Supporting Information

H-Atom-Forming Reaction Pathways in the Pyrolysis of Furan, 2-Methylfuran, and 2,5-Dimethylfuran: A Shock-Tube and Modeling Study

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Table S1. Detailed experimental conditions for furan pyrolysis experiments

T / K	p / bar	[Ar] / mol cm^{-3}	[furan]$_0$ / mol cm^{-3}
1540	1.06	8.3×10^{-6}	4.4×10^{-11}
1650	1.10	8.0×10^{-6}	3.7×10^{-11}
1770	1.05	7.1×10^{-6}	6.6×10^{-11}
1825	0.91	6.0×10^{-6}	5.6×10^{-11}

Table S2. Detailed experimental conditions for 2-MF pyrolysis experiments

T / K	p / bar	[Ar] / mol cm^{-3}	[2-MF]$_0$ / mol cm^{-3}
1480	1.12	9.1×10^{-6}	4.0×10^{-11}
1580	1.09	8.2×10^{-6}	3.6×10^{-11}
1690	0.93	6.6×10^{-6}	2.9×10^{-11}
1790	0.97	6.5×10^{-6}	6.6×10^{-11}

Table S3. Detailed experimental conditions for 2,5-DMF pyrolysis experiments

T / K	p / bar	[Ar] / mol cm^{-3}	[2,5-DMF]$_0$ / mol cm^{-3}
1290	1.64	1.5×10^{-5}	6.1×10^{-11}
1340	1.68	1.5×10^{-5}	6.6×10^{-11}
1400	1.61	1.4×10^{-5}	4.7×10^{-11}
1480	1.60	1.3×10^{-5}	5.2×10^{-11}

Figure S1. Local sensitivity analyses of the mechanism by Liu et al.[1] for H-atoms in F pyrolysis at different temperatures (blue: 1540 K, green: 1650 K, red: 1770K, black: 1825 K) and t_{react} ~ 50 µs. Only reactions with at least one sensitivity coefficient higher 0.01 are shown.

