

**GEOS-Chem**  
**Chemical Mechanism**  
**Version 8-02-04**

Jingqiu Mao<sup>1</sup>, Claire Carouge<sup>1</sup>, Mat Evans<sup>2</sup>, Dylan Millet<sup>3</sup>,  
and Paul Palmer group<sup>4</sup>

<sup>1</sup>Harvard University, Cambridge, MA, USA

<sup>2</sup>University of Leeds, Leeds, UK

<sup>3</sup>University of Minnesota, St. Paul, MN, USA

<sup>4</sup>University of Edinburgh, Edinburgh, UK

Oct 27, 2009

Updates in v8-02-04:

1. Change the branch ratio of HNO<sub>4</sub> photolysis in ratj.d

Line 13 HNO<sub>4</sub>+hv->OH+NO<sub>3</sub> from 33.3 to 5.0

Line 14 HNO<sub>4</sub>+hv->HO<sub>2</sub>+NO<sub>2</sub> from 66.7 to 95.0

This is based on Jimenez et al. (Quantum yields of OH, HO<sub>2</sub> and NO<sub>3</sub> in the UV photolysis of HO<sub>2</sub>NO<sub>2</sub>, PHYSICAL CHEMISTRY CHEMICAL PHYSICS, 2005), which shows that HO<sub>2</sub> yield should be 0.95 and OH yield should be 0.05 for wavelength above 290nm.

This way all the near-IR photolysis will have most weight on HO<sub>2</sub> channel (Stark et al., Overtone dissociation of peroxyntic acid (HO<sub>2</sub>NO<sub>2</sub>): Absorption cross sections and photolysis products, JOURNAL OF PHYSICAL CHEMISTRY A, 2008).

2. Comment out the near-IR calculation of HNO<sub>4</sub> photolysis in calcrate.f since FastJX already takes this into account.

No.	Reaction	Rate Constant	Reference	Notes
1	NO + O3 → NO2 + O2	3.00E-12 exp(-1500/T)	JPL00	
		Same	JPL06	
2	O3+OH = HO2+O2	1.70E-12 exp(-940/T)	JPL02	
		Same	JPL06	
3	O3+HO2 = OH+2O2	1.00E-14 exp(-490/T)	JPL02	
		Same	JPL06	
4	O3+NO2 = O2+NO3	1.20E-13 exp(-2450/T)	JPL97	
		Same	JPL06	
5	O3+MO2 = CH2O+HO2+2O2	2.90E-16 exp(-1000/T)	JPL02	
		Same	JPL06	
6	OH+OH = H2O+O3	4.20E-12 exp(-240/T)	JPL97	
		1.8E-12	JPL06	JMAO
7	OH+OH+M = H2O2	LPL: 6.9E-31(300/T)	JPL02	
		HPL: 2.60E-11		
		Fc:0.6		
		Same	JPL06	
8	OH+HO2 = H2O + O2	4.80E-11 exp(250/T)	JPL97	
		Same	JPL06	
9	OH+H2O2 = H2O + HO2	2.90E-12 exp(-160/T)	JPL97	
		1.8E-12	JPL06	JMAO
10	HO2+NO = OH + NO2	3.50E-12 exp(250/T)	JPL97	
		Same	JPL06	
11	HO2+HO2 = H2O2	K1=2.30E-13 exp(600/T)	JPL97	
	HO2+HO2+M=H2O2	K2=1.70E-33 [M]		
		exp(1000/T)		
		K = (K1 + K2)*(1+1.4E-21*[H2O]*EXP(2200/T))		
		K1=3.50E-13 exp(430/T)	JPL06	JMAO
		K2=1.70E-33 [M]exp(1000/T)		
		K = (K1 + K2)*(1+1.4E-21*[H2O]*EXP(2200/T))		
12	OH+H2 = H2O + HO2	5.50E-12 exp(-2000/T)	JPL97	
		2.80E-12 exp(-1800/T)	JPL06	JMAO
13	CO+OH = HO2 + CO2	K0=1.50E-13	JPL97	
		K = K0(1+0.6 Patm)		
	CO+OH = HOCO	LPL: 5.9E-33(300/T)^1.4 HPL:1.1E-12(300/T)^-1.3 Fc:0.6	JPL06	JMAO(in calcrate.f) Ignore the intermediate species HOCO and use two 3-body reactions
	HOCO + O2= HO2 + CO2	2.00E-12		
	CO+OH=HO2+CO2 (different formula)	LPL: 1.5E-13(300/T)^-0.6 HPL:2.10E9(300/T)^-6.1 Fc:0.6	JPL06	

14	OH+ CH4 = MO2+H2O	<del>1.26E-12 (300/T)^(-6.7E-01) exp(-1575/T)</del>	JPL97	This reaction coefficient was not found on JPL97.
		2.45E-12exp(-1775/T)	JPL06	JMAO:could also be 2.8E-14T^0.667 exp(-1575/T)
15	MO2+NO =CH2O+HO2+NO2	2.80E-12 exp(300/T)	Tyndall 2001	Tyndall et al., Atmospheric Chemistry of small organic peroxy radicals,JGR 106, 12157-12182, 2001.
		Same	JPL06	
16	MO2+HO2 = MP+O2	<del>K1=4.10E-13 exp(750/T) K2=2.00E-03exp(1160/T) K=K1/(1+K2)</del>	<del>Tyndall-2001&amp;Elrod 2001</del>	
		4.1E-13 exp(750/T)	JPL06	JMAO
17	MO2+HO2 = CH2O + O2	<del>K1=4.10E-13 exp(750/T) K2=4.98E+2 exp(-1160/T) K=K1/(1+K2)</del>	<del>Tyndall-2001&amp;Elrod 2001</del>	
		Not recommended in JPL06	JPL06(P1-59,D35)	JMAO
18	MO2+MO2 =MOH+CH2O+O2	K1=9.5E-14 exp(390/T)	Tyndall 2001	This reaction coefficient was not found on Tyndall.
		K2=2.62E+1 exp(-1130/T)		
		Same		
19	MO2+MO2 = 2CH2O + 2HO2	K1=9.5E-14 exp(390/T)	Tyndall 2001	This reaction coefficient was not found on Tyndall.
		K2=4.00E-02 exp(1130/T)		
		K=K1 / (1+K2)		
		Same		
20	MP+OH = MO2+H2O	2.66E-12 exp(200/T)	JPL97	
		Same	JPL06	
21	MP+OH = CH2O+OH+H2O	1.14E-12 exp(200/T)	JPL97	
		Same	JPL06	
22	CH2O+OH = CO+HO2+H2O	<del>9.00E-12</del>	<del>JPL02</del>	
	CH2O+OH = HCO +H2O	5.5E-12 exp(125/T)	JPL06	JMAO(use the first rate)
	HCO + O2 = CO + HO2	5.2E-12	JPL06	
23	NO2+OH+M = HNO3+M	<del>LPL: 2.00E-30(300/T)^3 HPL:2.50E-11(300/T)^0 Fc: 0.6</del>	<del>JPL02</del>	
	OH + NO2 + M = HONO2	LPL: 1.80E-30(300/T)^3 HPL:2.80E-11(300/T)^0 Fc:0.6	JPL06	JMAO: Ignore the HOONO channel for now.

	OH + NO2 + M=HOONO	LPL:9.10E-32(300/T)^3.9 HPL:4.20E-11(300/T)^0.5 Fc:0.6	JPL06	This adds a new species HOONO, should we include this reaction?
24	HNO3+OH = H2O+NO3	K0=2.41E-14 exp(460/T) K2=2.69E-17exp(2199/T) K3=6.51E-34exp(1335/T)	Brown 98	OH + HNO3: K = K0 + K3[M] / (1 + K3[M]/K2)
		Same	JPL06,same source	Brown, S. S., R. K. Talukdar and A. R. Ravishankara, 1999, J. Phys. Chem. A, 103, 3031-3037.
25	NO+OH+M = HNO2+M	LPL: 7.00E-31(300/T)^2.6 HPL: 3.60E-11(300/T)^0.1 Fc: 0.6	JPL97	
		LPL: 7.00E-31(300/T)^2.6 HPL: 3.60E-11(300/T)^0.1 Fc: 0.6	JPL06	
26	HNO2+OH = H2O+NO2	1.80E-11 exp(-390/T) Same	JPL97 JPL06	
27	HO2+NO2+M = HNO4+M	LPL: 1.80E-31(300/T)^3.2;- HPL:4.7E-12(300/T)^1.4; Fc= 0.6	JPL97	
		LPL: 2.0E-31(300/T)^3.4 HPL:2.9E-12(300/T)^1.1 Fc= 0.6	JPL06	JMAO
28	HNO4+M = HO2+NO2	LPL: 8.64E-5(300/T)^3.2* exp(-10900/T);- HPL:2.24E+15*(300/T)^1.4*exp(-10900/T); Fc=0.6	K=forward rxn/Keq Keq=2.1E-27exp(10900/T) JPL97	
		LPL: 9.52E-5(300/T)^3.2* exp(-10900/T) HPL:1.38E+15*(300/T)^1.4*exp(-10900/T); Fc=0.6	K=forward rxn/Keq Keq=2.1E-27exp(10900/T) JPL06	JMAO
29	HNO4+OH = H2O+NO2+O2	1.30E-12 exp(380/T) Same	JPL97 JPL06	
30	NO+NO3=2NO2	1.50E-11 exp(170/T) Same	JPL97 JPL06	
31	HO2+NO3 = OH+NO2+O2	3.50E-12 Same	JPL06	
32	OH+NO3 = HO2+NO2	2.20E-11 Same	JPL97 JPL06	
33	NO2+NO3+M = N2O5+M	LPL: 2.0E-30(300/T)^4.4; HPL:1.4E-12(300/T)^0.7; Fc=0.6	JPL00	

