

ESI Table of Content

Table S1. Parameters of the fitted modified Arrhenius expressions, $A \cdot T^{\alpha} \cdot \exp(-E_a/RT)$, for all considered reactions at pressures of 30 Torr, 1, 10, and 100 atm (Table S1.docx)

Input files for RKKM/ME calculations with MESS code:

c6h5_c3h4.inp
c6h6_c3h3.inp
c6h5_c3h6.inp
indene_ch3_1.inp
indene_ch3_2.inp
c10h9_methylindenyl.inp

Files containing two- and three-dimensional potentials for coupled hindered rotors:

A8_pes.dat	c9h11_i1.dat	c9h11_i4.dat	c9h11_i9.dat
TS9_pes1.dat	TS9_pes2.dat	TS9_pes3.dat	TS9_pes4.dat
TS9_pes5.dat	TS9_pes6.dat	TS9_pes7.dat	TS9_pes8.dat
TS9_pes9.dat	TS9_pes10.dat	TS9_pes11.dat	TS9_pes12.dat
TS9_pes13.dat	TS9_pes14.dat	TS9_pes15.dat	TS9_pes16.dat
TS9_pes17.dat	TS9_pes18.dat	TS9_pes19.dat	TS9_pes20.dat
TS9_pes21.dat	TS9_pes22.dat	TS9_pes23.dat	TS9_pes24.dat
TS9_pes25.dat	TS9_pes26.dat		

The files with extensions inp and dat can be viewed or edited by WordPad, other word processors, or Linux editors, and can be directly used to run rate constant calculations by the MESS code.

Table S1. Parameters of the fitted modified Arrhenius expressions, $A \cdot T^{\alpha} \cdot \exp(-E_a/RT)$, for all considered reactions at pressures of 30 Torr, 1, 10, and 100 atm.

The data are presented in the following order:

/ p , atm A , $\text{cm}^3 \text{mol}^{-1} \text{s}^{-1}$ 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

C₆H₅ + propyne → C₉H₉ (W1)				9.16E+20	-2.40	9287.0	
PLOG/3.947E-02	6.62E+67	-17.28	24570.0/				! fit btw. 500 and 1125 K with MAE of 7.9%, 15.1%
PLOG/1.000E+00	1.12E+49	-11.13	19650.0/				! fit btw. 500 and 1375 K with MAE of 15.4%, 25.1%
PLOG/1.000E+01	1.68E+33	-6.18	14030.0/				! fit btw. 500 and 1500 K with MAE of 15.7%, 31.0%
PLOG/1.000E+02	9.16E+20	-2.40	9287.0/				! fit btw. 500 and 1650 K with MAE of 12.8%, 31.1%
PLOG/3.947E-02	4.09E+95	-25.46	39640.0/				
PLOG/3.947E-02	1.27E+67	-17.61	20960.0/				! fit btw. 500 and 1125 K with MAE of 0.4%, 0.7%
PLOG/1.000E+00	6.57E+90	-23.21	45020.0/				
PLOG/1.000E+00	4.93E+53	-12.98	18690.0/				! fit btw. 500 and 1375 K with MAE of 0.8%, 1.8%
PLOG/1.000E+01	3.65E+80	-19.74	44800.0/				
PLOG/1.000E+01	1.58E+38	-8.00	14010.0/				! fit btw. 500 and 1500 K with MAE of 1.9%, 3.3%
PLOG/1.000E+02	9.13E+65	-15.15	41190.0/				
PLOG/1.000E+02	2.26E+26	-4.23	10160.0/				! fit btw. 500 and 1650 K with MAE of 2.3%, 4.4%
C₆H₅ + propyne → C₉H₉ (W4)				3.52E+22	-3.01	12990.0	
PLOG/3.947E-02	8.23E+63	-16.28	25100.0/				! fit btw. 500 and 1000 K with MAE of 3.3%, 6.2%
PLOG/1.000E+00	1.72E+42	-9.21	19610.0/				! fit btw. 500 and 1125 K with MAE of 8.8%, 13.8%
PLOG/1.000E+01	9.18E+34	-6.86	17610.0/				! fit btw. 500 and 1375 K with MAE of 13.0%, 22.7%
PLOG/1.000E+02	3.52E+22	-3.01	12990.0/				! fit btw. 500 and 1500 K with MAE of 11.0%, 23.2%
PLOG/3.947E-02	8.23E+63	-16.28	25100.0/				
PLOG/3.947E-02	0.00E+00	0.00	0.0/				! fit btw. 500 and 1000 K with MAE of 3.3%, 6.2%
PLOG/1.000E+00	5.23E+79	-20.21	40400.0/				
PLOG/1.000E+00	4.44E+48	-11.61	19460.0/				! fit btw. 500 and 1125 K with MAE of 0.7%, 1.5%
PLOG/1.000E+01	1.94E+74	-18.20	41990.0/				
PLOG/1.000E+01	1.33E+44	-10.04	18770.0/				! fit btw. 500 and 1375 K with MAE of 1.3%, 2.1%

PLOG/1.000E+02	3.07E+64	-14.99	41120.0/	
PLOG/1.000E+02	4.44E+28	-5.09	13940.0/	! fit btw. 500 and 1500 K with MAE of 1.6%, 2.7%

C₆H₅ + propyne → C₉H₉ (W6) 7.60E+39 -7.69 35790.0

PLOG/3.947E-02	5.29E+74	-18.76	35350.0/	! fit btw. 500 and 1650 K with MAE of 14.7%, 27.9%
PLOG/1.000E+00	2.39E+58	-13.52	34110.0/	! fit btw. 500 and 1800 K with MAE of 22.0%, 42.9%
PLOG/1.000E+01	2.87E+47	-10.08	33780.0/	! fit btw. 500 and 2000 K with MAE of 27.6%, 62.2%
PLOG/1.000E+02	7.60E+39	-7.69	35790.0/	! fit btw. 500 and 2500 K with MAE of 45.6%, 122.1%

PLOG/3.947E-02	1.35E+102	-26.57	53820.0/	
PLOG/3.947E-02	4.99E+77	-20.07	33890.0/	! fit btw. 500 and 1650 K with MAE of 2.5%, 5.7%
PLOG/1.000E+00	1.38E+84	-20.83	51510.0/	
PLOG/1.000E+00	2.99E+57	-13.86	29610.0/	! fit btw. 500 and 1800 K with MAE of 2.7%, 9.5%
PLOG/1.000E+01	1.44E+73	-17.32	51880.0/	
PLOG/1.000E+01	3.40E+44	-9.84	28100.0/	! fit btw. 500 and 2000 K with MAE of 4.6%, 12.8%
PLOG/1.000E+02	-1.49E+69	-16.47	47680.0/	
PLOG/1.000E+02	5.47E+49	-10.56	39160.0/	! fit btw. 500 and 2500 K with MAE of 16.4%, 45.6%

C₆H₅ + propyne → C₉H₉ (W9) 1.68E+09 0.96 20360.0

PLOG/3.947E-02	3.72E+71	-17.85	42430.0/	! fit btw. 800 and 1650 K with MAE of 2.1%, 3.3%
PLOG/1.000E+00	2.76E+52	-11.65	40080.0/	! fit btw. 800 and 2000 K with MAE of 2.5%, 5.2%
PLOG/1.000E+01	2.40E+11	0.08	15050.0/	! fit btw. 500 and 2500 K with MAE of 66.7%, 290.7%
PLOG/1.000E+02	1.68E+09	0.96	20360.0/	! fit btw. 500 and 2500 K with MAE of 83.4%, 462.5%

PLOG/3.947E-02	-1.34E+85	-21.99	45790.0/	
PLOG/3.947E-02	8.45E+74	-18.88	41140.0/	! fit btw. 800 and 1650 K with MAE of 0.2%, 0.6%
PLOG/1.000E+00	-4.88E+76	-18.54	55070.0/	
PLOG/1.000E+00	6.19E+66	-15.64	48780.0/	! fit btw. 800 and 2000 K with MAE of 0.8%, 1.3%
PLOG/1.000E+01	1.84E+45	-11.65	19250.0/	
PLOG/1.000E+01	4.07E+50	-10.78	45690.0/	! fit btw. 500 and 2500 K with MAE of 1.8%, 4.7%
PLOG/1.000E+02	1.26E+03	-6.66	-42200.0/	
PLOG/1.000E+02	6.10E+28	-4.51	34390.0/	! fit btw. 500 and 2500 K with MAE of 25.0%, 101.0%

C₆H₅ + propyne → indene + H (P1) 1.24E+10 0.75 37370.0

PLOG/3.947E-02	3.28E+41	-8.56	30610.0/	! fit btw. 500 and 2500 K with MAE of 8.8%, 17.5%
PLOG/1.000E+00	4.01E+38	-7.45	38820.0/	! fit btw. 500 and 2500 K with MAE of 8.6%, 23.4%
PLOG/1.000E+01	2.98E+28	-4.46	40710.0/	! fit btw. 500 and 2500 K with MAE of 31.2%, 92.8%
PLOG/1.000E+02	1.24E+10	0.75	37370.0/	! fit btw. 500 and 2500 K with MAE of 51.4%, 127.3%

PLOG/3.947E-02	7.20E+78	-19.50	52250.0/	
PLOG/3.947E-02	3.29E+33	-6.30	26200.0/	! fit btw. 500 and 2500 K with MAE of 2.1%, 4.3%
PLOG/1.000E+00	5.65E+41	-8.33	41100.0/	
PLOG/1.000E+00	9.54E+114	-33.58	52640.0/	! fit btw. 500 and 2500 K with MAE of 2.8%, 11.3%
PLOG/1.000E+01	1.70E+44	-8.84	52450.0/	
PLOG/1.000E+01	1.96E+48	-11.92	39280.0/	! fit btw. 500 and 2500 K with MAE of 2.0%, 4.3%
PLOG/1.000E+02	3.54E-04	4.01	25520.0/	
PLOG/1.000E+02	1.24E+41	-7.86	61110.0/	! fit btw. 500 and 2500 K with MAE of 7.4%, 14.9%

C₆H₅ + propyne → 1-phenylpropyne + H (P2)

2.28E+20 -1.67 25400.0

PLOG/3.947E-02	4.64E+25	-3.54	17460.0/	! fit btw. 500 and 2500 K with MAE of 12.1%, 20.0%
PLOG/1.000E+00	2.17E+32	-5.29	25250.0/	! fit btw. 500 and 2500 K with MAE of 12.2%, 28.5%
PLOG/1.000E+01	1.36E+30	-4.55	27450.0/	! fit btw. 500 and 2500 K with MAE of 23.4%, 65.1%
PLOG/1.000E+02	2.28E+20	-1.67	25400.0/	! fit btw. 500 and 2500 K with MAE of 40.4%, 85.3%

PLOG/3.947E-02	5.53E+37	-7.15	22960.0/	
PLOG/3.947E-02	6.16E+34	-5.72	36950.0/	! fit btw. 500 and 2500 K with MAE of 1.4%, 6.1%
PLOG/1.000E+00	4.07E+71	-16.72	48560.0/	
PLOG/1.000E+00	1.20E+21	-2.12	18960.0/	! fit btw. 500 and 2500 K with MAE of 1.8%, 4.3%
PLOG/1.000E+01	3.11E+41	-7.71	35890.0/	
PLOG/1.000E+01	1.61E+127	-36.20	53610.0/	! fit btw. 500 and 2500 K with MAE of 5.7%, 13.4%
PLOG/1.000E+02	3.57E+43	-8.09	43440.0/	
PLOG/1.000E+02	1.66E+35	-7.10	25120.0/	! fit btw. 500 and 2500 K with MAE of 6.3%, 12.5%

C₆H₅ + propyne → phenylallene + H (P3)

1.57E+18 -1.05 25370.0

PLOG/3.947E-02	1.24E+22	-2.52	16680.0/	! fit btw. 500 and 2500 K with MAE of 12.0%, 20.9%
PLOG/1.000E+00	1.36E+29	-4.38	24630.0/	! fit btw. 500 and 2500 K with MAE of 12.1%, 27.1%
PLOG/1.000E+01	2.90E+27	-3.79	27120.0/	! fit btw. 500 and 2500 K with MAE of 22.3%, 62.6%
PLOG/1.000E+02	1.57E+18	-1.05	25370.0/	! fit btw. 500 and 2500 K with MAE of 39.8%, 85.5%

PLOG/3.947E-02	1.81E+35	-6.47	22610.0/	
PLOG/3.947E-02	2.84E+29	-4.25	33130.0/	! fit btw. 500 and 2500 K with MAE of 1.3%, 5.4%
PLOG/1.000E+00	3.10E+72	-17.03	50020.0/	
PLOG/1.000E+00	1.23E+19	-1.54	19050.0/	! fit btw. 500 and 2500 K with MAE of 1.7%, 4.7%
PLOG/1.000E+01	9.83E+37	-6.72	34910.0/	
PLOG/1.000E+01	1.39E+142	-41.04	59060.0/	! fit btw. 500 and 2500 K with MAE of 6.0%, 13.8%
PLOG/1.000E+02	1.53E+41	-7.42	43220.0/	
PLOG/1.000E+02	6.05E+32	-6.41	24950.0/	! fit btw. 500 and 2500 K with MAE of 5.8%, 9.9%

C₆H₅ + propyne → phenylacetylene + CH₃ (P5)

4.79E+22 -2.31 27330.0

PLOG/3.947E-02	1.64E+23	-2.84	16460.0/	! fit btw. 500 and 2500 K with MAE of 19.5%, 38.2%
PLOG/1.000E+00	8.29E+30	-4.88	25080.0/	! fit btw. 500 and 2500 K with MAE of 14.6%, 26.3%
PLOG/1.000E+01	9.90E+29	-4.50	27990.0/	! fit btw. 500 and 2500 K with MAE of 15.5%, 41.5%
PLOG/1.000E+02	4.79E+22	-2.31	27330.0/	! fit btw. 500 and 2500 K with MAE of 30.2%, 71.2%

PLOG/3.947E-02	2.50E+44	-9.20	25970.0/	
PLOG/3.947E-02	1.65E+24	-2.85	25950.0/	! fit btw. 500 and 2500 K with MAE of 1.3%, 4.3%
PLOG/1.000E+00	3.29E+37	-6.83	28280.0/	
PLOG/1.000E+00	1.72E+92	-20.53	118800.0/	! fit btw. 500 and 2500 K with MAE of 6.5%, 22.2%
PLOG/1.000E+01	4.24E+35	-6.07	32100.0/	
PLOG/1.000E+01	1.53E+167	-49.31	65090.0/	! fit btw. 500 and 2500 K with MAE of 8.2%, 17.8%
PLOG/1.000E+02	2.82E+51	-10.35	48980.0/	
PLOG/1.000E+02	1.39E+09	1.30	18040.0/	! fit btw. 500 and 2500 K with MAE of 2.2%, 4.5%

C₆H₅ + propyne → total

4.37E+11 0.45 5465.0

PLOG/3.947E-02	6.05E+08	1.25	3785.0/	! fit btw. 500 and 2500 K with MAE of 1.3%, 2.4%
PLOG/1.000E+00	3.16E+09	1.05	4163.0/	! fit btw. 500 and 2500 K with MAE of 2.6%, 4.7%
PLOG/1.000E+01	3.34E+10	0.76	4756.0/	! fit btw. 500 and 2500 K with MAE of 3.3%, 7.4%
PLOG/1.000E+02	4.37E+11	0.45	5465.0/	! fit btw. 500 and 2500 K with MAE of 4.8%, 11.1%

PLOG/3.947E-02	9.27E+11	0.21	4872.0/	
PLOG/3.947E-02	2.85E+06	1.89	4109.0/	! fit btw. 500 and 2500 K with MAE of 0.7%, 1.5%
PLOG/1.000E+00	5.81E+70	-17.39	35740.0/	
PLOG/1.000E+00	2.16E+08	1.38	3577.0/	! fit btw. 500 and 2500 K with MAE of 0.5%, 0.9%
PLOG/1.000E+01	1.19E+20	-2.08	10240.0/	

PLOG/1.000E+01	1.16E+01	3.38	-313.8/	! fit btw. 500 and 2500 K with MAE of 1.4%, 2.9%
PLOG/1.000E+02	3.35E+85	-20.79	55750.0/	
PLOG/1.000E+02	5.00E+09	0.99	4300.0/	! fit btw. 500 and 2500 K with MAE of 1.8%, 7.3%

C₆H₅ + allene → C₉H₉ (W6) 1.73E+16 -0.89 8967.0

PLOG/3.947E-02	3.57E+49	-11.14	21750.0/	! fit btw. 500 and 1650 K with MAE of 25.7%, 55.7%
PLOG/1.000E+00	1.85E+28	-4.57	13750.0/	! fit btw. 500 and 1800 K with MAE of 23.0%, 59.8%
PLOG/1.000E+01	2.67E+18	-1.58	9671.0/	! fit btw. 500 and 2000 K with MAE of 19.5%, 61.2%
PLOG/1.000E+02	1.73E+16	-0.89	8967.0/	! fit btw. 500 and 2500 K with MAE of 22.6%, 81.3%

PLOG/3.947E-02	5.13E+101	-26.00	56380.0/	
PLOG/3.947E-02	2.43E+51	-12.10	19710.0/	! fit btw. 500 and 1650 K with MAE of 3.3%, 6.7%
PLOG/1.000E+00	9.78E-02	4.32	1317.0/	
PLOG/1.000E+00	-3.23E+25	-2.83	28270.0/	! fit btw. 500 and 1800 K with MAE of 0.9%, 1.6%
PLOG/1.000E+01	1.72E-03	4.83	493.2/	
PLOG/1.000E+01	-1.45E+14	0.38	21230.0/	! fit btw. 500 and 2000 K with MAE of 2.0%, 3.6%
PLOG/1.000E+02	2.57E+63	-13.79	51520.0/	
PLOG/1.000E+02	1.23E+20	-2.21	9425.0/	! fit btw. 500 and 2500 K with MAE of 6.6%, 12.4%

C₆H₅ + allene → C₉H₉ (W11) 1.67E+20 -2.51 8846.0

PLOG/3.947E-02	2.68E+55	-14.53	15760.0/	! fit btw. 500 and 900 K with MAE of 3.3%, 6.8%
PLOG/1.000E+00	2.63E+46	-10.92	16810.0/	! fit btw. 500 and 1125 K with MAE of 3.9%, 8.8%
PLOG/1.000E+01	1.11E+31	-5.93	12480.0/	! fit btw. 500 and 1375 K with MAE of 7.9%, 12.7%
PLOG/1.000E+02	1.67E+20	-2.51	8846.0/	! fit btw. 500 and 1650 K with MAE of 10.2%, 18.9%

PLOG/3.947E-02	2.68E+55	-14.53	15760.0/	
PLOG/3.947E-02	0.00E+00	0.00	0.0/	! fit btw. 500 and 900 K with MAE of 3.3%, 6.8%
PLOG/1.000E+00	6.47E+53	-13.11	20520.0/	
PLOG/1.000E+00	2.37E+38	-10.62	1329.0/	! fit btw. 500 and 1125 K with MAE of 1.0%, 2.7%
PLOG/1.000E+01	1.81E+91	-23.60	47000.0/	
PLOG/1.000E+01	8.36E+24	-4.19	9106.0/	! fit btw. 500 and 1375 K with MAE of 0.7%, 1.5%
PLOG/1.000E+02	3.07E+46	-9.95	27540.0/	

PLOG/1.000E+02	2.78E+27	-4.99	9962.0/	! fit btw. 500 and 1650 K with MAE of 1.0%, 1.9%
C₆H₅ + allene → indene + H (P1)				
			1.80E+30	-4.80 37860.0
PLOG/3.947E-02	2.30E+25	-3.89	15160.0/	! fit btw. 500 and 2500 K with MAE of 27.1%, 61.5%
PLOG/1.000E+00	3.50E+28	-4.69	20810.0/	! fit btw. 500 and 2500 K with MAE of 9.7%, 24.4%
PLOG/1.000E+01	7.27E+35	-6.59	31680.0/	! fit btw. 500 and 2500 K with MAE of 7.9%, 24.4%
PLOG/1.000E+02	1.80E+30	-4.80	37860.0/	! fit btw. 500 and 2500 K with MAE of 35.9%, 102.0%
PLOG/3.947E-02	4.03E+45	-9.49	31080.0/	
PLOG/3.947E-02	2.67E+69	-18.16	27450.0/	! fit btw. 500 and 2500 K with MAE of 5.2%, 10.2%
PLOG/1.000E+00	4.21E+68	-15.58	60540.0/	
PLOG/1.000E+00	5.43E+32	-6.02	22160.0/	! fit btw. 500 and 2500 K with MAE of 2.8%, 5.9%
PLOG/1.000E+01	1.73E+38	-7.25	33380.0/	
PLOG/1.000E+01	4.79E-27	5.62	-34580.0/	! fit btw. 500 and 2500 K with MAE of 4.2%, 11.2%
PLOG/1.000E+02	1.56E+47	-9.51	50470.0/	
PLOG/1.000E+02	1.32E+70	-18.57	43280.0/	! fit btw. 500 and 2500 K with MAE of 9.2%, 44.9%
C₆H₅ + allene → phenylallene + H (P3)				
			5.06E+09	1.07 21360.0
PLOG/3.947E-02	9.67E+20	-2.29	19920.0/	! fit btw. 500 and 2500 K with MAE of 25.5%, 70.3%
PLOG/1.000E+00	1.24E+16	-0.84	19490.0/	! fit btw. 500 and 2500 K with MAE of 20.9%, 42.9%
PLOG/1.000E+01	5.45E+14	-0.40	21310.0/	! fit btw. 500 and 2500 K with MAE of 16.0%, 38.9%
PLOG/1.000E+02	5.06E+09	1.07	21360.0/	! fit btw. 500 and 2500 K with MAE of 27.4%, 60.9%
PLOG/3.947E-02	6.27E+34	-6.13	30290.0/	
PLOG/3.947E-02	4.51E+100	-28.23	41500.0/	! fit btw. 500 and 2500 K with MAE of 5.9%, 13.0%
PLOG/1.000E+00	3.70E+68	-15.37	63390.0/	
PLOG/1.000E+00	7.26E+13	-0.32	17310.0/	! fit btw. 500 and 2500 K with MAE of 2.3%, 8.2%
PLOG/1.000E+01	3.81E+25	-3.40	29960.0/	
PLOG/1.000E+01	1.66E+15	-1.16	17440.0/	! fit btw. 500 and 2500 K with MAE of 4.2%, 10.5%
PLOG/1.000E+02	2.17E+29	-4.36	36830.0/	
PLOG/1.000E+02	1.00E+06	1.60	15580.0/	! fit btw. 500 and 2500 K with MAE of 2.1%, 5.0%

C₆H₅ + allene → 3-phenylpropyne + H (P4)

