Supporting Information

A Combined Experimental and Computational Study on the Unimolecular Decomposition of JP-8 Jet Fuel Surrogates II: *n*-Dodecane (*n*-$C_{12}H_{26}$)

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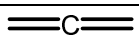
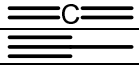
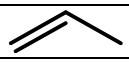
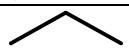
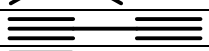
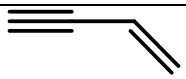
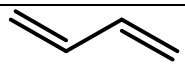
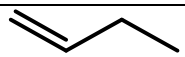
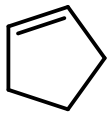
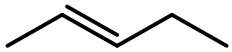
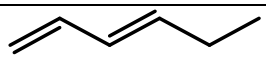
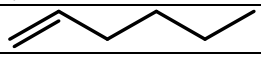
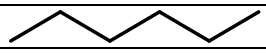
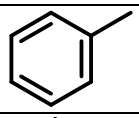
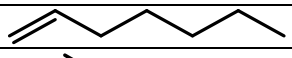
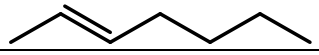
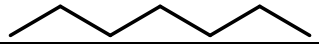
Table S1. Detected molecules in previous experimental studies of *n*-dodecane pyrolysis.

Molecule	Formula	Mass	Structure	Ref.
Hydrogen	H_2	2		1
Methane	CH_4	16		1-5
Acetylene	C_2H_2	26		1-3
Ethylene	C_2H_4	28		1-8
Ethane	C_2H_6	30		1-5
Allene	C_3H_4	40		1,3
Methylacetylene	C_3H_4	40		1,3
Propene	C_3H_6	42		1-5,7-8
Propane	C_3H_8	44		5,7-8
Diacetylene	C_4H_2	50		3
Vinylacetylene	C_4H_4	52		3
1,3-Butadiene	C_4H_6	54		1-3
1-Butene	C_4H_8	56		1-5,7-8
2-Butene	C_4H_8	56		5,7-8
Cyclopentadiene	C_5H_6	66		1
Cyclopentene	C_5H_8	68		1
1-Pentene	C_5H_{10}	70		1-4,7-8
2-Pentene	C_5H_{10}	70		5,7-8
n-Pentane	C_5H_{12}	72		5,7-8
Benzene	C_6H_6	78		1,3
1,3-Hexadiene	C_6H_{10}	82		2
1-Hexene	C_6H_{12}	84		1-5,7-8
2-Hexene	C_6H_{12}	84		5,7-8
n-Hexane	C_6H_{14}	86		7-8
Toluene	C_7H_8	92		1
1-Heptene	C_7H_{14}	98		1-4,7-8
2-Heptene	C_7H_{14}	98		5,7-8
n-Heptane	C_7H_{16}	100		7-8

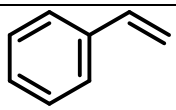
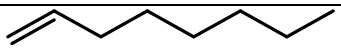
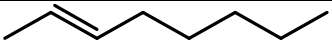
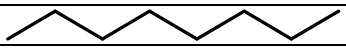
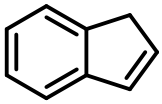
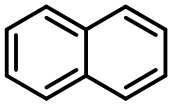
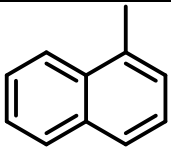
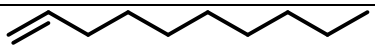
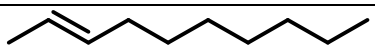
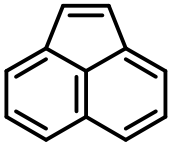
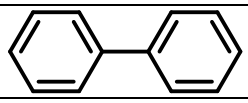
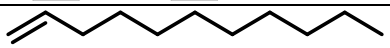
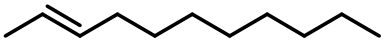
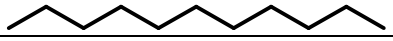
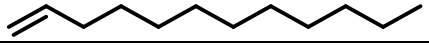
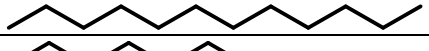
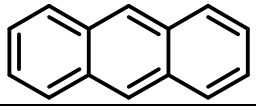
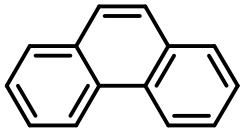
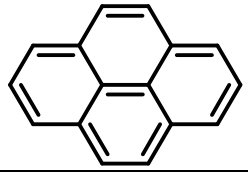
Styrene	C_8H_8	104		1
1-Octene	C_8H_{16}	112		1-3,5,7-8
2-Octene	C_8H_{16}	112		7-8
n-Octane	C_8H_{18}	114		5,7-8
Indene	C_9H_8	116		1
1-Nonene	C_9H_{18}	126		1-3,5,7-8
2-Nonene	C_9H_{18}	126		7-8
n-Nonane	C_9H_{20}	128		5,7-8
Naphthalene	$C_{10}H_8$	128		1
Methylnaphthalene	$C_{11}H_{10}$	142		1
1-Decene	$C_{10}H_{20}$	140		1-3,5,7-8
1-Decene	$C_{10}H_{20}$	140		7-8
n-Decane	$C_{10}H_{22}$	142		5,7-8
Acenaphthalene	$C_{12}H_8$	152		1
Biphenyl	$C_{12}H_{10}$	154		1
1-Undecene	$C_{11}H_{22}$	154		1,3,5,7-8
1-Undecene	$C_{11}H_{22}$	154		7-8
n-Undecane	$C_{11}H_{24}$	156		5,7-8
1-Dodecene	$C_{12}H_{24}$	168		5,7-8
n-Dodecane	$C_{12}H_{26}$	170		1-8
Anthracene	$C_{14}H_{10}$	178		1
Phenathrene	$C_{14}H_{10}$	178		1
Pyrene	$C_{16}H_{10}$	202		1