		Same	JPL06	
34	$\text{NCO}_5 + \text{M} = \text{NO}_2 + \text{NO}_3$	LPL: $6.67\text{E}-4(300/\text{T})^{4.4} \exp(-10990/\text{T})$ ; HPL: $4.67\text{E}+14*(300/\text{T})^{0.7} \exp(-10990/\text{T})$ ; Fc=0.6	K=forwardrxn/ Keq; Keq = $3.00\text{E}-27 \exp(10990/\text{T})$ ; JPL00	
		LPL: $7.4\text{E}-4(300/\text{T})^{4.4} \exp(-11000/\text{T})$ ; HPL: $5.18\text{E}+14*(300/\text{T})^{0.7} \exp(-11000/\text{T})$ ; Fc=0.6	K=forwardrxn/ Keq; Keq = $2.70\text{E}-27 \exp(11000/\text{T})$ ; JPL06	JMAO
35	$\text{HCOOH} + \text{OH} = \text{H}_2\text{O} + \text{CO}_2 + \text{HO}_2$	$4.00\text{E}-13$	JPL97	
		Same	JPL06	
36	$\text{MOH} + \text{OH} = \text{HO}_2 + \text{CH}_2\text{O}$	$7.30\text{E}-12 \exp(-620/\text{T})$	JPL02	
		$2.9\text{E}-12 \exp(-345/\text{T})$	JPL06	
37	$\text{NO}_2 + \text{NO}_3 = \text{NO} + \text{NO}_2 + \text{O}_2$	$4.50\text{E}-14 \exp(-1260/\text{T})$	JPL97	
		Same	JPL06	
38	$\text{NO}_3 + \text{CH}_2\text{O} = \text{HNO}_3 + \text{HO}_2 + \text{CO}$	$5.80\text{E}-16$	JPL97	
		Same	JPL06	
39	$\text{ALD}_2 + \text{OH} = \text{MCO}_3 + \text{H}_2\text{O}$	$5.60\text{E}-12 \exp(270/\text{T})$	JPL97	
		Same		JMAO: Can not find this reaction from JPL06, it was in JPL02. It is $4.4\text{E}-12 \exp(365/\text{T})$ in IUPAC06
	$\text{ALD}_2 + \text{OH} = \text{H}_2\text{O} + 0.95 \text{MCO}_3 + 0.05 \text{CH}_2\text{O} + 0.05 \text{CO} + 0.05 \text{HO}_2$	$4.4\text{E}-12 \exp(365/\text{T})$	IUPAC06	DBM
40	$\text{ALD}_2 + \text{NO}_3 = \text{HNO}_3 + \text{MCO}_3$	$1.40\text{E}-12 \exp(-1860/\text{T})$	IUPAC02	
		$1.40\text{E}-12 \exp(-1900/\text{T})$	JPL06	JMAO
41	$\text{MCO}_3 + \text{NO}_2 + \text{M} = \text{PAN}$	LPL: $8.50\text{E}-29(300/\text{T})^{6.5}$ ; HPL: $1.10\text{E}-11(300/\text{T})$ ; Fc: 0.6	Tyndall	
		LPL: $9.70\text{E}-29(300/\text{T})^{5.6}$ ; HPL: $9.3\text{E}-12(300/\text{T})^{1.5}$ ; Fc: 0.6	JPL06	JMAO
42	$\text{PAN} = \text{MCO}_3 + \text{NO}_2$	$9.30\text{E}-29 \exp(14000/\text{T})$	Tyndall	
			IUPAC06	
43	$\text{MCO}_3 + \text{NO} = \text{MO}_2 + \text{NO}_2 + \text{CO}_2$	$8.10\text{E}-12 \exp(270/\text{T})$	Tyndall	
		Same	JPL06	
44	$\text{C}_2\text{H}_6 + \text{OH} = \text{ETO}_2 + \text{H}_2\text{O}$	$8.7\text{E}-12 \exp(-1070/\text{T})$	JPL97	
		Same	JPL06	
45	$\text{ETO}_2 + \text{NO} = \text{ALD}_2 + \text{NO}_2 + \text{HO}_2$	$2.70\text{E}-12 \exp(350/\text{T})$	Tyndall	
		$2.60\text{E}-12 \exp(365/\text{T})$	JPL06	JMAO

46	C3H8+OH = B3O2	K1=7.60e-12 exp(-585/T); K2=5.87*(300/T)^0.64exp(-816/T); K=K1 / (1+K2)	IUPAC02	
	C3H8+OH = A3O2	K1=7.60E-12 exp(-585/T); K2=0.17*(300/T)^-0.64exp(816/T); K=K1 / (1+K2)	IUPAC02	Cant find from Tyndall
			IUPAC06	JMAO
47	A3O2+NO = NO2 + HO2 + RCHO	2.70E-12 exp(350/T)	Tyndall	The products is not from Tyndall
		2.90E-12 exp(350/T)	IUPAC06	JMAO
48	PO2+NO = NO2+HO2+CH2O+ALD2	2.70E-12 exp(350/T)	Tyndall	
49	ALK4+OH = R4O2	9.10E-12 exp(-405/T)	IUPAC02	
		Same	IUPAC06	
50	R4O2+NO = NO2 +0.32ACET + 0.19MEK +0.18MO2 + 0.27HO2 +0.32ALD2 + 0.13RCHO +0.50A3O2 + 0.18B3O2 + 0.32ETO2	K* (1-YN) where YN is returned from fyrno3.f; K=2.7E-12 exp(350/T) (Xcarbn=4.50E00)	Atkinson 97	
				A3O2 is 0.05 in the input file(Palmer)
51	R4O2+NO = R4N2	K* YN where YN is returned from fyrno3.f K=2.7E-12 exp(350/T) (Xcarbn=4.50E00)	Atkinson97	
52	ATO2+NO = 0.96NO2 + 0.960CH2O +0.960MCO3 + 0.04R4N2	2.80E-12 exp(300/T)	Tyndall	
53	KO2+NO = 0.93NO2+0.93NO + 0.93ALD2 +0.93MCO3 + 0.07R4N2	2.70E-12 exp(350/T)	Tyndall ETO2+NO	
54	<del>RIO2+NO = NO2+0.864HO2+0.690CH2O+ 0.402MVK+0.288MACR+0.136 RIO1+0.127IALD</del>	K* (1-YN) where YN is returned from fyrno3.f K=2.7E-12 exp(350/T) (Xcarbn=5.00E00)	<del>Atkinson 97</del>	
	RIO2 + NO = 0.90NO2 + 0.90HO2 + 0.34IALD + 0.34MVK + 0.22MACR + 0.56CH2O			DBM(MCM 3.1)

55	RIO2+NO = HNO3	K* YN where YN is returned from fyrno3.f K=2.7E-12 exp(350/T) (Xcarbn=5.00E00)	Atkinson 97	
56	IAO2+NO = 0.92HO2+0.61CO+0.17H2+0. 33HAC+0.24GLYC +0.53MGLY+0.92NO2 +0.35CH2O+0.08HNO3	2.7E-12 exp(350/T)	Tyndall ETO2+NO	
57	<del>ISN1+NO = 1.9NO2+0.95GLYC+0.95HAC +0.05HNO3+0.05NO2</del>	2.7E-12 exp(350/T)	Tyndall ETO2+NO	
	ISN1+NO = 1.9NO2+0.95GLYC+0.95HAC +0.05HNO3+0.05NO2+0.05HO 2		Paulson&Seinfeld 1992	HO2 term(Palmer, JMAO)
58	VRO2+NO = NO2+0.28HO2+0.28CH2O+0. 72MCO3+0.72GLYC+0.28MG LY	K* (1-YN) where YN is returned from fyrno3.f K=2.7E-12 exp(350/T) (Xcarbn=4.00E00)	Atkinson 97	
59	VRO2+NO = HNO3	K* YN where YN is returned from fyrno3.f K=2.7E-12 exp(350/T) (Xcarbn=4.00E00)	Atkinson 97	
60	<del>MRO2+NO = NO2+HO2- +0.17MGLY+0.83HAC- +0.83CO+0.17CH2O</del>	K* (1-YN) where YN is returned from fyrno3.f K=2.7E-12 exp(350/T) (Xcarbn=4.00E00)	Atkinson 97	
	MRO2 + NO = NO2 + HAC + CH2O + HO2			DBM(MCM 3.1)
61	MRO2+NO = HNO3	K* YN where YN is returned from fyrno3.f K=2.7E-12 exp(350/T) (Xcarbn=4.00E00)	Atkinson 97	
62	MVN2+NO = 1.90NO2 +0.30HO2+0.30CH2O+0.60M CO3+0.60GLYC+0.30MGLY+ 0.10HNO3	2.7E-12 exp(350/T)		
63	MAN2+NO = 2NO2+CH2O+MGLY	2.7E-12 exp(350/T)	Tyndall ETO2+NO	
64	B3O2+NO = NO2+HO2+ACET	2.7E-12 exp(350/T)		

65	INO2+NO = 1.10NO2+0.80HO2+0.85HNO 3+0.05NO2+0.10MACR+0.15 CH2O+0.05MVK	2.7E-12 exp(350/T)	Tyndall ETO2+NO	
66	PRN1+NO = 2NO2+CH2O+ALD2	2.7E-12 exp(350/T)	Tyndall ETO2+NO	
67	ALK4+NO3 = HNO3 + R4O2	2.8E-12 exp(-3280/T)	IUPAC02	
		Same	IUPAC06	? Can't find
68	R4N2+OH = R4N1+H2O	<del>1.30E-12</del>	<del>Atkinson 92</del>	HO + 1-C4H9ONO2 → products
		1.6E-12	IUPAC06	JMAO
69	ACTA+OH = MO2+CO2++H2O	<del>4.00E-13 exp(200/T)</del>	<del>DeMore et al., 1994</del>	
		4.20E-14 exp(855/T)	IUPAC06	JMAO
70	OH+RCHO= RCO3+H2O	<del>5.10E-12 exp(405/T)</del>	<del>IUPAC02</del>	HO + CH3CH2CH2CHO → products
		6.0E-12 exp(410/T)	IUPAC06	JMAO
71	RCO3+NO2 = PPN	LPL: 9.00E-28(300/T)^8.9 HPL:7.70E-12(300/T)^0.2 Fc: 0.6	JPL02	
		Same	JPL06	
72	PPN = RCO3+NO2	9e-29*exp(14000/T)	JPL02	
		Same	JPL06	
73	MAO3+NO2 = PMN	LPL: 9.00E-28(300/T)^8.9 HPL:7.70E-12(300/T)^0.2 Fc: 0.6	JPL02 Same	
		Same	as PPN	
74	PMN = MAO3+NO2	9e-29*exp(14000/T)	JPL02	
		Same		
75	GLCO3+NO2 = GLPAN	LPL: 9.00E-28(300/T)^8.9 HPL:7.70E-12(300/T)^0.2 Fc: 0.6	JPL02 Same as PPN	Should be same as RCO3???
76	GLPAN = GLCO3+NO2	9e-29*exp(14000/T)	JPL02 PPN	
77	GCO3+NO2 = GPAN	LPL: 9.00E-28(300/T)^8.9 HPL:7.70E-12(300/T)^0.2 Fc: 0.6	JPL02 Same as PPN	
78	GPAN = GCO3+NO2N	9e-29*exp(14000/T)	JPL02 PPN	
79	RCO3+NO = NO2+ETO2	6.70E-12 exp(340/T)	IUPAC02 C2H5CO3+NO	
		Same	IUPAC06	
80	GCO3+NO = NO2+HO2 +CH2O	6.70E-12 exp(340/T)	IUPAC02 C2H5CO3+NO	
		Same	IUPAC06	

