

171 **Chapter 6 Supplemental Tables 1-4 and Photocomp 2008 Instructions**

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173 **Table 6S-1. Chemical Species in CCMs** (1=AMTRAC3; 2=CAM3.5; 3=CCSRNIES; 4=CMAM; 5=CNRM-ACM; 6=E39CA;
 174 7=EMAC; 8=GEOSCCM; 9=LMDZrepro; 10=MRI; 11=NIWA-SOCOL; 12=SOCOL; 13=ULAQ; 14=UMETRAC;
 175 15=UMSLIMCAT; 16=UMUKCA-METO; 17=UMUKCA-UCAM; 18=WACCM; 19= PSS model).

#		1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	
1	O(³ P)	Y	Y	Y	Y	Y	Y	Y	Y*	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y
2	O(¹ D)	Y	Y	Y	Y	Y	Y	Y	Y*	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y
3	O ₃	Y	Y	Y	Y	Y	Y	Y	Y*	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y
4	O ₂	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y
5	H	Y	N	Y	Y	Y	Y	Y	Y*	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y
6	OH	Y	Y	Y	Y	Y	Y	Y	Y*	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y
7	HO ₂	Y	Y	Y	Y	Y	Y	Y	Y*	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y
8	H ₂	N	Y	Y	Y	N	Y	Y	N	N	Y	Y	Y	Y	N	Y	Y	Y	Y	Y	Y
9	H ₂ O ₂	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y
10	N	Y	Y	Y	Y	Y	Y	Y	Y*	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y
11	NO	Y	Y	Y	Y	Y	Y	Y	Y*	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y
12	NO ₂	Y	Y	Y	Y	Y	Y	Y	Y*	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y
13	NO ₃	Y	Y	Y	Y	Y	Y	Y	Y*	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y
14	N ₂ O ₅	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y
15	HONO	Y	N	N	N	N	Y	Y	N	N	N	N	N	N	Y	N	N	N	N	N	Y
16	HNO ₃	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y
17	HO ₂ NO ₂	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y
18	Cl	Y	Y	Y	Y	Y	Y	Y	Y*	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y
19	ClO	Y	Y	Y	Y	Y	Y	Y	Y*	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y
20	Cl ₂	N	Y	Y	Y	Y	Y	Y	Y	Y	N	Y	Y	N	N	N	N	N	N	Y	Y
21	OCIO	N	Y	Y	Y	Y	Y	Y	Y	Y	Y	N	N	N	N	Y	Y	Y	Y	Y	Y
22	Cl ₂ O ₂	Y	Y	Y	Y	Y	Y	Y	Y*	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y
23	HCl	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y
24	HOCl	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y

#		1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19
25	ClONO ₂	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y
26	Br	Y	Y	Y	Y	Y	Y*	Y	Y*	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y
27	BrO	Y	Y	Y	Y	Y	Y*	Y	Y*	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y
28	HOBr	Y	Y	Y	Y	Y	Y*	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y
29	HBr	Y	Y	Y	Y	Y	Y*	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y
30	BrONO ₂	Y	Y	Y	Y	Y	Y*	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y
31	BrCl	Y	Y	Y	Y	Y	Y*	Y	Y	Y	Y	Y	Y	N	Y	Y	Y	Y	Y	Y
32	Br ₂	N	N	Y	N	N	Y*	N	N	N	N	N	N	N	N	N	N	N	N	Y
33	CH ₄	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y
34	CH ₃ O ₂	Y	Y	Y	Y	Y	Y	Y	Y*	Y	N	Y	Y	Y	Y	Y	Y	Y	Y	Y
35	CH ₃ OOH	Y	Y	Y	Y	Y	Y	Y	Y	Y	N	Y	Y	Y	Y	Y	Y	Y	Y	Y
36	CH ₂ O	Y	Y	Y	Y	Y	Y	Y	Y*	Y	N	Y	Y	Y	Y	Y	Y	Y	Y	Y
37	CO	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y
38	H ₂ O	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y
39	N ₂ O	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	N
40	CO ₂	N	N	N	a	N	Y	Y	N	N	Y	Y	Y	Y	N	Y	Y	Y	Y	N
41	C ₂ H ₆	N	N	N	N	N	N	Y	N	N	N	N	N	Y	N	N	N	N	N	Y
42	CH ₃ Cl	N	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	N	N	N	N	Y	N
43	CFC-11	N	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	N	Y	Y	Y	Y	N
44	CFC-12	N	Y	Y	Y	Y	Y	Y	Y	Y*	Y	Y	Y	Y	N	Y	Y	Y	Y	N
45	CFC-113	N	Y	Y	N	Y	N	*	Y	Y	N	Y	Y	Y	N	N	N	N	Y	N
46	HCFC-22	N	Y	Y	Y	Y	N	*	Y	Y	N	Y	Y	Y	N	N	N	N	Y	N
47	HCFC141b	N	a	N	N	N	N	*	a	a	N	Y	Y	a	N	N	N	N	a	N
48	HCFC142b	N	b	N	N	N	N	*	a	b	N	Y	Y	b	N	N	N	N	b	N
49	CCl ₄	N	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	N	N	N	N	Y	N
50	CH ₃ CCl ₃	N	Y	Y	Y	Y	Y	Y	Y	Y	N	Y	Y	Y	N	N	N	N	Y	N
51	H-1202	N	c	N	N	N	N	N	N	c	N	N	N	c	N	N	N	N	c	N

#		1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19
52	H-1211	N	Y	Y	N	Y	N	Y	b	Y	Y	Y	Y	Y	N	N	N	N	Y	N
53	H-1301	N	Y	Y	N	Y	N	Y	Y	Y	Y	Y	Y	Y	N	N	N	N	Y	N
54	H-2402	N	d	N	N	N	N	N	b	d	N	Y	Y	d	N	N	N	N	d	N
55	CH ₃ Br	N	Y	Y	Y	Y	Y*	Y	Y	Y	Y	Y	Y	Y	N	Y	Y	Y	Y	N
56	NMHCs	N	e	N	N	N	N	Y	N	N	N	N	N	Y	N	N	N	N	N	N

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177 **Notes:**

178 Y = this species is explicitly derived. (O₂ specified as a constant volume mixing ratio).

179 N = this species is not explicitly derived.

180 NMHCs = the chemical mechanism includes a detailed representation of Non-Methane Hydrocarbons.

181

182 **Notes specific to each model:**

183 1: The halogen source molecules are parameterized to give realistic Cly and Bry.

184 2a-d: These species are not explicitly derived in CAM3.5. The time-dependent VMR lower boundary conditions for these species are added to surrogates with similar chemical lifetimes.

185 2e: CAM3.5 has a reduced NMHC mechanism for better representation of tropospheric chemistry.

186 3: The CCSRNIES model includes CHBr₃ with a constant surface mixing ratio of 1.8 pptv.

187 4a: For CMAM, photolysis of CO₂ is included (yielding CO + O(³P)) though the concentration of CO₂ is globally constant.

188 5: CNRM-ACM also includes ClNO₂ species.

189 6*: E39CA uses parameterization of bromine-catalyzed ozone loss (Appendix in Stenke *et al.*, 2009).

190 7*: Lumped into CFC-12 using weighting by amount of chlorine atoms.

191 8: GEOSCCM variables denoted by Y* are inferred from transported chemical families. CO₂, and H₂ are specified in the model.

192 8a: The surface boundary conditions of HCFC141b and HCFC142b are combined into one species defined as HCFC142b + 2*HCFC141b to account for total chlorine atoms involved.

193 8b: The surface boundary conditions of H-1211 and H-2402 are combined into one species defined as H-1211 + 2*H-2402 to account for the total bromine atoms involved.

194 9*: CFC-114 and CFC-115 are lumped into CFC-12 using weighting by number of chlorine atoms.

195 9a: Lumped into CH₃CCl₃ using weighting by number of chlorine atoms.

196 9b: Lumped into HCFC-22 using weighting by number of chlorine atoms.

200 9c: Lumped into CH₃Br using weighting by number of bromine atoms.
201 9d: Lumped into H-1301 using weighting by number of bromine atoms.
202 12: In the CCMVal SOCOL runs chlorine source gases were lumped in CFC-11 and CFC-12 (based on lifetimes) and bromine
203 source gases lumped into CH₃Br.
204 13: NMHC chemistry is included in ULAQ with a limited number of species (6), using lumping technique.
205 15-17: In the CCMVal UMSLIMCAT and UMUKCA runs chlorine source gases were lumped in CFC-11 and CFC-12 (based on
206 lifetimes) and bromine source gases lumped into CH₃Br.
207 18a-d: These species are not explicitly derived in WACCM. The time-dependent VMR lower boundary conditions for these species
208 are added to surrogates with similar chemical lifetimes.
209 19: The PSS model also includes: ClNO₂, ClONO, ClOO, HOONO; ClNO₂ is produced by N₂O₅+HCl(het) & Cl+NO₂; ClONO is
210 also produced by Cl+NO₂ and ClONO₂ photolysis; ClOO is produced by ClO+ClO; HOONO is produced by NO₂+OH. In this
211 model, Cl_y, NO_y, and Br_y are specified, rather than being produced from the organic source gases and N₂O. C₂H₆ from tracer
212 relations, with the focus on its production of HOx radicals and HCl, via reaction with OH and Cl, respectively.
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214 **Table 6S-2. Gas-phase Reactions in CCMs** (1=AMTRAC3; 2=CAM3.5; 3=CCSRNIES; 4=CMAM; 5=CNRM-ACM; 6=E39CA;
 215 7=EMAC; 8=GEOSCCM; 9=LMDZrepro; 10=MRI; 11=NIWA-SOCOL; 12=SOCOL; 13=ULAQ; 14=UMETRAC;
 216 15=UMSLIMCAT; 16=UMUKCA-METO; 17=UMUKCA-UCAM; 18=WACCM; 19= PSS model).