Table S2. Parameters of the fitted modified Arrhenius expressions, $A \cdot T^{\alpha} \cdot exp(-E_a/RT)$, for most important reactions involved in pyrolysis of *n*-dodecane at pressures of 0.03-0.04, 1, 10, and 100 atm.

The data are presented in the following order:

/*p*,atm A, $cm^3\ mol^{-1}\ s^{-1}$ α E_a, $cal\ mol^{-1}$/ ! fit btw. T_1 and T_2 with MAE = mean/max absolute error

The title line for each reaction shows A, α, and E_a at the high-pressure limit.

The fits are provided to a single Arrhenius expression and to a sum of two Arrhenius expressions

$C_{12}H_{26} \rightarrow C_2H_5 + C_{10}H_{21}$			3.81E+67	-14.27 110300.0
PLOG/3.000E-02	2.27E+107	-26.56	125300.0/	! fit btw. 500 and 2500 K with MAE of 44.6%, 153.4%
PLOG/3.947E-02	2.64E+106	-26.26	125100.0/	! fit btw. 500 and 2500 K with MAE of 44.5%, 155.5%
PLOG/1.000E+00	8.94E+92	-22.00	120800.0/	! fit btw. 500 and 2500 K with MAE of 49.3%, 165.1%
PLOG/1.000E+01	8.35E+80	-18.31	116100.0/	! fit btw. 500 and 2500 K with MAE of 53.7%, 157.2%
PLOG/1.000E+02	3.81E+67	-14.27	110300.0/	! fit btw. 500 and 2500 K with MAE of 53.0%, 124.8%
PLOG/3.000E-02	7.61E+253	-74.12	166000.0/	
PLOG/3.000E-02	2.28E+122	-30.73	136700.0/	! fit btw. 500 and 2500 K with MAE of 29.5%, 63.2%
PLOG/3.947E-02	2.00E+122	-30.67	137200.0/	
PLOG/3.947E-02	8.60E+256	-75.03	167400.0/	! fit btw. 500 and 2500 K with MAE of 28.3%, 60.4%
PLOG/1.000E+00	-2.37E+98	-23.91	118200.0/	
PLOG/1.000E+00	8.43E+86	-20.36	113800.0/	! fit btw. 500 and 2500 K with MAE of 38.0%, 63.1%
PLOG/1.000E+01	3.25E+109	-26.20	139000.0/	
PLOG/1.000E+01	1.22E+102	-25.86	116800.0/	! fit btw. 500 and 2500 K with MAE of 16.8%, 35.8%
PLOG/1.000E+02	2.48E+57	-11.63	102500.0/	
PLOG/1.000E+02	8.17E+142	-35.04	172800.0/	! fit btw. 500 and 2500 K with MAE of 8.1%, 20.9%
$C_{12}H_{26} \rightarrow C_3H_7 + C_9H_{19}$			3.14E+68	-14.45 111400.0
PLOG/3.000E-02	3.92E+108	-26.85	126500.0/	! fit btw. 500 and 2500 K with MAE of 45.0%, 154.5%
PLOG/3.947E-02	4.54E+107	-26.54	126300.0/	! fit btw. 500 and 2500 K with MAE of 44.9%, 156.7%
PLOG/1.000E+00	1.28E+94	-22.26	122000.0/	! fit btw. 500 and 2500 K with MAE of 49.6%, 166.8%
PLOG/1.000E+01	9.40E+81	-18.53	117200.0/	! fit btw. 500 and 2500 K with MAE of 54.1%, 159.5%
PLOG/1.000E+02	3.14E+68	-14.45	111400.0/	! fit btw. 500 and 2500 K with MAE of 53.5%, 126.8%
PLOG/3.000E-02	5.15E+254	-74.29	167000.0/	
PLOG/3.000E-02	3.09E+123	-30.98	137800.0/	! fit btw. 500 and 2500 K with MAE of 29.9%, 64.4%
PLOG/3.947E-02	2.84E+123	-30.93	138300.0/	
PLOG/3.947E-02	6.69E+255	-74.59	167700.0/	! fit btw. 500 and 2500 K with MAE of 28.7%, 61.5%

PLOG/1.000E+00 -4.90E+99 -24.21 119700.0/
PLOG/1.000E+00 1.91E+88 -20.67 115300.0/ ! fit btw. 500 and 2500 K with MAE of 37.8%, 62.1%
PLOG/1.000E+01 6.68E+110 -26.49 140400.0/
PLOG/1.000E+01 2.36E+102 -25.85 117600.0/ ! fit btw. 500 and 2500 K with MAE of 16.9%, 35.9%
PLOG/1.000E+02 1.31E+58 -11.75 103500.0/
PLOG/1.000E+02 1.77E+144 -35.34 174200.0/ ! fit btw. 500 and 2500 K with MAE of 8.2%, 20.9%