81	GLCO3+NO = NO2+HO2+CO	6.70E-12 exp(340/T)	IUPAC02 C2H5CO3+NO	
		Same	IUPAC06	
82	RCHO+NO3 = HNO3 +RCO3	1.82E-12exp(-1680/T)	IUPAC02 Mean of-	
			CH3CHO+NO3 and	
			C3H7CH+NO3	
		6.5E-15	IUPAC06	NO3+C2H5CHO → HNO3 + C2H5CO
83	ACET+OH = ATO2 + H2O	1.33E-13+ 3.82E-11 exp(-2000/T)	JPL 02 Implemented as 2 reactions	
		Same	JPL06	JMAO
84	A3O2+MO2 = HO2 +0.75CH2O+0.75RCHO+0.25 MOH + 0.25ROH	5.92E-13	Tyndall RateMO2+MO2 Atkinson97RO2+R O2	K(RO2+MO2) = 2*sqrt(k(MO2+MO2)*k( RO2+RO2)).
85	PO2+MO2 = HO2 + 0.5ALD2+1.25CH2O +0.16HAC + 0.09RCHO +0.25MOH + 0.25ROH	5.92E-13	Tyndall RateMO2+MO2 Atkinson97RO2+R O2	
86	R4O2+HO2 = R4P	7.40E-13 exp(700/T)	Tyndall	
			ETO2+HO2	
87	R4N1+HO2 = R4N2	7.40E-13 exp(700/T)	Tyndall	
			ETO2+HO2	
88	ATO2+HO2 = MCO3 + MO2	8.60E-13 exp(700/T)		
89	KO2+HO2 = MO2 + MGLY	7.40E-13 exp(700/T)	Tyndall	Tyndall forms CH3C(O)CH2OOH ,this must then split and go to MCO3+MO2, the products in chem..dat ??
			ETO2+HO2	
90	RIO2+HO2 = RIP	7.40E-13 exp(700/T)	Tyndall	
			ETO2+HO2	
91	RIO1+HO2 = RIP	7.40E-13 exp(700/T)	Tyndall	
			ETO2+HO2	
92	IAO2 + HO2 = IAP	7.40E-13 exp(700/T)	Tyndall	
			ETO2+HO2	
93	ISN1+HO2 = ISNP	7.40E-13 exp(700/T)	Tyndall	
			ETO2+HO2	
94	VRO2+HO2 = VRP	7.40E-13 exp(700/T)	Tyndall	
			ETO2+HO2	
95	MRO2+HO2 = MRP	7.40E-13 exp(700/T)	Tyndall	
			ETO2+HO2	

96	MVN2 + HO2 = ISNP	7.40E-13 exp(700/T)	Tyndall	
			ETO2+HO2	
97	MAN2 + HO2 = ISNP	7.40E-13 exp(700/T)	Tyndall	
			ETO2+HO2	
98	B3O2+HO2 = RB3P	7.40E-13 exp(700/T)	Tyndall	
			ETO2+HO2	
99	INO2 + HO2 = INPN	7.40E-13 exp(700/T)	Tyndall	
			ETO2+HO2	
100	PRN1 + HO2 = PRPN	7.40E-13 exp(700/T)	Tyndall	
			ETO2+HO2	
101	MEK+OH = KO2+H2O	<del>2.28E-13 * (300/T)<sup>-2</sup> * exp(503/T)</del>	IUPAC02	
		1.3 E-12 exp(-25/T)	IUPAC06	JMAO
102	MO2+ETO2 = 0.75CH2O+0.75ALD2+HO2+0.25MOH+0.25EOH	3.00E-13	Horowitz 98, Atkinson 92& 94	
103	MEK+NO3 = HNO3+ KO2	8.00E-16	Lurmann et al., 1986.	
104	R4O2+MO2 = 0.16ACET+0.10MEK+0.09MO2+0.14HO2+0.16ALD2+0.07RCHO+0.03A3O2+0.09B3O2+0.16ETO2+0.25MEK+0.75CH2O+0.25MOH+0.25ROH+0.50HO2	8.37E-14	Tyndall MO2+MO2 Atkinson97 RO2+RO2 (See note 11 below)	
105	R4N1+MO2 = NO2+0.20CH2O+0.38ALD2 +0.29RCHO+0.15R4O2+0.25RCHO+0.75CH2O+0.25MOH+0.25ROH+0.50HO2	8.37E-14	Tyndall MO2+MO2 Atkinson97 RO2+RO2 (See note 11 below)	
106	ATO2+MO2 = 0.30HO2+0.30CH2O+0.30MCO3+0.20HAC+0.20CH2O+0.50MGLY+0.50MOH	7.5E-13 exp(500/T)	Tyndall,2001	
107	KO2+MO2 = 0.5ALD2+0.50MCO3+0.25MEK+0.75CH2O+0.25MOH+0.25ROH+0.5HO2	8.37E-14		
108	RIO2+MO2 = 0.42HO2+0.35CH2O+0.2MVK+0.14MACR + 0.07RIO1+0.06IALD+0.25MEK+0.75CH2O+0.25MOH+0.25ROH + 0.5HO2	8.37E-14	Tyndall MO2+MO2 Atkinson97 RO2+RO2 (See note 11 below)	

				HO2 term is 0.43 in input file, need to be changed back to 0.42(Palmer, JMAO)
109	RIO1+MO2 = 0.50IALD+0.50HO2+0.38CH2O+0.25MEK+0.75CH2O+0.25MOH+0.25ROH+ 0.5HO2	8.37E-14	Tyndall MO2+MO2 Atkinson97 RO2+RO2 (See note 11 below)	
110	IAO2+MO2 = 0.50HO2+0.33CO+0.09H2+0.18HAC+0.13GLYC+0.29MGLY+0.25MEK+0.95CH2O+0.25MOH+0.25ROH+0.5HO2	8.37E-14	Tyndall MO2+MO2 Atkinson97 RO2+RO2 (See note 11 below)	
111	ISN1+MO2 = NO2+0.50GLYC+0.50HAC+0.25RCHO+0.75CH2O+0.25MOH+ 0.25ROH+0.50HO2	8.37E-14	Tyndall MO2+MO2 Atkinson97 RO2+RO2 (See note 11 below)	
112	VRO2+MO2 = 0.14HO2+0.14CH2O+0.36MCO3+0.36GLYC+0.14MGLY+0.25MEK+0.75CH2O+0.25MOH+0.25ROH+0.50HO2	8.37E-14	Tyndall MO2+MO2 Atkinson97 RO2+RO2 (See note 11 below)	
113	<del>MRO2+MO2 = 0.50HO2+0.09MGLY+0.42HAC+0.42CO+0.09CH2O+0.25MEK+0.75CH2O+0.25MOH+0.25ROH+0.50HO2</del>	<del>8.37E-14</del>	<del>Tyndall MO2+MO2 Atkinson97 RO2+RO2 (See note 11 below)</del>	
	MRO2 + MO2 = HAC + 0.85CH2O + 1.15HO2 + 0.15CO			DBM(MCM 3.1)
114	MVN2+MO2 = NO2+0.50CH2O+0.25MCO3+0.25MGLY+0.25HO2+0.25RCHO+0.75CH2O+0.25MOH+0.25ROH+0.50HO2	8.37E-14	Tyndall MO2+MO2 Atkinson97 RO2+RO2 (See note 11 below)	
115	MAN2+MO2= NO2+0.50CH2O+0.50MGLY+0.25RCHO+0.75CH2O+0.25MOH+0.25ROH+0.50HO2	8.37E-14	Tyndall MO2+MO2 Atkinson97 RO2+RO2 (See note 11 below)	

116	B3O2+MO2 = 0.50HO2+0.50ACET+0.25AC ET +0.75CH2O+0.25MOH+0.25R OH+0.50HO2	8.37E-14	Tyndall MO2+MO2 Atkinson97 RO2+RO2 (See note 11 below)	
117	INO2+MO2 = 0.55NO2+0.40HO2+0.425HNO 3+0.025NO2+0.05MACR+0.08 CH2O+0.03MVK+0.25RCHO+0 .75CH2O+0.25MOH+0.25ROH +0.05HO2	8.37E-14	Tyndall MO2+MO2 Atkinson97 RO2+RO2 (See note 11 below)	
				NISOP02(in MCM), HO2 term is 0.5 in the input file, need to be fixed. (Palmer, JMAO)
118	PRN1+MO2 = NO2+0.50CH2O+ 0.50ALD2+0.25RCHO+0.75C H2O+0.25MOH+0.25ROH+0.5 0HO2	8.37E-14	Tyndall MO2+MO2 Atkinson97 RO2+RO2 (See note 11 below)	
119	EOH+OH = HO2+ALD2	6.90E-12 exp(-230/T)	JPL02	
120	ROH+OH = HO2+RCHO	4.6E-12 exp(70/T)	IUPAC	not in JPL06
		Same	IUPAC06	
121	ETO2+ETO2 = 2ALD2 +2HO2	4.10E-14	JPL97	
		Same	JPL06	
122	ETO2+ETO2 = EOH + ALD2	2.70E-14	JPL97	
		Same	JPL06	
123	HO2+ETO2 = ETP	7.40E-13 exp(700/T)	Tyndall (see note 4)	
			Not JPL 03	
124	A3O2+HO2 = RA3P	7.40E-13 exp(700/T)	Tyndall	
			ETO2+HO2	
125	PO2+HO2 = PP	7.40E-13 exp(700/T)	Tyndall	
			ETO2+HO2	
126	HO2+MCO3 =ACTA+O3	K=K1/(1+K2); K1=4.30E- 13exp(1040/T) K2=3.70E+1 exp(- 660/T)	RateTyndall:br- crawford&- moortgart	
127	HO2+MCO3 = MAP	K=K1/(1+K2); K1=4.30E- 13exp(1040/T) K2=2.70E-2- exp(660/T)	RateTyndall:br- crawford&- moortgart	

	MCO3 + HO2 = 0.15 ACTA + 0.15 O3 + 0.44 OH + 0.44 MO2 + 0.41 MAP	5.2e-13exp(980/T)	IUPAC(Feb2009)	DBM
128	RCO3+HO2=0.3RCOOH+0.3 O3+ 0.7RP	4.30E-13 exp(1040/T)		
129	<del>GCO3+HO2=0.3RCOOH+0.3O3 +0.7GP</del>	4.30E-13 exp(1040/T)		
	GCO3 + HO2 = 0.71GP + 0.29O3 + 0.29CH2O			DBM(MCM 3.1)
130	MAO3+HO2=0.3RCOOH+0.3 O3 + 0.7MAOP	4.30E-13 exp(1040/T)		
131	GLCO3+HO2=0.3RCOOH+0.3 O3+0.7GLP	4.30E-13 exp(1040/T)		
132	PRPE+OH+M = PO2	<del>LPL: 8.00E-27(300/T)^3.5</del>	<del>Atkinson-92&amp;IUPAC 03</del>	
		<del>HPL:3.00E-11</del>	<del>for Fc.</del>	
		<del>Fc: 0.5</del>		
		LPL: 8.00E-27(300/T)^3.5	IUPAC06	JMAO
		HPL:3.00E-11(300/T)		
		Fc: 0.5		
133	PRPE+O3 = 0.535CH2O+0.500ALD2+0.42 OCO+0.300HO2+0.135OH+0.065H2+0.305MO2	<del>6.50E-15 exp(-1880/T)</del>	<del>Paulson &amp; Seinfeld-92</del>	
		5.50E-15 exp(-1880/T)	IUPAC06	JMAO
134	GLYX+OH = HO2+2CO	<del>K1=1.10E-11</del>	<del>Atkinson 92,94</del>	
		<del>K = K1*([O2]+3.5D18)/</del>		
		<del>(2*[O2]+3.5D18)</del>		
		1.1E-11	IUPAC06	Already updated
135	MGLY+OH = MCO3+CO	<del>1.70E-11</del>	<del>Atkinson 92,94</del>	
		1.50E-11	IUPAC06	JMAO
136	GLYX+NO3 = HNO3 + HO2+ 2CO	K1=1.40E-12exp(-1860/T) K=K1*([O2]+3.5D18)/(2*[O2]+3.5D18)	Atkinson92&94, (ALD2)	
137	MGLY+NO3 = HNO3 + CO +MCO3	1.40E-12 exp(-1860/T)	Atkinson92&94, (ALD2)	
		Same	IUPAC06	
138	ISOP+OH = RIO2	2.70E-11 exp(390/T)	IUPAC02	

