Supplement of

CAPRAM reduction towards an operational multiphase halogen and dimethyl sulfide chemistry treatment in the chemistry transport model COSMO-MUSCAT(5.04e)

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Figure S1 Modelled concentration time-profile of key compounds within the pristine marine boundary layer for the summer simulations at 15° latitude. Red: simulation at rel. humidity of 50% (red). Orange: simulation at relative humidity of 70% and cloud occurrence at early morning and evening of the first model day. Dark green: simulation at relative humidity of 70% and cloud occurrence at noon and midnight. Blue: simulation at relative humidity of 90% and cloud occurrence at noon and midnight.
Figure S2  Modelled concentration time-profile of key compounds within the pristine marine boundary layer for the winter simulations at 15° latitude. Red: simulation at rel. humidity of 50% (red). Orange: simulation at relative humidity of 70% and cloud occurrence at early morning and evening of the first model day. Dark green: simulation at relative humidity of 70% and cloud occurrence at noon and midnight. Blue: simulation at relative humidity of 90% and cloud occurrence at noon and midnight.
Figure S3  Modelled concentration time-profile of key compounds within the pristine marine boundary layer for the summer simulations at 30° latitude. Red: simulation at rel. humidity of 50% (red). Orange: simulation at relative humidity of 70% and cloud occurrence at early morning and evening of the first model day. Dark green: simulation at relative humidity of 70% and cloud occurrence at noon and midnight. Blue: simulation at relative humidity of 90% and cloud occurrence at noon and midnight.
Figure S4  Modelled concentration time-profile of key compounds within the pristine marine boundary layer for the winter simulations at 30° latitude. Red: simulation at rel. humidity of 50% (red). Orange: simulation at rel. humidity of 70% and cloud occurrence at early morning and evening of the first model day. Dark green: simulation at rel. humidity of 70% and cloud occurrence at noon and midnight. Blue: simulation at rel. humidity of 90% and cloud occurrence at noon and midnight.
Figure S5  Modelled concentration time-profile of key compounds within the pristine marine boundary layer for the summer simulations at 45° latitude. Red: simulation at rel. humidity of 50% (red). Orange: simulation at relative humidity of 70% and cloud occurrence at early morning and evening of the first model day. Dark green: simulation at relative humidity of 70% and cloud occurrence at noon and midnight. Blue: simulation at relative humidity of 90% and cloud occurrence at noon and midnight.
Figure S6  Modelled concentration time-profile of key compounds within the pristine marine boundary layer for the winter simulations at 45° latitude. Red: simulation at rel. humidity of 50% (red). Orange: simulation at relative humidity of 70% and cloud occurrence at early morning and evening of the first model day. Dark green: simulation at relative humidity of 70% and cloud occurrence at noon and midnight. Blue: simulation at relative humidity of 90% and cloud occurrence at noon and midnight.
Figure S7  Modelled concentration time-profile of key compounds within the pristine marine boundary layer for the summer simulations at 60° latitude. Red: simulation at relative humidity of 50% (red). Orange: simulation at relative humidity of 70% and cloud occurrence at early morning and evening of the first model day. Dark green: simulation at relative humidity of 70% and cloud occurrence at noon and midnight. Blue: simulation at relative humidity of 90% and cloud occurrence at noon and midnight.
Figure S8  Modelled concentration time-profile of key compounds within the pristine marine boundary layer for the winter simulations at 60° latitude. Red: simulation at rel. humidity of 50% (red). Orange: simulation at relative humidity of 70% and cloud occurrence at early morning and evening of the first model day. Dark green: simulation at relative humidity of 70% and cloud occurrence at noon and midnight. Blue: simulation at relative humidity of 90% and cloud occurrence at noon and midnight.
Figure S9  Modelled concentration time-profile of key compounds within the pristine marine boundary layer for the summer simulations at 75° latitude. Red: simulation at rel. humidity of 50% (red). Orange: simulation at relative humidity of 70% and cloud occurrence at early morning and evening of the first model day. Dark green: simulation at relative humidity of 70% and cloud occurrence at noon and midnight. Blue: simulation at relative humidity of 90% and cloud occurrence at noon and midnight.
Figure S10  Modelled concentration time-profile of key compounds within the pristine marine boundary layer for the winter simulations at 75° latitude. Red: simulation at rel. humidity of 50% (red). Orange: simulation at relative humidity of 70% and cloud occurrence at early morning and evening of the first model day. Dark green: simulation at relative humidity of 70% and cloud occurrence at noon and midnight. Blue: simulation at relative humidity of 90% and cloud occurrence at noon and midnight.
Figure S11  Modelled formation rate of DMSO in (a) the gas phase and (c) the aqueous phase together with the modelled oxidation rate in (b) the gas phase and (d) the aqueous phase in the ‘stable meteorological condition’ simulation with stratiform clouds after 12 hours of modelling time. The x-axis represents the innermost horizontal grid cells divided by 100. The black contour lines represent the simulated clouds. The black line corresponds to a liquid water content of 0.01 g m$^{-3}$ and the white line to 0.1 g m$^{-3}$. The area framed by the white line includes LWC above 0.1 g m$^{-3}$. 

Figure S12  Simulated aqueous-phase concentration of bromide in the ‘stable meteorological condition’ simulation with stratiform clouds after 12 hours of modelling time. The x-axis represents the innermost horizontal grid cells divided by 100. The black contour lines represent the simulated clouds. The black line corresponds to a liquid water content of 0.01 g m$^{-3}$ and the white line to 0.1 g m$^{-3}$. The area framed by the white line includes LWC above 0.1 g m$^{-3}$. The initial background concentration is at about 16 ng m$^{-3}$. 
Details on the dry deposition velocities are given in the previous CAPRAM studies Bräuer et al. (2013), Hoffmann et al. (2016) and Hoffmann et al. (2019a). Details on the initial concentrations and emission rates are given in Bräuer et al. (2013) and Hoffmann et al. (2016). In the term of I$_2$ and HOI, emission rates are derived from Prados-Roman et al. (2015). Aerosol initial concentrations are calculated from the SPACCIM simulations and were provided in the previous CAPRAM study Bräuer et al. (2013).

