

# The Chemical Mechanism of MECCA1

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Table 1: Gas phase reactions

| #      | labels | reaction  | rate coefficient  | reference  |
|--------|--------|---|---|--|
| G1000  | StTrG  | $\text{O}_2 + \text{O}(^1\text{D}) \rightarrow \text{O}(^3\text{P}) + \text{O}_2$ | $3.2\text{E-}11*\text{EXP}(70./\text{temp})$  | Sander et al. (2003)                                     |
| G1001  | StTrG  | $\text{O}_2 + \text{O}(^3\text{P}) \rightarrow \text{O}_3$                        | $6.\text{E-}34*((\text{temp}/300.)**(-2.4))*\text{cair}$                                | Sander et al. (2003)                                     |
| G1002  | StG    | $\text{O}_3 + \text{O}(^1\text{D}) \rightarrow 2 \text{O}_2$                      | 1.2E-10   | Sander et al. (2003)*                                    |
| G1003  | StG    | $\text{O}_3 + \text{O}(^3\text{P}) \rightarrow 2 \text{O}_2$                      | $8.\text{E-}12*\text{EXP}(-2060./\text{temp})$  | Sander et al. (2003)                                     |
| G2100  | StTrG  | $\text{H} + \text{O}_2 \rightarrow \text{HO}_2$                                   | $\text{k\_3rd}(\text{temp}, \text{cair}, 5.7\text{E-}32, 1.6, 7.5\text{E-}11, 0., 0.6)$ | Sander et al. (2003)                                     |
| G2101  | StG    | $\text{H} + \text{O}_3 \rightarrow \text{OH}$                                     | $1.4\text{E-}10*\text{EXP}(-470./\text{temp})$  | Sander et al. (2003)                                     |
| G2102  | StG    | $\text{H}_2 + \text{O}(^1\text{D}) \rightarrow \text{H} + \text{OH}$              | 1.1E-10   | Sander et al. (2003)                                     |
| G2103  | StG    | $\text{OH} + \text{O}(^3\text{P}) \rightarrow \text{H}$                           | $2.2\text{E-}11*\text{EXP}(120./\text{temp})$   | Sander et al. (2003)                                     |
| G2104  | StTrG  | $\text{OH} + \text{O}_3 \rightarrow \text{HO}_2$                                  | $1.7\text{E-}12*\text{EXP}(-940./\text{temp})$  | Sander et al. (2003)                                     |
| G2105  | StTrG  | $\text{OH} + \text{H}_2 \rightarrow \text{H}_2\text{O} + \text{H}$                | $5.5\text{E-}12*\text{EXP}(-2000./\text{temp})$   | Sander et al. (2003)                                     |
| G2106  | StG    | $\text{HO}_2 + \text{O}(^3\text{P}) \rightarrow \text{OH}$                        | $3.\text{E-}11*\text{EXP}(200./\text{temp})$  | Sander et al. (2003)                                     |
| G2107  | StTrG  | $\text{HO}_2 + \text{O}_3 \rightarrow \text{OH}$                                  | $1.\text{E-}14*\text{EXP}(-490./\text{temp})$   | Sander et al. (2003)                                     |
| G2108a | StG    | $\text{HO}_2 + \text{H} \rightarrow 2 \text{OH}$                                  | $0.69*8.1\text{E-}11$   | Sander et al. (2003)*                                    |
| G2108b | StG    | $\text{HO}_2 + \text{H} \rightarrow \text{H}_2$                                   | $0.29*8.1\text{E-}11$   | Sander et al. (2003)*                                    |
| G2108c | StG    | $\text{HO}_2 + \text{H} \rightarrow \text{O}(^3\text{P}) + \text{H}_2\text{O}$    | $0.02*8.1\text{E-}11$   | Sander et al. (2003)*                                    |
| G2109  | StTrG  | $\text{HO}_2 + \text{OH} \rightarrow \text{H}_2\text{O}$                          | $4.8\text{E-}11*\text{EXP}(250./\text{temp})$   | Sander et al. (2003)                                     |
| G2110  | StTrG  | $\text{HO}_2 + \text{HO}_2 \rightarrow \text{H}_2\text{O}_2$                      | $\text{k\_H02\_H02}$  | Christensen et al. (2002),<br>Kircher and Sander (1984)* |
| G2111  | StTrG  | $\text{H}_2\text{O} + \text{O}(^1\text{D}) \rightarrow 2 \text{OH}$               | 2.2E-10   | Sander et al. (2003)                                     |
| G2112  | StTrG  | $\text{H}_2\text{O}_2 + \text{OH} \rightarrow \text{H}_2\text{O} + \text{HO}_2$   | $2.9\text{E-}12*\text{EXP}(-160./\text{temp})$  | Sander et al. (2003)                                     |
| G3100  | StGN   | $\text{N} + \text{O}_2 \rightarrow \text{NO} + \text{O}(^3\text{P})$              | $1.5\text{E-}11*\text{EXP}(-3600./\text{temp})$   | Sander et al. (2003)                                     |
| G3101  | StTrG  | $\text{N}_2 + \text{O}(^1\text{D}) \rightarrow \text{O}(^3\text{P}) + \text{N}_2$ | $1.8\text{E-}11*\text{EXP}(110./\text{temp})$   | Sander et al. (2003)                                     |
| G3102a | StGN   | $\text{N}_2\text{O} + \text{O}(^1\text{D}) \rightarrow 2 \text{NO}$               | 6.7E-11   | Sander et al. (2003)                                     |
| G3102b | StGN   | $\text{N}_2\text{O} + \text{O}(^1\text{D}) \rightarrow \text{N}_2 + \text{O}_2$   | 4.9E-11   | Sander et al. (2003)                                     |

Table 1: Gas phase reactions (... continued)