		Same	IUPAC06	
139	MVK+OH = VRO2	<del>4.13E-12 exp(452/T)</del>	<del>Atkinson92,94;- Tuazon- &amp;Atkinson-89,90</del>	
		2.6e-12exp(610/T)	IUPAC06	JMAO
140	MACR+OH = 0.5MAO3 +0.5MRO2	<del>1.86E-11 exp(175/T)</del>	<del>Atkinson92,94;- Tuazon- &amp;Atkinson89,90</del>	
	MACR + OH = 0.57MAO3 + 0.43MRO2	8.0E-12exp(380/T)	IUPAC06	JMAO,DBM(MCM3.1)
141	HAC+OH = MGLY+HO2	3E-12	Atkinson 92,94	
		Same	IUPAC06	
142	MCO3+A3O2 = MO2+RCHO+HO2	1.68E-12 exp(500/T)	T dep & B.R.Tyndall K298Villenave 98 See note 12	
143	MCO3+PO2 = MO2 +ALD2+CH2O+HO2	1.68E-12 exp(500/T)	T dep & B.R.Tyndall K298Villenave 98 See note 12	
144	MCO3+A3O2 = ACTA +RCHO	1.87E-13 exp(500/T)	T dep & B.R.Tyndall K298Villenave 98 See note 12	k 298 = 1e-11cm3 molec-1. Use T dep. From MCO3+MO2 according to Tyndall, and apply branching ratio from Tyndall. Keeping rate constant at 298K equal to 1E- 11,means that A factor is 1.87E-12. Branching ratio from Tyndall sends 90% to the radical branch(A = 0.9*1.87E-12 = 1.68E- 12), and 10% to molecular branch (A = 0.1* 1.87E-12 =1.87E- 13).
145	MCO3+PO2 = ACTA + 0.35RCHO+0.65HAC	1.87E-13 exp(500/T)	T dep & B.R.Tyndall K298Villenave 98 See note 12	

146	ISOP+O3 = 0.387MACR + 0.159MVK+0.100O3+0.270OH +0.070PRPE+0.900CH2O+0.0 60HO2+0.150CO2+0.050CO	1.05E-14 exp(-2000/T)	Paulson & Seinfeld, 92 Aschmann & Atkinson, 94	
147	MVK+O3 = 0.82MGLY+ 0.80CH2O+0.20O2+0.05CO+0 .06HO2+ 0.04ALD2	<del>4.00E-15 exp(-2000/T)</del>	<del>Paulson &amp; Seinfeld 92</del>	
	0.20O2->0.20O3(Palmer, JMAO, according to Paulson & Seinfeld 92)	8.5 E-16exp(-1520/T)	IUPAC06	JMAO, 0.20O2- >0.20O3(Palmer, JMAO, according to Paulson & Seinfeld 92)
148	MACR+O3 = 0.800MGLY +0.700CH2O+0.200O3+0.200 CO+0.275HO2+0.215OH+0.16 0CO2	<del>4.40E-15 exp(-2500/T)</del>	<del>Paulson &amp; Seinfeld 92</del>	
		1.4 E-15exp(-2100/T)	IUPAC06	JMAO
149	ISOP+NO3 = INO2	<del>3.03E-12 exp(-446/T)</del>	<del>Atkinson 92,94</del>	
		3.15E-12 exp(-450/T)	IUPAC06	JMAO
150	MVK+NO3 = MVN2	<del>2.00E-14</del>	<del>Horowitz et al., 1998, Lurmann et al., 1986</del>	
		REMOVED (<6E-16,IUPAC06)		JMAO
151	MACR+NO3 = MAN2	<del>6.70E-15</del>	<del>Lurmann et al., 1986</del>	
		2.3E-15	IUPAC06	JMAO
152	MACR+NO3 = MAO3+HNO3	<del>3.30E-15</del>	<del>Lurmann et al., 1986</del>	IUPAC06 total rate is 3.4E-15, so use the ratio from Lurmann et al., 1986
		1.1E-15	IUPAC06	JMAO
153	RCO3+MO2 = CH2O+HO2+ETO2	1.68E-12 exp(500/T)	T dep & B.R.Tyndall K298Villenave 98 See note 12	
154	GCO3+MO2 = 2CH2O +2HO2	1.68E-12 exp(500/T)	T dep & B.R.Tyndall K298Villenave 98 See note 12	

155	MAO3+MO2 = CH2O+HO2+CH2O+MCO3	1.68E-12 exp(500/T)	T dep & B.R.Tyndall K298Villenave 98 See note 12	
156	GLCO3+MO2 = CH2O +2HO2+CO	1.68E-12 exp(500/T)	T dep & B.R.Tyndall K298Villenave 98 See note 12	
157	RCO3+MO2 = RCOOH +CH2O	1.87E-13 exp(500/T)	T dep & B.R.Tyndall K298Villenave 98 See note 12	
158	GCO3+MO2 = RCOOH + CH2O	1.87E-13 exp(500/T)	T dep & B.R.Tyndall K298Villenave 98 See note 12	
159	MAO3+MO2 = RCOOH + CH2O	1.87E-13 exp(500/T)	T dep & B.R.Tyndall K298Villenave 98 See note 12	
160	GLCO3+MO2 = RCOOH + CH2O	1.87E-13 exp(500/T)	T dep & B.R.Tyndall K298Villenave 98 See note 12	
161	INPN+OH = INO2	3.80E-12 exp(200/T)	DeMore,reported in Horowitz as MP+OH	
162	PRPN+OH = PRN1	3.80E-12 exp(200/T)	JPL97,MP+OH	
163	ETP+OH = 0.50OH+ 0.50ETO2+0.50ALD2	3.80E-12 exp(200/T)	JPL97,MP+OH	
164	RA3P+OH = 0.50OH + 0.50A3O2+0.50RCHO	3.80E-12 exp(200/T)	JPL97,MP+OH	
165	<del>RB3P+OH =</del> <del>0.50OH+0.50B3O2+0.50RCHO</del>	3.80E-12 exp(200/T)	JPL97,MP+OH	
	RB3P + OH = 0.50OH + 0.5B3O2 + 0.5ACET			DBM,lumping from MCM3.1
166	R4P+OH = 0.50OH+0.50R4O2 + 0.50RCHO	3.80E-12 exp(200/T)	JPL97,MP+OH	

167	RP+OH = 0.50OH+0.50RCO3+0.50ALD 2	3.80E-12 exp(200/T)	JPL97,MP+OH	
168	<del>PP+OH =</del> <del>0.50OH+0.50PO2+0.50RCHO</del>	3.80E-12 exp(200/T)	JPL97,MP+OH	
	PP + OH = PO2			DBM(MCM 3.1)
169	<del>GP+OH =</del> <del>0.50OH+0.50GCO3+0.50CH2O</del>	3.80E-12 exp(200/T)	<del>JPL97,MP+OH</del>	
	GP + OH = GCO3			DBM(MCM 3.1)
170	GLP+OH = 0.50OH+0.50GLCO3+0.50CO	3.80E-12 exp(200/T)	JPL97,MP+OH	
171	<del>RIP+OH = 0.50IAO2 + 0.40RIO2 + 0.20RIO1</del>	3.80E-12 exp(200/T)	JPL97,MP+OH	
	RIP + OH = 0.509IALD + 0.509OH + 0.491RIO2			DBM,lumping from MCM3.1
172	<del>IAP+OH = 0.50OH + 0.50RCHO + 0.50IAO2</del>	3.80E-12 exp(200/T)	<del>JPL97,MP+OH</del>	
	IAP + OH = IAO2			DBM(MCM 3.1)
173	ISNP+OH = 0.50OH+0.50RCHO+0.50NO2 +0.50ISN1	3.80E-12 exp(200/T)	JPL97,MP+OH	
174	VRP+OH = 0.50OH+0.50RCHO+0.50VRO 2	3.80E-12 exp(200/T)	JPL97,MP+OH	
175	<del>MRP+OH = 0.50OH + 0.50RCHO + 0.50MRO2</del>	3.80E-12 exp(200/T)	<del>JPL97,MP+OH</del>	
	MRP + OH = MRO2			DBM(MCM 3.1)
176	<del>MAOP+OH =</del> <del>0.50OH+0.50RCHO +</del> <del>0.50MAO3</del>	3.80E-12 exp(200/T)	JPL97,MP+OH	
	MAOP + OH = MAO3			DBM(MCM 3.1)
177	OH+MAP = 0.50OH+0.50CH2O + 0.50MCO3	3.80E-12 exp(200/T)	JPL97,MP+OH	

178	C2H6+NO3 = ETO2+HNO3	1.40E-18 <1E-17	Atkinson,92	
179	MNO3+OH =CH2O+NOMNO32	5.00E-13 exp(-810/T)	JPL02	
		8.0E-13exp(-1000/T)	JPL06	JMAO, The product is NO2 in the input file instead of NOMNO32.
180	IALD+OH = 0.44IAO2 +0.41MAO3+0.15HO2	3.70E-11	Paulson &Seinfeld, 92	
181	IALD+O3 = 0.60MGLY+0.10OH+0.12CH2 O+0.28GLYC+0.30O3+0.40C O+0.20H2+0.20HAC+0.20HC OOH	6.16E-15 exp(-1814/T)	Paulson &Seinfeld, 92	MCO3+NO,MCO3,HO2 ,RCO3,GCO3,MAO3,G LCO3 rates are used for other radicals.
182	MCO3+MCO3 = 2MO2	2.50E-12 exp(500/T)	Tyndall; See note 6.	RCO3+HO2 same as MCO3+HO2, RCO3+NO same as MCO3+NO, RCO3+MCO3 same asMCO3+MCO3
183	MCO3+MO2 = CH2O+MO2+HO2	1.80E-12 exp(500/T)	Tyndall	
184	MCO3+MO2 = ACTA +CH2O	2.00E-13 exp(500/T)	Tyndall	
185	R4O2+MCO3 = MO2 +0.32ACET+0.19MEK+0.18M O2+0.27HO2+0.32ALD2+0.13 RCHO+0.05A3O2+0.18B3O2+ 0.32ETO2	1.68E-12 exp(500/T)	T dep & B.R.Tyndall K298Villenave 98 See note 12	
186	ATO2+MCO3 = MO2 +0.8HO2+0.2CH2O+0.2MCO3 +0.8MGLY	1.68E-12 exp(500/T)	Ibid.	
187	KO2+MCO3 = MO2 +ALD2+MCO3	1.68E-12 exp(500/T)	Ibid.	

