

Supplementary Material for PCCP
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ELEMENTS H O C N HE AR END

SPECIES

B1O	B2CO	B5CH2	H2	H2O
O2	H2O2	CH4	HCHO	CH3OH
CO2	CH3OOH	C2H2T	C2H4Z	C2H6
CH2CO	CH3CHO	C2H5OH	C2H5OOH	C3H6Y
C3H8	C4H8Y	C2H3CHOZ	C2H5COOOH	C3H7OOH
C3H5OOHY	C4H7OOHY	C2H4O#3	C3H6O#3	C3H6O#4
R1H	R2OH	R3OOH	R4CH3	R5CHO
R7CH3O	R8CH3OO	R10C2H3V	R11C2H5	R12CHCOV
R14CH3CO	R15C2H5O	R17C2H5OO	R19C3H7	R21C3H7
R22C3H7OO	R24C3H7OO	R25C3H6OOH	R26C3H6OOH	R30C3H6OOH
R31C3H6OOOOH	R32C3H6OOOOH	R37C3H6OOOOH	ZC3H5Y	ZC4H7Y
ZC3H5O#4	ZOOC3H5O#4	ZC3H4O#4OOH	ZOOC3H4O#4OOH	N2

END

!

! Heat-of-formation, entropy, and heat capacity of species at 298.15K

!

!

! species	dH kJ/mole	S J/K_mole	Cp kJ/mole	Tlow K	Tmid K	Thigh K
! B1O	249.185	160.937	21.898	300.	1000.	5000.
! B2CO	-110.535	197.538	29.070	300.	1000.	5000.
! B5CH2	386.973	195.474	34.484	300.	1000.	5000.
! H2	-0.053	130.568	28.910	300.	1000.	5000.
! H2O	-241.904	188.689	33.514	300.	1000.	5000.
! O2	-0.054	205.023	29.260	300.	1000.	5000.
! H2O2	-136.206	232.870	43.221	300.	1000.	5000.
! CH4	-74.971	186.263	35.408	300.	1000.	5000.
! HCHO	-115.987	218.645	35.147	300.	1000.	5000.
! CH3OH	-201.307	239.689	43.543	300.	1000.	5000.
! CO2	-393.556	213.792	37.412	300.	1000.	5000.
! CH3OOH	-131.130	282.406	64.891	300.	1000.	5000.
! C2H2T	226.634	200.822	44.182	300.	1000.	5000.
! C2H4Z	52.159	219.440	44.156	300.	1000.	5000.
! C2H6	-84.873	229.481	52.437	300.	1000.	5000.
! CH2CO	-47.808	241.781	51.933	300.	1000.	5000.
! CH3CHO	-177.298	264.252	58.431	300.	1399.	5000.
! C2H5OH	-235.014	282.573	65.285	300.	1000.	5000.
! C2H5OOH	-163.205	320.706	83.609	300.	1000.	5000.
! C3H6Y	20.209	266.926	63.710	300.	1000.	5000.
! C3H8	-104.104	269.896	73.386	300.	1000.	5000.
! C4H8Y	-0.284	305.053	85.576	300.	1000.	5000.
! C2H3CHOZ	-74.821	296.966	76.789	300.	1000.	5000.
! C2H5COOOH	-264.862	351.967	114.925	300.	1382.	5000.
! C3H7OOH	-204.192	351.779	108.571	300.	1000.	5000.
! C3H5OOHY	-60.293	345.736	98.046	300.	1386.	5000.
! C4H7OOHY	-99.795	376.398	121.251	300.	1394.	5000.
! C2H4O#3	-62.803	242.431	48.400	300.	1387.	5000.
! C3H6O#3	-92.990	286.716	72.083	300.	1000.	5000.
! C3H6O#4	-80.355	267.857	60.113	300.	1000.	5000.
! R1H	217.949	114.636	20.920	300.	1000.	5000.
! R2OH	39.274	183.669	30.125	300.	1000.	5000.
! R3OOH	14.437	222.902	35.987	300.	1000.	5000.
! R4CH3	143.408	194.128	36.678	300.	1000.	5000.
! R5CHO	37.590	224.455	34.695	300.	1000.	5000.
! R7CH3O	17.533	227.382	36.372	300.	1000.	5000.
! R8CH3OO	21.606	263.667	57.487	300.	1000.	5000.
! R10C2H3V	298.278	235.377	40.309	300.	1000.	5000.

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! R11C2H5	118.487	246.337	47.564	300.	1000.	5000.
! R12CHCOV	177.596	254.145	52.864	300.	1000.	5000.
! R14CH3CO	-10.097	270.027	50.563	300.	1000.	5000.
! R15C2H5O	-17.010	269.624	58.061	300.	1000.	5000.
! R17C2H5OO	-23.281	301.954	76.560	300.	1407.	5000.
! R19C3H7	100.931	284.094	73.114	300.	1000.	5000.
! R21C3H7	90.051	278.996	72.132	300.	1000.	5000.
! R22C3H7OO	-40.852	341.406	99.075	300.	1392.	5000.
! R24C3H7OO	-63.873	333.086	101.684	300.	1393.	5000.
! R25C3H6OOH	6.500	369.497	106.090	300.	1393.	5000.
! R26C3H6OOH	18.091	368.827	106.939	300.	1394.	5000.
! R30C3H6OOH	5.530	366.257	109.565	300.	1394.	5000.
! R31C3H6OOOOH	-138.492	417.650	133.409	300.	1000.	5000.
! R32C3H6OOOOH	-120.795	425.970	131.304	300.	1000.	5000.
! R37C3H6OOOOH	-138.492	417.642	133.422	300.	1000.	5000.
! ZC3H5Y	163.584	258.871	63.383	200.	1000.	6000.
! ZC4H7Y	126.501	295.959	83.326	300.	1000.	3000.
! ZC3H5O#4	110.325	293.950	69.055	298.	1000.	3000.
! ZOOC3H5O#4	-52.972	324.735	97.657	300.	1369.	5000.
! ZC3H4O#4OOH	-10.080	348.416	96.940	300.	1372.	5000.
! ZOOC3H4O#4OOH	-156.617	395.159	130.146	300.	1383.	5000.

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! Thermodynamic summary was printed by program MECHMOD
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THERMO ALL

	300.000	1000.000	5000.000									
B1O			O	1	0	0	OG	300.00	5000.00	1000.00	0	1
	2.54206000E+00	-2.75506200E-05	-3.10280300E-09		4.55106700E-12	-4.36805200E-16					2	
	2.92308000E+04	4.92030800E+00	2.94642900E+00	-1.63816600E-03	2.42103200E-06						3	
	-1.60284300E-09	3.89069600E-13	2.91476400E+04	2.96399500E+00							4	
B2CO			O	1C	1	0	OG	300.00	5000.00	1000.00	0	1
	3.02507800E+00	1.44268900E-03	-5.63082800E-07	1.01858100E-10	-6.91095200E-15						2	
	-1.42683500E+04	6.10821800E+00	3.26245200E+00	1.51194100E-03	-3.88175500E-06						3	
	5.58194400E-09	-2.47495100E-12	-1.43105400E+04	4.84889700E+00							4	
B5CH2			H	2C	1	0	OG	300.00	5000.00	1000.00	0	1
	3.63640800E+00	1.93305700E-03	-1.68701600E-07	-1.00989900E-10	1.80825600E-14						2	
	4.53413400E+04	2.15656100E+00	3.76223700E+00	1.15981900E-03	2.48958500E-07						3	
	8.80083600E-10	-7.33243500E-13	4.53679100E+04	1.71257800E+00							4	
H2			H	2	0	0	OG	300.00	5000.00	1000.00	0	1
	2.50170000E+00	1.78083000E-03	-7.80013000E-07	1.48437000E-10	-1.03401000E-14						2	
	-6.86891000E+02	1.25553000E+00	3.43853000E+00	1.44314000E-04	-1.08191000E-07						3	
	2.16839000E-10	-5.54307000E-14	-1.03749000E+03	-3.92682000E+00							4	
H2O			H	2O	1	0	OG	300.00	5000.00	1000.00	0	1
	2.68039000E+00	3.09623000E-03	-9.31393000E-07	1.34865000E-10	-7.70007000E-15						2	
	-2.99236000E+04	6.77857000E+00	3.97559000E+00	-4.41834000E-04	2.45596000E-06						3	
	-1.24431000E-09	2.26702000E-13	-3.02810000E+04	7.71523000E-02							4	
O2			O	2	0	0	OG	300.00	5000.00	1000.00	0	1
	3.19345000E+00	1.56657000E-03	-6.90657000E-07	1.32082000E-10	-9.23577000E-15						2	
	-1.05228000E+03	5.96618000E+00	3.08809000E+00	1.60342000E-03	-5.34550000E-07						3	
	2.80793000E-11	2.98899000E-15	-9.93828000E+02	6.61069000E+00							4	
H2O2			H	2O	2	0	OG	300.00	5000.00	1000.00	0	1
	5.20269000E+00	3.07820000E-03	-8.47786000E-07	1.14867000E-10	-6.24436000E-15						2	
	-1.81737000E+04	-2.81106000E+00	2.79724000E+00	9.30806000E-03	-3.27081000E-06						3	
	-3.91853000E-09	2.63341000E-12	-1.75951000E+04	9.47142000E+00							4	
CH4			H	4C	1	0	OG	300.00	5000.00	1000.00	0	1
	1.61991000E+00	1.03080000E-02	-3.71228000E-06</									

