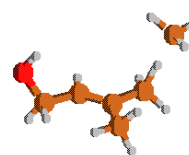
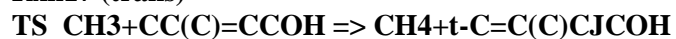
Geometry [Angstroms]

6	0.000805	0.024895	-0.006655
6	-0.020118	0.036775	1.468893
6	1.079825	-0.007167	2.248243
6	2.515604	-0.011164	1.819605
8	3.279247	0.980341	2.516802
6	-1.395950	0.032177	2.093703
1	0.948217	-0.021253	3.328358
1	-0.200036	-1.159210	-0.418342
1	-0.827556	0.569035	-0.463907
1	0.947840	0.290335	-0.473176
1	-1.967551	-0.845317	1.770259
1	-1.345846	0.021375	3.183792
1	-1.969039	0.913071	1.783641
1	2.988663	-0.962320	2.083804
1	2.617955	0.109513	0.734445
1	2.837569	1.824274	2.376342
6	-0.401154	-2.510159	-0.960318
1	0.184054	-3.123657	-0.281455
1	-1.475385	-2.658586	-0.899151
1	-0.008406	-2.443530	-1.970770

Rotational Constants [GHz] = 0.973 1.212 3.082

Frequencies [cm⁻¹]

-1482.8964	22.5035	41.1333
59.7657	102.7945	147.7469
187.4684	264.9830	350.7019
368.0638	371.6489	423.7422
470.9473	498.9883	512.2453
614.1380	697.7364	805.2258
864.9082	958.5068	988.9225
1025.9373	1036.5433	1058.3600
1085.6481	1119.4987	1134.6866
1192.3422	1244.5490	1337.7056
1376.4615	1393.5741	1397.7899
1413.2679	1419.5033	1431.5593
1434.1813	1472.4482	1484.4814
1495.5121	1505.5765	1675.1353
3006.7053	3011.3669	3048.5935
3055.0977	3063.6836	3067.8320
3104.1631	3127.8901	3142.3242
3205.1548	3206.4744	3817.0010

Rxn17 (trans)

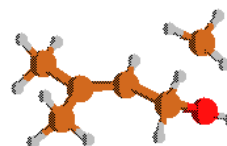
Geometry [Angstroms]

6	-0.004475	-0.010259	0.026239
1	-0.113246	0.022202	1.106614
1	1.022350	-0.063792	-0.323876
1	-0.634344	0.688972	-0.516232
1	-0.568967	-1.310196	-0.353682
6	-1.003310	-2.445059	-0.728682
1	-0.449730	-3.125807	-0.078690
1	-0.665574	-2.521158	-1.762037
6	-2.469611	-2.487023	-0.555863
6	-2.939041	-2.672047	0.867879
1	-2.636474	-3.655514	1.244153
1	-4.019470	-2.592025	0.981395
1	-2.471050	-1.928553	1.522227
6	-3.288588	-2.332509	-1.615975
1	-2.834982	-2.207129	-2.597584
6	-4.786454	-2.292316	-1.642424
1	-5.217308	-2.355673	-0.636587
1	-5.178956	-3.137511	-2.216441
8	-5.271334	-1.131661	-2.329830
1	-4.870572	-0.366343	-1.904658

Rotational Constants [GHz] = 0.990 1.123 3.283

Frequencies [cm⁻¹]

-1488.6895	23.7167	44.9724
72.1193	83.5369	131.8750
174.5983	266.9833	349.3227
368.3662	370.6437	435.1843
445.0168	494.3732	536.4490
599.7086	699.3083	802.1062
874.9753	957.8187	982.5848
1022.7860	1035.3337	1057.7474
1086.1691	1120.8802	1139.1029
1192.4774	1248.0637	1337.4811
1378.6589	1394.9694	1397.6125
1416.3207	1420.8801	1432.6194
1435.2114	1469.4392	1487.8995
1489.5479	1508.6150	1678.2538
3010.6975	3019.0874	3051.1501
3058.9536	3060.8496	3062.9392
3122.1511	3123.6421	3134.7512
3203.2144	3204.6860	3816.4861