| #      | labels | reaction  | rate coefficient   | reference                 |
|--------|--------|---|--|---------------------------|
| G3103  | StTrGN | $\text{NO} + \text{O}_3 \rightarrow \text{NO}_2 + \text{O}_2$   | $3. \text{E} - 12 * \text{EXP}(-1500./\text{temp})$  | Sander et al. (2003)      |
| G3104  | StGN   | $\text{NO} + \text{N} \rightarrow \text{O}({}^3\text{P}) + \text{N}_2$  | $2.1 \text{E} - 11 * \text{EXP}(100./\text{temp})$   | Sander et al. (2003)      |
| G3105  | StGN   | $\text{NO}_2 + \text{O}({}^3\text{P}) \rightarrow \text{NO} + \text{O}_2$   | $5.6 \text{E} - 12 * \text{EXP}(180./\text{temp})$   | Sander et al. (2003)      |
| G3106  | StTrGN | $\text{NO}_2 + \text{O}_3 \rightarrow \text{NO}_3 + \text{O}_2$   | $1.2 \text{E} - 13 * \text{EXP}(-2450./\text{temp})$   | Sander et al. (2003)      |
| G3107  | StGN   | $\text{NO}_2 + \text{N} \rightarrow \text{N}_2\text{O} + \text{O}({}^3\text{P})$  | $5.8 \text{E} - 12 * \text{EXP}(220./\text{temp})$   | Sander et al. (2003)      |
| G3108  | StTrGN | $\text{NO}_3 + \text{NO} \rightarrow 2 \text{NO}_2$   | $1.5 \text{E} - 11 * \text{EXP}(170./\text{temp})$   | Sander et al. (2003)      |
| G3109  | StTrGN | $\text{NO}_3 + \text{NO}_2 \rightarrow \text{N}_2\text{O}_5$  | k_NO3_NO2  | Sander et al. (2003)*     |
| G3110  | StTrGN | $\text{N}_2\text{O}_5 \rightarrow \text{NO}_2 + \text{NO}_3$  | $\text{k\_NO3\_NO2}/(3. \text{E} - 27 * \text{EXP}(10990./\text{temp}))$                             | Sander et al. (2003)*     |
| G3200  | TrG    | $\text{NO} + \text{OH} \rightarrow \text{HONO}$   | $\text{k\_3rd}(\text{temp}, \text{cair}, 7. \text{E} - 31, 2.6, 3.6 \text{E} - 11, 0.1, 0.6)$        | Sander et al. (2003)      |
| G3201  | StTrGN | $\text{NO} + \text{HO}_2 \rightarrow \text{NO}_2 + \text{OH}$   | $3.5 \text{E} - 12 * \text{EXP}(250./\text{temp})$   | Sander et al. (2003)      |
| G3202  | StTrGN | $\text{NO}_2 + \text{OH} \rightarrow \text{HNO}_3$  | $\text{k\_3rd}(\text{temp}, \text{cair}, 2. \text{E} - 30, 3., 2.5 \text{E} - 11, 0., 0.6)$          | Sander et al. (2003)      |
| G3203  | StTrGN | $\text{NO}_2 + \text{HO}_2 \rightarrow \text{HNO}_4$  | k_NO2_HO2  | Sander et al. (2003)      |
| G3204  | TrGN   | $\text{NO}_3 + \text{HO}_2 \rightarrow \text{NO}_2 + \text{OH} + \text{O}_2$  | 3.5E-12  | Sander et al. (2003)      |
| G3205  | TrG    | $\text{HONO} + \text{OH} \rightarrow \text{NO}_2 + \text{H}_2\text{O}$  | $1.8 \text{E} - 11 * \text{EXP}(-390./\text{temp})$  | Sander et al. (2003)      |
| G3206  | StTrGN | $\text{HNO}_3 + \text{OH} \rightarrow \text{H}_2\text{O} + \text{NO}_3$   | k_HNO3_OH  | Sander et al. (2003)*     |
| G3207  | StTrGN | $\text{HNO}_4 \rightarrow \text{NO}_2 + \text{HO}_2$  | $\text{k\_NO2\_HO2}/(2.1 \text{E} - 27 * \text{EXP}(10900./\text{temp}))$                            | Sander et al. (2003)*     |
| G3208  | StTrGN | $\text{HNO}_4 + \text{OH} \rightarrow \text{NO}_2 + \text{H}_2\text{O}$   | $1.3 \text{E} - 12 * \text{EXP}(380./\text{temp})$   | Sander et al. (2003)      |
| G4100  | StG    | $\text{CH}_4 + \text{O}({}^1\text{D}) \rightarrow .75 \text{CH}_3\text{O}_2 + .75 \text{OH} + .25 \text{HCHO} + .4 \text{H} + .05 \text{H}_2$ | 1.5E-10  | Sander et al. (2003)      |
| G4101  | StTrG  | $\text{CH}_4 + \text{OH} \rightarrow \text{CH}_3\text{O}_2 + \text{H}_2\text{O}$  | $1.85 \text{E} - 20 * \text{EXP}(2.82 * \log(\text{temp}) - 987./\text{temp})$                       | Atkinson (2003)*          |
| G4102  | TrG    | $\text{CH}_3\text{OH} + \text{OH} \rightarrow \text{HCHO} + \text{HO}_2$  | $7.3 \text{E} - 12 * \text{EXP}(-620./\text{temp})$  | Sander et al. (2003)      |
| G4103a | StTrG  | $\text{CH}_3\text{O}_2 + \text{HO}_2 \rightarrow \text{CH}_3\text{OOH}$   | $4.1 \text{E} - 13 * \text{EXP}(750./\text{temp}) / (1. + 1./497.7 * \text{EXP}(1160./\text{temp}))$ | Sander et al. (2003)*     |
| G4103b | StTrG  | $\text{CH}_3\text{O}_2 + \text{HO}_2 \rightarrow \text{HCHO} + \text{H}_2\text{O} + \text{O}_2$   | $4.1 \text{E} - 13 * \text{EXP}(750./\text{temp}) / (1. + 497.7 * \text{EXP}(-1160./\text{temp}))$   | Sander et al. (2003)*     |
| G4104  | StTrGN | $\text{CH}_3\text{O}_2 + \text{NO} \rightarrow \text{HCHO} + \text{NO}_2 + \text{HO}_2$   | $2.8 \text{E} - 12 * \text{EXP}(300./\text{temp})$   | Sander et al. (2003)      |
| G4105  | TrGN   | $\text{CH}_3\text{O}_2 + \text{NO}_3 \rightarrow \text{HCHO} + \text{HO}_2 + \text{NO}_2$   | 1.3E-12  | Atkinson et al. (1999)    |
| G4106a | StTrG  | $\text{CH}_3\text{O}_2 + \text{CH}_3\text{O}_2 \rightarrow 2 \text{HCHO} + 2 \text{HO}_2$   | $9.5 \text{E} - 14 * \text{EXP}(390./\text{temp}) / (1. + 1./26.2 * \text{EXP}(1130./\text{temp}))$  | Sander et al. (2003)      |
| G4106b | StTrG  | $\text{CH}_3\text{O}_2 + \text{CH}_3\text{O}_2 \rightarrow \text{HCHO} + \text{CH}_3\text{OH}$  | $9.5 \text{E} - 14 * \text{EXP}(390./\text{temp}) / (1. + 26.2 * \text{EXP}(-1130./\text{temp}))$    | Sander et al. (2003)      |
| G4107  | StTrG  | $\text{CH}_3\text{OOH} + \text{OH} \rightarrow .7 \text{CH}_3\text{O}_2 + .3 \text{HCHO} + .3 \text{OH} + \text{H}_2\text{O}$                 | k_CH300H_OH  | Sander et al. (2003)*     |
| G4108  | StTrG  | $\text{HCHO} + \text{OH} \rightarrow \text{CO} + \text{H}_2\text{O} + \text{HO}_2$  | $9.52 \text{E} - 18 * \text{EXP}(2.03 * \log(\text{temp}) + 636./\text{temp})$                       | Sivakumaran et al. (2003) |

Table 1: Gas phase reactions (... continued)