188	RIO2+MCO3 = MO2+0.864HO2+0.690CH2O +0.402MVK+0.288MACR+0.1 36RIO1+0.127IALD	1.68E-12 exp(500/T)	ibid.	
189	RIO1+MCO3 = MO2 +IALD+HO2+0.75CH2O	1.68E-12 exp(500/T)	ibid.	
190	IAO2+MCO3 = MO2 +HO2+0.65CO+0.18H2+0.36H AC+0.26GLYC+0.58MGLY+0. 4CH2O	1.68E-12 exp(500/T)	ibid.	
191	ISN1+MCO3 = MO2+NO2+GLYC+HAC	1.68E-12 exp(500/T)	ibid.	
192	VRO2+MCO3 = MO2+0.28HO2+0.28CH2O+0. 72MCO3+0.72GLYC+0.28MG LY	1.68E-12 exp(500/T)	ibid.	
193	MRO2+MCO3 = MO2+HO2+0.17MGLY+0.83H AC+0.83CO+0.17CH2O	1.68E-12 exp(500/T)	ibid.	
194	B3O2+MCO3 = MO2+HO2+ACET	1.68E-12 exp(500/T)	ibid.	
195	R4N1+MCO3 = MO2+NO2+0.39CH2O+0.75A LD2+0.57RCHO+0.30R4O2	1.68E-12 exp(500/T)	ibid.	
196	MVN2+MCO3 = MO2 +NO2+CH2O+0.5MCO3+0.5M GLY+0.5HO2	1.68E-12 exp(500/T)	ibid.	
197	MAN2+MCO3 = MO2 +NO2+CH2O+MGLY	1.68E-12 exp(500/T)	ibid.	
198	INO2+MCO3 = MO2 +0.10NO2 + 0.80HO2 +0.85HNO3 + 0.05NO2 +0.10MACR + 0.15CH2O +0.05MVK	1.68E-12 exp(500/T)	ibid.	
199	PRN1+MCO3 = MO2 +NO2+CH2O+ALD2	1.68E-12 exp(500/T)	ibid.	

200	R4O2+MCO3 = MEK +ACTA	1.87E-13 exp(500/T)	Ibid.	
201	ATO2+MCO3 = MEK +ACTA	1.87E-13 exp(500/T)	Ibid.	
202	KO2+MCO3 = MEK + ACTA	1.87E-13 exp(500/T)	Ibid.	
203	RIO2+MCO3 = MEK +ACTA	1.87E-13 exp(500/T)	Ibid.	
204	RIO1+MCO3 = MEK +ACTA	1.87E-13 exp(500/T)	Ibid.	
205	IAO2+MCO3 = MEK+ ACTA	1.87E-13 exp(500/T)	Ibid.	
206	VRO2+MCO3 = MEK +ACTA	1.87E-13 exp(500/T)	Ibid.	
207	MRO2+MCO3 = MEK +ACTA	1.87E-13 exp(500/T)	Ibid.	
208	R4N1+MCO3 = RCHO +ACTA + NO2	1.87E-13 exp(500/T)	Ibid.	
209	ISN1+MCO3 = RCHO +ACTA + NO2	1.87E-13 exp(500/T)	Ibid.	
210	MVN2+MCO3 = RCHO +ACTA + NO2	1.87E-13 exp(500/T)	Ibid.	
211	MAN2+MCO3 = RCHO +ACTA + NO2	1.87E-13 exp(500/T)	Ibid.	
212	INO2+MCO3 = RCHO +ACTA + NO2	1.87E-13 exp(500/T)	Ibid.	
213	PRN1 + MCO3 = RCHO +ACTA + NO2	1.87E-13 exp(500/T)	Ibid.	
214	B3O2+MCO3 = ACET +ACTA	1.87E-13 exp(500/T)	Ibid.	
215	MCO3+ETO2 = MO2+ALD2+HO2	1.68E-12 exp(500/T)	Ibid.	
216	MCO3+ETO2 = ACTA +ALD2	1.87E-13 exp(500/T)	Ibid.	
217	RCO3+MCO3 = MO2 + ETO2	2.50E-12 exp(500/T)	Tyndall,MCO3+MC O3	
218	GCO3+MCO3 = MO2 + HO2+ CH2O	2.50E-12 exp(500/T)	Tyndall,MCO3+MC O3	

219	MAO3+MCO3 = MO2 + CH2O + MCO3	2.50E-12 exp(500/T)	Tyndall,MCO3+MC O3	
220	GLCO3+MCO3 = MO2+ HO2+ CO	2.50E-12 exp(500/T)	Tyndall,MCO3+MC O3	
221	NO3+NO3 = 2NO2 + O2	8.50E-13 exp(-2450/T) Same	JPL 97 JPL06	
222	HO2 = 0.50H2O2	gamma=2E-1	Jacob, 2000	
223	NO2 = 0.50HNO3 +0.50HNO2	gamma=1E-4	Jacob, 2000	
224	NO3 = HNO3	gamma=1E-3	Jacob, 2000	
225	N2O5 = 2HNO3	gamma= fct(aerosol type, rh, temp)	See Appendix	
226	DMS+OH = SO2+MO2+CH2O	<del>1.20E-11 exp(-260/T)</del> 1.1E-11exp(-240/T)	<del>JPL 2003</del> JPL06	JMAO
227	DMS+OH+O2 = 0.75SO2+0.25MSA+MO2	<del>K1 = 1.7E-42exp(7810/T)- K2=5.5E-31exp(7460/T) K = K1/(1.0+K2*[O2])</del> K1=1.0E-39exp(5820/T) K2=5.0E-30exp(6280/T) K=K1*[O2]/(1.0+K2*[O2])	<del>Atkinson 89,yields from Chatfield and Crutzen 90,as- reported by Chin- et al., 1996.</del>	MJE
228	DMS+NO3 = SO2+HNO3 +MO2+CH2O	1.90E-13 exp(500/T)	JPL2003	
229	SO2+OH+M = SO4+HO2	<del>LPL: 3.00E-31(300/T)^3.3- HPL:1.50E-12 Fc: 0.6</del> LPL: 3.30E-31(300/T)^4.3 HPL:1.60E-12 Fc: 0.6	<del>JPL97</del> JPL06	JMAO
230	MAO3+NO=1.0NO2+4.0CH2O +1.0HO2	6.7E-12exp(340/T)	IUPAC2006	This reaction doesn't exist in the manual but is in the input The rate is from IUPAC2006 (or 2003), using the rate of CH3CH2C(O)O2+NO=C 2H5C(O)O+NO2.
	MAO3 + NO=MCO3 + CH2O + NO2			Palmer, May, JMAO



Photolysis reaction

Photolysis reaction	reference	Date updated	Flag
$O_3 = 2OH$	JPL97 and Atkinson97 as reported by Wild et al., 2000; See also notes with Q flag	1/2002	Q
$NO_2 = NO + O_3$	As in Wild et al., 2000		
$H_2O_2 = 2OH$	As in Wild et al., 2000		
$MP = CH_2O + HO_2 + OH$	As in Wild et al., 2000.		
$CH_2O = 2HO_2 + CO$	As in Wild et al., 2000.		
$CH_2O = H_2 + CO$	As in Wild et al., 2000.		
$HNO_3 = OH+NO_2$	As in Wild et al., 2000.		
$HNO_2 = OH+NO$	As in Wild et al., 2000.		
$HNO_4 = OH+NO_3$	As in Wild et al., 2000.		
$NO_3 = NO_2 + O_3$	As in Wild et al., 2000.		
$NO_3 = NO + O_2$	As in Wild et al., 2000.		
$N_2O_5 = NO_2 + NO_2$	As in Wild et al., 2000.		
$N_2O_5 = NO_3 + NO + O_3$	As in Wild et al., 2000.		
$HNO_4 = HO_2 + NO_2$	As in Wild et al., 2000.; See also T flag notes [Roehl, 2002]	1/2002	T
$ALD_2 = MO_2 + HO_2 + CO$	As in Wild et al., 2000.		
$ALD_2 = CH_4 + CO$	As in Wild et al., 2000.		
<del>PAN = MCO<sub>3</sub> + NO<sub>2</sub></del>	<del>As in Wild et al.</del>		
PAN = 0.6 MCO <sub>3</sub> + 0.6 NO <sub>2</sub> + 0.4 MO <sub>2</sub> + 0.4 NO <sub>3</sub>	JPL06		DBM
$RCHO = ETO_2 + HO_2 + CO$	As in Wild et al.		
<del>ACET = MCO<sub>3</sub> + MO<sub>2</sub></del>	<del>Pressure dependent crosssections from Cameron-Smith et al., 2000</del>		
ACET = MCO <sub>3</sub> + MO <sub>2</sub> ; ACET = 2MO <sub>2</sub> +CO	FAST_JX		Prather
<del>MEK = MCO<sub>3</sub> + ETO<sub>2</sub></del>	As in Wild et al., 2000.		
MEK = 0.15MO <sub>2</sub> +0.15RCO <sub>3</sub> +0.85MC O <sub>3</sub> + 0.85ETO <sub>2</sub>	FAST_JX		Prather
$MNO_3 = CH_2O + H_2O + NO_2$	As in Wild et al., 2000.		
<del>GLYC = CH<sub>2</sub>O + HO<sub>2</sub> + CO</del>	<del>As in Wild et al.</del>		
GLYC =CH <sub>2</sub> O + 2.0 HO <sub>2</sub> + CO	JPL06,Lurman1986	GLYC + hv → CH <sub>2</sub> OH + HCO; CH <sub>2</sub> OH + O <sub>2</sub> → CH <sub>2</sub> O + HO <sub>2</sub> ; HCO + O <sub>2</sub> → CO + HO <sub>2</sub>	Palmer,JMAO
<del>GLYX = H<sub>2</sub> + 2CO</del>	<del>As in Wild et al.</del>		
<del>GLYX = 2CO + 2HO<sub>2</sub></del>	<del>As in Wild et al.</del>		
<del>GLYX = CH<sub>2</sub>O + CO</del>	<del>As in Wild et al.</del>		
GLYX=0.5H <sub>2</sub> +CO+0.5CH <sub>2</sub> O+0. 5CO;	FAST_JX		Prather
GLYX=2CO+2HO <sub>2</sub>			