-1.52827000E+04	7.43680000E+00	2.41049000E+00	7.02041000E-03	-4.22947000E-06	3
4.40116000E-09	-2.12647000E-12	-1.49519000E+04	1.06246000E+01		4
CH3OH	H	4O	1C	1	OG
			300.00	5000.00	1000.00
3.27626000E+00	1.05432000E-02	-3.54918000E-06	5.58743000E-10	-3.39236000E-14	2
-2.58917000E+04	6.60656000E+00	1.85957000E+00	1.25312000E-02	-4.47107000E-06	3
1.73293000E-09	-8.71066000E-13	-2.52879000E+04	1.46835000E+01		4
CO2	O	2C	1	0	OG
			300.00	5000.00	1000.00
2.73827000E+00	6.09914000E-03	-2.81755000E-06	5.57282000E-10	-3.99470000E-14	2
-4.82637000E+04	8.67355000E+00	2.67844000E+00	6.31159000E-03	1.20975000E-06	3
-7.46647000E-09	3.79399000E-12	-4.84134000E+04	8.57691000E+00		4
CH3OOH	H	4O	2C	1	OG
			300.00	5000.00	1000.00
6.37596000E+00	1.07372000E-02	-3.68666000E-06	5.88827000E-10	-3.61266000E-14	2
-1.84341000E+04	-6.12840000E+00	3.09218000E+00	1.80223000E-02	-7.11862000E-06	3
-1.47978000E-09	1.45517000E-12	-1.74300000E+04	1.13028000E+01		4
C2H2T	H	2C	2	0	OG
			300.00	5000.00	1000.00
3.00338000E+00	7.58476000E-03	-3.11008000E-06	5.64312000E-10	-3.79570000E-14	2
2.62468000E+04	5.29247000E+00	2.54593000E+00	1.14007000E-02	-7.07123000E-06	3
-6.00363000E-10	1.71894000E-12	2.60564000E+04	6.56609000E+00		4
C2H4Z	H	4C	2	0	OG
			300.00	5000.00	1000.00
3.99720000E-01	1.67299000E-02	-6.80909000E-06	1.22922000E-09	-8.23928000E-14	2
5.63749000E+03	1.97729000E+01	1.31810000E+00	1.44460000E-02	-2.74335000E-06	3
-3.10835000E-09	1.52772000E-12	5.26817000E+03	1.47233000E+01		4
C2H6	H	6C	2	0	OG
			300.00	5000.00	1000.00
3.94109000E-01	2.11928000E-02	-8.08560000E-06	1.39339000E-09	-9.03005000E-14	2
-1.10714000E+04	1.96366000E+01	9.75454000E-01	1.88110000E-02	-1.46453000E-06	3
-6.38247000E-09	2.84067000E-12	-1.13111000E+04	1.65514000E+01		4
CH2CO	H	2O	1C	2	OG
			300.00	5000.00	1000.00
5.35267000E+00	6.94209000E-03	-2.50061000E-06	4.13231000E-10	-2.59692000E-14	2
-7.81007000E+03	-3.80283000E+00	2.99539000E+00	1.23540000E-02	-4.06499000E-06	3
-3.34608000E-09	2.24152000E-12	-7.15097000E+03	8.53716000E+00		4
CH3CHO	H	4O	1C	2	OG
			300.00	5000.00	1399.00
4.51972824E+00	1.17700048E-02	-3.75830216E-06	5.44798539E-10	-2.98230765E-14	2
-2.34197108E+04	2.18555589E+00	3.41239058E+00	1.33720451E-02	-4.31103682E-06	3
4.43492976E-10	2.89819827E-14	-2.28998293E+04	8.54236977E+00		4
C2H5OH	H	6O	1C	2	OG
			300.00	5000.00	1000.00
5.62516000E+00	1.59916000E-02	-5.36799000E-06	8.43422000E-10	-5.11406000E-14	2
-3.10498000E+04	-3.61961000E+00	9.39858000E-01	2.61811000E-02	-9.25134000E-06	3
-3.45825000E-09	2.62098000E-12	-2.96238000E+04	2.12634000E+01		4
C2H5OOH	H	6O	2C	2	OG
			300.00	5000.00	1000.00
8.86549000E+00	1.46991000E-02	-4.66630000E-06	7.03129000E-10	-4.13262000E-14	2
-2.34663000E+04	-1.74646000E+01	2.03266000E+00	3.20310000E-02	-1.79773000E-05	3
2.38766000E-09	1.07206000E-12	-2.15063000E+04	1.82187000E+01		4
C3H6Y	H	6C	3	0	OG
			300.00	5000.00	1000.00
5.00264930E+00	1.76389930E-02	-6.22663080E-06	1.01514330E-09	-6.32359770E-14	2
-2.70561520E+02	-2.47234340E+00	5.55982830E-01	2.70915310E-02	-1.07521040E-05	3
-9.75392100E-10	1.43147210E-12	1.15701900E+03	2.13441730E+01		4
C3H8	H	8C	3	0	OG
			300.00	5000.00	1000.00
5.46388480E+00	2.21605690E-02	-7.72962810E-06	1.24954760E-09	-7.73776050E-14	2
-1.56293740E+04	-6.23091510E+00	-3.18318960E-01	3.47464050E-02	-1.28850180E-05	3
-3.50570370E-09	3.01653580E-12	-1.38515940E+04	2.45145950E+01		4
C4H8Y	H	8C	4	0	OG
			300.00	5000.00	1000.00
9.30019470E+00	1.98714620E-02	-6.57139750E-06	1.02588880E-09	-6.21603940E-14	2
-4.66497070E+03	-2.42603000E+01	-2.58697420E-01	4.14754970E-02	-2.13176860E-05	3
2.79188210E-09	8.57493110E-13	-1.61809580E+03	2.67207180E+01		4
C2H3CHOZ	H	4O	1C	3	OG
			300.00	5000.00	1000.00
1.23118860E+01	1.29615880E-02	-6.17746540E-06	1.25014050E-09	-9.11699710E-14	2
-1.52189510E+04	-4.23031770E+01	9.31374370E-01	3.55744180E-02	-3.33472640E-05	3
2.83980340E-08	-1.13956440E-11	-1.06143290E+04	2.10594920E+01		4
C2H5COOOH	H	6O	3C	3	OG
			300.00	5000.00	1382.00
1.55011716E+01	1.41508466E-02	-4.91558149E-06	7.71160485E-10	-4.50686845E-14	2

-3.87511819E+04-5.34551375E+01	4.33718410E+00	3.87006528E-02-2.56101058E-05	3
8.82869519E-09-1.28056545E-12-3.46612406E+04	7.14689908E+00		4
C3H7OOH	H 8O 2C 3 OG	300.00 5000.00 1000.00	0 1
1.15500000E+01 2.00116000E-02-6.48304000E-06		9.93973000E-10-5.92885000E-14	2
-2.95948000E+04-3.09692000E+01 1.41922000E+00		4.71105000E-02-2.83636000E-05	3
3.70396000E-09 2.12765000E-12-2.68348000E+04		2.14033000E+01	4
C3H5OOHY	H 6O 2C 3 OG	300.00 5000.00 1386.00	0 1
1.38848040E+01 1.34942718E-02-4.70978184E-06		7.41183011E-10-4.34097816E-14	2
-1.36631099E+04-4.48841928E+01 1.86604908E+00		4.11015023E-02-2.92829961E-05	3
1.08977747E-08-1.69153504E-12-9.39718504E+03		1.99070231E+01	4
C4H7OOHY	H 8O 2C 4 OG	300.00 5000.00 1394.00	0 1
1.79375119E+01 1.72174384E-02-5.98236489E-06		9.38625383E-10-5.48584632E-14	2
-2.02800828E+04-6.64460150E+01-8.02160384E-01		6.65653438E-02-5.74809844E-05	3
2.59065677E-08-4.71885440E-12-1.42637965E+04		3.23319826E+01	4
C2H4O#3	H 4O 1C 2 OG	300.00 5000.00 1387.00	0 1
6.92819484E+00 1.03517910E-02-3.59464333E-06		5.63735765E-10-3.29363477E-14	2
-1.12398916E+04-1.56957700E+01-1.01424206E+00		2.78706260E-02-1.83781735E-05	3
6.30188267E-09-9.04898236E-13-8.33990233E+03		2.73914997E+01	4
C3H6O#3	H 6O 1C 3 OG	300.00 5000.00 1000.00	0 1
7.29482000E+00 1.84105000E-02-6.54108000E-06		1.07188000E-09-6.70432000E-14	2
-1.50956000E+04-1.44063000E+01 9.39739000E-02		3.50454000E-02-2.55405000E-05	3
1.69102000E-08-6.38433000E-12-1.25752000E+04		2.45001000E+01	4
C3H6O#4	H 6O 1C 3 OG	300.00 5000.00 1000.00	0 1
-2.80859000E-01 3.28683000E-02-1.41730000E-05		2.66755000E-09-1.84356000E-13	2
-1.13051000E+04 2.38104000E+01 1.54114000E+00		1.02641000E-02 4.43080000E-05	3
-5.54504000E-08 2.02306000E-11-1.08722000E+04		1.88571000E+01	4
R1H	H 1 0 0 OG	300.00 5000.00 1000.00	0 1
2.51382000E+00 4.09189000E-06-2.41082000E-09		5.71874000E-13-4.70917000E-17	2
2.54654000E+04-5.34746000E-01 2.51984000E+00-2.59920000E-05		6.27898000E-08	3
-6.29951000E-11 2.23973000E-14 2.54641000E+04-5.63259000E-01			4
R2OH	H 1O 1 0 OG	300.00 5000.00 1000.00	0 1
3.04144000E+00 6.51385000E-04-1.91218000E-08-1.04196000E-13		4.00330000E-17	2
3.90412000E+03 4.81762000E+00 3.67780000E+00-2.14153000E-04		5.70231000E-08	3
1.71404000E-10-1.84629000E-14 3.63597000E+03		1.19670000E+00	4
R3OOH	H 1O 2 0 OG	300.00 5000.00 1000.00	0 1
5.23478510E+00 7.78144870E-04-7.06623310E-08		5.46766930E-12-2.85448520E-16	2
-2.95903320E+01-3.67735670E+00 1.48979600E+00		1.35345300E-02-1.58687740E-05	3
8.62084450E-09-1.82699880E-12 8.14742070E+02		1.49196660E+01	4
R4CH3	H 3C 1 0 OG	300.00 5000.00 1000.00	0 1
1.02702000E+00 9.49641000E-03-3.82860000E-06		6.86498000E-10-4.57900000E-14	2
1.67624000E+04 1.53006000E+01 2.94974000E+00		5.11940000E-03-8.75334000E-07	3
6.64224000E-10-5.42393000E-13 1.61486000E+04		5.05087000E+00	4
R5CHO	H 1O 1C 1 OG	300.00 5000.00 1000.00	0 1
3.60940910E+00 2.87452620E-03-9.87888140E-07		1.58403230E-10-9.77351760E-15	2
3.23210350E+03 5.43047140E+00 3.53402730E+00		2.02347310E-03 5.18340810E-07	3
-3.72460760E-10-6.08028570E-14 3.37385740E+03		6.23884010E+00	4
R7CH3O	H 3O 1C 1 OG	300.00 5000.00 1000.00	0 1
5.59226800E+00 4.39604740E-03-8.63939190E-07		9.20933470E-11-4.30128070E-15	2
-4.39009280E+02-7.28133010E+00 7.20297100E-01		1.51383550E-02-1.16431340E-05	3
7.33661310E-09-2.33887870E-12 1.31065820E+03		1.91891500E+01	4
R8CH3OO	H 3O 2C 1 OG	300.00 5000.00 1000.00	0 1
8.02230640E+00 5.44526060E-03-1.22918850E-06		1.45793450E-10-7.33809040E-15	2
-6.40058590E+02-1.69487950E+01 1.77592210E+00		2.19173360E-02-1.81584020E-05	3
8.81693470E-09-1.97437680E-12 1.23898170E+03		1.57936120E+01	4
R10C2H3V	H 3C 2 0 OG	300.00 5000.00 1000.00	0 1
5.05883600E+00 5.40125560E-03-1.21193580E-06		1.42714060E-10-7.12726560E-15	2
3.37216950E+04-3.00214770E+00 1.23165540E+00		1.46593540E-02-9.51360200E-06	3
3.64669490E-09-6.26403390E-13 3.49349100E+04		1.73146400E+01	4
R11C2H5	H 5C 2 0 OG	300.00 5000.00 1000.00	0 1
3.50261000E+00 1.26143000E-02-3.65730000E-06		5.16642000E-10-2.90469000E-14	2