$C_{12}H_{26} \rightarrow C_4H_9 + C_8H_{17}$ 1.96E+68 -14.42 111300.0

PLOG/3.000E-02 2.18E+108 -26.80 126300.0/ ! fit btw. 500 and 2500 K with MAE of 45.0%, 154.4%
PLOG/3.947E-02 2.53E+107 -26.50 126100.0/ ! fit btw. 500 and 2500 K with MAE of 44.8%, 156.6%
PLOG/1.000E+00 7.35E+93 -22.22 121800.0/ ! fit btw. 500 and 2500 K with MAE of 49.6%, 166.6%
PLOG/1.000E+01 5.59E+81 -18.49 117000.0/ ! fit btw. 500 and 2500 K with MAE of 54.1%, 159.2%
PLOG/1.000E+02 1.96E+68 -14.42 111300.0/ ! fit btw. 500 and 2500 K with MAE of 53.5%, 126.5%

PLOG/3.000E-02 3.58E+254 -74.27 166800.0/
PLOG/3.000E-02 1.81E+123 -30.94 137700.0/ ! fit btw. 500 and 2500 K with MAE of 29.9%, 64.2%
PLOG/3.947E-02 1.63E+123 -30.89 138100.0/
PLOG/3.947E-02 1.15E+257 -75.01 168000.0/ ! fit btw. 500 and 2500 K with MAE of 28.6%, 61.3%
PLOG/1.000E+00 -1.62E+99 -24.11 119100.0/
PLOG/1.000E+00 8.39E+87 -20.60 114900.0/ ! fit btw. 500 and 2500 K with MAE of 39.1%, 64.3%
PLOG/1.000E+01 2.35E+110 -26.39 140000.0/
PLOG/1.000E+01 8.48E+102 -26.06 117700.0/ ! fit btw. 500 and 2500 K with MAE of 16.9%, 36.1%
PLOG/1.000E+02 8.70E+57 -11.73 103300.0/
PLOG/1.000E+02 9.51E+143 -35.29 174000.0/ ! fit btw. 500 and 2500 K with MAE of 8.2%, 20.9%

$C_{12}H_{26} \rightarrow C_5H_{11} + C_7H_{15}$ 2.14E+68 -14.43 111300.0

PLOG/3.000E-02 2.46E+108 -26.82 126400.0/ ! fit btw. 500 and 2500 K with MAE of 45.0%, 154.4%
PLOG/3.947E-02 2.85E+107 -26.52 126200.0/ ! fit btw. 500 and 2500 K with MAE of 44.8%, 156.6%
PLOG/1.000E+00 8.22E+93 -22.23 121800.0/ ! fit btw. 500 and 2500 K with MAE of 49.6%, 166.6%
PLOG/1.000E+01 6.19E+81 -18.51 117100.0/ ! fit btw. 500 and 2500 K with MAE of 54.1%, 159.2%
PLOG/1.000E+02 2.14E+68 -14.43 111300.0/ ! fit btw. 500 and 2500 K with MAE of 53.5%, 126.5%

PLOG/3.000E-02 3.81E+254 -74.28 166900.0/
PLOG/3.000E-02 1.97E+123 -30.96 137700.0/ ! fit btw. 500 and 2500 K with MAE of 29.9%, 64.3%
PLOG/3.947E-02 1.79E+123 -30.90 138200.0/
PLOG/3.947E-02 1.32E+257 -75.03 168100.0/ ! fit btw. 500 and 2500 K with MAE of 28.7%, 61.4%
PLOG/1.000E+00 -1.40E+99 -24.07 119300.0/
PLOG/1.000E+00 1.34E+88 -20.66 115000.0/ ! fit btw. 500 and 2500 K with MAE of 38.3%, 65.8%

PLOG/1.000E+01	4.25E+110	-26.46	140200.0/	
PLOG/1.000E+01	1.64E+102	-25.84	117500.0/	! fit btw. 500 and 2500 K with MAE of 16.8%, 35.9%
PLOG/1.000E+02	9.37E+57	-11.74	103400.0/	
PLOG/1.000E+02	1.09E+144	-35.31	174100.0/	! fit btw. 500 and 2500 K with MAE of 8.2%, 21.1%