| Specie | Dry deposition / s$^{-1}$ | Initial concentration / molecules cm$^{-3}$ | Emission rates / mol m$^{-2}$ s$^{-1}$ | Aerosol initial concentration / mol m$^{-3}$ |
|--------|-----------------------------|---------------------------------------------|----------------------------------------|---------------------------------------------|
| NH$_3$ | $1.0\cdot10^{-2}$           | $1.28\cdot10^{9}$                           | $7.589\cdot10^{-10}$                  |                                             |
| NO     | $2.0\cdot10^{-4}$           | $2.50\cdot10^{8}$                           | $4.151\cdot10^{-12}$                  |                                             |
| NO$_2$ | $2.0\cdot10^{-4}$           | $5.00\cdot10^{8}$                           |                                        |                                             |
| NO$_3$ | $1.0\cdot10^{-2}$           |                                             |                                        |                                             |
| N$_2$O$_5$ | $1.0\cdot10^{-2}$ |                                             |                                        |                                             |
| HONO   |                             | $2.50\cdot10^{8}$                           |                                        |                                             |
| HNO$_3$| $7.0\cdot10^{-3}$           | $2.00\cdot10^{9}$                           |                                        |                                             |
| HO$_2$NO$_2$ | $5.0\cdot10^{-3}$ |                                             |                                        |                                             |
| O$_3$  | $1.5\cdot10^{-3}$           | $7.50\cdot10^{11}$                          |                                        |                                             |
| CO     | $1.0\cdot10^{-3}$           | $4.25\cdot10^{12}$                          | $1.416\cdot10^{9}$                    |                                             |
| CO$_2$ |                             | $1.02\cdot10^{16}$                          |                                        |                                             |
| SO$_2$ | $8.7\cdot10^{-3}$           | $2.55\cdot10^{9}$                           |                                        |                                             |
| SULF   | $1.0\cdot10^{-2}$           |                                             |                                        |                                             |
| H$_2$  |                             | $1.28\cdot10^{13}$                          |                                        |                                             |
| H$_2$O$_2$ | $5.0\cdot10^{-3}$ |                                             |                                        |                                             |
| CH$_4$ | $4.50\cdot10^{-13}$         | $2.923\cdot10^{-11}$                        |                                        |                                             |
| C$_2$H$_6$ | $1.28\cdot10^{-10}$ |                                             |                                        |                                             |
| C$_2$H$_8$ | $2.31\cdot10^{-10}$ |                                             |                                        |                                             |
| C$_3$H$_2$ | $2.42\cdot10^{-9}$   |                                             |                                        |                                             |
| C$_3$H$_4$ | $2.55\cdot10^{-9}$ |                                             |                                        |                                             |
| C$_3$H$_6$ | $5.13\cdot10^{3}$  | $9.083\cdot10^{11}$                        |                                        |                                             |
| HYAC   |                             | $3.83\cdot10^{8}$                           |                                        | $4.151\cdot10^{-12}$                        |
| Specie     | Dry deposition / s^{-1} | Initial concentration / molecules cm^{-3} | Emission rates / mol m^{-2} s^{-1} | Aerosol initial concentration / mol m^{-3} |
|------------|-------------------------|------------------------------------------|-----------------------------------|-------------------------------------------|
| CH\_3COCH\_3 |                         | 1.10\cdot 10^{10}                       |                                   | 6.320\cdot 10^{-12}                      |
| MEK        |                         | 6.89\cdot 10^{8}                        |                                   | 7.124\cdot 10^{-16}                      |
| GLYOXAL    |                         | 2.55\cdot 10^{8}                        |                                   |                                           |
| CH\_3COCHO  |                         | 2.55\cdot 10^{8}                        |                                   |                                           |
| CH\_3OOH   | 2.5\cdot 10^{-3}        | 5.00\cdot 10^{9}                        |                                   |                                           |
| CH\_3CH\_2OOH |                    | 2.55\cdot 10^{9}                       |                                   |                                           |
| CH\_3COOOH |                         | 2.55\cdot 10^{7}                        |                                   |                                           |
| PAN        | 1.0\cdot 10^{-4}        | 2.50\cdot 10^{8}                        |                                   |                                           |
| CH\_3OH    | 1.0\cdot 10^{-2}        | 1.40\cdot 10^{10}                       |                                   | 9.797\cdot 10^{-16}                      |
| CH\_3CH\_2OH |                    | 5.0\cdot 10^{-3}                       | 2.00\cdot 10^{9}                 | 1.015\cdot 10^{-11}                      |
| HCOOH      | 1.0\cdot 10^{-2}        |                                           | 6.25\cdot 10^{6}                 |                                           |
| CH\_3COOH  | 1.0\cdot 10^{-2}        | 5.00\cdot 10^{9}                        |                                   | 1.278\cdot 10^{-12}                      |
| C\_4H\_8    |                         | 1.28\cdot 10^{9}                        |                                   | 2.341\cdot 10^{-12}                      |
| APIN       |                         | 4.53\cdot 10^{8}                        |                                   | 2.541\cdot 10^{-14}                      |
| BPIN       |                         | 3.02\cdot 10^{8}                        |                                   |                                           |
| CHBr\_3    |                         | 3.83\cdot 10^{7}                        |                                   | 2.225\cdot 10^{-13}                      |
| C\_6H\_7I  |                         | 1.63\cdot 10^{7}                        |                                   | 8.170\cdot 10^{-15}                      |
| CH\_2I     |                         | 2.55\cdot 10^{6}                        |                                   | 1.876\cdot 10^{-13}                      |
| CH\_3I     |                         | 2.04\cdot 10^{7}                        |                                   | 2.458\cdot 10^{-13}                      |
| CH\_2ClI   |                         | 2.55\cdot 10^{6}                        |                                   | 1.524\cdot 10^{-13}                      |
| CH\_2BrI   |                         | 8.93\cdot 10^{4}                        |                                   | 8.751\cdot 10^{-14}                      |
| HCl        | 2.0\cdot 10^{-2}        | 2.50\cdot 10^{9}                        |                                   |                                           |
| HOCl       | 2.0\cdot 10^{-3}        |                                           |                                   |                                           |
| ClNO\_2    | 1.0\cdot 10^{-2}        |                                           |                                   |                                           |
| ClNO\_3    | 1.0\cdot 10^{-2}        |                                           |                                   |                                           |
| HBr        | 2.0\cdot 10^{-2}        |                                           |                                   |                                           |
| HOBr       | 1.6\cdot 10^{-3}        |                                           |                                   |                                           |
| BrNO\_2    | 1.0\cdot 10^{-2}        |                                           |                                   |                                           |
| BrNO\_3    | 5.0\cdot 10^{-3}        |                                           |                                   |                                           |
| I\_2       |                         |                                           |                                   | 1.744\cdot 10^{-14}                      |
| HOI        | 1.0\cdot 10^{-2}        |                                           |                                   | 3.321\cdot 10^{-13}                      |
| Specie       | Dry deposition / s⁻¹ | Initial concentration / molecules cm⁻³ | Emission rates / mol m⁻² s⁻¹ | Aerosol initial concentration / mol m⁻³ |
|--------------|----------------------|----------------------------------------|----------------------------|----------------------------------------|
| INO₃         | 1.0·10⁻²             |                                        |                            |                                        |
| I₂O₂         | 1.0·10⁻²             |                                        |                            |                                        |
| I₂O₃         | 1.0·10⁻²             |                                        |                            |                                        |
| I₂O₄         | 1.0·10⁻²             |                                        |                            |                                        |
| DMS          |                      | 1.53·10⁹                              | 1.026·10⁻¹⁰                |                                        |
| DMSO         | 5.0·10⁻³             |                                        |                            |                                        |
| DMSO₂        | 5.0·10⁻³             |                                        |                            |                                        |
| MSA          | 5.0·10⁻³             |                                        |                            |                                        |
| SO₄²⁻        |                      |                                        |                            | 1.05·10⁻⁸                              |
| NO₃⁻         |                      |                                        |                            | 2.05·10⁻⁹                              |
| Cl⁻          |                      |                                        |                            | 9.76·10⁻⁸                              |
| Br⁻          |                      |                                        |                            | 2.14·10⁻⁹                              |
| NH₄⁺         |                      |                                        |                            | 5.72·10⁻⁹                              |
| Mn³⁺         |                      |                                        |                            | 3.93·10⁻¹⁵                             |
| Fe³⁺         |                      |                                        |                            | 4.80·10⁻¹⁵                             |
| Cu²⁺         |                      |                                        |                            | 1.72·10⁻¹³                             |
| H₂C₂O₄⁻      |                      |                                        |                            | 3.94·10⁻¹¹                             |
| MSA          |                      |                                        |                            | 3.26·10⁻¹⁰                             |
| H⁺           |                      |                                        |                            | 1.00·10⁻¹¹                             |
| Nr. | Reaction | Rate constant$^{(a)}$ | Reference |
|-----|----------|-----------------------|-----------|
| D1  | DMS + OH $\rightarrow$ CH$_3$SCH$_2$O$_2$ - O$_2$ | $k = 1.12 \cdot 10^{-11} \exp(-250/T)$ | IUPAC, Atkinson et al. (2004) |
| D2  | DMS + OH $\rightarrow$ 0.9 DMSO + 0.9 HO$_2$ + 0.1 CH$_3$SOH + 0.1 CH$_3$O$_2$ - O$_2$ | $k = 1.90 \cdot 10^{-13} \exp(520/T)$ | see description at the table end |
| D3  | DMS + NO$_1$ $\rightarrow$ CH$_3$SCH$_2$O$_2$ - O$_2$ | $k = 5.00 \cdot 10^{-13} \exp(400/T)$ | IUPAC, Atkinson et al. (2004) |
| D4  | DMS + Cl$_2$ $\rightarrow$ 0.82 CH$_3$SCH$_2$O$_2$ + 0.82 HCl + 0.18 DMSO + 0.18 ClO + O$_2$ | $k = 1.88 \cdot 10^{-10}$ | IUPAC, Urbanski and Wine (1999) |
| D5  | DMS + ClO $\rightarrow$ 0.73 Cl + 0.73 DMSO + 0.27 HClO + 0.27 CH$_3$SCH$_2$O$_2$ - 0.27 O$_2$ | $k = 1.70 \cdot 10^{-15} \exp(340/T)$ | IUPAC |
| D6  | DMS + BrO $\rightarrow$ DMSO + Br | $k = 1.50 \cdot 10^{-14} \exp(1000/T)$ | IUPAC |
| D7  | DMS + Cl$_2$ $\rightarrow$ CH$_3$S$\times$Cl + HCl | $k = 3.40 \cdot 10^{-14}$ | Dyke et al. (2005) |
| D8  | DMS + IO $\rightarrow$ DMSO + I | $k = 3.30 \cdot 10^{-13} \exp(-925/T)$ | IUPAC |
| D9  | CH$_3$SCH$_2$O$_2$ + HO$_2$ $\rightarrow$ CH$_3$SCH$_2$OOH + O$_2$ | $k = 9.00 \times 10^{-13}$ | MCMv3.2, Rickard et al. (21.10.2013) |
| D10 | CH$_3$SCH$_2$O$_2$ + NO $\rightarrow$ CH$_3$S + HCHO + NO$_2$ | $k = 4.90 \cdot 10^{-12} \exp(260/T)$ | MCMv3.2, Rickard et al. (21.10.2013) |
| D11 | CH$_3$SCH$_2$O$_2$ + NO$_3$ $\rightarrow$ CH$_3$S + HCHO + NO$_2$ + O$_2$ | $k = 2.30 \cdot 10^{-12}$ | MCMv3.2, Rickard et al. (21.10.2013) |
| D12 | CH$_3$SCH$_2$O$_2$ + CH$_2$O$_2$ $\rightarrow$ 0.89 CH$_3$S + 0.89 HCHO + 0.11 CH$_3$SCHO + O$_2$ | $k = 5.00 \cdot 10^{-13} \exp(400/T)$ | In accordance to MCMv3.2 RO$_2$ reaction |
| D13 | CH$_3$SCH$_2$Cl + OH $\rightarrow$ CH$_3$SOH + ClCH$_2$O$_2$ - O$_2$ | $k = 2.50 \cdot 10^{-12}$ | Shallcross et al. (2006) |
| D14 | CH$_3$SCH$_2$O + OH $\rightarrow$ CH$_3$SCHO + OH + H$_2$O | $k = 7.03 \cdot 10^{-11}$ | MCMv3.2, Rickard et al. (21.10.2013) |
| D15 | CH$_3$SCHO + OH $\rightarrow$ CH$_3$S + CO + H$_2$O | $k = 1.11 \cdot 10^{-11}$ | MCMv3.2, Rickard et al. (21.10.2013) |
| D16 | DMSO + OH $\rightarrow$ MSIA + CH$_3$O$_2$ - O$_2$ | $k = 6.10 \cdot 10^{-12} \exp(800/T)$ | MCMv3.2, Rickard et al. (21.10.2013) |
| D17 | DMSO + NO$_3$ $\rightarrow$ DMSO$_2$ + NO$_2$ | $k = 2.90 \cdot 10^{-13}$ | Sander et al. (2006) |
| D18 | DMSO + Cl $\rightarrow$ 0.43 DM$_2$SO + 0.43 CIO + 0.57 CH$_3$SO + 0.57 HCHO + 0.57 HCl - 0.43 O$_2$ | $k = 1.45 \cdot 10^{-11}$ | Falbe-Hansen et al. (2000); Nicovich et al. (2006); Kleissas et al. (2007) |
| D19 | DMSO + BrO $\rightarrow$ CH$_3$SO$\times$CH$_3$ + Br | $k = 1.00 \cdot 10^{-14}$ | Ballesteros et al. (2002) |
| D20 | CH$_3$SOH + OH $\rightarrow$ CH$_3$SO + H$_2$O | $k = 4.00 \cdot 10^{-13}$ | Lucas and Prinn (2002a) |
| D21 | CH$_3$S + O$_3$ $\rightarrow$ CH$_3$SO + O$_2$ | $k = 1.15 \cdot 10^{-12} \exp(430/T)$ | see description at the table end |
| D22 | CH$_3$S + O$_2$ $\rightarrow$ CH$_3$O$_2$ + SO$_2$ - O$_2$ | $k = 9.00 \cdot 10^{-11}$ | see description at the table end |
| D23 | CH$_3$S + O$_2$ $\rightarrow$ CH$_3$SO | $k = 4.00 \cdot 10^{-13}$ | MCMv3.2, Rickard et al. (21.10.2013) |
| D24 | MSIA + OH $\rightarrow$ CH$_3$O$_2$ + SO$_2$ + H$_2$O - O$_2$ | $k = 3.00 \cdot 10^{-13}$ | MCMv3.2, Rickard et al. (21.10.2013) |
Table S3  Implemented phase transfers in the CAPRAM-DM1.0red