Rxn18

Geometry [Angstroms]

6	-0.010855	-0.086706	0.031913
6	0.007130	0.020547	1.535147
6	1.123645	0.127568	2.273110
6	2.522149	0.116064	1.805694
8	3.334596	0.846397	2.701530
6	-1.350540	-0.009830	2.188702

1	1.030603	0.184947	3.355275
1	-0.699794	0.649449	-0.397814
1	0.969515	0.062592	-0.420940
1	-0.374587	-1.072866	-0.281065
1	-1.883915	-0.937340	1.946674
1	-1.279788	0.067573	3.275042
1	-1.978081	0.813240	1.826167
1	2.929381	-1.050492	1.802059
1	2.654020	0.438491	0.765736
1	4.251285	0.731631	2.433009
6	3.567884	-2.463110	1.850773
1	2.786350	-3.080111	1.418607
1	4.472807	-2.377805	1.256001
1	3.722896	-2.589721	2.917831

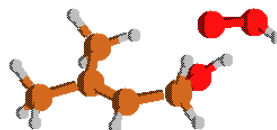
Rotational Constants [GHz] = 1.083 1.227 3.072

Frequencies [cm-1]

-1145.4313	38.1919	41.2162
63.7522	129.6104	140.6004
180.0505	207.2368	258.6426
308.7158	351.1411	418.3337
462.6835	484.6169	509.6861
530.3090	593.4530	821.5462
862.2053	962.2918	1006.7633
1012.1708	1060.9304	1073.9053
1098.5706	1111.3396	1131.0496
1208.3885	1274.8335	1314.0054
1360.9114	1410.3419	1418.8630
1420.4836	1423.9360	1454.7880
1463.7566	1473.2467	1486.6216
1491.8850	1497.9318	1710.9514
3001.6553	3006.2002	3011.1052
3041.3220	3048.1069	3064.3447
3102.0190	3113.2285	3135.6418
3206.2876	3212.6785	3829.7590

Rxn22 (cis)

TS HO₂+C₂C=CCOH => H₂O₂+c-CC(C)=CCJOH

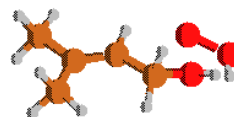
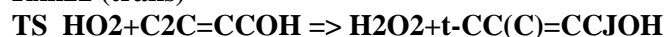


Geometry [Angstroms]

6	-0.024153	0.065091	0.000023
1	-0.039766	0.024843	1.247722
1	1.056059	-0.033040	-0.189057
8	-0.508692	1.333246	-0.312834
1	-0.181943	1.936199	0.373872
8	-0.003614	0.485870	2.512246
8	0.326851	1.845502	2.345919
1	1.275404	1.865919	2.542161
6	-0.772825	-1.087237	-0.504873
1	-0.169934	-1.992425	-0.539285
6	-2.071427	-1.203572	-0.861293
6	-2.600168	-2.531713	-1.337190
1	-1.830745	-3.305650	-1.345789
1	-3.011278	-2.444574	-2.349915
1	-3.423571	-2.870881	-0.697384

6	-3.086269	-0.093978	-0.831028			
1	-3.450703	0.110959	-1.845366			
1	-3.959528	-0.407612	-0.247009			
1	-2.685648	0.825287	-0.416736			
Rotational Constants [GHz] =		0.815	0.851	3.676		
Frequencies [cm-1]						
-1234.7256	33.4602	62.6797				
92.9078	110.3208	172.3608				
190.6429	245.5167	271.4249				
305.5137	356.0374	393.7926				
436.0243	477.4000	581.0376				
600.2036	702.5616	798.7990				
843.1559	959.4883	976.3205				
999.2780	1005.1023	1012.9154				
1088.0970	1098.2722	1187.9225				
1226.3903	1300.8931	1340.0690				
1358.7679	1378.5599	1409.2889				
1418.1233	1429.6617	1472.3361				
1477.3136	1493.2821	1498.7887				
1572.1884	1665.4935	2966.8191				
3004.1455	3010.4160	3043.8535				
3048.8245	3102.5276	3127.3403				
3174.7878	3686.9937	3721.4375				