	1.24032000E+04	5.44236000E+00	5.46580000E-01	2.04368000E-02	-1.16694000E-05	3
	4.82541000E-09	-1.19281000E-12	1.32743000E+04	2.09001000E+01		4
R12CHCOV	H	10	1C	2	OG	300.00 5000.00 1000.00 0 1
	6.75807300E+00	2.00040000E-03	-2.02760700E-07	-1.04113200E-10	1.96516500E-14	2
	1.90151300E+04	-9.07126200E+00	5.04796500E+00	4.45347800E-03	2.26828300E-07	3
	-1.48209500E-09	2.25074200E-13	1.96589200E+04	4.81843900E-01		4
R14CH3CO	H	30	1C	2	OG	300.00 5000.00 1000.00 0 1
	1.09371840E+01	5.44143490E-04	-1.58658760E-08	-2.31073920E-13	4.62528230E-17	2
	-6.07338090E+03	-3.33421250E+01	3.85792660E+00	5.40231490E-03	9.49966670E-06	3
	-9.34900250E-09	2.06671940E-12	-2.67119410E+03	8.54330640E+00		4
R15C2H5O	H	50	1C	2	OG	300.00 5000.00 1000.00 0 1
	8.79327000E+00	8.37917000E-03	-1.93446000E-06	2.29371000E-10	-1.13191000E-14	2
	-6.03107000E+03	-2.23324000E+01	-6.00093000E-01	3.17670000E-02	-2.42586000E-05	3
	1.08137000E-08	-2.26856000E-12	-3.08491000E+03	2.73650000E+01		4
R17C2H5OO	H	50	2C	2	OG	300.00 5000.00 1407.00 0 1
	9.14240068E+00	1.27542434E-02	-4.24151458E-06	6.45607741E-10	-3.69255491E-14	2
	-6.97579168E+03	-2.13194222E+01	9.01075086E-01	3.53849497E-02	-2.89014798E-05	3
	1.30444255E-08	-2.41434493E-12	-4.41092930E+03	2.18088870E+01		4
R19C3H7	H	7C	3	0	OG	300.00 5000.00 1000.00 0 1
	4.90850000E+00	1.95492000E-02	-6.09862000E-06	9.08986000E-10	-5.30994000E-14	2
	9.72711000E+03	2.41566000E-01	-9.97049000E-01	4.22637000E-02	-3.67683000E-05	3
	1.83985000E-08	-3.66617000E-12	1.08489000E+04	2.87294000E+01		4
R21C3H7	H	7C	3	0	OG	300.00 5000.00 1000.00 0 1
	6.86823000E+00	1.61443000E-02	-4.60387000E-06	6.41404000E-10	-3.56487000E-14	2
	7.53026000E+03	-1.15057000E+01	7.75611000E-01	3.08041000E-02	-1.47528000E-05	3
	5.39690000E-10	1.67448000E-12	9.35939000E+03	2.06017000E+01		4
R22C3H7OO	H	7O	2C	3	OG	300.00 5000.00 1392.00 0 1
	1.36152355E+01	1.54856586E-02	-5.29653835E-06	8.58043338E-10	-5.20491162E-14	2
	-1.12872035E+04	-4.43946340E+01	5.77276290E-01	4.75704860E-02	-3.61204834E-05	3
	1.45739973E-08	-2.42057865E-12	-6.90864049E+03	2.50732368E+01		4
R24C3H7OO	H	7O	2C	3	OG	300.00 5000.00 1393.00 0 1
	1.42125805E+01	1.51915551E-02	-5.35268994E-06	8.90393261E-10	-5.49823461E-14	2
	-1.42534776E+04	-4.87886410E+01	5.74488480E-01	4.92541727E-02	-3.85714205E-05	3
	1.58709804E-08	-2.66959437E-12	-9.73238987E+03	2.36843304E+01		4
R25C3H6OOH	H	7O	2C	3	OG	300.00 5000.00 1393.00 0 1
	1.36435123E+01	1.45580710E-02	-4.87405385E-06	7.93445831E-10	-4.87443480E-14	2
	-5.28647810E+03	-4.03274923E+01	3.12745634E+00	3.99439256E-02	-2.88033029E-05	3
	1.12667479E-08	-1.83417457E-12	-1.69290631E+03	1.58988310E+01		4
R26C3H6OOH	H	7O	2C	3	OG	300.00 5000.00 1394.00 0 1
	1.40620950E+01	1.45235277E-02	-5.03881569E-06	8.44287285E-10	-5.28085231E-14	2
	-4.08004247E+03	-4.29224890E+01	2.75659469E+00	4.22502526E-02	-3.16070765E-05	3
	1.26473142E-08	-2.08922654E-12	-2.68579798E+02	1.73565547E+01		4
R30C3H6OOH	H	7O	2C	3	OG	300.00 5000.00 1394.00 0 1
	1.45405806E+01	1.44550560E-02	-5.23355641E-06	9.06948302E-10	-5.78989023E-14	2
	-5.74306895E+03	-4.59703493E+01	2.78233148E+00	4.37882032E-02	-3.38271815E-05	3
	1.38030120E-08	-2.30936979E-12	-1.83795193E+03	1.65311464E+01		4
R31C3H6OOOOH	H	7O	4C	3	OG	300.00 5000.00 1000.00 0 1
	1.90484000E+01	1.26718000E-02	-2.97004000E-06	3.54256000E-10	-1.74466000E-14	2
	-2.42266000E+04	-6.50764000E+01	2.13126000E+00	5.97630000E-02	-4.91660000E-05	3
	1.81720000E-08	-1.82122000E-12	-1.95501000E+04	2.23015000E+01		4
R32C3H6OOOOH	H	7O	4C	3	OG	300.00 5000.00 1000.00 0 1
	1.83522000E+01	1.33235000E-02	-3.20553000E-06	3.94529000E-10	-2.01319000E-14	2
	-2.19050000E+04	-6.02423000E+01	2.64693000E+00	5.58589000E-02	-4.42549000E-05	3
	1.66943000E-08	-2.10627000E-12	-1.74420000E+04	2.13235000E+01		4
R37C3H6OOOOH	H	7O	4C	3	OG	300.00 5000.00 1000.00 0 1
	1.89993000E+01	1.27598000E-02	-3.02203000E-06	3.66603000E-10	-1.84641000E-14	2
	-2.42072000E+04	-6.48045000E+01	2.22168000E+00	5.91333000E-02	-4.76472000E-05	3
	1.66500000E-08	-1.28068000E-12	-1.95597000E+04	2.19180000E+01		4
ZC3H5Y	H	5C	3	0	OG	200.00 6000.00 1000.00 0 1
	7.00945680E+00	1.31066290E-02	-4.65334420E-06	7.45143230E-10	-4.43500510E-14	2

```

1.64129090E+04-1.39461140E+01 1.46980360E+00 1.90343650E-02 1.44804250E-05 3
-3.54686520E-08 1.66475940E-11 1.83258310E+04 1.67241140E+01 4
ZC4H7Y H 7C 4 0 OG 300.00 3000.00 1000.00 0 1
5.52142000E+00 2.68368400E-02-1.28643000E-05 3.08864000E-09-3.03085600E-13 2
1.19804400E+04-4.48244700E+00-1.08051400E+00 4.63868600E-02-3.46469700E-05 3
1.40137400E-08-2.39504000E-12 1.37553800E+04 2.93446600E+01 4
ZC3H5O#4 H 5O 1C 3 OG 298.15 3000.00 1000.00 0 1
9.12069910E+00 1.21961170E-02-4.29297770E-06 1.26168920E-09-1.57053670E-13 2
9.17650120E+03-2.20714470E+01 7.05993930E-01 2.56297970E-02 7.10804110E-06 3
-2.96934950E-08 1.43607210E-11 1.19092680E+04 2.36100390E+01 4
ZOOC3H5O#4 H 5O 3C 3 OG 300.00 5000.00 1369.00 0 1
1.54292894E+01 1.34713554E-02-4.80458893E-06 7.67113305E-10-4.53837038E-14 2
-1.37760602E+04-5.72932611E+01 1.08911058E+00 4.31068369E-02-2.69371387E-05 3
7.75608875E-09-8.09158566E-13-8.38912109E+03 2.11315823E+01 4
ZC3H4O#4OOH H 5O 3C 3 OG 300.00 5000.00 1372.00 0 1
1.54851015E+01 1.29806531E-02-4.63101831E-06 7.39557652E-10-4.37600615E-14 2
-8.57748809E+03-5.45652299E+01 7.11475084E-01 4.49231777E-02-3.03649748E-05 3
9.95831187E-09-1.29093246E-12-3.17208804E+03 2.57238494E+01 4
ZOOC3H4O#4OOH H 5O 5C 3 OG 300.00 5000.00 1383.00 0 1
2.19261622E+01 1.22967381E-02-4.42322044E-06 7.10259257E-10-4.21876990E-14 2
-2.85261302E+04-8.64513194E+01 2.46130593E-01 6.67669100E-02-5.75657952E-05 3
2.45760582E-08-4.18014287E-12-2.14167573E+04 2.85701475E+01 4
N2 N 2 0 0 OG 300.00 5000.00 1000.00 0 1
2.92664000E+00 1.48797700E-03-5.68476030E-07 1.00970400E-10-6.75335090E-15 2
-9.22767600E+02 5.98052900E+00 3.29867700E+00 1.40823990E-03-3.96322180E-06 3
5.64151480E-09-2.44485400E-12-1.02090000E+03 3.95037200E+00 4
END
REACTIONS MOLECULES KELVINS
!
! 1
R11C2H5+O2 = R17C2H5OO 2.545E+27 -13.1000 4200.00
DUPLICATE
!
! 2
R11C2H5+O2 = R17C2H5OO 5.299E+38 -16.0000 8090.00
DUPLICATE
!
! 3
R11C2H5+O2 = C2H4Z+R3OOH 1.181E-04 -2.6900 2340.00
DUPLICATE
!
! 4
R11C2H5+O2 = C2H4Z+R3OOH 4.140E-01 -3.0700 10500.00
DUPLICATE
!
! 5
R11C2H5+O2 = C2H4Z+R3OOH 1.614E-31 5.1900 4070.00
DUPLICATE
!
! 6
R11C2H5+O2 = C2H4O#3+R2OH 1.140E-02 -3.8300 3850.00
DUPLICATE
!
! 7
R11C2H5+O2 = C2H4O#3+R2OH 2.529E-14 0.1540 5060.00
DUPLICATE
!
! 8
R11C2H5+O2 = CH3CHO+R2OH 1.130E-25 3.5700 1330.00
!
```

Supplementary Material for PCCP
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!	9					
R17C2H5OO	=	C2H4Z+R3OOH	5.854E+27	-5.6300	16300.00	
DUPLICATE						
!	10					
R17C2H5OO	=	C2H4Z+R3OOH	3.112E+65	-17.0000	24200.00	
DUPLICATE						
!	11					
R17C2H5OO	=	C2H4O#3+R2OH	6.796E+46	-11.8000	22200.00	
!	12					
R17C2H5OO	=	CH3CHO+R2OH	5.344E+37	-9.5400	20300.00	
DUPLICATE						
!	13					
R17C2H5OO	=	CH3CHO+R2OH	-1.164E+72	-19.2000	33900.00	
DUPLICATE						
!	14					
R19C3H7+O2	=	R22C3H7OO	3.669E+27	-13.1000	4380.00	
DUPLICATE						
!	15					
R19C3H7+O2	=	R22C3H7OO	1.705E+53	-20.0000	12900.00	
DUPLICATE						
!	16					
R19C3H7+O2	=	R25C3H6OOH	3.628E-06	-3.2500	1990.00	
!	17					
R19C3H7+O2	=	R26C3H6OOH	5.284E-19	1.7800	84.50	
!	18					
R19C3H7+O2	=	C3H6Y+R3OOH	7.588E-04	-2.6300	4520.00	
DUPLICATE						
!	19					
R19C3H7+O2	=	C3H6Y+R3OOH	2.180E-33	5.6600	3050.00	
DUPLICATE						
!	20					
R19C3H7+O2	=	C3H6Y+R3OOH	1.337E-23	3.3200	6470.00	
DUPLICATE						
!	21					
R19C3H7+O2	=	C3H6O#3+R2OH	6.991E-13	-0.2980	2640.00	
DUPLICATE						
!	22					
R19C3H7+O2	=	C3H6O#3+R2OH	2.962E+23	-11.0000	10600.00	
DUPLICATE						
!	23					
R19C3H7+O2	=	C3H6O#4+R2OH	1.637E-18	1.5200	3760.00	
DUPLICATE						
!	24					
R19C3H7+O2	=	C3H6O#4+R2OH	2.112E+09	-6.5100	9750.00	
DUPLICATE						