| #      | labels | reaction  | rate coefficient   | reference   |
|--------|--------|---|--|---|
| G4109  | TrGN   | $\text{HCHO} + \text{NO}_3 \rightarrow \text{HNO}_3 + \text{CO} + \text{HO}_2$  | $3.4\text{E-}13 \cdot \text{EXP}(-1900./\text{temp})$  | Sander et al. (2003)*                                     |
| G4110  | StTrG  | $\text{CO} + \text{OH} \rightarrow \text{H} + \text{CO}_2$  | $1.57\text{E-}13 + \text{cair} \cdot 3.54\text{E-}33$  | McCabe et al. (2001)                                      |
| G4111  | TrG    | $\text{HCOOH} + \text{OH} \rightarrow \text{HO}_2$  | 4.E-13   | Sander et al. (2003)                                      |
| G4200  | TrGC   | $\text{C}_2\text{H}_6 + \text{OH} \rightarrow \text{C}_2\text{H}_5\text{O}_2 + \text{H}_2\text{O}$  | $1.49\text{E-}17 \cdot \text{temp} \cdot \text{temp} \cdot \text{EXP}(-499./\text{temp})$            | Atkinson (2003)   |
| G4203  | TrGC   | $\text{C}_2\text{H}_5\text{O}_2 + \text{HO}_2 \rightarrow \text{C}_2\text{H}_5\text{OOH}$   | $7.5\text{E-}13 \cdot \text{EXP}(700./\text{temp})$  | Sander et al. (2003)                                      |
| G4204  | TrGNC  | $\text{C}_2\text{H}_5\text{O}_2 + \text{NO} \rightarrow \text{CH}_3\text{CHO} + \text{HO}_2 + \text{NO}_2$  | $2.6\text{E-}12 \cdot \text{EXP}(365./\text{temp})$  | Sander et al. (2003)                                      |
| G4205  | TrGNC  | $\text{C}_2\text{H}_5\text{O}_2 + \text{NO}_3 \rightarrow \text{CH}_3\text{CHO} + \text{HO}_2 + \text{NO}_2$  | 2.3E-12  | Atkinson et al. (1999)                                    |
| G4206  | TrGC   | $\text{C}_2\text{H}_5\text{O}_2 + \text{CH}_3\text{O}_2 \rightarrow .75 \text{ HCHO} + \text{HO}_2 + .75 \text{ CH}_3\text{CHO}$<br>$+ .25 \text{ CH}_3\text{OH}$   | $1.6\text{E-}13 \cdot \text{EXP}(195./\text{temp})$  | see note  |
| G4207  | TrGC   | $\text{C}_2\text{H}_5\text{OOH} + \text{OH} \rightarrow .3 \text{ C}_2\text{H}_5\text{O}_2 + .7 \text{ CH}_3\text{CHO} + .7 \text{ OH}$   | k_CH300H_OH  | see note  |
| G4208  | TrGC   | $\text{CH}_3\text{CHO} + \text{OH} \rightarrow \text{CH}_3\text{C(O)OO} + \text{H}_2\text{O}$   | $5.6\text{E-}12 \cdot \text{EXP}(270./\text{temp})$  | Sander et al. (2003)                                      |
| G4209  | TrGNC  | $\text{CH}_3\text{CHO} + \text{NO}_3 \rightarrow \text{CH}_3\text{C(O)OO} + \text{HNO}_3$   | $1.4\text{E-}12 \cdot \text{EXP}(-1900./\text{temp})$  | Sander et al. (2003)                                      |
| G4210  | TrGC   | $\text{CH}_3\text{COOH} + \text{OH} \rightarrow \text{CH}_3\text{O}_2$  | $4.\text{E-}13 \cdot \text{EXP}(200./\text{temp})$   | Sander et al. (2003)                                      |
| G4211a | TrGC   | $\text{CH}_3\text{C(O)OO} + \text{HO}_2 \rightarrow \text{CH}_3\text{C(O)OOH}$  | $4.3\text{E-}13 \cdot \text{EXP}(1040./\text{temp}) / (1.+1./$<br>$37.\text{EXP}(660./\text{temp}))$ | Tyndall et al. (2001)                                     |
| G4211b | TrGC   | $\text{CH}_3\text{C(O)OO} + \text{HO}_2 \rightarrow \text{CH}_3\text{COOH} + \text{O}_3$  | $4.3\text{E-}13 \cdot \text{EXP}(1040./\text{temp}) / (1.+$<br>$37.\text{EXP}(-660./\text{temp}))$   | Tyndall et al. (2001)                                     |
| G4212  | TrGNC  | $\text{CH}_3\text{C(O)OO} + \text{NO} \rightarrow \text{CH}_3\text{O}_2 + \text{NO}_2$  | $8.1\text{E-}12 \cdot \text{EXP}(270./\text{temp})$  | Tyndall et al. (2001)                                     |
| G4213  | TrGNC  | $\text{CH}_3\text{C(O)OO} + \text{NO}_2 \rightarrow \text{PAN}$   | k_PA_NO2   | Tyndall et al. (2001)                                     |
| G4214  | TrGNC  | $\text{CH}_3\text{C(O)OO} + \text{NO}_3 \rightarrow \text{CH}_3\text{O}_2 + \text{NO}_2$  | 4.E-12   | Canosa-Mas et al. (1996)                                  |
| G4215a | TrGC   | $\text{CH}_3\text{C(O)OO} + \text{CH}_3\text{O}_2 \rightarrow \text{HCHO} + \text{HO}_2 + \text{CH}_3\text{O}_2 + \text{CO}_2$  | $0.9 \cdot 2.\text{E-}12 \cdot \text{EXP}(500./\text{temp})$   | Sander et al. (2003)                                      |
| G4215b | TrGC   | $\text{CH}_3\text{C(O)OO} + \text{CH}_3\text{O}_2 \rightarrow \text{CH}_3\text{COOH} + \text{HCHO} + \text{CO}_2$   | $0.1 \cdot 2.\text{E-}12 \cdot \text{EXP}(500./\text{temp})$   | Sander et al. (2003)                                      |
| G4216  | TrGC   | $\text{CH}_3\text{C(O)OO} + \text{C}_2\text{H}_5\text{O}_2 \rightarrow .82 \text{ CH}_3\text{O}_2 + \text{CH}_3\text{CHO} + .82$<br>$\text{HO}_2 + .18 \text{ CH}_3\text{COOH}$   | $4.9\text{E-}12 \cdot \text{EXP}(211./\text{temp})$  | Atkinson et al. (1999), Kirchner<br>and Stockwell (1996)* |
| G4217  | TrGC   | $\text{CH}_3\text{C(O)OO} + \text{CH}_3\text{C(O)OO} \rightarrow 2 \text{ CH}_3\text{O}_2 + 2 \text{ CO}_2 + \text{O}_2$  | $2.5\text{E-}12 \cdot \text{EXP}(500./\text{temp})$  | Tyndall et al. (2001)                                     |
| G4218  | TrGC   | $\text{CH}_3\text{C(O)OOH} + \text{OH} \rightarrow \text{CH}_3\text{C(O)OO}$  | k_CH300H_OH  | see note  |
| G4220  | TrGNC  | $\text{PAN} + \text{OH} \rightarrow \text{HCHO} + \text{NO}_2$  | 2.E-14   | see note  |
| G4221  | TrGNC  | $\text{PAN} \rightarrow \text{CH}_3\text{C(O)OO} + \text{NO}_2$   | k_PAN_M  | Sander et al. (2003)*                                     |
| G4301a | TrGC   | $\text{C}_3\text{H}_6 + \text{O}_3 \rightarrow .57 \text{ HCHO} + .47 \text{ CH}_3\text{CHO} + .33 \text{ OH} + .26$<br>$\text{HO}_2 + .07 \text{ CH}_3\text{O}_2 + .06 \text{ C}_2\text{H}_5\text{O}_2 + .23 \text{ CH}_3\text{C(O)OO} +$<br>$.06 \text{ CH}_4 + .31 \text{ CO} + .22 \text{ HCOOH} + .03 \text{ CH}_3\text{OH}$ | $6.5\text{E-}15 \cdot \text{EXP}(-1900./\text{temp})$  | Sander et al. (2003)*                                     |
| G4302a | TrGC   | $\text{C}_3\text{H}_6 + \text{OH} \rightarrow .98 \text{ CH}_3\text{CHO} + .98 \text{ HCHO}$  | k_3rd(temp, cair, 8.E-27, 3.5, 3.E-11, 0.,<br>0.5)   | Atkinson et al. (1999)                                    |
| G4311  | TrGC   | $\text{CH}_3\text{COCH}_3 + \text{OH} \rightarrow \text{CH}_3\text{COCH}_2\text{O}_2 + \text{H}_2\text{O}$  | $1.33\text{E-}13 + 3.82\text{E-}11 \cdot \text{EXP}(-2000./\text{temp})$                             | Sander et al. (2003)                                      |
| G4312a | TrGC   | $\text{CH}_3\text{COCH}_2\text{O}_2 + \text{HO}_2 \rightarrow \text{CH}_3\text{C(O)OO}$   | $8.6\text{E-}13 \cdot \text{EXP}(700./\text{temp})$  | Tyndall et al. (2001)                                     |