	MGLY = MCO3 + CO + HO2	As in Wild et al.		
	<del>MGLY = ALD2 + CO</del>	<del>As in Wild et al.</del>	Removed; JPL06	Not important according to JPL06,DBM
				Updated in ratj.d for the yield
	MVK = PRPE + CO	As in Wild et al.		
	MVK = MCO3+CH2O+CO+HO2	As in Wild et al.		
	MVK = MO2+MAO3	As in Wild et al.		
	MACR = MAO3 + HO2	As in Wild et al.		
	<del>MACR = CO + HO2 + 0.8MGLY + 0.8HO2 + 0.2MCO3 + 0.2CH2O</del>	<del>As in Wild et al.</del>		
	MACR = CO + HO2 + CH2O + MCO3			DBM(MCM3.1)
	HAC = MCO3 + CH2O + HO2	Uses pressure-dependent acetone cross-section;Cameron-Smith et al., 2000.		
	INPN = OH + HO2 + RCHO + NO2	Uses MP cross-section		
	PRPN = OH + HO2 + RCHO + NO2	Uses MP cross-section		
	ETP = OH + HO2 + ALD2	Uses MP cross-section		
	RA3P = OH + HO2 + RCHO	Uses MP cross-section		
	<del>RB3P = OH + HO2 + RCHO</del>	Uses MP cross-section		
	RB3P = OH + HO2 + ACET			DBM
	R4P = OH + HO2 + RCHO	Uses MP cross-section		
	<del>PP = OH + HO2 + RCHO</del>	Uses MP cross-section		
	PP = OH + HO2 + ALD2 + CH2O			DBM(MCM 3.1)
	RP = OH + HO2 + ALD2	Uses MP cross-section		
	GP = OH + HO2 + CH2O	Uses MP cross-section		
	GLP = OH + HO2 + CO	Uses MP cross-section		
	<del>RIP = OH + 0.864HO2 + 0.69CH2O + 0.402MVK + 0.288MACR + 0.136RIO1 + 0.127IALD</del>	<del>Uses MP cross-section</del>		
	RIP = OH + HO2 + 0.627CH2O + 0.368MVK + 0.259MACR + 0.373IALD	J(41)???		DBM(MCM3.1)
	IAP = OH + HO2 + 0.67CO + 0.19H2 + 0.36HAC + 0.26GLYC + 0.58MGLY	Uses MP cross-section		
	ISNP = OH + HO2 + RCHO + NO2	Uses MP cross-section		

	<del>VRP = OH + 0.28HO2 + 0.28CH2O + 0.72MCO3 + 0.72GLYC + 0.28MGLY</del>	Uses MP cross-section		
	VRP = OH + 0.3HO2 + 0.3CH2O + 0.7MCO3 + 0.7GLYC + 0.3MGLY			DBM(MCM3.1)
	<del>MRP = OH + HO2 + 0.17MGLY + 0.83HAC + 0.83CO + 0.17CH2O</del>	Uses MP cross-section		
	MRP = OH + HO2 + HAC + 0.5CO + 0.5CH2O			DBM(MCM3.1)
	<del>MAOP = OH + HO2 + RCHO</del>	Uses MP cross-section		
	MAOP = OH + MCO3 + CH2O			DBM(MCM3.1)
	R4N2 = NO2 + 0.32ACET + 0.19MEK + 0.18MO2 + 0.27HO2 + 0.18B3O2 + 0.32ETO2 + 0.32ALD2 + 0.13RCHO + 0.05A3O2 + 0.18B3O2 + 0.32ETO2	Uses MNO3 cross-section		
	MAP = OH + MO2	Uses MP cross-section		

# PHOTOLYSIS REACTIONS - MASTER RATEFILE - Paul Brown, Oliver Wild & David Rowley  
 # Centre for Atmospheric Science, Cambridge, U.K. Release date: 22 November 1993  
 # SCCS version information: @(#)photol.d 1.2 5/11/94  
 #  
 # Modified for Harvard chemistry: several reactions added, re-ordered per chem.dat  
 # Also putting in the Harvard names in col 1, the UCI x-sec names in last col !!!  
 # -Prashant Murti [4/13/98]

# The new peroxide recycling now activates the following photolysis species:  
 # GP, IAP, INPN, ISN1, ISNP, MAOP, MRP, PP, PRPN, RIP, VRP.  
 # Also be sure to set parameter JPMAX = 55 in "cmn\_fj.h".  
 # - Randall Martin & Bob Yantosca [12/20/00]  
 # New updates from FASTJX.(jmao,ccarouge, 04/20/09)

#	Harvard species	Products - UCI notation						UCI xsec
#	=====	=====						=====
1	H2O	PHOTON	OH	HO2	0.00E+00	0.00	0.0	
2	HO2	PHOTON	OH	O(3P)	0.00E+00	0.00	0.0	
3	O2	PHOTON	O(3P)	O(3P)	0.00E+00	0.00	100.0 O2	
4	O3_P	PHOTON	O2	O(3P)	0.00E+00	0.00	100.0 O3	
5	O3	PHOTON	O2	O(1D)	0.00E+00	0.00	100.0 O3_1d	
6	NO2	PHOTON	NO	O(3P)	0.00E+00	0.00	100.0 NO2	
7	H2O2	PHOTON	OH	OH	0.00E+00	0.00	100.0 H2O2	
8	MP	PHOTON	HCHO	OH HO2	0.00E+00	0.00	100.0 ROOH	
9	CH2O	PHOTON	CO	HO2 HO2	0.00E+00	0.00	100.0 HCHO=H+	
10	CH2O	PHOTON	CO	H2	0.00E+00	0.00	100.0 HCHO=H2	
11	HNO3	PHOTON	OH	NO2	0.00E+00	0.00	100.0 HONO2	
12	HNO2	PHOTON	OH	NO	0.00E+00	0.00	100.0 HONO	
13	HNO4	PHOTON	OH	NO3	0.00E+00	0.00	5.0 HO2NO2	
14	HNO4	PHOTON	HO2	NO2	0.00E+00	0.00	95.0 HO2NO2	
15	NO3	PHOTON	NO	O2	0.00E+00	0.00	100.0 NO3=O2+	
16	NO3	PHOTON	NO2	O(3P)	0.00E+00	0.00	100.0 NO3=O+	
17	N2O5	PHOTON	NO3	NO O(3P)	0.00E+00	0.00	0.0 N2O5	
18	N2O5	PHOTON	NO3	NO2	0.00E+00	0.00	100.0 N2O5	
19	ALD2	PHOTON	CH4	CO	0.00E+00	0.00	100.0 Acet=R+	
20	ALD2	PHOTON	MeOO	HO2 CO	0.00E+00	0.00	100.0 Acet=RO	
21	PAN	PHOTON	MeCO3	NO2	0.00E+00	0.00	100.0 PAN	
22	RCHO	PHOTON	EtO2	HO2 CO	0.00E+00	0.00	100.0 RCHO	
23	ACET	PHOTON	MeCO3	MeOO	0.00E+00	0.00	100.0 AcetA	
24	ACET	PHOTON	MeOO	MeOO CO	0.00E+00	0.00	100.0 AcetB	
25	MEK	PHOTON	MeCO3	EtOO	0.00E+00	0.00	100.0 EtCOMe	
26	MNO3	PHOTON	HCHO	H2O NO2	0.00E+00	0.00	100.0 MeNO3	
27	GLYC	PHOTON	HCHO	HO2 CO	0.00E+00	0.00	100.0 HOMeCHO	
28	GLYX	PHOTON	H2	CO HCHO	0.00E+00	0.00	100.0 Glyxla	
29	GLYX	PHOTON	CO	HO2	0.00E+00	0.00	100.0 Glyxlb	
30	MGLY	PHOTON	MeCO3	CO HO2	0.00E+00	0.00	100.0 MeCOCHO	
31	MGLY	PHOTON	Acet	CO	0.00E+00	0.00	0.0 MeCOCHO	
32	MVK	PHOTON	PRPE	CO	0.00E+00	0.00	60.0 MeCOVi	
33	MVK	PHOTON	MeCO3	HCHO CO HO2	0.00E+00	0.00	20.0 MeCOVi	
34	MVK	PHOTON	MeOO	MAO3	0.00E+00	0.00	20.0 MeCOVi	
35	MACR	PHOTON	MAO3	HO2	0.00E+00	0.00	50.0 MACR	
36	MACR	PHOTON	CO HO2 MGLY HO2 MeCO3 HCHO		0.00E+00	0.00	50.0 MACR	
37	HAC	PHOTON	MeCO3	HCHO HO2	0.00E+00	0.00	100.0 AcetA	
38	ETP	PHOTON	OH	HO2 Acet	0.00E+00	0.00	100.0 ROOH	
39	RA3P	PHOTON	OH	HO2 RCHO	0.00E+00	0.00	100.0 ROOH	
40	RB3P	PHOTON	OH	HO2 RCHO	0.00E+00	0.00	100.0 ROOH	
41	R4P	PHOTON	OH	HO2 RCHO	0.00E+00	0.00	100.0 ROOH	
42	RP	PHOTON	OH	HO2 Acet	0.00E+00	0.00	100.0 ROOH	
43	R4N2	PHOTON	NO2 MeCOMe MEK MO2 HO2 ALD2 ...		0.00E+00	0.00	100.0 MeNO3	
44	MAP	PHOTON	OH	MO2	0.00E+00	0.00	100.0 ROOH	
45	INPN	PHOTON	OH	HO2 RCHO NO2	0.00E+00	0.00	100.0 ROOH	
46	PRPN	PHOTON	OH	HO2 RCHO NO2	0.00E+00	0.00	100.0 ROOH	
47	PP	PHOTON	OH	HO2 RCHO	0.00E+00	0.00	100.0 ROOH	

48 GP	PHOTON	OH		HO2		RCHO		0.00E+00	0.00	100.0	ROOH	
49 GLP	PHOTON	OH		HO2		RCHO		0.00E+00	0.00	100.0	ROOH	
50 RIP	PHOTON	OH	HO2	CH2O	MVK	MACR	RIO1	IALD	0.00E+00	0.00	100.0	ROOH
51 IAP	PHOTON	OH	HO2	CO	H2	HAC	GLYC	MGLY	0.00E+00	0.00	100.0	ROOH
52 ISNP	PHOTON	OH		HO2		RCHO	NO2		0.00E+00	0.00	100.0	ROOH
53 VRP	PHOTON	OH	HO2	CH2O	MCO3	GLYC	MGLY		0.00E+00	0.00	100.0	ROOH
54 MRP	PHOTON	OH	HO2	MGLY	HAC	CO	CH2O		0.00E+00	0.00	100.0	ROOH
55 MAOP	PHOTON	OH		HO2		RCHO			0.00E+00	0.00	100.0	ROOH
9999									0.00E-00	0.00	0.0	

NOTES:

-----

[4/15/98]

Oliver Wild: All reaction data from JPL '97, IUPAC IV. IUPAC V is soon expected. - ppm

All reaction data taken from IUPAC supplement IV unless otherwise indicated.

JPL - data from JPL (latest assessment as far as possible)

? - reaction products unknown

\* - user strongly advised to consult source material

B - branching ratio assumed equal for all channels in the absence of more information

U - upper limit for rate coefficient

Changes since 08/3/93 release:

O now written as O(3P)

(Note that the second of the acetaldehyde channels above occurs at wavelengths less than 289 nm, and therefore doesn't appear in the Fast-J region at all - I've simply included it here for completeness) - [from Oliver, 3/7/98]

JV\_SPEC.dat updates(mostly cut from the visible wavelength bins of FASTJX 6.4, except Solar Flux, O3 cross section, NO2 cross section are from Huisheng Bian and Michael Prather's latest updates in 2009): Green is the value to be updated.Red is the value significantly changed.