#	Reactions	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19
Oxygen Reactions																				
1	O + O ₂ + M	J6	J6	J6	J6	J6	J2	J2	J2	J6	J6	J6	J6	J6	J2	J6	J6	14	J6	J6
2	O + O ₃	J6	J6	J6	J6	J6	J2	J2	J2	J6	J6	J6	J6	J6	J2	J6	J6	14	J6	J6
3	O + O + M	N	N	J6	J6	N	N	N	J2	J6	J6	J6	J6	J6	N	J6	N	N	J6	J6
4	O(¹ D) + N ₂	J6	J6	J6	J6	J6	J2	J2	J2	J6	J6	J6	J6	J6	J2	J6	J6	14	J6	J6
5	O(¹ D) + O ₂	J6	J6	J6	J6	J6	J2	J2	J2	J6	J6	J6	J6	J6	J2	J6	J6	14	J6	J6
6	O(¹ D) + O ₃	N	J6	J6	J6	J6	J2	J2	J2	N	N	J6	J6	J6	N	J6	J6	14	J6	J6
7	O(¹ D) + H ₂ O	J6	J6	J6	J6	J6	J2	J2	J2	J6	J6	J6	J6	J6	J2	J6	J6	14	J6	J6
8	O(¹ D) + N ₂ O (NO)	J6	J6	J6	J6	J6	J2	J2	J2	J6	J6	J6	J6	J6	J2	J6	J6	J2	J6	N
9	O(¹ D) + N ₂ O (N ₂)	J6	J6	J6	J6	J6	J2	J2	J2	J6	J6	J6	J6	J6	J2	J6	J6	J2	J6	N
10	O(¹ D) + CH ₄ (tot)	J6	J6	J6	J6	J6	J2	J2	J2	J6	N	J6	J6	J6	J2	J6	J6	14	J6	J6
11	O(¹ D) + H ₂	N	J6	J6	J6	J6	J2	J2	J2	N	J6	J6	J6	J6	N	J6	J6	14	J6	J6
12	O(¹ D) + HCl	N	J6	N	N	J6	N	N	N	N	N	J6	J6	N	N	N	J6	14	J6	N
13	O(¹ D) + HBr	N	N	J6	N	J6	N	N	N	J6	N	J6	J6	N	N	J6	J6	J2	J6	J6
14	O(¹ D) + CFC-11	N	J6	J6	J6	J6	J2	J2	J2	J6	J6	J6	J6	J6	N	J6	J6	J2	J6	N
15	O(¹ D) + CFC-12	N	J6	J6	J6	J6	J2	J2	J2	J6	J6	J6	J6	J6	N	J6	J6	J2	J6	N
16	O(¹ D) + CFC-113	N	J6	J6	N	J6	N	N	J2	J6	N	J6	J6	J6	N	N	N	N	J6	N
17	O(¹ D) + CFC-114	N	N	N	N	N	N	N	J2	N	N	J6	J6	J6	N	N	N	N	J6	N
18	O(¹ D) + CFC-115	N	N	N	N	N	N	N	J2	N	N	J6	J6	J6	N	N	N	N	J6	N
19	O(¹ D) + HCFC22	N	J6	J6	J6	J6	N	N	N	J6	N	J6	J6	J6	N	N	N	N	J6	N
20	O(¹ D) + HCFC-141b	N	N	N	N	N	N	N	N	N	N	J6	J6	N	N	N	N	N	N	N
21	O(¹ D) + HCFC-142b	N	N	N	N	N	N	N	N	N	N	J6	J6	N	N	N	N	N	N	N
22	O(¹ D) + CCl ₄	N	N	J6	J6	J6	J2	J2	J2	J6	J6	J6	J6	J6	N	N	N	N	J6	N
23	O(¹ D) + CH ₃ Br	N	N	J6	J6	J6	N	N	J2	J6	J6	J6	J6	J6	N	N	J6	J2	J6	N

#	Reactions	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19
24	O(¹ D) + H-1211	N	N	J6	N	J6	N	N	J2	J6	J6	J6	J6	J6	N	N	N	N	J6	N
25	O(¹ D) + H-1301	N	N	J6	N	J6	N	N	J2	J6	J6	J6	J6	J6	N	N	N	N	J6	N
26	O(¹ D) + H-1202	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N
Nitrogen Radicals																				
27	H + NO ₂	N	N	N	J6	J6	N	N	J2	N	N	J6	J6	N	N	N	J6	J2	N	J6
28	N + O ₂	J6	J6	J6	J6	J6	J2	J2	J2	J6	J6	J6	J6	J6	J2	J6	J6	J2	J6	J6
29	N + NO	J6	J6	J6	J6	J6	J2	J2	J2	J6	J6	J6	J6	J6	J2	J6	J6	J2	J6	N
30	N + NO ₂	J6	N	N	N	J6	J2	J2	J2	J6	N	J6	J6	N	J2	N	J6	J2	J6	N
31	N + O ₃	N	N	J6	N	J6	N	N	N	N	N	N	N	N	N	J6	N	N	N	N
32	NO + O + M	N	N	N	J6	J6	N	N	J2	N	N	J6	J6	N	J2	N	J6	J2	J6	J6
33	NO + OH + M (HONO)	J6	N	N	N	N	J2	J2	N	J6	N	N	N	N	J2	N	N	N	N	J6
34	NO + HO ₂	J6	J6	J6	J6	J6	J2	J2	J2	J6	J6	J6	J6	J6	J2	J6	J6	J2	J6	J6
35	NO + O ₃	J6	J6	J6	J6	J6	J2	J2	J2	J6	J6	J6	J6	J6	J2	J6	J6	14	J6	J6
36	NO ₂ + O	J6	J6	J6	J6	J6	J2	J2	J2	J6	J6	J6	J6	J6	J2	J6	J6	14	J6	J6
37	NO ₂ + O + M	N	N	N	N	J6	N	N	J2	N	N	J6	J6	N	N	N	J6	14	J6	J6
38	NO ₂ + O ₃	J6	J6	J6	J6	J6	J2	J2	J2	J6	J6	J6	J6	J6	J2	J6	J6	14	J6	J6
39	NO ₂ + NO ₃ + M	J6	J6	J6	J6	J6	J2	J2	J2	J6	J6	J6	J6	J6	J2	J6	J6	14	J6	J6
40	N ₂ O ₅ + M	J6	J6	J6	J6	J6	J2	J2	J2	J6	J6	J6	J6	J6	J2	J6	J6	14	J6	J6
41	NO ₂ + OH + M	J6	J6	J6	J6	J6	J2	J2	J2	J6	J6	J6	J6	J6	J2	J6	J6	14	J6	J6
42	NO ₂ + HO ₂ + M	J6	J6	J6	J6	J6	J2	J2	J2	J6	J6	J6	J6	J6	J2	J6	J6	14	J6	J6
43	NO ₃ + NO	J6	J6	N	N	J6	J2	J2	J2	N	N	J6	J6	N	J2	J6	J6	14	J6	J6
44	NO ₃ + O	N	N	N	J6	N	N	N	N	N	N	J6	J6	N	N	J6	J6	14	J6	J6
45	NO ₃ + OH	N	N	N	N	J6	N	N	N	N	N	J6	J6	N	N	N	J6	J2	J6	J6
46	NO ₃ + HO ₂	N	J6	N	N	N	J2	J2	N	N	N	J6	J6	N	N	N	J6	14	J6	J6
47	HONO + OH	J6	N	N	N	N	J2	J2	N	N	N	N	N	N	J2	N	N	N	N	J6
48	HO ₂ NO ₂ + OH	N	J6	J6	J6	J6	J2	J2	J2	J6	J6	J6	J6	J6	J2	J6	J6	J2	J6	J6
49	HO ₂ NO ₂ + M	J6	J6	J6	J6	J6	J2	J2	J2	J6	J6	J6	J6	J6	J2	J6	J6	14	J6	J6