Rxn22 (trans)

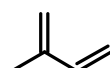


Geometry [Angstroms]

6	-0.134778	0.097122	-0.025471			
6	-0.019453	0.050868	1.474703			
6	1.147747	-0.060096	2.141187			
6	2.488289	-0.183545	1.569791			
8	3.486541	0.181228	2.471757			
6	-1.325446	0.122196	2.218887			
8	3.420116	-2.511534	1.136988			
8	4.752951	-2.078374	1.286989			
1	1.129864	-0.115246	3.226502			
1	0.829134	0.141493	-0.531783			
1	-0.663437	-0.789946	-0.393924			
1	-0.726372	0.964713	-0.338676			
1	-1.987289	-0.701758	1.925813			
1	-1.181442	0.076538	3.299368			
1	-1.859858	1.049579	1.980831			
1	2.719177	-1.388896	1.327531			
1	2.622476	0.259692	0.573116			
1	4.294113	-0.287043	2.209813			
1	5.060392	-1.999763	0.371644			
Rotational Constants [GHz] =		0.746	0.814	3.467		
Frequencies [cm-1]						
-1262.9999	43.3089	66.2281				
86.8729	116.1027	170.7544				
195.3581	200.4452	271.6172				
295.7166	355.5277	419.5837				
458.5129	468.9524	518.4820				

572.4368	609.1164	824.3916
859.5575	961.4686	984.2647
1002.3051	1007.9543	1056.8921
1095.2601	1109.9731	1144.1136
1216.5005	1290.6855	1327.6182
1356.1130	1360.2328	1410.1736
1419.0295	1424.2773	1470.9980
1483.1971	1490.0292	1492.8735
1560.2354	1681.2645	2986.0044
3004.9731	3014.2256	3045.5945
3053.3386	3107.5388	3119.2578
3147.3611	3704.1230	3721.9021

C=C(C)C=C



Geometry [Angstroms]

6	-0.000028	0.000084	0.000040
1	-0.002707	0.000342	1.094796
1	1.047434	0.002647	-0.318265
1	-0.457899	-0.929122	-0.341765
6	-0.735498	1.198756	-0.544613
6	-1.805780	1.062633	-1.340946
6	-0.259797	2.540325	-0.188221
1	-2.332435	1.927005	-1.731022
1	-2.185484	0.087906	-1.625255
6	0.788149	2.824115	0.591616
1	-0.832283	3.362291	-0.612348
1	1.067793	3.849652	0.801584
1	1.400297	2.053036	1.045314

Rotational Constants [GHz] = 2.850 4.168 8.537

Frequencies [cm-1]

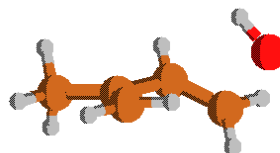
159.8516	200.3661	280.2193
409.0172	427.9214	537.0587
643.8355	786.1387	791.0768
922.0821	933.4094	959.7651
1010.8891	1028.3893	1070.3127
1088.4780	1325.5746	1328.3258
1411.0972	1429.7859	1458.8708
1482.9919	1503.0266	1659.3724
1698.7388	3022.3003	3069.6616
3109.9868	3128.9170	3134.0471
3143.9062	3215.2292	3222.3938

Rxn31 (cis)

TS c-C=C(C)CJOH => C=C(C)C=C+OH

Geometry [Angstroms] @ UQCISD-FC\6-31G(d)

6	0.029378	0.036668	0.009547
6	0.037283	0.010137	1.351354
6	1.300883	0.128667	2.113788
6	2.339147	0.928075	1.755583
8	3.357851	-0.354701	0.295226
6	-1.218331	-0.159329	2.174309
1	1.391123	-0.484527	3.014284