Notes:1.Acetone photolysis is implemented by Claire.2. Pressure dependence is updated for MVK,MEK, MGLY by Claire. 3.Glyoxal reactions and branching ratio have been changed here and ratj.d

Species	Unit	FAST-J std	JPL	0 (mje 4/02)			aer/dust(rvm,3/02)	
NW-JValue	27	7	1	7	NJVAL,	NWWW,	NW1:NW2	
w-beg(nm)		289	298.25	307.45	312.45	320.3	345	412.45
w-end(nm)		298.25	307.45	312.45	320.3	345	412.45	850
w-eff(nm)		294	303	310	316	333	380	574
SOL#/cm2/s		7.352E+14	7.332E+14	5.022E+14	8.709E+14	3.786E+15	1.544E+16	2.11E+17
	New	5.882E+14	7.686E+14	5.046E+14	8.906E+14	3.854E+15	1.548E+16	2.131E+17
Raylay	cm2	6.180E-26	5.430E-26	4.920E-26	4.540E-26	3.630E-26	2.09E-26	3.830E-27
		6.131E-26	5.422E-26	4.923E-26	4.514E-26	3.643E-26	2.087E-26	3.848E-27
BCarb	m2/g	10.08	9.96	9.87	9.79	9.58	9	6.5
O2	180							
O2	260							
O2	300							
O3	180	8.693E-19	2.365E-19	8.722E-20	3.694E-20	4.295E-21	1.804E-23	1.630E-21
	180	7.561E-19	2.367E-19	8.756E-20	3.69E-20	4.256E-21	1.806E-23	1.625E-21
O3	260	9.189E-19	2.571E-19	9.673E-20	4.141E-20	5.457E-21	2.775E-23	1.630E-21
	260	8.016E-19	2.572E-19	9.71E-20	4.136E-20	5.409E-21	2.784E-23	1.625E-21
O3	300	9.574E-19	2.777E-19	1.075E-19	4.725E-20	6.782E-21	4.824E-23	1.630E-21
	300	8.391E-19	2.778E-19	1.079E-19	4.72E-20	6.725E-21	4.845E-23	1.625E-21
O3_1d	180	0.9	0.9	0.3824	0.08092	0.0765	0	0
	180	0.9	0.8941	0.4501	0.09189	0.07915	0.065	0
O3_1d	260	0.9	0.9	0.4531	0.1438	0.07654	0	0
	260	0.9	0.8948	0.4992	0.1463	0.08728	0.07017	0
O3_1d	300	0.9	0.9	0.5273	0.2395	0.07659	0	0
	300	0.9	0.8965	0.5636	0.2349	0.1002	0.07435	0
NO2	200	1.048E-19	1.494E-19	1.898E-19	2.295E-19	3.391E-19	4.230E-19	4.047E-22
	220	1.173E-19	1.603E-19	1.966E-19	2.349E-19	3.354E-19	4.473E-19	2.339E-22
NO2	300	1.039E-19	1.462E-19	1.845E-19	2.223E-19	3.256E-19	4.150E-19	4.02E-22
	298	1.165E-19	1.617E-19	2.021E-19	2.455E-19	3.619E-19	4.680E-19	4.291E-22
H2O2	200	8.838E-21	4.991E-21	3.190E-21	2.099E-21	7.716E-22	1.707E-23	0
	200	8.360E-21	5.008E-21	3.220E-21	2.115E-21	7.984E-22	2.101E-23	0
H2O2	300	9.801E-21	5.718E-21	3.773E-21	2.568E-21	1.02E-21	2.287E-23	0
	300	9.300E-21	5.735E-21	3.803E-21	2.583E-21	1.046E-21	2.715E-23	0
ROOH	300	5.883E-21	3.573E-21	2.437E-21	1.756E-21	7.428E-22	4.194E-23	0
	297	5.621E-21	3.573E-21	2.441E-21	1.755E-21	7.405E-22	4.261E-23	0
ROOH	300	5.883E-21	3.573E-21	2.437E-21	1.756E-21	7.428E-22	4.194E-23	0
	298	5.621E-21	3.573E-21	2.441E-21	1.755E-21	7.405E-22	4.261E-23	0
HCHO=H+	223	0	1.969E-20	1.274E-20	1.971E-20	4.354E-21	0	0
	223	0	1.945E-20	1.289E-20	1.969E-20	4.324E-21	5.105E-26	0
HCHO=H+	293	0	1.873E-20	1.304E-20	1.896E-20	3.949E-21	0	0
	293	0	1.85E-20	1.317E-20	1.895E-20	3.922E-21	4.467E-26	0
HCHO=H2	223	0	6.475E-21	4.392E-21	9.027E-21	1.041E-20	1.946E-22	0
	223	0	6.397E-21	4.443E-21	9.027E-21	1.04E-20	1.960E-22	0
HCHO=H2	293	0	6.163E-21	4.500E-21	8.715E-21	9.434E-21	1.883E-22	0
	293	0	6.086E-21	4.543E-21	8.717E-21	9.424E-21	1.903E-22	0
HONO2	200	3.706E-21	1.377E-21	5.451E-22	2.102E-22	2.154E-23	8.105E-26	0
	200	3.396E-21	1.377E-21	5.474E-22	2.100E-22	2.131E-23	8.822E-26	0
HONO2	300	4.747E-21	1.923E-21	8.314E-22	3.589E-22	4.764E-23	2.499E-25	0

	300	4.384E-21	1.923E-21	8.345E-22	3.586E-22	4.720E-23	2.683E-25	0
HONO	300	0	0	1.265E-20	3.469E-20	1.09E-19	8.644E-20	0
	297	0	0	1.175E-20	3.47E-20	1.093E-19	8.764E-20	0
HONO	300	0	0	1.265E-20	3.469E-20	1.09E-19	8.644E-20	0
	298	0	0	1.175E-20	3.47E-20	1.093E-19	8.764E-20	0
HO2NO2	300	2.869E-20	1.102E-20	5.222E-21	2.794E-21	3.255E-22	0	0
	297	2.601E-20	1.103E-20	5.239E-21	2.793E-21	2.250E-22	0	4.792E-23
HO2NO2	300	2.869E-20	1.102E-20	5.222E-21	2.794E-21	3.255E-22	0	0
	298	2.601E-20	1.103E-20	5.239E-21	2.793E-21	2.250E-22	0	4.792E-23
NO3=O+	298	0	0	0	0	0	0	7.428E-19
	297	0	0	0	0	0	0	7.321E-19
NO3=O+	298	0	0	0	0	0	0	7.428E-19
	298	0	0	0	0	0	0	7.321E-19
NO3=O2+	298	0	0	0	0	0	0	9.569E-20
	297	0	0	0	0	0	0	9.435E-20
NO3=O2+	298	0	0	0	0	0	0	9.569E-20
	298	0	0	0	0	0	0	9.435E-20
N2O5	225	4.13E-20	1.998E-20	1.167E-20	7.250E-21	2.296E-21	1.161E-22	0
	225	3.823E-20	1.998E-20	1.17E-20	7.246E-21	2.286E-21	1.173E-22	0
N2O5	300	5.718E-20	3.317E-20	2.223E-20	1.552E-20	6.409E-21	5.415E-22	0
	300	5.404E-20	3.317E-20	2.226E-20	1.551E-20	6.389E-21	5.481E-22	0
Acet=RO	298	4.008E-20	2.869E-20	1.84E-20	3.626E-21	0	0	0
with yield?	298	2.161E-20	1.46E-20	8.410E-21	3.335E-21	1.751E-22	0	0
Acet=RO	298	4.008E-20	2.869E-20	1.84E-20	3.626E-21	0	0	0
	298	2.161E-20	1.46E-20	8.410E-21	3.335E-21	1.751E-22	0	0
Acet=R+	298	0	0	0	0	0	0	0
	298	0	0	0	0	0	0	0
Acet=R+	298	0	0	0	0	0	0	0
	298	0	0	0	0	0	0	0
PAN	250	2.714E-21	9.251E-22	4.342E-22	2.290E-22	5.508E-23	6.551E-25	0
	250	2.438E-21	9.252E-22	4.355E-22	2.288E-22	5.480E-23	6.941E-25	0
PAN	298	3.931E-21	1.399E-21	6.730E-22	3.630E-22	9.301E-23	1.193E-24	0
	298	3.555E-21	1.399E-21	6.750E-22	3.627E-22	9.257E-23	1.265E-24	0
RCHO	298	5.203E-20	3.671E-20	2.22E-20	1.17E-20	1.569E-21	0	0
	297	5.548E-20	4.63E-20	3.578E-20	2.441E-20	5.853E-21	1.257E-23	0
RCHO	298	5.203E-20	3.671E-20	2.22E-20	1.17E-20	1.569E-21	0	0
	298	5.548E-20	4.63E-20	3.578E-20	2.441E-20	5.853E-21	1.257E-23	0
Acetone	235	2.98E-20	1.30E-20	4.32E-21	1.04E-21	5.88E-23	1.53E-25	0.00E+00
Acetone	298	3.26E-20	1.48E-20	5.18E-21	1.30E-21	9.62E-23	2.67E-25	0.00E+00
AcetA	220	3.100E-20	1.944E-20	1.088E-20	5.532E-21	4.637E-22	3.425E-25	0
AcetA	300	3.439E-20	2.255E-20	1.356E-20	7.273E-21	8.481E-22	6.682E-25	0
AcetB	240	5.156E-03	1.931E-03	8.022E-04	4.144E-04	4.156E-05	0	0
AcetB	300	8.564E-02	5.100E-02	3.298E-02	2.214E-02	3.533E-03	0	0
EtCOMe	298	1.432E-20	4.217E-21	1.150E-21	3.394E-22	4.706E-23	0	0
	297	4.170E-20	2.684E-20	1.57E-20	7.721E-21	8.142E-22	3.734E-25	0
EtCOMe	298	1.432E-20	4.217E-21	1.150E-21	3.394E-22	4.706E-23	0	0
	298	4.170E-20	2.684E-20	1.57E-20	7.721E-21	8.142E-22	3.734E-25	0