$C_{12}H_{26} \rightarrow C_6H_{13} + C_6H_{13}$ 2.43E+68 -14.43 111300.0

PLOG/3.000E-02	2.80E+108	-26.82	126400.0/	! fit btw. 500 and 2500 K with MAE of 45.0%, 154.4%
PLOG/3.947E-02	3.25E+107	-26.51	126200.0/	! fit btw. 500 and 2500 K with MAE of 44.8%, 156.6%
PLOG/1.000E+00	9.36E+93	-22.23	121800.0/	! fit btw. 500 and 2500 K with MAE of 49.6%, 166.6%
PLOG/1.000E+01	7.04E+81	-18.50	117100.0/	! fit btw. 500 and 2500 K with MAE of 54.1%, 159.2%
PLOG/1.000E+02	2.43E+68	-14.43	111300.0/	! fit btw. 500 and 2500 K with MAE of 53.5%, 126.6%
PLOG/3.000E-02	4.12E+254	-74.27	166900.0/	
PLOG/3.000E-02	2.28E+123	-30.96	137700.0/	! fit btw. 500 and 2500 K with MAE of 29.9%, 64.2%
PLOG/3.947E-02	2.06E+123	-30.90	138200.0/	
PLOG/3.947E-02	1.42E+257	-75.02	168100.0/	! fit btw. 500 and 2500 K with MAE of 28.7%, 61.4%
PLOG/1.000E+00	-2.13E+99	-24.12	119200.0/	
PLOG/1.000E+00	9.64E+87	-20.60	114800.0/	! fit btw. 500 and 2500 K with MAE of 39.7%, 66.2%
PLOG/1.000E+01	4.86E+110	-26.46	140200.0/	
PLOG/1.000E+01	1.83E+102	-25.83	117500.0/	! fit btw. 500 and 2500 K with MAE of 16.8%, 35.9%
PLOG/1.000E+02	1.06E+58	-11.74	103400.0/	
PLOG/1.000E+02	1.23E+144	-35.30	174000.0/	! fit btw. 500 and 2500 K with MAE of 8.1%, 21.1%

C_9H_{21} (1-nonyl) $\rightarrow C_2H_4 + C_7H_{15}$[b] 1.51E+29 -4.56 37640.0

PLOG/3.000E-02	5.15E+33	-6.79	33390.0/	! fit btw. 500 and 2500 K with MAE of 29.6%, 88.7%
PLOG/1.000E+00	1.74E+37	-7.34	38490.0/	! fit btw. 500 and 2500 K with MAE of 18.3%, 31.0%
PLOG/1.000E+01	1.11E+35	-6.45	39240.0/	! fit btw. 500 and 2500 K with MAE of 10.6%, 17.6%
PLOG/1.000E+02	1.51E+29	-4.56	37640.0/	! fit btw. 500 and 2500 K with MAE of 8.7%, 22.8%
PLOG/3.000E-02	1.61E+77	-19.82	53500.0/	
PLOG/3.000E-02	9.57E+22	-3.67	29830.0/	! fit btw. 500 and 2500 K with MAE of 3.1%, 5.7%
PLOG/1.000E+00	4.64E+48	-10.72	44080.0/	
PLOG/1.000E+00	7.47E+67	-14.95	92450.0/	! fit btw. 500 and 2500 K with MAE of 4.7%, 18.3%
PLOG/1.000E+01	8.47E+79	-19.50	66240.0/	
PLOG/1.000E+01	1.08E+26	-3.91	34190.0/	! fit btw. 500 and 2500 K with MAE of 1.4%, 3.4%
PLOG/1.000E+02	1.15E+70	-16.20	66790.0/	
PLOG/1.000E+02	1.81E+23	-2.92	33990.0/	! fit btw. 500 and 2500 K with MAE of 0.6%, 2.0%

$C_{10}H_{21}$ (1-decyl) → C_2H_4 + C_8H_{17}[b]				7.78E+27	-4.19	37110.0
PLOG/3.000E-02	1.83E+36	-7.50	35050.0/	! fit btw. 500 and 2500 K with MAE of 33.0%, 70.9%		
PLOG/1.000E+00	1.73E+38	-7.61	39310.0/	! fit btw. 500 and 2500 K with MAE of 17.9%, 33.0%		
PLOG/1.000E+01	4.70E+34	-6.33	39280.0/	! fit btw. 500 and 2500 K with MAE of 11.0%, 18.7%		
PLOG/1.000E+02	7.78E+27	-4.19	37110.0/	! fit btw. 500 and 2500 K with MAE of 10.7%, 21.0%		
PLOG/3.000E-02	1.57E+81	-20.97	55830.0/			
PLOG/3.000E-02	9.22E+22	-3.66	29670.0/	! fit btw. 500 and 2500 K with MAE of 3.3%, 5.5%		
PLOG/1.000E+00	3.24E+47	-10.36	43780.0/			
PLOG/1.000E+00	2.71E+74	-16.63	102300.0/	! fit btw. 500 and 2500 K with MAE of 6.3%, 19.0%		
PLOG/1.000E+01	6.57E+82	-20.31	68740.0/			
PLOG/1.000E+01	3.22E+26	-4.04	34640.0/	! fit btw. 500 and 2500 K with MAE of 1.4%, 3.3%		
PLOG/1.000E+02	4.98E+67	-15.50	65840.0/			
PLOG/1.000E+02	6.14E+22	-2.79	33870.0/	! fit btw. 500 and 2500 K with MAE of 0.8%, 2.1%		
$C_{12}H_{25}$ (1-dodecyl) → C_2H_4 + $C_{10}H_{21}$[b]				2.13E+28	-4.31	37400.0
PLOG/3.000E-02	6.15E+34	-7.06	34320.0/	! fit btw. 500 and 2500 K with MAE of 30.4%, 86.1%		
PLOG/3.947E-02	1.86E+35	-7.16	34830.0/	! fit btw. 500 and 2500 K with MAE of 29.6%, 79.5%		
PLOG/1.000E+00	3.62E+37	-7.41	39020.0/	! fit btw. 500 and 2500 K with MAE of 17.5%, 30.4%		
PLOG/1.000E+01	4.96E+34	-6.33	39350.0/	! fit btw. 500 and 2500 K with MAE of 10.5%, 20.5%		
PLOG/1.000E+02	2.13E+28	-4.31	37400.0/	! fit btw. 500 and 2500 K with MAE of 9.4%, 22.9%		
PLOG/3.000E-02	6.14E+81	-21.11	56370.0/			
PLOG/3.000E-02	6.46E+22	-3.60	29640.0/	! fit btw. 500 and 2500 K with MAE of 3.3%, 6.6%		
PLOG/3.947E-02	1.48E+82	-21.17	57020.0/			
PLOG/3.947E-02	7.33E+22	-3.59	29720.0/	! fit btw. 500 and 2500 K with MAE of 3.2%, 6.3%		
PLOG/1.000E+00	4.07E+47	-10.37	43950.0/			
PLOG/1.000E+00	3.27E+70	-15.59	97770.0/	! fit btw. 500 and 2500 K with MAE of 5.2%, 19.9%		
PLOG/1.000E+01	4.27E+85	-21.09	70880.0/			
PLOG/1.000E+01	3.94E+26	-4.05	34750.0/	! fit btw. 500 and 2500 K with MAE of 1.2%, 3.5%		
PLOG/1.000E+02	1.07E+67	-15.29	65680.0/			
PLOG/1.000E+02	3.93E+22	-2.73	33800.0/	! fit btw. 500 and 2500 K with MAE of 0.7%, 2.1%		
$C_{12}H_{25}$ (2-dodecyl) → C_3H_6 + C_9H_{19}[b]				3.49E+28	-4.36	37550.0
PLOG/3.000E-02	6.83E+34	-7.07	34360.0/	! fit btw. 500 and 2500 K with MAE of 30.5%, 86.6%		
PLOG/3.947E-02	2.08E+35	-7.17	34870.0/	! fit btw. 500 and 2500 K with MAE of 29.7%, 80.0%		