1.49E+12 0.66 23170.0

PLOG/3.947E-02	2.92E+21	-2.14	20750.0/	! fit btw. 500 and 2500 K with MAE of 26.8%, 70.1%
PLOG/1.000E+00	1.20E+18	-1.12	20990.0/	! fit btw. 500 and 2500 K with MAE of 21.0%, 43.7%
PLOG/1.000E+01	1.41E+17	-0.80	23050.0/	! fit btw. 500 and 2500 K with MAE of 16.1%, 39.7%
PLOG/1.000E+02	1.49E+12	0.66	23170.0/	! fit btw. 500 and 2500 K with MAE of 27.6%, 61.3%

PLOG/3.947E-02	6.12E+36	-6.40	32330.0/	
PLOG/3.947E-02	1.02E+91	-24.80	39400.0/	! fit btw. 500 and 2500 K with MAE of 5.3%, 11.2%
PLOG/1.000E+00	3.14E+70	-15.63	65030.0/	
PLOG/1.000E+00	1.12E+16	-0.66	18920.0/	! fit btw. 500 and 2500 K with MAE of 2.3%, 8.2%
PLOG/1.000E+01	1.30E+29	-4.11	32700.0/	
PLOG/1.000E+01	3.48E+16	-1.15	19210.0/	! fit btw. 500 and 2500 K with MAE of 4.5%, 9.4%
PLOG/1.000E+02	7.88E+31	-4.80	38710.0/	
PLOG/1.000E+02	3.64E+08	1.16	17410.0/	! fit btw. 500 and 2500 K with MAE of 2.1%, 4.6%

C₆H₅ + allene → phenylacetylene + CH₃ (P5)

2.29E+17 -0.54 40540.0

PLOG/3.947E-02	3.51E+38	-7.08	31620.0/	! fit btw. 500 and 2500 K with MAE of 16.1%, 42.6%
PLOG/1.000E+00	3.37E+34	-5.73	36180.0/	! fit btw. 500 and 2500 K with MAE of 30.1%, 57.6%
PLOG/1.000E+01	1.10E+28	-3.72	38890.0/	! fit btw. 500 and 2500 K with MAE of 33.6%, 86.1%
PLOG/1.000E+02	2.29E+17	-0.54	40540.0/	! fit btw. 500 and 2500 K with MAE of 46.5%, 126.6%

PLOG/3.947E-02	1.02E+45	-8.88	36360.0/	
PLOG/3.947E-02	4.98E+182	-53.81	72770.0/	! fit btw. 500 and 2500 K with MAE of 7.5%, 17.6%
PLOG/1.000E+00	2.22E+69	-15.43	63210.0/	
PLOG/1.000E+00	3.02E+25	-3.37	29510.0/	! fit btw. 500 and 2500 K with MAE of 3.2%, 8.8%
PLOG/1.000E+01	2.56E+57	-11.84	62600.0/	
PLOG/1.000E+01	1.49E+26	-3.62	34650.0/	! fit btw. 500 and 2500 K with MAE of 6.9%, 16.8%
PLOG/1.000E+02	-3.97E+47	-9.63	52720.0/	
PLOG/1.000E+02	1.57E+26	-3.12	43380.0/	! fit btw. 500 and 2500 K with MAE of 17.5%, 53.1%

C₆H₅ + allene → total

5.55E+10 0.74 5983.0

PLOG/3.947E-02	3.28E+12	0.16	6387.0/	! fit btw. 500 and 2500 K with MAE of 4.4%, 9.2%
PLOG/1.000E+00	2.54E+13	-0.09	6965.0/	! fit btw. 500 and 2500 K with MAE of 8.0%, 13.5%
PLOG/1.000E+01	3.78E+13	-0.11	7226.0/	! fit btw. 500 and 2500 K with MAE of 12.5%, 19.6%
PLOG/1.000E+02	5.55E+10	0.74	5983.0/	! fit btw. 500 and 2500 K with MAE of 11.7%, 33.4%

PLOG/3.947E-02	3.56E+32	-5.63	21210.0/	
PLOG/3.947E-02	4.65E+09	0.93	4522.0/	! fit btw. 500 and 2500 K with MAE of 0.1%, 0.2%
PLOG/1.000E+00	3.83E+57	-12.62	40190.0/	
PLOG/1.000E+00	4.50E+10	0.66	5143.0/	! fit btw. 500 and 2500 K with MAE of 0.9%, 2.4%
PLOG/1.000E+01	1.15E+50	-10.26	38190.0/	
PLOG/1.000E+01	1.87E+12	0.17	5823.0/	! fit btw. 500 and 2500 K with MAE of 2.3%, 7.6%
PLOG/1.000E+02	3.11E+27	-3.83	21540.0/	
PLOG/1.000E+02	2.41E+20	-2.40	8504.0/	! fit btw. 500 and 2500 K with MAE of 3.1%, 7.3%

benzyl + C₂H₂ → C₉H₉ (W18) 4.40E+27 -4.54 25630.0

PLOG/3.947E-02	1.35E+44	-11.67	17270.0/	! fit btw. 500 and 800 K with MAE of 4.5%, 7.7%
PLOG/1.000E+00	2.01E+44	-10.50	23370.0/	! fit btw. 500 and 1000 K with MAE of 16.9%, 37.3%
PLOG/1.000E+01	3.08E+54	-13.00	32670.0/	! fit btw. 500 and 1125 K with MAE of 4.9%, 10.0%
PLOG/1.000E+02	4.40E+27	-4.54	25630.0/	! fit btw. 500 and 1375 K with MAE of 15.9%, 47.8%

PLOG/3.947E-02	1.35E+44	-11.67	17270.0/	
PLOG/3.947E-02	0.00E+00	0.00	0.0/	! fit btw. 500 and 800 K with MAE of 4.5%, 7.7%
PLOG/1.000E+00	2.01E+44	-10.50	23370.0/	
PLOG/1.000E+00	0.00E+00	0.00	0.0/	! fit btw. 500 and 1000 K with MAE of 16.9%, 37.3%
PLOG/1.000E+01	1.22E+58	-14.06	34460.0/	
PLOG/1.000E+01	5.06E+38	-16.57	-23690.0/	! fit btw. 500 and 1125 K with MAE of 4.1%, 10.5%
PLOG/1.000E+02	1.29E+55	-12.74	38780.0/	
PLOG/1.000E+02	1.12E-104	34.28	-35320.0/	! fit btw. 500 and 1375 K with MAE of 7.2%, 16.0%

benzyl + C₂H₂ → C₉H₉ (W20) 9.51E+23 -3.50 18170.0

PLOG/3.947E-02	2.31E+08	0.00	7226.0/	! fit btw. 500 and 700 K with MAE of 14.8%, 24.0%
PLOG/1.000E+00	1.13E+45	-10.73	22220.0/	! fit btw. 500 and 800 K with MAE of 0.3%, 0.5%

PLOG/1.000E+01	5.46E+34	-7.04	20920.0/	! fit btw. 500 and 1000 K with MAE of 2.5%, 4.3%
PLOG/1.000E+02	9.51E+23	-3.50	18170.0/	! fit btw. 500 and 1250 K with MAE of 5.9%, 9.4%
PLOG/3.947E-02	2.31E+08	0.00	7226.0/	
PLOG/3.947E-02	0.00E+00	0.00	0.0/	! fit btw. 500 and 700 K with MAE of 14.8%, 24.0%
PLOG/1.000E+00	1.13E+45	-10.73	22220.0/	
PLOG/1.000E+00	0.00E+00	0.00	0.0/	! fit btw. 500 and 800 K with MAE of 0.3%, 0.5%
PLOG/1.000E+01	5.46E+34	-7.04	20920.0/	
PLOG/1.000E+01	0.00E+00	0.00	0.0/	! fit btw. 500 and 1000 K with MAE of 2.5%, 4.3%
PLOG/1.000E+02	3.04E+54	-12.32	37160.0/	
PLOG/1.000E+02	1.93E+32	-6.31	19770.0/	! fit btw. 500 and 1250 K with MAE of 0.4%, 0.8%
benzyl + C₂H₂ → C₉H₉ (W21)			1.90E+18	-1.52 22800.0
PLOG/3.947E-02	1.68E+08	0.00	6765.0/	! fit btw. 500 and 600 K with MAE of 0.0%, 0.0%
PLOG/1.000E+00	1.63E+26	-4.53	18620.0/	! fit btw. 500 and 900 K with MAE of 8.3%, 18.2%
PLOG/1.000E+01	4.81E+25	-3.91	22740.0/	! fit btw. 500 and 1125 K with MAE of 8.0%, 23.6%
PLOG/1.000E+02	1.90E+18	-1.52	22800.0/	! fit btw. 500 and 1500 K with MAE of 13.7%, 33.3%
PLOG/3.947E-02	1.68E+08	0.00	6765.0/	
PLOG/3.947E-02	0.00E+00	0.00	0.0/	! fit btw. 500 and 600 K with MAE of 0.0%, 0.0%
PLOG/1.000E+00	1.63E+26	-4.53	18620.0/	
PLOG/1.000E+00	0.00E+00	0.00	0.0/	! fit btw. 500 and 900 K with MAE of 8.3%, 18.2%
PLOG/1.000E+01	6.23E+35	-7.01	26770.0/	
PLOG/1.000E+01	1.01E+32	4.16	183900.0/	! fit btw. 500 and 1125 K with MAE of 3.3%, 7.3%
PLOG/1.000E+02	1.96E+26	-3.84	27640.0/	
PLOG/1.000E+02	1.03E+14	-1.22	15320.0/	! fit btw. 500 and 1500 K with MAE of 9.7%, 34.4%
benzyl + C₂H₂ → C₉H₉ (W22)			4.98E+30	-5.38 33490.0
PLOG/3.947E-02	7.48E+87	-24.39	37360.0/	! fit btw. 500 and 1125 K with MAE of 3.7%, 7.9%
PLOG/1.000E+00	1.69E+77	-19.96	42020.0/	! fit btw. 500 and 1250 K with MAE of 10.6%, 24.4%
PLOG/1.000E+01	1.03E+58	-13.62	40850.0/	! fit btw. 500 and 1500 K with MAE of 16.7%, 40.6%
PLOG/1.000E+02	4.98E+30	-5.38	33490.0/	! fit btw. 500 and 1800 K with MAE of 60.8%, 430.5%

PLOG/3.947E-02	2.64E+96	-26.92	41750.0/	
PLOG/3.947E-02	1.17E+82	-23.99	27470.0/	! fit btw. 500 and 1125 K with MAE of 1.0%, 2.4%
PLOG/1.000E+00	8.97E+150	-41.33	86580.0/	
PLOG/1.000E+00	1.99E+86	-22.94	44280.0/	! fit btw. 500 and 1250 K with MAE of 5.0%, 11.7%
PLOG/1.000E+01	2.78E+84	-21.18	58100.0/	
PLOG/1.000E+01	4.34E+63	-15.71	40630.0/	! fit btw. 500 and 1500 K with MAE of 13.2%, 37.3%
PLOG/1.000E+02	3.41E+29	-3.82	66230.0/	
PLOG/1.000E+02	9.37E+33	-6.39	34700.0/	! fit btw. 500 and 1800 K with MAE of 55.9%, 346.7%

PLOG/1.000E+00	2.24E+36	-6.98	27250.0/	
PLOG/1.000E+00	1.08E+55	-11.29	72720.0/	! fit btw. 500 and 2500 K with MAE of 1.0%, 3.7%
PLOG/1.000E+01	6.32E+194	-47.77	254800.0/	
PLOG/1.000E+01	1.85E+42	-8.50	34890.0/	! fit btw. 500 and 2500 K with MAE of 4.9%, 14.6%
PLOG/1.000E+02	5.70E+44	-8.96	43510.0/	
PLOG/1.000E+02	7.19E+175	-52.00	76360.0/	! fit btw. 500 and 2500 K with MAE of 5.6%, 15.5%

benzyl + C₂H₂ → 3-phenylpropyne + H (P4)

2.67E+21 -2.02 38860.0

PLOG/3.947E-02	3.36E+16	-0.81	30440.0/	! fit btw. 500 and 2500 K with MAE of 3.8%, 6.7%
PLOG/1.000E+00	1.04E+19	-1.48	32980.0/	! fit btw. 500 and 2500 K with MAE of 5.0%, 9.3%
PLOG/1.000E+01	1.67E+21	-2.05	35990.0/	! fit btw. 500 and 2500 K with MAE of 6.0%, 11.3%
PLOG/1.000E+02	2.67E+21	-2.02	38860.0/	! fit btw. 500 and 2500 K with MAE of 10.6%, 27.6%

PLOG/3.947E-02	3.69E+42	-8.50	46080.0/	
PLOG/3.947E-02	1.18E+12	0.44	27940.0/	! fit btw. 500 and 2500 K with MAE of 1.1%, 1.9%
PLOG/1.000E+00	6.19E+42	-8.50	46840.0/	
PLOG/1.000E+00	1.98E+12	0.41	29280.0/	! fit btw. 500 and 2500 K with MAE of 0.2%, 0.6%
PLOG/1.000E+01	3.01E+37	-6.78	46170.0/	
PLOG/1.000E+01	5.19E+10	0.87	29940.0/	! fit btw. 500 and 2500 K with MAE of 0.8%, 2.0%
PLOG/1.000E+02	2.34E+26	-3.40	42490.0/	
PLOG/1.000E+02	1.91E+161	-47.33	79190.0/	! fit btw. 500 and 2500 K with MAE of 2.2%, 5.5%

benzyl + C₂H₂ → total

4.50E+16 -1.25 15200.0

PLOG/3.947E-02	4.34E+12	-0.12	12920.0/	! fit btw. 500 and 2500 K with MAE of 13.7%, 28.8%
PLOG/1.000E+00	6.03E+12	-0.16	12980.0/	! fit btw. 500 and 2500 K with MAE of 14.0%, 29.2%
PLOG/1.000E+01	4.75E+13	-0.41	13450.0/	! fit btw. 500 and 2500 K with MAE of 16.0%, 31.3%
PLOG/1.000E+02	4.50E+16	-1.25	15200.0/	! fit btw. 500 and 2500 K with MAE of 16.5%, 43.9%

PLOG/3.947E-02	1.25E+20	-2.32	16530.0/	
PLOG/3.947E-02	4.19E+46	-8.54	74410.0/	! fit btw. 500 and 2500 K with MAE of 1.9%, 4.8%
PLOG/1.000E+00	3.16E+20	-2.44	16710.0/	
PLOG/1.000E+00	1.37E+44	-7.89	71030.0/	! fit btw. 500 and 2500 K with MAE of 1.8%, 5.1%

PLOG/1.000E+01	2.02E+22	-2.97	17620.0/	
PLOG/1.000E+01	4.27E+47	-8.84	74040.0/	! fit btw. 500 and 2500 K with MAE of 3.2%, 7.5%
PLOG/1.000E+02	2.96E+23	-3.26	18550.0/	
PLOG/1.000E+02	1.45E+147	-34.88	200800.0/	! fit btw. 500 and 2500 K with MAE of 7.0%, 15.1%

1-phenylpropyne + H → C₉H₉ (W1) 1.65E+22 -2.57 9984.0

PLOG/3.947E-02	3.56E+61	-14.97	23380.0/	! fit btw. 500 and 1125 K with MAE of 9.3%, 16.5%
PLOG/1.000E+00	2.08E+45	-9.73	18670.0/	! fit btw. 500 and 1375 K with MAE of 15.0%, 25.5%
PLOG/1.000E+01	1.31E+32	-5.62	13850.0/	! fit btw. 500 and 1500 K with MAE of 14.0%, 29.4%
PLOG/1.000E+02	1.65E+22	-2.57	9984.0/	! fit btw. 500 and 1650 K with MAE of 11.2%, 28.2%

PLOG/3.947E-02	3.75E+92	-24.10	40150.0/	
PLOG/3.947E-02	6.39E+61	-15.62	20010.0/	! fit btw. 500 and 1125 K with MAE of 0.7%, 1.3%
PLOG/1.000E+00	3.03E+90	-22.77	46360.0/	
PLOG/1.000E+00	7.44E+50	-11.80	18420.0/	! fit btw. 500 and 1375 K with MAE of 1.1%, 2.1%
PLOG/1.000E+01	4.27E+74	-17.77	41800.0/	
PLOG/1.000E+01	4.79E+42	-9.17	15950.0/	! fit btw. 500 and 1500 K with MAE of 2.1%, 3.2%
PLOG/1.000E+02	1.32E+66	-15.00	41520.0/	
PLOG/1.000E+02	6.17E+27	-4.44	11100.0/	! fit btw. 500 and 1650 K with MAE of 2.2%, 4.1%

1-phenylpropyne + H → C₉H₉ (W5) 1.59E+29 -4.61 11070.0

PLOG/3.947E-02	6.14E+74	-19.09	25870.0/	! fit btw. 500 and 1125 K with MAE of 8.5%, 16.4%
PLOG/1.000E+00	2.23E+52	-11.88	19100.0/	! fit btw. 500 and 1250 K with MAE of 12.9%, 20.7%
PLOG/1.000E+01	2.62E+37	-7.19	13900.0/	! fit btw. 500 and 1375 K with MAE of 13.6%, 24.3%
PLOG/1.000E+02	1.59E+29	-4.61	11070.0/	! fit btw. 500 and 1650 K with MAE of 14.9%, 34.5%

PLOG/3.947E-02	6.37E+97	-25.88	38050.0/	
PLOG/3.947E-02	2.26E+70	-18.51	19450.0/	! fit btw. 500 and 1125 K with MAE of 0.7%, 1.5%
PLOG/1.000E+00	2.19E+96	-24.69	44600.0/	
PLOG/1.000E+00	6.91E+59	-14.62	19230.0/	! fit btw. 500 and 1250 K with MAE of 0.5%, 0.9%
PLOG/1.000E+01	7.91E+84	-20.88	43420.0/	
PLOG/1.000E+01	6.53E+43	-9.46	14390.0/	! fit btw. 500 and 1375 K with MAE of 1.3%, 2.3%

PLOG/1.000E+02 1.58E+69 -15.95 38960.0/
PLOG/1.000E+02 6.87E+37 -7.52 12680.0/

! fit btw. 500 and 1650 K with MAE of 2.4%, 4.3%

1-phenylpropyne + H → C₆H₅ + propyne (R1)

1.58E+27 -3.18 34730.0

PLOG/3.947E-02 3.22E+32 -5.05 26790.0/
PLOG/1.000E+00 1.51E+39 -6.81 34580.0/
PLOG/1.000E+01 9.46E+36 -6.06 36780.0/
PLOG/1.000E+02 1.58E+27 -3.18 34730.0/

! fit btw. 500 and 2500 K with MAE of 12.5%, 20.7%
! fit btw. 500 and 2500 K with MAE of 12.4%, 28.4%
! fit btw. 500 and 2500 K with MAE of 23.2%, 64.5%
! fit btw. 500 and 2500 K with MAE of 40.0%, 84.6%

PLOG/3.947E-02 7.30E+44 -8.75 32420.0/
PLOG/3.947E-02 8.23E+40 -7.03 45570.0/
PLOG/1.000E+00 1.66E+79 -18.46 58270.0/
PLOG/1.000E+00 9.05E+27 -3.64 28320.0/
PLOG/1.000E+01 1.36E+48 -9.17 45060.0/
PLOG/1.000E+01 2.69E+138 -39.11 64390.0/
PLOG/1.000E+02 1.85E+50 -9.57 52670.0/
PLOG/1.000E+02 1.05E+42 -8.60 34460.0/

! fit btw. 500 and 2500 K with MAE of 1.5%, 6.1%

! fit btw. 500 and 2500 K with MAE of 1.7%, 4.0%

! fit btw. 500 and 2500 K with MAE of 5.9%, 13.8%

! fit btw. 500 and 2500 K with MAE of 6.1%, 12.2%

1-phenylpropyne + H → phenylallene + H (P3)

2.71E+21 -1.75 29260.0

PLOG/3.947E-02 1.49E+30 -4.59 23200.0/
PLOG/1.000E+00 3.35E+35 -5.96 30470.0/
PLOG/1.000E+01 1.72E+32 -4.91 32060.0/
PLOG/1.000E+02 2.71E+21 -1.75 29260.0/

! fit btw. 500 and 2500 K with MAE of 18.5%, 32.9%
! fit btw. 500 and 2500 K with MAE of 16.0%, 32.3%
! fit btw. 500 and 2500 K with MAE of 23.9%, 66.3%
! fit btw. 500 and 2500 K with MAE of 39.1%, 84.0%

PLOG/3.947E-02 9.94E+44 -9.01 30090.0/
PLOG/3.947E-02 6.00E+29 -4.11 35990.0/
PLOG/1.000E+00 2.47E+74 -17.26 53280.0/
PLOG/1.000E+00 1.52E+20 -1.63 21930.0/
PLOG/1.000E+01 8.80E+42 -7.89 39970.0/
PLOG/1.000E+01 1.36E+181 -52.95 75590.0/
PLOG/1.000E+02 1.67E+44 -8.06 46950.0/
PLOG/1.000E+02 4.27E+35 -6.97 28750.0/

! fit btw. 500 and 2500 K with MAE of 2.6%, 9.6%

! fit btw. 500 and 2500 K with MAE of 0.9%, 2.2%

! fit btw. 500 and 2500 K with MAE of 8.0%, 19.7%

! fit btw. 500 and 2500 K with MAE of 5.9%, 12.0%

1-phenylpropyne + H → phenylacetylene + CH₃ (P5)

2.58E+28 -3.55 27980.0

PLOG/3.947E-02	8.52E+32	-5.26	19280.0/	! fit btw. 500 and 2500 K with MAE of 13.4%, 26.7%
PLOG/1.000E+00	3.94E+40	-7.31	27510.0/	! fit btw. 500 and 2500 K with MAE of 11.3%, 22.7%
PLOG/1.000E+01	2.02E+40	-7.11	30740.0/	! fit btw. 500 and 2500 K with MAE of 18.4%, 52.9%
PLOG/1.000E+02	7.57E+31	-4.61	29420.0/	! fit btw. 500 and 2500 K with MAE of 35.2%, 80.1%

PLOG/3.947E-02	2.22E+62	-14.16	32590.0/	
PLOG/3.947E-02	3.83E+20	-1.64	14340.0/	! fit btw. 500 and 2500 K with MAE of 1.1%, 1.8%
PLOG/1.000E+00	3.95E+42	-7.88	28610.0/	
PLOG/1.000E+00	3.89E+88	-19.28	108800.0/	! fit btw. 500 and 2500 K with MAE of 6.3%, 22.8%
PLOG/1.000E+01	2.67E+41	-7.32	32780.0/	
PLOG/1.000E+01	1.42E+171	-50.11	64410.0/	! fit btw. 500 and 2500 K with MAE of 8.9%, 19.8%
PLOG/1.000E+02	8.00E+59	-12.37	51330.0/	
PLOG/1.000E+02	3.30E+13	0.47	18100.0/	! fit btw. 500 and 2500 K with MAE of 2.5%, 5.0%