!					
!	25				
R22C3H7OO	=	C3H6Y+R3OOH	7.957E+24	-4.4100	16200.00
DUPLICATE					
!					
!	26				
R22C3H7OO	=	C3H6Y+R3OOH	5.053E+67	-17.1000	26400.00
DUPLICATE					
!					
!	27				
R22C3H7OO	=	C3H6O#3+R2OH	2.747E+28	-5.6400	17800.00
DUPLICATE					
!					
!	28				
R22C3H7OO	=	C3H6O#3+R2OH	5.842E+62	-15.9000	25300.00
DUPLICATE					
!					
!	29				
R22C3H7OO	=	C3H6O#4+R2OH	8.768E+36	-8.1400	22200.00
DUPLICATE					
!					
!	30				
R22C3H7OO	=	C3H6O#4+R2OH	3.123+100	-27.2000	36600.00
DUPLICATE					
!					
!	31				
R25C3H6OOH	=	C3H6Y+R3OOH	1.810E+40	-9.4000	12600.00
!					
!	32				
R25C3H6OOH	=	C3H6O#3+R2OH	1.040E+33	-6.8200	9970.00
!					
!	33				
R25C3H6OOH	=	C3H6O#4+R2OH	2.324E+15	-2.5500	14800.00
!					
!	34				
R25C3H6OOH	=	R22C3H7OO	2.810E-03	2.5100	2700.00
DUPLICATE					
!					
!	35				
R25C3H6OOH	=	R22C3H7OO	4.108E+32	-7.8100	10300.00
DUPLICATE					
!					
!	36				
R26C3H6OOH	=	C3H6Y+R3OOH	1.003E-06	5.4400	7150.00
!					
!	37				
R26C3H6OOH	=	C3H6O#3+R2OH	1.556E+07	1.1500	10100.00
!					
!	38				
R26C3H6OOH	=	C3H6O#4+R2OH	1.795E+26	-5.1700	12800.00
!					
!	39				
R26C3H6OOH	=	R22C3H7OO	4.297E+01	2.5900	1470.00
!					
!	40				
R26C3H6OOH	=	R25C3H6OOH	7.658E+06	0.3120	7320.00
!					
!	41				
R21C3H7+O2	=	R24C3H7OO	5.633E+38	-16.7000	5510.00
DUPLICATE					

!					
!	42				
R21C3H7+O2 =	R24C3H7OO	7.999E+54	-20.8000	11300.00	
DUPLICATE					
!					
!	43				
R21C3H7+O2 =	R30C3H6OOH	3.493E+13	-8.8000	4800.00	
!					
!	44				
R21C3H7+O2 =	C3H6Y+R3OOH	3.442E-04	-2.6000	2680.00	
DUPLICATE					
!					
!	45				
R21C3H7+O2 =	C3H6Y+R3OOH	3.169E+56	-18.3000	39000.00	
DUPLICATE					
!					
!	46				
R21C3H7+O2 =	C3H6Y+R3OOH	2.651E-29	4.6300	2480.00	
DUPLICATE					
!					
!	47				
R21C3H7+O2 =	C3H6Y+R3OOH	8.786E-23	3.2300	5330.00	
DUPLICATE					
!					
!	48				
R21C3H7+O2 =	C3H6O#3+R2OH	3.376E-01	-3.6800	4630.00	
DUPLICATE					
!					
!	49				
R21C3H7+O2 =	C3H6O#3+R2OH	1.588E+15	-7.2600	19600.00	
DUPLICATE					
!					
!	50				
R24C3H7OO =	C3H6Y+R3OOH	1.873E+32	-6.5700	17800.00	
DUPLICATE					
!					
!	51				
R24C3H7OO =	C3H6Y+R3OOH	3.124E+81	-21.4000	28400.00	
DUPLICATE					
!					
!	52				
R24C3H7OO =	C3H6O#3+R2OH	6.742E+04	1.1200	15000.00	
DUPLICATE					
!					
!	53				
R24C3H7OO =	C3H6O#3+R2OH	4.585E+58	-14.6000	25600.00	
DUPLICATE					
!					
!	54				
R30C3H6OOH =	C3H6Y+R3OOH	4.574E+35	-7.6700	12000.00	
!					
!	55				
R30C3H6OOH =	C3H6O#3+R2OH	8.014E+26	-4.9400	9220.00	
!					
!	56				
R30C3H6OOH =	R24C3H7OO	1.291E+07	-0.2910	4040.00	
DUPLICATE					
!					
!	57				
R30C3H6OOH =	R24C3H7OO	9.978E+52	-13.9000	14000.00	

DUPLICATE

!				
!	58			
C3H8 =	R4CH3+R11C2H5	5.000E+16	0.0000	43011.33
!				
!	59			
C3H8+O2 =	R3OOH+R21C3H7	3.321E-11	0.0000	24157.02
!				
!	60			
C3H8+O2 =	R3OOH+R19C3H7	4.151E-11	0.0000	24660.29
!				
!	61			
R25C3H6OOH+O2 =	R31C3H6OOOOH	3.653E-05	-2.5000	0.00
!				
!	62			
R26C3H6OOH+O2 =	R32C3H6OOOOH	3.653E-05	-2.5000	0.00
!				
!	63			
R30C3H6OOH+O2 =	R37C3H6OOOOH	3.653E-05	-2.5000	0.00
!				
!	64			
R31C3H6OOOOH =	R2OH+C2H5COOOH	5.000E+09	1.0000	17866.13
DUPLICATE				
!				
!	65			
R31C3H6OOOOH =	R2OH+C2H5COOOH	3.300E+09	1.0000	15349.77
DUPLICATE				
!				
!	66			
R32C3H6OOOOH =	R2OH+C2H5COOOH	3.300E+09	1.0000	16356.32
DUPLICATE				
!				
!	67			
R32C3H6OOOOH =	R2OH+C2H5COOOH	5.700E+08	1.0000	11826.88
DUPLICATE				
!				
!	68			
R37C3H6OOOOH =	R2OH+C2H5COOOH	1.700E+09	1.0000	13839.96
DUPLICATE				
!				
!	69			
R37C3H6OOOOH =	R2OH+C2H5COOOH	8.600E+08	1.0000	14343.23
DUPLICATE				
!				
!	70			
R19C3H7 =	R4CH3+C2H4Z	2.000E+13	0.0000	15601.41
!				
!	71			
B1O+C3H8 =	R2OH+R21C3H7	4.317E-11	0.0000	2617.01
!				
!	72			
B1O+C3H8 =	R2OH+R19C3H7	1.660E-10	0.0000	3950.68
!				
!	73			
C3H8+R1H =	H2+R21C3H7	1.494E-17	2.0000	2516.36
!				
!	74			
C3H8+R1H =	H2+R19C3H7	9.464E-17	2.0000	3875.19
!				
!	75			

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C3H8+R2OH = H2O+R21C3H7	4.317E-18	2.0000	-385.00
!			
! 76			
C3H8+R2OH = H2O+R19C3H7	8.966E-18	2.0000	226.47
!			
! 77			
C3H8+R3OOH = H2O2+R21C3H7	6.641E-13	0.0000	7800.70
!			
! 78			
C3H8+R3OOH = H2O2+R19C3H7	1.992E-12	0.0000	8555.61
!			
! 79			
C3H8+R4CH3 = CH4+R21C3H7	3.321E-13	0.0000	4831.40
!			
! 80			
C3H8+R4CH3 = CH4+R19C3H7	9.962E-25	4.0000	4126.82
!			
! 81			
C3H8+R5CHO = HCHO+R21C3H7	1.826E-17	1.9000	8555.61
!			
! 82			
C3H8+R5CHO = HCHO+R19C3H7	3.321E-19	2.5000	9310.52
!			
! 83			
C3H8+R7CH3O = CH3OH+R21C3H7	2.490E-13	0.0000	2264.72
!			
! 84			
C3H8+R7CH3O = CH3OH+R19C3H7	5.313E-13	0.0000	3673.88
!			
! 85			
C3H8+R8CH3OO = CH3OOH+R21C3H7	4.981E-12	0.0000	8807.25
!			
! 86			
C3H8+R8CH3OO = CH3OOH+R19C3H7	1.992E-11	0.0000	10065.43
!			
! 87			
C3H8+R11C2H5 = C2H6+R21C3H7	3.321E-13	0.0000	5535.98
!			
! 88			
C3H8+R11C2H5 = C2H6+R19C3H7	9.962E-13	0.0000	6794.16
!			
! 89			
C3H8+R21C3H7 = C3H8+R19C3H7	1.395E-26	4.2000	4378.46
!			
! 90			
C3H8+R22C3H7OO = C3H7OOH+R21C3H7	4.981E-12	0.0000	8807.25
!			
! 91			
C3H8+R22C3H7OO = C3H7OOH+R19C3H7	1.992E-11	0.0000	10065.43
!			
! 92			
C3H8+R24C3H7OO = C3H7OOH+R21C3H7	4.981E-12	0.0000	8807.25
!			
! 93			
C3H8+R24C3H7OO = C3H7OOH+R19C3H7	1.992E-11	0.0000	10065.43
!			
! 94			
R1H+R21C3H7 = C3H8	1.046E-11	0.0000	0.00
!			
! 95			

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R3OOH+R21C3H7 = C3H7OOH	6.641E-12	0.0000	0.00
!			
! 96			
R22C3H7OO+R3OOH = C3H7OOH+O2	3.321E-13	0.0000	-654.25
!			
! 97			
R24C3H7OO+R3OOH = C3H7OOH+O2	3.321E-13	0.0000	-654.25
!			
! 98			
C3H7OOH = R2OH+HCHO+R11C2H5	1.500E+16	0.0000	21137.39
!			
! 99			
C3H5OOHY = R2OH+HCHO+R10C2H3V	1.500E+16	0.0000	21137.39
!			
! 100			
C4H7OOHY = R2OH+CH3CHO+R10C2H3V	1.500E+16	0.0000	21137.39
!			
! 101			
C2H5COOOH = R2OH+HCHO+B2CO+R4CH3	1.500E+16	0.0000	21137.39
!			
! 102			
C3H6O#3+R1H = H2+CH2CO+R4CH3	4.483E-17	2.0000	2516.36
!			
! 103			
C3H6O#3+R2OH = H2O+CH2CO+R4CH3	1.295E-17	2.0000	-385.00
!			
! 104			
C3H6O#3+R3OOH = H2O2+CH2CO+R4CH3	1.992E-12	0.0000	7800.70
!			
! 105			
C3H6O#3+R4CH3 = CH4+CH2CO+R4CH3	9.962E-13	0.0000	4831.40
!			
! 106			
C3H6O#3+R8CH3OO = CH3OOH+CH2CO+R4CH3	9.962E-13	0.0000	4831.40
!			
! 107			
C3H6O#3+R11C2H5 = C2H6+CH2CO+R4CH3	9.962E-13	0.0000	5535.98
!			
! 108			
C3H6O#3+B1O = R2OH+R5CHO+C2H4Z	1.295E-10	0.0000	2617.01
!			
! 109			
C3H6O#4+R1H = H2+CH2CO+R4CH3	4.483E-17	2.0000	2516.36
!			
! 110			
C3H6O#4+R2OH = H2O+CH2CO+R4CH3	1.295E-17	2.0000	-385.00
!			
! 111			
C3H6O#4+R3OOH = H2O2+CH2CO+R4CH3	1.992E-12	0.0000	7800.70
!			
! 112			
C3H6O#4+R4CH3 = CH4+CH2CO+R4CH3	9.962E-13	0.0000	4831.40
!			
! 113			
C3H6O#4+R8CH3OO = CH3OOH+CH2CO+R4CH3	9.962E-13	0.0000	4831.40
!			
! 114			
C3H6O#4+R11C2H5 = C2H6+CH2CO+R4CH3	9.962E-13	0.0000	5535.98
!			
! 115			