Table 1: Gas phase reactions (... continued)

| #      | labels   | reaction  | rate coefficient  | reference              |
|--------|----------|---|---|------------------------|
| G4313  | TrGNC    | $\text{CH}_3\text{COCH}_2\text{O}_2 + \text{NO} \rightarrow \text{NO}_2 + \text{CH}_3\text{C}(\text{O})\text{OO} + \text{HCHO}$   | $2.9\text{E-}12*\text{EXP}(300./\text{temp})$   | Sander et al. (2003)   |
| G4314a | TrGC     | $\text{CH}_3\text{COCH}_2\text{O}_2 + \text{CH}_3\text{O}_2 \rightarrow .5 \text{CH}_3\text{OH} + \text{CH}_3\text{C}(\text{O})\text{OO} + .8 \text{HCHO} + .3 \text{HO}_2$ | $7.5\text{E-}13*\text{EXP}(500./\text{temp})$   | Tyndall et al. (2001)  |
| G4400a | TrGC     | $\text{C}_4\text{H}_{10} + \text{OH} \rightarrow 0.8 \text{CH}_3\text{C}(\text{O})\text{OO} + .85 \text{CH}_3\text{CHO} + .1 \text{HCHO}$                                   | $1.81\text{E-}17*\text{temp}*\text{temp}*\text{EXP}(114./\text{temp})$                    | Atkinson (2003)        |
| G6100  | StTrGCl  | $\text{Cl} + \text{O}_3 \rightarrow \text{ClO}$   | $2.3\text{E-}11*\text{EXP}(-200./\text{temp})$  | Sander et al. (2003)   |
| G6101  | StGCl    | $\text{ClO} + \text{O}(^3\text{P}) \rightarrow \text{Cl}$   | $3.\text{E-}11*\text{EXP}(70./\text{temp})$   | Sander et al. (2003)   |
| G6102  | StTrGCl  | $\text{ClO} + \text{ClO} \rightarrow \text{Cl}_2\text{O}_2$   | k_C10_C10   | Atkinson et al. (2005) |
| G6103  | StTrGCl  | $\text{Cl}_2\text{O}_2 \rightarrow \text{ClO} + \text{ClO}$   | $k_{\text{ClO}_2}/(1.27\text{E-}27*\text{EXP}(8744./\text{temp}))$                        | Sander et al. (2003)*  |
| G6200  | StGCl    | $\text{Cl} + \text{H}_2 \rightarrow \text{HCl} + \text{H}$  | $3.7\text{E-}11*\text{EXP}(-2300./\text{temp})$   | Sander et al. (2003)   |
| G6201a | StGCl    | $\text{Cl} + \text{HO}_2 \rightarrow \text{HCl}$  | $1.8\text{E-}11*\text{EXP}(170./\text{temp})$   | Sander et al. (2003)   |
| G6201b | StGCl    | $\text{Cl} + \text{HO}_2 \rightarrow \text{ClO} + \text{OH}$  | $4.1\text{E-}11*\text{EXP}(-450./\text{temp})$  | Sander et al. (2003)   |
| G6202  | StTrGCl  | $\text{Cl} + \text{H}_2\text{O}_2 \rightarrow \text{HCl} + \text{HO}_2$   | $1.1\text{E-}11*\text{EXP}(-980./\text{temp})$  | Sander et al. (2003)   |
| G6203a | StGCl    | $\text{ClO} + \text{OH} \rightarrow \text{Cl} + \text{HO}_2$  | $7.4\text{E-}12*\text{EXP}(270./\text{temp})$   | Sander et al. (2003)   |
| G6203b | StGCl    | $\text{ClO} + \text{OH} \rightarrow \text{HCl}$   | $6.\text{E-}13*\text{EXP}(230./\text{temp})$  | Sander et al. (2003)   |
| G6204  | StTrGCl  | $\text{ClO} + \text{HO}_2 \rightarrow \text{HOCl}$  | $2.7\text{E-}12*\text{EXP}(220./\text{temp})$   | Sander et al. (2003)   |
| G6205  | StTrGCl  | $\text{HCl} + \text{OH} \rightarrow \text{Cl} + \text{H}_2\text{O}$   | $2.6\text{E-}12*\text{EXP}(-350./\text{temp})$  | Sander et al. (2003)   |
| G6206  | StGCl    | $\text{HOCl} + \text{OH} \rightarrow \text{ClO} + \text{H}_2\text{O}$   | $3.\text{E-}12*\text{EXP}(-500./\text{temp})$   | Sander et al. (2003)   |
| G6300  | StTrGNCl | $\text{ClO} + \text{NO} \rightarrow \text{NO}_2 + \text{Cl}$  | $6.4\text{E-}12*\text{EXP}(290./\text{temp})$   | Sander et al. (2003)   |
| G6301  | StTrGNCl | $\text{ClO} + \text{NO}_2 \rightarrow \text{ClNO}_3$  | $k_{\text{3rd}}(\text{temp}, \text{cair}, 1.8\text{E-}31, 3.4, 1.5\text{E-}11, 1.9, 0.6)$ | Sander et al. (2003)   |
| G6303  | StGNCl   | $\text{ClNO}_3 + \text{O}(^3\text{P}) \rightarrow \text{ClO} + \text{NO}_3$   | $2.9\text{E-}12*\text{EXP}(-800./\text{temp})$  | Sander et al. (2003)   |
| G6304  | StTrGNCl | $\text{ClNO}_3 + \text{Cl} \rightarrow \text{Cl}_2 + \text{NO}_3$   | $6.5\text{E-}12*\text{EXP}(135./\text{temp})$   | Sander et al. (2003)   |
| G6400  | StTrGCl  | $\text{Cl} + \text{CH}_4 \rightarrow \text{HCl} + \text{CH}_3\text{O}_2$  | $9.6\text{E-}12*\text{EXP}(-1360./\text{temp})$   | Sander et al. (2003)   |
| G6401  | StTrGCl  | $\text{Cl} + \text{HCHO} \rightarrow \text{HCl} + \text{CO} + \text{HO}_2$  | $8.1\text{E-}11*\text{EXP}(-30./\text{temp})$   | Sander et al. (2003)   |
| G6402  | StTrGCl  | $\text{Cl} + \text{CH}_3\text{OOH} \rightarrow \text{CH}_3\text{O}_2 + \text{HCl}$  | $5.7\text{E-}11$  | Sander et al. (2003)   |
| G6403  | StTrGCl  | $\text{ClO} + \text{CH}_3\text{O}_2 \rightarrow \text{HO}_2 + \text{Cl} + \text{HCHO}$  | $3.3\text{E-}12*\text{EXP}(-115./\text{temp})$  | Sander et al. (2003)   |
| G6404  | StGCl    | $\text{CCl}_4 + \text{O}(^1\text{D}) \rightarrow \text{ClO} + 3 \text{Cl}$  | $3.3\text{E-}10$  | Sander et al. (2003)   |
| G6405  | StGCl    | $\text{CH}_3\text{Cl} + \text{O}(^1\text{D}) \rightarrow \text{OH} + \text{Cl}$   | $1.65\text{E-}10$   | Sander et al. (2003)*  |
| G6406  | StGCl    | $\text{CH}_3\text{Cl} + \text{OH} \rightarrow \text{H}_2\text{O} + \text{Cl}$   | $2.4\text{E-}12*\text{EXP}(-1250./\text{temp})$   | Sander et al. (2003)   |
| G6407  | StGCCl   | $\text{CH}_3\text{CCl}_3 + \text{O}(^1\text{D}) \rightarrow \text{OH} + 3 \text{Cl}$  | $3.\text{E-}10$   | Sander et al. (2003)*  |
| G6408  | StTrGCCl | $\text{CH}_3\text{CCl}_3 + \text{OH} \rightarrow \text{H}_2\text{O} + 3 \text{Cl}$  | $1.6\text{E-}12*\text{EXP}(-1520./\text{temp})$   | Sander et al. (2003)   |
| G6500  | StGFCl   | $\text{CF}_2\text{Cl}_2 + \text{O}(^1\text{D}) \rightarrow \text{ClO} + \text{Cl}$  | $1.4\text{E-}10$  | Sander et al. (2003)   |
| G6501  | StGFCl   | $\text{CFCl}_3 + \text{O}(^1\text{D}) \rightarrow \text{ClO} + 2 \text{Cl}$   | $2.3\text{E-}10$  | Sander et al. (2003)   |
| G7100  | StTrGBr  | $\text{Br} + \text{O}_3 \rightarrow \text{BrO}$   | $1.7\text{E-}11*\text{EXP}(-800./\text{temp})$  | Sander et al. (2003)   |