1-phenylpropyne + H → total

4.01E+11 0.77 3751.0

PLOG/3.947E-02	1.46E+10	1.17	2932.0/	! fit btw. 500 and 2500 K with MAE of 1.0%, 2.4%
PLOG/1.000E+00	4.65E+10	1.03	3193.0/	! fit btw. 500 and 2500 K with MAE of 1.7%, 3.0%
PLOG/1.000E+01	1.42E+11	0.89	3471.0/	! fit btw. 500 and 2500 K with MAE of 1.6%, 3.1%
PLOG/1.000E+02	4.01E+11	0.77	3751.0/	! fit btw. 500 and 2500 K with MAE of 1.4%, 4.0%

PLOG/3.947E-02	9.40E+15	-0.35	13200.0/	
PLOG/3.947E-02	2.84E+14	-0.15	4578.0/	! fit btw. 500 and 2500 K with MAE of 0.2%, 0.4%
PLOG/1.000E+00	3.04E+12	0.48	4013.0/	
PLOG/1.000E+00	3.33E+34	-5.27	38480.0/	! fit btw. 500 and 2500 K with MAE of 0.4%, 1.0%
PLOG/1.000E+01	3.77E+45	-9.54	22070.0/	
PLOG/1.000E+01	8.52E+09	1.24	2841.0/	! fit btw. 500 and 2500 K with MAE of 0.4%, 0.8%
PLOG/1.000E+02	8.96E+44	-9.17	24360.0/	
PLOG/1.000E+02	2.55E+10	1.10	3074.0/	! fit btw. 500 and 2500 K with MAE of 0.7%, 2.5%

phenylallene + H → C₉H₉ (W1)

1.93E+22 -2.54 8197.0

PLOG/3.947E-02	9.78E+63	-15.71	22300.0/	! fit btw. 500 and 1125 K with MAE of 9.5%, 17.1%
PLOG/1.000E+00	1.08E+47	-10.22	17460.0/	! fit btw. 500 and 1375 K with MAE of 15.7%, 26.6%
PLOG/1.000E+01	1.02E+33	-5.85	12370.0/	! fit btw. 500 and 1500 K with MAE of 15.0%, 31.3%
PLOG/1.000E+02	1.93E+22	-2.54	8197.0/	! fit btw. 500 and 1650 K with MAE of 12.2%, 30.7%
PLOG/3.947E-02	4.70E+94	-24.74	38820.0/	
PLOG/3.947E-02	3.68E+63	-16.16	18520.0/	! fit btw. 500 and 1125 K with MAE of 0.7%, 1.4%
PLOG/1.000E+00	6.19E+92	-23.44	45390.0/	
PLOG/1.000E+00	1.73E+52	-12.20	16950.0/	! fit btw. 500 and 1375 K with MAE of 1.1%, 2.3%
PLOG/1.000E+01	1.64E+82	-19.93	44570.0/	
PLOG/1.000E+01	3.35E+38	-7.81	12730.0/	! fit btw. 500 and 1500 K with MAE of 2.2%, 3.7%
PLOG/1.000E+02	1.08E+68	-15.50	40820.0/	
PLOG/1.000E+02	7.51E+27	-4.43	9239.0/	! fit btw. 500 and 1650 K with MAE of 2.4%, 4.4%
phenylallene + H → C₉H₉ (W6)				
	1.53E+34	-5.83	27070.0	
PLOG/3.947E-02	9.35E+69	-16.91	32700.0/	! fit btw. 500 and 1650 K with MAE of 19.1%, 37.5%
PLOG/1.000E+00	3.06E+54	-11.98	30580.0/	! fit btw. 500 and 1800 K with MAE of 23.0%, 48.5%
PLOG/1.000E+01	4.27E+42	-8.33	28380.0/	! fit btw. 500 and 2000 K with MAE of 32.7%, 80.5%
PLOG/1.000E+02	1.53E+34	-5.83	27070.0/	! fit btw. 500 and 2500 K with MAE of 49.1%, 150.4%
PLOG/3.947E-02	2.70E+103	-26.45	54870.0/	
PLOG/3.947E-02	1.41E+72	-18.02	30540.0/	! fit btw. 500 and 1650 K with MAE of 3.0%, 5.8%
PLOG/1.000E+00	1.56E+85	-20.68	51620.0/	
PLOG/1.000E+00	1.51E+55	-12.70	27360.0/	! fit btw. 500 and 1800 K with MAE of 4.0%, 7.3%
PLOG/1.000E+01	1.79E+77	-18.07	53070.0/	
PLOG/1.000E+01	7.85E+41	-8.68	24040.0/	! fit btw. 500 and 2000 K with MAE of 5.8%, 11.9%
PLOG/1.000E+02	-2.32E+64	-14.79	40020.0/	
PLOG/1.000E+02	2.65E+46	-9.36	31890.0/	! fit btw. 500 and 2500 K with MAE of 17.9%, 57.7%
phenylallene + H → C₉H₉ (W9)				
	4.35E+13	0.12	5322.0	
PLOG/3.947E-02	2.46E+62	-14.39	30040.0/	! fit btw. 800 and 1650 K with MAE of 4.4%, 6.5%
PLOG/1.000E+00	3.74E+31	-5.10	15860.0/	! fit btw. 800 and 2000 K with MAE of 8.0%, 15.5%

PLOG/1.000E+01	3.90E+14	-0.25	4502.0/	! fit btw. 500 and 2500 K with MAE of 26.3%, 65.8%
PLOG/1.000E+02	4.35E+13	0.12	5322.0/	! fit btw. 500 and 2500 K with MAE of 12.6%, 53.4%

PLOG/3.947E-02	-1.15E+87	-21.70	40580.0/	
PLOG/3.947E-02	1.80E+73	-17.56	33610.0/	! fit btw. 800 and 1650 K with MAE of 0.5%, 1.1%
PLOG/1.000E+00	-3.90E+66	-15.11	36320.0/	
PLOG/1.000E+00	1.37E+53	-11.18	28240.0/	! fit btw. 800 and 2000 K with MAE of 1.8%, 3.6%
PLOG/1.000E+01	1.95E+14	-0.25	4502.0/	
PLOG/1.000E+01	1.95E+14	-0.25	4502.0/	! fit btw. 500 and 2500 K with MAE of 26.3%, 65.8%
PLOG/1.000E+02	7.18E+32	-5.71	13530.0/	
PLOG/1.000E+02	7.85E+38	-6.58	34280.0/	! fit btw. 500 and 2500 K with MAE of 10.6%, 45.1%

phenylallene + H → C₉H₉ (W11) 1.33E+25 -3.54 11370.0

PLOG/3.947E-02	5.79E+72	-19.23	23700.0/	! fit btw. 500 and 900 K with MAE of 0.8%, 1.6%
PLOG/1.000E+00	1.53E+51	-11.86	19600.0/	! fit btw. 500 and 1125 K with MAE of 7.0%, 12.5%
PLOG/1.000E+01	1.18E+36	-6.98	15140.0/	! fit btw. 500 and 1375 K with MAE of 11.1%, 18.6%
PLOG/1.000E+02	1.33E+25	-3.54	11370.0/	! fit btw. 500 and 1650 K with MAE of 12.6%, 28.9%

PLOG/3.947E-02	5.79E+72	-19.23	23700.0/	
PLOG/3.947E-02	0.00E+00	0.00	0.0/	! fit btw. 500 and 900 K with MAE of 0.8%, 1.6%
PLOG/1.000E+00	1.49E+80	-20.37	35670.0/	
PLOG/1.000E+00	7.42E+53	-13.12	17940.0/	! fit btw. 500 and 1125 K with MAE of 0.1%, 0.4%
PLOG/1.000E+01	2.14E+72	-17.44	37820.0/	
PLOG/1.000E+01	2.86E+42	-9.27	15520.0/	! fit btw. 500 and 1375 K with MAE of 0.7%, 1.3%
PLOG/1.000E+02	5.68E+63	-14.50	38610.0/	
PLOG/1.000E+02	2.79E+30	-5.39	12020.0/	! fit btw. 500 and 1650 K with MAE of 1.9%, 3.6%

phenylallene + H → C₆H₅ + propyne (R1) 1.38E+27 -3.10 32660.0

PLOG/3.947E-02	1.09E+31	-4.57	23980.0/	! fit btw. 500 and 2500 K with MAE of 13.1%, 23.1%
PLOG/1.000E+00	1.19E+38	-6.43	31930.0/	! fit btw. 500 and 2500 K with MAE of 12.6%, 26.6%
PLOG/1.000E+01	2.55E+36	-5.84	34410.0/	! fit btw. 500 and 2500 K with MAE of 21.5%, 60.4%
PLOG/1.000E+02	1.38E+27	-3.10	32660.0/	! fit btw. 500 and 2500 K with MAE of 38.6%, 83.0%

PLOG/3.947E-02	3.18E+45	-8.91	30480.0/	
PLOG/3.947E-02	5.25E+35	-5.58	37420.0/	! fit btw. 500 and 2500 K with MAE of 1.3%, 5.5%
PLOG/1.000E+00	6.33E+82	-19.49	57860.0/	
PLOG/1.000E+00	9.33E+27	-3.57	26350.0/	! fit btw. 500 and 2500 K with MAE of 1.4%, 3.8%
PLOG/1.000E+01	1.95E+46	-8.59	41710.0/	
PLOG/1.000E+01	4.58E+184	-53.69	77710.0/	! fit btw. 500 and 2500 K with MAE of 6.3%, 14.6%
PLOG/1.000E+02	6.94E+49	-9.39	50300.0/	
PLOG/1.000E+02	1.05E+41	-8.22	32090.0/	! fit btw. 500 and 2500 K with MAE of 5.4%, 9.3%

phenylallene + H → indene + H (P1)

2.56E+09 1.49 22490.0

PLOG/3.947E-02	2.60E+26	-3.41	18270.0/	! fit btw. 500 and 2500 K with MAE of 26.5%, 52.9%
PLOG/1.000E+00	9.06E+18	-1.21	18380.0/	! fit btw. 500 and 2500 K with MAE of 12.5%, 45.5%
PLOG/1.000E+01	1.19E+20	-1.52	23520.0/	! fit btw. 500 and 2500 K with MAE of 13.4%, 44.2%
PLOG/1.000E+02	2.56E+09	1.49	22490.0/	! fit btw. 500 and 2500 K with MAE of 37.1%, 101.3%

PLOG/3.947E-02	1.07E+57	-11.91	42680.0/	
PLOG/3.947E-02	2.67E+20	-1.93	13200.0/	! fit btw. 500 and 2500 K with MAE of 0.9%, 2.3%
PLOG/1.000E+00	1.06E+76	-16.67	74870.0/	
PLOG/1.000E+00	2.16E+24	-2.89	20290.0/	! fit btw. 500 and 2500 K with MAE of 3.9%, 11.7%
PLOG/1.000E+01	3.67E+24	-2.77	26750.0/	
PLOG/1.000E+01	7.19E+72	-21.59	20380.0/	! fit btw. 500 and 2500 K with MAE of 6.5%, 14.6%
PLOG/1.000E+02	6.43E+30	-4.46	38740.0/	
PLOG/1.000E+02	1.26E+36	-7.83	25310.0/	! fit btw. 500 and 2500 K with MAE of 7.3%, 23.4%

phenylallene + H → 1-phenylpropyne + H (P2)

3.43E+23 -2.28 27220.0

PLOG/3.947E-02	1.88E+32	-5.12	21160.0/	! fit btw. 500 and 2500 K with MAE of 19.2%, 34.0%
PLOG/1.000E+00	4.24E+37	-6.49	28430.0/	! fit btw. 500 and 2500 K with MAE of 16.3%, 31.8%
PLOG/1.000E+01	2.17E+34	-5.44	30030.0/	! fit btw. 500 and 2500 K with MAE of 23.4%, 64.7%
PLOG/1.000E+02	3.43E+23	-2.28	27220.0/	! fit btw. 500 and 2500 K with MAE of 38.3%, 82.2%

PLOG/3.947E-02	5.24E+47	-9.73	28340.0/	
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PLOG/3.947E-02 2.42E+30 -4.24 32290.0/
PLOG/1.000E+00 1.41E+74 -17.12 49750.0/
PLOG/1.000E+00 1.70E+21 -1.87 19340.0/
PLOG/1.000E+01 4.99E+44 -8.33 37680.0/
PLOG/1.000E+01 4.65E+181 -53.01 72970.0/
PLOG/1.000E+02 1.33E+46 -8.54 44770.0/
PLOG/1.000E+02 2.00E+37 -7.36 26640.0/

! fit btw. 500 and 2500 K with MAE of 2.6%, 9.4%

! fit btw. 500 and 2500 K with MAE of 1.1%, 2.5%

! fit btw. 500 and 2500 K with MAE of 8.2%, 20.2%

! fit btw. 500 and 2500 K with MAE of 5.7%, 11.6%

phenylallene + H → 3-phenylpropyne + H (P4)

2.30E+24 -2.46 30970.0

PLOG/3.947E-02 8.10E+21 -2.04 20950.0/
PLOG/1.000E+00 1.50E+27 -3.46 26220.0/
PLOG/1.000E+01 9.64E+29 -4.16 30770.0/
PLOG/1.000E+02 2.30E+24 -2.46 30970.0/

! fit btw. 500 and 2500 K with MAE of 7.6%, 16.8%

! fit btw. 500 and 2500 K with MAE of 4.2%, 10.9%

! fit btw. 500 and 2500 K with MAE of 13.3%, 37.1%

! fit btw. 500 and 2500 K with MAE of 30.9%, 70.6%

PLOG/3.947E-02 2.74E+25 -3.02 23580.0/
PLOG/3.947E-02 3.46E+175 -51.33 68500.0/
PLOG/1.000E+00 4.36E+35 -5.93 31260.0/
PLOG/1.000E+00 6.54E+10 1.06 17150.0/
PLOG/1.000E+01 5.01E+35 -5.76 34960.0/
PLOG/1.000E+01 2.29E+172 -50.42 70850.0/
PLOG/1.000E+02 1.05E+54 -10.75 53440.0/
PLOG/1.000E+02 4.06E+11 0.92 22070.0/

! fit btw. 500 and 2500 K with MAE of 3.5%, 8.0%

! fit btw. 500 and 2500 K with MAE of 0.6%, 1.4%

! fit btw. 500 and 2500 K with MAE of 5.1%, 12.4%

! fit btw. 500 and 2500 K with MAE of 2.3%, 5.1%

phenylallene + H → phenylacetylene + CH₃ (P5)

2.08E+41 -7.31 44540.0

PLOG/3.947E-02 1.41E+41 -7.83 25570.0/
PLOG/1.000E+00 1.73E+52 -10.77 38250.0/
PLOG/1.000E+01 1.45E+53 -10.84 44840.0/
PLOG/1.000E+02 2.08E+41 -7.31 44540.0/

! fit btw. 500 and 2500 K with MAE of 25.8%, 45.2%

! fit btw. 500 and 2500 K with MAE of 23.4%, 46.9%

! fit btw. 500 and 2500 K with MAE of 25.1%, 60.2%

! fit btw. 500 and 2500 K with MAE of 48.5%, 135.6%

PLOG/3.947E-02 9.51E+60 -13.74 34820.0/
PLOG/3.947E-02 7.03E+28 -4.11 27090.0/
PLOG/1.000E+00 5.32E+62 -13.87 43370.0/

! fit btw. 500 and 2500 K with MAE of 1.9%, 6.0%

PLOG/1.000E+00	4.85E+110	-25.41	135800.0/	! fit btw. 500 and 2500 K with MAE of 8.1%, 28.5%
PLOG/1.000E+01	5.74E+59	-12.69	49620.0/	
PLOG/1.000E+01	4.05E+148	-43.12	63700.0/	! fit btw. 500 and 2500 K with MAE of 15.0%, 33.8%
PLOG/1.000E+02	-3.26E+78	-18.59	59270.0/	
PLOG/1.000E+02	4.44E+47	-9.18	46030.0/	! fit btw. 500 and 2500 K with MAE of 16.3%, 39.8%

phenylallene + H → total 2.07E+10 1.18 3101.0

PLOG/3.947E-02	2.66E+11	0.83	3481.0/	! fit btw. 500 and 2500 K with MAE of 1.8%, 3.0%
PLOG/1.000E+00	5.67E+11	0.74	3701.0/	! fit btw. 500 and 2500 K with MAE of 2.7%, 5.0%
PLOG/1.000E+01	1.33E+11	0.93	3453.0/	! fit btw. 500 and 2500 K with MAE of 2.2%, 6.7%
PLOG/1.000E+02	2.07E+10	1.18	3101.0/	! fit btw. 500 and 2500 K with MAE of 1.2%, 3.0%

PLOG/3.947E-02	3.46E+53	-11.11	39680.0/	
PLOG/3.947E-02	1.57E+11	0.88	3273.0/	! fit btw. 500 and 2500 K with MAE of 0.1%, 0.5%
PLOG/1.000E+00	1.53E+20	-1.60	13710.0/	
PLOG/1.000E+00	2.15E+13	0.20	3962.0/	! fit btw. 500 and 2500 K with MAE of 0.7%, 2.0%
PLOG/1.000E+01	3.14E+19	-1.38	13860.0/	
PLOG/1.000E+01	1.26E+13	0.28	3931.0/	! fit btw. 500 and 2500 K with MAE of 0.9%, 1.7%
PLOG/1.000E+02	1.67E+13	0.30	7083.0/	
PLOG/1.000E+02	2.78E+10	1.06	2748.0/	! fit btw. 500 and 2500 K with MAE of 0.4%, 1.2%

3-phenylpropyne + H → C₉H₉ (W6) 1.73E+36 -6.21 24770.0

PLOG/3.947E-02	1.53E+61	-14.20	25020.0/	! fit btw. 500 and 1650 K with MAE of 21.0%, 45.7%
PLOG/1.000E+00	5.81E+53	-11.60	26600.0/	! fit btw. 500 and 1800 K with MAE of 19.5%, 43.4%
PLOG/1.000E+01	2.35E+44	-8.65	25780.0/	! fit btw. 500 and 2000 K with MAE of 29.9%, 72.2%
PLOG/1.000E+02	1.73E+36	-6.21	24770.0/	! fit btw. 500 and 2500 K with MAE of 47.3%, 140.9%

PLOG/3.947E-02	6.89E+110	-28.33	58570.0/	
PLOG/3.947E-02	2.87E+64	-15.52	24120.0/	! fit btw. 500 and 1650 K with MAE of 2.6%, 5.6%
PLOG/1.000E+00	1.47E+25	-2.88	14760.0/	
PLOG/1.000E+00	-2.26E+44	-8.05	34330.0/	! fit btw. 500 and 1800 K with MAE of 2.7%, 8.4%
PLOG/1.000E+01	2.66E+76	-17.67	48690.0/	

PLOG/1.000E+01	8.97E+43	-9.08	21710.0/	! fit btw. 500 and 2000 K with MAE of 5.4%, 12.6%
PLOG/1.000E+02	7.02E+59	-12.75	43270.0/	
PLOG/1.000E+02	2.30E+52	-12.04	24920.0/	! fit btw. 500 and 2500 K with MAE of 11.6%, 47.8%

3-phenylpropyne + H → C₉H₉ (W11) 2.52E+28 -4.26 10400.0

PLOG/3.947E-02	1.63E+76	-20.14	22130.0/	! fit btw. 500 and 900 K with MAE of 0.6%, 1.1%
PLOG/1.000E+00	1.14E+56	-13.10	19000.0/	! fit btw. 500 and 1125 K with MAE of 6.5%, 11.8%
PLOG/1.000E+01	1.34E+40	-7.95	14420.0/	! fit btw. 500 and 1375 K with MAE of 10.9%, 18.0%
PLOG/1.000E+02	2.52E+28	-4.26	10400.0/	! fit btw. 500 and 1650 K with MAE of 12.5%, 28.1%

PLOG/3.947E-02	1.63E+76	-20.14	22130.0/	
PLOG/3.947E-02	0.00E+00	0.00	0.0/	! fit btw. 500 and 900 K with MAE of 0.6%, 1.1%
PLOG/1.000E+00	3.47E+73	-18.25	28320.0/	
PLOG/1.000E+00	2.50E+51	-12.45	12660.0/	! fit btw. 500 and 1125 K with MAE of 0.8%, 1.4%
PLOG/1.000E+01	8.36E+74	-17.98	36160.0/	
PLOG/1.000E+01	2.71E+46	-10.22	14700.0/	! fit btw. 500 and 1375 K with MAE of 0.6%, 1.1%
PLOG/1.000E+02	1.39E+66	-14.96	36990.0/	
PLOG/1.000E+02	3.80E+33	-6.06	10970.0/	! fit btw. 500 and 1650 K with MAE of 1.8%, 3.4%

3-phenylpropyne + H → C₉H₉ (W20) 6.70E+35 -6.83 14290.0

PLOG/3.947E-02	1.57E+10	0.00	3317.0/	! fit btw. 500 and 700 K with MAE of 38.8%, 70.0%
PLOG/1.000E+00	1.57E+43	-10.00	12890.0/	! fit btw. 500 and 800 K with MAE of 0.5%, 0.9%
PLOG/1.000E+01	7.50E+42	-9.35	14990.0/	! fit btw. 500 and 1000 K with MAE of 2.0%, 3.1%
PLOG/1.000E+02	6.70E+35	-6.83	14290.0/	! fit btw. 500 and 1250 K with MAE of 7.1%, 11.2%

PLOG/3.947E-02	1.57E+10	0.00	3317.0/	
PLOG/3.947E-02	0.00E+00	0.00	0.0/	! fit btw. 500 and 700 K with MAE of 38.8%, 70.0%
PLOG/1.000E+00	1.57E+43	-10.00	12890.0/	
PLOG/1.000E+00	0.00E+00	0.00	0.0/	! fit btw. 500 and 800 K with MAE of 0.5%, 0.9%
PLOG/1.000E+01	7.50E+42	-9.35	14990.0/	
PLOG/1.000E+01	0.00E+00	0.00	0.0/	! fit btw. 500 and 1000 K with MAE of 2.0%, 3.1%
PLOG/1.000E+02	7.51E+67	-16.12	33850.0/	