| Species | $K_T$ ($298 \text{ K}$) | $\Delta H / R$ | Reference | $\alpha$ | Reference | $D_g$ ($298 \text{ K}$) | Reference |
|---------|-------------------------|----------------|------------|---------|------------|-------------------------|------------|
| D33© DMS | 0.56 | 4480 | Campolongo et al. (1999) | 0.001 | Zhu et al. (2006) | 1.08·10⁻⁵ | Fuller et al. (1966) |
| D34© DMSO | 1.00·10⁷ | 2580 | Campolongo et al. (1999) | 0.1 | De Bruyn et al. (1994) | 1.01·10⁻⁵ | Fuller et al. (1966) |
| D35© DMSO₂ | 1.00·10⁷ | 5390 | Campolongo et al. (1999) | 0.1 | De Bruyn et al. (1994) | 9.55·10⁻⁶ | Fuller et al. (1966) |
| D36© MSA | 1.00·10⁸ | 1760 | between DMSO₂ and MSA | 0.1 | as for MSAa | 1.11·10⁻⁵ | Fuller et al. (1966) |
| D37© MSA | 5.09·10¹³ | 1760 | Campolongo et al. (1999) | 0.1 | De Bruyn et al. (1994) | 1.04·10⁻⁵ | Fuller et al. (1966) |

(a) in M atm⁻¹; (b) in K; (c) in m² s⁻¹
Table S4  Implemented aqueous-phase reactions in the CAPRAM-DM1.0red

| Nr. | Reaction | Rate constant(a) | Reference |
|-----|----------|------------------|-----------|
| D38 | DMS + O3 → DMSO + O2 | k = 8.61·10^{08}\exp(-2600/T) | Gershenzon et al. (2001) |
| D39 | DMSO + OH → MSIA + CH3 | k = 6.65·10^{09}\exp(-1270/T) | Zhu et al. (2003a) |
| D40② | DMSO + SO4^− → MSIA + CH3 + H^+ + SO4^2− | k = 2.97·10^{09}\exp(-1440/T) | Zhu et al. (2003b) |
| D41② | DMSO + HCl → MSIA + CH3 + H^− + Cl^− | k = 1.60·10^{07} | Zhu (2004) |
| D42② | MSIA + O3 → MSA + O2 | k = 3.50·10^{07} | Herrmann and Zellner (1997) |
| D43 | MSI^− + OH → CH3 + 0.135 SO2 + 0.765 MS^− + 0.765 SO3 - 0.765 MS^− + 0.9 OH^- + 0.1 HSO^- | k = 1.20·10^{−10} | Bardouki et al. (2002) |
| D44② | MSI^− + Cl2^- → CH3 + 0.15 SO2 + 0.85 MS^− + 0.85 SO3 - 0.85 MS^− + 2 Cl^- | k = 8.00·10^{−08} | Zhu et al. (2005) |
| D45② | MSI^− + O3 → CH3SO3^- + O2 | k = 2.00·10^{−06} | Flyunt et al. (2001) |
| D46 | MS^− + OH → HCHO + SO3^- + H2O - 0.5 O2 | k = 1.29·10^{−07}\exp(-2630/T) | Zhu et al. (2003a) |
| D47② | MS^− + Cl2^- → CH3 + SO3^- + 2 Cl^- | k = 3.89·10^{−03} | Zhu (2004) |

(a) k^{2nd} in l^3 mol^{-1} s^{-1}

Table S5  Implemented aqueous-phase equilibria in the CAPRAM-DM1.0red

| Equilibrium | K^{(a)} | k_f, 298(b) | E_A/R^{(c)} | k_b, 298(b) | E_A/R^{(c)} | Reference |
|-------------|---------|-------------|-------------|-------------|-------------|-----------|
| D48② | MSIA ⇌ MSI^− + H^+ | 5.0·10^{−03} | 2.50·10^{06} | 5.00·10^{10} | 5.00·10^{10} | Wudl et al. (1967) |
| D49② | MSA ⇌ MS^− + H^+ | 73 | 3.65·10^{13} | 5.00·10^{10} | 5.00·10^{10} | Clarke and Woodward (1966) |

(a) in M^{m-n}, n order of reaction of forward reaction, m order of reaction of backward reaction; (b) k^{2nd} in l^3 mol^{-1} s^{-1}, k^{1st} in s^{-1}; (c) in K

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Table S6    Implemented gas-phase reactions in the CAPRAM-HM3.0red