Table 1: Gas phase reactions (... continued)

| #      | labels    | reaction   | rate coefficient                                 | reference               |
|--------|-----------|--|--|-------------------------|
| G7101  | StGBr     | $\text{BrO} + \text{O}(^3\text{P}) \rightarrow \text{Br} + \text{O}_2$   | $1.9\text{E-}11*\text{EXP}(230./\text{temp})$    | Sander et al. (2003)    |
| G7200  | StTrGBr   | $\text{Br} + \text{HO}_2 \rightarrow \text{HBr}$   | $1.5\text{E-}11*\text{EXP}(-600./\text{temp})$   | Sander et al. (2003)    |
| G7201  | StTrGBr   | $\text{BrO} + \text{HO}_2 \rightarrow \text{HOBr}$   | $3.4\text{E-}12*\text{EXP}(540./\text{temp})$    | Sander et al. (2003)    |
| G7202  | StTrGBr   | $\text{HBr} + \text{OH} \rightarrow \text{Br} + \text{H}_2\text{O}$  | 1.1E-11  | Sander et al. (2003)    |
| G7203  | StGBr     | $\text{HOBr} + \text{O}(^3\text{P}) \rightarrow \text{OH} + \text{BrO}$  | $1.2\text{E-}10*\text{EXP}(-430./\text{temp})$   | Sander et al. (2003)    |
| G7301  | StTrGNBr  | $\text{BrO} + \text{NO} \rightarrow \text{Br} + \text{NO}_2$   | $8.8\text{E-}12*\text{EXP}(260./\text{temp})$    | Sander et al. (2003)    |
| G7302  | StTrGNBr  | $\text{BrO} + \text{NO}_2 \rightarrow \text{BrNO}_3$   | k_BrO_NO2  | Sander et al. (2003)*   |
| G7400  | StTrGBr   | $\text{Br} + \text{HCHO} \rightarrow \text{HBr} + \text{CO} + \text{HO}_2$   | $1.7\text{E-}11*\text{EXP}(-800./\text{temp})$   | Sander et al. (2003)    |
| G7403  | StTrGBr   | $\text{CH}_3\text{Br} + \text{OH} \rightarrow \text{H}_2\text{O} + \text{Br}$  | $2.35\text{E-}12*\text{EXP}(-1300./\text{temp})$ | Sander et al. (2003)    |
| G7603a | StTrGClBr | $\text{BrO} + \text{ClO} \rightarrow \text{Br} + \text{OClO}$  | $9.5\text{E-}13*\text{EXP}(550./\text{temp})$    | Sander et al. (2003)    |
| G7603b | StTrGClBr | $\text{BrO} + \text{ClO} \rightarrow \text{Br} + \text{Cl}$  | $2.3\text{E-}12*\text{EXP}(260./\text{temp})$    | Sander et al. (2003)    |
| G7603c | StTrGClBr | $\text{BrO} + \text{ClO} \rightarrow \text{BrCl}$  | $4.1\text{E-}13*\text{EXP}(290./\text{temp})$    | Sander et al. (2003)    |
| G9200  | TrStGS    | $\text{SO}_2 + \text{OH} \rightarrow \text{H}_2\text{SO}_4 + \text{HO}_2$  | k_3rd(temp, cair, 3.E-31, 3.3, 1.5E-12, 0., 0.6) | Sander et al. (2003)    |
| G9400a | TrGS      | $\text{DMS} + \text{OH} \rightarrow \text{CH}_3\text{SO}_2 + \text{HCHO}$  | $1.13\text{E-}11*\text{EXP}(-253./\text{temp})$  | Atkinson et al. (2003)* |
| G9400b | TrGS      | $\text{DMS} + \text{OH} \rightarrow \text{DMSO} + \text{HO}_2$   | k_DMS_OH   | Atkinson et al. (2003)* |
| G9401  | TrGNS     | $\text{DMS} + \text{NO}_3 \rightarrow \text{CH}_3\text{SO}_2 + \text{HNO}_3 + \text{HCHO}$   | $1.9\text{E-}13*\text{EXP}(520./\text{temp})$    | Atkinson et al. (2003)  |
| G9402  | TrGS      | $\text{DMSO} + \text{OH} \rightarrow .6 \text{SO}_2 + \text{HCHO} + .6 \text{CH}_3\text{O}_2 + .4 \text{HO}_2 + .4 \text{CH}_3\text{SO}_3\text{H}$ | 1.E-10   | Hynes and Wine (1996)   |
| G9403  | TrGS      | $\text{CH}_3\text{SO}_2 \rightarrow \text{SO}_2 + \text{CH}_3\text{O}_2$   | $1.9\text{E}13*\text{EXP}(-8661./\text{temp})$   | Barone et al. (1995)    |
| G9404  | TrGS      | $\text{CH}_3\text{SO}_2 + \text{O}_3 \rightarrow \text{CH}_3\text{SO}_3$   | 3.E-13   | Barone et al. (1995)    |
| G9405  | TrGS      | $\text{CH}_3\text{SO}_3 + \text{HO}_2 \rightarrow \text{CH}_3\text{SO}_3\text{H}$  | 5.E-11   | Barone et al. (1995)    |

\*Notes:

Rate coefficients for three-body reactions are defined via the function  $\text{k\_3rd}(T, M, k_0^{300}, n, k_{\text{inf}}^{300}, m, f_c)$ . In the code, the temperature  $T$  is called `temp` and the concentration of “air molecules”  $M$  is called `cair`. Using the auxiliary variables  $k_0(T)$ ,  $k_{\text{inf}}(T)$ , and  $k_{\text{ratio}}$ ,  $\text{k\_3rd}$  is defined as:

$$k_0(T) = k_0^{300} \times \left(\frac{300\text{K}}{T}\right)^n \quad (1)$$

$$k_{\text{inf}}(T) = k_{\text{inf}}^{300} \times \left(\frac{300\text{K}}{T}\right)^m \quad (2)$$

$$k_{\text{ratio}} = \frac{k_0(T)M}{k_{\text{inf}}(T)} \quad (3)$$

$$\text{k\_3rd} = \frac{k_0(T)M}{1 + k_{\text{ratio}}} \times f_c \left( \frac{1}{1 + (\log_{10}(k_{\text{ratio}}))^2} \right) \quad (4)$$

A similar function, called  $\text{k\_3rd\_iupac}$  here, is used by Atkinson et al. (2005) for three-body reactions. It has the same function parameters as  $\text{k\_3rd}$  and it is defined as:

$$k_0(T) = k_0^{300} \times \left(\frac{300\text{K}}{T}\right)^n \quad (5)$$

$$k_{\text{inf}}(T) = k_{\text{inf}}^{300} \times \left(\frac{300\text{K}}{T}\right)^m \quad (6)$$

$$k_{\text{ratio}} = \frac{k_0(T)M}{k_{\text{inf}}(T)} \quad (7)$$

$$N = 0.75 - 1.27 \times \log_{10}(f_c) \quad (8)$$

$$\text{k\_3rd\_iupac} = \frac{k_0(T)M}{1 + k_{\text{ratio}}} \times f_c \left( \frac{1}{1 + (\log_{10}(k_{\text{ratio}})/N)^2} \right) \quad (9)$$

G1002: path leading to  $2 \text{O}(^3\text{P}) + \text{O}_2$  neglectedG01Diag: `k_03s` =  $(1.7\text{E-}12*\text{EXP}(-940./$

temp)) \* C(KPP\_OH) + (1.E-14\*EXP(-490./temp)) \* C(KPP\_H02) + J\_01D \* 2.2E-10 \* C(KPP\_H2O) / ( 3.2E-11\*EXP(70./temp)\*C(KPP\_O2) + 1.8E-11\*EXP(110./temp)\*C(KPP\_N2) + 2.2E-10\*EXP(1000./temp)\*C(KPP\_H2O) )

G2108: branching ratio from Hack et al., see note B5 of Sander et al. (2003)

G2110: The rate coefficient is:  $k_{H02_H02} = (1.5E-12*EXP(19./temp)+1.7E-33*EXP(1000./temp)*c_{air}) * (1.+1.4E-21*EXP(2200./temp)*C(KPP_H2O))$ . The value for the first (pressure-independent) part is from Christensen et al. (2002), the water term from Kircher and Sander (1984)

G3109: The rate coefficient is:  $k_{N03_N02} = k_{3rd}(temp, c_{air}, 2.E-30, 4.4, 1.4E-12, 0.7, 0.6)$ .