PLOG/1.000E+02	9.58E+43	-9.63	15580.0/	! fit btw. 500 and 1250 K with MAE of 0.6%, 1.2%
3-phenylpropyne + H → C₉H₉ (W21)				1.66E+20 -1.75 14120.0
PLOG/3.947E-02	4.23E+09	0.00	1241.0/	! fit btw. 500 and 600 K with MAE of 0.0%, 0.0%
PLOG/1.000E+00	2.27E+17	-1.60	5714.0/	! fit btw. 500 and 900 K with MAE of 4.4%, 8.5%
PLOG/1.000E+01	5.36E+25	-3.65	12890.0/	! fit btw. 500 and 1125 K with MAE of 2.8%, 6.9%
PLOG/1.000E+02	1.66E+20	-1.75	14120.0/	! fit btw. 500 and 1500 K with MAE of 10.8%, 29.2%
PLOG/3.947E-02	4.23E+09	0.00	1241.0/	
PLOG/3.947E-02	0.00E+00	0.00	0.0/	! fit btw. 500 and 600 K with MAE of 0.0%, 0.0%
PLOG/1.000E+00	2.27E+17	-1.60	5714.0/	
PLOG/1.000E+00	0.00E+00	0.00	0.0/	! fit btw. 500 and 900 K with MAE of 4.4%, 8.5%
PLOG/1.000E+01	1.97E+29	-4.74	14310.0/	
PLOG/1.000E+01	1.47E+30	3.48	151900.0/	! fit btw. 500 and 1125 K with MAE of 0.9%, 2.2%
PLOG/1.000E+02	6.85E+44	-8.78	30640.0/	
PLOG/1.000E+02	5.15E+26	-4.05	14690.0/	! fit btw. 500 and 1500 K with MAE of 4.9%, 18.5%
3-phenylpropyne + H → C₆H₅ + allene (R2)				7.48E+18 -0.94 26090.0
PLOG/3.947E-02	1.47E+28	-3.75	23670.0/	! fit btw. 500 and 2500 K with MAE of 26.1%, 68.5%
PLOG/1.000E+00	6.05E+24	-2.73	23910.0/	! fit btw. 500 and 2500 K with MAE of 20.2%, 41.5%
PLOG/1.000E+01	7.10E+23	-2.40	25970.0/	! fit btw. 500 and 2500 K with MAE of 15.4%, 37.6%
PLOG/1.000E+02	7.48E+18	-0.94	26090.0/	! fit btw. 500 and 2500 K with MAE of 26.8%, 59.7%
PLOG/3.947E-02	9.44E+42	-7.86	34850.0/	
PLOG/3.947E-02	2.47E+102	-27.88	43930.0/	! fit btw. 500 and 2500 K with MAE of 5.4%, 11.6%
PLOG/1.000E+00	2.98E+76	-17.04	67400.0/	
PLOG/1.000E+00	7.02E+22	-2.29	21910.0/	! fit btw. 500 and 2500 K with MAE of 2.2%, 7.6%
PLOG/1.000E+01	1.64E+35	-5.55	35130.0/	
PLOG/1.000E+01	3.36E+22	-2.54	21860.0/	! fit btw. 500 and 2500 K with MAE of 4.3%, 9.1%
PLOG/1.000E+02	2.50E+36	-5.80	39780.0/	
PLOG/1.000E+02	4.59E+26	-4.07	24050.0/	! fit btw. 500 and 2500 K with MAE of 2.3%, 3.9%

3-phenylpropyne + H → benzyl + C₂H₂ (R3)

1.53E+25 -2.83 21500.0

PLOG/3.947E-02 1.92E+20 -1.62 13070.0/
PLOG/1.000E+00 5.92E+22 -2.29 15620.0/
PLOG/1.000E+01 9.53E+24 -2.86 18630.0/
PLOG/1.000E+02 1.53E+25 -2.83 21500.0/

! fit btw. 500 and 2500 K with MAE of 3.9%, 6.7%
! fit btw. 500 and 2500 K with MAE of 5.1%, 9.7%
! fit btw. 500 and 2500 K with MAE of 6.2%, 11.7%
! fit btw. 500 and 2500 K with MAE of 10.8%, 28.1%

PLOG/3.947E-02 1.74E+16 -0.48 10800.0/
PLOG/3.947E-02 2.23E+50 -10.48 31240.0/
PLOG/1.000E+00 5.58E+177 -42.43 235700.0/
PLOG/1.000E+00 1.05E+24 -2.66 16230.0/
PLOG/1.000E+01 6.80E+16 -3.03 -15.8/
PLOG/1.000E+01 3.13E+26 -3.28 19720.0/
PLOG/1.000E+02 1.57E+30 -4.22 25180.0/
PLOG/1.000E+02 3.23E+165 -48.28 61960.0/

! fit btw. 500 and 2500 K with MAE of 1.1%, 1.7%

! fit btw. 500 and 2500 K with MAE of 3.2%, 10.0%

! fit btw. 500 and 2500 K with MAE of 3.8%, 9.2%

! fit btw. 500 and 2500 K with MAE of 2.3%, 5.7%

3-phenylpropyne + H → indene + H (P1)

2.10E+32 -5.17 24530.0

PLOG/3.947E-02 5.61E+27 -4.15 11750.0/
PLOG/1.000E+00 1.82E+31 -5.09 15660.0/
PLOG/1.000E+01 7.51E+33 -5.73 20370.0/
PLOG/1.000E+02 2.10E+32 -5.17 24530.0/

! fit btw. 500 and 2500 K with MAE of 3.2%, 5.9%
! fit btw. 500 and 2500 K with MAE of 5.4%, 10.9%
! fit btw. 500 and 2500 K with MAE of 6.0%, 11.9%
! fit btw. 500 and 2500 K with MAE of 12.2%, 27.4%

PLOG/3.947E-02 1.82E+145 -37.72 94340.0/
PLOG/3.947E-02 6.59E+26 -3.89 11180.0/
PLOG/1.000E+00 1.48E+44 -8.85 23450.0/
PLOG/1.000E+00 9.89E+17 -1.40 8221.0/
PLOG/1.000E+01 2.82E+74 -17.37 49100.0/
PLOG/1.000E+01 8.25E+30 -4.91 18530.0/
PLOG/1.000E+02 2.78E+36 -6.32 27530.0/
PLOG/1.000E+02 1.14E+144 -42.15 52000.0/

! fit btw. 500 and 2500 K with MAE of 0.8%, 2.9%

! fit btw. 500 and 2500 K with MAE of 0.8%, 2.0%

! fit btw. 500 and 2500 K with MAE of 2.3%, 5.0%

! fit btw. 500 and 2500 K with MAE of 5.2%, 20.7%

3-phenylpropyne + H → phenylallene + H (P3)

4.81E+22 -2.09 25710.0

PLOG/3.947E-02	1.69E+20	-1.66	15690.0/	! fit btw. 500 and 2500 K with MAE of 7.8%, 17.2%
PLOG/1.000E+00	3.13E+25	-3.08	20970.0/	! fit btw. 500 and 2500 K with MAE of 4.1%, 11.0%
PLOG/1.000E+01	2.01E+28	-3.79	25520.0/	! fit btw. 500 and 2500 K with MAE of 13.5%, 37.7%
PLOG/1.000E+02	4.81E+22	-2.09	25710.0/	! fit btw. 500 and 2500 K with MAE of 31.2%, 71.3%

PLOG/3.947E-02	8.66E+23	-2.69	18460.0/	
PLOG/3.947E-02	4.35E+173	-50.86	63270.0/	! fit btw. 500 and 2500 K with MAE of 3.5%, 7.7%
PLOG/1.000E+00	9.08E+32	-5.26	25450.0/	
PLOG/1.000E+00	2.70E+07	1.90	10900.0/	! fit btw. 500 and 2500 K with MAE of 0.6%, 1.3%
PLOG/1.000E+01	1.53E+34	-5.42	29830.0/	
PLOG/1.000E+01	1.15E+171	-50.14	65880.0/	! fit btw. 500 and 2500 K with MAE of 4.9%, 12.0%
PLOG/1.000E+02	1.99E+52	-10.36	48190.0/	
PLOG/1.000E+02	9.70E+09	1.27	16800.0/	! fit btw. 500 and 2500 K with MAE of 2.3%, 5.2%

3-phenylpropyne + H → phenylacetylene + CH₃ (P5)

1.62E+42 -7.41 56600.0

PLOG/3.947E-02	1.01E+58	-12.54	38610.0/	! fit btw. 500 and 2500 K with MAE of 20.2%, 52.6%
PLOG/1.000E+00	2.57E+56	-11.85	45860.0/	! fit btw. 500 and 2500 K with MAE of 27.2%, 48.8%
PLOG/1.000E+01	7.43E+52	-10.63	52300.0/	! fit btw. 500 and 2500 K with MAE of 29.6%, 69.3%
PLOG/1.000E+02	1.62E+42	-7.41	56600.0/	! fit btw. 500 and 2500 K with MAE of 55.4%, 142.8%

PLOG/3.947E-02	4.13E+67	-15.22	45740.0/	
PLOG/3.947E-02	1.65E+191	-55.53	77640.0/	! fit btw. 500 and 2500 K with MAE of 6.4%, 15.7%
PLOG/1.000E+00	5.80E+84	-19.72	68460.0/	
PLOG/1.000E+00	2.03E+50	-10.37	40550.0/	! fit btw. 500 and 2500 K with MAE of 3.8%, 8.3%
PLOG/1.000E+01	2.73E+73	-16.32	68430.0/	
PLOG/1.000E+01	4.60E+48	-9.98	46080.0/	! fit btw. 500 and 2500 K with MAE of 6.2%, 9.6%
PLOG/1.000E+02	3.75E+30	-4.79	45110.0/	
PLOG/1.000E+02	1.27E+74	-16.26	81020.0/	! fit btw. 500 and 2500 K with MAE of 7.1%, 16.4%

3-phenylpropyne + H → total 1.86E+17 -0.84 5908.0

PLOG/3.947E-02	1.33E+15	-0.24	4554.0/	! fit btw. 500 and 2500 K with MAE of 4.6%, 9.6%
PLOG/1.000E+00	5.99E+15	-0.43	4948.0/	! fit btw. 500 and 2500 K with MAE of 4.1%, 9.6%

PLOG/1.000E+01	2.29E+16	-0.59	5308.0/	! fit btw. 500 and 2500 K with MAE of 4.0%, 8.9%
PLOG/1.000E+02	1.86E+17	-0.84	5908.0/	! fit btw. 500 and 2500 K with MAE of 5.4%, 11.3%

PLOG/3.947E-02	3.93E+74	-15.61	92820.0/	
PLOG/3.947E-02	3.63E+17	-0.97	5730.0/	! fit btw. 500 and 2500 K with MAE of 1.5%, 3.2%
PLOG/1.000E+00	1.60E+25	-3.22	10200.0/	
PLOG/1.000E+00	1.95E+03	3.05	-1641.0/	! fit btw. 500 and 2500 K with MAE of 0.9%, 2.0%
PLOG/1.000E+01	2.04E+26	-3.52	11040.0/	
PLOG/1.000E+01	6.75E+03	2.89	-1480.0/	! fit btw. 500 and 2500 K with MAE of 1.2%, 2.9%
PLOG/1.000E+02	2.97E+16	-2.00	-1796.0/	
PLOG/1.000E+02	2.94E+18	-1.17	6801.0/	! fit btw. 500 and 2500 K with MAE of 4.0%, 12.3%

phenylacetylene + CH₃ → C₉H₉ (W4) 2.28E+20 -1.97 17740.0

PLOG/3.947E-02	4.95E+63	-16.04	30050.0/	! fit btw. 500 and 1000 K with MAE of 1.9%, 4.0%
PLOG/1.000E+00	6.37E+44	-9.70	25890.0/	! fit btw. 500 and 1125 K with MAE of 8.0%, 13.4%
PLOG/1.000E+01	1.40E+34	-6.25	22880.0/	! fit btw. 500 and 1375 K with MAE of 12.3%, 20.9%
PLOG/1.000E+02	2.28E+20	-1.97	17740.0/	! fit btw. 500 and 1500 K with MAE of 10.0%, 21.2%

PLOG/3.947E-02	4.95E+63	-16.04	30050.0/	
PLOG/3.947E-02	0.00E+00	0.00	0.0/	! fit btw. 500 and 1000 K with MAE of 1.9%, 4.0%
PLOG/1.000E+00	1.53E+74	-18.34	42020.0/	
PLOG/1.000E+00	4.27E+46	-10.76	23590.0/	! fit btw. 500 and 1125 K with MAE of 0.7%, 1.1%
PLOG/1.000E+01	8.68E+73	-17.73	47620.0/	
PLOG/1.000E+01	2.80E+40	-8.52	23170.0/	! fit btw. 500 and 1375 K with MAE of 0.8%, 1.7%
PLOG/1.000E+02	3.64E+60	-13.45	44920.0/	
PLOG/1.000E+02	2.87E+26	-4.04	18790.0/	! fit btw. 500 and 1500 K with MAE of 1.5%, 2.5%

phenylacetylene + CH₃ → C₉H₉ (W5) 1.18E+23 -2.65 14850.0

PLOG/3.947E-02	8.16E+66	-16.55	29230.0/	! fit btw. 500 and 1125 K with MAE of 8.9%, 16.9%
PLOG/1.000E+00	6.92E+44	-9.48	22420.0/	! fit btw. 500 and 1250 K with MAE of 12.9%, 20.3%
PLOG/1.000E+01	4.15E+30	-5.02	17440.0/	! fit btw. 500 and 1375 K with MAE of 13.4%, 23.9%
PLOG/1.000E+02	1.18E+23	-2.65	14850.0/	! fit btw. 500 and 1650 K with MAE of 14.6%, 34.0%

PLOG/3.947E-02	1.19E+92	-23.96	42600.0/	
PLOG/3.947E-02	1.95E+63	-16.16	23440.0/	! fit btw. 500 and 1125 K with MAE of 0.7%, 1.5%
PLOG/1.000E+00	4.57E+89	-22.52	48450.0/	
PLOG/1.000E+00	2.59E+52	-12.23	22660.0/	! fit btw. 500 and 1250 K with MAE of 0.5%, 1.1%
PLOG/1.000E+01	1.38E+78	-18.72	47050.0/	
PLOG/1.000E+01	1.37E+37	-7.31	18030.0/	! fit btw. 500 and 1375 K with MAE of 1.3%, 2.3%
PLOG/1.000E+02	9.83E+66	-15.11	45520.0/	
PLOG/1.000E+02	1.86E+28	-4.46	15370.0/	! fit btw. 500 and 1650 K with MAE of 2.3%, 4.4%

phenylacetylene + CH₃ → C₉H₉ (W6)

8.15E+39 -7.24 44240.0

PLOG/3.947E-02	6.77E+59	-13.94	36590.0/	! fit btw. 500 and 1650 K with MAE of 15.7%, 33.4%
PLOG/1.000E+00	1.09E+53	-11.53	39270.0/	! fit btw. 500 and 1800 K with MAE of 16.2%, 32.5%
PLOG/1.000E+01	2.67E+48	-9.89	42880.0/	! fit btw. 500 and 2000 K with MAE of 30.6%, 150.7%
PLOG/1.000E+02	8.15E+39	-7.24	44240.0/	! fit btw. 500 and 2500 K with MAE of 44.5%, 115.1%

PLOG/3.947E-02	1.03E+97	-24.51	62050.0/	
PLOG/3.947E-02	6.22E+63	-15.45	36140.0/	! fit btw. 500 and 1650 K with MAE of 2.7%, 5.6%
PLOG/1.000E+00	8.88E+26	-3.56	28590.0/	
PLOG/1.000E+00	-2.03E+44	-8.24	46480.0/	! fit btw. 500 and 1800 K with MAE of 4.0%, 14.3%
PLOG/1.000E+01	1.17E+63	-14.05	52400.0/	
PLOG/1.000E+01	9.40E+32	-13.59	-15930.0/	! fit btw. 500 and 2000 K with MAE of 5.9%, 14.2%
PLOG/1.000E+02	-5.06E+69	-16.21	56120.0/	
PLOG/1.000E+02	2.54E+48	-9.72	46870.0/	! fit btw. 500 and 2500 K with MAE of 16.7%, 46.6%

phenylacetylene + CH₃ → C₆H₅ + propyne (R1)

4.77E+23 -2.16 42240.0

PLOG/3.947E-02	1.63E+24	-2.68	31360.0/	! fit btw. 500 and 2500 K with MAE of 19.8%, 39.2%
PLOG/1.000E+00	8.26E+31	-4.72	39990.0/	! fit btw. 500 and 2500 K with MAE of 14.7%, 26.6%
PLOG/1.000E+01	9.85E+30	-4.34	42890.0/	! fit btw. 500 and 2500 K with MAE of 15.3%, 40.6%
PLOG/1.000E+02	4.77E+23	-2.16	42240.0/	! fit btw. 500 and 2500 K with MAE of 29.9%, 70.1%
PLOG/3.947E-02	1.35E+46	-9.27	41180.0/	
PLOG/3.947E-02	1.80E+24	-2.44	39620.0/	! fit btw. 500 and 2500 K with MAE of 1.2%, 4.2%

PLOG/1.000E+00	5.00E+38	-6.73	43270.0/	
PLOG/1.000E+00	1.21E+91	-19.81	130800.0/	! fit btw. 500 and 2500 K with MAE of 6.4%, 21.7%
PLOG/1.000E+01	2.97E+36	-5.87	46890.0/	
PLOG/1.000E+01	1.80E+168	-49.20	79930.0/	! fit btw. 500 and 2500 K with MAE of 8.2%, 17.8%
PLOG/1.000E+02	2.48E+52	-10.19	63850.0/	
PLOG/1.000E+02	2.07E+10	1.41	33060.0/	! fit btw. 500 and 2500 K with MAE of 2.2%, 4.3%

phenylacetylene + CH₃ → indene + H (P1)

3.46E+21 -2.03 53930.0

PLOG/3.947E-02	4.18E+40	-7.79	40570.0/	! fit btw. 500 and 2500 K with MAE of 11.7%, 25.3%
PLOG/1.000E+00	1.53E+35	-6.01	46210.0/	! fit btw. 500 and 2500 K with MAE of 12.1%, 27.6%
PLOG/1.000E+01	3.63E+25	-3.20	47630.0/	! fit btw. 500 and 2500 K with MAE of 27.0%, 74.1%
PLOG/1.000E+02	3.46E+21	-2.03	53930.0/	! fit btw. 600 and 2500 K with MAE of 18.7%, 41.8%

PLOG/3.947E-02	5.45E+44	-8.94	43600.0/	
PLOG/3.947E-02	4.52E+190	-56.26	84840.0/	! fit btw. 500 and 2500 K with MAE of 6.9%, 15.4%
PLOG/1.000E+00	4.37E+40	-7.54	50240.0/	
PLOG/1.000E+00	8.28E+73	-19.50	51580.0/	! fit btw. 500 and 2500 K with MAE of 3.2%, 11.2%
PLOG/1.000E+01	1.34E+40	-7.25	58570.0/	
PLOG/1.000E+01	4.67E+57	-14.32	51840.0/	! fit btw. 500 and 2500 K with MAE of 2.5%, 6.3%
PLOG/1.000E+02	1.83E+153	-43.73	97260.0/	
PLOG/1.000E+02	1.43E+32	-4.97	62340.0/	! fit btw. 600 and 2500 K with MAE of 6.6%, 22.3%

phenylacetylene + CH₃ → 1-phenylpropyne + H (P2)

3.70E+22 -1.88 33550.0

PLOG/3.947E-02	2.03E+22	-2.17	22670.0/	! fit btw. 500 and 2500 K with MAE of 18.6%, 38.3%
PLOG/1.000E+00	1.05E+30	-4.22	30930.0/	! fit btw. 500 and 2500 K with MAE of 14.3%, 26.3%
PLOG/1.000E+01	9.68E+29	-4.09	34280.0/	! fit btw. 500 and 2500 K with MAE of 16.6%, 43.3%
PLOG/1.000E+02	3.70E+22	-1.88	33550.0/	! fit btw. 500 and 2500 K with MAE of 30.7%, 74.5%

PLOG/3.947E-02	9.66E+14	-0.04	20050.0/	
PLOG/3.947E-02	1.01E+57	-12.65	38350.0/	! fit btw. 500 and 2500 K with MAE of 1.0%, 1.7%
PLOG/1.000E+00	5.48E+36	-6.21	34180.0/	
PLOG/1.000E+00	1.57E+82	-17.47	113300.0/	! fit btw. 500 and 2500 K with MAE of 6.2%, 22.2%

PLOG/1.000E+01 3.79E+35 -5.65 38360.0/
PLOG/1.000E+01 4.67E+164 -48.22 69900.0/
PLOG/1.000E+02 8.46E+53 -10.66 56850.0/
PLOG/1.000E+02 7.87E+07 2.08 23790.0/

! fit btw. 500 and 2500 K with MAE of 8.7%, 19.4%

! fit btw. 500 and 2500 K with MAE of 2.5%, 5.3%

phenylacetylene + CH₃ → phenylallene + H (P3)

2.36E+33 -5.10 52150.0

PLOG/3.947E-02 1.59E+33 -5.63 33170.0/
PLOG/1.000E+00 1.96E+44 -8.56 45860.0/
PLOG/1.000E+01 1.64E+45 -8.64 52450.0/
PLOG/1.000E+02 2.36E+33 -5.10 52150.0/

! fit btw. 500 and 2500 K with MAE of 25.0%, 43.7%

! fit btw. 500 and 2500 K with MAE of 22.6%, 45.3%

! fit btw. 500 and 2500 K with MAE of 24.9%, 61.4%

! fit btw. 500 and 2500 K with MAE of 49.3%, 137.3%

PLOG/3.947E-02 2.99E+52 -11.38 42160.0/
PLOG/3.947E-02 4.42E+22 -2.37 36430.0/
PLOG/1.000E+00 2.21E+54 -11.53 50770.0/
PLOG/1.000E+00 5.07E+106 -24.26 148100.0/
PLOG/1.000E+01 1.40E+52 -10.57 57470.0/
PLOG/1.000E+01 1.39E+159 -46.58 78560.0/
PLOG/1.000E+02 -3.89E+38 -6.95 49540.0/
PLOG/1.000E+02 2.37E+27 -3.46 45270.0/

! fit btw. 500 and 2500 K with MAE of 1.8%, 5.6%

! fit btw. 500 and 2500 K with MAE of 8.1%, 28.1%

! fit btw. 500 and 2500 K with MAE of 14.5%, 33.0%

! fit btw. 500 and 2500 K with MAE of 34.7%, 125.5%

phenylacetylene + CH₃ → 3-phenylpropyne + H (P4)

8.77E+35 -5.58 69460.0

PLOG/3.947E-02 5.50E+51 -10.72 51480.0/
PLOG/1.000E+00 1.39E+50 -10.02 58720.0/
PLOG/1.000E+01 4.03E+46 -8.80 65160.0/
PLOG/1.000E+02 8.77E+35 -5.58 69460.0/

! fit btw. 500 and 2500 K with MAE of 20.4%, 53.1%

! fit btw. 500 and 2500 K with MAE of 27.7%, 50.6%

! fit btw. 500 and 2500 K with MAE of 30.0%, 71.3%

! fit btw. 500 and 2500 K with MAE of 55.9%, 143.5%

PLOG/3.947E-02 6.45E+61 -13.52 58970.0/
PLOG/3.947E-02 9.50E+142 -40.45 76290.0/
PLOG/1.000E+00 3.86E+78 -17.91 81460.0/
PLOG/1.000E+00 2.27E+44 -8.64 53520.0/
PLOG/1.000E+01 4.49E+67 -14.63 81700.0/
PLOG/1.000E+01 3.60E+42 -8.20 59050.0/