1	0.954299	0.106634	-0.557619
1	-0.899891	-0.032240	-0.553463
1	-2.100943	-0.262688	1.533423
1	-1.149568	-1.052923	2.810774
1	-1.370695	0.700981	2.839876
1	2.236964	1.654830	0.955493
1	2.929212	-1.190865	0.580998
1	3.226048	1.007237	2.377322

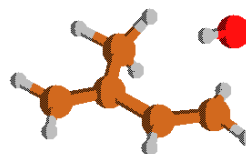
Rotational Constants [GHz] = 1.673 1.998 6.152

Frequencies [cm-1] @ UQCISD-FC\6-31G(d)

-323.0577	73.5137	124.7225
177.9684	192.1577	204.9022
282.3913	395.0139	436.7675
555.6780	696.8066	700.6796
798.5319	821.0638	937.1937
956.0150	989.1354	1002.2410
1043.6943	1090.5936	1125.2086
1303.2581	1330.0590	1457.0175
1482.5591	1493.3809	1530.0306
1545.9164	1641.1469	1739.1357
3056.3911	3117.8601	3151.7400
3161.0869	3180.9905	3204.7549
3271.2244	3293.6365	3664.4814

Rxn31 (trans)

TS t-C=C(C)CJCOH => C=C(C)C=C+OH



Geometry [Angstroms] @ UQCISD-FC\6-31G(d)

6	0.022072	0.135337	0.092898
6	-0.028746	0.034969	1.432476
6	1.216553	-0.010442	2.284058
6	-1.334237	-0.011330	2.109581
6	-1.510584	-0.132854	3.449069
8	-1.129927	1.986094	4.056404
1	-2.212821	0.100066	1.470343
1	-0.882352	0.175226	-0.512494
1	0.967480	0.176527	-0.444145
1	2.114470	0.103826	1.667334
1	1.190920	0.792276	3.031308
1	1.291012	-0.963835	2.824200
1	-2.508133	-0.189270	3.875375
1	-1.393169	2.374735	3.193807
1	-0.688252	-0.341473	4.125238

Rotational Constants [GHz] = 1.877 2.076 5.100

Frequencies [cm-1] @ UQCISD-FC\6-31G(d)

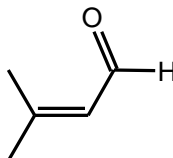
-274.1259	76.0016	95.5481
184.5604	232.6282	239.5029
292.4149	427.2358	444.0406
538.5678	663.9436	667.6134
786.8163	809.7228	923.7290
931.5377	985.1123	1002.4285
1036.1259	1101.3770	1114.4768
1334.0709	1364.3702	1452.5186
1470.0251	1499.8521	1530.5630

1558.4108	1640.6559	1714.8140
3065.4114	3133.9507	3158.9751
3168.7593	3176.0601	3210.0288
3257.0847	3295.6533	3665.1511

c-CC(C)=CC=O

Geometry [Angstroms]

6	0.002914	-0.002165	0.003644
6	-0.001770	-0.008115	1.508183
6	1.171665	0.003181	-0.671340
6	-1.353259	-0.002734	-0.642417
6	1.375477	0.009437	-2.129611
1	2.095812	0.003026	-0.098343
1	-0.535284	-0.888252	1.884693
1	1.005648	-0.007586	1.926355
1	-0.539069	0.866718	1.891610
1	-1.922879	0.871590	-0.305905
1	-1.291653	0.001943	-1.726107
1	-1.918601	-0.882627	-0.313281
1	2.449976	0.013079	-2.416873
8	0.527333	0.010910	-2.999293



Rotational Constants [GHz] = 1.817 2.351 7.281

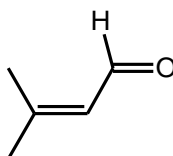
Frequencies [cm-1]

