Supporting information for: A theoretical and Computational Analysis of the Methyl-vinyl + O_2 Reaction and Its Effects on Propene Combustion

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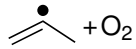
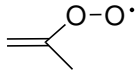
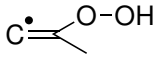
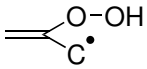
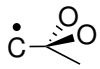
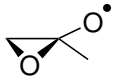
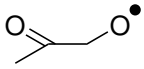
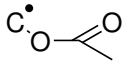
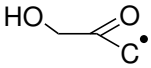
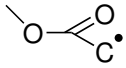
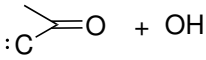
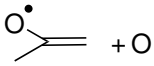
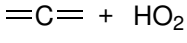
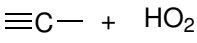
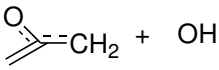
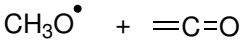
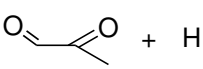
Table S1: Intermediates and products on the $CH_3C(OO)CH_2$ Potential Energy Surface

#	Species Name	Structure	Relative Energy (kcal/mol)	T1 diagnostic
R	$CH_3CCH_2 + O_2$		0.0	0.0153
W1	$CH_3C(OO)CH_2$		-41.27	0.0335
W2	$CH_3C(OOH)CH$		-14.15	0.0146
W3	$CH_2C(OOH)CH_2$		-37.41	0.0231
W4	$c{-}CH_3(COO)CH_2$		-33.38	0.0165
W5	$c{-}(CH_2OOC)CH_3$		-22.71	0.0194
W6	$c{-}(CH_2OC)CH_3O$		-77.33	0.0353
W7	$CH_3C(=O)CH_2O$		-90.12	0.0444
W8	$CH_3C(=O)OCH_2$		-108.37	0.0170
W9	$CH_2C(=O)CH_2OH$		-101.75	0.0182
W10	CH_2COOCH_3		-108.88	0.0167
P1	$CH_3C(=O)CH + OH$		-0.38	0.0258 0.0078
P2	$CH_3C(=O)CH_2 + O$		-6.38	0.0191 0.0078
P3	$CH_2CCH_2 + HO_2$		-9.53	0.0129 0.0372
P4	$CH_3CCH + HO_2$		-10.63	0.0122 0.0372
P5	$CH_2C(=O)CH_2 + OH$		-13.28	0.0230 0.0078
P6	$CH_3O + CH_2CO$		-66.97	0.0208 0.0163
P7	$CH_3C(=O)CHO + H$		-71.81	0.0150

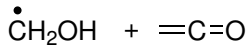
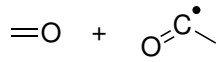
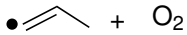
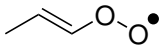
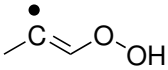
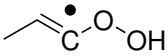
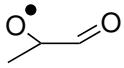
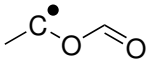
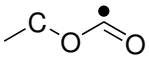
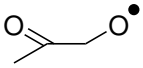
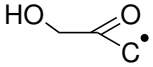
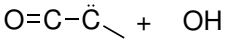
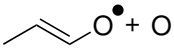
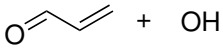
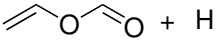
P8	$CH_2OH + CH_2CO$		-75.93	0.0175 0.0163
P9	$CH_2O + CH_3CO$		-87.45	0.0150 0.0217

Table S2: Intermediates and products on the $CH_3CHCHOO$ Potential Energy Surface

#	Species Name	Structure	Relative Energy (kcal/mol)	T1 diagnostic
R2	$CH_3CHCH + O_2$		4.09	0.0149
W11	$CH_3CHCHOO$		-38.19	0.0334
W12	$CH_3CCHOOH$		-13.98	0.0157
W13	$CH_3CHCOOH$		-15.26	0.0193
W14	$c-(CHOO)CHCH_3$		-29.52	0.0164
W15	$c-(CHOOCH)CH_3$		-21.64	0.0206
W16	$c-CH_3(CHOCH)O$		-79.01	0.0282
W17	$CH_3CHOCHO$		-85.89	0.0318
W18	$HCOOCHCH_3$		-105.23	0.0177
W19	CH_3CH_2OCO		-104.31	0.0202
W7	$CH_3C(=O)CH_2O$		-90.12	0.0444
W9	$CH_2C(=O)CH_2OH$		-101.75	0.0182
P10	$CH_3CCHO + OH$		-0.72	0.0250 0.0078
P11	$CH_3CHCHO + O$		-4.86	0.0204 0.0050
P12	$CH_3CHCO + OH$		-64.62	0.0149 0.0078
P13	$CH_2CHCHO + OH$		-65.2	0.0148 0.0078
P14	$CH_2CHOCHO + H$		-68.55	0.0154