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C3H6O#4+R1H = H2+ZC3H5O#4	4.483E-17	2.0000	2516.36
!			
! 116			
C3H6O#4+R2OH = H2O+ZC3H5O#4	1.295E-17	2.0000	-385.00
!			
! 117			
C3H6O#4+R3OOH = H2O2+ZC3H5O#4	1.992E-12	0.0000	7800.70
!			
! 118			
C3H6O#4+R4CH3 = CH4+ZC3H5O#4	9.962E-13	0.0000	4831.40
!			
! 119			
C3H6O#4+R8CH3OO = CH3OOH+ZC3H5O#4	9.962E-13	0.0000	4831.40
!			
! 120			
C3H6O#4+R11C2H5 = C2H6+ZC3H5O#4	9.962E-13	0.0000	5535.98
!			
! 121			
ZC3H5O#4 = R5CHO+C2H4Z	5.000E+13	0.0000	12481.13
!			
! 122			
ZC3H5O#4+O2 = ZOOC3H5O#4	3.653E-05	-2.5000	0.00
!			
! 123			
ZOOC3H5O#4 = ZC3H4O#4OOH	8.000E+13	0.0000	12833.42
!			
! 124			
ZC3H4O#4OOH+O2 = ZOOC3H4O#4OOH	3.653E-05	-2.5000	0.00
!			
! 125			
C3H6Y+R1H = C2H4Z+R4CH3	1.195E-11	0.0000	1459.49
!			
! 126			
C4H8Y+R1H = C2H4Z+R11C2H5	1.195E-11	0.0000	1459.49
!			
! 127			
C3H6Y+R2OH = R4CH3+CH3CHO	2.324E-12	0.0000	-452.94
!			
! 128			
C3H6Y+R2OH = HCHO+R11C2H5	2.324E-12	0.0000	-452.94
!			
! 129			
C4H8Y+R2OH = HCHO+R4CH3+C2H4Z	2.324E-12	0.0000	-452.94
!			
! 130			
C3H6Y+B1O = CH2CO+R4CH3+R1H	5.645E-17	1.8300	276.80
!			
! 131			
C4H8Y+B1O = CH2CO+R11C2H5+R1H	5.645E-17	1.8300	276.80
!			
! 132			
C3H6Y+R3OOH = R2OH+C3H6O#3	1.660E-12	0.0000	7247.11
!			
! 133			
C3H6Y+R1H = ZC3H5Y+H2	9.464E-20	2.5000	145.95
!			
! 134			
C3H6Y+R2OH = ZC3H5Y+H2O	4.981E-18	2.0000	-762.46
!			
! 135			

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C3H6Y+R3OOH = ZC3H5Y+H2O2 ! ! 136	1.046E-20	2.6000	6240.56
C3H6Y+R4CH3 = ZC3H5Y+CH4 ! ! 137	2.158E-24	3.5000	1799.19
C3H6Y+R8CH3OO = ZC3H5Y+CH3OOH ! ! 138	3.321E-12	0.0000	8580.78
C3H6Y+R11C2H5 = ZC3H5Y+C2H6 ! ! 139	2.324E-24	3.5000	2181.68
C4H8Y+R1H = ZC4H7Y+H2 ! ! 140	9.464E-20	2.5000	145.95
C4H8Y+R2OH = ZC4H7Y+H2O ! ! 141	4.981E-18	2.0000	-762.46
C4H8Y+R3OOH = ZC4H7Y+H2O2 ! ! 142	1.046E-20	2.6000	6240.56
C4H8Y+R4CH3 = ZC4H7Y+CH4 ! ! 143	2.158E-24	3.5000	1799.19
C4H8Y+R8CH3OO = ZC4H7Y+CH3OOH ! ! 144	3.321E-12	0.0000	8580.78
C4H8Y+R11C2H5 = ZC4H7Y+C2H6 ! ! 145	2.324E-24	3.5000	2181.68
C3H6Y+B1O = ZC3H5Y+R2OH ! ! 146	1.511E-13	0.7000	1927.53
C4H8Y+B1O = ZC4H7Y+R2OH ! ! 147	1.511E-13	0.7000	1927.53
ZC3H5Y+C4H8Y = R4CH3+C2H2T+2C2H4Z ! ! 148	9.962E-15	0.0000	5737.29
ZC3H5Y+C3H6Y = R10C2H3V+2C2H4Z ! ! 149	9.962E-15	0.0000	5737.29
ZC4H7Y+C4H8Y = R10C2H3V+3C2H4Z ! ! 150	9.962E-15	0.0000	5737.29
ZC4H7Y+C3H6Y = R4CH3+C2H2T+2C2H4Z ! ! 151	9.962E-15	0.0000	5737.29
ZC3H5Y+R1H = C3H6Y ! ! 152	1.660E-11	0.0000	0.00
ZC3H5Y+R3OOH = C3H5OOHY ! ! 153	8.302E-12	0.0000	0.00
ZC3H5Y+R4CH3 = C4H8Y ! ! 154	1.660E-11	0.0000	0.00
ZC4H7Y+R1H = C4H8Y ! ! 155	1.660E-11	0.0000	0.00

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ZC4H7Y+R3OOH = C4H7OOHY	8.302E-12	0.0000	0.00
!			
! 156			
2R1H+M = H2+M	5.155E-30	-1.0000	0.00
O2/0.4/ N2/0.4/ B2CO/0.75/ CO2/1.5/ H2O/6.5/ CH4/3/ H2/0/ C2H6/3/			
!			
! 157			
2B5CH2 = C2H2T+2R1H	1.992E-10	0.0000	402.62
!			
! 158			
R4CH3+M = B5CH2+R1H+M	4.831E-08	0.0000	45646.71
O2/0.4/ N2/0.4/ B2CO/0.75/ CO2/1.5/ H2O/6.5/ CH4/3/ C2H6/3/			
!			
! 159			
R4CH3+B5CH2 = C2H4Z+R1H	6.973E-11	0.0000	0.00
!			
! 160			
2R4CH3(+M) = C2H6(+M)	5.994E-11	0.0000	0.00
O2/0.4/ N2/0.4/ B2CO/0.75/ CO2/1.5/ H2O/6.5/ CH4/3/ C2H6/3/			
LOW / 1.001E-06 -7.00 1389.03 /			
TROE / 6.2000E-01 7.3000E+01 1.1800E+03 /			
!			
! 161			
2R4CH3 = R11C2H5+R1H	4.981E-11	0.0000	6794.16
!			
! 162			
2R4CH3 = C2H4Z+H2	3.487E-10	0.0000	9713.14
!			
! 163			
R1H+R4CH3(+M) = CH4(+M)	2.773E-10	0.0000	0.00
O2/0.4/ N2/0.4/ B2CO/0.75/ CO2/1.5/ H2O/6.5/ CH4/3/ C2H6/3/			
LOW / 3.881E-24 -1.80 0.00 /			
TROE / 3.7000E-01 3.3150E+03 6.1000E+01 /			
!			
! 164			
CH4(+CH4) = R4CH3+R1H(+CH4)	2.400E+16	0.0000	52843.48
LOW / 1.400E-06 0.00 45747.36 /			
TROE / 6.9000E-01 9.0000E+01 2.2100E+03 /			
!			
! 165			
CH4+R1H = R4CH3+H2	2.158E-20	3.0000	4026.17
!			
! 166			
R10C2H3V(+M) = C2H2T+R1H(+M)	2.000E+14	0.0000	20030.20
O2/0.4/ N2/0.4/ B2CO/0.75/ CO2/1.5/ H2O/6.5/ CH4/3/			
LOW / 1.976E+18 -7.50 22924.01 /			
TROE / 3.5000E-01 1.0000E+00 1.0000E+08 /			
!			
! 167			
R10C2H3V+R1H = C2H2T+H2	1.992E-11	0.0000	0.00
!			
! 168			
R10C2H3V+B5CH2 = C2H2T+R4CH3	2.989E-11	0.0000	0.00
!			
! 169			
R10C2H3V+R4CH3 = CH4+C2H2T	6.475E-13	0.0000	0.00
!			
! 170			
2R10C2H3V = C2H4Z+C2H2T	1.594E-12	0.0000	0.00
!			

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!	171			
C2H4Z+M =	C2H2T+H2+M	1.655E-07	0.0000	36034.22
O2/0.4/	N2/0.4/ B2CO/0.75/ CO2/1.5/ H2O/6.5/ CH4/3/ C2H6/3/			
!				
!	172			
C2H4Z+M =	R10C2H3V+R1H+M	1.229E-06	0.0000	48666.33
O2/0.4/	N2/0.4/ B2CO/0.75/ CO2/1.5/ H2O/6.5/ CH4/3/ C2H6/3/			
!				
!	173			
C2H4Z+R1H =	R10C2H3V+H2	8.302E-17	1.9300	6542.53
!				
!	174			
C2H4Z+R4CH3 =	CH4+R10C2H3V	1.046E-12	0.0000	8052.34
!				
!	175			
R11C2H5(+M) =	C2H4Z+R1H(+M)	8.200E+13	0.0000	20130.85
O2/0.4/	N2/0.4/ B2CO/0.75/ CO2/1.5/ H2O/6.5/ CH4/3/ C2H6/3/			
LOW /	5.645E-07 0.00 16809.26 /			
TROE /	7.5000E-01 9.7000E+01 1.3790E+03 /			
!				
!	176			
R11C2H5+R1H =	C2H4Z+H2	2.989E-12	0.0000	0.00
!				
!	177			
R11C2H5+R1H =	C2H6	5.977E-11	0.0000	0.00
!				
!	178			
R11C2H5+B5CH2 =	C2H4Z+R4CH3	2.989E-11	0.0000	0.00
!				
!	179			
R11C2H5+R4CH3 =	C2H4Z+CH4	1.826E-12	0.0000	0.00
!				
!	180			
R11C2H5+R10C2H3V =	2C2H4Z	7.969E-13	0.0000	0.00
!				
!	181			
R11C2H5+R10C2H3V =	C2H2T+C2H6	7.969E-13	0.0000	0.00
!				
!	182			
2R11C2H5 =	C2H4Z+C2H6	2.324E-12	0.0000	0.00
!				
!	183			
C2H6+M =	C2H4Z+H2+M	3.819E-07	0.0000	33920.48
!				
!	184			
C2H6+R1H =	R11C2H5+H2	2.324E-15	1.5000	3724.21
!				
!	185			
C2H6+R4CH3 =	R11C2H5+CH4	2.490E-31	6.0000	2918.97
!				
!	186			
C2H6+R10C2H3V =	R11C2H5+C2H4Z	9.962E-22	3.3000	5284.35
!				
!	187			
B1O+H2 =	R2OH+R1H	8.468E-20	2.6700	3120.28
!				
!	188			
B1O+B5CH2 =	B2CO+2R1H	1.195E-10	0.0000	0.00
!				
!	189			