83.2772	113.3168	168.0311
242.1650	242.1786	375.2135
395.8217	486.5647	731.4472
833.9577	849.4372	955.0478
993.6698	1003.0093	1037.5189
1107.0259	1116.7750	1228.4399
1377.2880	1408.8529	1413.2703
1442.7145	1468.4056	1474.5212
1486.7332	1506.8606	1663.9999
1771.2211	2867.7417	3010.4285
3017.1609	3051.4685	3059.9746
3111.3999	3136.8274	3169.9500

t-CC(C)=CC=O

Geometry [Angstroms]

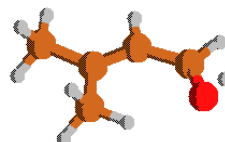
6	0.016661	-0.002129	-0.000090
6	-0.002063	-0.008224	1.504627
6	1.187160	0.003007	-0.666997
6	-1.346180	-0.002412	-0.641320
6	1.367580	0.009269	-2.121612
1	2.120894	0.002708	-0.111218
1	-0.536288	-0.888870	1.879272
1	1.003545	-0.007901	1.926282
1	-0.539807	0.867235	1.886330
1	-1.915285	0.872533	-0.308325
1	-1.322962	0.002136	-1.728912
1	-1.911490	-0.882538	-0.315590
1	0.448240	0.009888	-2.741570



8	2.457672	0.013680	-2.655402			
Rotational Constants [GHz] =				1.592	1.944	7.941
Frequencies [cm-1]						
117.2768	130.3355	185.8472				
222.9414	232.6464	367.2280				
470.5475	477.4172	535.9862				
847.5639	866.2675	956.3340				
1006.1034	1021.9833	1062.2509				
1102.6460	1141.9362	1215.1062				
1341.2762	1409.5958	1415.0789				
1433.0081	1470.7183	1482.7563				
1489.5219	1492.4940	1692.8730				
1758.5513	2898.4189	3012.5752				
3022.2473	3056.0779	3062.7104				
3115.2695	3139.9353	3150.7830				

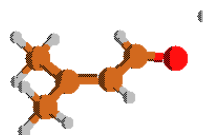
Rxn33 (cis)

TS CC(C)=CCJOH => c-CC(C)=CC=O+H



Geometry [Angstroms]

6	0.036584	-0.007135	-0.019053			
6	-0.012085	0.006822	1.483962			
6	1.231160	0.008763	-0.658473			
6	-1.299784	-0.039646	-0.703201			
6	1.494946	-0.001417	-2.088718			
1	2.130807	0.037902	-0.048342			
1	-0.550382	-0.871639	1.858192			
1	0.982344	0.020492	1.932031			
1	-0.566668	0.882831	1.839968			
1	-1.919817	0.790080	-0.343852			
1	-1.211520	0.014027	-1.783619			
1	-1.832105	-0.959498	-0.432539			
1	2.568505	-0.016982	-2.350971			
8	0.658373	-0.015232	-3.003921			
1	0.313427	-1.405140	-3.772853			
Rotational Constants [GHz] =				1.761	2.257	6.937
Frequencies [cm-1]						
-1055.6949	74.5718	106.3125				
113.5507	167.8923	241.9655				
258.8773	372.2068	395.4566				
485.8950	496.7398	729.2581				
839.6325	846.0785	957.2410				
997.0938	1003.3203	1011.8020				
1102.6395	1120.7715	1230.2917				
1378.7035	1406.6552	1413.6199				
1426.8636	1467.3044	1473.4956				
1485.9210	1504.1072	1590.1923				
1675.7863	2940.3872	3008.5647				
3015.0342	3048.9204	3055.9609				
3110.4988	3136.3040	3171.4612				

Rxn33 (trans)**TS CC(C)=CCJOH => t-CC(C)=CC=O+H**

Geometry [Angstroms]