#	Reactions	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19
50	HNO ₃ + OH	J6	J6	J6	J6	J6	J2	J2	J2	J6	J6	J6	J6	J6	J2	J6	a	14	J6	J6
	Hydrogen Radicals																			
51	H + O ₂ + M	J6	N	J6	J6	J6	J2	J2	J2	J6	J6	J6	J6	J6	J2	J6	J6	J2	J6	J6
52	H + O ₃	J6	N	J6	J6	J6	J2	J2	J2	J6	J6	J6	J6	J6	J2	J6	J6	14	J6	J6
53	H + HO ₂ (OH)	N	N	J6	J6	J6	J2	a	J2	J6	J6	J6	J6	J6	N	J6	J6	J2	J6	J6
54	H + HO ₂ (H ₂ O)	N	N	J6	J6	J6	J2	a	J2	J6	J6	N	N	J6	N	J6	J6	J2	J6	J6
55	H + HO ₂ (H ₂)	N	N	J6	J6	J6	J2	a	J2	J6	J6	J6	J6	J6	N	J6	J6	J2	J6	J6
56	OH + O	J6	J6	J6	J6	J6	J2	J2	J2	J6	J6	J6	J6	J6	J2	J6	J6	14	J6	J6
57	OH + O ₃	J6	J6	J6	J6	J6	J2	J2	J2	J6	J6	J6	J6	J6	J2	J6	J6	14	J6	J6
58	OH + HO ₂	J6	J6	J6	J6	J6	J2	J2	J2	J6	J6	J6	J6	J6	J2	J6	J6	14	J6	J6
59	OH + OH (tot)	J6	J6	J6	J6	J6	N	N	J2	J6	N	J6	J6	J6	J2	J6	J6	J2	J6	J6
60	OH + OH + M	J6	J6	N	J6	J6	N	N	J2	N	N	J6	J6	J6	J2	J6	J6	14	J6	J6
61	OH + H ₂	J6	J6	J6	J6	J6	J2	J2	J2	J6	J6	J6	J6	J6	J2	J6	J6	14	J6	J6
62	OH + H ₂ O ₂	J6	J6	J6	J6	J6	J2	J2	J2	J6	J6	J6	J6	J6	J2	J6	J6	14	J6	J6
63	HO ₂ + O	J6	J6	J6	J6	J6	J2	J2	J2	J6	J6	J6	J6	J6	J2	J6	J6	14	J6	J6
64	HO ₂ + O ₃	J6	J6	J6	J6	J6	J2	J2	J2	J6	J6	J6	J6	J6	J2	J6	J6	14	J6	J6
65	HO ₂ + HO ₂	J6	J6	J6	J6	J6	J2	b	J2	J6	J6	J6	J6	J6	J2	J6	J6	14	J6	J6
66	H ₂ O ₂ + O	N	N	N	J6	N	N	N	J2	N	N	J6	J6	N	N	N	J6	14	J6	J6
	Chlorine Radicals																			
67	Cl + O ₃	J6	J6	J6	J6	J6	J2	J2	J2	J6	J6	J6	J6	J6	J2	J6	J6	14	J6	J6
68	Cl + H ₂	N	J6	J6	J6	J6	J2	J2	J2	J6	J6	J6	J6	J6	N	J6	J6	14	J6	J6
69	Cl + H ₂ O ₂	N	J6	J6	J6	N	J2	J2	J2	N	N	J6	J6	N	N	J6	J6	14	J6	J6
70	Cl + HO ₂ (HCl)	J6	J6	J6	J6	J6	J2	J2	J2	J6	J6	J6	J6	J6	J2	J6	J6	14	J6	J6
71	Cl + HO ₂ (ClO)	N	J6	J6	J6	J6	J2	J2	J2	N	N	J6	J6	J6	N	J6	J6	14	J6	J6
72	Cl + CH ₂ O	J6	J6	J6	J6	J6	J2	J2	J2	J6	N	J6	J6	J6	J2	J6	J6	14	J6	J6
73	Cl + CH ₄	J6	J6	J6	J6	J6	J2	J2	J2	J6	J6	J6	J6	J6	J2	J6	J6	14	J6	J6
74	ClO + O	J6	J6	J6	J6	J6	J2	J2	J2	J6	J6	J6	J6	J6	J2	J6	J6	14	J6	J6

#	Reactions	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19
75	ClO + OH (Cl)	J6	J6	J6	J6	J6	J2	J2	J2	J6	J6	J6	J6	J6	J2	J6	J6	J2	J6	J6
76	ClO + OH (HCl)	J6	J6	J6	J6	J6	J2	J2	J2	J6	N	J6	J6	J6	N	J6	J6	J2	J6	J6
77	ClO + HO ₂	J6	J6	J6	J6	J6	J2	J2	J2	J6	J6	J6	J6	J6	J2	J6	J6	14	J6	J6
78	ClO + NO	J6	J6	J6	J6	J6	J2	J2	J2	J6	J6	J6	J6	J6	J2	J6	J6	14	J6	J6
79	ClO + NO ₂ + M	J6	J6	J6	J6	J6	J2	J2	J2	J6	J6	J6	J6	J6	J2	J6	J6	14	J6	J6
80	ClO + ClO (Cl ₂)	N	J6	J6	J6	J6	N	N	N	J6	N	J6	J6	J6	N	J6	J6	14	J6	J6
81	ClO + ClO (ClOO)	J6	J6	N	N	a	N	N	N	N	N	N	N	J6	N	J6	J6	14	J6	J6
82	ClO + ClO (OCIO)	N	J6	J6	N	J6	N	N	N	N	N	N	N	J6	N	J6	J6	14	J6	J6
83	ClO + ClO + M	N	J6	J6	J6	J6	J2	15	J2	J6	J6	J6	J6	J6	J2	J6	J6	14	J6	J6
84	OCIO + O	N	N	J6	J6	N	N	N	N	N	J6	N	N	N	N	N	J6	14	N	J6
85	OCIO + NO	N	N	J6	J6	N	N	N	N	N	J6	N	N	N	N	N	J6	14	N	J6
86	OCIO + Cl	N	N	J6	J6	N	N	N	N	N	J6	N	N	N	N	N	J6	14	N	J6
87	Cl ₂ O ₂ + M	J6	J6	J6	J6	J6	J2	J2	J2	J6	J6	J6	J6	J6	J2	J6	J6	14	J6	J6
88	Cl ₂ O ₂ + Cl	N	N	N	N	N	N	N	N	N	N	J6	J6	N	N	J6	J6	14	N	J6
89	HCl + OH	J6	J6	J6	J6	J6	J2	J2	J2	J6	J6	J6	J6	J6	J2	J6	J6	14	J6	J6
90	HCl + O	N	J6	J6	J6	N	N	N	N	N	N	J6	J6	N	N	N	J6	J2	J6	J6
91	HOCl + O	N	N	J6	J6	J6	N	N	N	J6	J6	J6	J6	N	N	J6	J6	14	J6	J6
92	HOCl + Cl	N	J6	J6	J6	J6	N	N	N	J6	N	J6	J6	N	N	J6	J6	J2	J6	J6
93	HOCl + OH	N	N	J6	J6	J6	J2	J2	J2	J6	J6	J6	J6	J6	N	J6	J6	J2	J6	J6
94	ClONO ₂ + O	J6	J6	J6	J6	J6	J2	J2	J2	J6	J6	J6	J6	J6	J2	J6	J6	J2	J6	J6
95	ClONO ₂ + OH	N	J6	N	N	N	N	N	J2	N	N	J6	J6	N	N	J6	J6	J2	J6	J6
96	ClONO ₂ + Cl	N	J6	N	N	N	J2	J2	N	N	N	J6	J6	N	N	J6	J6	J2	J6	J6
Bromine Radicals																				
97	Br + O ₃	J6	J6	J6	J6	J6	*	J2	J2	J6	J6	J6	J6	J6	J2	J6	J6	14	J6	J6
98	Br + HO ₂	J6	J6	J6	J6	J6	*	J2	J2	J6	J6	J6	J6	J6	J2	J6	J6	14	J6	J6
99	Br + CH ₂ O	J6	J6	J6	N	J6	*	J2	J2	J6	N	J6	J6	N	J2	J6	J6	J2	J6	J6
100	BrO + O	J6	J6	J6	J6	J6	*	J2	J2	J6	J6	J6	J6	J6	N	J6	J6	14	J6	J6
101	BrO + OH	N	J6	J6	J6	J6	*	N	N	N	N	J6	J6	J6	N	J6	J6	14	J6	J6