! fit btw. 500 and 2500 K with MAE of 6.1%, 15.5%

! fit btw. 500 and 2500 K with MAE of 3.8%, 8.5%

! fit btw. 500 and 2500 K with MAE of 6.4%, 10.6%

PLOG/1.000E+02	2.66E+24	-3.00	58050.0/	
PLOG/1.000E+02	1.71E+68	-14.55	94200.0/	! fit btw. 500 and 2500 K with MAE of 7.5%, 16.8%

phenylacetylene + CH₃ → total

5.36E+18 -1.34 12880.0

PLOG/3.947E-02	1.38E-01	4.17	1553.0/	! fit btw. 500 and 2500 K with MAE of 20.8%, 55.8%
PLOG/1.000E+00	1.85E+07	1.85	5889.0/	! fit btw. 500 and 2500 K with MAE of 29.5%, 80.9%
PLOG/1.000E+01	3.09E+13	0.10	9497.0/	! fit btw. 500 and 2500 K with MAE of 29.0%, 108.2%
PLOG/1.000E+02	5.36E+18	-1.34	12880.0/	! fit btw. 500 and 2500 K with MAE of 19.2%, 88.0%

PLOG/3.947E-02	6.03E+45	-10.01	21210.0/	
PLOG/3.947E-02	3.24E+12	0.65	17350.0/	! fit btw. 500 and 2500 K with MAE of 2.3%, 5.8%
PLOG/1.000E+00	2.78E+33	-5.96	18000.0/	
PLOG/1.000E+00	1.24E+45	-7.94	56400.0/	! fit btw. 500 and 2500 K with MAE of 6.3%, 17.5%
PLOG/1.000E+01	1.52E+29	-4.55	17050.0/	
PLOG/1.000E+01	2.74E+107	-24.28	134800.0/	! fit btw. 500 and 2500 K with MAE of 12.1%, 42.2%
PLOG/1.000E+02	5.33E+31	-5.11	20350.0/	
PLOG/1.000E+02	7.58E-32	12.65	-14500.0/	! fit btw. 500 and 2500 K with MAE of 12.4%, 47.0%

1-phenylallyl (W8 + W9) → C₉H₉ (W6)

3.92E-32 11.81 28300.0

PLOG/3.947E-02	1.13E+101	-26.40	106700.0/	! fit btw. 800 and 1650 K with MAE of 3.1%, 7.0%
PLOG/1.000E+00	8.86E+81	-20.25	103400.0/	! fit btw. 800 and 1800 K with MAE of 7.0%, 10.0%
PLOG/1.000E+01	3.45E-73	23.53	89.3/	! fit btw. 500 and 2000 K with MAE of 436.3%, 3732.9%
PLOG/1.000E+02	3.92E-32	11.81	28300.0/	! fit btw. 600 and 2500 K with MAE of 516.5%, 4783.1%

PLOG/3.947E-02	-8.92E+112	-30.41	104300.0/	
PLOG/3.947E-02	1.09E+89	-23.19	93200.0/	! fit btw. 800 and 1650 K with MAE of 1.2%, 2.4%
PLOG/1.000E+00	2.32E+113	-28.95	129800.0/	
PLOG/1.000E+00	1.55E+87	-22.18	102100.0/	! fit btw. 800 and 1800 K with MAE of 1.7%, 4.7%
PLOG/1.000E+01	3.05E-71	23.18	5177.0/	
PLOG/1.000E+01	2.41E-73	22.38	-8530.0/	! fit btw. 500 and 2000 K with MAE of 288.9%, 1472.3%
PLOG/1.000E+02	1.72E-137	36.32	-78690.0/	
PLOG/1.000E+02	2.43E+31	-5.61	76640.0/	! fit btw. 600 and 2500 K with MAE of 59.1%, 303.4%

1-phenylallyl (W8 + W9) → C₆H₅ + propyne (R1)

PLOG/3.947E-02 1.73E+83 -20.76 106300.0/
PLOG/1.000E+00 1.50E+67 -15.47 105700.0/
PLOG/1.000E+01 9.83E+18 -1.77 74980.0/
PLOG/1.000E+02 3.78E+19 -1.68 81690.0/

3.78E+19 -1.68 81690.0

! fit btw. 800 and 1650 K with MAE of 1.2%, 2.2%
! fit btw. 800 and 2000 K with MAE of 1.0%, 2.2%
! fit btw. 500 and 2500 K with MAE of 79.9%, 452.0%
! fit btw. 500 and 2500 K with MAE of 86.4%, 438.1%

PLOG/3.947E-02 6.79E-290 84.89 -129500.0/
PLOG/3.947E-02 1.56E+86 -21.61 108200.0/
PLOG/1.000E+00 5.50E+81 -19.84 112700.0/
PLOG/1.000E+00 1.07E+85 -20.24 126100.0/
PLOG/1.000E+01 1.72E+23 -2.88 79750.0/
PLOG/1.000E+01 6.49E+20 -3.73 66200.0/
PLOG/1.000E+02 5.29E+12 -9.92 13750.0/
PLOG/1.000E+02 4.55E+37 -6.74 94650.0/

! fit btw. 800 and 1650 K with MAE of 0.3%, 1.0%

! fit btw. 800 and 2000 K with MAE of 0.6%, 1.5%

! fit btw. 500 and 2500 K with MAE of 59.1%, 213.8%

! fit btw. 500 and 2500 K with MAE of 33.9%, 167.7%

1-phenylallyl (W8 + W9) → C₆H₅ + allene (R2)

PLOG/3.947E-02 1.33E+93 -23.42 119000.0/
PLOG/1.000E+00 9.01E+52 -11.40 101100.0/
PLOG/1.000E+01 4.64E-02 3.83 63180.0/
PLOG/1.000E+02 1.54E+24 -3.14 86480.0/

1.54E+24 -3.14 86480.0

! fit btw. 800 and 1650 K with MAE of 4.5%, 9.3%
! fit btw. 800 and 2000 K with MAE of 12.1%, 21.0%
! fit btw. 500 and 2500 K with MAE of 98.3%, 460.5%
! fit btw. 600 and 2500 K with MAE of 32.2%, 141.2%

PLOG/3.947E-02 -5.55E+101 -26.33 115500.0/
PLOG/3.947E-02 8.39E+86 -21.87 108600.0/
PLOG/1.000E+00 -6.93E+73 -16.03 144000.0/
PLOG/1.000E+00 6.64E+10 0.85 76670.0/
PLOG/1.000E+01 2.48E-15 6.64 48950.0/
PLOG/1.000E+01 2.25E+51 -10.76 104400.0/
PLOG/1.000E+02 1.30E+26 -3.66 90460.0/
PLOG/1.000E+02 9.71E+25 -3.80 86430.0/

! fit btw. 800 and 1650 K with MAE of 1.8%, 4.7%

! fit btw. 800 and 2000 K with MAE of 1.3%, 2.8%

! fit btw. 500 and 2500 K with MAE of 8.2%, 21.8%

! fit btw. 600 and 2500 K with MAE of 31.9%, 135.2%

1-phenylallyl (W8 + W9) → benzyl + C₂H₂ (R3)

1.63E+22 -2.64 74770.0

PLOG/3.947E-02 4.31E+75 -18.57 99580.0/
PLOG/1.000E+00 1.70E+49 -10.50 88960.0/
PLOG/1.000E+01 1.75E+11 0.25 63050.0/
PLOG/1.000E+02 1.63E+22 -2.64 74770.0/

! fit btw. 800 and 1650 K with MAE of 2.3%, 4.6%
! fit btw. 800 and 2000 K with MAE of 5.0%, 8.7%
! fit btw. 500 and 2500 K with MAE of 52.2%, 240.7%
! fit btw. 700 and 2500 K with MAE of 27.9%, 101.2%

PLOG/3.947E-02 -2.82E+85 -21.86 97460.0/
PLOG/3.947E-02 2.18E+68 -16.68 89740.0/
PLOG/1.000E+00 -8.76E+53 -12.18 84110.0/
PLOG/1.000E+00 5.55E+43 -9.10 79380.0/
PLOG/1.000E+01 -1.03E+28 -4.71 68590.0/
PLOG/1.000E+01 3.75E+19 -2.14 64910.0/
PLOG/1.000E+02 1.65E+24 -3.17 78210.0/
PLOG/1.000E+02 7.69E+23 -3.36 73920.0/

! fit btw. 800 and 1650 K with MAE of 1.1%, 2.1%
! fit btw. 800 and 2000 K with MAE of 3.5%, 7.1%
! fit btw. 500 and 2500 K with MAE of 24.1%, 73.4%
! fit btw. 700 and 2500 K with MAE of 27.7%, 96.9%

1-phenylallyl (W8 + W9) → indene + H (P1)

1.07E+28 -4.55 52400.0

PLOG/3.947E-02 1.27E+42 -9.11 50180.0/
PLOG/1.000E+00 2.83E+37 -7.50 51480.0/
PLOG/1.000E+01 2.05E+30 -5.35 49520.0/
PLOG/1.000E+02 1.07E+28 -4.55 52400.0/

! fit btw. 800 and 1650 K with MAE of 0.8%, 2.4%
! fit btw. 800 and 2000 K with MAE of 3.0%, 8.2%
! fit btw. 500 and 2500 K with MAE of 20.2%, 81.0%
! fit btw. 500 and 2500 K with MAE of 21.1%, 72.4%

PLOG/3.947E-02 4.53E+43 -9.55 51270.0/
PLOG/3.947E-02 4.21E+02 -10.87 -108500.0/
PLOG/1.000E+00 3.75E+140 -35.04 167400.0/
PLOG/1.000E+00 2.39E+45 -9.80 56170.0/
PLOG/1.000E+01 2.36E+29 -5.11 49770.0/
PLOG/1.000E+01 1.70E+32 -6.07 49990.0/
PLOG/1.000E+02 2.47E+30 -5.21 54090.0/
PLOG/1.000E+02 2.53E+10 -8.51 -11670.0/

! fit btw. 800 and 1650 K with MAE of 0.3%, 0.9%
! fit btw. 800 and 2000 K with MAE of 1.5%, 5.3%
! fit btw. 500 and 2500 K with MAE of 20.5%, 81.6%
! fit btw. 500 and 2500 K with MAE of 17.3%, 72.7%

1-phenylallyl (W8 + W9) → 1-phenylpropyne + H (P2)

4.41E+14 -0.46 73040.0

PLOG/3.947E-02 7.46E+75 -18.77 97430.0/
PLOG/1.000E+00 1.68E+59 -13.38 95540.0/

! fit btw. 800 and 1650 K with MAE of 1.2%, 2.1%
! fit btw. 800 and 2000 K with MAE of 1.3%, 2.5%

PLOG/1.000E+01	9.64E+25	-3.86	75490.0/	! fit btw. 600 and 2500 K with MAE of 53.1%, 261.4%
PLOG/1.000E+02	4.41E+14	-0.46	73040.0/	! fit btw. 500 and 2500 K with MAE of 90.9%, 563.0%

PLOG/3.947E-02	1.01E+38	-19.88	-48060.0/	
PLOG/3.947E-02	1.30E+77	-19.12	98310.0/	! fit btw. 800 and 1650 K with MAE of 0.8%, 1.9%
PLOG/1.000E+00	2.40E+80	-19.72	105700.0/	
PLOG/1.000E+00	1.24E+79	-18.72	116700.0/	! fit btw. 800 and 2000 K with MAE of 0.6%, 1.3%
PLOG/1.000E+01	4.75E+33	-5.93	82770.0/	
PLOG/1.000E+01	1.70E+13	-9.60	-4167.0/	! fit btw. 600 and 2500 K with MAE of 28.1%, 78.5%
PLOG/1.000E+02	1.13E+07	-9.03	1222.0/	
PLOG/1.000E+02	2.46E+34	-5.98	87200.0/	! fit btw. 500 and 2500 K with MAE of 27.0%, 135.1%

1-phenylallyl (W8 + W9) → phenylallene + H (P3)

1.18E+15 -0.48 59370.0

PLOG/3.947E-02	1.04E+65	-15.22	86670.0/	! fit btw. 800 and 1650 K with MAE of 2.6%, 4.8%
PLOG/1.000E+00	4.18E+37	-6.94	74380.0/	! fit btw. 800 and 2000 K with MAE of 6.5%, 11.9%
PLOG/1.000E+01	2.48E+13	-0.09	57210.0/	! fit btw. 500 and 2500 K with MAE of 37.1%, 107.3%
PLOG/1.000E+02	1.18E+15	-0.48	59370.0/	! fit btw. 500 and 2500 K with MAE of 20.0%, 66.3%

PLOG/3.947E-02	-1.13E+72	-17.61	83380.0/	
PLOG/3.947E-02	2.62E+60	-14.08	78110.0/	! fit btw. 800 and 1650 K with MAE of 2.1%, 5.9%
PLOG/1.000E+00	-1.57E+42	-8.57	69350.0/	
PLOG/1.000E+00	3.73E+32	-5.67	64840.0/	! fit btw. 800 and 2000 K with MAE of 4.8%, 9.9%
PLOG/1.000E+01	1.57E+15	-0.57	61240.0/	
PLOG/1.000E+01	1.58E+15	-0.75	57270.0/	! fit btw. 500 and 2500 K with MAE of 36.7%, 99.1%
PLOG/1.000E+02	1.24E+59	-13.91	77510.0/	
PLOG/1.000E+02	2.14E+37	-6.45	82110.0/	! fit btw. 500 and 2500 K with MAE of 16.3%, 60.2%

1-phenylallyl (W8 + W9) → 3-phenylpropyne + H (P4)

2.34E+31 -4.94 88580.0

PLOG/3.947E-02	1.85E+82	-20.32	107800.0/	! fit btw. 800 and 1650 K with MAE of 3.2%, 6.2%
PLOG/1.000E+00	1.00E+57	-12.51	98940.0/	! fit btw. 800 and 2000 K with MAE of 5.0%, 7.8%
PLOG/1.000E+01	1.51E+06	1.86	64720.0/	! fit btw. 500 and 2500 K with MAE of 94.5%, 471.9%
PLOG/1.000E+02	2.34E+31	-4.94	88580.0/	! fit btw. 600 and 2500 K with MAE of 31.9%, 144.7%

PLOG/3.947E-02	-1.22E+91	-24.16	147000.0/	
PLOG/3.947E-02	1.66E+76	-18.59	103900.0/	! fit btw. 800 and 1650 K with MAE of 5.1%, 8.9%
PLOG/1.000E+00	-2.72E+62	-14.42	94520.0/	
PLOG/1.000E+00	8.20E+50	-10.94	89190.0/	! fit btw. 800 and 2000 K with MAE of 4.3%, 7.8%
PLOG/1.000E+01	1.84E+17	-3.13	58000.0/	
PLOG/1.000E+01	9.76E+54	-11.66	102700.0/	! fit btw. 500 and 2500 K with MAE of 2.1%, 5.1%
PLOG/1.000E+02	2.07E+33	-5.46	92600.0/	
PLOG/1.000E+02	1.52E+33	-5.60	88570.0/	! fit btw. 600 and 2500 K with MAE of 31.5%, 139.0%

1-phenylallyl (W8 + W9) → phenylacetylene + CH₃ (P5)

2.25E+24 -3.07 77780.0

PLOG/3.947E-02	1.79E+72	-17.60	93430.0/	! fit btw. 800 and 1650 K with MAE of 1.0%, 2.0%
PLOG/1.000E+00	3.18E+56	-12.50	91650.0/	! fit btw. 800 and 2000 K with MAE of 1.6%, 3.7%
PLOG/1.000E+01	1.86E+23	-3.00	71410.0/	! fit btw. 500 and 2500 K with MAE of 50.8%, 276.6%
PLOG/1.000E+02	2.25E+24	-3.07	77780.0/	! fit btw. 500 and 2500 K with MAE of 57.0%, 252.9%

PLOG/3.947E-02	1.45E+65	-18.70	60330.0/	
PLOG/3.947E-02	7.58E+73	-18.06	94590.0/	! fit btw. 800 and 1650 K with MAE of 0.7%, 1.5%
PLOG/1.000E+00	8.95E+55	-12.36	91840.0/	
PLOG/1.000E+00	1.78E+58	-13.21	92120.0/	! fit btw. 800 and 2000 K with MAE of 1.6%, 3.7%
PLOG/1.000E+01	2.06E+25	-3.52	74030.0/	
PLOG/1.000E+01	4.56E+23	-4.02	65740.0/	! fit btw. 500 and 2500 K with MAE of 44.1%, 182.6%
PLOG/1.000E+02	5.52E+36	-6.53	86670.0/	
PLOG/1.000E+02	1.29E+07	-7.74	8591.0/	! fit btw. 500 and 2500 K with MAE of 24.6%, 127.8%

C₆H₆ + C₃H₃ → C₉H₉ (W1)

3.77E+22 -3.35 19580.0

PLOG/3.947E-02	8.64E+07	0.00	8334.0/	! fit btw. 500 and 600 K with MAE of 0.0%, 0.0%
PLOG/1.000E+00	6.06E+09	0.00	11300.0/	! fit btw. 500 and 700 K with MAE of 7.5%, 10.8%
PLOG/1.000E+01	4.61E+36	-7.97	23340.0/	! fit btw. 500 and 800 K with MAE of 0.7%, 1.2%
PLOG/1.000E+02	3.77E+22	-3.35	19580.0/	! fit btw. 500 and 1000 K with MAE of 2.4%, 4.1%

PLOG/3.947E-02 8.64E+07 0.00 8334.0/

PLOG/3.947E-02	0.00E+00	0.00	0.0/	! fit btw. 500 and 600 K with MAE of 0.0%, 0.0%
PLOG/1.000E+00	6.06E+09	0.00	11300.0/	
PLOG/1.000E+00	0.00E+00	0.00	0.0/	! fit btw. 500 and 700 K with MAE of 7.5%, 10.8%
PLOG/1.000E+01	4.61E+36	-7.97	23340.0/	
PLOG/1.000E+01	0.00E+00	0.00	0.0/	! fit btw. 500 and 800 K with MAE of 0.7%, 1.2%
PLOG/1.000E+02	3.77E+22	-3.35	19580.0/	
PLOG/1.000E+02	0.00E+00	0.00	0.0/	! fit btw. 500 and 1000 K with MAE of 2.4%, 4.1%

C₆H₆ + C₃H₃ → C₉H₉ (W2) 6.74E+19 -2.41 20790.0

PLOG/3.947E-02	4.47E+08	0.00	10750.0/	! fit btw. 500 and 700 K with MAE of 9.9%, 14.0%
PLOG/1.000E+00	9.96E+48	-11.93	28840.0/	! fit btw. 500 and 800 K with MAE of 0.7%, 1.2%
PLOG/1.000E+01	1.76E+32	-6.42	24480.0/	! fit btw. 500 and 900 K with MAE of 2.3%, 3.7%
PLOG/1.000E+02	6.74E+19	-2.41	20790.0/	! fit btw. 500 and 1125 K with MAE of 4.4%, 6.6%

PLOG/3.947E-02	4.47E+08	0.00	10750.0/	
PLOG/3.947E-02	0.00E+00	0.00	0.0/	! fit btw. 500 and 700 K with MAE of 9.9%, 14.0%
PLOG/1.000E+00	9.96E+48	-11.93	28840.0/	
PLOG/1.000E+00	0.00E+00	0.00	0.0/	! fit btw. 500 and 800 K with MAE of 0.7%, 1.2%
PLOG/1.000E+01	1.76E+32	-6.42	24480.0/	
PLOG/1.000E+01	0.00E+00	0.00	0.0/	! fit btw. 500 and 900 K with MAE of 2.3%, 3.7%
PLOG/1.000E+02	4.70E+35	-7.06	29730.0/	
PLOG/1.000E+02	1.16E+19	-2.65	17790.0/	! fit btw. 500 and 1125 K with MAE of 0.9%, 1.5%

C₆H₆ + C₃H₃ → phenylallene + H (P1) 2.68E+16 -0.97 36050.0

PLOG/3.947E-02	1.57E+01	3.17	21840.0/	! fit btw. 500 and 2500 K with MAE of 0.9%, 2.0%
PLOG/1.000E+00	3.98E+05	1.95	25200.0/	! fit btw. 500 and 2500 K with MAE of 6.8%, 17.7%
PLOG/1.000E+01	1.74E+12	0.12	30770.0/	! fit btw. 500 and 2500 K with MAE of 11.1%, 20.2%
PLOG/1.000E+02	2.68E+16	-0.97	36050.0/	! fit btw. 500 and 2500 K with MAE of 7.2%, 14.5%

PLOG/3.947E-02	2.34E+03	2.58	24110.0/	
PLOG/3.947E-02	6.03E+18	-2.60	26980.0/	! fit btw. 500 and 2500 K with MAE of 0.1%, 0.2%
PLOG/1.000E+00	1.17E+33	-6.60	35840.0/	

PLOG/1.000E+00	8.78E+05	1.90	26920.0/	! fit btw. 500 and 2500 K with MAE of 0.5%, 1.4%
PLOG/1.000E+01	1.09E+24	-3.42	36100.0/	
PLOG/1.000E+01	1.44E+22	-2.30	50060.0/	! fit btw. 500 and 2500 K with MAE of 1.3%, 4.1%
PLOG/1.000E+02	1.49E+33	-5.86	45890.0/	
PLOG/1.000E+02	1.05E+03	2.78	28620.0/	! fit btw. 500 and 2500 K with MAE of 1.8%, 8.0%

C₆H₆ + C₃H₃ → 3- phenylpropyne + H (P2)

3.13E+12 0.18 33550.0

PLOG/3.947E-02	2.24E+02	2.96	24960.0/	! fit btw. 500 and 2500 K with MAE of 1.3%, 2.9%
PLOG/1.000E+00	8.80E+02	2.80	25400.0/	! fit btw. 500 and 2500 K with MAE of 0.8%, 2.0%
PLOG/1.000E+01	2.66E+06	1.83	28080.0/	! fit btw. 500 and 2500 K with MAE of 5.1%, 12.6%
PLOG/1.000E+02	3.13E+12	0.18	33550.0/	! fit btw. 500 and 2500 K with MAE of 6.6%, 12.2%

PLOG/3.947E-02	2.58E+06	1.81	31160.0/	
PLOG/3.947E-02	5.04E+03	2.50	25180.0/	! fit btw. 500 and 2500 K with MAE of 0.1%, 0.2%
PLOG/1.000E+00	1.94E+15	-1.20	29140.0/	
PLOG/1.000E+00	1.23E+06	1.97	29200.0/	! fit btw. 500 and 2500 K with MAE of 0.1%, 0.3%
PLOG/1.000E+01	2.88E+27	-4.76	35970.0/	
PLOG/1.000E+01	1.11E+07	1.71	30080.0/	! fit btw. 500 and 2500 K with MAE of 0.3%, 1.0%
PLOG/1.000E+02	7.74E+16	-1.13	35620.0/	
PLOG/1.000E+02	2.02E+42	-7.43	81790.0/	! fit btw. 500 and 2500 K with MAE of 1.3%, 3.9%