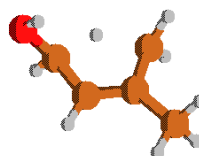
6	0.011911	0.008053	0.006127
6	-0.008236	-0.016216	1.509531
6	1.187875	0.030665	-0.661423
6	-1.346485	-0.001757	-0.641553
6	1.369247	0.030777	-2.098506
1	2.117928	0.027485	-0.099533
1	-0.528847	-0.909392	1.874530
1	0.996726	-0.005493	1.932765
1	-0.560039	0.845927	1.901932
1	-1.934792	0.853584	-0.291054
1	-1.317166	0.029617	-1.728794
1	-1.897871	-0.900344	-0.342432
1	0.472766	0.078429	-2.737871
8	2.489564	-0.002417	-2.625804
1	3.045100	1.299150	-3.423377

Rotational Constants [GHz] =

1.529 1.841 7.730

Frequencies [cm-1]

-1061.4971	104.9615	116.6559
133.0586	177.7832	219.1968
243.6553	364.0088	453.4223
475.5626	512.5404	536.0450
846.7097	874.4831	957.6596
982.9819	1008.7309	1066.1711
1098.1840	1157.0479	1217.4359
1342.8398	1406.2208	1410.2616
1423.3777	1469.7069	1481.6998
1487.9645	1491.1118	1611.2811
1667.4026	2969.4480	3009.6953
3019.7942	3051.8721	3059.2107
3114.1267	3137.6921	3151.1665

Rxn34**TS CC(C)=CCJOH => C=C(C)CJCOH**

Geometry [Angstroms]

-1783.2719	127.2646	156.4852
193.8014	305.2725	394.1734
408.4386	438.3267	522.1052
560.0742	633.1541	827.2442
876.7899	928.1936	964.8164
986.6165	1032.2192	1049.9836
1101.7760	1132.3596	1206.2129
1241.2953	1315.5890	1392.0754
1409.7472	1426.8165	1441.0721
1477.5972	1485.5046	1639.2054
1703.4283	3011.7617	3058.2595
3059.6448	3081.4395	3091.7405
3128.3064	3142.6667	3804.5623

Rotational Constants [GHz] =

1.762 2.041 7.657

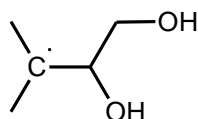
Frequencies [cm-1]

6	0.002407	-0.000101	0.000664
6	-0.000470	-0.004295	1.499329
6	1.235678	0.000629	-0.529256
6	-1.281755	-0.012465	-0.775464
6	2.327715	-0.016332	0.489182
1	1.442675	0.009299	-1.596499
1	-0.344150	-0.917616	1.986375
1	1.447011	0.028789	1.497636
1	-0.381285	0.892861	1.990481
1	-1.909293	0.842306	-0.499939
1	-1.104644	0.018994	-1.853322
1	-1.864272	-0.912324	-0.548753
1	2.877590	-0.951693	0.609376
8	3.259565	1.020768	0.445913
1	2.788373	1.828410	0.211493

C2CJC(OH)COH

Geometry [Angstroms]

6	0.258031	-0.249291	0.223321
6	-0.099112	0.446002	1.496540
6	1.630075	-0.082688	-0.341920
6	-0.659827	-1.305772	-0.313384
1	-1.171257	0.392189	1.707213
1	0.424599	0.020616	2.369151
1	0.185186	1.505124	1.463840
1	1.697631	-0.520108	-1.337856
1	1.903538	0.977630	-0.407218
1	2.399669	-0.555440	0.291935
1	-1.702716	-1.006822	-0.115005
8	-0.463583	-1.465000	-1.714942
6	-0.451417	-2.666332	0.370929
8	-1.345424	-3.584769	-0.270933
1	0.591545	-2.977695	0.234471
1	-0.669045	-2.590220	1.443583
1	-0.899245	-2.297082	-1.939947
1	-1.072622	-4.481411	-0.058595



Rotational Constants [GHz] = 1.402 1.661 4.030

Frequencies [cm-1]