G3110: The rate coefficient is defined as backward reaction divided by equilibrium constant.

G3203: The rate coefficient is:  $k_{N02_H02} = k_{3rd}(temp, c_{air}, 1.8E-31, 3.2, 4.7E-12, 1.4, 0.6)$ .

G3206: The rate coefficient is:  $k_{HN03_OH} = 2.4E-14 * EXP(460./temp) + 1./ ( 1./ (6.5E-34 * EXP(1335./temp)*c_{air}) + 1./ (2.7E-17 * EXP(2199./temp)) )$

G3207: The rate coefficient is defined as backward reaction divided by equilibrium constant.

G4103: product distribution is from Elrod et al. (2001)

G4107: The rate coefficient is:  $k_{CH300H_OH} = 3.8E-12*EXP(200./temp)$

G4109: same temperature dependence assumed as for CH<sub>3</sub>CHO+NO<sub>3</sub>

G4201: product distribution is from von Kuhlmann (2001) (see also Neeb et al. (1998))

G4206: Rate coefficient calculated by von Kuhlmann (pers. comm. 2004) using self reactions of CH<sub>3</sub>OO and C<sub>2</sub>H<sub>5</sub>OO from Sander et al. (2003) and geometric mean as suggested by Madronich and Calvert (1990) and Kirchner and Stockwell (1996). The product distribution branching=0.5/0.25/0.25) is calculated by von Kuhlmann (pers. comm. 2004) based on Villenave and Lesclaux (1996) and Tyndall et al. (2001).

G4207: same value as for G4107: CH<sub>3</sub>OOH+OH assumed

G4213: The rate coefficient is:  $k_{PA_N02} = k_{3rd}(temp, c_{air}, 8.5E-29, 6.5, 1.1E-11, 1., 0.6)$ .

G4216: 1.0E-11 from Atkinson et al. (1999), temperature dependence from Kirchner and Stockwell (1996)

G4218: same value as for G4107: CH<sub>3</sub>OOH+OH assumed

G4219: according to Pöschl et al. (2000), the same value as for CH<sub>3</sub>CHO+OH can be assumed

G4220: 50% of the upper limit given by Sander et al. (2003), as suggested by von Kuhlmann (2001)

G4221: The rate coefficient is:  $k_{PAN_M} = k_{PA_N02}/9.E-29*EXP(-14000./temp)$ , i.e. the rate coefficient is defined as backward reaction divided by equilibrium constant.

G4301: product distribution is for terminal olefin carbons from Zaveri and Peters (1999)

G4304: The rate coefficient is:  $k_{Pr02_H02} = 1.9E-13*EXP(1300./temp)$ . Value for generic RO<sub>2</sub> + HO<sub>2</sub> reaction from Atkinson (1997) is used.

G4305: The rate coefficient is:  $k_{Pr02_N0} = 2.7E-12*EXP(360./temp)$

G4306: The rate coefficient is:  $k_{Pr02_CH302} = 9.46E-14*EXP(431./temp)$ . The product distribution is from von Kuhlmann (2001).

G4307: same value as for G4107: CH<sub>3</sub>OOH+OH assumed

G4309: products are from von Kuhlmann (2001)

G4315: same value as for G4107: CH<sub>3</sub>OOH+OH assumed

G4319: same value as for PAN assumed

G4401: same value as for propyl group assumed ( $k_{Pr02_CH302}$ )

G4402: same value as for propyl group assumed ( $k_{Pr02_H02}$ )

G4403: same value as for propyl group assumed ( $k_{Pr02_N0}$ )

G4404: same value as for G4107: CH<sub>3</sub>OOH+OH assumed

G4409: The factor 0.25 was recommended by Uli Poeschl (pers. comm. 2004).

G4414: same value as for propyl group assumed ( $k_{Pr02_H02}$ )

G4415: same value as for propyl group assumed ( $k_{Pr02_N0}$ )

G4416: same value as for G4107: CH<sub>3</sub>OOH+OH assumed

G4417: value for C<sub>4</sub>H<sub>9</sub>ONO<sub>2</sub> used here

G4503: same temperature dependence assumed as for other RO<sub>2</sub>+HO<sub>2</sub> reactions

G4504: Yield of 12 % RONO<sub>2</sub> assumed as suggested in Table 2 of Sprengnether et al. (2002).

G6102: The rate coefficient is:  $k_{C10_C10} = k_{3rd\_iupac}(temp, c_{air}, 2.E-32, 4., 1.E-11, 0., 0.45)$ .

G6103: The rate coefficient is defined as backward reaction divided by equilibrium constant.

G6204: At low temperatures, there may be a minor reaction channel leading to O<sub>3</sub>+HCl. See Finkbeiner et al. (1995) for details. It is neglected here.

G6405: average of reactions with CH<sub>3</sub>Br and CH<sub>3</sub>F (B. Steil, pers. comm., see also note A15 in Sander et al. (2003)).

G6407: extrapolated from reactions with  $\text{CH}_3\text{CF}_3$ ,  $\text{CH}_3\text{CClF}_2$ , and  $\text{CH}_3\text{CCl}_2\text{F}$  (B. Steil, pers. comm., see also note A15 in Sander et al. (2003)).

G7302: The rate coefficient is:  $k_{\text{BrO}_2} = k_{\text{3rd}}(\text{temp}, \text{cair}, 5.2\text{E-}31, 3.2, 6.9\text{E-}12, 2.9, 0.6)$ .

G7303: The rate coefficient is defined as backward reaction (Sander et al., 2003) divided by equilibrium constant (Orlando and Tyndall, 1996).

G8101: This value was assumed by Jimenez et al. (2003).

G8102: The product as well as the reaction were assumed by von Glasow et al. (2002). An alternative pathway is the formation of new particles. This reaction needs to be updated when laboratory measurements become available.

G8103: product distribution is from Bloss et al. (2001)

G8203: assumed (J. Crowley, pers. comm. 2004)

G8300: The rate coefficient is:  $k_{\text{I}_2} = k_{\text{3rd}}(\text{temp}, \text{cair}, 3.0\text{E-}31, 1., 6.6\text{E-}11, 0., 0.6)$ .

G8304: J. Moldanova and J. Plane, pers. comm.

G8305: The rate coefficient is defined as backward reaction (Sander et al., 2003) divided by equilibrium constant (van den Bergh and Troe, 1976).

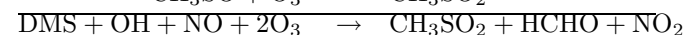
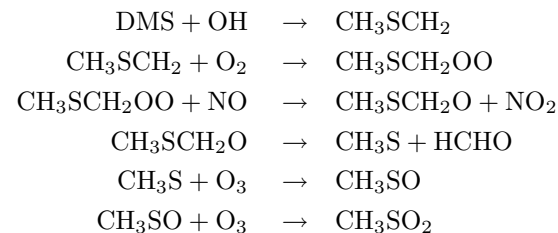
G8306: Note that in an earlier study by Jenkin et al. (1985), a value of  $5\text{E-}3 \text{ s}^{-1}$  was assumed.

G8600: Turnipseed et al. (1997) found a branching ratio of 14% for the sum of channels which do not produce I atoms. We assume that OIO and Cl are produced in this case.