#	Reactions	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	
102	BrO + HO ₂	J6	J6	J6	J6	J6	*	J2	J2	J6	J6	J6	J6	J6	J2	J6	J6	J2	J6	J6	
103	BrO + NO	J6	J6	J6	J6	J6	*	J2	J2	J6	N	J6	J6	J6	J2	J6	J6	14	J6	J6	
104	BrO + NO ₂ + M	J6	J6	J6	J6	J6	*	J2	J2	J6	J6	J6	J6	J6	J2	J6	J6	14	J6	J6	
105	BrO + ClO (OCIO)	N	J6	J6	J6	J6	*	J2	J2	J6	J6	J6*	J6*	J6	N	J6	J6	14	J6	J6	
106	BrO + ClO (ClOO)	J6	J6	J6	a	b	*	J2	J2	N	J6	J6*	J6*	J6	J2	J6	J6	14	J6	J6	
107	BrO + ClO (BrCl)	J6	J6	J6	J6	J6	*	J2	J2	J6	J6	J6	J6	J6	J2	J6	J6	14	J6	J6	
108	BrO + BrO	N	J6	J6	J6	J6	*	N	J2	N	N	J6	J6	J6	N	J6	J6	J2	J6	J6	
109	BrO+BrO → Br ₂ + O ₂	N	N	J6	N	c	*	N	N	J6	N	N	N	J6	N	N	N	N	N	J6	
110	Br ₂ + OH	N	N	N	N	N	*	N	N	N	N	N	N	N	N	N	N	N	N	N	J6
111	HBr + O	N	N	J6	N	N	*	N	N	N	N	J6	J6	J6	N	J6	J6	J2	J6	J6	
112	HBr + OH	J6	J6	J6	J6	J6	*	J2	J2	J6	J6	J6	J6	J6	J2	J6	J6	14	J6	J6	
113	HOBr + O	J6	N	N	N	J6	*	J2	N	J6	N	J6	J6	J6	J2	J6	N	N	J6	J6	
114	BrONO ₂ + O	N	N	N	N	N	*	N	N	J6	N	N	N	N	N	J6	N	N	J6	J6	
	Organic Halogen Reactions																				
115	CH ₃ Cl + Cl	N	J6	N	J6	N	N	N	N	N	N	N	N	N	N	N	N	N	N	J6	N
116	CH ₃ Cl + OH	N	J6	J6	J6	J6	J2	J2	J2	J6	J6	J6	J6	J6	N	N	N	N	N	J6	N
117	CH ₃ CCl ₃ + OH	N	J6	J6	J6	J6	J2	J2	J2	J6	N	J6	J6	J6	N	N	N	N	N	J6	N
118	HCFC22 + OH	N	J6	N	J6	J6	N	N	J2	J6	N	J6	J6	J6	N	N	N	N	N	J6	N
119	CH ₃ Br + OH	N	J6	J6	J6	J6	N	J2	J2	J6	N	J6	J6	J6	N	J6	J6	J2	J6	J6	N
	CH ₄ and Derivatives																				
120	CH ₄ + OH	J6	J6	J6	J6	J6	J2	c	J2	J6	J6	J6	J6	J6	J2	J6	J6	14	J6	J6	
121	CH ₃ O ₂ + NO	J6	J6	J6	J6	J6	J2	J2	J2	J6	N	J6	J6	J6	J2	J6	J6	14	J6	J6	
122	CH ₃ O ₂ + HO ₂	J6	J6	J6	J6	J6	J2	J2	J2	J6	N	J6	J6	J6	J2	J6	J6	14	J6	J6	
123	CH ₃ O ₂ + ClO	N	N	J6	J6	J6	J2	J2	N	N	N	N	N	N	N	J6	J6	J2	N	J6	
124	CH ₃ O ₂ + CH ₃ O ₂	J6	J6	J6	J6	J6	J2	J2	N	J6	N	J6	J6	J6	J2	J6	J6	J2	N	J6	
125	CH ₃ OOH + OH	J6	J6	J6	J6	J6	J2	J2	J2	J6	N	J6	J6	J6	J2	J6	J6	14	J6	J6	
126	CH ₂ O + NO ₃	N	J6	N	N	J6	J2	J2	N	N	N	J6	J6	N	J2	N	J6	14	J6	J6	

#	Reactions	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19
127	CH ₂ O + OH	J6	J6	J6	J6	J6	J2	d	J2	J6	N	J6	J6	J6	J2	J6	J6	I4	J6	J6
128	CH ₂ O + O	N	N	J6	J6	J6	N	N	J2	J6	N	J6	J6	J6	N	J6	J6	I4	J6	J6
128	CO + OH +M (CO ₂)	J6	J6	N	J6	J6	J2	e	J2	J6	N	J6	J6	J6	J2	J6	I4	I4	J6	J6
129	CO + OH +M (HOCO)	N	N	N	b	J6	N	N	N	N	N	N	N	N	N	N	N	N	J6	J6
	C ₂ H ₆ chemistry																			
130	C ₂ H ₆ +OH	N	N	N	N	N	N	c	N	N	N	N	N	J6	N	N	N	N	N	J6
131	C ₂ H ₆ +Cl	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N	J6

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218

219 **Notes:**

220 I4 = IUPAC, 2004.

221 I5 = IUPAC, 2005.

222 J2 = Chemical Kinetics and Photochemical Data for Use in Atmospheric Studies, Eval#14 (JPL-02).

223 J6 = Chemical Kinetics and Photochemical Data for Use in Atmospheric Studies, Eval#15 (JPL-06).

224 N = This reaction is not explicitly represented.

225

226 **Notes specific to each model:**

227 3: rxn#101: BrO + OH → Br + HO₂ (98%), → HBr + O₂ (2%) is assumed.

228 3: rxn#108: BrO + BrO → 2Br + O₂ is assumed.

229 3: The CCSRNIES model includes the reactions Cl + O₂ + M → ClOO + M, OClO + OH → HOCl + O₂, CHBr₃ + OH → 3Br + products, and CO + OH → H + CO₂.

231 4a: JPL-06 but forms Cl + O₂

232 4b: Both channels of OH + CO included, but both yield CO₂ + H.

233 5: "a" produces OClO; "b" produces OClO; "c" produces 2xBr instead of Br₂.

234 6*: Uses parameterization of bromine-catalyzed ozone loss (Appendix in Stenke *et al.*, 2009).

235 7a: Hack *et al.* (1978), listed in JPL-02.

236 7b: Christensen *et al.* (2002), Kircher and Sander (1984).

237 7c: Atkinson (2003).

238 7d: Sivakumaran *et al.* (2003).

239 7e: McCabe *et al.* (2001).
240 12: The products of 105 and 106 are Cl + Br + O₂.
241 16a: The OH + HNO₃ reaction rate is amalgamated from JPL-06 and IUPAC (2002).
242 17: The IUPAC 2004 (I4) reference is used for many of the reactions; however, the rate constants were set in 2002 using the
243 online version of IUPAC.
244

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Table 6S-3. Photolytic Reactions in CCMs (1=AMTRAC3; 2=CAM3.5; 3=CCSRNIES; 4=CMAM; 5=CNRM-ACM; 6=E39CA; 7=EMAC; 8=GEOSCCM; 9=LMDZrepro; 10=MRI; 11=NIWA-SOCOL; 12=SOCOL; 13=ULAQ; 14=UMETRAC; 15=UMSLIMCAT; 16=UMUKCA-METO; 17=UMUKCA-UCAM; 18=WACCM; 19= PSS model).

#	Reaction	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	
1	O ₂ + hv (O ¹ D)	N	N	N	N	N	N	N	J2	N	N	La	La	N	N	N	J	J	J6	N	
2	O ₂ + hv (O ³ P)	J6	J6	J6	J6	J6	a	a	J2	J6	J6	Af	Af	J6	Y	Mi	J	J	J6	J6	
3	1.0 O ₃ + hv (O ¹ D)	J6	J6	J0	J6	J6	b	b	J2	J6	J6	J0	J0	J6	Y	J2	J	J	J6	J6	
4	O ₃ + hv (O ³ P)	J6	J6	J0	J6	J6	b	b	J2	J6	J6	J0	J0	J6	Y	J2	J	J	J6	J6	
5	N ₂ O + hv	J6	J6	J6	J6	J6	J7	J7	J2	J6	J6	J2	J2	J6	Y	J0	J	J	J6	N	
6	NO + hv	J6	Mi	Af	Mi	J6	c	c	J2	J6	J6	Ni	Ni	J6	Y	Mi	J	J	Mi	J6	
7	NO ₂ + hv	J6	J6	J2	J6	J6	J7	J7	J2	J6	J6	J2	J2	J6	Y	J0	J	J	J6	J6	
8	N ₂ O ₅ + hv (NO)	N	N	N	N	A	N	N	N	N	N	N	N	N	N	N	N	N	N	J6	N
9	N ₂ O ₅ + hv (NO ₂)	J6	J6	J2	J6	A	J7	J7	J2	J6	J6	J6	J6	J6	Y	J0	J	J	J6	J6	
10	HONO + hv	J6	N	N	N	N	J7	J7	N	J6	N	N	N	N	Y	N	N	N	N	J6	
11	HNO ₃ + hv	J6	J6	J6	J6	J6	J7	J7	J2	J6	J6	J6	J6	J6	Y	J0	J	J	J6	J6	
12	NO ₃ + hv (NO)	J6	J6	J2	J6	J6	J7	J7	J2	J6	J6	J2	J2	J6	Y	J0	J	J	J6	J6	
13	NO ₃ + hv (NO ₂)	J6	J6	J2	J6	J6	J7	J7	J2	J6	J6	J2	J2	J6	Y	J0	J	J	J6	J6	
14	HO ₂ NO ₂ + hv (NO ₂)	J6	a	J2	J6	J6	d	d	J2	J6	J6	J6	J6	J6	Y	J0	J	J	a	J6	
15	HO ₂ NO ₂ + hv (NO ₃)	N	a	J2	N	J6	N	N	N	N	N	N	N	N	N	N	J	J	a	J6	
16	CH ₃ OOH + hv	J6	J6	J6	J6	J6	J7	J7	J2	J6	N	J6	J6	J6	Y	J0	J	J	J6	J6	
17	CH ₂ O + hv (H)	J6	J6	J2	J6	J6	J7	J7	J2	J6	N	J2	J2	J6	Y	J0	J	J	J6	J6	
18	CH ₂ O + hv (H ₂)	J6	J6	J2	J6	J6	J7	J7	J2	J6	N	J2	J2	J6	Y	J0	J	J	J6	J6	
19	H ₂ O + hv	J6	N	a	J	J6	J7	J7	J2	J6	J6	La	La	J6	Y	J	J	J	b	J6	
20	HO ₂ + hv	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N	J6	
21	H ₂ O ₂ + hv	J6	J6	J6	J6	J6	J7	J7	J2	J6	J6	J2	J2	J6	Y	J0	J	J	J6	J6	
22	Cl ₂ + hv	Y	J6	J2	J6	J6	J7	J7	N	J6	J6	J6	J6	N	N	N	N	N	J6	J6	
23	ClO + hv	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N	J6	J6	