C₆H₆ + C₃H₃ → total

9.14E-02 3.40 6014.0

PLOG/3.947E-02	2.47E-44	15.69	-13020.0/	! fit btw. 500 and 2500 K with MAE of 95.2%, 675.3%
PLOG/1.000E+00	1.91E-40	14.47	-13760.0/	! fit btw. 500 and 2500 K with MAE of 106.1%, 703.1%
PLOG/1.000E+01	6.64E-28	10.84	-8146.0/	! fit btw. 500 and 2500 K with MAE of 133.3%, 830.5%
PLOG/1.000E+02	9.14E-02	3.40	6014.0/	! fit btw. 500 and 2500 K with MAE of 145.8%, 830.3%

PLOG/3.947E-02	1.66E-42	15.24	-10090.0/	
PLOG/3.947E-02	2.63E-43	14.75	-16810.0/	! fit btw. 500 and 2500 K with MAE of 86.3%, 496.8%
PLOG/1.000E+00	4.33E-40	14.44	-8109.0/	
PLOG/1.000E+00	4.61E-38	13.70	-13130.0/	! fit btw. 500 and 2500 K with MAE of 105.5%, 676.6%
PLOG/1.000E+01	7.96E-29	11.46	4414.0/	

PLOG/1.000E+01	6.27E-25	9.88	-7434.0/	! fit btw. 500 and 2500 K with MAE of 122.7%, 722.5%
PLOG/1.000E+02	7.56E+82	-21.67	44640.0/	
PLOG/1.000E+02	5.03E+46	-8.86	70930.0/	! fit btw. 500 and 2500 K with MAE of 40.5%, 220.0%

C₆H₅ + C₃H₆ → C₉H₁₁ (W1) 4.32E+16 -1.27 6407.0

PLOG/3.947E-02	9.35E+50	-12.14	17880.0/	! fit btw. 500 and 1125 K with MAE of 13.6%, 23.7%
PLOG/1.000E+00	1.15E+26	-4.29	9224.0/	! fit btw. 500 and 1250 K with MAE of 8.0%, 17.1%
PLOG/1.000E+01	5.62E+22	-3.19	8528.0/	! fit btw. 500 and 1500 K with MAE of 10.4%, 15.0%
PLOG/1.000E+02	4.32E+16	-1.27	6407.0/	! fit btw. 500 and 1800 K with MAE of 11.5%, 17.8%

PLOG/3.947E-02	3.02E+142	-38.93	69060.0/	
PLOG/3.947E-02	9.15E+69	-18.30	23250.0/	! fit btw. 500 and 1125 K with MAE of 4.6%, 10.6%
PLOG/1.000E+00	7.17E+65	-15.80	33880.0/	
PLOG/1.000E+00	1.16E+36	-7.60	11630.0/	! fit btw. 500 and 1250 K with MAE of 4.4%, 12.3%
PLOG/1.000E+01	9.90E+125	-33.20	70750.0/	
PLOG/1.000E+01	1.76E+18	-1.91	5994.0/	! fit btw. 500 and 1500 K with MAE of 2.9%, 8.1%
PLOG/1.000E+02	3.34E+38	-7.42	22580.0/	
PLOG/1.000E+02	1.73E+30	-5.76	9640.0/	! fit btw. 500 and 1800 K with MAE of 2.9%, 12.0%

C₆H₅ + C₃H₆ → C₉H₁₁ (W2) 1.83E+10 0.53 5196.0

PLOG/3.947E-02	7.82E+27	-5.04	10240.0/	! fit btw. 500 and 800 K with MAE of 1.1%, 1.8%
PLOG/1.000E+00	7.72E+14	-0.84	7092.0/	! fit btw. 500 and 1000 K with MAE of 5.3%, 7.5%
PLOG/1.000E+01	6.90E+15	-1.16	7528.0/	! fit btw. 500 and 1375 K with MAE of 11.2%, 22.1%
PLOG/1.000E+02	1.83E+10	0.53	5196.0/	! fit btw. 500 and 1650 K with MAE of 8.3%, 21.2%

PLOG/3.947E-02	7.82E+27	-5.04	10240.0/	
PLOG/3.947E-02	0.00E+00	0.00	0.0/	! fit btw. 500 and 800 K with MAE of 1.1%, 1.8%
PLOG/1.000E+00	7.72E+14	-0.84	7092.0/	
PLOG/1.000E+00	0.00E+00	0.00	0.0/	! fit btw. 500 and 1000 K with MAE of 5.3%, 7.5%
PLOG/1.000E+01	2.51E+71	-17.14	43000.0/	
PLOG/1.000E+01	7.01E+22	-3.51	8951.0/	! fit btw. 500 and 1375 K with MAE of 1.7%, 2.6%
PLOG/1.000E+02	6.26E+51	-11.20	35890.0/	

PLOG/1.000E+02	2.75E+15	-1.17	6464.0/	! fit btw. 500 and 1650 K with MAE of 1.7%, 3.1%
C₆H₅ + C₃H₆ → styrene + CH₃ (P1)				3.46E+08 1.56 19560.0
PLOG/3.947E-02	2.82E+26	-3.90	17400.0/	! fit btw. 500 and 2500 K with MAE of 24.0%, 40.6%
PLOG/1.000E+00	3.95E+31	-5.18	25560.0/	! fit btw. 500 and 2500 K with MAE of 18.4%, 39.2%
PLOG/1.000E+01	4.76E+23	-2.81	24890.0/	! fit btw. 500 and 2500 K with MAE of 29.1%, 78.5%
PLOG/1.000E+02	3.46E+08	1.56	19560.0/	! fit btw. 500 and 2500 K with MAE of 36.9%, 82.4%
PLOG/3.947E-02	1.44E+45	-9.48	26150.0/	
PLOG/3.947E-02	8.41E+36	-6.29	42400.0/	! fit btw. 500 and 2500 K with MAE of 3.6%, 12.9%
PLOG/1.000E+00	5.49E-05	-5.97	-60910.0/	
PLOG/1.000E+00	3.73E+34	-6.01	27690.0/	! fit btw. 500 and 2500 K with MAE of 14.1%, 29.8%
PLOG/1.000E+01	5.98E+38	-7.01	36220.0/	
PLOG/1.000E+01	4.47E+81	-22.03	38250.0/	! fit btw. 500 and 2500 K with MAE of 6.4%, 14.6%
PLOG/1.000E+02	1.19E+39	-6.89	43940.0/	
PLOG/1.000E+02	1.59E+04	2.37	13990.0/	! fit btw. 500 and 2500 K with MAE of 5.3%, 18.6%
C₆H₅ + C₃H₆ → 3-phenylpropene + H (P2)				1.09E+14 0.23 23930.0
PLOG/3.947E-02	6.86E+23	-2.90	18490.0/	! fit btw. 500 and 2500 K with MAE of 15.2%, 25.6%
PLOG/1.000E+00	8.55E+28	-4.20	25560.0/	! fit btw. 500 and 2500 K with MAE of 14.8%, 33.8%
PLOG/1.000E+01	1.58E+25	-3.03	26890.0/	! fit btw. 500 and 2500 K with MAE of 26.6%, 72.4%
PLOG/1.000E+02	1.09E+14	0.23	23930.0/	! fit btw. 500 and 2500 K with MAE of 40.6%, 84.0%
PLOG/3.947E-02	3.71E+36	-6.71	24390.0/	
PLOG/3.947E-02	5.94E+33	-5.23	41020.0/	! fit btw. 500 and 2500 K with MAE of 2.7%, 10.6%
PLOG/1.000E+00	1.07E+32	-5.07	27790.0/	
PLOG/1.000E+00	5.15E+13	-7.20	-27340.0/	! fit btw. 500 and 2500 K with MAE of 10.1%, 21.5%
PLOG/1.000E+01	5.55E+38	-6.80	37010.0/	
PLOG/1.000E+01	7.20E+93	-25.66	43720.0/	! fit btw. 500 and 2500 K with MAE of 6.1%, 14.3%
PLOG/1.000E+02	3.77E+37	-6.29	42270.0/	
PLOG/1.000E+02	3.42E+29	-5.38	23980.0/	! fit btw. 500 and 2500 K with MAE of 6.3%, 11.4%

C₆H₅ + C₃H₆ → cis-1-phenylpropene + H (P3)

1.50E+13 0.13 23720.0

PLOG/3.947E-02	2.51E+23	-3.12	18510.0/	! fit btw. 500 and 2500 K with MAE of 15.4%, 26.1%
PLOG/1.000E+00	2.17E+28	-4.38	25510.0/	! fit btw. 500 and 2500 K with MAE of 15.1%, 34.2%
PLOG/1.000E+01	2.85E+24	-3.16	26760.0/	! fit btw. 500 and 2500 K with MAE of 26.9%, 72.9%
PLOG/1.000E+02	1.50E+13	0.13	23720.0/	! fit btw. 500 and 2500 K with MAE of 40.7%, 83.8%

PLOG/3.947E-02	1.14E+36	-6.90	24380.0/	
PLOG/3.947E-02	6.16E+33	-5.56	41870.0/	! fit btw. 500 and 2500 K with MAE of 2.8%, 11.0%
PLOG/1.000E+00	3.24E+31	-5.26	27790.0/	
PLOG/1.000E+00	3.23E+13	-7.33	-26240.0/	! fit btw. 500 and 2500 K with MAE of 10.1%, 21.6%
PLOG/1.000E+01	1.57E+38	-6.98	37030.0/	
PLOG/1.000E+01	3.58E+90	-24.97	42750.0/	! fit btw. 500 and 2500 K with MAE of 6.0%, 14.3%
PLOG/1.000E+02	5.34E+36	-6.39	42080.0/	
PLOG/1.000E+02	5.31E+28	-5.50	23810.0/	! fit btw. 500 and 2500 K with MAE of 6.4%, 11.4%

C₆H₅ + C₃H₆ → 2-phenylpropene + H (P4)

1.72E+01 3.54 19720.0

PLOG/3.947E-02	1.42E+25	-3.61	20990.0/	! fit btw. 500 and 2500 K with MAE of 21.2%, 35.9%
PLOG/1.000E+00	1.53E+27	-4.00	27520.0/	! fit btw. 500 and 2500 K with MAE of 17.8%, 42.4%
PLOG/1.000E+01	3.36E+17	-1.14	25830.0/	! fit btw. 500 and 2500 K with MAE of 32.8%, 82.4%
PLOG/1.000E+02	1.72E+01	3.54	19720.0/	! fit btw. 500 and 2500 K with MAE of 37.6%, 97.3%

PLOG/3.947E-02	3.01E+38	-7.57	27340.0/	
PLOG/3.947E-02	2.64E+53	-10.65	69490.0/	! fit btw. 500 and 2500 K with MAE of 4.8%, 17.1%
PLOG/1.000E+00	7.36E+31	-5.31	30890.0/	
PLOG/1.000E+00	1.63E+03	0.92	3134.0/	! fit btw. 500 and 2500 K with MAE of 11.0%, 22.2%
PLOG/1.000E+01	6.10E+49	-10.17	49760.0/	
PLOG/1.000E+01	5.18E+01	3.13	15340.0/	! fit btw. 500 and 2500 K with MAE of 2.1%, 5.0%
PLOG/1.000E+02	3.66E+24	-2.91	38190.0/	
PLOG/1.000E+02	5.07E+16	-1.92	20760.0/	! fit btw. 500 and 2500 K with MAE of 7.5%, 23.0%

C₆H₅ + C₃H₆ → total

2.04E+05 2.19 1629.0

PLOG/3.947E-02	1.41E+04	2.51	938.5/	! fit btw. 500 and 2500 K with MAE of 1.0%, 2.0%
PLOG/1.000E+00	3.41E+04	2.40	1143.0/	! fit btw. 500 and 2500 K with MAE of 1.6%, 3.1%
PLOG/1.000E+01	9.17E+04	2.28	1396.0/	! fit btw. 500 and 2500 K with MAE of 1.4%, 3.6%
PLOG/1.000E+02	2.04E+05	2.19	1629.0/	! fit btw. 500 and 2500 K with MAE of 1.3%, 3.0%

PLOG/3.947E-02	1.96E+06	1.86	1834.0/	
PLOG/3.947E-02	1.78E+11	0.64	15180.0/	! fit btw. 500 and 2500 K with MAE of 0.2%, 0.4%
PLOG/1.000E+00	1.08E+09	1.00	3379.0/	
PLOG/1.000E+00	5.64E-01	3.71	-918.1/	! fit btw. 500 and 2500 K with MAE of 0.7%, 1.6%
PLOG/1.000E+01	1.98E+25	-3.89	13000.0/	
PLOG/1.000E+01	9.62E+02	2.84	343.9/	! fit btw. 500 and 2500 K with MAE of 0.5%, 1.4%
PLOG/1.000E+02	3.11E+71	-17.00	47220.0/	
PLOG/1.000E+02	5.86E+04	2.34	1303.0/	! fit btw. 500 and 2500 K with MAE of 0.4%, 2.0%

C₆H₆ + C₃H₅ → C₉H₁₁ (W11) 3.25E+17 -1.62 21510.0

PLOG/3.947E-02	1.40E+03	0.00	0.0/	! fit btw. 500 and 500 K with MAE of 0.0%, 0.0%
PLOG/1.000E+00	3.40E+10	0.00	15750.0/	! fit btw. 500 and 700 K with MAE of 6.9%, 10.0%
PLOG/1.000E+01	2.68E+31	-6.14	25490.0/	! fit btw. 500 and 800 K with MAE of 0.8%, 1.4%
PLOG/1.000E+02	3.25E+17	-1.62	21510.0/	! fit btw. 500 and 1000 K with MAE of 2.2%, 3.5%

PLOG/3.947E-02	1.40E+03	0.00	0.0/	
PLOG/3.947E-02	0.00E+00	0.00	0.0/	! fit btw. 500 and 500 K with MAE of 0.0%, 0.0%
PLOG/1.000E+00	3.40E+10	0.00	15750.0/	
PLOG/1.000E+00	0.00E+00	0.00	0.0/	! fit btw. 500 and 700 K with MAE of 6.9%, 10.0%
PLOG/1.000E+01	2.68E+31	-6.14	25490.0/	
PLOG/1.000E+01	0.00E+00	0.00	0.0/	! fit btw. 500 and 800 K with MAE of 0.8%, 1.4%
PLOG/1.000E+02	3.25E+17	-1.62	21510.0/	
PLOG/1.000E+02	0.00E+00	0.00	0.0/	! fit btw. 500 and 1000 K with MAE of 2.2%, 3.5%

C₆H₆ + C₃H₅ → 3-phenylpropene + H (P2) 4.72E+15 -0.50 39010.0

PLOG/3.947E-02	9.49E+03	2.69	28660.0/	! fit btw. 500 and 2500 K with MAE of 1.9%, 4.0%
PLOG/1.000E+00	1.58E+05	2.35	29570.0/	! fit btw. 500 and 2500 K with MAE of 1.2%, 3.1%

PLOG/1.000E+01	1.02E+10	1.02	33350.0/	! fit btw. 500 and 2500 K with MAE of 6.4%, 14.0%
PLOG/1.000E+02	4.72E+15	-0.50	39010.0/	! fit btw. 500 and 2500 K with MAE of 5.4%, 13.3%

PLOG/3.947E-02	3.96E+08	1.38	34640.0/	
PLOG/3.947E-02	8.24E+04	2.33	28580.0/	! fit btw. 500 and 2500 K with MAE of 0.1%, 0.2%
PLOG/1.000E+00	9.50E+23	-3.72	35470.0/	
PLOG/1.000E+00	3.44E+07	1.73	32160.0/	! fit btw. 500 and 2500 K with MAE of 0.1%, 0.3%
PLOG/1.000E+01	1.30E+15	-0.24	43140.0/	
PLOG/1.000E+01	4.41E+22	-2.83	38610.0/	! fit btw. 500 and 2500 K with MAE of 0.6%, 2.7%
PLOG/1.000E+02	3.53E+27	-4.00	45730.0/	
PLOG/1.000E+02	4.71E+02	3.13	32030.0/	! fit btw. 500 and 2500 K with MAE of 2.0%, 9.3%

C₆H₆ + C₃H₅ → total 1.40E-10 6.06 5046.0

PLOG/3.947E-02	9.60E-40	14.71	-2172.0/	! fit btw. 500 and 2500 K with MAE of 370.5%, 4085.5%
PLOG/1.000E+00	1.06E-47	16.72	-13090.0/	! fit btw. 500 and 2500 K with MAE of 172.6%, 1484.7%
PLOG/1.000E+01	3.11E-37	13.67	-8963.0/	! fit btw. 500 and 2500 K with MAE of 157.2%, 1155.8%
PLOG/1.000E+02	1.40E-10	6.06	5046.0/	! fit btw. 500 and 2500 K with MAE of 158.9%, 960.6%

PLOG/3.947E-02	6.94E-44	8.30	-54660.0/	
PLOG/3.947E-02	5.74E+04	2.47	29240.0/	! fit btw. 500 and 2500 K with MAE of 0.9%, 1.9%
PLOG/1.000E+00	6.77E-46	16.29	-9433.0/	
PLOG/1.000E+00	2.92E-46	15.98	-14610.0/	! fit btw. 500 and 2500 K with MAE of 159.1%, 1252.0%
PLOG/1.000E+01	4.86E-38	14.04	-2154.0/	
PLOG/1.000E+01	1.23E-34	12.83	-8271.0/	! fit btw. 500 and 2500 K with MAE of 154.2%, 1095.9%
PLOG/1.000E+02	2.27E+107	-29.18	57340.0/	
PLOG/1.000E+02	4.84E+32	-5.03	57550.0/	! fit btw. 500 and 2500 K with MAE of 47.9%, 314.3%

indene + CH₃ → C₁₀H₁₁ (W1) 1.79E+15 -0.97 13080.0

PLOG/3.947E-02	1.13E+58	-14.58	26890.0/	! fit btw. 500 and 900 K with MAE of 4.3%, 7.1%
PLOG/1.000E+00	2.05E+38	-8.19	21230.0/	! fit btw. 500 and 1125 K with MAE of 9.6%, 14.8%
PLOG/1.000E+01	1.38E+23	-3.43	15900.0/	! fit btw. 500 and 1250 K with MAE of 8.9%, 14.7%
PLOG/1.000E+02	1.79E+15	-0.97	13080.0/	! fit btw. 500 and 1500 K with MAE of 8.4%, 18.3%

PLOG/3.947E-02	1.13E+58	-14.58	26890.0/	
PLOG/3.947E-02	0.00E+00	0.00	0.0/	! fit btw. 500 and 900 K with MAE of 4.3%, 7.1%
PLOG/1.000E+00	5.00E+79	-20.33	44140.0/	
PLOG/1.000E+00	1.02E+46	-10.98	21550.0/	! fit btw. 500 and 1125 K with MAE of 0.6%, 1.1%
PLOG/1.000E+01	3.04E+68	-16.57	43370.0/	
PLOG/1.000E+01	1.20E+32	-6.44	17710.0/	! fit btw. 500 and 1250 K with MAE of 0.8%, 1.3%
PLOG/1.000E+02	3.20E+54	-12.16	40120.0/	
PLOG/1.000E+02	2.42E+21	-3.01	14390.0/	! fit btw. 500 and 1500 K with MAE of 1.4%, 2.3%
indene + CH₃→ total via 1-addition				
	7.54E+12	-0.28	11770.0	
PLOG/3.947E-02	2.32E-10	6.08	-912.8/	! fit btw. 500 and 2500 K with MAE of 27.0%, 103.6%
PLOG/1.000E+00	2.05E+00	3.24	4300.0/	! fit btw. 500 and 2500 K with MAE of 33.5%, 109.5%
PLOG/1.000E+01	5.90E+06	1.41	7969.0/	! fit btw. 500 and 2500 K with MAE of 35.5%, 133.4%
PLOG/1.000E+02	7.54E+12	-0.28	11770.0/	! fit btw. 500 and 2500 K with MAE of 22.6%, 106.7%
PLOG/3.947E-02	1.10E-11	6.57	6862.0/	
PLOG/3.947E-02	5.68E-08	5.34	0.0/	! fit btw. 500 and 2500 K with MAE of 26.7%, 100.4%
PLOG/1.000E+00	4.84E+36	-7.67	20740.0/	
PLOG/1.000E+00	7.21E+38	-6.87	50960.0/	! fit btw. 500 and 2500 K with MAE of 9.2%, 34.4%
PLOG/1.000E+01	2.51E+29	-5.32	18640.0/	
PLOG/1.000E+01	1.46E+78	-17.20	99380.0/	! fit btw. 500 and 2500 K with MAE of 14.9%, 56.8%
PLOG/1.000E+02	1.45E+17	-0.48	51900.0/	
PLOG/1.000E+02	2.02E+20	-2.47	15420.0/	! fit btw. 500 and 2500 K with MAE of 17.6%, 64.6%
indene + CH₃→ 3-methylindene + H (P1)				
	2.17E+19	-1.59	34520.0	
PLOG/3.947E-02	3.18E+18	-1.72	23290.0/	! fit btw. 500 and 2500 K with MAE of 18.4%, 42.2%
PLOG/1.000E+00	1.92E+27	-4.08	32100.0/	! fit btw. 500 and 2500 K with MAE of 14.9%, 26.5%
PLOG/1.000E+01	4.32E+27	-4.06	35720.0/	! fit btw. 500 and 2500 K with MAE of 16.6%, 42.4%
PLOG/1.000E+02	2.17E+19	-1.59	34520.0/	! fit btw. 500 and 2500 K with MAE of 30.5%, 69.6%
PLOG/3.947E-02	2.15E+13	-0.19	22110.0/	

PLOG/3.947E-02	7.01E+55	-13.05	39630.0/	! fit btw. 500 and 2500 K with MAE of 1.0%, 2.4%
PLOG/1.000E+00	1.96E+35	-6.45	35950.0/	
PLOG/1.000E+00	1.16E+69	-14.66	98750.0/	! fit btw. 500 and 2500 K with MAE of 5.6%, 22.4%
PLOG/1.000E+01	1.14E+33	-5.57	39660.0/	
PLOG/1.000E+01	2.56E+161	-47.95	70720.0/	! fit btw. 500 and 2500 K with MAE of 9.0%, 19.2%
PLOG/1.000E+02	8.30E+45	-9.00	54820.0/	
PLOG/1.000E+02	1.49E+07	1.59	25730.0/	! fit btw. 500 and 2500 K with MAE of 3.4%, 13.3%

indene + CH₃→ 1-methylindene + H (P2)

9.12E+18 -1.44 35520.0

PLOG/3.947E-02	6.43E+16	-1.19	23680.0/	! fit btw. 500 and 2500 K with MAE of 16.7%, 39.4%
PLOG/1.000E+00	8.94E+25	-3.66	32590.0/	! fit btw. 500 and 2500 K with MAE of 14.7%, 25.7%
PLOG/1.000E+01	6.24E+26	-3.78	36460.0/	! fit btw. 500 and 2500 K with MAE of 16.0%, 40.5%
PLOG/1.000E+02	9.12E+18	-1.44	35520.0/	! fit btw. 500 and 2500 K with MAE of 30.2%, 69.8%