| Nr. | Reaction | Rate constant(a) | Comment |
|-----|----------|------------------|---------|
| H1  | Cl + O₃ → ClO | k = 2.80·10⁻¹¹ exp(-250/T) | Atkinson et al. (2007) |
| H2  | ClO + HO₂ → HOCl | k = 2.20·10⁻¹² exp(340/T) | Atkinson et al. (2007) |
| H3  | HCl + OH → Cl | k = 1.70·10⁻¹² exp(-230/T) | Atkinson et al. (2007) |
| H4  | ClO + NO → Cl + NO₂ | k = 6.20·10⁻¹² exp(295/T) | Atkinson et al. (2007) |
| H5  | Cl + NO₂ → CINO₂ | k = [M]*2.75·10⁻⁶ exp(11438/T) | Anderson and Fahey (1990) |
| H6  | ClO + NO₂ → CINO₃ | k = 6.60·10⁻¹² exp(-1240/T) | IUPAC, Atkinson et al. (2006) |
| H7  | ClNO₃ → ClO + NO₂ | k = 8.30·10⁻¹¹ exp(-100/T) | IUPAC, Atkinson et al. (2006) |
| H8  | Cl + CH₄ → CH₂O₂ + HCl | k = 1.40·10⁻¹⁰ | IUPAC, Atkinson et al. (2006) |
| H9  | Cl + C₂H₆ → C₂H₅O₂ + HCl | k = 2.05·10⁻¹⁰ | IUPAC, Atkinson et al. (2006) |
| H10 | Cl + BIGALKANE → ALKO₂ + HCl | k = 7.10·10⁻¹¹ exp(-75/T) | IUPAC, Atkinson et al. (2006) |
| H11 | Cl + CH₂OH → HCHO + HO₂ + HCl | k = 6.05·10⁻¹¹ exp(155/T) | IUPAC, Atkinson et al. (2006) |
| H12 | Cl + CH₂OH → HCHO + HO₂ + HCl | k = 5.90·10⁻¹¹ | IUPAC, Atkinson et al. (2006) |
| H13 | Cl + C₂H₅OH → 0.92 CH₃CHO + 0.92 HO₂ + 0.08 EO₂ + HCl | k = 7.20·10⁻¹¹ exp(525/T) | IUPAC, Atkinson et al. (2006) |
| H14 | Cl + ALKOH → 1.25 MEK + HO₂ + HCl | k = 1.07·10⁻¹⁰ | Wallington et al. (1989) |
| H15 | Cl + CH₃OOH → HCl + 0.6 CH₂O₂ + 0.4 HCHO + 0.4 OH | k = 1.80·10⁻¹¹ exp(-600/T) | Burkholder et al. (2015) |
| H16 | Cl + C₂H₅OOH → HCl + CH₃CHO + OH | k = 8.10·10⁻¹¹ exp(-34/T) | IUPAC, Atkinson et al. (2006) |
| H17 | ClO + CH₂O₂ → Cl + O₂ + HCHO + HO₂ | k = 8.00·10⁻¹¹ | IUPAC, Atkinson et al. (2006) |
| H18 | CL + CH₃CHO → HCl + CH₃CO₃ | k = 1.30·10⁻¹⁰ | IUPAC, Atkinson et al. (2006) |
| H19 | Cl + HYAC → HCl + MGLY + HO₂ | k = 5.70·10⁻¹¹ | Orlando et al. (1999) |
| H20 | Cl + CH₃COHO → HCl + CH₃CO₃ + CO | k = 4.80·10⁻¹¹ | Green et al. (1990) |
| H21 | Cl + GLYOX → HCl + 2.0 CO + HO₂ | k = 3.80·10⁻¹¹ | Niki et al. (1985) |
| H22 | Cl + MEK → HCl + MEKO₂ | k = 3.05·10⁻¹¹ exp(80/T) | IUPAC, Atkinson et al. (2006) |
| H23 | Cl + MACR → 0.2 MACRO₂ + 0.8 CC(O)(O)(CCl)C=O + 0.2 HCl | k = 2.55·10⁻¹⁰ | Rate constant average Canosa-Mas et al. (2001), Wang et al. (2002), Orlando et al. (2003) & Kaiser et al. (2010),
| H24 | CC(O)(O)(CCl)C=O + HO₂ → CH₂COC₂H₂Cl + CO + HO₂ + OH | k = 1.00·10⁻¹¹ | Hasson et al. (2012) |
| H25 | CC(O)(O)(CCl)C=O + NO → CH₂COC₂H₂Cl + CO + HO₂ + NO₂ | k = 1.17·10⁻¹¹ | Hsin and Elrod (2007) |
| Nr. | Reaction | Rate constant<sup>(a)</sup> | Comment |
|-----|----------|-----------------------------|---------|
| H28 | CC(O(O))(CCl)C=O + CH₃O₂ → CH₃COCH₂Cl + CO + HO₂ + HCHO | k = 1.00×10⁻¹² | Hasson et al. (2012) |
| H29 | CC(O(O))(CCl)C=O + CH₃CO₂ → CH₃COCH₂Cl + CO + HO₂ + CH₂O₂ | k = 1.00×10⁻¹¹ | estimated |
| H30 | OH + CC(OO)(CCl)C=O → CH₃COCH₂Cl + CO + OH | k = 3.77×10⁻¹¹ | estimated |
| H31 | Cl + MVK → CC(O(O))CCl | k = 2.10×10⁻¹⁰ | Canosa-Mas et al. (2001) |
| H32 | CC(=O)CCl + HO₂ → CC(=O)(OO)CCl | k = 1.82×10⁻¹² exp(1300/T) | MCMv3.2, Rickard et al. (21.10.2013) |
| H33 | CC(=O)CCl + NO → ClCH₂CHO + NO₂ + CH₃CO₂ | k = 2.70×10⁻¹² exp(360/T) | MCMv3.2, Rickard et al. (21.10.2013) |
| H34 | CC(=O)CCl + NO₃ → ClCH₂CHO + NO₂ + CH₃CO₂ | k = 2.30×10⁻¹² | MCMv3.2, Rickard et al. (21.10.2013) |
| H35 | CC(=O)CCl + CH₂O₂ → ClCH₂CHO + CH₂CO₂ + HCHO | k = 1.00×10⁻¹² | estimated |
| H36 | CC(=O)CCl + CH₂O₂ → ClCH₂CHO + CH₂CO₂ + CH₃O₂ | k = 1.00×10⁻¹¹ | estimated |
| H37 | OH + CC(O(O))CCl → ClCH₂CHO + CH₂CO₂ + OH | k = 3.95×10⁻¹¹ | after MVKOOH in MCMv3.2, Rickard et al. (21.10.2013) |
| H38 | Cl + BIGALD1 → MALO₂ + HO₂ + HCl | k = 1.35×10⁻¹⁰ | Martín et al. (2013) |
| H39 | Cl + TOL → HCl + TOLO₂ | k = 6.20×10⁻¹¹ | Wang et al. (2005) |
| H40 | Cl + XYL → HCl + XYLNO₂ | k = 1.40×10⁻¹⁰ | Wang et al. (2005) |
| H41 | Cl + BZALD → HCl + ACBZO₂ | k = 1.00×10⁻¹⁰ | Thiault et al. (2002) |
| H42 | Cl + GLYALD → HCl + HOCH₂CO₂ | k = 7.00×10⁻¹¹ | Niki et al. (1987) |
| H43 | Cl + CH₂COCH₂ → HCl + CH₂COCH₂O₂ | k = 3.20×10⁻¹¹ exp(-815/T) | Atkinson et al. (2006) |
| H44 | Cl + C₂H₂ → 0.26 ClCHO + 0.21 Cl + 0.53 HCl + 0.21 GLYOXAL + 1.32 CO + 0.79 HO₂ | | TROE |
| H45 | Cl + C₂H₄ → ClCH₂CH₂O₂ | | TROE |
| H46 | ClCH₂CH₂O₂ + HO₂ → ClCH₂CH₂OOH | k = 3.30×10⁻¹³ exp(820/T) | MCMv3.2, Rickard et al. (21.10.2013) |
| H47 | ClCH₂CH₂O₂ + NO → ClCH₂CHO + HO₂ + NO₂ | k = 3.24×10⁻¹² exp(360/T) | Atkinson et al. (2008) |
| H48 | ClCH₂CH₂O₂ + NO₃ → ClCH₂CHO + HO₂ + NO₂ | k = 2.30×10⁻¹² | MCMv3.2, Rickard et al. (21.10.2013) |
| H49 | ClCH₂CH₂O₂ + CH₂O₂ → ClCH₂CHO + 0.8 HCHO + 0.2 CH₂OH + 1.4 HO₂ | k = 2.00×10⁻¹² | estimated |
| H50 | ClCH₂CHO + NO → ClCH₂CO₂ + HNO₃ | k = 1.40×10⁻¹² exp(-1860/T) | MCMv3.2, Rickard et al. (21.10.2013) |
| H51 | ClCH₂CHO + OH → ClCH₂CO₂ + H₂O | k = 2.09×10⁻¹¹ | Atkinson et al. (2008) |
| H52 | ClCH₂CO₂ + HO₂ → 0.44 ClCH₂O₂ + 0.44 OH + 0.15 ClCH₂COOH + 0.15 O₃ + 0.41 ClCH₂(OOOH) | k = 5.20×10⁻¹³ exp(980/T) | MCMv3.2, Rickard et al. (21.10.2013) |
| H53 | ClCH₂CO₂ + NO → ClCH₂O₂ + NO₂ | k = 7.50×10⁻¹² exp(290/T) | MCMv3.2, Rickard et al. (21.10.2013) |
| H54 | ClCH₂CO₂ + NO₂ → CIPAN | TROE | MCMv3.2, Rickard et al. (21.10.2013) |
| H55 | ClCH₂CO₂ + NO₃ → ClCH₂O₂ + NO₂ | k = 4.00×10⁻¹² | MCMv3.2, Rickard et al. (21.10.2013) |
| Nr. | Reaction                                                                 | Rate constant\(^{(a)}\) | Comment                                                                 |
|-----|---------------------------------------------------------------------------|---------------------------|-------------------------------------------------------------------------|
| H56 | CH<sub>2</sub>CO<sub>3</sub> + CH<sub>3</sub>O<sub>2</sub> → 0.7 ClCH<sub>2</sub>O<sub>2</sub> + 0.3 ClCH<sub>2</sub>COOH + 0.7 HO<sub>2</sub> + HCHO | k = 1.00·10<sup>-11</sup> | estimated                                                               |
| H57 | CH<sub>2</sub>COOH + OH → ClCH<sub>2</sub>O<sub>2</sub>                   | k = 1.90·10<sup>-12</sup>exp(190/T) | MCMv3.2, Rickard et al. (21.10.2013)                                    |
| H58 | ClCH<sub>2</sub>(O)OOH + OH → ClCH<sub>2</sub>O<sub>2</sub>              | k = 4.29·10<sup>-12</sup> | MCMv3.2, Rickard et al. (21.10.2013)                                    |
| H59 | CIPAN + OH → CICH<sub>2</sub>OH + CO + NO<sub>2</sub>                    | k = 6.26·10<sup>-13</sup> | MCMv3.2, Rickard et al. (21.10.2013)                                    |
| H60 | CIPAN → ClCH<sub>2</sub>CO<sub>2</sub> + NO<sub>2</sub>                   | TROE                      | MCMv3.2, Rickard et al. (21.10.2013)                                    |
| H61 | ClCH<sub>2</sub>O<sub>2</sub> + HO<sub>2</sub> → 0.3 ClCH<sub>2</sub>OOH + 0.7 ClCHO | k = 3.20·10<sup>-15</sup>exp(820/T) | MCMv3.2, Rickard et al. (21.10.2013)                                    |
| H62 | ClCH<sub>2</sub>O<sub>2</sub> + NO → CICH<sub>2</sub>OH + HO<sub>2</sub> + NO<sub>2</sub> | k = 4.05·10<sup>-12</sup>exp(360/T) | MCMv3.2, Rickard et al. (21.10.2013)                                    |