MeNO3	298	2.871E-20	1.08E-20	5.497E-21	3.460E-21	2.919E-22	0	0
	240	4.679E-21	2.022E-21	9.381E-22	3.730E-22	3.755E-23	0	0
MeNO3	298	2.871E-20	1.08E-20	5.497E-21	3.460E-21	2.919E-22	0	0
	298	6.029E-21	2.735E-21	1.346E-21	5.734E-22	6.957E-23	0	0
HOMeCHO	296	2.322E-20	1.773E-20	1.139E-20	5.584E-21	3.639E-22	0	0
	297	2.784E-20	1.706E-20	9.411E-21	4.388E-21	4.937E-22	0	0
HOMeCHO	296	2.322E-20	1.773E-20	1.139E-20	5.584E-21	3.639E-22	0	0
	298	2.784E-20	1.706E-20	9.411E-21	4.388E-21	4.937E-22	0	0
HCOCHO	298	9.701E-22	1.498E-21	8.257E-21	1.434E-21	2.078E-22	6.393E-22	3.277E-22
HCOCHO	298	9.701E-22	1.498E-21	8.257E-21	1.434E-21	2.078E-22	6.393E-22	3.277E-22
Glyxla	297	0	0	0	0	0	5.914E-22	2.199E-22
Glyxla	298	0	0	0	0	0	5.914E-22	2.199E-22
Glyxlb	297	1.333E-20	1.238E-20	1.117E-20	8.335E-21	2.625E-21	0	0
Glyxlb	298	1.333E-20	1.238E-20	1.117E-20	8.335E-21	2.625E-21	0	0
MeCOCHO	298	2.381E-21	1.853E-21	1.296E-21	9.572E-22	3.327E-22	2.004E-21	4.255E-22
	297	4.384E-20	3.465E-20	2.428E-20	1.788E-20	6.194E-21	2.237E-20	1.435E-21
MeCOCHO	298	2.381E-21	1.853E-21	1.296E-21	9.572E-22	3.327E-22	2.004E-21	4.255E-22
	298	4.384E-20	3.465E-20	2.428E-20	1.788E-20	6.194E-21	2.237E-20	1.435E-21
MeCOVi	298	1.388E-21	1.985E-21	2.587E-21	2.837E-21	3.115E-21	6.627E-22	0
	297	5.521E-21	7.955E-21	8.828E-21	7.236E-21	3.374E-21	1.790E-22	0
MeCOVi	298	1.388E-21	1.985E-21	2.587E-21	2.837E-21	3.115E-21	6.627E-22	0
	298	5.521E-21	7.955E-21	8.828E-21	7.236E-21	3.374E-21	1.790E-22	0
MACR	298	7.862E-22	1.215E-21	1.645E-21	1.804E-21	1.998E-21	3.654E-22	0
	297	2.107E-22	3.151E-22	3.995E-22	4.742E-22	5.222E-22	1.064E-22	0
MACR	298	7.862E-22	1.215E-21	1.645E-21	1.804E-21	1.998E-21	3.654E-22	0
	298	2.107E-22	3.151E-22	3.995E-22	4.742E-22	5.222E-22	1.064E-22	0
CH3I	225	3.289E-20	9.071E-21	4.037E-21	2.073E-21	3.577E-22	1.551E-24	0
	210	2.781E-20	8.253E-21	3.557E-21	1.826E-21	3.437E-22	2.347E-24	0
CH3I	298	5.024E-20	1.479E-20	6.296E-21	3.199E-21	6.783E-22	6.121E-24	0
	298	4.648E-20	1.511E-20	6.466E-21	3.293E-21	6.699E-22	9.781E-24	0
Q1A-Ac	240	1.00E+00	1.21E+00	4.133E+00	2.498E+01	9.452E+01	1.000E+02	1.00E+02
Q1A-Ac	300	1.01E+00	1.22E+00	2.411E+00	6.656E+00	1.969E+01	2.100E+01	2.10E+01
Q1B-Ac	240	1.03E+00	1.07E+01	5.202E+01	2.632E+02	2.760E+03	3.210E+03	3.21E+03
Q1B-Ac	300	8.79E-01	4.90E+00	1.617E+01	5.268E+01	3.023E+02	3.420E+02	3.42E+02

=====**Pressure Dependencies**=====

Pressure Dep: 5

MeCOVi	1	1.67E-19	1.67E-19	1.670E-19	1.670E-19	1.670E-19	1.670E-19	1.67E-19
EtCOMe	1	8.00E-20	8.00E-20	8.000E-20	8.000E-20	8.000E-20	8.000E-20	8.00E-20
MeCOCHO	1	1.66E-19	1.66E-19	1.660E-19	1.660E-19	1.660E-19	1.660E-19	1.66E-19
AcetA	2	1.00E+00	1.00E+00	1.000E+00	1.000E+00	1.000E+00	1.000E+00	1.00E+00
AcetB	3	1.00E+00	1.00E+00	1.000E+00	1.000E+00	1.000E+00	1.000E+00	1.00E+00

=====**Pressure Dependencies**=====

From Fast-JX(Michael Prather)

NO3 => NO+O2 [0.11414] fixed

=> NO2+O [0.88586]

Acet=RO is multiplied by the branching ratio

PAN = Peroxyacetyl nitrate =  $\text{CH}_3\text{C}(\text{O})\text{COONO}_2$   
 $\Rightarrow \text{CH}_3\text{C}(\text{O})\text{O}_2 + \text{NO}_2$

CH3NO3 =  $\text{CH}_3\text{ONO}_2$  = Methyl nitrate  
 $\Rightarrow \text{CH}_3\text{O} + \text{NO}_2$

ActAld = Acetaldehyde =  $\text{CH}_3\text{CHO}$   
 $\Rightarrow \text{CH}_3 + \text{HCO}$

MeVK = Methylvinyl ketone =  $\text{CH}_3\text{C}(\text{O})\text{CH}=\text{CH}_2$   
 $\Rightarrow \text{C}_3\text{H}_6 + \text{CO}$  [0.6]  
 $\Rightarrow \text{CH}_2\text{CHCO} + \text{CH}_3$  [0.4]  
 to be scaled by density  $1/(1 + 1.67\text{e-}19*\text{M})$

MeAcr = Methacrolein  $\text{CH}_2\text{C}(\text{CH}_3)\text{CHO}$   
 $\Rightarrow \text{CH}_2=\text{C}(\text{CH}_3) + \text{HCO}$   
 X-sect includes q-yld = 0.008

GlyAld = Glycol aldehyde =  $\text{HOCH}_2\text{CHO}$   
 $\Rightarrow \text{HOCH}_2 + \text{HCO}$   
 X-sect includes q-yld = 0.75

MEKeto = Methyl ethyl ketone =  $\text{CH}_3\text{COC}_2\text{H}_5$   
 $\Rightarrow \text{C}_2\text{H}_5 + \text{CH}_3\text{CO}$  [.85]  
 $\Rightarrow \text{CH}_3 + \text{C}_2\text{H}_5\text{CO}$  [.15]  
 to be scaled by pressure  $1/(1 + 2.0*\text{M}(\text{bar}))$

EAld = Ethyl aldehyde =  $\text{C}_2\text{H}_5\text{CHO}$   
 $\Rightarrow \text{C}_2\text{H}_5 + \text{HCO}$

MGlyxl = Methyl glyoxal =  $\text{CH}_3\text{COCHO}$   
 $\Rightarrow \text{CH}_3\text{CO} + \text{HCO}$   
 includes \*qyld-0(wvl)  
 to be scaled by pressure  $1/(1 + 4.15*\text{M}(\text{bar}))$

Glyxl = Glyoxal  $(\text{CHO})_2$

Glyxla  $\Rightarrow \text{H}_2 + \text{CO} + \text{CO}$  or  $\text{CO} + \text{CH}_2\text{O}$  wvl > 340 nm  
 X-sect includes qyld-2 [0.029]

Glyxlb  $\Rightarrow \text{HCO} + \text{HCO}$  wvl < 340 nm  
 X-sect includes qyld-1 [0.40]

C3H6O = Acet = Acetone =  $\text{CH}_3\text{C}(\text{O})\text{CH}_3$

Acet-A  $\Rightarrow \text{CH}_3\text{CO} + \text{CH}_3$

Acet-B  $\Rightarrow \text{CH}_3 + \text{CH}_3 + \text{CO}$   
 q-ylds scale with T and density

Q1A-Ac and Q1B-Ac are for the pressure dependence of Acetone.

Updates from Randall Martin

15 Mdust 0.15 = mineral dust (R.V.Martin)

300	4.0154	0.151	0.964	1.000	2.104	2.573	2.380	1.837	1.226	0.608	0.153
400	3.0582	0.151	0.986	1.000	2.021	2.061	1.505	0.757	0.210	0.057	0.010
600	1.2133	0.151	0.994	1.000	1.712	1.120	0.368	0.096	0.015	0.002	0.000
999	0.2195	0.151	0.988	1.000	0.628	0.573	0.113	0.011	0.001	0.000	0.000

16 Mdust 0.25 = mineral dust (R.V.Martin)

300	2.6560	0.253	0.905	1.000	1.666	2.248	1.871	2.248	2.056	2.231	2.048
400	3.9669	0.253	0.980	1.000	2.060	2.715	2.658	2.515	2.163	1.591	1.024
600	3.2556	0.253	0.996	1.000	2.077	2.287	1.790	1.017	0.388	0.147	0.031
999	1.1019	0.253	0.994	1.000	1.708	1.120	0.374	0.096	0.015	0.002	0.000

17 Mdust 0.4 = mineral dust (R.V.Martin)

300	2.6071	0.402	0.862	1.000	2.190	3.255	3.624	4.518	4.572	5.092	4.820
400	2.1923	0.402	0.941	1.000	1.517	2.098	1.515	2.102	1.809	2.234	2.079
600	3.9815	0.402	0.993	1.000	2.085	2.791	2.764	2.694	2.379	1.855	1.308
999	2.9227	0.402	0.996	1.000	2.079	2.211	1.661	0.887	0.289	0.090	0.018

18 Mdust 0.8 = mineral dust (R.V.Martin)

300	2.3459	0.818	0.784	1.000	2.411	3.560	4.213	5.255	5.832	6.783	7.227
400	2.3417	0.818	0.907	1.000	2.223	3.180	3.372	4.151	4.298	5.044	5.206
600	2.4688	0.818	0.978	1.000	1.987	2.992	3.061	4.004	3.935	4.526	4.272
999	3.3741	0.818	0.992	1.000	1.984	2.703	2.614	2.793	2.687	2.533	2.298

19 Mdust 1.5 = mineral dust (R.V.Martin)

300	2.1925	1.491	0.694	1.000	2.582	3.893	4.901	6.101	7.097	8.288	9.215
400	2.2457	1.491	0.860	1.000	2.380	3.497	3.982	5.010	5.498	6.555	7.020
600	2.3919	1.491	0.964	1.000	2.237	3.288	3.523	4.492	4.768	5.704	5.996
999	2.6314	1.491	0.980	1.000	2.133	3.236	3.499	4.489	4.582	5.171	5.055

20 Mdust 2.5 = mineral dust (R.V.Martin)

300	2.1427	2.417	0.627	1.000	2.698	4.194	5.526	6.930	8.263	9.655	10.931
400	2.1881	2.417	0.805	1.000	2.493	3.713	4.426	5.563	6.301	7.494	8.213
600	2.1559	2.417	0.944	1.000	2.293	3.361	3.606	4.583	4.849	5.859	6.157
999	2.3282	2.417	0.967	1.000	2.240	3.252	3.437	4.274	4.506	5.346	5.708

21 Mdust 4.0 = mineral dust (R.V.Martin)

300	2.1045	3.721	0.582	1.000	2.769	4.422	5.990	7.568	9.129	10.687	12.200
400	2.1191	3.721	0.742	1.000	2.580	3.887	4.812	6.027	7.005	8.295	9.268
600	2.2094	3.721	0.925	1.000	2.402	3.575	4.016	5.102	5.567	6.724	7.229
999	2.3429	3.721	0.956	1.000	2.358	3.499	3.877	4.861	5.221	6.222	6.690