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B1O+B5CH2 = B2CO+H2	7.969E-11	0.0000	0.00
!			
! 190			
B1O+R4CH3 = HCHO+R1H	1.395E-10	0.0000	0.00
!			
! 191			
B1O+R4CH3 = R7CH3O	1.328E-08	-2.1200	301.96
!			
! 192			
B1O+CH4 = R4CH3+R2OH	1.195E-15	1.5600	4227.48
!			
! 193			
B1O+C2H2T = B5CH2+B2CO	3.603E-18	2.1000	805.23
!			
! 194			
B1O+C2H2T = R12CHCOV+R1H	8.401E-18	2.1000	805.23
!			
! 195			
B1O+R10C2H3V = R4CH3+B2CO	4.981E-11	0.0000	0.00
!			
! 196			
B1O+R10C2H3V = CH2CO+R1H	1.594E-10	0.0000	0.00
!			
! 197			
B1O+C2H4Z = R4CH3+R5CHO	1.345E-17	1.8800	100.65
!			
! 198			
B1O+C2H4Z = HCHO+B5CH2	6.641E-19	1.8800	100.65
!			
! 199			
B1O+C2H4Z = CH2CO+H2	1.096E-18	1.8800	100.65
!			
! 200			
B1O+C2H4Z = R2OH+R10C2H3V	2.490E-17	1.9100	1862.10
!			
! 201			
B1O+R11C2H5 = HCHO+R4CH3	1.826E-11	0.0000	0.00
!			
! 202			
B1O+R11C2H5 = CH3CHO+R1H	9.132E-11	0.0000	0.00
!			
! 203			
B1O+R11C2H5 = C2H4Z+R2OH	4.981E-11	0.0000	0.00
!			
! 204			
B1O+C2H6 = R11C2H5+R2OH	1.660E-15	1.5000	2918.97
!			
! 205			
R1H+B1O+M = R2OH+M	3.253E-29	-1.0000	0.00
O2/0.4/ N2/0.4/ B2CO/0.75/ CO2/1.5/ H2O/6.5/ CH4/3/ C2H6/3/			
!			
! 206			
R1H+R2OH+M = H2O+M	1.524E-25	-2.0000	0.00
O2/0.4/ N2/0.4/ B2CO/0.75/ CO2/1.5/ H2O/2.54/ CH4/3/ C2H6/3/			
!			
! 207			
R2OH+H2 = R1H+H2O	1.660E-16	1.6000	1660.80
!			
! 208			
R2OH+B5CH2 = HCHO+R1H	2.989E-11	0.0000	0.00

!				
!	209			
	R2OH+R4CH3 (+M) = CH3OH (+M)	9.962E-11	0.0000	0.00
	LOW / 3.859E-04 -8.20 0.00 /			
	TROE / 8.2000E-01 2.0000E+02 1.4380E+03 /			
!				
!	210			
	R2OH+R4CH3 = HCHO+H2	5.313E-12	-0.5300	5435.33
!				
!	211			
	R2OH+R4CH3 = R7CH3O+R1H	9.464E-12	-0.2300	6995.47
!				
!	212			
	R2OH+CH4 = R4CH3+H2O	2.656E-17	1.8300	1358.83
!				
!	213			
	R2OH+C2H2T = CH2CO+R1H	3.653E-28	4.5000	-503.27
!				
!	214			
	R2OH+C2H2T = R4CH3+B2CO	7.969E-28	4.0000	-1006.54
!				
!	215			
	R2OH+R10C2H3V = C2H2T+H2O	4.981E-11	0.0000	0.00
!				
!	216			
	R2OH+R10C2H3V = CH3CHO	4.981E-11	0.0000	0.00
!				
!	217			
	R2OH+C2H4Z = R10C2H3V+H2O	3.321E-11	0.0000	2969.30
!				
!	218			
	R2OH+C2H4Z = R4CH3+HCHO	3.321E-12	0.0000	452.94
!				
!	219			
	R2OH+R11C2H5 = C2H4Z+H2O	3.985E-11	0.0000	0.00
!				
!	220			
	R2OH+R11C2H5 = R4CH3+R1H+HCHO	3.985E-11	0.0000	0.00
!				
!	221			
	R2OH+C2H6 = R11C2H5+H2O	1.195E-17	2.0000	452.94
!				
!	222			
	2R2OH = H2O+B1O	2.490E-15	1.1400	50.33
!				
!	223			
	B2CO+R4CH3 (+M) = R14CH3CO (+M)	8.302E-13	0.0000	3472.57
	LOW / 3.032E-34 0.00 1912.43 /			
	TROE / 5.0000E-01 1.0000E+00 1.0000E+08 /			
!				
!	224			
	B2CO+B1O+M = CO2+M	4.245E-33	0.0000	1509.81
	O2/0.4/ N2/0.4/ B2CO/0.75/ CO2/1.5/ H2O/6.5/ CH4/3/ C2H6/3/			
!				
!	225			
	B2CO+R2OH = CO2+R1H	1.046E-17	1.5000	-251.64
!				
!	226			
	R5CHO+M = R1H+B2CO+M	3.155E-07	-1.0000	8555.61
	H2/2/ B2CO/1.5/ CO2/2/ H2O/6/			

!				
!	227			
R5CHO+R1H =	H2+B2CO	1.494E-10	0.0000	0.00
!				
!	228			
R5CHO+R1H =	B1O+B5CH2	6.641E-11	0.0000	51585.31
!				
!	229			
R5CHO+B5CH2 =	R4CH3+B2CO	2.989E-11	0.0000	0.00
!				
!	230			
R5CHO+R4CH3 =	CH4+B2CO	1.992E-10	0.0000	0.00
!				
!	231			
R5CHO+R4CH3 =	CH3CHO	2.989E-11	0.0000	0.00
!				
!	232			
R4CH3+HCHO =	R5CHO+CH4	1.278E-31	6.1000	991.44
!				
!	233			
R5CHO+R10C2H3V =	C2H4Z+B2CO	1.494E-10	0.0000	0.00
!				
!	234			
R10C2H3V+HCHO =	R5CHO+C2H4Z	8.966E-21	2.8100	2969.30
!				
!	235			
R5CHO+R11C2H5 =	C2H6+B2CO	1.992E-10	0.0000	0.00
!				
!	236			
R11C2H5+HCHO =	R5CHO+C2H6	9.248E-21	2.8100	2949.17
!				
!	237			
R5CHO+B1O =	R1H+CO2	4.981E-11	0.0000	0.00
!				
!	238			
R5CHO+B1O =	R2OH+B2CO	4.981E-11	0.0000	0.00
!				
!	239			
R5CHO+R2OH =	H2O+B2CO	1.826E-10	0.0000	0.00
!				
!	240			
2R5CHO =	HCHO+B2CO	4.981E-11	0.0000	0.00
!				
!	241			
HCHO+M =	R5CHO+R1H+M	2.324E+12	-5.5400	48716.66
	O2/0.4/ N2/0.4/ B2CO/0.75/ CO2/1.5/ H2O/6.5/ CH4/3/ C2H6/3/			
!				
!	242			
HCHO+M =	H2+B2CO+M	5.413E+12	-5.5400	48716.66
	O2/0.4/ N2/0.4/ B2CO/0.75/ CO2/1.5/ H2O/6.5/ CH4/3/ C2H6/3/			
!				
!	243			
HCHO+R1H =	R5CHO+H2	2.158E-16	1.6200	1056.87
!				
!	244			
HCHO+B1O =	R5CHO+R2OH	6.807E-13	0.5700	1358.83
!				
!	245			
HCHO+R2OH =	R5CHO+H2O	5.645E-15	1.1800	-201.31
!				

!	246			
	R7CH3O+M =	HCHO+R1H+M	2.573E-10	0.0000
		O2/0.4/ N2/0.4/ B2CO/0.75/ CO2/1.5/ H2O/6.5/ CH4/3/ C2H6/3/		6794.16
!				
!	247			
	R7CH3O+R1H =	HCHO+H2	2.989E-11	0.0000
!				0.00
!				
!	248			
	R7CH3O+B5CH2 =	R4CH3+HCHO	2.989E-11	0.0000
!				0.00
!				
!	249			
	R7CH3O+R4CH3 =	HCHO+CH4	3.985E-11	0.0000
!				0.00
!				
!	250			
	R7CH3O+CH4 =	R4CH3+CH3OH	2.656E-13	0.0000
!				4428.79
!				
!	251			
	R7CH3O+R10C2H3V =	HCHO+C2H4Z	3.985E-11	0.0000
!				0.00
!				
!	252			
	R7CH3O+C2H4Z =	HCHO+R11C2H5	1.992E-13	0.0000
!				3371.92
!				
!	253			
	R7CH3O+R11C2H5 =	HCHO+C2H6	3.985E-11	0.0000
!				0.00
!				
!	254			
	R7CH3O+C2H6 =	R11C2H5+CH3OH	3.985E-13	0.0000
!				3522.90
!				
!	255			
	R7CH3O+B1O =	HCHO+R2OH	2.989E-12	0.0000
!				0.00
!				
!	256			
	R7CH3O+R2OH =	HCHO+H2O	2.989E-11	0.0000
!				0.00
!				
!	257			
	R7CH3O+B2CO =	R4CH3+CO2	2.656E-11	0.0000
!				5888.27
!				
!	258			
	R7CH3O+R5CHO =	CH3OH+B2CO	1.511E-10	0.0000
!				0.00
!				
!	259			
	R7CH3O+HCHO =	CH3OH+R5CHO	1.660E-13	0.0000
!				1509.81
!				
!	260			
	2R7CH3O =	CH3OH+HCHO	9.962E-11	0.0000
!				0.00
!				
!	261			
	CH3OH+R1H =	R4CH3+H2O	3.321E-10	0.0000
!				2667.34
!				
!	262			
	CH3OH+R1H =	R7CH3O+H2	6.973E-18	2.1000
!				2466.03
!				
!	263			
	CH3OH+B5CH2 =	R4CH3+R7CH3O	2.391E-23	3.1000
!				3472.57
!				
!	264			
	CH3OH+R10C2H3V =	C2H4Z+R7CH3O	2.391E-23	3.1000
!				3472.57
!				
!	265			
	CH3OH+B1O =	R7CH3O+R2OH	1.660E-11	0.0000
!				2365.38

!				
!	266			
	CH3OH+R2OH =	R7CH3O+H2O	8.966E-19	2.0000 -171.11
!				
!	267			
	R12CHCOV+R1H =	B5CH2+B2CO	2.490E-10	0.0000 0.00
!				
!	268			
	R12CHCOV+B5CH2 =	R10C2H3V+B2CO	4.981E-11	0.0000 0.00
!				
!	269			
	R12CHCOV+B1O =	2B2CO+R1H	1.594E-10	0.0000 0.00
!				
!	270			
	R12CHCOV+R2OH =	R5CHO+B2CO+R1H	1.660E-11	0.0000 0.00
!				
!	271			
	CH2CO+M =	R12CHCOV+R1H+M	4.483E-07	0.0000 43784.60
	O2/0.4/ N2/0.4/ B2CO/0.75/ CO2/1.5/ H2O/6.5/ CH4/3/ C2H6/3/			
!				
!	272			
	CH2CO+R1H =	R4CH3+B2CO	2.989E-11	0.0000 1711.12
!				
!	273			
	CH2CO+R1H =	R12CHCOV+H2	8.302E-11	0.0000 4026.17
!				
!	274			
	CH2CO+B5CH2 =	C2H4Z+B2CO	2.158E-10	0.0000 0.00
!				
!	275			
	CH2CO+B1O =	B5CH2+CO2	2.989E-12	0.0000 654.25
!				
!	276			
	CH2CO+B1O =	R12CHCOV+R2OH	1.660E-11	0.0000 4026.17
!				
!	277			
	CH2CO+R2OH =	R12CHCOV+H2O	1.245E-11	0.0000 1006.54
!				
!	278			
	CH2CO+R2OH =	R4CH3+CO2	4.184E-12	0.0000 0.00
!				
!	279			
	R14CH3CO+R1H =	R4CH3+R5CHO	1.594E-10	0.0000 0.00
!				
!	280			
	R14CH3CO+B5CH2 =	R4CH3+CH2CO	2.989E-11	0.0000 0.00
!				
!	281			
	R14CH3CO+B1O =	R4CH3+CO2	1.594E-11	0.0000 0.00
!				
!	282			
	R14CH3CO+R2OH =	CH2CO+H2O	1.992E-11	0.0000 0.00
!				
!	283			
	R14CH3CO+R2OH =	R4CH3+B2CO+R2OH	4.981E-11	0.0000 0.00
!				
!	284			
	R14CH3CO+R5CHO =	CH3CHO+B2CO	1.494E-11	0.0000 0.00
!				
!	285			