24	OCIO + hv	N	J6	J2	J6	J6	e	e	J2	J6	J6	N	N	N	N	J	J	J	J6	J6
25	Cl ₂ O ₂ + hv	J6	b	J6	J6	J6	f	f	J2	J6	J6	J6	J6	a	Y	a	a	a	c	J6
26	HOCl + hv	J6	J6	J2	J6	J6	J7	J7	J2	J6	J6	J6	J6	J6	Y	J0	J	J	J6	J6
27	2.0 HCl + hv	J6	J6	J2	J6	J6	J7	J7	J2	J6	J6	J6	J6	J6	N	J0	J	J	J6	J6
28	ClONO ₂ + hv ClONO)	N	J6	J6	N	B	N	N	N	J6	N	N	N	N	N	N	N	N	J6	J6
29	ClONO ₂ + hv (NO ₃)	J6	J6	J6	J6	J6	J7	J7	J2	J6	J6	J6	J6	J6	Y	J0	J	J	J6	J6
30	BrCl + hv	J6	J6	J6	J6	J6	N	J7	N	J6	J6	J6	J6	N	Y	J0	J	J	J6	J6
31	BrO + hv	J6	J6	J2	J6	J6	N	N	J2	J6	N	J6	J6	J6	Y	J0	J	J	J6	J6
32	HOBr + hv	J6	J6	J2	J6	J6	N	J2	J2	J6	J6	J6	J6	J6	Y	J0	J	J	J6	J6
33	HBr + hv	N	N	b	J6	N	N	N	N	N	N	N	N	N	N	N	N	N	N	J6
34	Br ₂ + hv	N	N	J6	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N	J6
35	BrONO ₂ + hv (NO ₂)	N	J6	J2	N	N	N	N	J2	N	J6	J6	J6	N	N	N	J	J	J6	J6
36	BrONO ₂ + hv (NO ₃)	J6	J6	J2	J6	J6	N	J7	N	J6	J6	J6	J6	J6	Y	J0	J	J	J6	J6
37	CH ₄ + hv	J6	J	N	J	N	N	N	J2	J6	J6	La	La	N	N	J	J	J	J	J6
38	CO ₂ + hv	N	N	N	J	J6	J7	J7	J2	J6	J6	La	La	J6	N	J	J	J	J	N
39	CH ₃ Cl + hv	N	J6	J0	J6	J6	J7	J7	J2	J6	J6	15	15	J6	N	N	N	N	J6	N
40	CCl ₄ + hv	N	J6	J0	J6	J6	J7	J7	J2	J6	J6	15	15	J6	N	N	N	N	J6	N
41	CH ₃ CCl ₃ + hv	N	J6	J0	J6	J6	J7	J7	J2	J6	N	15	15	J6	N	N	N	N	J6	N
42	CFC-11 + hv	N	J6	J0	J6	J6	J7	J7	J2	J6	J6	15	15	J6	N	J0	J	J	J6	N
43	CFC-12 + hv	N	J6	J0	J6	J6	J7	J7	J2	J6	J6	J2	J2	J6	N	J0	J	J	J6	N
44	CFC-113 + hv	N	J6	J0	N	J6	N	N	J2	J6	N	15	15	J6	N	N	N	N	J6	N
45	CFC-114 + hv	N	N	N	N	N	N	N	J2	N	N	15	15	J6	N	N	N	N	N	N
46	CFC-115 + hv	N	N	N	N	N	N	N	J2	N	N	15	15	J6	N	N	N	N	N	N
47	HCFC-22 + hv	N	J6	J6	J6	J6	N	N	J2	J6	N	15	15	J6	N	N	N	N	J6	N
48	HCFC-141b + hv	N	N	N	N	N	N	N	N	N	N	15	15	N	N	N	N	N	J6	N
49	HCFC-142b + hv	N	N	N	N	N	N	N	N	N	N	15	15	N	N	N	N	N	J6	N
50	CH ₃ Br + hv	N	J6	J0	J6	J6	N	J7	J2	J6	J6	14	14	J6	N	J0	J	J	J6	N
51	H-1202 + hv	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N

52	H-1211 + hv	N	J6	J6	N	J6	N	J7	J2	J6	J6	I4	I4	J6	N	N	N	N	J6	N
53	H-1301 + hv	N	J6	J6	N	J6	N	J7	J2	J6	J6	J2	J2	J6	N	N	N	N	J6	N
54	H-2402 + hv	N	N	N	N	N	N	N	N	N	N	I4	I4	N	N	N	N	N	N	N

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250 **Notes:**

251 J7 = Chemical Kinetics and Photochemical Data for Use in Atmospheric Studies, Eval#12 (JPL-97).

252 J0 = Chemical Kinetics and Photochemical Data for Use in Atmospheric Studies, Eval#13 (JPL-00).

253 J2 = Chemical Kinetics and Photochemical Data for Use in Atmospheric Studies, Eval#14 (JPL-02).

254 J6 = Chemical Kinetics and Photochemical Data for Use in Atmospheric Studies, Eval#15 (JPL-06).

255 I4 = IUPAC, 2004.

256 I5 = IUPAC, 2005.

257

258 J = Data taken from a variety of sources.

259 N = This reaction is not explicitly represented.

260

261 **Notes specific to each model:**

262 1: Cl₂ is photolysed, but lumped with Cl₂O₂.

263 2a: CAM3.5 does not include the near-IR photolysis of HO₂NO₂.

264 2b: JCl₂O₂ uses Burkholder *et al.*, (1990) [with log-linear extrapolation to 450nm].

265 2Mi: On-line calculation of J_{NO} using parameterization of Minschwaner and Siskind (1993).

266

266

267 3Af: Allen and Frederick (1982).

268 3a: Equations (4.98) and (4.99) on p.157, Brasseur and Solomon (1986).

269 3b: Assumed to be the same values as those for J_{HCl} .

270 4Mi: On-line calculation of J_{NO} using parameterization of Minschwaner and Siskind (1993).

271 5a: Produces 2x NO_x according to JPL-06.

272 5b: Produces $\text{ClO} + \text{NO}_2$ according to JPL-06.

273 6a/7a: JPL-97 + Koppers and Murtagh (1996) + Chabrilla and Kockarts (1997).

274 6b/7b: JPL-97 + Talukdar *et al.* (1998).

275 6c/7c: Allen and Frederick (1982).

276 6d/7d: JPL-97 + Roehl *et al.* (2002).

277 6e/7e: Wahner *et al.* (1987).

278 6f/7f: JPL-97, j-value scaled by 1.4 (close to Burkholder *et al.* 1990). See PhotoComp. Some values marked with N can be

279 calculated by the model but are not used.

280 11Af: Allen and Frederick (1982).

281 12Af: Allen and Frederick (1982).

282 12Ni: Nicolet (1979); Nicolet and Cieslik, (1980).

283 14: The code contains no information on when the rates were last updated, so only existence or not could be established.

284 15Mi: Minschwaner *et al.* (1993), Minschwaner and Siskind (1993);

285 15a: Burkholder *et al.*, (1990) [with log-linear extrapolation to 450nm].

286 16-17: Photolysis in UMUKCA (both versions) is based on an earlier version of the SLIMCAT CTM but the cross sections have not

287 been updated. Exceptions are the photolysis of HO_2NO_2 , ClONO_2 , and BrONO_2 . Here the cross sections are unchanged but

288 new information on branching ratios has been adopted. Also we have introduced a reaction $\text{O}_2 + h\nu \Rightarrow \text{O}(^1\text{D}) + \text{O}(^3\text{P})$ with a

289 branching ratio following JPL-06. The cross sections and quantum yields for oxygen photolysis follow WMO (1985).

290 18 For JO_2 , the Ly-a and SRB is derived using Chabrilat and Kockarts (1997) and Kopper and Murtagh (1996), respectively.

291 18a: WACCM does not include the near-IR photolysis of JHO_2NO_2 .

292 18b: JH_2O cross sections are taken from JPL-06, plus Lyman alpha photolysis.

293 18c: JCl_2O_2 uses Burkholder *et al.*, (1990) [with log-linear extrapolation to 450nm].

294 18Mi: On-line calculation of J_{NO} using parameterization of Minschwaner and Siskind (1993).

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Table 6S-4. Description of models in PhotoComp 2008.