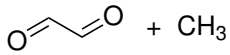
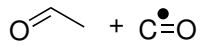
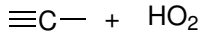
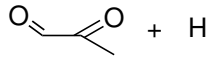
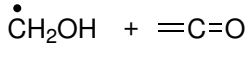
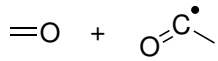
P15	$OCHCHO + CH_3$		-75.2	0.0063 0.0157
P16	$CH_3CHO + HCO$		-88.49	0.0141 0.0253
P17	$CO_2 + C_2H_5$		-126.69	0.0175 0.0105
P4	$CH_3CCH + HO_2$		-10.63	0.0122 0.0372
P7	$CH_3C(=O)CHO + H$		-71.81	0.0150
P8	$CH_2OH + CH_2CO$		-75.93	0.0175 0.0163
P9	$CH_2O + CH_3CO$		-87.45	0.0150 0.0217

Table S3: Transition state barrier heights on the $CH_3C(OO)CH_2$ potential energy surface

#	Reaction	Relative Energy (kcal/mol)	T1
TS1 [1]	R to W1		
TS2 [2]	W1 to P2	-4.84	
TS3	W1 to P3	0.31	0.0324
TS4	W1 to P4	-0.93	0.0337
TS5	W1 to W2	-4.39	0.0277
TS6	W1 to W3	-4.44	0.0255
TS7	W1 to W4	-19.60	0.0437
TS8	W1 to W5	-5.35	0.0318
TS9[2]	W2 to P1	-1.28	
TS10	W2 to P4	4.66	0.0240
TS11	W3 to P3	3.89	0.0284
TS12	W3 to P5	-22.24	0.0883
TS13[2]	W4 to W6	-16.53	
TS14	W5 to W7	-20.96	0.0890
TS15	W6 to W7	-77.77	0.0245
TS16	W6 to W8	-78.49	0.0330
TS17	W7 to W9	-72.95	0.0279
TS18	W7 to P7	-66.90	0.0194
TS19	W7 to P9	-85.15	0.0216
TS20	W8 to W10	-80.18	0.0165
TS21	W8 to P9	-75.91	0.0347
TS22	W9 to P8	-68.38	0.0209
TS23	W10 to P6	-60.33	0.0351

[1] Barrierless transition states. The partition function were calculated using VRC-TST;

[2] Barrier heights based on multi-reference calculation. Details are discussed in the following subsections

Table S4: Transition state barrier heights on the $CH_3CHCHOO$ potential energy surface

#	Reaction	Relative Energy (kcal/mol)	T1
TS24[1]	R2 to W11		
TS25	W11 to W12	-2.21	0.0260
TS26	W11 to W13	11.59	0.0585
TS27	W11 to W14	-15.73	0.0348
TS28	W11 to W15	-3.94	0.0351
TS29[2]	W11 to P11	-3.58	
TS30	W11 to P13	-13.04	0.0314
TS31[2]	W12 to P10	-0.74	
TS32	W12 to P4	4.45	0.0175
TS33	W13 to P12	-12.03	0.0339
TS34[2]	W14 to W16	-14.41	
TS35	W15to W17	-18.58	0.0846
TS36	W16 to W17	-77.86	0.0302
TS37	W16 to W18	-79.77	0.0152
TS38	W17 to W7	-71.62	0.0199
TS39	W17 to P15	-66.51	0.0210
TS40	W17 to P16	-79.61	0.0210
TS41	W18 to W19	-67.48	0.0212
TS42	W18 to P14	-66.02	0.0182
TS43	W18 to P16	-76.52	0.0336
TS44	W19 to P17	-89.80	0.0403
TS17	W7 to W9	-72.95	0.0279
TS18	W7 to P7	-66.90	0.0194
TS19	W7 to P9	-85.15	0.0216
TS22	W9 to P8	-68.38	0.0209

[1] Barrierless transition states. The partition function were calculated using VRC-TST;

[2] Barrier heights based on multi-reference calculation. Details are discussed in the following subsections