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R14CH3CO+HCHO = CH3CHO+R5CHO ! ! 286	2.989E-13	0.0000	6492.20
R14CH3CO+R7CH3O = CH3OH+CH2CO ! ! 287	9.962E-12	0.0000	0.00
R14CH3CO+R7CH3O = HCHO+CH3CHO ! ! 288	9.962E-12	0.0000	0.00
2R14CH3CO = CH2CO+CH3CHO ! ! 289	1.992E-11	0.0000	0.00
CH3CHO+R1H = H2+R14CH3CO ! ! 290	6.641E-11	0.0000	2113.74
CH3CHO+R4CH3 = R14CH3CO+CH4 ! ! 291	3.321E-30	5.6000	1258.18
CH3CHO+R10C2H3V = C2H4Z+R14CH3CO ! ! 292	1.345E-13	0.0000	1862.10
CH3CHO+R11C2H5 = C2H6+R14CH3CO ! ! 293	2.158E-12	0.0000	4277.81
CH3CHO+B1O = R14CH3CO+R2OH ! ! 294	2.324E-11	0.0000	1157.52
CH3CHO+R2OH = R14CH3CO+H2O ! ! 295	6.973E-12	0.0000	251.64
CH3CHO+R7CH3O = R14CH3CO+CH3OH ! ! 296	3.985E-13	0.0000	905.89
C2H4O#3 = CH4+B2CO ! ! 297	1.200E+13	0.0000	28787.12
C2H4O#3 = CH3CHO ! ! 298	7.300E+13	0.0000	28787.12
C2H4O#3 = R4CH3+R5CHO ! ! 299	3.600E+13	0.0000	28787.12
C2H4O#3+R1H = H2O+R10C2H3V ! ! 300	8.302E-15	0.0000	2516.36
C2H4O#3+R1H = C2H4Z+R2OH ! ! 301	1.577E-13	0.0000	2516.36
C2H4O#3+R4CH3 = R11C2H5+HCHO ! ! 302	2.324E-13	0.0000	3824.86
C2H4O#3+R4CH3 = C2H4Z+R7CH3O ! ! 303	2.490E-14	0.0000	3824.86
R15C2H5O = HCHO+R4CH3 ! ! 304	8.000E+13	0.0000	10820.33
R15C2H5O = CH3CHO+R1H ! ! 305	2.000E+14	0.0000	11726.22

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C2H5OH(+M) = R11C2H5+R2OH(+M)	1.200E+23	-1.5400	48314.04
CO2/3/ H2O/5/ B2CO/2/ H2/2/			
LOW / 5.313E+61 -18.81 57825.87 /			
TROE / 5.0000E-01 3.0000E+02 9.0000E+02 5.0000E+03 /			
!			
! 306			
C2H5OH(+M) = C2H4Z+H2O(+M)	2.800E+13	0.0900	33266.23
H2O/5/			
LOW / 4.317E+59 -18.85 43532.97 /			
TROE / 7.0000E-01 3.5000E+02 8.0000E+02 3.8000E+03 /			
!			
! 307			
C2H5OH(+M) = CH3CHO+H2(+M)	7.200E+11	0.0950	45797.69
H2O/5/			
LOW / 7.471E+63 -19.42 58178.16 /			
TROE / 9.0000E-01 9.0000E+02 1.1000E+03 3.5000E+03 /			
!			
! 308			
C2H5OH+R1H = H2+R15C2H5O	2.490E-17	1.6000	1529.94
!			
! 309			
C2H5OH+B1O = R2OH+R15C2H5O	2.656E-17	2.0000	2239.56
!			
! 310			
C2H5OH+R2OH = H2O+R15C2H5O	1.245E-12	0.3000	805.23
!			
! 311			
C2H5OH+R3OOH = H2O2+R15C2H5O	4.151E-12	0.0000	12078.51
!			
! 312			
C2H5OH+R4CH3 = CH4+R15C2H5O	2.324E-22	2.9900	3850.03
!			
! 313			
C2H5OH+R1H = H2+R2OH+C2H4Z	1.992E-17	1.8000	2566.68
!			
! 314			
C2H5OH+B1O = 2R2OH+C2H4Z	1.561E-16	1.7000	2747.86
!			
! 315			
C2H5OH+R2OH = H2O+R2OH+C2H4Z	2.823E-13	0.2700	301.96
!			
! 316			
C2H5OH+R3OOH = H2O2+R2OH+C2H4Z	1.992E-20	2.5500	7901.36
!			
! 317			
C2H5OH+R4CH3 = CH4+R2OH+C2H4Z	3.653E-22	3.1800	4831.40
!			
! 318			
C2H5OH+R1H = H2+CH3CHO+R1H	4.317E-17	1.6500	1409.16
!			
! 319			
C2H5OH+B1O = R2OH+CH3CHO+R1H	3.155E-17	1.8500	915.95
!			
! 320			
C2H5OH+R2OH = H2O+CH3CHO+R1H	7.637E-13	0.1500	0.00
!			
! 321			
C2H5OH+R3OOH = H2O2+CH3CHO+R1H	1.361E-20	2.5500	5385.00
!			
! 322			

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C2H5OH+R4CH3 = CH4+CH3CHO+R1H	1.212E-21	2.9900	3975.84
!			
! 323			
2B1O+M = O2+M	1.489E-34	0.0000	-900.86
O2/0.4/ N2/0.4/ B2CO/0.75/ CO2/1.5/ H2O/6.5/ CH4/3/ C2H6/3/			
!			
! 324			
O2+R1H = R2OH+B1O	1.627E-10	0.0000	7448.41
!			
! 325			
O2+R1H(+M) = R3OOH(+M)	7.505E-11	0.0000	0.00
O2/0.4/ N2/0.4/ B2CO/0.75/ CO2/1.5/ H2O/0/ CH4/3/ C2H6/3/			
LOW / 4.962E-30 -0.80 0.00 /			
TROE / 5.0000E-01 1.0000E+00 1.0000E+08 /			
!			
! 326			
O2+R1H(+H2O) = R3OOH(+H2O)	7.505E-11	0.0000	0.00
LOW / 1.902E-32 0.00 -1046.80 /			
TROE / 4.5000E-01 1.0000E+00 1.0000E+08 /			
!			
! 327			
O2+B5CH2 = R5CHO+R2OH	7.139E-14	0.0000	-251.64
!			
! 328			
O2+B5CH2 = CO2+H2	1.146E-12	0.0000	251.64
!			
! 329			
O2+B5CH2 = CO2+2R1H	2.656E-12	0.0000	503.27
!			
! 330			
O2+B5CH2 = B2CO+H2O	3.155E-14	0.0000	-503.27
!			
! 331			
O2+B5CH2 = B2CO+R2OH+R1H	1.428E-13	0.0000	-251.64
!			
! 332			
O2+B5CH2 = HCHO+B1O	1.660E-10	0.0000	2264.72
!			
! 333			
O2+R4CH3(+M) = R8CH3OO(+M)	1.295E-15	1.2000	0.00
LOW / 1.544E-22 -3.30 0.00 /			
TROE / 3.6000E-01 1.0000E+00 1.0000E+08 /			
!			
! 334			
O2+R4CH3 = R7CH3O+B1O	2.158E-10	0.0000	15752.39
!			
! 335			
O2+R4CH3 = HCHO+R2OH	4.981E+06	-4.6900	18419.73
!			
! 336			
O2+CH4 = R4CH3+R3OOH	6.641E-11	0.0000	28535.48
!			
! 337			
O2+C2H2T = 2R5CHO	1.162E-16	1.8000	15400.10
!			
! 338			
O2+R10C2H3V = C2H2T+R3OOH	2.225E-18	1.6100	-201.31
!			
! 339			
O2+R10C2H3V = HCHO+R5CHO	7.471E-08	-1.3900	503.27

!				
!	340			
O2+C2H4Z =	R10C2H3V+R3OOH	6.973E-11	0.0000	28887.77
!				
!	341			
O2+R11C2H5 =	R15C2H5O+B1O	1.992E-11	-0.2000	14041.27
!				
!	342			
O2+C2H6 =	R11C2H5+R3OOH	9.962E-11	0.0000	26019.13
!				
!	343			
O2+R2OH =	R3OOH+B1O	3.653E-11	0.0000	26421.74
!				
!	344			
O2+B2CO =	CO2+B1O	4.151E-12	0.0000	24006.04
!				
!	345			
O2+R5CHO =	B2CO+R3OOH	1.262E-11	0.0000	206.34
!				
!	346			
O2+HCHO =	R5CHO+R3OOH	3.321E-11	0.0000	19526.93
!				
!	347			
O2+R7CH3O =	HCHO+R3OOH	3.653E-14	0.0000	855.56
!				
!	348			
O2+R12CHCOV =	2B2CO+R2OH	2.490E-12	0.0000	1258.18
!				
!	349			
O2+CH3CHO =	R14CH3CO+R3OOH	8.302E-11	0.0000	18319.07
!				
!	350			
O2+R15C2H5O =	CH3CHO+R3OOH	9.962E-14	0.0000	855.56
!				
!	351			
R3OOH+R1H =	H2+O2	7.139E-11	0.0000	704.58
!				
!	352			
R3OOH+R1H =	2R2OH	2.823E-10	0.0000	452.94
!				
!	353			
R3OOH+R1H =	H2O+B1O	4.981E-11	0.0000	855.56
!				
!	354			
R3OOH+B5CH2 =	HCHO+R2OH	2.989E-11	0.0000	0.00
!				
!	355			
R3OOH+R4CH3 =	R7CH3O+R2OH	2.989E-11	0.0000	0.00
!				
!	356			
R3OOH+CH4 =	R4CH3+H2O2	1.494E-11	0.0000	12380.47
!				
!	357			
R3OOH+C2H2T =	CH2CO+R2OH	9.962E-15	0.0000	4026.17
!				
!	358			
R3OOH+R10C2H3V =	R2OH+R4CH3+B2CO	4.981E-11	0.0000	0.00
!				
!	359			
R3OOH+C2H4Z =	CH3CHO+R2OH	9.962E-15	0.0000	3975.84