| H63 | ClCH<sub>2</sub>O<sub>2</sub> + NO<sub>1</sub> → CICH<sub>2</sub>OH + HO<sub>2</sub> + NO<sub>2</sub> | k = 2.30·10<sup>-12</sup> | MCMv3.2, Rickard et al. (21.10.2013)                                    |
| H64 | ClCH<sub>2</sub>O<sub>2</sub> + CH<sub>3</sub>OH → 1.4 HO<sub>2</sub> + ClCHO + 0.8 HCHO + 0.2 CH<sub>3</sub>OH | k = 2.50·10<sup>-12</sup> | estimated                                                              |
| H65 | Cl + C<sub>2</sub>H<sub>6</sub> → 0.4 CH<sub>3</sub>CH(O)<sub>2</sub>CH<sub>2</sub>Cl + 0.5 CH<sub>3</sub>CH(Cl)CH<sub>2</sub>O<sub>2</sub> + 0.1 HYAC | k = 1.43·10<sup>-14</sup>exp(2886/T) | Atkinson et al. (2006)                                                  |
| H66 | CH<sub>3</sub>CH(O)<sub>2</sub>CH<sub>2</sub>Cl + NO → CH<sub>3</sub>COCH<sub>2</sub>Cl + HO<sub>2</sub> + NO<sub>2</sub> | k = 2.70·10<sup>-12</sup>exp(360/T) | Atkinson et al. (2008)                                                  |
| H67 | CH<sub>3</sub>CH(Cl)CH<sub>2</sub>O<sub>2</sub> + NO → CH<sub>3</sub>CH(Cl)CHO + NO<sub>2</sub> + HO<sub>2</sub> | k = 2.70·10<sup>-12</sup>exp(360/T) | MCMv3.2, Rickard et al. (21.10.2013)                                    |
| H68 | CH<sub>3</sub>CH(O)<sub>2</sub>CH<sub>2</sub>Cl + CH<sub>3</sub>O<sub>2</sub> → CH<sub>3</sub>COCH<sub>2</sub>Cl + 0.8 HCHO + 0.2 CH<sub>3</sub>OH + 1.4 HO<sub>2</sub> | k = 4.00·10<sup>-14</sup> | estimated                                                              |
| H69 | CH<sub>3</sub>CH(Cl)CH<sub>2</sub>O<sub>2</sub> + CH<sub>3</sub>OH → CH<sub>3</sub>CH(Cl)CHO + 0.8 HCHO + 0.2 CH<sub>3</sub>OH + 1.4 HO<sub>2</sub> | k = 6.48·10<sup>-13</sup> | estimated                                                              |
| H70 | CH<sub>3</sub>COCH<sub>2</sub>Cl + OH → CH<sub>3</sub>COCHClO<sub>2</sub> | k = 3.68·10<sup>-13</sup> | Atkinson et al. (2008)                                                  |
| H71 | CH<sub>3</sub>COCHClO<sub>2</sub> + HO<sub>2</sub> → CH<sub>3</sub>COCHClOOH | k = 3.30·10<sup>-12</sup>exp(820/T) | MCMv3.2, Rickard et al. (21.10.2013)                                    |
| H72 | CH<sub>3</sub>COCHClO<sub>2</sub> + NO → CICH<sub>2</sub>OH + CH<sub>3</sub>CO + NO<sub>2</sub> | k = 2.70·10<sup>-12</sup>exp(360/T) | Atkinson et al. (2008)                                                  |
| H73 | CH<sub>3</sub>COCHClO<sub>2</sub> + NO<sub>3</sub> → CICH<sub>2</sub>OH + CH<sub>3</sub>CO + NO<sub>2</sub> | k = 2.30·10<sup>-12</sup> | MCMv3.2, Rickard et al. (21.10.2013)                                    |
| H74 | CH<sub>3</sub>COCHClO<sub>2</sub> + CH<sub>3</sub>O<sub>2</sub> → CICH<sub>2</sub>OH + CH<sub>3</sub>CO + 0.8 HCHO + 0.2 CH<sub>3</sub>OH + NO<sub>2</sub> | k = 2.00·10<sup>-12</sup> | estimated                                                              |
| H75 | CH<sub>3</sub>COCHClOOH + OH → CH<sub>3</sub>COCHClO<sub>2</sub> | k = 8.34·10<sup>-12</sup> | MCMv3.2, Rickard et al. (21.10.2013)                                    |
| H76 | CICH<sub>2</sub>OH + NO<sub>3</sub> → CO + Cl + HNO<sub>3</sub> | k = 1.40·10<sup>-12</sup>exp(-1860/T) | Atkinson et al. (2008)                                                  |
| H77 | CICH<sub>2</sub>OH + OH → CO + Cl + H<sub>2</sub>O | k = 6.12·10<sup>-12</sup> | Atkinson et al. (2008)                                                  |
| H78 | CH<sub>3</sub>CH(Cl)CHO + OH → CH<sub>3</sub>CH( Cl)( C)( O)<sub>2</sub> | k = 4.90·10<sup>-12</sup>exp(405/T) | MCMv3.2, Rickard et al. (21.10.2013)                                    |
| H79 | CH<sub>3</sub>CH(Cl)CHO + NO<sub>3</sub> → CH<sub>3</sub>CH( Cl)( C)( O)<sub>2</sub> + HNO<sub>3</sub> | k = 3.24·10<sup>-12</sup>exp(-1860/T) | MCMv3.2, Rickard et al. (21.10.2013)                                    |
| H80 | CH<sub>3</sub>CH(Cl)( C)( O)<sub>2</sub> + HO<sub>2</sub> → 0.15 CH<sub>3</sub>CH(Cl)COOH + 0.15 O<sub>3</sub> + 0.41 CH<sub>3</sub>CH(Cl)( C)( O)OOH + 0.44 CH<sub>3</sub>CH(Cl)<sub>2</sub>O<sub>2</sub> + 0.44 OH | k = 5.20·10<sup>-13</sup>exp(980/T) | MCMv3.2, Rickard et al. (21.10.2013)                                    |
| H81 | CH<sub>3</sub>CH(Cl)( C)( O)<sub>2</sub> + NO → CH<sub>3</sub>CH(Cl)<sub>2</sub>O<sub>2</sub> + NO<sub>2</sub> | k = 7.50·10<sup>-12</sup>exp(290/T) | MCMv3.2, Rickard et al. (21.10.2013)                                    |
| H82 | CH<sub>3</sub>CH(Cl)CO<sub>3</sub> + NO<sub>2</sub> → CH<sub>3</sub>CIPAN | TROE                      | MCMv3.2, Rickard et al. (21.10.2013)                                    |
| Nr. | Reaction                                                                 | Rate constant(a)          | Comment                                      |
|-----|--------------------------------------------------------------------------|---------------------------|----------------------------------------------|
| H83 | CH3CIPAN → CH3CH(Cl)CO3 + NO2                                             | TROE                      | MCMv3.2, Rickard et al. (21.10.2013)         |
| H84 | CH3CH(Cl)(O)O2 + NO2 → CH3CH(Cl)O2 + NO2                                  | k = 4.00·10^{-12}         | MCMv3.2, Rickard et al. (21.10.2013)         |
| H85 | CH3CH(Cl)(C)(O)2 + CH3O2 → 0.3 CH3CH(Cl)COOH + 0.7 CH3CH(Cl)O2 + HCHO + HO2 | k = 1.00·10^{-11}         | estimated                                    |
| H86 | CC(Cl)(=O)OO + OH → CC(Cl)(=O)O[O]                                        | k = 4.42·10^{-12}         | MCMv3.2, Rickard et al. (21.10.2013)         |
| H87 | CH3CH(Cl)COOH + OH → CH3CH(Cl)O2                                         | k = 1.20·10^{-12}         | MCMv3.2, Rickard et al. (21.10.2013)         |
| H88 | CH3CH(Cl)O2 + NO2 → CH3CHO + Cl + NO2                                    | k = 3.30·10^{-13}exp(820/T)| MCMv3.2, Rickard et al. (21.10.2013)         |
| H89 | CH3CH(Cl)O2 + NO → CH3CHO + Cl + NO2                                     | k = 4.05·10^{-12}exp(360/T)| MCMv3.2, Rickard et al. (21.10.2013)         |
| H90 | CH3CH(Cl)O2 + NO2 → CH3CHO + Cl + NO2                                    | k = 2.30·10^{-12}         | MCMv3.2, Rickard et al. (21.10.2013)         |
| H91 | CH3CH(Cl)O2 + CH3O2 → 0.6 CH3CHO + 0.6 Cl + 0.4 CH3C(O)Cl + 0.8 HCHO + 0.2 CH3OH + 0.8 HO2 | k = 2.65·10^{-12}         | MCMv3.2, Rickard et al. (21.10.2013)         |
| H92 | CH3CH(Cl)OOH + OH → CH3CH(Cl)O2 + H2O                                    | k = 1.90·10^{-12}exp(190/T)| MCMv3.2, Rickard et al. (21.10.2013)         |
| H93 | CH3CH(Cl)OOH + OH → CH3C(O)Cl + OH + H2O                                 | k = 9.95·10^{-12}         | MCMv3.2, Rickard et al. (21.10.2013)         |
| H94 | CH3C(O)Cl + OH → CICOCH2O2 + H2O                                        | k = 3.88·10^{-14}         | MCMv3.2, Rickard et al. (21.10.2013)         |
| H95 | CICOCH2O2 + HO2 → CICOCH3OOH                                            | k = 3.30·10^{-13}exp(820/T)| MCMv3.2, Rickard et al. (21.10.2013)         |