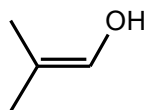
49.3953	84.9284	114.7962
134.4374	162.8078	255.5216
284.5584	297.5390	328.2179
421.9480	493.3085	508.4544
551.3571	795.6683	887.5086
949.6274	975.3082	986.4591
1008.8839	1043.0105	1048.6864
1102.1254	1197.6046	1234.1674
1265.0769	1284.5778	1325.5450
1360.4406	1396.4033	1410.9117
1425.6385	1439.2953	1470.4689
1473.9312	1487.0171	1499.0596
1505.2936	2933.6519	2936.6978
2941.6189	2993.5312	3011.8997
3017.1716	3040.3679	3072.6799

3119.8811 3777.5095 3848.4194

C2C=COH

Geometry [Angstroms]

6	0.011077	-0.018435	-0.042501
6	-0.007181	-0.158173	1.457443
6	1.170939	-0.055190	-0.706225
6	-1.329531	0.158873	-0.707055
8	1.377687	0.053967	-2.053260
1	2.116327	-0.184510	-0.191657
1	-0.604065	-1.023844	1.770180
1	0.999068	-0.282543	1.863996
1	-0.454688	0.722425	1.934676
1	-1.839000	1.054013	-0.331545
1	-1.274741	0.257778	-1.795720
1	-1.987768	-0.692439	-0.497639
1	0.530664	0.168078	-2.497360



Rotational Constants [GHz] =

2.651 3.729 8.236

Frequencies [cm-1]

77.3932	194.3130	279.4630
286.7536	338.2336	365.7105
488.7004	575.7484	803.5699
885.7677	974.2265	1014.8379
1041.0736	1096.8408	1173.5275
1201.8408	1313.1622	1405.2354
1416.7430	1428.8317	1468.6907
1485.4146	1496.3425	1504.0724
1743.7111	2996.9009	3003.6177
3034.1382	3046.2441	3064.6128
3091.1633	3182.3616	3818.3799

CH2OH

Geometry [Angstroms]

6	0.071889	0.120362	0.048723
1	-0.030680	-0.005885	1.116927
1	1.019016	-0.067945	-0.445944
8	-0.770960	1.064386	-0.468638
1	-0.582479	1.175272	-1.405401

Rotational Constants [GHz] =

26.113 29.864 192.561

Frequencies [cm-1]

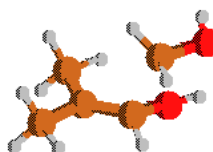
441.1690	587.2377	1061.8090
1207.2646	1367.2296	1487.7806
3111.3669	3255.5083	3840.8074

Rxn43

TS C2CJC(OH)COH => C2C=COH+CH2OH

Geometry [Angstroms]

6	-0.121940	-0.077167	0.034485
6	0.046310	-0.023678	1.524062



6	1.295088	0.159937	2.070347
6	2.347913	-1.821193	2.159023
8	2.881907	-1.832837	3.444267
6	-1.157557	-0.295274	2.374973
8	1.415869	0.456656	3.413968
1	0.812770	0.132883	-0.491776
1	-0.480220	-1.061968	-0.296792
1	-0.867847	0.651583	-0.308317
1	-0.918588	-0.214060	3.434918
1	-1.965285	0.413345	2.152435
1	-1.567252	-1.297500	2.181889
1	2.089385	0.547900	1.434191
1	1.587122	-2.571080	1.956303
1	3.133698	-1.722542	1.417656
1	2.249539	0.069991	3.719310
1	2.212588	-2.170642	4.048412

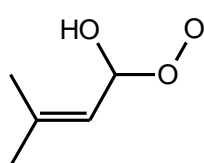
Rotational Constants [GHz] = 1.330 1.510 3.699
 Frequencies [cm-1]