PLOG/1.000E+00	4.72E+37	-7.44	39090.0/	! fit btw. 500 and 2500 K with MAE of 17.6%, 30.6%
PLOG/1.000E+01	7.40E+34	-6.38	39470.0/	! fit btw. 500 and 2500 K with MAE of 10.7%, 20.7%
PLOG/1.000E+02	3.49E+28	-4.36	37550.0/	! fit btw. 500 and 2500 K with MAE of 9.5%, 23.5%
PLOG/3.000E-02	8.43E+81	-21.15	56440.0/	
PLOG/3.000E-02	6.95E+22	-3.60	29670.0/	! fit btw. 500 and 2500 K with MAE of 3.4%, 6.5%
PLOG/3.947E-02	2.17E+82	-21.22	57100.0/	
PLOG/3.947E-02	7.98E+22	-3.59	29760.0/	! fit btw. 500 and 2500 K with MAE of 3.2%, 6.3%
PLOG/1.000E+00	7.26E+47	-10.44	44090.0/	
PLOG/1.000E+00	1.55E+70	-15.50	97230.0/	! fit btw. 500 and 2500 K with MAE of 5.3%, 20.5%
PLOG/1.000E+01	4.71E+85	-21.10	70860.0/	
PLOG/1.000E+01	4.20E+26	-4.06	34780.0/	! fit btw. 500 and 2500 K with MAE of 1.2%, 3.5%
PLOG/1.000E+02	1.92E+67	-15.36	65780.0/	
PLOG/1.000E+02	4.44E+22	-2.74	33850.0/	! fit btw. 500 and 2500 K with MAE of 0.7%, 2.1%

$C_{12}H_{25}$ (3-dodecyl) → $C_{11}H_{22}$ (1-undecene) + CH_3[b] 1.46E+32 -5.40 39600.0

PLOG/3.000E-02	1.63E+34	-6.96	33710.0/	! fit btw. 500 and 2500 K with MAE of 33.4%, 108.2%
PLOG/3.947E-02	6.61E+34	-7.10	34280.0/	! fit btw. 500 and 2500 K with MAE of 32.6%, 101.5%
PLOG/1.000E+00	6.32E+38	-7.81	39450.0/	! fit btw. 500 and 2500 K with MAE of 21.9%, 36.5%
PLOG/1.000E+01	2.52E+37	-7.13	40720.0/	! fit btw. 500 and 2500 K with MAE of 12.9%, 22.5%
PLOG/1.000E+02	1.46E+32	-5.40	39600.0/	! fit btw. 500 and 2500 K with MAE of 9.6%, 26.4%
PLOG/3.000E-02	1.70E+82	-21.34	55800.0/	
PLOG/3.000E-02	3.89E+23	-3.86	30550.0/	! fit btw. 500 and 2500 K with MAE of 4.1%, 8.2%
PLOG/3.947E-02	7.54E+82	-21.48	56540.0/	
PLOG/3.947E-02	3.28E+23	-3.81	30430.0/	! fit btw. 500 and 2500 K with MAE of 3.9%, 7.2%
PLOG/1.000E+00	8.20E+53	-12.28	46770.0/	
PLOG/1.000E+00	3.39E+54	-11.50	74430.0/	! fit btw. 500 and 2500 K with MAE of 5.2%, 21.5%
PLOG/1.000E+01	4.61E+41	-8.39	42870.0/	
PLOG/1.000E+01	5.63E+140	-33.62	195800.0/	! fit btw. 500 and 2500 K with MAE of 7.0%, 24.8%
PLOG/1.000E+02	1.92E+78	-18.58	71250.0/	
PLOG/1.000E+02	9.88E+24	-3.41	35300.0/	! fit btw. 500 and 2500 K with MAE of 0.7%, 2.3%