| H96 | CICOCH2O2 + NO2 → HCHO + Cl + CO + NO2                                   | k = 3.24·10^{-12}exp(360/T)| MCMv3.2, Rickard et al. (21.10.2013)         |
| H97 | CICOCH2O2 + NO3 → HCHO + Cl + CO + NO3                                   | k = 2.30·10^{-12}         | MCMv3.2, Rickard et al. (21.10.2013)         |
| H98 | CICOCH2O2 + CH3O2 → 2 HCHO + Cl + CO + HO2                               | k = 2.00·10^{-12}         | MCMv3.2, Rickard et al. (21.10.2013)         |
| H99 | Br + O1 → BrO                                                            | k = 1.70·10^{-11}exp(-800/T)| Atkinson et al. (2007)                        |
| H100| BrO + HO2 → HOBr                                                         | k = 4.50·10^{-12}exp(-500/T)| Atkinson et al. (2007)                        |
| H101| BrO + BrO → 1.7 Br + 0.15 Br2                                            | k = 1.60·10^{-12}exp(-210/T)| Atkinson et al. (2007)                        |
| H102| Br + NO2 → BrNO2                                                          | TROE                      | Atkinson et al. (2007)                        |
| H103| BrO + NO → Br + NO2                                                      | k = 8.70·10^{-12}exp(-260/T)| Atkinson et al. (2007)                        |
| H104| BrO + NO2 → BrNO3                                                        | TROE                      | Atkinson et al. (2007)                        |
| H105| BrNO3 → BrO + NO2                                                        | k = 2.79·10^{-3}exp(-12360/T)| Orlando and Tyndall (1996)                   |
| H106| Br + BrNO3 → Br2 + NO3                                                   | k = 4.90·10^{-11}         | Orlando and Tyndall (1996)                   |
| H107| BrO + ClO → 0.95 Br + 0.5 OCIO + 0.45 Cl + 0.05 BrCl                      | k = 7.32·10^{-12}exp(-200/T)| Summation A-Factor Burkholder et al. (2015)   |
| H108| BrO + CH3O2 → 0.25 Br + 0.25 HCHO + 0.25 HO2 + 0.75 HOB + 0.75 HCOOH    | k = 4.10·10^{-13}exp(-800/T)| Bräuer et al. (2013)                         |
| H109| Br + CH3O2 → 0.17 BrCHO + 0.09 Br + 0.74 HBr + 0.09 GLYOXAL + 1.65 CO + 0.91 HO2 | k = 6.35·10^{-15}exp(-440/T)| Atkinson et al. (2006)                        |
| Nr. | Reaction | Rate constant$^{(a)}$ | Comment |
|-----|----------|-----------------------|---------|
| H110 | Br + HCHO → HBr + CO + HO2 | k = 1.70·10^{-13} exp(-800/T) | Sander et al. (2006) |
| H111 | BrO + HCHO → HOBr + CO + HO2 | k = 1.50·10^{-14} | Hansen et al. (1999) |
| H112 | Br + CH₃CHO → HBr + CH₃CO₂ | k = 1.80·10^{-11} exp(-460/T) | Atkinson et al. (2006) |
| H113 | Br + C₂H₃CHO → HBr + 1.5 CH₂CO₂ | k = 5.75·10^{-11} exp(-610/T) | Ramacher et al. (2000) |
| H114 | Br + C₂H₄ → BrCH₂CH₂O₂ | k = 2.25·10^{-12} exp(-277/T) | Atkinson et al. (2006) |
| H115 | BrCH₂CH₂O₂ + NO → BrCH₂CHO + HO₂ + NO₂ | k = 9.70·10^{-12} | Atkinson et al. (2008) |
| H116 | BrCH₂CH₂O₂ + CH₃O₂ → BrCH₂CHO + 0.8 HCHO + 0.2 CH₃OH + 1.4 HO₂ | k = 2.00·10^{-12} | Bräuer et al. (2013) |
| H117 | BrCH₂CHO + OH → BrCH₂CO₂ + H₂O | k = 2.05·10^{-12} | Atkinson et al. (2008) |
| H118 | BrCH₂CO₂ + HO₂ → 0.15 BrCH₂COOH + 0.15 O₃ + 0.41 BrCH₂C(O)OOH + 0.44 BrCH₂O₂ + 0.44 OH | k = 5.20·10^{-13} exp(980/T) | MCMv3.2, Rickard et al. (21.10.2013) |
| H119 | BrCH₂CO₂ + NO → BrCH₂O₂ + NO₂ | k = 7.50·10^{-12} exp(290/T) | MCMv3.2, Rickard et al. (21.10.2013) |
| H120 | BrCH₂CO₂ + CH₃O₂ → 0.7 BrCH₂O₂ + 0.3 BrCH₂COOH + 0.7 HO₂ + HCHO | k = 1.00·10^{-11} | Bräuer et al. (2013) |
| H121 | BrCH₂COOH + H₂O → BrCH₂O₂ + H₂O | k = 1.90·10^{-12} exp(190/T) | MCMv3.2, Rickard et al. (21.10.2013) |
| H122 | BrCH₂C(O)OOH + OH → BrCH₂CO₂ + H₂O | k = 3.79·10^{-12} | MCMv3.2, Rickard et al. (21.10.2013) |
| H123 | BrCH₂O₂ + HO₂ → BrCH₂OOH | k = 4.28·10^{-13} exp(820/T) | MCMv3.2, Rickard et al. (21.10.2013) |
| H124 | BrCH₂O₂ + NO → BrCHO + HO₂ + NO₂ | k = 4.05·10^{-12} exp(360/T) | MCMv3.2, Rickard et al. (21.10.2013) |
| H125 | BrCH₂O₂ + NO → BrCHO + HO₂ + NO₂ | k = 2.30·10^{-12} | MCMv3.2, Rickard et al. (21.10.2013) |
| H126 | BrCH₂O₂ + CH₃O₂ → 1.4 HO₂ + BrCHO + 0.8 HCHO + 0.2 CH₃OH | k = 2.00·10^{-12} | Bräuer et al. (2013) |
| H127 | BrCH₂OOH + OH → BrCH₂O₂ + H₂O | k = 1.90·10^{-12} exp(190/T) | MCMv3.2, Rickard et al. (21.10.2013) |
| H128 | BrCH₂OOH + OH → BrCHO + OH + H₂O | k = 5.79·10^{-12} | MCMv3.2, Rickard et al. (21.10.2013) |
| H129 | BrCHO + NO₂ → CO + Br + HNO₂ | k = 1.40·10^{-12} exp(-1860/T) | Atkinson et al. (2008) |
| H130 | BrCHO + OH → CO + Br + H₂O | k = 1.16·10^{-12} | Atkinson et al. (2008) |
| H131 | Br + C₂H₆ → CH₂CH(OC₂H₃)Br | k = 3.60·10^{-12} | Atkinson et al. (2006) |
| H132 | CH₃CH(OC₂H₅)CH₂Br + NO → CH₃COCH₂Br + HO₂ + NO₂ | k = 2.70·10^{-12} exp(360/T) | Atkinson et al. (2008) |
| H133 | CH₃CH(OC₂H₅)CH₂Br + CH₃O₂ → CH₃COCH₂Br + 0.8 HCHO + 0.2 CH₃OH + 1.4 HO₂ | k = 4.00·10^{-14} | Bräuer et al. (2013) |
| H134 | CH₃COCH₂Br + OH → CH₃COCH₂BrO₂ | k = 8.80·10^{-12} exp(-1320/T) | Atkinson et al. (2008) |
| H135 | CH₃COCH₂BrO₂ + NO → CH₃CO₂ + BrCHO + NO₂ | k = 8.00·10^{-12} | Atkinson et al. (2008) |
| H136 | CH₃COCH₂BrO₂ + CH₃O₂ → 0.4 CH₃COC(O)Br + 0.6 CH₃CO₂ + 0.6 BrCHO + 0.8 HO₂ + 0.8 HCHO + 0.2 CH₃OH | k = 2.00·10^{-12} | Bräuer et al. (2013) |
| Nr. | Reaction | Rate constant*(a) | Comment |
|-----|----------|-------------------|---------|
| H137 | I + O₃ → IO | k = 2.10·10⁻¹¹ exp(-830/T) | Atkinson et al. (2007) |
| H138 | I₂ + OH → I + HOI | k = 2.10·10⁻¹⁰ | Atkinson et al. (2007) |
| H139 | IO + HO₂ → HOI | k = 1.40·10⁻¹¹ exp(540/T) | Atkinson et al. (2007) |
| H140 | IO + IO → 0.38 OIO + 0.46 IO₂ + 0.6 I + 0.05 I₂ | k = 5.40·10⁻¹¹ exp(180/T) | Sander et al. (2006) |
| H141 | OIO + OH → HIO₃ | k = 2.20·10⁻¹⁰ exp(243/T) | von Glasow et al. (2002) |
| H142 | IO + O₁ → 0.83 I + 0.17 OIO | k = 1.20·10⁻¹⁵ | (Larin et al., 1999) |
| H143 | IO + OIO → I₂O₃ | k = 1.00·10⁻¹⁰ | (Gómez Martin et al., 2007) |
| H144 | I₂O₁ → IO + OIO | k = 2.78·10⁻¹¹ | (Kaltsoyannis and Plane, 2008) |
| H145 | OIO + OIO → I₂O₄ | k = 1.00·10⁻¹⁰ | (Saunders and Plane, 2005) |
| H146 | I₂O₄ → OIO + OIO | k = 1.67·10⁻⁰⁰ | (Kaltsoyannis and Plane, 2008) |
| H147 | I₂ + O₁ → IO + I | k = 4.02·10⁻¹⁵ exp(-2050/T) | (Vikis and Macfarlane, 1985) |
| H148 | I₂O₂ → 0.995 OIO + 0.995 I + 0.01 IO | k = 1.00·10⁻⁰¹ | (Kaltsoyannis and Plane, 2008) |
| H149 | I₂ + NO₁ → I + INO₃ | k = 1.50·10⁻¹² | Atkinson et al. (2007) |
| H150 | IO + NO → I + NO₂ | k = 7.15·10⁻¹² exp(300/T) | Atkinson et al. (2007) |
| H151 | IO + NO₂ → INO₂ | k = 1.50·10⁻¹¹ exp(510/T) | Atkinson et al. (2007) |
| H152 | INO₃ → IO + NO₂ | k = [M]*4.40·10⁻⁰⁵ exp(12060/T) | Atkinson et al. (2007) |
| H153 | IO + CH₂O → I + HO₂ + HCHO | k = 2.00·10⁻¹² | (Dillon et al., 2006) |
| H154 | IO + ClO → 0.8 I + 0.55 OCIIO + 0.25 Cl + 0.2 ICl | k = 4.70·10⁻¹² exp(280/T) | Atkinson et al. (2007) |
| H155 | IO + BrO → 0.8 OIO + Br + 0.2 I | k = 1.50·10⁻¹¹ exp(510/T) | Atkinson et al. (2007) |