-491.9630	62.5040	106.7106
115.6556	143.5377	182.6487
233.5205	278.9000	283.5547
338.8100	388.1857	436.1457
537.7986	580.8569	616.8349
799.5107	873.9691	953.2153
969.5306	995.9578	1038.5934
1077.6941	1079.9216	1112.7668
1158.0525	1229.9700	1341.9293
1361.9945	1378.8031	1404.5415
1416.4983	1471.7097	1479.2889
1483.3486	1489.0077	1493.2351
1572.4746	2976.2786	2982.6636
3015.9009	3019.6340	3080.7153
3081.6743	3095.4580	3122.2024
3201.6973	3714.6670	3829.2920

CC(C)=CC(OO)OH

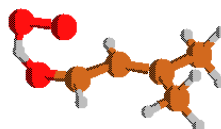
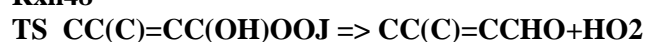
Geometry [Angstroms]

6	-0.064156	-0.030786	-0.028438
6	0.017532	0.049471	1.473546
6	0.993567	-0.429235	-0.744884
6	-1.391399	0.378438	-0.611688
6	1.066688	-0.535888	-2.222029
1	1.923642	-0.684892	-0.247260
1	-0.184233	1.069979	1.817770
1	-0.739820	-0.593288	1.936314
1	0.998166	-0.250890	1.844879
1	-2.202906	-0.197446	-0.153975
1	-1.588561	1.432425	-0.387280
1	-1.450289	0.256719	-1.692498
8	1.467870	0.850106	-2.754263
8	2.023101	-1.444641	-2.599681
1	0.105012	-0.697081	-2.719371
1	2.161583	-1.315490	-3.550298



8	1.896978	0.745474	-3.988512			
Rotational Constants [GHz] =				0.962	1.072	3.933
Frequencies [cm-1]						
32.1010	79.0981	109.6265				
128.5335	186.3923	215.7218				
307.5567	357.3730	386.0785				
458.9609	476.8784	508.0403				
509.0415	659.6394	702.3635				
841.3404	871.5357	961.5666				
1007.4074	1045.3696	1104.3628				
1115.2285	1159.5734	1189.8005				
1214.7469	1283.6250	1328.7605				
1357.2858	1412.4062	1422.0560				
1471.8196	1473.3661	1487.0594				
1492.4800	1498.4061	1733.2793				
3013.6880	3022.0137	3037.9353				
3058.1250	3064.2693	3111.6526				
3125.8113	3162.1089	3729.8401				

Rxn48



Geometry [Angstroms]

6	0.012772	0.000806	-0.014425			
6	-0.004844	-0.039507	1.488366			
6	1.350835	-0.002411	2.138592			
6	-1.176638	-0.091175	2.154431			
6	-1.347408	-0.148025	3.590254			
8	-2.504368	-0.419197	4.088263			
8	-1.448694	1.846814	4.229108			
8	-2.527308	1.758075	4.919240			
1	-2.109471	-0.098394	1.598600			
1	0.520780	0.905111	-0.368710			
1	0.575458	-0.849594	-0.416413			
1	-0.992469	-0.018427	-0.436625			
1	1.978993	-0.811420	1.750172			
1	1.857459	0.935377	1.884725			
1	1.321662	-0.081522	3.223567			
1	-0.467560	-0.270455	4.225683			
1	-2.769501	0.505230	4.680159			
Rotational Constants [GHz] =				0.925	0.982	3.864
Frequencies [cm-1]						
-633.8458	56.2452	72.8101				
111.0562	136.7485	169.6417				
222.9082	276.5411	355.4767				
450.4925	481.4202	497.0307				
499.6849	611.0162	798.4984				
849.8149	879.4098	958.8356				
979.9663	1004.7710	1068.1799				
1099.4039	1101.2852	1164.1870				
1223.3960	1309.6941	1342.0300				
1382.2034	1411.0496	1420.3528				
1469.0549	1480.6738	1487.0044				
1490.5291	1555.2930	1689.2025				

1886.9437	3012.2512	3022.1260
3055.4712	3063.1575	3074.1658
3114.9185	3137.2900	3158.3381

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