Supplementary Material

Auto-ignition of oxymethylene ethers (OME_n, n = 2–4) as promising synthetic e-fuels from renewable electricity: shock tube experiments and automatic mechanism generation

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Class	Rate rules	f_k	x^*
C1	Unimolecular Fuel decomposition ↔ R' + R"	4.0	-0.0133
C2	Fuel decomposition ↔ H and fuel radical (R)	4.0	1.0000
C3	H-atom abstraction from the fuel by H (primary carbon sites)	4.0	-0.8300
C3	H-atom abstraction from the fuel by H (secondary carbon sites)	4.0	-1.0000
C3	H-atom abstraction from the fuel by OH (primary carbon sites)	4.0	0.0415
C3	H-atom abstraction from the fuel by OH (secondary carbon sites)	4.0	-1.0000
C3	H-atom abstraction from the fuel by CH_3 (primary carbon sites)	4.0	1.0000
C3	H-atom abstraction from the fuel by CH_3 (secondary carbon sites)	4.0	1.0000
C3	H-atom abstraction from the fuel by HO_2 (primary carbon sites)	4.0	1.0000
C3	H-atom abstraction from the fuel by HO_2 (secondary carbon sites)	4.0	1.0000
C3	H-atom abstraction from the fuel by CH_3O (primary carbon sites)	4.0	-0.7890
C3	H-atom abstraction from the fuel by CH_3O (secondary carbon sites)	4.0	0.0860
C3	H-atom abstraction from the fuel by O_2 (secondary carbon sites)	4.0	1.0000
C3	H-atom abstraction from the fuel by CH_3O_2 (secondary carbon sites)	4.0	0.5721
C3	H-atom abstraction from the fuel by CH_3O_2 (secondary carbon sites)	4.0	-1.0000
C4	CO β-scission of R radicals	4.0	1.000
C5	OCO β-scission of R radicals	4.0	-0.3020
C8	R + CH_3O_2 ↔ RO + CH_3O	4.0	0.1077
C9	Peroxy (RO_2) radical isomerization (8 member ring, H-abstraction from primary sites)	4.0	-0.3964
C10	RO_2+ HO_2 ↔ ROOH + O_2	4.0	-0.1421
C16	QOOH → cyclic ether + OH (4 member ring)	4.0	0.8154
C16	QOOH → cyclic ether + OH (6 member ring)	4.0	-1.0000
C17	QOOH → β-Scission products	4.0	0.1267
C18	Addition of O_2 to QOOH (primary carbon sites)	4.0	1.0000
C18	Addition of O_2 to QOOH (secondary carbon sites)	4.0	-1.0000
C19	Isomerization of O_2QOOH (6 member ring, H-abstraction from primary sites)	4.0	0.9784
C19	Isomerization of O_2QOOH (6 member ring, H-abstraction from secondary sites)	4.0	0.9784
C20	Decomposition of carbonylhydroperoxide	4.0	0.7925

Table S1: Optimized rate rules. f_k and x_k^* denote the uncertainty factor and the calibrated normalized rate parameters of the rate rule k, respectively. The optimized Arrhenius pre-exponential factor A_k^* can be determined based on its nominal value in the prior mechanism (A_k) following $A_k^* = A_k \times f_k^{x_k^*}$.

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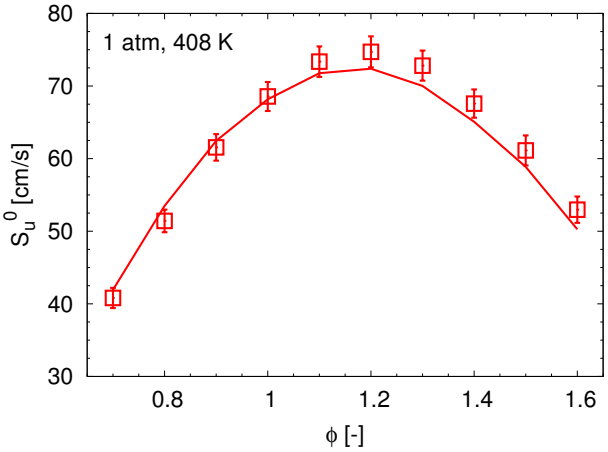

Figure S1: Flame speeds of OME_3/air mixtures at 1 atm. Symbols denote experiments from [14] and lines show results calculated using the optimized mechanism.

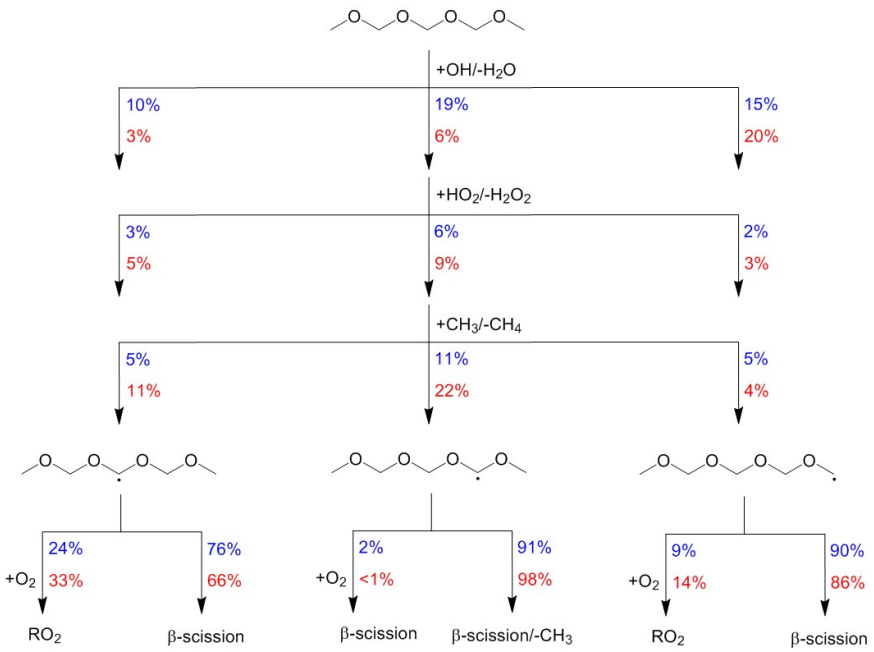

Figure S2: Reaction pathways during the auto-ignition of OME_3/air mixture at 20 bar, 1150 K, ϕ = 1.0, and 20% fuel consumption. Blue and red values are results predicted using the prior and optimized mechanisms, respectively.