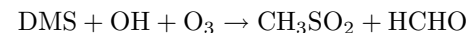
G8701: Gilles et al. (1997) found an upper limit of 35% for I atom production. We assume 35% I and 65% OIO as products. See also Rowley et al. (2001) for info about products.

G9400a: Abstraction path. The assumed reaction sequence (omitting  $\text{H}_2\text{O}$  and  $\text{O}_2$  as products) according

to Yin et al. (1990) is:



Neglecting the effect on  $\text{O}_3$  and  $\text{NO}_x$ , the remaining reaction is:



G9400b: Addition path. The rate coefficient is:  $k_{\text{DMS-OH}} = 1.0\text{E-}39 * \text{EXP}(5820./\text{temp}) * \text{C}(\text{KPP}_02) / (1. + 5.0\text{E-}30 * \text{EXP}(6280./\text{temp}) * \text{C}(\text{KPP}_02))$ .

Table 2: Photolysis reactions

| #      | labels    | reaction   | rate coefficient | reference |
|--------|-----------|--|------------------|-----------|
| J1000  | StTrGJ    | $O_2 + h\nu \rightarrow O(^3P) + O(^3P)$                               | JX(ip_02)        | see note  |
| J1001a | StTrGJ    | $O_3 + h\nu \rightarrow O(^1D)$  | JX(ip_01D)       | see note  |
| J1001b | StTrGJ    | $O_3 + h\nu \rightarrow O(^3P)$  | JX(ip_03P)       | see note  |
| J2100  | StGJ      | $H_2O + h\nu \rightarrow H + OH$                                       | JX(ip_H2O)       | see note  |
| J2101  | StTrGJ    | $H_2O_2 + h\nu \rightarrow 2 OH$                                       | JX(ip_H2O2)      | see note  |
| J3100  | StGNJ     | $N_2O + h\nu \rightarrow O(^1D)$                                       | JX(ip_N2O)       | see note  |
| J3101  | StTrGNJ   | $NO_2 + h\nu \rightarrow NO + O(^3P)$                                  | JX(ip_NO2)       | see note  |
| J3102  | StGNJ     | $NO + h\nu \rightarrow N + O(^3P)$                                     | JX(ip_NO)        | see note  |
| J3103a | StTrGNJ   | $NO_3 + h\nu \rightarrow NO_2 + O(^3P)$                                | JX(ip_NO2O)      | see note  |
| J3103b | StTrGNJ   | $NO_3 + h\nu \rightarrow NO$   | JX(ip_NOO2)      | see note  |
| J3104a | StTrGNJ   | $N_2O_5 + h\nu \rightarrow NO_2 + NO_3$                                | JX(ip_N2O5)      | see note  |
| J3104b | StGNJ     | $N_2O_5 + h\nu \rightarrow NO + O(^3P) + NO_3$                         | JX(ip_NO3NOO)    | see note  |
| J3200  | TrGJ      | $HONO + h\nu \rightarrow NO + OH$                                      | JX(ip_HONO)      | see note  |
| J3201  | StTrGNJ   | $HNO_3 + h\nu \rightarrow NO_2 + OH$                                   | JX(ip_HNO3)      | see note  |
| J3202  | StTrGNJ   | $HNO_4 + h\nu \rightarrow .667 NO_2 + .667 HO_2 + .333 NO_3 + .333 OH$ | JX(ip_HNO4)      | see note  |
| J4100  | StTrGJ    | $CH_3OOH + h\nu \rightarrow HCHO + OH + HO_2$                          | JX(ip_CH3OOH)    | see note  |
| J4101a | StTrGJ    | $HCHO + h\nu \rightarrow H_2 + CO$                                     | JX(ip_COH2)      | see note  |
| J4101b | StTrGJ    | $HCHO + h\nu \rightarrow H + CO + HO_2$                                | JX(ip_CHOH)      | see note  |
| J4102  | StGJ      | $CO_2 + h\nu \rightarrow CO + O(^3P)$                                  | JX(ip_CO2)       | see note  |
| J4103  | StGJ      | $CH_4 + h\nu \rightarrow CO + 0.31 H + 0.69 H_2 + 1.155 H_2O$          | JX(ip_CH4)       | see note  |
| J4200  | TrGCJ     | $C_2H_5OOH + h\nu \rightarrow CH_3CHO + HO_2 + OH$                     | JX(ip_CH3OOH)    | see note  |
| J4201  | TrGCJ     | $CH_3CHO + h\nu \rightarrow CH_3O_2 + HO_2 + CO$                       | JX(ip_CH3CHO)    | see note  |
| J4202  | TrGCJ     | $CH_3C(O)OOH + h\nu \rightarrow CH_3O_2 + OH$                          | JX(ip_PAA)       | see note  |
| J4204  | TrGNCLJ   | $PAN + h\nu \rightarrow CH_3C(O)OO + NO_2$                             | JX(ip_PAN)       | see note  |
| J4301  | TrGCJ     | $CH_3COCH_3 + h\nu \rightarrow CH_3C(O)OO + CH_3O_2$                   | JX(ip_CH3COCH3)  | see note  |
| J6000  | StTrGCLJ  | $Cl_2 + h\nu \rightarrow Cl + Cl$                                      | JX(ip_Cl2)       | see note  |
| J6100  | StTrGCLJ  | $Cl_2O_2 + h\nu \rightarrow 2 Cl$                                      | 1.4*JX(ip_Cl2O2) | see note  |
| J6101  | StTrGCLJ  | $OCIO + h\nu \rightarrow ClO + O(^3P)$                                 | JX(ip_OC10)      | see note  |
| J6200  | StGCLJ    | $HCl + h\nu \rightarrow Cl + H$  | JX(ip_HCl)       | see note  |
| J6201  | StTrGCLJ  | $HOCl + h\nu \rightarrow OH + Cl$                                      | JX(ip_HOCl)      | see note  |
| J6301a | StTrGNCLJ | $ClNO_3 + h\nu \rightarrow Cl + NO_3$                                  | JX(ip_Cl1NO3)    | see note  |
| J6301b | StTrGNCLJ | $ClNO_3 + h\nu \rightarrow ClO + NO_2$                                 | JX(ip_Cl1NO2)    | see note  |
| J6400  | StGCLJ    | $CH_3Cl + h\nu \rightarrow Cl + CH_3O_2$                               | JX(ip_CH3Cl)     | see note  |
| J6401  | StGCLJ    | $CCl_4 + h\nu \rightarrow 4 Cl$  | JX(ip_CC14)      | see note  |



Table 2: Photolysis reactions (... continued)

| #     | labels     | reaction  | rate coefficient | reference |
|-------|------------|---|------------------|-----------|
| J6402 | StGCClJ    | $\text{CH}_3\text{CCl}_3 + h\nu \rightarrow 3 \text{Cl}$                    | JX(ip_CH3CCl3)   | see note  |
| J6500 | StGFClJ    | $\text{CFCl}_3 + h\nu \rightarrow 3 \text{Cl}$                              | JX(ip_CFCl3)     | see note  |
| J6501 | StGFClJ    | $\text{CF}_2\text{Cl}_2 + h\nu \rightarrow 2 \text{Cl}$                     | JX(ip_CF2Cl2)    | see note  |
| J7200 | StTrGBrJ   | $\text{HOBr} + h\nu \rightarrow \text{Br} + \text{OH}$                      | JX(ip_HOBr)      | see note  |
| J7301 | StTrGNBrJ  | $\text{BrNO}_3 + h\nu \rightarrow \text{Br} + \text{NO}_3$                  | JX(ip_BrNO3)     | see note  |
| J7400 | StGBrJ     | $\text{CH}_3\text{Br} + h\nu \rightarrow \text{Br} + \text{CH}_3\text{O}_2$ | JX(ip_CH3Br)     | see note  |
| J7500 | StGFBBrJ   | $\text{CF}_3\text{Br} + h\nu \rightarrow \text{Br}$                         | JX(ip_CF3Br)     | see note  |
| J7600 | StTrGClBrJ | $\text{BrCl} + h\nu \rightarrow \text{Br} + \text{Cl}$                      | JX(ip_BrCl)      | see note  |
| J7601 | StGFClBrJ  | $\text{CF}_2\text{ClBr} + h\nu \rightarrow \text{Br} + \text{Cl}$           | JX(ip_CF2ClBr)   | see note  |
| J9002 | StGSJ      | $\text{SF}_6 + h\nu \rightarrow \text{products}$                            | JX(ip_SF6)       | see note  |