PLOG/3.947E-02	2.53E+53	-12.32	39460.0/	
PLOG/3.947E-02	5.25E+12	0.03	23120.0/	! fit btw. 500 and 2500 K with MAE of 0.9%, 2.2%
PLOG/1.000E+00	1.66E+34	-6.11	36550.0/	
PLOG/1.000E+00	1.37E+63	-13.06	92600.0/	! fit btw. 500 and 2500 K with MAE of 5.2%, 20.9%
PLOG/1.000E+01	7.84E+29	-4.64	38770.0/	
PLOG/1.000E+01	1.90E+01	-0.00	1582.0/	! fit btw. 500 and 2500 K with MAE of 9.7%, 18.3%
PLOG/1.000E+02	3.55E+45	-8.86	55740.0/	
PLOG/1.000E+02	1.83E+06	1.90	26500.0/	! fit btw. 500 and 2500 K with MAE of 3.1%, 11.8%

3-methylindene + H (P1) → C₁₀H₁₁ (W1)

5.91E+21 -2.50 10260.0

PLOG/3.947E-02	6.68E+69	-17.84	25440.0/	! fit btw. 500 and 900 K with MAE of 4.2%, 7.0%
PLOG/1.000E+00	1.17E+48	-10.76	19450.0/	! fit btw. 500 and 1125 K with MAE of 10.3%, 16.4%
PLOG/1.000E+01	8.99E+30	-5.38	13520.0/	! fit btw. 500 and 1250 K with MAE of 10.0%, 16.4%
PLOG/1.000E+02	5.91E+21	-2.50	10260.0/	! fit btw. 500 and 1500 K with MAE of 9.6%, 20.7%

PLOG/3.947E-02	6.68E+69	-17.84	25440.0/	
PLOG/3.947E-02	0.00E+00	0.00	0.0/	! fit btw. 500 and 900 K with MAE of 4.2%, 7.0%
PLOG/1.000E+00	3.28E+89	-22.93	42210.0/	

PLOG/1.000E+00	4.09E+54	-13.23	19130.0/	! fit btw. 500 and 1125 K with MAE of 0.6%, 1.1%
PLOG/1.000E+01	8.29E+72	-17.55	38600.0/	
PLOG/1.000E+01	1.17E+42	-9.13	15680.0/	! fit btw. 500 and 1250 K with MAE of 0.9%, 1.7%
PLOG/1.000E+02	3.48E+62	-14.14	37980.0/	
PLOG/1.000E+02	8.84E+27	-4.59	11440.0/	! fit btw. 500 and 1500 K with MAE of 1.6%, 2.5%

3-methylindene + H (P1) → indene + CH₃ (R1)

2.29E+26 -3.11 28660.0

PLOG/3.947E-02	3.36E+25	-3.24	17440.0/	! fit btw. 500 and 2500 K with MAE of 18.4%, 41.8%
PLOG/1.000E+00	2.02E+34	-5.60	26250.0/	! fit btw. 500 and 2500 K with MAE of 15.0%, 26.7%
PLOG/1.000E+01	4.56E+34	-5.58	29860.0/	! fit btw. 500 and 2500 K with MAE of 16.8%, 42.8%
PLOG/1.000E+02	2.29E+26	-3.11	28660.0/	! fit btw. 500 and 2500 K with MAE of 30.5%, 70.1%

PLOG/3.947E-02	2.41E+53	-11.68	29430.0/	
PLOG/3.947E-02	2.81E+24	-2.78	21540.0/	! fit btw. 500 and 2500 K with MAE of 1.4%, 2.8%
PLOG/1.000E+00	1.94E+42	-7.96	30090.0/	
PLOG/1.000E+00	2.99E+76	-16.28	93640.0/	! fit btw. 500 and 2500 K with MAE of 5.7%, 22.8%
PLOG/1.000E+01	1.25E+40	-7.09	33820.0/	
PLOG/1.000E+01	2.35E+169	-49.78	65080.0/	! fit btw. 500 and 2500 K with MAE of 9.1%, 19.5%
PLOG/1.000E+02	1.04E+53	-10.54	48980.0/	
PLOG/1.000E+02	8.69E+13	0.15	19750.0/	! fit btw. 500 and 2500 K with MAE of 3.4%, 13.4%

3-methylindene + H (P1) → total

8.49E+09 1.11 5388.0

PLOG/3.947E-02	1.93E+09	1.29	5030.0/	! fit btw. 500 and 2500 K with MAE of 1.0%, 2.5%
PLOG/1.000E+00	2.71E+09	1.25	5100.0/	! fit btw. 500 and 2500 K with MAE of 0.6%, 1.8%
PLOG/1.000E+01	4.40E+09	1.19	5216.0/	! fit btw. 500 and 2500 K with MAE of 0.6%, 1.2%
PLOG/1.000E+02	8.49E+09	1.11	5388.0/	! fit btw. 500 and 2500 K with MAE of 1.1%, 2.3%

PLOG/3.947E-02	1.15E+11	0.71	5516.0/	
PLOG/3.947E-02	8.22E+13	0.00	12540.0/	! fit btw. 500 and 2500 K with MAE of 0.0%, 0.2%
PLOG/1.000E+00	6.88E+69	-15.48	66180.0/	
PLOG/1.000E+00	3.59E+09	1.21	5134.0/	! fit btw. 500 and 2500 K with MAE of 0.2%, 0.6%
PLOG/1.000E+01	6.74E+09	1.14	5353.0/	

PLOG/1.000E+01	5.13E-01	2.54	-6007.0/	! fit btw. 500 and 2500 K with MAE of 0.4%, 1.2%
PLOG/1.000E+02	8.76E+42	-8.59	28960.0/	
PLOG/1.000E+02	1.91E+09	1.29	4986.0/	! fit btw. 500 and 2500 K with MAE of 0.3%, 1.2%

3-methylindene + H (P1) → 1-methylindene + H (P2)

2.59E+23 -2.39 30770.0

PLOG/3.947E-02	2.15E+19	-1.58	18020.0/	! fit btw. 500 and 2500 K with MAE of 14.2%, 34.6%
PLOG/1.000E+00	7.98E+28	-4.18	27020.0/	! fit btw. 500 and 2500 K with MAE of 14.2%, 24.4%
PLOG/1.000E+01	3.02E+30	-4.51	31260.0/	! fit btw. 500 and 2500 K with MAE of 15.2%, 38.1%
PLOG/1.000E+02	2.59E+23	-2.39	30770.0/	! fit btw. 500 and 2500 K with MAE of 29.8%, 70.8%

PLOG/3.947E-02	3.72E+16	-0.74	18110.0/	
PLOG/3.947E-02	3.01E+55	-12.63	33310.0/	! fit btw. 500 and 2500 K with MAE of 0.8%, 1.7%
PLOG/1.000E+00	2.74E+37	-6.71	31080.0/	
PLOG/1.000E+00	8.69E+60	-12.26	79400.0/	! fit btw. 500 and 2500 K with MAE of 4.8%, 19.1%
PLOG/1.000E+01	5.37E+34	-5.69	34320.0/	
PLOG/1.000E+01	2.30E+06	0.51	7215.0/	! fit btw. 500 and 2500 K with MAE of 9.1%, 18.0%
PLOG/1.000E+02	7.90E+51	-10.35	52140.0/	
PLOG/1.000E+02	4.50E+09	1.29	21380.0/	! fit btw. 500 and 2500 K with MAE of 2.6%, 8.9%

1-methylindene + H (P2) → C₁₀H₁₁ (W1)

2.29E+23 -2.91 9452.0

PLOG/3.947E-02	4.01E+74	-19.30	25450.0/	! fit btw. 500 and 900 K with MAE of 4.0%, 6.7%
PLOG/1.000E+00	5.06E+51	-11.82	19300.0/	! fit btw. 500 and 1125 K with MAE of 10.4%, 17.0%
PLOG/1.000E+01	2.69E+33	-6.06	13020.0/	! fit btw. 500 and 1250 K with MAE of 10.4%, 17.0%
PLOG/1.000E+02	2.29E+23	-2.91	9452.0/	! fit btw. 500 and 1500 K with MAE of 10.0%, 21.5%

PLOG/3.947E-02	4.01E+74	-19.30	25450.0/	
PLOG/3.947E-02	0.00E+00	0.00	0.0/	! fit btw. 500 and 900 K with MAE of 4.0%, 6.7%
PLOG/1.000E+00	9.16E+96	-25.10	44210.0/	
PLOG/1.000E+00	1.42E+60	-14.85	19820.0/	! fit btw. 500 and 1125 K with MAE of 0.2%, 0.5%
PLOG/1.000E+01	3.35E+80	-19.73	41120.0/	
PLOG/1.000E+01	1.50E+42	-9.05	14480.0/	! fit btw. 500 and 1250 K with MAE of 0.8%, 1.4%
PLOG/1.000E+02	6.05E+64	-14.74	37490.0/	

PLOG/1.000E+02 3.30E+29 -5.00 10570.0/

! fit btw. 500 and 1500 K with MAE of 1.6%, 2.6%

1-methylindene + H (P2) → indene + CH₃ (R1)

3.72E+26 -3.12 26710.0

PLOG/3.947E-02 2.62E+24 -2.87 14860.0/
PLOG/1.000E+00 3.65E+33 -5.34 23770.0/
PLOG/1.000E+01 2.55E+34 -5.46 27640.0/
PLOG/1.000E+02 3.72E+26 -3.12 26710.0/

! fit btw. 500 and 2500 K with MAE of 17.1%, 39.9%
! fit btw. 500 and 2500 K with MAE of 15.1%, 26.4%
! fit btw. 500 and 2500 K with MAE of 16.1%, 40.2%
! fit btw. 500 and 2500 K with MAE of 29.9%, 69.4%

PLOG/3.947E-02 1.49E+60 -13.74 30310.0/
PLOG/3.947E-02 1.29E+20 -1.59 14250.0/
PLOG/1.000E+00 1.08E+42 -7.85 27830.0/
PLOG/1.000E+00 8.86E+69 -14.52 83020.0/
PLOG/1.000E+01 1.84E+39 -6.81 31160.0/
PLOG/1.000E+01 3.12E+153 -44.95 56280.0/
PLOG/1.000E+02 7.14E+53 -10.74 47350.0/
PLOG/1.000E+02 3.97E+13 0.31 17640.0/

! fit btw. 500 and 2500 K with MAE of 1.0%, 2.4%

! fit btw. 500 and 2500 K with MAE of 5.3%, 21.0%

! fit btw. 500 and 2500 K with MAE of 9.2%, 19.2%

! fit btw. 500 and 2500 K with MAE of 3.1%, 11.9%

1-methylindene + H (P2) → 3-methylindene + H (P1)

1.00E+24 -2.55 27810.0

PLOG/3.947E-02 8.34E+19 -1.74 15060.0/
PLOG/1.000E+00 3.09E+29 -4.34 24050.0/
PLOG/1.000E+01 1.17E+31 -4.67 28290.0/
PLOG/1.000E+02 1.00E+24 -2.55 27810.0/

! fit btw. 500 and 2500 K with MAE of 14.5%, 35.4%
! fit btw. 500 and 2500 K with MAE of 14.5%, 24.9%
! fit btw. 500 and 2500 K with MAE of 15.2%, 37.4%
! fit btw. 500 and 2500 K with MAE of 29.5%, 70.0%

PLOG/3.947E-02 1.28E+17 -0.89 15200.0/
PLOG/3.947E-02 4.83E+55 -12.67 30190.0/
PLOG/1.000E+00 1.93E+38 -6.95 28240.0/
PLOG/1.000E+00 3.38E+60 -12.16 75190.0/
PLOG/1.000E+01 1.55E+35 -5.82 31260.0/
PLOG/1.000E+01 2.82E+06 0.39 3365.0/
PLOG/1.000E+02 2.94E+52 -10.51 49140.0/
PLOG/1.000E+02 1.89E+10 1.12 18470.0/

! fit btw. 500 and 2500 K with MAE of 0.8%, 1.8%

! fit btw. 500 and 2500 K with MAE of 4.8%, 19.0%

! fit btw. 500 and 2500 K with MAE of 9.2%, 18.3%

! fit btw. 500 and 2500 K with MAE of 2.6%, 9.2%

1-methylindene + H (P2) → total				4.05E+10	0.98	4222.0	
PLOG/3.947E-02	1.47E+10	1.10	3974.0/				! fit btw. 500 and 2500 K with MAE of 1.1%, 2.6%
PLOG/1.000E+00	1.77E+10	1.08	4012.0/				! fit btw. 500 and 2500 K with MAE of 0.9%, 2.3%
PLOG/1.000E+01	2.44E+10	1.04	4089.0/				! fit btw. 500 and 2500 K with MAE of 0.8%, 1.9%
PLOG/1.000E+02	4.05E+10	0.98	4222.0/				! fit btw. 500 and 2500 K with MAE of 1.2%, 2.6%
PLOG/3.947E-02	5.75E+11	0.57	4321.0/				
PLOG/3.947E-02	1.23E+14	0.00	10310.0/				! fit btw. 500 and 2500 K with MAE of 0.1%, 0.2%
PLOG/1.000E+00	1.04E+14	0.00	10490.0/				
PLOG/1.000E+00	3.25E+11	0.66	4299.0/				! fit btw. 500 and 2500 K with MAE of 0.2%, 0.5%
PLOG/1.000E+01	2.77E+11	0.71	5797.0/				
PLOG/1.000E+01	2.11E+10	0.91	3447.0/				! fit btw. 500 and 2500 K with MAE of 0.3%, 0.8%
PLOG/1.000E+02	2.43E+31	-5.15	20260.0/				
PLOG/1.000E+02	8.60E+09	1.16	3772.0/				! fit btw. 500 and 2500 K with MAE of 0.2%, 1.0%
indene + CH₃→ C₁₀H₁₁ (W2)				1.26E+15	-0.83	10880.0	
PLOG/3.947E-02	5.60E+53	-12.95	24400.0/				! fit btw. 500 and 1125 K with MAE of 11.7%, 19.6%
PLOG/1.000E+00	1.43E+29	-5.22	15860.0/				! fit btw. 500 and 1250 K with MAE of 11.5%, 19.1%
PLOG/1.000E+01	4.07E+21	-2.85	13310.0/				! fit btw. 500 and 1500 K with MAE of 12.4%, 27.1%
PLOG/1.000E+02	1.26E+15	-0.83	10880.0/				! fit btw. 500 and 1800 K with MAE of 12.1%, 31.9%
PLOG/3.947E-02	1.71E+97	-25.73	48000.0/				
PLOG/3.947E-02	1.32E+59	-15.11	23300.0/				! fit btw. 500 and 1125 K with MAE of 0.6%, 1.0%
PLOG/1.000E+00	1.70E+82	-20.64	47400.0/				
PLOG/1.000E+00	6.34E+37	-8.17	17320.0/				! fit btw. 500 and 1250 K with MAE of 1.1%, 1.9%
PLOG/1.000E+01	1.65E+70	-16.73	45710.0/				
PLOG/1.000E+01	4.89E+27	-4.92	14250.0/				! fit btw. 500 and 1500 K with MAE of 2.0%, 3.5%
PLOG/1.000E+02	9.96E+55	-12.32	41860.0/				
PLOG/1.000E+02	1.26E+20	-2.51	11820.0/				! fit btw. 500 and 1800 K with MAE of 2.6%, 4.6%
indene + CH₃→ total via 2-addition				3.81E+21	-2.75	14000.0	

PLOG/3.947E-02	3.80E-01	3.35	311.8/	! fit btw. 500 and 2500 K with MAE of 45.8%, 148.3%
PLOG/1.000E+00	3.01E+10	0.26	6450.0/	! fit btw. 500 and 2500 K with MAE of 54.4%, 228.6%
PLOG/1.000E+01	5.57E+18	-2.03	11600.0/	! fit btw. 500 and 2500 K with MAE of 34.4%, 179.9%
PLOG/1.000E+02	3.81E+21	-2.75	14000.0/	! fit btw. 500 and 2500 K with MAE of 27.4%, 114.9%

PLOG/3.947E-02	1.22E+51	-12.12	23470.0/	
PLOG/3.947E-02	2.32E+32	-5.21	40900.0/	! fit btw. 500 and 2500 K with MAE of 9.5%, 31.1%
PLOG/1.000E+00	1.59E+42	-9.17	21450.0/	
PLOG/1.000E+00	7.72E+81	-18.27	99950.0/	! fit btw. 500 and 2500 K with MAE of 21.8%, 87.7%
PLOG/1.000E+01	5.55E+19	-1.07	58270.0/	
PLOG/1.000E+01	3.18E+24	-3.75	14280.0/	! fit btw. 500 and 2500 K with MAE of 25.2%, 118.3%
PLOG/1.000E+02	1.31E+135	-34.56	100800.0/	
PLOG/1.000E+02	1.15E+17	-1.51	11020.0/	! fit btw. 500 and 2500 K with MAE of 14.7%, 86.0%

indene + CH₃→ 2-methylindene + H (P3)

2.28E+11 0.81 31400.0

PLOG/3.947E-02	2.46E+25	-3.53	27980.0/	! fit btw. 500 and 2500 K with MAE of 19.5%, 30.5%
PLOG/1.000E+00	4.86E+29	-4.59	34950.0/	! fit btw. 500 and 2500 K with MAE of 16.5%, 37.3%
PLOG/1.000E+01	1.89E+24	-2.94	35420.0/	! fit btw. 500 and 2500 K with MAE of 28.8%, 76.6%
PLOG/1.000E+02	2.28E+11	0.81	31400.0/	! fit btw. 500 and 2500 K with MAE of 40.3%, 87.9%

PLOG/3.947E-02	3.30E+41	-8.34	35460.0/	
PLOG/3.947E-02	1.73E+39	-6.89	54820.0/	! fit btw. 500 and 2500 K with MAE of 3.7%, 13.6%
PLOG/1.000E+00	1.32E+33	-5.55	37410.0/	
PLOG/1.000E+00	8.75E+14	-7.59	-16970.0/	! fit btw. 500 and 2500 K with MAE of 11.2%, 23.1%
PLOG/1.000E+01	3.32E+39	-7.18	46870.0/	
PLOG/1.000E+01	5.36E+75	-20.09	46650.0/	! fit btw. 500 and 2500 K with MAE of 5.9%, 13.7%
PLOG/1.000E+02	8.97E+34	-5.72	49890.0/	
PLOG/1.000E+02	3.82E+26	-4.67	31710.0/	! fit btw. 500 and 2500 K with MAE of 7.3%, 14.5%

2-methylindene + H (P3)→ C₁₀H₁₁ (W2)

1.55E+21 -2.41 8117.0

PLOG/3.947E-02	1.96E+65	-16.28	23320.0/	! fit btw. 500 and 1125 K with MAE of 11.8%, 20.7%
PLOG/1.000E+00	9.03E+37	-7.66	14030.0/	! fit btw. 500 and 1250 K with MAE of 12.7%, 20.9%

PLOG/1.000E+01	7.25E+28	-4.80	10960.0/	! fit btw. 500 and 1500 K with MAE of 13.9%, 30.0%
PLOG/1.000E+02	1.55E+21	-2.41	8117.0/	! fit btw. 500 and 1800 K with MAE of 13.6%, 35.6%

PLOG/3.947E-02	1.63E+106	-28.32	45390.0/	
PLOG/3.947E-02	2.99E+68	-17.81	21130.0/	! fit btw. 500 and 1125 K with MAE of 0.6%, 0.9%
PLOG/1.000E+00	8.43E+91	-23.35	45800.0/	
PLOG/1.000E+00	2.09E+46	-10.56	15160.0/	! fit btw. 500 and 1250 K with MAE of 1.1%, 1.9%
PLOG/1.000E+01	7.79E+78	-19.10	43980.0/	
PLOG/1.000E+01	5.36E+34	-6.83	11650.0/	! fit btw. 500 and 1500 K with MAE of 2.2%, 3.8%
PLOG/1.000E+02	4.45E+63	-14.36	39910.0/	
PLOG/1.000E+02	1.45E+26	-4.11	8910.0/	! fit btw. 500 and 1800 K with MAE of 2.8%, 5.2%

2-methylindene + H (P3)→ indene + CH₃

6.36E+17 -0.70 24910.0

PLOG/3.947E-02	6.84E+31	-5.04	21490.0/	! fit btw. 500 and 2500 K with MAE of 19.5%, 30.7%
PLOG/1.000E+00	1.35E+36	-6.10	28460.0/	! fit btw. 500 and 2500 K with MAE of 16.7%, 37.9%
PLOG/1.000E+01	5.26E+30	-4.45	28930.0/	! fit btw. 500 and 2500 K with MAE of 28.9%, 77.2%
PLOG/1.000E+02	6.36E+17	-0.70	24910.0/	! fit btw. 500 and 2500 K with MAE of 40.4%, 87.4%

PLOG/3.947E-02	5.72E+47	-9.79	28890.0/	
PLOG/3.947E-02	6.72E+45	-8.43	48710.0/	! fit btw. 500 and 2500 K with MAE of 3.7%, 14.0%
PLOG/1.000E+00	4.06E+39	-7.07	30950.0/	
PLOG/1.000E+00	2.46E+21	-9.10	-23500.0/	! fit btw. 500 and 2500 K with MAE of 11.4%, 23.4%
PLOG/1.000E+01	8.95E+45	-8.68	40370.0/	
PLOG/1.000E+01	1.06E+83	-21.87	40400.0/	! fit btw. 500 and 2500 K with MAE of 6.0%, 14.0%
PLOG/1.000E+02	1.76E+41	-7.19	43270.0/	
PLOG/1.000E+02	2.36E+33	-6.29	25280.0/	! fit btw. 500 and 2500 K with MAE of 7.3%, 14.4%

2-methylindene + H (P3)→ total

6.31E+09 1.02 3151.0

PLOG/3.947E-02	2.02E+09	1.16	2852.0/	! fit btw. 500 and 2500 K with MAE of 0.8%, 2.3%
PLOG/1.000E+00	2.90E+09	1.12	2936.0/	! fit btw. 500 and 2500 K with MAE of 0.6%, 1.7%
PLOG/1.000E+01	4.41E+09	1.06	3044.0/	! fit btw. 500 and 2500 K with MAE of 0.9%, 1.9%
PLOG/1.000E+02	6.31E+09	1.02	3151.0/	! fit btw. 500 and 2500 K with MAE of 1.7%, 2.9%

PLOG/3.947E-02 2.94E+13 -0.00 10020.0/
PLOG/3.947E-02 1.26E+11 0.58 3356.0/
PLOG/1.000E+00 1.82E+11 0.53 6837.0/
PLOG/1.000E+00 9.60E+09 0.92 2920.0/
PLOG/1.000E+01 9.51E+11 0.34 5239.0/
PLOG/1.000E+01 7.88E+07 1.46 1769.0/
PLOG/1.000E+02 3.26E+35 -6.41 24540.0/
PLOG/1.000E+02 2.31E+09 1.13 2815.0/