!				
!	360			
R3OOH+C2H4Z =	C2H4O#3+R2OH	3.653E-12	0.0000	8656.27
!				
!	361			
R3OOH+R11C2H5 =	R4CH3+HCHO+R2OH	3.985E-11	0.0000	0.00
!				
!	362			
R3OOH+R11C2H5 =	C2H4Z+H2O2	4.981E-13	0.0000	0.00
!				
!	363			
R3OOH+C2H6 =	R11C2H5+H2O2	2.158E-11	0.0000	10266.73
!				
!	364			
R3OOH+R2OH =	H2O+O2	4.815E-11	0.0000	-251.64
!				
!	365			
R3OOH+B2CO =	CO2+R2OH	2.490E-10	0.0000	11877.20
!				
!	366			
R3OOH+R5CHO =	R2OH+R1H+CO2	4.981E-11	0.0000	0.00
!				
!	367			
R3OOH+HCHO =	R5CHO+H2O2	4.981E-12	0.0000	6542.53
!				
!	368			
R3OOH+R7CH3O =	HCHO+H2O2	4.981E-13	0.0000	0.00
!				
!	369			
R3OOH+R14CH3CO =	R4CH3+CO2+R2OH	4.981E-11	0.0000	0.00
!				
!	370			
R3OOH+CH3CHO =	R14CH3CO+H2O2	1.660E-12	0.0000	5032.71
!				
!	371			
2R3OOH =	H2O2+O2	2.158E-13	0.0000	-820.33
DUPLICATE				
!				
!	372			
2R3OOH =	H2O2+O2	6.973E-10	0.0000	6029.19
DUPLICATE				
!				
!	373			
H2O2 (+M) =	2R2OH (+M)	3.000E+14	0.0000	24408.66
O2/0.4/ N2/0.4/ B2CO/0.75/ CO2/1.5/ H2O/6.5/ CH4/3/ C2H6/3/				
LOW /	4.981E-07 0.00 22898.84 /			
TROE /	5.0000E-01 1.0000E+00 1.0000E+08 /			
!				
!	374			
H2O2+R1H =	H2+R3OOH	2.823E-12	0.0000	1862.10
!				
!	375			
H2O2+R1H =	H2O+R2OH	1.660E-11	0.0000	1811.78
!				
!	376			
H2O2+R10C2H3V =	C2H4Z+R3OOH	1.992E-14	0.0000	-301.96
!				
!	377			
H2O2+B1O =	R2OH+R3OOH	1.096E-12	0.0000	2013.09
!				

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!	378			
H2O2+R2OH =	H2O+R3OOH	1.295E-11	0.0000	654.25
!				
!	379			
CO2+B5CH2 =	HCHO+B2CO	3.819E-14	0.0000	0.00
!				
!	380			
R8CH3OO =	HCHO+R2OH	1.500E+13	0.0000	23653.75
!				
!	381			
R8CH3OO+R1H =	R7CH3O+R2OH	1.594E-10	0.0000	0.00
!				
!	382			
R8CH3OO+H2 =	CH3OOH+R1H	4.981E-11	0.0000	13085.05
!				
!	383			
R8CH3OO+B5CH2 =	HCHO+R7CH3O	2.989E-11	0.0000	0.00
!				
!	384			
R8CH3OO+R4CH3 =	2R7CH3O	8.302E-12	0.0000	-704.58
!				
!	385			
R8CH3OO+CH4 =	CH3OOH+R4CH3	2.989E-13	0.0000	9310.52
!				
!	386			
R8CH3OO+C2H4Z =	R7CH3O+C2H4O#3	1.826E-09	0.0000	10065.43
!				
!	387			
R8CH3OO+C2H4Z =	CH3OOH+R10C2H3V	6.475E-12	0.0000	12330.15
!				
!	388			
R8CH3OO+R11C2H5 =	R7CH3O+R15C2H5O	3.985E-11	0.0000	0.00
!				
!	389			
R8CH3OO+C2H6 =	CH3OOH+R11C2H5	4.815E-13	0.0000	7498.74
!				
!	390			
R8CH3OO+B1O =	R7CH3O+O2	5.977E-11	0.0000	0.00
!				
!	391			
R8CH3OO+R2OH =	CH3OH+O2	9.962E-11	0.0000	0.00
!				
!	392			
R8CH3OO+R2OH =	R7CH3O+R3OOH	4.981E-12	0.0000	0.00
!				
!	393			
R8CH3OO+B2CO =	R7CH3O+CO2	1.660E-10	0.0000	12078.51
!				
!	394			
R8CH3OO+R5CHO =	R7CH3O+R1H+CO2	4.981E-11	0.0000	0.00
!				
!	395			
R8CH3OO+HCHO =	CH3OOH+R5CHO	1.660E-12	0.0000	6089.58
!				
!	396			
R8CH3OO+R7CH3O =	HCHO+CH3OOH	4.981E-13	0.0000	0.00
!				
!	397			
R8CH3OO+CH3OH =	CH3OOH+R7CH3O	4.649E-13	0.0000	9461.50
!				

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!	398				
R8CH3OO+CH2CO =	CH3OOH+R12CHCOV	2.823E-12	0.0000	13588.32	
!					
!	399				
R8CH3OO+R14CH3CO =	R4CH3+CO2+R7CH3O	3.985E-11	0.0000	0.00	
!					
!	400				
R8CH3OO+CH3CHO =	CH3OOH+R14CH3CO	1.660E-12	0.0000	6089.58	
!					
!	401				
R8CH3OO+R3OOH =	CH3OOH+O2	4.151E-13	0.0000	-805.23	
!					
!	402				
R8CH3OO+R3OOH =	O2+HCHO+H2O	8.302E-14	0.0000	0.00	
!					
!	403				
R8CH3OO+H2O2 =	CH3OOH+R3OOH	3.985E-12	0.0000	4982.39	
!					
!	404				
2R8CH3OO =	CH3OH+HCHO+O2	4.151E-14	0.0000	-402.62	
!					
!	405				
2R8CH3OO =	2R7CH3O+O2	4.151E-14	0.0000	-402.62	
!					
!	406				
CH3OOH =	R7CH3O+R2OH	6.000E+14	0.0000	21288.38	
!					
!	407				
CH3OOH+B1O =	R8CH3OO+R2OH	3.321E-11	0.0000	2415.70	
!					
!	408				
CH3OOH+R2OH =	H2O+R8CH3OO	2.989E-12	0.0000	-186.21	
!					
!	409				
CH3OOH+R7CH3O =	CH3OH+R2OH+HCHO	2.490E-13	0.0000	3271.26	
!					
!	410				
R17C2H5OO+H2 =	C2H5OOH+R1H	1.312E-11	0.0000	10568.70	
!					
!	411				
R17C2H5OO+R4CH3 =	R15C2H5O+R7CH3O	3.321E-12	0.0000	-603.93	
!					
!	412				
R17C2H5OO+CH4 =	C2H5OOH+R4CH3	6.475E-12	0.0000	12078.51	
!					
!	413				
R17C2H5OO+C2H4Z =	C2H5OOH+R10C2H3V	6.475E-12	0.0000	12279.82	
!					
!	414				
R17C2H5OO+C2H4Z =	R15C2H5O+C2H4O#3	3.819E-08	0.0000	11021.64	
!					
!	415				
R17C2H5OO+C2H6 =	C2H5OOH+R11C2H5	8.468E-12	0.0000	9813.79	
!					
!	416				
R17C2H5OO+H2O =	C2H5OOH+R2OH	9.298E-12	0.0000	15400.10	
!					
!	417				
R17C2H5OO+B2CO =	CO2+R15C2H5O	1.660E-10	0.0000	12078.51	
!					

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!	418			
R17C2H5OO+HCHO =	C2H5OOH+R5CHO	7.471E-12	0.0000	7247.11
!				
!	419			
R17C2H5OO+CH3OH =	C2H5OOH+R7CH3O	4.649E-13	0.0000	9260.19
!				
!	420			
R17C2H5OO+CH2CO =	C2H5OOH+R12CHCOV	2.823E-12	0.0000	12279.82
!				
!	421			
R17C2H5OO+CH3CHO =	C2H5OOH+R14CH3CO	6.475E-12	0.0000	7247.11
!				
!	422			
R17C2H5OO+R3OOH =	O2+C2H5OOH	6.475E-13	0.0000	-654.25
!				
!	423			
R17C2H5OO+H2O2 =	C2H5OOH+R3OOH	7.471E-13	0.0000	5435.33
!				
!	424			
R17C2H5OO+R8CH3OO =	R15C2H5O+R7CH3O+O2	3.321E-13	0.0000	0.00
!				
!	425			
R17C2H5OO+CH3OOH =	C2H5OOH+R8CH3OO	1.826E-12	0.0000	8203.32
!				
!	426			
2R17C2H5OO =	2R15C2H5O+O2	6.807E-14	0.0000	100.65
!				
!	427			
2R17C2H5OO =	C2H5OH+CH3CHO+O2	2.989E-14	0.0000	100.65
!				
!	428			
C2H5OOH =	R15C2H5O+R2OH	4.000E+15	0.0000	21590.34
!				
!	429			
C2H5OOH+R1H =	CH3CHO+R2OH+H2	5.313E-11	0.0000	3875.19
!				
!	430			
C2H5OOH+R4CH3 =	CH3CHO+R2OH+CH4	9.464E-13	0.0000	4378.46
!				
!	431			
C2H5OOH+R10C2H3V =	CH3CHO+R2OH+C2H4Z	1.660E-12	0.0000	4378.46
!				
!	432			
C2H5OOH+R11C2H5 =	CH3CHO+R2OH+C2H6	5.645E-13	0.0000	5737.29
!				
!	433			
C2H5OOH+R2OH =	CH3CHO+R2OH+H2O	9.796E-12	0.0000	452.94
!				
!	434			
C2H5OOH+R5CHO =	CH3CHO+R2OH+HCHO	2.989E-12	0.0000	8404.63
!				
!	435			
C2H5OOH+R7CH3O =	CH3CHO+R2OH+CH3OH	1.046E-12	0.0000	2767.99
!				
!	436			
C2H5OOH+R14CH3CO =	2CH3CHO+R2OH	3.321E-12	0.0000	9310.52
!				
!	437			
C2H5OOH+R3OOH =	CH3CHO+R2OH+H2O2	1.328E-12	0.0000	8152.99
!				

! 438			
C2H5OOH+R8CH3OO = CH3CHO+R2OH+CH3OOH	1.826E-12	0.0000	8404.63
! 439			
C2H5OOH+R17C2H5OO = CH3CHO+R2OH+C2H5OOH	1.826E-12	0.0000	8404.63
! 440			
R11C2H5+R10C2H3V = C4H8Y	2.490E-11	0.0000	0.00
! 441			
R5CHO+R10C2H3V = C2H3CHOZ	2.989E-11	0.0000	0.00
! 442			
C2H3CHOZ+R2OH = B2CO+R10C2H3V+H2O	1.660E-11	0.0000	0.00
! 443			
C2H3CHOZ+B1O = B2CO+R10C2H3V+R2OH	1.195E-11	0.0000	1006.54
! 444			
C2H3CHOZ+B1O = CH2CO+R5CHO+R1H	8.302E-17	1.7600	40.26
! 445			
C2H3CHOZ+R1H = B2CO+R10C2H3V+H2	6.641E-11	0.0000	2113.74
! 446			
C2H3CHOZ+R1H = C2H4Z+R5CHO	3.321E-11	0.0000	1761.45
! 447			
C2H3CHOZ+O2 = B2CO+R10C2H3V+R3OOH	4.981E-11	0.0000	18117.77
! 448			
ZC3H5Y+R3OOH = C2H3CHOZ+R1H+R2OH	1.162E-05	-2.0000	0.00
! 449			
ZC3H5Y+O2 = C2H3CHOZ+R2OH	2.989E-11	-0.4100	11524.91
! 450			
ZC3H5Y+B1O = C2H3CHOZ+R1H	2.989E-10	0.0000	0.00
END			
!-----!			
! The mechanism was reprinted by program MECHMOD v1.5 !			
!-----!			