\*Notes: J-values are calculated with an external module and then supplied to the MECCA1 chemistry

J6100: Stimpfle et al. (2004) claim that the combination of absorption cross sections from Burkholder et al. (1990) and the  $\text{Cl}_2\text{O}_2$  formation rate coefficient by Sander et al. (2003) can approximately reproduce the observed  $\text{Cl}_2\text{O}_2/\text{ClO}$  ratios and ozone depletion. They give an almost zenith-angle independent ratio of 1.4 for Burkholder et al. (1990) to Sander et al. (2003) J-values. The IUPAC recommendation for the  $\text{Cl}_2\text{O}_2$  formation rate is about 5 to 15 % less than the value by Sander et al. (2003) but more than 20 % larger than the value by Sander et al. (2000). The J-values by Burkholder et al. (1990) are within the uncertainty range of the IUPAC recommendation.

Table 3: Heterogeneous reactions

| # | labels | reaction | rate coefficient | reference |
|---|--------|----------|------------------|-----------|
|---|--------|----------|------------------|-----------|

\*Notes:

The forward (`k_exf`) and backward (`k_exb`) rate coefficients are calculated in the file `messy_mecca1_aero.f90` using the accommodation coefficients in subroutine `mecca1_aero_alpha` and Henry's law constants in subroutine `mecca1_aero_henry`.

$k_{mt}$  = mass transfer coefficient

`lwc` = liquid water content of aerosol mode

H3201, H6300, H6301, H6302, H7300, H7301, H7302, H7601, H7602: For uptake of  $X$  ( $= \text{N}_2\text{O}_5, \text{ClNO}_3, \text{BrNO}_3$ ) and subsequent reaction with  $\text{H}_2\text{O}$ ,  $\text{Cl}^-$ , and  $\text{Br}^-$ , we define  $k_{\text{exf}}(X) = k_{\text{mt}}(X) \times lwc / ([\text{H}_2\text{O}] + 5.0E2[\text{Cl}^-] + 3.0E5[\text{Br}^-])$ .

H6301, H6302, H7601: The total uptake is determined by  $k_{\text{mt}}(\text{ClNO}_3)$ . The relative rates are assumed to be the same as for  $\text{N}_2\text{O}_5$  (H3201, H6300, H7300).

H7301, H7302, H7602: The total uptake is determined by  $k_{\text{mt}}(\text{BrNO}_3)$ . The relative rates are assumed to be the same as for  $\text{N}_2\text{O}_5$  (H3201, H6300, H7300).

Table 4: PSC reactions

| #      | labels     | reaction  | rate coefficient | reference |
|--------|------------|---|------------------|-----------|
| PSC200 | StPscN     | $\text{N}_2\text{O}_5 + \text{H}_2\text{O} \rightarrow \text{HNO}_3 + \text{HNO}_3$ | khet_N2O5_H2O    | see note  |
| PSC410 | StPscCl    | $\text{HOCl} + \text{HCl} \rightarrow \text{Cl}_2 + \text{H}_2\text{O}$             | khet_HOCl_HCl    | see note  |
| PSC420 | StPscNCl   | $\text{ClNO}_3 + \text{HCl} \rightarrow \text{Cl}_2 + \text{HNO}_3$                 | khet_ClNO3_HCl   | see note  |
| PSC421 | StPscNCl   | $\text{ClNO}_3 + \text{H}_2\text{O} \rightarrow \text{HOCl} + \text{HNO}_3$         | khet_ClNO3_H2O   | see note  |
| PSC520 | StPscNBr   | $\text{BrNO}_3 + \text{H}_2\text{O} \rightarrow \text{HOBr} + \text{HNO}_3$         | khet_BrNO3_H2O   | see note  |
| PSC541 | StPscNClBr | $\text{BrNO}_3 + \text{HCl} \rightarrow \text{BrCl} + \text{HNO}_3$                 | khet_BrNO3_HCl   | see note  |
| PSC543 | StPscClBr  | $\text{HOBr} + \text{HCl} \rightarrow \text{BrCl} + \text{H}_2\text{O}$             | khet_HOBr_HCl    | see note  |

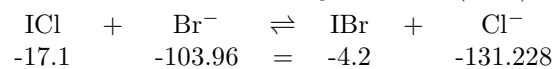
\*Notes: PSC reaction rates are calculated with an external module and then supplied to the MECCA1 chemistry (see <http://www.messy-interface.org> for details)

Table 5: Acid-base and other equilibria

| # | labels | reaction | $K_0[M^{m-n}]$ | $-\Delta H/R[K]$ | reference |
|---|--------|----------|----------------|------------------|-----------|
|---|--------|----------|----------------|------------------|-----------|

\*Notes:

EQ82 and EQ83: Thermodynamic calculations on the IBr/ICl equilibrium according to the data tables from Wagman et al. (1982):



$$\frac{\Delta G}{[\text{kJ/mol}]} = -4.2 - 131.228 - (-17.1 - 103.96) = -14.368$$

$$K = \frac{[\text{IBr}] \times [\text{Cl}^-]}{[\text{ICl}] \times [\text{Br}^-]} = \exp\left(\frac{-\Delta G}{RT}\right) = \exp\left(\frac{14368}{8.314 \times 298}\right) = 330$$

This means we have equal amounts of IBr and ICl when the  $[\text{Cl}^-]/[\text{Br}^-]$  ratio equals 330.

Table 6: Aqueous phase reactions

| #      | labels   | reaction   | $k_0$ [ $M^{1-n}s^{-1}$ ] | $-E_a/R[K]$ | reference |
|--------|--|--|---------------------------|-------------|-----------|
| A6102: | Jacobi (1996)  | found an upper limit of 6E9 and cite an upper limit from another study of 2E9. Here, we set the rate coefficient to 1E9. |                           |             |           |
| A6301: | There is also an earlier study by Exner et al. (1992) which found a smaller rate coefficient but did not consider the back reaction.   |  |                           |             |           |
| A7400: | assumed to be the same as for $\text{Br}_2^- + \text{H}_2\text{O}_2$ .   |  |                           |             |           |
| A9106: | see also: (Huie and Neta, 1987; Warneck, 1991). If this reaction produces a lot of $\text{SO}_4^-$ , it will have an effect. However, we currently assume only the stable $\text{S}_2\text{O}_8^{2-}$ as product. Since $\text{S}_2\text{O}_8^{2-}$ is not treated explicitly in the mechanism, we use $\text{SO}_4^{2-}$ as a proxy. Note that this destroys the mass consistency for sulfur species. |  |                           |             |           |
| A9205: | D. Sedlak, pers. comm. (1993)  |  |                           |             |           |
| A9208: | D. Sedlak, pers. comm. (1993)  |  |                           |             |           |
| A9105: | The rate coefficient for the sum of the paths (leading to either $\text{HSO}_5^-$ or $\text{SO}_4^{2-}$ ) is from Huie and Neta (1987), the ratio 0.28/0.72 is from Deister and Warneck (1990).  |  |                           |             |           |
| A9605: | assumed to be the same as for $\text{SO}_3^{2-} + \text{HOCl}$ .   |  |                           |             |           |
| A9705: | assumed to be the same as for $\text{SO}_3^{2-} + \text{HOBr}$ .   |  |                           |             |           |

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