$C_{12}H_{25}$ (3-dodecyl) → C_4H_8 (1-butene) + C_8H_{17}[b] 5.90E+31 -5.36 38970.0

PLOG/3.000E-02	8.40E+33	-6.92	33300.0/	! fit btw. 500 and 2500 K with MAE of 32.8%, 105.5%
PLOG/3.947E-02	3.24E+34	-7.05	33860.0/	! fit btw. 500 and 2500 K with MAE of 32.1%, 99.0%
PLOG/1.000E+00	2.06E+38	-7.72	38870.0/	! fit btw. 500 and 2500 K with MAE of 21.6%, 35.8%
PLOG/1.000E+01	8.11E+36	-7.05	40080.0/	! fit btw. 500 and 2500 K with MAE of 12.6%, 22.2%

PLOG/1.000E+02	5.90E+31	-5.36	38970.0/	! fit btw. 500 and 2500 K with MAE of 9.3%, 25.3%
PLOG/3.000E-02	5.95E+80	-20.95	54840.0/	
PLOG/3.000E-02	3.07E+23	-3.87	30300.0/	! fit btw. 500 and 2500 K with MAE of 4.0%, 7.9%
PLOG/3.947E-02	2.74E+81	-21.10	55580.0/	
PLOG/3.947E-02	2.22E+23	-3.80	30120.0/	! fit btw. 500 and 2500 K with MAE of 3.7%, 7.0%
PLOG/1.000E+00	1.59E+53	-12.13	46080.0/	
PLOG/1.000E+00	1.88E+54	-11.48	74040.0/	! fit btw. 500 and 2500 K with MAE of 5.0%, 20.9%
PLOG/1.000E+01	1.39E+41	-8.30	42210.0/	
PLOG/1.000E+01	6.88E+138	-33.17	193300.0/	! fit btw. 500 and 2500 K with MAE of 6.8%, 23.9%
PLOG/1.000E+02	3.58E+78	-18.73	71040.0/	
PLOG/1.000E+02	7.97E+24	-3.44	34850.0/	! fit btw. 500 and 2500 K with MAE of 0.7%, 2.2%
$C_{12}H_{25}$ (4-dodecyl) → $C_{10}H_{20}$ (1-decene) + C_2H_5[b]				1.72E+29 -4.66 37730.0
PLOG/3.000E-02	9.80E+33	-6.94	33640.0/	! fit btw. 500 and 2500 K with MAE of 31.1%, 93.0%
PLOG/3.947E-02	3.21E+34	-7.05	34170.0/	! fit btw. 500 and 2500 K with MAE of 30.4%, 86.5%
PLOG/1.000E+00	2.58E+37	-7.47	38680.0/	! fit btw. 500 and 2500 K with MAE of 19.0%, 31.9%
PLOG/1.000E+01	1.36E+35	-6.56	39370.0/	! fit btw. 500 and 2500 K with MAE of 11.2%, 18.8%
PLOG/1.000E+02	1.72E+29	-4.66	37730.0/	! fit btw. 500 and 2500 K with MAE of 9.1%, 23.9%
PLOG/3.000E-02	1.28E+81	-21.04	55550.0/	
PLOG/3.000E-02	4.28E+22	-3.64	29540.0/	! fit btw. 500 and 2500 K with MAE of 3.5%, 6.4%
PLOG/3.947E-02	4.80E+81	-21.15	56280.0/	
PLOG/3.947E-02	4.28E+22	-3.62	29550.0/	! fit btw. 500 and 2500 K with MAE of 3.3%, 6.1%
PLOG/1.000E+00	1.44E+49	-10.94	44420.0/	
PLOG/1.000E+00	6.88E+62	-13.69	86940.0/	! fit btw. 500 and 2500 K with MAE of 5.1%, 20.6%
PLOG/1.000E+01	2.13E+83	-20.56	68480.0/	
PLOG/1.000E+01	1.29E+26	-4.01	34300.0/	! fit btw. 500 and 2500 K with MAE of 1.4%, 3.7%
PLOG/1.000E+02	4.19E+71	-16.73	67940.0/	
PLOG/1.000E+02	1.27E+23	-2.96	33960.0/	! fit btw. 500 and 2500 K with MAE of 0.7%, 2.3%
$C_{12}H_{25}$ (4-dodecyl) → C_5H_{10} (1-pentene) + C_7H_{15}[b]				4.40E+29 -4.73 38240.0
PLOG/3.000E-02	2.05E+34	-7.00	34010.0/	! fit btw. 500 and 2500 K with MAE of 31.5%, 95.2%
PLOG/3.947E-02	6.97E+34	-7.12	34550.0/	! fit btw. 500 and 2500 K with MAE of 30.9%, 88.6%
PLOG/1.000E+00	7.37E+37	-7.56	39160.0/	! fit btw. 500 and 2500 K with MAE of 19.3%, 32.3%
PLOG/1.000E+01	3.94E+35	-6.65	39880.0/	! fit btw. 500 and 2500 K with MAE of 11.3%, 18.9%
PLOG/1.000E+02	4.40E+29	-4.73	38240.0/	! fit btw. 500 and 2500 K with MAE of 9.2%, 24.2%