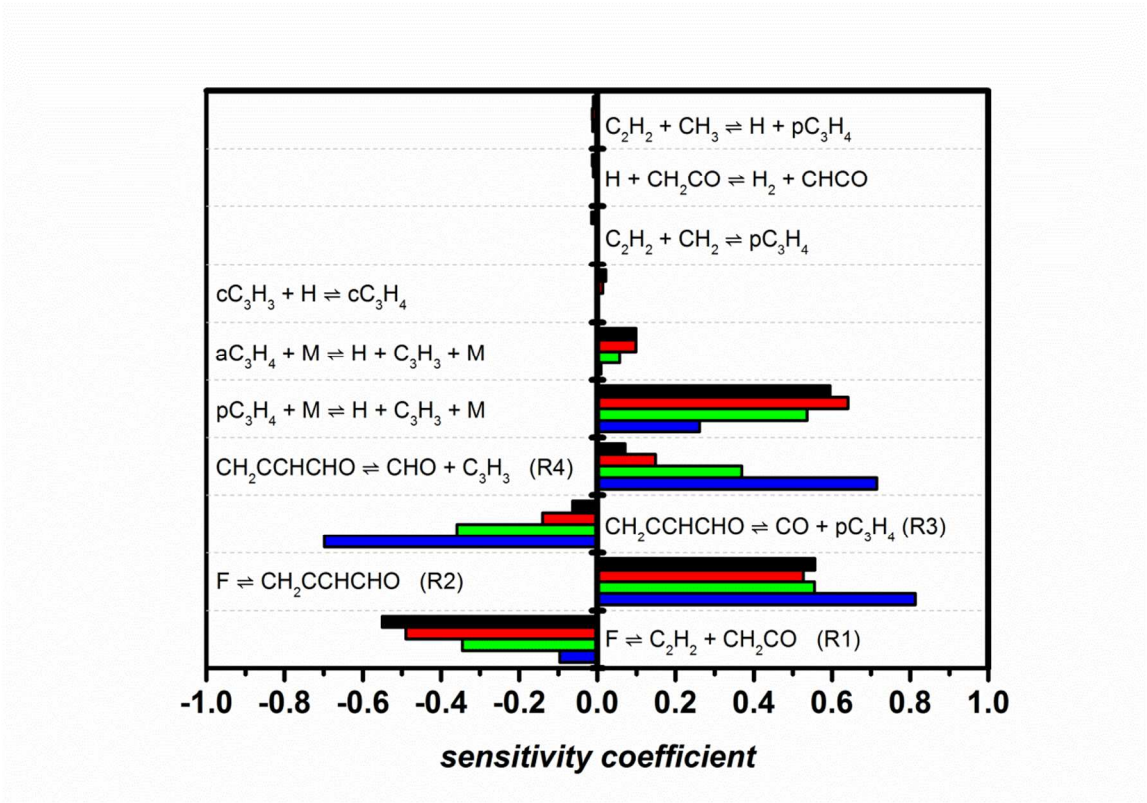


Figure S2. Local sensitivity analyses of the mechanism by Liu et al.[1, 2] for H-atoms in 2-MF pyrolysis at different temperatures (blue: 1480 K, green: 1580 K, red: 1690K, black: 1790 K) and t_{react} ~ 30 µs. Only reactions with at least one sensitivity coefficient higher 0.01 are shown.