Label	Model	Method	Bins	Scattering code	SR Bands	Solar Irradiance and CS/QY comments	Low Sun	Cloud (P1c)	Aerosol(P1b)
AMTR	AMTRAC	LUT from Groves & Tuck 1980	?	?	?	JPL 2002	Spherical solar rays, no refraction.		
CCSR	CCSRNIES	Inline RT	16 [200 – 690nm] + 2 [>690 nm], SR param for O ₂ &NO	Two-stream, plane-parallel	O ₂ : M93 NO: AF82	Sep86+Nov89 from L97	Spherical solar rays, no refraction.		Own aerosol scattering, same tau
EMAC	EMAC	Inline RT (v1.5)	7 [202-682 nm] + Ly-alpha + SR param.	Delta 2-stream (PIFM) + LUT	O ₂ : KM96 NO: AF82	JPL1997 + updates: O(¹ D), HNO ₄ , acetone, OCIO, HOBr, ...	Extrapolation when SZA 88–94.5° (L03)	OD match PC08, LWC and scattering from EMAC	
GFJX	UCI Fast-JX (v6.2)	Standalone RT	18 [177.4 - 850nm], not contiguous.	8-stream, asymmetric Feautrier, plane-parallel	Redo SR ODFs in UCIR by BP02	JPL 2002, IUPAC 2005 + updates (O ¹ D, HNO ₄ , acetone, NO ₂ (JPL O3 from AFGL/Molina. SUSIM solar fluxes (Mar 92+Nov 94)	Spherical solar rays, no refraction.	per PC08	per PC08
Gtbl	GEOSCCM	LUT (p,col-O ₃ ,SZA, λ)	79 [176.215-652.5 nm] +Lyman-alpha	Matrix inversion, isotropic scattering	KM96	JPL 2002	Spherical solar rays with refraction		
LMDZ	LMDZRepro	LUT from TUV 4.1		LUT (p, col-O ₃ , SZA, λ)	See TUV	See TUV 4.1	See TUV	?	?
NIWA	NIWA-SOCOL v2.0	LUT from Mezon CTM	73 total [120-750 nm] with Lyman-alpha	LUT (XO ₂ & XO ₃)	O ₂ and NO: AF82	Mostly JPL 2006 + IUPAC. Solar: CCMVal2 see Lean 2005.	Spherical solar rays, no refraction	OD match PC08, LWC and scattering from S78	

SLIM	UMSLIMCAT	LUT(p,col-O ₃ ,SZA, T)	203 total [120-850 nm] with Lyman-alpha	Plane parallel isotropic multiple scattering.	O ₂ : M93 NO: MS93	JPL 2002. Solar: WMO (1985) for PhotoComp. Lean (2005) for CCMVal runs.	Spherical solar rays, no refraction.		
SOCL	SOCOL v2.0	Inline RT (Mezon CTM)	73 [120-750nm]	Delta-Eddington, plane-parallel	NO & O ₂ : AF82	Mostly JPL 2006 + IUPAC. Solar: CCMVal2 see Lean 2005	Spherical solar rays, no refraction		
TUVM	NCAR TUV (v4.6)	Standalone RT	For campaign: fixed bins SR and 8 bins [208-735 nm], with Lα	4-stream discrete-ordinates, plane-parallel, St88.	KM96	mostly JPL06 Solar irradiance: SUSIM: $\lambda < 150$ nm Atlas 3: 150 ~ 400 nm Neckel and Labs 1984: > 400 nm	Spherical solar rays, no refraction	per PC08	per PC08
UCIJ	UCI Fast-JX (v6.5)	Standalone RT	18 [177.4 - 850nm], not contiguous	8-stream, asymmetric Feautrier, plane-parallel	Redo SR ODFs in UCIr by BP02	JPL 2002, IUPAC 2005 + updates (O ¹ D, HNO ₄ , acetone, NO ₂ (JPL O ₃ from AFGL/Molina. SUSIM solar fluxes (Mar 92+Nov 94)	Spherical solar rays, no refraction	per PC08	per PC08
UCIr	UCI ref J-code (2005)	Standalone RT	62 [202-850 nm] +83 ODFs [177-202 nm]	6-stream, symmetric Feautrier, plane-parallel	O ₂ & NO ODFs derived from M93 & MS93	JPL 2002, IUPAC 2005, hi-res O ₃ + updates (O ¹ D, HNO ₄ , acetone, NO ₂). SUSIM solar fluxes (Mar 92+Nov 94)	Spherical solar rays, no refraction		
WACC	WACCM	LUT [SZA, ALB, colO ₃ , temp, press]	100 total [120-750 nm] 33: [120-200 nm] 67: [200-750 nm] with Lα	4-stream discrete-ordinates, St98.	In line: O ₂ : KM96 NO: MS93	CS and QY: mostly JPL06 Solar irradiance model of Lean <i>et al.</i> (2005) interpolated to the 100 bins used in WACCM. A solar average file was used for the photocomp 2008.	Spherical solar rays, no refraction ; SZA $\leq 97^\circ$		

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Abbreviations:

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CS = Cross Sections; QY= Quantum yield; SZA: Solar zenith angle; ALB = surface albedo; RT=radiative transfer; SR = Schumann-Runge; L α =

353

Lyman-Alpha; LUT: Lookup Table, λ : wavelength

- 354
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SPARC CCMVal PhotoComp-2008 (1 June 2008, MJP)

GOALS. Evaluate how models calculate photolysis (and indirectly heating) rates in the stratosphere and troposphere with the incentive of locating errors or biases and identifying improved and practical methods. There are three basic parts to PhotoComp2008:

(1) Basic test of *all* J- values for high sun (SZA=15°), w/ & w/o additional scattering layers (stratiform clouds & stratospheric volcanic aerosols).

(2) Test of twilight, sphericity, and 24-hour averages (SZA = 84° - 96°).

(3) Test of wavelength integration w/o scattering (SZA = 15°).

There will be one standard atmosphere, whose primary definition will include air mass, ozone mass, and temperature in each layer. This atmosphere is typical of the tropics, ozone column = 260 DU. For efficiency, we will use this same atmosphere in all sections, even the low-sun, polar cases.

PARTICIPATION. This study is designed to aid development and testing of the photolysis and short-wave heating codes used in chemistry-transport models and coupled chemistry-climate models. This project is open: any research group can participate by running the experiments and reporting the results as specified below. We also encourage participation from groups (without CTMs or CCMs) who have participated in other model-measurement studies (e.g., IPMMI, POLARIS). Many CTM/CCMs will be using “the same” photolysis scheme (e.g., fast-TUV, fast-J) and think their participation redundant – this is false. The implementation of a standard scheme into any CTM/CCM will likely alter (intended or inadvertent) how the J-values are calculated: thus it is very important when you perform these tests that the photolysis module that is as close a possible to that embedded within the CTM/CCM and not the original, standalone version that you used to derive your inline model.

EXPERIMENTS.

Part 1 is a basic test of all J-values for high sun (SZA = 15°) over the ocean (albedo = 0.10, Lambertian). **Part 1a: Clear sky** (only Rayleigh scattering) and no aerosols. **Part 1b: Pinatubo aerosol** in the stratosphere (layer 10). **Part 1c: Stratus cloud** (layer 2). The primary atmosphere (Table 1a) is specified in terms of pressure layers, mean temperature, and column O₃ in each layer. Please do not include absorption by NO₂ or other species in calculating optical depths. For 1b and 1c we recommend that you use the specified optical properties in Table 1c, interpolating across the 5 specified wavelengths.

414 **Part 2** tests the simulation of a spherical atmosphere and twilight conditions that are critical to the polar regions. Use the same
415 atmosphere as Part 1 without clouds or aerosols. Assume equinox (solar declination = 0°) and a latitude of 84°N. The surface SZA
416 (not including refraction) varies from 84° (noon) to 96° (midnight). Report all J-values at noon, midnight, and the 24-hour average
417 (integrating as you would in your CTM/CCM). With a spherical atmosphere, the local solar zenith angle changes with altitude and if
418 refraction is included it will change the surface angle. Please note how you treat the solar ray path in your model description.
419

420 **Part 3** tests the accuracy of wavelength binning in the critical region 290-400 nm that dominates tropospheric photolysis. Shut off all
421 Rayleigh scattering and surface reflection (albedo = 0) giving effectively a simple Beer's Law calculation. Repeat the calculation in
422 Part 1, but report only J-values for J-O3 (i.e., total), J-O3(1d) [$O_3 \Rightarrow O_2 + O(^1D)$], and J-NO2 [$NO_2 \Rightarrow NO + O$]. These are the two
423 critical J-values for the troposphere, and they both have unusual structures in absorption cross section and quantum yields. The
424 organizers will make these calculations using very high resolution (0.05 nm) cross sections and solar fluxes and for different options
425 (e.g., JPL-06 vs. IUPAC cross sections) to provide a benchmark. NOTE that we will only use results below 20 km (L=1:11) for this
426 comparison.
427

428 **DIAGNOSTICS.**

430
431 **Model Documentation** should include a brief outline of the methods and any references (limit: one page). Please include brief notes
432 on: how you treat sphericity and refraction, the Schumann-Runge bands (J-O₂ and J-NO), Rayleigh scattering, multiple scattering,
433 clouds and aerosols, seasonal changes in sun-earth distance, solar variability, and any specific parameterizations. Default cross
434 sections are JPL-2006, please note if you are using alternate.
435

436 **Report** all J-values and all standard model layers since this is a check on all modeled J-values, not just the radiative transfer solution.
437 See Appendix for data formatting. We are not specifying the day-of-the-year, so use solar fluxes for sun-earth distance = 1.0 au and
438 average over the 11-yr solar cycle if possible. UCI's high-resolution solar spectrum used in these experiments is the average of two
439 high and low SUSIM spectra (29 Mar 1992 and 11 Nov 1994), this is not meant to be the 11-yr average. It will be provided at 0.05
440 nm resolution, but we encourage you to use your own solar fluxes for the primary tests since changing solar fluxes will mostly likely
441 require a complete re-averaging of all cross-sections (see Fast-J paper, Wild, Zhu, Prather, 2000). Please report in model
442 documentation what you are using for the solar spectrum and how the solar cycle is represented in your submissions, and if possible
443 submit it as a separate file so that it may be used to address differences later. (With different wavelength binning, this will not be
444 trivial.) Reported photolysis rates should be calculated for the mass mid-point of each layer, this brings PhotoComp closer to current

445 CTM usage rather than the original grid-point formulation used in M&M. Results in the form of clearly labeled ascii text files should
446 be sent to the organizers (see web posting for specific details).