PLOG/3.000E-02	3.93E+81	-21.15	55980.0/	
PLOG/3.000E-02	7.55E+22	-3.68	29920.0/	! fit btw. 500 and 2500 K with MAE of 3.6%, 6.4%
PLOG/3.947E-02	1.62E+82	-21.28	56730.0/	
PLOG/3.947E-02	7.48E+22	-3.65	29920.0/	! fit btw. 500 and 2500 K with MAE of 3.4%, 6.7%
PLOG/1.000E+00	4.96E+49	-11.06	44950.0/	
PLOG/1.000E+00	1.10E+70	-15.57	95270.0/	! fit btw. 500 and 2500 K with MAE of 5.3%, 20.1%
PLOG/1.000E+01	5.25E+83	-20.63	68920.0/	
PLOG/1.000E+01	2.69E+26	-4.07	34730.0/	! fit btw. 500 and 2500 K with MAE of 1.5%, 3.7%
PLOG/1.000E+02	4.44E+70	-16.41	67430.0/	
PLOG/1.000E+02	2.06E+23	-2.98	34340.0/	! fit btw. 500 and 2500 K with MAE of 0.7%, 2.1%

$C_{12}H_{25}$ (5-dodecyl) → C_9H_{18} (1-nonene) + C_3H_7[b] 8.86E+30 -5.14 38830.0

PLOG/3.000E-02	7.43E+33	-6.93	33550.0/	! fit btw. 500 and 2500 K with MAE of 32.6%, 103.5%
PLOG/3.947E-02	2.79E+34	-7.06	34110.0/	! fit btw. 500 and 2500 K with MAE of 31.8%, 96.9%
PLOG/1.000E+00	1.21E+38	-7.68	39060.0/	! fit btw. 500 and 2500 K with MAE of 20.9%, 34.8%
PLOG/1.000E+01	2.52E+36	-6.93	40140.0/	! fit btw. 500 and 2500 K with MAE of 12.2%, 21.1%
PLOG/1.000E+02	8.86E+30	-5.14	38830.0/	! fit btw. 500 and 2500 K with MAE of 9.1%, 24.8%
PLOG/3.000E-02	2.68E+81	-21.17	55480.0/	
PLOG/3.000E-02	1.32E+23	-3.79	30180.0/	! fit btw. 500 and 2500 K with MAE of 3.9%, 7.5%
PLOG/3.947E-02	1.19E+82	-21.31	56230.0/	
PLOG/3.947E-02	1.11E+23	-3.75	30080.0/	! fit btw. 500 and 2500 K with MAE of 3.7%, 6.7%
PLOG/1.000E+00	9.05E+51	-11.78	45810.0/	
PLOG/1.000E+00	1.77E+62	-13.60	84310.0/	! fit btw. 500 and 2500 K with MAE of 5.2%, 20.5%
PLOG/1.000E+01	1.00E+190	-46.61	257700.0/	
PLOG/1.000E+01	1.26E+40	-8.01	42000.0/	! fit btw. 500 and 2500 K with MAE of 6.9%, 23.9%
PLOG/1.000E+02	1.85E+76	-18.08	70290.0/	
PLOG/1.000E+02	2.09E+24	-3.30	34830.0/	! fit btw. 500 and 2500 K with MAE of 0.7%, 2.2%

$C_{12}H_{25}$ (5-dodecyl) → C_6H_{12} (1-hexene) + C_6H_{13}[b] 1.31E+31 -5.12 38690.0

PLOG/3.000E-02	1.17E+34	-6.91	33450.0/	! fit btw. 500 and 2500 K with MAE of 32.4%, 102.8%
PLOG/3.947E-02	4.37E+34	-7.04	34010.0/	! fit btw. 500 and 2500 K with MAE of 31.7%, 96.2%
PLOG/1.000E+00	1.74E+38	-7.65	38930.0/	! fit btw. 500 and 2500 K with MAE of 20.8%, 34.6%
PLOG/1.000E+01	3.60E+36	-6.90	39990.0/	! fit btw. 500 and 2500 K with MAE of 12.2%, 21.0%
PLOG/1.000E+02	1.31E+31	-5.12	38690.0/	! fit btw. 500 and 2500 K with MAE of 9.1%, 24.8%
PLOG/3.000E-02	3.61E+81	-21.13	55350.0/	
PLOG/3.000E-02	2.14E+23	-3.78	30070.0/	! fit btw. 500 and 2500 K with MAE of 3.9%, 7.5%