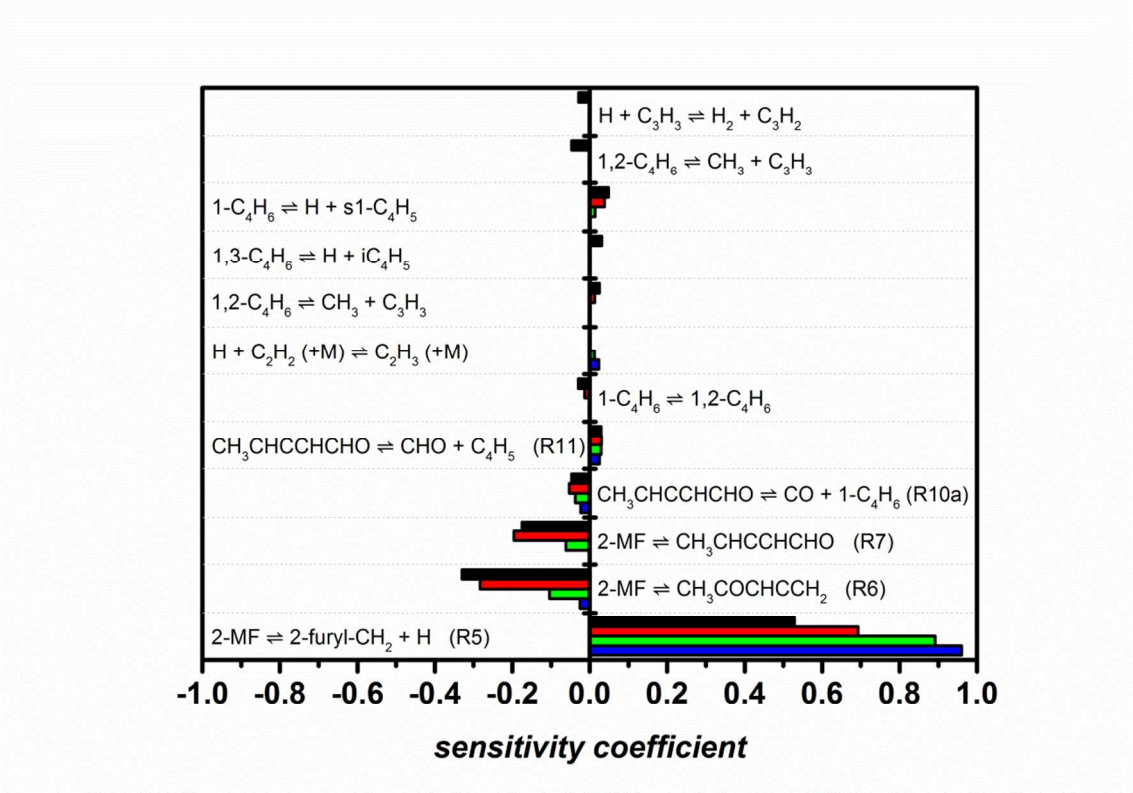
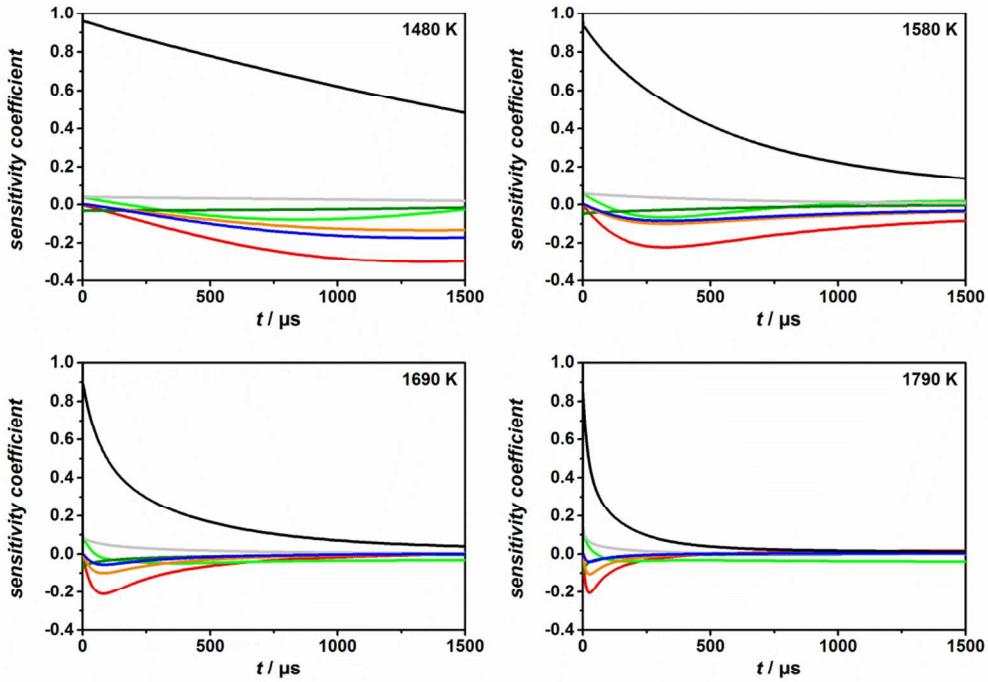


Figure S3. Time-resolved sensitivity analyses of the mechanism by Liu et al.[1, 2] for H-atoms in 2-MF pyrolysis at different temperatures. Reactions: R5 (black), R6 (red), R7 (green), R8 (blue), R10a (dark green), R11 (light grey), R18 (orange).



References

1. Liu, D.; Togbé, C.; Tran, L.-S.; Felsmann, D.; Oßwald, P.; Nau, P.; Koppmann, J.; Lackner, A.; Glaude, P.-A.; Sirjean, B., et al., Combustion chemistry and flame structure of furan group biofuels using molecular-beam mass spectrometry and gas chromatography – Part I: Furan. *Combust. Flame* **2014,** *161* (3), 748-765.
2. Tran, L.-S.; Togbé, C.; Liu, D.; Felsmann, D.; Oßwald, P.; Glaude, P.-A.; Fournet, R.; Sirjean, B.; Battin-Leclerc, F.; Kohse-Höinghaus, K., Combustion chemistry and flame structure of furan group biofuels using molecular-beam mass spectrometry and gas chromatography – Part II: 2-Methylfuran. *Combust. Flame* **2014,** *161* (3), 766-779.