

Supplementary Materials (SM)

Experimental and kinetic modeling of combustion chemistry of high-energy density fuel JP-10

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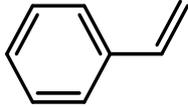
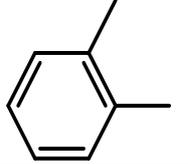
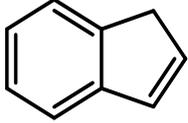
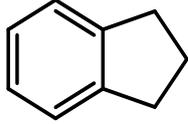
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NSRL flow reactor at low pressure (30 Torr):

Table. S1 Compilation of hydrocarbons observed in the pyrolysis of JP-10.

Species	Formula	Mass	Structure
Acetylene	C ₂ H ₂	26	
Ethylene	C ₂ H ₄	28	
Allene	C ₃ H ₄	40	
Propyne	C ₃ H ₄	40	
Allyl	C ₃ H ₅	41	
Propene	C ₃ H ₆	42	
Vinylacetylene	C ₄ H ₄	52	
1,3-Butadiene	C ₄ H ₆	54	
1-Butene	C ₄ H ₈	56	
Cyclopentadienyl radical	C ₅ H ₅	65	
Cyclopentadiene	C ₅ H ₆	66	
Cyclopentene	C ₅ H ₈	68	
Benzene	C ₆ H ₆	78	
1,3-Cyclohexadiene	C ₆ H ₈	80	
Cyclohexene	C ₆ H ₁₀	82	
Toluene	C ₇ H ₈	92	

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Styrene	C_8H_8	104	
<i>o</i> -Xylene	C_8H_{10}	106	
Indene	C_9H_8	116	
Indane	C_9H_{10}	118	

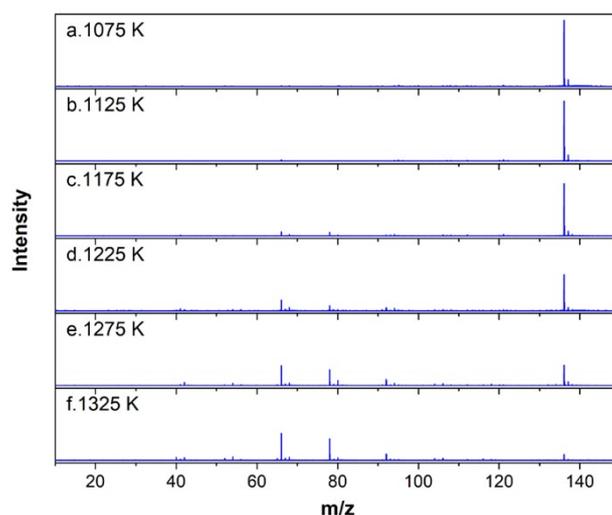
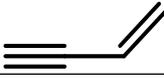


Fig. S1 Mass spectra of the products obtained from the decomposition of JP-10 pyrolysis recorded in NSRL at a photon energy of 10.5 eV at different temperatures from 1075 K to 1325 K.

Table.S2 Compilation of hydrocarbons observed in the oxidation of JP-10.

Species	Formula	Mass	Structure
Acetylene	C_2H_2	26	
Ethylene	C_2H_4	28	
Allene	C_3H_4	40	
Propyne	C_3H_4	40	
Allyl	C_3H_5	41	
Propene	C_3H_6	42	
Vinylacetylene	C_4H_4	52	
1,3-Butadiene	C_4H_6	54	
1-Butene	C_4H_8	56	

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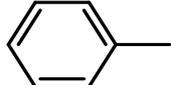
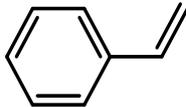
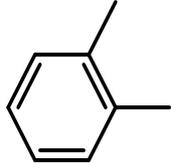
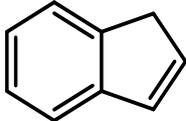
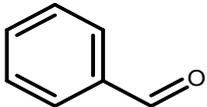
Cyclopentadienyl radical	C_5H_5	65	
Cyclopentadiene	C_5H_6	66	
1,4-Pentadiene	C_5H_8	68	
Benzene	C_6H_6	78	
1,3-Cyclohexadiene	C_6H_8	80	
Toluene	C_7H_8	92	
Styrene	C_8H_8	104	
<i>o</i> -Xylene	C_8H_{10}	106	
Indene	C_9H_8	116	

Table. S3 Compilation of oxygenated species observed in the oxidation of JP-10.

Species	Formula	Mass	Structure
Carbon monoxide	CO	28	$+o \equiv c^-$
Formaldehyde	CH ₂ O	30	$H_2C=O$
Ketene	C ₂ H ₂ O	42	$O=C=CH_2$
Benzaldehyde	C ₇ H ₆ O	106	

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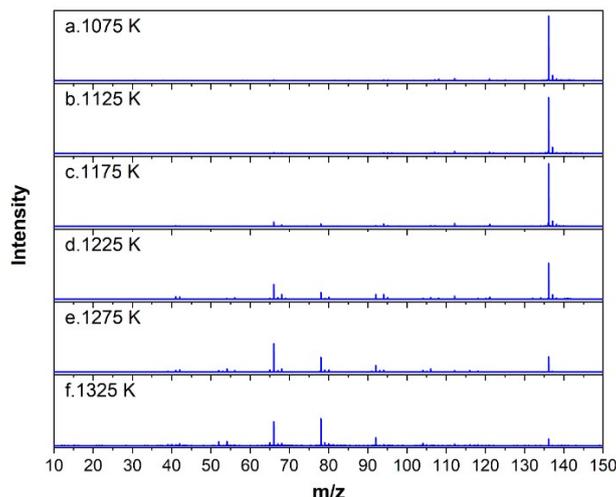


Fig. S2 Mass spectra of the products obtained from the decomposition of JP-10 oxidation $\phi = 1$ recorded in NSRL at a photon energy of 10.5 eV at different temperatures from 1075 K to 1325 K.

Table. S4 Comparison of Key Species in Tao model, Jiang model, and the present HyChem Models

Species	Tao model [1]	Jiang model [2]	Present Model
H ₂	✓		✓
CO		✓	✓
CH ₂ O			✓
CH ₃	✓	✓	✓
C ₂ H ₂		✓	
CH ₃ CHO		✓	
C ₂ H ₄	✓	✓	✓
aC ₃ H ₅ ·	✓		✓
C ₃ H ₆	✓	✓	✓
C ₄ H ₆			✓
C ₅ H ₆	✓	✓	✓
C ₅ H ₈		✓	✓
C ₆ H ₆	✓	✓	✓
C ₇ H ₈	✓	✓	✓

References:

- [1] Y. Tao, R. Xu, K. Wang, J. Shao, S.E. Johnson, A. Movaghar, X. Han, J.-W. Park, T. Lu, K. Brezinsky, F.N. Egolfopoulos, D.F. Davidson, R.K. Hanson, C.T. Bowman, H. Wang, A Physics-based approach to modeling real-fuel combustion chemistry – III. Reaction kinetic model of JP10, *Combust. Flame* 198 (2018) 466–476.
- [2] H. Jiang, W. Shen, S. Bai, D. Chen, C. Wang, X. Liang, K. Wang, Revised HyChem modeling combustion chemistry of air-breathing high-energy density jet fuel: JP-10, *Combust. Flame* 248 (2023) 112578.