**Photolysis reactions**

| Nr. | Reaction | Rate constant*(a) | Comment |
|-----|----------|-------------------|---------|
| H156 | Cl₂ → Cl + Cl | J = 3.827·10⁰⁺ cos(χ)cos(0.54² cos(0.024 cos(χ))) | Bräuer et al. (2013) |
| H157 | ClO → Cl + O(¹P) | J = 4.755·10⁰⁺ cos(χ)cos(0.588 cos(χ)) | Bräuer et al. (2013) |
| H158 | OCIO → ClO + O(³P) | J = 1.332·10⁻¹ cos(χ)exp(-0.244 cos(χ)) | Bräuer et al. (2013) |
| H159 | HOCl → Cl + OH | J = 4.615·10⁻⁰⁺ cos(χ)exp(-0.240 cos(χ)) | Bräuer et al. (2013) |
| H160 | CINO₂ → Cl + NO₂ | J = 6.219·10⁻⁰⁺ cos(χ)exp(-0.255 cos(χ)) | Bräuer et al. (2013) |
| H161 | CINO₃ → Cl + NO₃ | J = 6.420·10⁻⁰⁺ cos(χ)exp(-0.217 cos(χ)) | Bräuer et al. (2013) |
| H162 | CINO₃ → ClO + NO₂ | J = 1.393·10⁻⁰⁺ cos(χ)exp(-0.243 cos(χ)) | Bräuer et al. (2013) |
| H163 | CC(=O)ClOCCl → CICH₂CHO + CH₂CO₃ + OH | J = 7.649·10⁻⁰⁺ cos(χ)exp(-0.279 cos(χ)) | Bräuer et al. (2013) |
| H164 | CICH₂CHO + HO₂ + OH | J = 7.649·10⁻⁰⁺ cos(χ)exp(-0.279 cos(χ)) | Bräuer et al. (2013) |
| H165 | CICH₂CHO → CICH₂O₂ + HO₂ + CO | J = 4.642·10⁻⁰⁺ cos(χ)exp(-0.353 cos(χ)) | Bräuer et al. (2013) |
| Nr. | Reaction | Rate constant<sup>(a)</sup> | Comment |
|-----|----------|-----------------------------|---------|
| H166 | CH₂C(O)OOH → CH₂O₂ + OH | J = 7.649·10⁻⁶cos(χ)⁰·₆₈²exp(-0.279/cos(χ)) | Bräuer et al. (2013) |
| H167 | CH₂OOH → CICHO + HO₂ + OH | J = 7.649·10⁻⁶cos(χ)⁰·₆₈²exp(-0.279/cos(χ)) | Bräuer et al. (2013) |
| H168 | CH₃CH(O)CH₂Cl → CH₃O₂ + CHCl₂CO₂⁺ | J = 5.804·10⁻⁶cos(χ)⁰·₁₀⁹exp(-0.377/cos(χ)) | Bräuer et al. (2013) |
| H169 | CH₃CH(O)CH₂OOH → CICHO + CH₂CO₂⁺ + OH | J = 7.649·10⁻⁶cos(χ)⁰·₆₈²exp(-0.279/cos(χ)) | Bräuer et al. (2013) |
| H170 | CICCHO → HO₂ + CO + Cl | J = 4.642·10⁻⁶cos(χ)⁰·₇₆²exp(-0.353/cos(χ)) | Bräuer et al. (2013) |
| H171 | CH₃CH(Cl)CHO → CH₃CH(Cl)O₂ + HO₂ + CO | J = 2.879·10⁻⁶cos(χ)⁰·₁₀⁹exp(-0.358/cos(χ)) | Bräuer et al. (2013) |
| H172 | CH₃CH(Cl)OOH → CH₃CHO + Cl + OH | J = 7.649·10⁻⁶cos(χ)⁰·₆₈²exp(-0.279/cos(χ)) | Bräuer et al. (2013) |
| H173 | CH₃C(O)Cl → CH₃CO + Cl | J = 5.804·10⁻⁶cos(χ)⁰·₁₀⁹exp(-0.377/cos(χ)) | Bräuer et al. (2013) |
| H174 | CICOCH₂OOH → ClCOCH₂O₂ + OH | J = 7.649·10⁻⁶cos(χ)⁰·₆₈²exp(-0.279/cos(χ)) | Bräuer et al. (2013) |
| H175 | Br₂ → Br + Br | J = 4.773·10⁻⁷cos(χ)⁰·₁⁹⁹exp(-0.213/cos(χ)) | Bräuer et al. (2013) |
| H176 | BrO → Br + O(P) | J = 6.368·10⁻⁷cos(χ)⁰·₁⁶⁹exp(-0.269/cos(χ)) | Bräuer et al. (2013) |
| H177 | HOBr → Br + OH | J = 3.464·10⁻⁷cos(χ)⁰·₄⁴⁴exp(-0.214/cos(χ)) | Bräuer et al. (2013) |
| H178 | BrNO₂ → Br + NO₂ | J = 7.443·10⁻⁷cos(χ)⁰·₃⁵⁵exp(-0.236/cos(χ)) | Bräuer et al. (2013) |
| H179 | BrNO₂ → 0.29 Br + 0.29 NO₃ + 0.71 BrO + 0.71 NO₂ | J = 2.194·10⁻⁷cos(χ)⁰·₄⁹⁹exp(-0.215/cos(χ)) | Bräuer et al. (2013) |
| H180 | BrCl → Br + Cl | J = 1.650·10⁻⁷cos(χ)⁰·₂⁹⁷exp(-0.224/cos(χ)) | Bräuer et al. (2013) |
| H181 | BrCH₂CHO → BrCH₂O₂ + HO₂ + CO | J = 4.642·10⁻⁷cos(χ)⁰·₇₆²exp(-0.353/cos(χ)) | Bräuer et al. (2013) |
| H182 | BrCH₂C(O)OOH → BrCH₂O₂ + OH | J = 7.649·10⁻⁷cos(χ)⁰·₆₈²exp(-0.279/cos(χ)) | Bräuer et al. (2013) |
| H183 | BrCH₂OOH → BrCHO + OH + HO₂ | J = 7.649·10⁻⁷cos(χ)⁰·₆₈²exp(-0.279/cos(χ)) | Bräuer et al. (2013) |
| H184 | BrCHO → HO₂ + CO + Br | J = 4.642·10⁻⁷cos(χ)⁰·₇₆²exp(-0.353/cos(χ)) | Bräuer et al. (2013) |
| H185 | CH₃COCOHBr → 0.7 CO + 0.7 Br + 0.7 CH₃CO₂⁺ + 0.3 BrCH₂CO₂⁺ + 0.3 CH₃O₂⁺ | J = 3.523·10⁻⁷cos(χ)⁰·₈₃₈exp(-0.283/cos(χ)) | Bräuer et al. (2013) |
| H186 | CH₃COC(O)Br → CO + Br + CH₂CO₂⁺ | J = 1.853·10⁻⁷cos(χ)⁰·₅₈⁸exp(-0.225/cos(χ)) | Bräuer et al. (2013) |
| H187 | CHBr₃ → 3 Br + CO + HO₂ | J = 2.228·10⁻⁷cos(χ)¹·₄⁷¹exp(-0.2³⁰/cos(χ)) | Bräuer et al. (2013) |
| H188 | I₂ → I + I | J = 2.165·10⁻⁶cos(χ)⁰·₁²²exp(-0.1₈⁵/cos(χ)) | Bräuer et al. (2013) |
| H189 | IO → I⁺ + O(P) | J = 2.640·10⁻⁶cos(χ)⁰·₂⁴⁹exp(-0.2₄⁰/cos(χ)) | Bräuer et al. (2013) |
| H190 | OIO → 0.₉₆ I + 0.₀₄ IO + 0.₀₄ O(P) | J = 4.0₅₄·10⁻⁶cos(χ)⁰·₁₁⁹exp(-0.₁₈⁵/cos(χ)) | Bräuer et al. (2013) |
| H191 | HOI → I + OH | J = 1.₄₆₉·10⁻⁶cos(χ)⁰·₃₄²exp(-0.₂₃₆/cos(χ)) | Bräuer et al. (2013) |
| H192 | INO₂ → 0.₈₅ I + 0.₈₅ NO₂ + 0.₁₅ IO + 0.₁₅ NO₂ | J = 6.₉₉₉·10⁻⁶cos(χ)⁰·₅₃₈exp(-0.₂₄₃/cos(χ)) | Bräuer et al. (2013) |
| H193 | ICl → I⁺ + Cl | J = 3.₄₀₃·10⁻⁶cos(χ)⁰·₁₇⁷exp(-0.₂₀⁷/cos(χ)) | Bräuer et al. (2013) |
| H194 | IBr → I⁺ + Br | J = 1.₀₀₀·10⁻⁶cos(χ)⁰·₁₄⁹exp(-0.₁₉⁷/cos(χ)) | Bräuer et al. (2013) |
| H195 | C₃H₂I → 1 + C₃H₂O₂ | J = 3.₇₃₁·10⁻⁶cos(χ)¹·₂₉⁸exp(-0.₂₁⁷/cos(χ)) | Bräuer et al. (2013) |
| H196 | CH₃I₂ → 2 I + 2 HO₂ | J = 1.₄₉₆·10⁻⁶cos(χ)⁰·₈₃⁰exp(-0.₂₆₅/cos(χ)) | Bräuer et al. (2013) |
| Nr. | Reaction | Rate constant\(^{(a)}\) | Comment |
|-----|----------|--------------------------|---------|
| H197 | CH$_3$I $\rightarrow$ I + CH$_3$O$_2$ | \[ J = 1.206 \times 10^{0.5} \cos(\chi) \times 1.25 \times \exp(-0.231 / \cos(\chi)) \] | Bräuer et al. (2013) |
| H198 | ClCH$_3$I $\rightarrow$ I + ClCH$_2$O$_2$ | \[ J = 6.910 \times 10^{0.4} \cos(\chi) \times 1.85 \times \exp(-0.238 / \cos(\chi)) \] | Bräuer et al. (2013) |
| H199 | BrCH$_3$I $\rightarrow$ I + BrCH$_2$O$_2$ | \[ J = 4.261 \times 10^{0.4} \cos(\chi) \times 0.976 \times \exp(-0.250 / \cos(\chi)) \] | Bräuer et al. (2013) |