447

448

449 **DISCUSSION.**

450

451 Implementation into a particular model's code will up to the participant. For example, at UCI we have two models that we will use in
452 PhotoComp: a fast-JX model within the CTM that uses layers of uniform composition defined by mass (kg/m^2); and a stand-alone
453 photochemical box model that defines altitude (in cm) as the vertical grid and uses number densities for air and ozone. For the latter,
454 we have re-mapped the primary atmosphere (Table 1a) onto a grid-point structure (Table 1b) that has the same mid-layer properties as
455 the layer mean value and the same columns of O_2 and O_3 .

456 One question will be: What is the correct answer? In some cases we may be able to define a "best" answer based on obvious physics
457 or convergence of some of the more resolved models, but in others we may not. Thus in all of our proposed experiments we will
458 begin with a "standard model" result (not necessarily the best answer) from one of the models and then determine a best answer, if
459 possible, after analysis of the results.

460

461 One approach to defining the correct answer would be to merge observed radiation fields or photolysis rates (e.g., IPMMI, POLARIS,
462 see references below), but we feel this may be too difficult to match the exact observing conditions. One way to include the
463 knowledge gained by these field studies is to ensure participation from some of the models (e.g., NCAR-TUV, APL).

464

465 We do not recommend reporting detailed actinic fluxes as a function of wavelength since everyone selects different ways of
466 integrating over wavelength (e.g., bins) and trying to reconcile the different wavelength scales is not worthwhile. If major problems
467 show up, then a subgroup of models can consider how to resolve the differences.

468

469 Another major issue with photolysis and heating rates is the treatment of clouds and cloud fraction. This is very important, but
470 probably beyond the current PhotoComp. It would require a special workshop. We do include an option for a plane-parallel volcanic
471 aerosol layer (aka Pinatubo) and a stratiform cloud.

472

473 **APPENDIX**

474

Standard Atmosphere & Other Specifications

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Table 1a. PhotoComp 2008 standard atmosphere =====

L edge p(hPa) T O3(mass/mass) DU(**redundant)

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1	1000.0	299.9	3.844E-08	2.4532
2^^	866.0	289.5	4.704E-08	4.8514
3	649.4	278.8	4.720E-08	3.6498
4	487.0	267.2	4.972E-08	2.8831
5	365.2	253.9	5.551E-08	2.4140
6	273.8	239.7	5.977E-08	1.9491
7	205.4	224.6	6.390E-08	1.5627
8	154.0	209.4	9.012E-08	1.6527
9	115.5	198.2	1.486E-07	2.0441
10**	86.60	195.8	3.885E-07	4.0065
11	64.94	203.1	1.533E-06	11.8582
12	48.70	209.9	3.790E-06	21.9783
13	36.52	215.5	6.849E-06	29.7855
14	27.38	220.1	1.034E-05	33.7361
15	20.54	224.5	1.326E-05	32.4219
16	15.40	228.9	1.577E-05	28.9124
17	11.55	233.3	1.653E-05	22.7293
18	8.660	237.8	1.670E-05	17.2239
19	6.494	242.6	1.578E-05	12.2053
20	4.870	248.3	1.363E-05	7.9054
21	3.652	254.1	1.236E-05	5.3734
22	2.738	259.5	9.733E-06	3.1740
23	2.054	262.9	8.158E-06	1.9951
24	1.540	265.1	6.721E-06	1.2325
25	1.155	266.9	5.511E-06	0.7578
26	0.8660	264.7	4.810E-06	0.4960
27	0.6494	261.8	4.009E-06	0.3100
28	0.4870	259.7	3.325E-06	0.1928
29	0.3652	254.3	2.820E-06	0.1226
30	0.2738	247.0	2.323E-06	0.0758
31	0.2054	239.4	1.909E-06	0.0467
32	0.1540	234.4	1.585E-06	0.0291
33	0.1155	232.7	1.335E-06	0.0184
34	0.08660	226.4	1.102E-06	0.0114

513 35 0.06494 216.4 8.927E-07 0.0069
514 36 0.04870 210.8 7.372E-07 0.0043
515 37 0.03652 208.0 6.168E-07 0.0027
516 38 0.02738 205.2 5.162E-07 0.0017
517 39 0.02054 202.4 4.317E-07 0.0011
518 40 0.01540 199.4 3.607E-07 0.00066
519 41 0.01155 197.6 3.032E-07 0.00042
520 42 0.00866
521 above model top layer=41 @ 0.0866 hPa, assume uniform T & O3
522 42 0.00866 197.6 3.032E-07 0.00125
523 43 0.00000

524 =====
525 ^^ layer for stratiform cloud: OD (600 nm) = 20.0
526 ** layer for Pinatubo sulfate aerosol: OD(600 nm) = 1.00
527 see Table 1c.
528 =====

529
530
531 **Table 1b.** Standard atmosphere shown mapped into grid points
532 =====

L	alt(km)	air(#/cm ³)	O3(#/cm ³)	T(K)
533	1	2.416E+19	5.611E+11	299.9
534	2	1.877E+19	5.335E+11	289.5
535	3	1.462E+19	4.169E+11	278.8
536	4	1.144E+19	3.436E+11	267.2
537	5	9.025E+18	3.027E+11	253.9
538	6	7.169E+18	2.589E+11	239.7
539	7	5.737E+18	2.215E+11	224.6
540	8	4.615E+18	2.513E+11	209.4
541	9	3.656E+18	3.283E+11	198.2
542	10	2.775E+18	6.514E+11	195.8
543	11	2.006E+18	1.858E+12	203.1
544	12	1.456E+18	3.334E+12	209.9
545	13	1.063E+18	4.399E+12	215.5
546	14	7.807E+17	4.879E+12	220.1
547	15	5.740E+17	4.598E+12	224.5
548	16	4.222E+17	4.022E+12	228.9
549	17	3.106E+17	3.102E+12	233.3
550	18	2.285E+17	2.306E+12	237.8
551	19	1.680E+17	1.602E+12	242.6
552				

553	20	37.5	1.231E+17	1.014E+12	248.3
554	21	39.6	9.018E+16	6.732E+11	254.1
555	22	41.7	6.622E+16	3.894E+11	259.5
556	23	43.9	4.902E+16	2.416E+11	262.9
557	24	46.2	3.645E+16	1.480E+11	265.1
558	25	48.4	2.715E+16	9.039E+10	266.9
559	26	50.6	2.053E+16	5.966E+10	264.7
560	27	52.8	1.557E+16	3.771E+10	261.8
561	28	55.0	1.177E+16	2.364E+10	259.7
562	29	57.2	9.011E+15	1.535E+10	254.3
563	30	59.3	6.957E+15	9.766E+09	247.0
564	31	61.4	5.383E+15	6.210E+09	239.4
565	32	63.4	4.123E+15	3.949E+09	234.4
566	33	65.3	3.114E+15	2.512E+09	232.7
567	34	67.3	2.400E+15	1.597E+09	226.4
568	35	69.1	1.883E+15	1.016E+09	216.4
569	36	70.9	1.450E+15	6.458E+08	210.8
570	37	72.7	1.102E+15	4.107E+08	208.0
571	38	74.4	8.374E+14	2.612E+08	205.2
572	39	76.1	6.367E+14	1.661E+08	202.4
573	40	77.8	4.846E+14	1.056E+08	199.4
574	41	79.5	3.667E+14	6.717E+07	197.6

```

=====
576 above-top extend with 6.3-km scale-height for air & O3
577     columns:  air(#/cm^2)  O3(#/cm^2)
578             2.129E+25   6.985E+18
579 =====

```

Table 1c. Scattering properties of Pinatubo and stratus layers

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=====
585 Definitions:
586     W = wavelength (nm)
587
588     Q = scattering efficiency (average of cross-section / (pi * r**2) )
589         typically Q ~ 2 for large clouds and large aerosols
590         fn of aerosol size distrib N(r), index of refraction, wavelength.
591
592     K = extinction (m2/g), the cross-sectional area per gram of material

```

593 $K(m^2/g) = Q / [4/3 * Reff(micron) * Rho(g/cm^3)]$
594
595 Reff = effective radius (microns)
596 = Average[N(r) * r**3] / Average[N(r) * r**2]
597
598 Rho = density of particles (g/cm3)
599
600 n = index of refraction
601
602 OD = optical depth (column) = column mass (g/m2) * K (m2/g)
603
604 SSA = single scattering abledo
605
606 LG(1:8) = coefficients of Legendre expansion of scattering phase fn.
607 both polarizations are added. By definition SLEG(1) = 1.
608 Fast-JX uses these first 8 terms to define the scattering.
609
610 g = asymmetry factor = LG(2) / 3.
611
612
613 Pinatubo: OD = 1.0 in layer 10 (86.6 to 64.9 hPa)
614 =====
615 Stratospheric aerosol composed of 75%-wt H2SO4.
616 Rho = 1.630
617 n = 1.514 + 0.000i (200 nm)
618 1.473 + 0.000i (300 nm)
619 1.459 + 0.000i (400 nm)
620 1.448 + 0.000i (600 nm)
621 1.435 + 0.000i (999 nm)
622 Log-normal distribution with R0 = 0.08 micron & sigma = 0.800
623 **check that you are using the right log-normal by deriving Reff
624 Reff = 0.386 micron
625
626 K (600nm) = 2.610
627 OD (@600nm) = 1.00 ==> aerosol = 1.00/K = 0.3832 g/m2
628
629 W Q SSA LG(2) LG(3) LG(4) LG(5) LG(6) LG(7) LG(8)
630 200 2.5935 1.0000 2.092 2.914 2.880 3.295 3.185 3.430 3.379
631 300 2.6669 1.0000 2.121 2.861 2.792 2.936 2.733 2.703 2.568
632 400 2.5588 1.0000 2.144 2.813 2.711 2.695 2.425 2.257 2.069