! fit btw. 500 and 2500 K with MAE of 0.1%, 0.4%

! fit btw. 500 and 2500 K with MAE of 0.3%, 0.7%

! fit btw. 500 and 2500 K with MAE of 0.2%, 0.6%

! fit btw. 500 and 2500 K with MAE of 0.2%, 0.7%

1-methylindenyl (W101) → naphthalene + H (P1)

1.25E+40 -7.11 81540.0

PLOG/3.947E-02 1.82E+48 -10.48 66750.0/
PLOG/1.000E+00 1.08E+53 -11.48 74650.0/
PLOG/1.000E+01 1.36E+52 -10.88 80400.0/
PLOG/1.000E+02 1.25E+40 -7.11 81540.0/

! fit btw. 500 and 1500 K with MAE of 14.0%, 29.2%

! fit btw. 500 and 1800 K with MAE of 12.5%, 26.7%

! fit btw. 500 and 2000 K with MAE of 20.7%, 43.0%

! fit btw. 500 and 2250 K with MAE of 33.7%, 99.2%

PLOG/3.947E-02 5.96E+96 -24.34 98890.0/
PLOG/3.947E-02 5.56E+59 -14.28 69460.0/
PLOG/1.000E+00 3.41E+77 -18.39 92580.0/
PLOG/1.000E+00 4.47E+56 -12.87 74200.0/
PLOG/1.000E+01 3.06E+74 -17.17 96450.0/
PLOG/1.000E+01 1.68E+51 -11.13 76410.0/
PLOG/1.000E+02 3.55E+65 -14.22 100500.0/
PLOG/1.000E+02 9.29E+38 -7.43 76460.0/

! fit btw. 500 and 1500 K with MAE of 2.0%, 3.7%

! fit btw. 500 and 1800 K with MAE of 3.5%, 6.0%

! fit btw. 500 and 2000 K with MAE of 4.7%, 11.6%

! fit btw. 500 and 2250 K with MAE of 11.2%, 34.5%

1-methylindenyl (W101) → benzofulvene + H (P2)

4.18E+18 -1.14 56390.0

PLOG/3.947E-02 2.40E+43 -8.77 65980.0/
PLOG/1.000E+00 1.19E+32 -5.24 61940.0/
PLOG/1.000E+01 1.52E+24 -2.83 58750.0/
PLOG/1.000E+02 4.18E+18 -1.14 56390.0/

! fit btw. 500 and 1500 K with MAE of 21.2%, 41.4%

! fit btw. 500 and 1800 K with MAE of 22.8%, 54.4%

! fit btw. 500 and 2000 K with MAE of 19.8%, 56.7%

! fit btw. 500 and 2250 K with MAE of 15.5%, 50.7%

PLOG/3.947E-02 2.38E+62 -15.14 69840.0/

PLOG/3.947E-02	1.29E+87	-21.32	93570.0/	! fit btw. 500 and 1500 K with MAE of 3.2%, 5.7%
PLOG/1.000E+00	3.08E+03	3.42	49750.0/	
PLOG/1.000E+00	-1.74E+34	-4.88	80650.0/	! fit btw. 500 and 1800 K with MAE of 1.4%, 2.7%
PLOG/1.000E+01	5.88E+02	3.64	49410.0/	
PLOG/1.000E+01	-7.83E+24	-2.22	75240.0/	! fit btw. 500 and 2000 K with MAE of 2.0%, 3.5%
PLOG/1.000E+02	3.59E+56	-11.61	89040.0/	
PLOG/1.000E+02	1.57E+23	-2.67	57250.0/	! fit btw. 500 and 2250 K with MAE of 4.3%, 7.0%

1-methylene-indan-3-yl (W102) → naphthalene + H (P1)

3.71E+34 -5.53 65410.0

PLOG/3.947E-02	2.60E+64	-15.65	58790.0/	! fit btw. 500 and 1125 K with MAE of 5.0%, 9.5%
PLOG/1.000E+00	4.88E+63	-14.83	65330.0/	! fit btw. 500 and 1375 K with MAE of 9.4%, 20.1%
PLOG/1.000E+01	2.57E+52	-11.04	66880.0/	! fit btw. 500 and 1500 K with MAE of 15.8%, 31.6%
PLOG/1.000E+02	3.71E+34	-5.53	65410.0/	! fit btw. 500 and 1800 K with MAE of 25.2%, 44.6%

PLOG/3.947E-02	1.58E+82	-20.88	68560.0/	
PLOG/3.947E-02	7.79E+61	-15.43	54630.0/	! fit btw. 500 and 1125 K with MAE of 0.5%, 0.7%
PLOG/1.000E+00	3.26E+81	-20.00	75860.0/	
PLOG/1.000E+00	5.54E+59	-14.30	59600.0/	! fit btw. 500 and 1375 K with MAE of 1.1%, 2.8%
PLOG/1.000E+01	7.89E+77	-18.38	82580.0/	
PLOG/1.000E+01	4.36E+52	-11.77	62710.0/	! fit btw. 500 and 1500 K with MAE of 3.1%, 7.4%
PLOG/1.000E+02	6.68E+38	-6.73	68320.0/	
PLOG/1.000E+02	2.25E+08	-2.14	26530.0/	! fit btw. 500 and 1800 K with MAE of 16.9%, 29.7%

1-methylene-indan-3-yl (W102) → benzofulvene + H (P2)

2.94E+20 -1.81 44010.0

PLOG/3.947E-02	1.70E+49	-10.87	53830.0/	! fit btw. 500 and 1125 K with MAE of 8.6%, 14.1%
PLOG/1.000E+00	8.50E+35	-6.61	49750.0/	! fit btw. 500 and 1375 K with MAE of 11.9%, 19.9%
PLOG/1.000E+01	2.17E+25	-3.32	45790.0/	! fit btw. 500 and 1500 K with MAE of 10.1%, 21.0%
PLOG/1.000E+02	2.94E+20	-1.81	44010.0/	! fit btw. 500 and 1800 K with MAE of 10.1%, 24.1%

PLOG/3.947E-02	1.99E+82	-20.58	72030.0/	
PLOG/3.947E-02	5.85E+52	-12.42	52320.0/	! fit btw. 500 and 1125 K with MAE of 0.6%, 1.2%
PLOG/1.000E+00	3.00E+76	-18.30	75050.0/	

PLOG/1.000E+00	4.85E+41	-8.69	49980.0/	! fit btw. 500 and 1375 K with MAE of 0.7%, 1.6%
PLOG/1.000E+01	9.72E+65	-14.93	73220.0/	
PLOG/1.000E+01	1.51E+31	-5.32	46730.0/	! fit btw. 500 and 1500 K with MAE of 1.4%, 2.5%
PLOG/1.000E+02	3.48E+53	-11.11	69310.0/	
PLOG/1.000E+02	1.02E+25	-3.35	44770.0/	! fit btw. 500 and 1800 K with MAE of 1.7%, 3.3%

1-methylene-indan-2-yl (W119) → naphthalene + H (P1)

5.43E+42 -7.62 85780.0

PLOG/3.947E-02	2.74E+80	-19.87	78040.0/	! fit btw. 500 and 1250 K with MAE of 13.1%, 26.6%
PLOG/1.000E+00	3.83E+70	-16.39	82190.0/	! fit btw. 500 and 1500 K with MAE of 20.3%, 37.2%
PLOG/1.000E+01	4.66E+57	-12.19	84280.0/	! fit btw. 500 and 1650 K with MAE of 28.1%, 55.7%
PLOG/1.000E+02	5.43E+42	-7.62	85780.0/	! fit btw. 500 and 2000 K with MAE of 49.2%, 126.9%

PLOG/3.947E-02	5.76E+97	-24.96	87330.0/	
PLOG/3.947E-02	2.19E+73	-19.16	66400.0/	! fit btw. 500 and 1250 K with MAE of 4.9%, 14.9%
PLOG/1.000E+00	1.32E+79	-18.86	87240.0/	
PLOG/1.000E+00	3.34E+43	-68.53	-301400.0/	! fit btw. 500 and 1500 K with MAE of 11.6%, 34.8%
PLOG/1.000E+01	9.97E+140	-36.34	134000.0/	
PLOG/1.000E+01	6.95E+37	-6.51	73590.0/	! fit btw. 500 and 1650 K with MAE of 8.9%, 30.5%
PLOG/1.000E+02	1.93E+55	-12.61	82930.0/	
PLOG/1.000E+02	1.09E+76	-17.02	108500.0/	! fit btw. 500 and 2000 K with MAE of 18.2%, 85.4%

1-methylene-indan-2-yl (W119) → benzofulvene + H (P2)

2.15E+21 -2.00 47790.0

PLOG/3.947E-02	1.75E+51	-11.30	58810.0/	! fit btw. 500 and 1250 K with MAE of 14.4%, 24.1%
PLOG/1.000E+00	3.34E+35	-6.38	53280.0/	! fit btw. 500 and 1500 K with MAE of 16.5%, 27.8%
PLOG/1.000E+01	1.60E+25	-3.21	49210.0/	! fit btw. 500 and 1650 K with MAE of 13.4%, 28.5%
PLOG/1.000E+02	2.15E+21	-2.00	47790.0/	! fit btw. 500 and 2000 K with MAE of 13.3%, 32.4%

PLOG/3.947E-02	2.55E+126	-33.35	100600.0/	
PLOG/3.947E-02	3.18E+42	-8.87	53640.0/	! fit btw. 500 and 1250 K with MAE of 0.8%, 1.6%
PLOG/1.000E+00	8.03E+92	-22.86	90070.0/	
PLOG/1.000E+00	8.05E+34	-6.43	51360.0/	! fit btw. 500 and 1500 K with MAE of 1.8%, 3.0%
PLOG/1.000E+01	2.19E+64	-14.29	76860.0/	

PLOG/1.000E+01 9.87E+33 -6.13 51110.0/
PLOG/1.000E+02 5.13E+53 -11.03 73750.0/
PLOG/1.000E+02 4.01E+26 -3.78 48710.0/

! fit btw. 500 and 1650 K with MAE of 2.1%, 3.9%

! fit btw. 500 and 2000 K with MAE of 2.4%, 4.5%

2-methylindenyl (W106) → naphthalene + H (P1)

9.44E+30 -4.61 84230.0

PLOG/3.947E-02 7.42E+27 -4.22 71860.0/
PLOG/1.000E+00 3.82E+30 -4.87 75250.0/
PLOG/1.000E+01 8.92E+34 -5.94 81300.0/
PLOG/1.000E+02 9.44E+30 -4.61 84230.0/

! fit btw. 500 and 1800 K with MAE of 23.3%, 64.2%

! fit btw. 500 and 2250 K with MAE of 16.4%, 62.1%

! fit btw. 500 and 2500 K with MAE of 9.9%, 24.8%

! fit btw. 500 and 2500 K with MAE of 24.1%, 57.3%

PLOG/3.947E-02 6.49E+61 -13.80 95790.0/
PLOG/3.947E-02 8.45E+52 -12.38 78580.0/
PLOG/1.000E+00 8.35E+97 -23.39 134400.0/
PLOG/1.000E+00 6.81E+34 -6.25 76330.0/
PLOG/1.000E+01 4.16E+41 -7.79 86810.0/
PLOG/1.000E+01 1.72E+34 -6.24 77790.0/
PLOG/1.000E+02 4.21E+46 -8.95 96470.0/
PLOG/1.000E+02 3.38E+28 -4.54 78560.0/

! fit btw. 500 and 1800 K with MAE of 7.7%, 20.2%

! fit btw. 500 and 2250 K with MAE of 4.2%, 7.2%

! fit btw. 500 and 2500 K with MAE of 5.6%, 11.4%

! fit btw. 500 and 2500 K with MAE of 3.8%, 11.2%

2-methylindenyl (W106) → benzofluvene + H (P2)

2.34E+13 0.50 81210.0

PLOG/3.947E-02 1.19E+36 -6.38 86180.0/
PLOG/1.000E+00 4.45E+24 -2.94 82160.0/
PLOG/1.000E+01 1.39E+19 -1.28 80930.0/
PLOG/1.000E+02 2.34E+13 0.50 81210.0/

! fit btw. 500 and 1800 K with MAE of 37.1%, 92.3%

! fit btw. 500 and 2250 K with MAE of 50.9%, 169.4%

! fit btw. 500 and 2500 K with MAE of 43.5%, 138.8%

! fit btw. 500 and 2500 K with MAE of 29.0%, 97.2%

PLOG/3.947E-02 7.72E+35 -6.80 82710.0/
PLOG/3.947E-02 1.97E+92 -22.30 124800.0/
PLOG/1.000E+00 7.52E+23 -3.21 78090.0/
PLOG/1.000E+00 1.68E+78 -17.85 123300.0/
PLOG/1.000E+01 3.81E+45 -8.57 102300.0/
PLOG/1.000E+01 2.31E+38 -7.79 84080.0/
PLOG/1.000E+02 3.33E+33 -5.06 97760.0/

! fit btw. 500 and 1800 K with MAE of 7.8%, 17.1%

! fit btw. 500 and 2250 K with MAE of 10.3%, 19.8%

! fit btw. 500 and 2500 K with MAE of 14.2%, 46.4%

PLOG/1.000E+02	5.67E+25	-3.80	82580.0/	! fit btw. 500 and 2500 K with MAE of 9.6%, 36.7%
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2-methylindenyl (W106) → 2-benzofluvene + H (P109)

4.36E+12 0.52 68060.0

PLOG/3.947E-02	1.68E+30	-4.80	75620.0/	! fit btw. 500 and 1800 K with MAE of 24.0%, 67.1%
PLOG/1.000E+00	4.00E+24	-3.05	73610.0/	! fit btw. 500 and 2250 K with MAE of 25.8%, 89.5%
PLOG/1.000E+01	1.23E+19	-1.39	71180.0/	! fit btw. 500 and 2500 K with MAE of 20.3%, 70.3%
PLOG/1.000E+02	4.36E+12	0.52	68060.0/	! fit btw. 500 and 2500 K with MAE of 8.3%, 32.4%

PLOG/3.947E-02	1.14E+02	3.72	63500.0/	
PLOG/3.947E-02	-2.83E+35	-5.28	97520.0/	! fit btw. 500 and 1800 K with MAE of 2.1%, 3.9%
PLOG/1.000E+00	7.31E+80	-18.60	120500.0/	
PLOG/1.000E+00	3.89E+28	-4.45	73850.0/	! fit btw. 500 and 2250 K with MAE of 6.4%, 10.2%
PLOG/1.000E+01	1.33E+67	-14.52	115000.0/	
PLOG/1.000E+01	5.05E+22	-2.62	71700.0/	! fit btw. 500 and 2500 K with MAE of 5.9%, 9.7%
PLOG/1.000E+02	1.31E+28	-3.68	83290.0/	
PLOG/1.000E+02	2.65E+21	-2.30	70660.0/	! fit btw. 500 and 2500 K with MAE of 3.6%, 11.9%

benzofulvene + H → C₁₀H₉ (W101)

5.57E+18 -1.28 5738.0

PLOG/3.947E-02	5.12E+44	-9.28	15820.0/	! fit btw. 500 and 1500 K with MAE of 22.0%, 46.7%
PLOG/1.000E+00	2.26E+33	-5.73	11800.0/	! fit btw. 500 and 1800 K with MAE of 24.5%, 65.7%
PLOG/1.000E+01	7.22E+24	-3.13	8346.0/	! fit btw. 500 and 2000 K with MAE of 21.1%, 67.1%
PLOG/1.000E+02	5.57E+18	-1.28	5738.0/	! fit btw. 500 and 2250 K with MAE of 16.2%, 58.4%

PLOG/3.947E-02	1.63E+49	-10.56	18750.0/	
PLOG/3.947E-02	2.96E+35	-8.88	-2568.0/	! fit btw. 500 and 1500 K with MAE of 14.8%, 47.5%
PLOG/1.000E+00	1.31E+03	3.44	-1094.0/	
PLOG/1.000E+00	-5.29E+31	-4.28	27780.0/	! fit btw. 500 and 1800 K with MAE of 1.5%, 2.7%
PLOG/1.000E+01	3.49E+03	3.30	-1000.0/	
PLOG/1.000E+01	-6.31E+24	-2.31	24490.0/	! fit btw. 500 and 2000 K with MAE of 2.3%, 3.7%
PLOG/1.000E+02	3.46E+63	-13.62	44500.0/	
PLOG/1.000E+02	3.06E+23	-2.85	6768.0/	! fit btw. 500 and 2250 K with MAE of 5.1%, 9.5%

benzofulvene + H → C₁₀H₉ (W102)				1.13E+19	-1.51	6197.0	
PLOG/3.947E-02	1.78E+49	-11.01	16560.0/				! fit btw. 500 and 1125 K with MAE of 9.4%, 14.8%
PLOG/1.000E+00	5.66E+35	-6.69	12440.0/				! fit btw. 500 and 1375 K with MAE of 13.3%, 24.0%
PLOG/1.000E+01	1.49E+24	-3.10	8072.0/				! fit btw. 500 and 1500 K with MAE of 10.7%, 23.8%
PLOG/1.000E+02	1.13E+19	-1.51	6197.0/				! fit btw. 500 and 1800 K with MAE of 10.9%, 28.9%
PLOG/3.947E-02	4.73E+88	-22.58	38350.0/				
PLOG/3.947E-02	9.18E+55	-13.51	16460.0/				! fit btw. 500 and 1125 K with MAE of 0.7%, 1.5%
PLOG/1.000E+00	3.42E+82	-20.17	41590.0/				
PLOG/1.000E+00	2.99E+42	-9.05	13090.0/				! fit btw. 500 and 1375 K with MAE of 1.4%, 2.3%
PLOG/1.000E+01	3.03E+69	-16.03	38630.0/				
PLOG/1.000E+01	2.45E+30	-5.20	9218.0/				! fit btw. 500 and 1500 K with MAE of 1.9%, 3.2%
PLOG/1.000E+02	8.70E+52	-11.01	32160.0/				
PLOG/1.000E+02	3.43E+26	-3.96	8026.0/				! fit btw. 500 and 1800 K with MAE of 2.4%, 4.1%
benzofulvene + H → C₁₀H₉ (W119)				9.93E+17	-1.16	5650.0	
PLOG/3.947E-02	1.13E+47	-10.18	16390.0/				! fit btw. 500 and 1250 K with MAE of 13.0%, 21.8%
PLOG/1.000E+00	1.95E+32	-5.56	11220.0/				! fit btw. 500 and 1500 K with MAE of 15.2%, 22.7%
PLOG/1.000E+01	2.55E+21	-2.22	6891.0/				! fit btw. 500 and 1650 K with MAE of 11.2%, 16.8%
PLOG/1.000E+02	9.93E+17	-1.16	5650.0/				! fit btw. 500 and 2000 K with MAE of 11.4%, 18.2%
PLOG/3.947E-02	8.02E+15	-3.36	-12180.0/				
PLOG/3.947E-02	1.45E+56	-12.85	21300.0/				! fit btw. 500 and 1250 K with MAE of 6.0%, 10.8%
PLOG/1.000E+00	2.07E+126	-32.76	69120.0/				
PLOG/1.000E+00	1.16E+27	-4.11	8016.0/				! fit btw. 500 and 1500 K with MAE of 3.0%, 6.9%
PLOG/1.000E+01	5.77E+49	-10.24	27130.0/				
PLOG/1.000E+01	2.48E+29	-4.91	8395.0/				! fit btw. 500 and 1650 K with MAE of 2.8%, 10.4%
PLOG/1.000E+02	1.38E+17	-0.98	4662.0/				
PLOG/1.000E+02	3.18E+82	-19.33	54680.0/				! fit btw. 500 and 2000 K with MAE of 2.9%, 8.1%
benzofulvene + H → naphthalene + H (P1)				1.67E+28	-3.53	30080.0	

PLOG/3.947E-02	1.66E+25	-3.06	14940.0/	! fit btw. 500 and 2500 K with MAE of 17.1%, 45.8%
PLOG/1.000E+00	1.48E+26	-3.25	18150.0/	! fit btw. 500 and 2500 K with MAE of 10.8%, 18.8%
PLOG/1.000E+01	1.46E+31	-4.54	25240.0/	! fit btw. 500 and 2500 K with MAE of 7.4%, 17.1%
PLOG/1.000E+02	1.67E+28	-3.53	30080.0/	! fit btw. 500 and 2500 K with MAE of 21.8%, 51.9%
PLOG/3.947E-02	2.00E+34	-5.59	21730.0/	
PLOG/3.947E-02	1.85E+155	-44.83	54340.0/	! fit btw. 500 and 2500 K with MAE of 4.3%, 9.4%
PLOG/1.000E+00	6.25E+40	-7.26	30950.0/	
PLOG/1.000E+00	1.23E+48	-10.27	24860.0/	! fit btw. 500 and 2500 K with MAE of 2.8%, 4.5%
PLOG/1.000E+01	7.34E+35	-5.85	28980.0/	
PLOG/1.000E+01	2.66E+26	-3.77	19320.0/	! fit btw. 500 and 2500 K with MAE of 2.6%, 6.3%
PLOG/1.000E+02	7.52E+41	-7.32	40700.0/	
PLOG/1.000E+02	5.21E+25	-3.49	24160.0/	! fit btw. 500 and 2500 K with MAE of 3.5%, 15.6%
benzofulvene + H → total				
	1.90E+26	-3.41	9470.0	
PLOG/3.947E-02	3.39E+22	-2.55	5706.0/	! fit btw. 500 and 2500 K with MAE of 16.9%, 37.2%
PLOG/1.000E+00	1.22E+28	-4.09	9214.0/	! fit btw. 500 and 2500 K with MAE of 15.5%, 35.1%
PLOG/1.000E+01	3.52E+29	-4.44	10550.0/	! fit btw. 500 and 2500 K with MAE of 20.1%, 44.1%
PLOG/1.000E+02	1.90E+26	-3.41	9470.0/	! fit btw. 500 and 2500 K with MAE of 29.6%, 122.1%
PLOG/3.947E-02	9.19E+31	-5.35	10240.0/	
PLOG/3.947E-02	5.31E+86	-19.08	97260.0/	! fit btw. 500 and 2500 K with MAE of 6.2%, 12.7%
PLOG/1.000E+00	1.25E+93	-22.79	51020.0/	
PLOG/1.000E+00	2.30E+20	-1.92	4713.0/	! fit btw. 500 and 2500 K with MAE of 6.8%, 20.4%
PLOG/1.000E+01	1.97E+93	-22.32	59340.0/	
PLOG/1.000E+01	1.56E+24	-2.99	6946.0/	! fit btw. 500 and 2500 K with MAE of 5.8%, 19.9%
PLOG/1.000E+02	3.53E+77	-17.45	54860.0/	
PLOG/1.000E+02	4.70E+30	-4.94	9803.0/	! fit btw. 500 and 2500 K with MAE of 9.5%, 22.3%