PLOG/3.947E-02	1.64E+82	-21.28	56100.0/	
PLOG/3.947E-02	1.80E+23	-3.73	29970.0/	! fit btw. 500 and 2500 K with MAE of 3.6%, 6.8%
PLOG/1.000E+00	1.65E+52	-11.78	45710.0/	
PLOG/1.000E+00	3.42E+56	-12.01	77350.0/	! fit btw. 500 and 2500 K with MAE of 5.1%, 21.0%
PLOG/1.000E+01	4.86E+190	-46.72	258300.0/	
PLOG/1.000E+01	1.69E+40	-7.98	41850.0/	! fit btw. 500 and 2500 K with MAE of 6.9%, 23.9%
PLOG/1.000E+02	2.14E+76	-18.03	70080.0/	
PLOG/1.000E+02	3.14E+24	-3.28	34690.0/	! fit btw. 500 and 2500 K with MAE of 0.7%, 2.2%

$C_{12}H_{25}$ (6-dodecyl) → C_8H_{16} (1-octene) + C_4H_9[b] 4.39E+31 -5.29 38890.0

PLOG/3.000E-02	3.76E+33	-6.80	33040.0/	! fit btw. 500 and 2500 K with MAE of 33.0%, 107.7%
PLOG/3.947E-02	1.55E+34	-6.94	33620.0/	! fit btw. 500 and 2500 K with MAE of 32.3%, 101.1%
PLOG/1.000E+00	1.50E+38	-7.66	38740.0/	! fit btw. 500 and 2500 K with MAE of 21.7%, 36.0%
PLOG/1.000E+01	6.48E+36	-7.00	40000.0/	! fit btw. 500 and 2500 K with MAE of 12.5%, 22.3%
PLOG/1.000E+02	4.39E+31	-5.29	38890.0/	! fit btw. 500 and 2500 K with MAE of 9.2%, 24.8%
PLOG/3.000E-02	9.65E+80	-21.01	54810.0/	
PLOG/3.000E-02	2.08E+23	-3.80	30170.0/	! fit btw. 500 and 2500 K with MAE of 4.1%, 7.9%
PLOG/3.947E-02	4.00E+81	-21.14	55520.0/	
PLOG/3.947E-02	1.72E+23	-3.75	30030.0/	! fit btw. 500 and 2500 K with MAE of 3.8%, 6.9%
PLOG/1.000E+00	1.40E+53	-12.09	46000.0/	
PLOG/1.000E+00	3.96E+58	-12.61	78870.0/	! fit btw. 500 and 2500 K with MAE of 5.0%, 20.4%
PLOG/1.000E+01	1.29E+41	-8.26	42170.0/	
PLOG/1.000E+01	6.03E+135	-32.35	189200.0/	! fit btw. 500 and 2500 K with MAE of 6.7%, 23.5%
PLOG/1.000E+02	3.29E+76	-18.13	69620.0/	
PLOG/1.000E+02	5.31E+24	-3.36	34740.0/	! fit btw. 500 and 2500 K with MAE of 0.7%, 1.7%

$C_{12}H_{25}$ (6-dodecyl) → C_7H_{14} (1-heptene) + C_5H_{11}[b] 4.13E+31 -5.29 38860.0

PLOG/3.000E-02	3.62E+33	-6.80	33020.0/	! fit btw. 500 and 2500 K with MAE of 32.9%, 107.5%
PLOG/3.947E-02	1.48E+34	-6.94	33600.0/	! fit btw. 500 and 2500 K with MAE of 32.2%, 100.9%
PLOG/1.000E+00	1.41E+38	-7.65	38720.0/	! fit btw. 500 and 2500 K with MAE of 21.7%, 35.9%
PLOG/1.000E+01	6.09E+36	-6.99	39980.0/	! fit btw. 500 and 2500 K with MAE of 12.5%, 22.3%
PLOG/1.000E+02	4.13E+31	-5.29	38860.0/	! fit btw. 500 and 2500 K with MAE of 9.2%, 24.8%
PLOG/3.000E-02	9.49E+80	-21.01	54800.0/	
PLOG/3.000E-02	1.99E+23	-3.79	30140.0/	! fit btw. 500 and 2500 K with MAE of 4.1%, 7.9%
PLOG/3.947E-02	3.75E+81	-21.13	55500.0/	
PLOG/3.947E-02	1.65E+23	-3.75	30010.0/	! fit btw. 500 and 2500 K with MAE of 3.8%, 6.9%

PLOG/1.000E+00	1.26E+53	-12.08	45970.0/	
PLOG/1.000E+00	4.22E+58	-12.61	78910.0/	! fit btw. 500 and 2500 K with MAE of 5.0%, 20.3%
PLOG/1.000E+01	1.19E+41	-8.25	42140.0/	
PLOG/1.000E+01	8.35E+135	-32.39	189400.0/	! fit btw. 500 and 2500 K with MAE of 6.7%, 23.4%
PLOG/1.000E+02	1.35E+78	-18.59	70740.0/	
PLOG/1.000E+02	7.07E+24	-3.40	34800.0/	! fit btw. 500 and 2500 K with MAE of 0.7%, 2.2%

[a]Fits have been carried out using the auxiliary MESS_TPfit written by Franklin Goldsmith; see http://tcg.cse.anl.gov/papr/codes/mess.html.
[b]The calculations of the rate constant have been performed using a simplified PES including only the direct C-C bond β-scission channel.

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