```

633      600 2.1893 1.0000 2.149 2.713 2.547 2.362 2.018 1.740 1.499
634      999 1.4540 1.0000 2.118 2.537 2.277 1.951 1.555 1.229 0.972
635      (fast-JX v61 scatter #15)
636
637      Stratus: OD = 20.0 in layer 2 (866 to 649 hPa)
638      =====
639      Pure water cloud
640      Rho = 1.000
641      n = 1.335 + 0.000i (assumed 200-999 nm)
642      Deirmendjian Cumulus C1 (Gamma, n(r) = a r**alpha exp[-b r**gamma])
643      mode radius Rc = 4 microns, alpha=6, b=3/2, gamma = 1
644      Reff = 6.00 micron
645
646      K (600nm) = 0.2668
647      OD (@600nm) = 20.0 ==> aerosol = 20.0/K = 75.0 g/m2
648
649      W   Q   SSA LG(2) LG(3) LG(4) LG(5) LG(6) LG(7) LG(8)
650      200 2.0650 1.0000 2.610 3.998 4.771 5.450 6.196 6.829 7.721
651      300 2.0835 1.0000 2.596 3.973 4.725 5.406 6.129 6.751 7.607
652      400 2.1064 1.0000 2.571 3.936 4.660 5.345 6.056 6.670 7.492
653      600 2.1345 1.0000 2.557 3.902 4.596 5.263 5.923 6.507 7.267
654      999 2.1922 1.0000 2.499 3.799 4.418 5.081 5.667 6.213 6.851
655      (fast-JX v61 scatter #08)
656      =====
657
658
659      =====
660      Table 2. Standard diagnostics and file names
661      =====
662      Ascii tables will be fine given small data sets.
663      Report J-values at the mid-point of Layers 1 through 40.
664      File names: PC08_{model name + version if need be}_{PhotoPart#}
665      Write format: J-title, J-value(1:41) '(a8,1x,41e9.2)'
666
667      File Examples:
668      PC08_UCIref_doc.txt (or .pdf or .doc if need formatting)
669      UCI old reference code, documentation
670      PC08_UCI-JX_doc.txt
671      UCI version of fast-JX, documentation
672      PC08_UCIref_P1a.txt

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673 PC08_UCIref_P1b.txt
 674 PC08_UCIref_P1c.txt
 675 UCI-ref results for Part 1 clear, Pinatubo & stratus (see sample below)
 676 PC08_UCIref_P2n.txt
 677 PC08_UCIref_P2m.txt
 678 PC08_UCIref_P2a.txt
 679 UCI-ref results for Part 2 noon, midnight and average
 680 PC08_UCIref_P3.txt
 681 UCI-ref results for Part 3 (J-O3(1d) and J-NO2 only).
 682
 683 PC08_UCIref_P1.txt
 684 -----file: PC08_UCIref_P1a.txt -----
 685 PhotoComp2008: UCI pratmo P1a '(a8,1x,41e9.2)' ** note that UCIref does not calculate L=1(933) but at surface(1000)
 686 pressure 933.** 750. 562.0237 .0178 .0133 .0100
 687 J-NO 7.02E-31 6.85E-28 7.42E-25 4.71E-06 4.91E-06 5.10E-06 5.26E-06
 688 J-O2 1.16E-23 6.49E-22 4.67E-20 4.80E-09 5.57E-09 6.45E-09 7.51E-09
 689 J-O3 4.55E-04 5.09E-04 5.37E-04
 690 J-O3(1D) 4.84E-05 7.00E-05 8.02E-05
 691 J-H2COa 3.08E-05 4.43E-05 5.22E-05
 692
 693 J-Acet-b 4.26E-07 3.94E-07 2.79E-07

=====
Table 3. Standard J-value names.
 =====

700 Please use these abbreviations (if possible in the following order) so that J's can be sorted. For new J's please add with unique name. (available as PC08_J-
 701 labels.txt)

702 Note that for some J's, the branching ratios do not have different cross-sections associated with them and the branching ratios are fixed, hence we report only
 703 one J.

704 For many organics, the quantum yields are complex and have been incorporated into
 705 these J's. If you do not calculate one of these, please keep that row in your table with zero or blank values.

- =====
 707 1 J-NO NO =N+O
 708 2 J-O2 O2 =O+O
 709 3 J-O3 O3 =O+O2 (total = both O(3P) and O(1D))*
 710 4 J-O3(1d) O3 =O(1D)+O2
 711 5 J-H2COa H2COa =H+HCO
 712 6 J-H2COb H2COb =H2+CO

713 7 J-H2O2 H2O2 =OH+OH
714 8 J-CH3OOH CH3OOH =CH3O+OH
715 9 J-NO2 NO2 =NO+O
716 10 J-NO3 NO3 =NO+O2(11.4%) & NO2+O(88.6%)*
717 11 J-N2O5 N2O5 =NO2+NO3
718 12 J-HNO2 HONO =OH+NO
719 13 J-HNO3 HNO3 =OH+NO2
720 14 J-HNO4 HO2NO2 =OH+NO3
721 15 J-ClNO3a ClNO3a =Cl+NO3
722 16 J-ClNO3b ClNO3b =ClO+NO2
723 17 J-Cl2 Cl2 =Cl+Cl
724 18 J-HOCl HOCl =OH+Cl
725 19 J-OCIO OCIO =O+ClO
726 20 J-Cl2O2 Cl2O2 =Cl+Cl+O2
727 21 J-ClO ClO =Cl+O
728 22 J-BrO BrO =Br+O
729 23 J-BrNO3 BrNO3 =Br+NO3(29%) & BrO+NO2(71%)*
730 24 J-HOBr HOBr =OH+Br
731 25 J-BrCl BrCl =Br+Cl
732 26 J-N2O N2O =N2+O
733 27 J-CFCl3 CFCl3 =...
734 28 J-CF2Cl2 CF2Cl2 =...
735 29 J-F113 CF2ClCFCl2=...
736 30 J-F114 CF2ClCF2Cl=...
737 31 J-F115 CF3CF2Cl=...
738 32 J-CCl4 CCl4 =...
739 33 J-CH3Cl CH3Cl =CH3+Cl
740 34 J-MeCCl3 CH3CCl3=...
741 35 J-CH2Cl2 CH2Cl2 =...
742 36 J-CHF2Cl CHF2Cl =...
743 37 J-F123 CF3CHCl2=...
744 38 J-F141b CH3CFCl2=...
745 39 J-F142b CH3CF2Cl=...
746 40 J-CH3Br CH3Br =CH3+Br
747 41 J-H1211 CF2ClBr=...
748 42 J-H1301 CF3Br =...
749 43 J-H2402 C2F4Br2=...
750 44 J-CH2Br2 CH2Br2 =...
751 45 J-CHBr3 CHBr3 =...
752 46 J-CH3I CH3I =CH3+I

753 47 J-CF3I CF3I =CF3+I
 754 48 J-OCS OCS =CO+S
 755 49 J-PAN CH3C(O)O2NO2 =CH3C(O)O2+NO2(60%) & CH3C(O)O+NO3(40%)*
 756 50 J-CH3NO3 CH3ONO2=CH3O+NO2
 757 51 J-ActAld CH3CHO =CH3+HCO
 758 52 J-MeVK CH3C(O)CH=CH2 =C3H6+CO(60%) & CH2=CHCO+CH3(40%)*
 759 53 J-MeAcr CH2C(CH3)CHO =CH2=C(CH3)+HCO
 760 54 J-GlyAld HOCH2CHO =HOCH2+HCO
 761 55 J-MEKeto CH3COC2H5 =CH3+C2H5CO(15%) & C2H5+CH3CO(85%)*
 762 56 J-EAld C2H5CHO =C2H5+HCO
 763 57 J-MGlyxl CH3COCHO =CH3CO+HCO
 764 58 J-Glyxla (CHO)2 =HCO+HCO
 765 59 J-Glyxlb (CHO)2 =H2+CO+CO
 766 61 J-Acet-a C3H6O =CH3CO+CH3
 767 62 J-Acet-b C3H6O =CH3+CH3+CO

=====

* In preliminary comparisons, we have found it best to compare
 the total O3 photolysis rate and the rate leading to O(1D),
 skipping the O(3P) path. When branching paths with % are
 indicated in the table, they indicate the values derived for
 fast-JX, please just report the total J-value.