(a) \(k^{2nd}\) in cm$^3$ molecules$^{-1}$ s$^{-1}$; \(k^{1st}\) in s$^{-1}$; \(J\) in s$^{-1}$

Table S7  Parameters for pressure dependent reactions.

| Reaction | TYPE | \(k_0^{(a)}\) | \(k_\infty^{(a)}\) | \(F_c\) |
|----------|------|----------------|-----------------|-------|
| H5       | Cl + NO$_2$ $\rightarrow$ ClNO$_2$ | TROE | 1.80 \times 10^{-31} \times (T/298)^{2.0} | 1.00 \times 10^{-10} \times (T/298)^{1.0} | 0.6 |
| H6       | ClO + NO$_2$ $\rightarrow$ ClNO$_3$ | TROE | 1.60 \times 10^{-31} \times (T/298)^{3.4} | 7.00 \times 10^{-11} | 0.4 |
| H44      | Cl + C$_2$H$_2$ $\rightarrow$ 0.26 ClCHO + 0.21 Cl + 0.53 HCl + 0.21 GLYOXAL + 1.32 CO + 0.79 HO$_2$ | TROE | 6.10 \times 10^{-30} \times (T/298)^{3.0} | 2.00 \times 10^{-10} | 0.6 |
| H45      | Cl + C$_2$H$_4$ $\rightarrow$ ClCH$_2$CH$_2$O$_2$ | TROE | 1.85 \times 10^{-29} \times (T/298)^{3.3} | 6.00 \times 10^{-10} | 0.4 |
| H54      | ClCH$_2$CO$_2$ + NO$_2$ $\rightarrow$ CIPAN | TROE | 2.70 \times 10^{-28} \times (T/298)^{7.1} | 1.20 \times 10^{-11} \times (T/298)^{9.9} | 0.3 |
| H60      | CIPAN $\rightarrow$ ClCH$_2$CO$_3$ + NO$_2$ | TROE | 4.90 \times 10^{-10} \times \exp(-12100/T) | 5.40 \times 10^{-16} \times \exp(-13830/T) | 0.3 |
| H82      | CH$_2$CH(Chi)CO$_3$ + NO$_2$ $\rightarrow$ CH$_2$CIPAN | TROE | 2.70 \times 10^{-28} \times (T/298)^{7.1} | 1.20 \times 10^{-11} \times (T/298)^{9.9} | 0.3 |
| H83      | CH$_2$CIPAN $\rightarrow$ CH$_2$CH(Chi)CO$_3$ + NO$_2$ | TROE | 4.90 \times 10^{-10} \times \exp(-12100/T) | 5.40 \times 10^{-16} \times \exp(-13830/T) | 0.3 |
| H102     | Br + NO$_2$ $\rightarrow$ BrNO$_2$ | TROE | 4.20 \times 10^{-31} \times (T/298)^{2.4} | 2.70 \times 10^{-11} | 0.55 |
| H104     | BrO + NO$_2$ $\rightarrow$ BrNO$_3$ | TROE | 4.70 \times 10^{-31} \times (T/298)^{3.1} | 1.80 \times 10^{-11} | 0.4 |
| H151     | IO + NO$_2$ $\rightarrow$ IO$_3$ | TROE | 7.70 \times 10^{-31} \times (T/300)^{3.0} | 1.60 \times 10^{-11} | 0.6 |

(a) \(k^{2nd}\) in cm$^3$ molecules$^{-1}$ s$^{-1}$; \(k^{1st}\) in s$^{-1}$

Rate constants calculated with TROE formula: \(k(T) = \frac{k_0(T)[M]}{k_\infty(T)[M]} \times F_c \times \left[ \frac{1 + \ln(\frac{k_0(T)[M]}{k_\infty(T)[M]})}{1 + \ln(\frac{k_0(T)[M]}{k_\infty(T)[M]})} \right]^{1/10} \)
| Species | $K_H$ (298 K)$^\text{[a]}$ | $\Delta H/R$ | $\alpha$ | $D_g$ (298 K)$^\text{[c]}$ | Comment |
|---------|-----------------|----------|-----|-----------------|--------|
| H200$^\circledR$ Cl$_2$ | $9.15 \cdot 10^{-2}$ | 2490 | 0.08 | 1.28 | Bräuer et al. (2013) |
| H201 | Cl | $2.00 \cdot 10^{-3}$ | 0.05 | 1.82 | Bräuer et al. (2013) |
| H202$^\circledR$ HCl | $1.10 \cdot 10^8$ | 2020 | 0.1026 | 1.89 | Bräuer et al. (2013) |
| H203$^\circledR$ HOCl | $6.60 \cdot 10^2$ | 5862 | 0.5 | 1.51 | Bräuer et al. (2013) |
| H204$^\circledR$ CINO$_2$ | $2.40 \cdot 10^{-2}$ | 0.01 | 1.27 | 1.27 | Bräuer et al. (2013) |
| H205$^\circledR$ CINO$_3$ | $2.10 \cdot 10^8$ | 8700 | 0.1 | 1.18 | Bräuer et al. (2013) |
| H206 | CICHO | $3.00 \cdot 10^3$ | 7216 | 0.02 | 1.23 | Bräuer et al. (2013) |
| H207$^\circledR$ Br$_2$ | $7.60 \cdot 10^{-3}$ | 4100 | 0.08 | 1.00 | Bräuer et al. (2013) |
| H208 | Br | $1.20 \cdot 10^{-3}$ | 0.05 | 1.29 | Bräuer et al. (2013) |
| H209$^\circledR$ HBr | $1.30 \cdot 10^8$ | 10239 | 0.0481 | 1.26 | Bräuer et al. (2013) |
| H210 | HOBr | $9.30 \cdot 10^4$ | 5862 | 0.5 | 1.16 | Bräuer et al. (2013) |
| H211 | BrNO$_3$ | $2.10 \cdot 10^8$ | 8700 | 0.8 | 1.01 | Bräuer et al. (2013) |
| H212 | BrCl | $9.40 \cdot 10^{-3}$ | -5600 | 0.33 | 1.05 | Bräuer et al. (2013) |
| H213 | BrCH$_2$CO$_2$ | $6.69 \cdot 10^2$ | 5893 | 0.019 | 0.84 | Bräuer et al. (2013) |
| H214$^\circledR$ BrCH$_2$COOH | $1.52 \cdot 10^3$ | 9300 | 0.0322 | 0.84 | Bräuer et al. (2013); Sander (2015) |
| H215 | BrCHO | $7.40 \cdot 10^3$ | 0.02 | 1.02 | Bräuer et al. (2013) |
| H216 | I$_2$ | $3.00 \cdot 10^8$ | 4431 | 0.0126 | 0.86 | Bräuer et al. (2013) |
| H217$^\circledR$ HI | $4.50 \cdot 10^2$ | 5862 | 0.5 | 1.08 | Bräuer et al. (2013) |
| H218 | HIO$_3$ | $2.10 \cdot 10^8$ | 8700 | 0.0126 | 0.98 | Bräuer et al. (2013) |
| H219$^\circledR$ INO$_3$ | $2.10 \cdot 10^8$ | 8700 | 0.123 | 0.96 | Bräuer et al. (2013) |
| H220$^\circledR$ I$_2$O$_2$ | $1.00 \cdot 10^8$ | 0.123 | 1.20 | 0.80 | Bräuer et al. (2013); Sander (2015) |
| H221$^\circledR$ ICl | $1.10 \cdot 10^2$ | 5600 | 0.0126 | 0.98 | Bräuer et al. (2013) |
| H222$^\circledR$ IBr | $2.40 \cdot 10^4$ | 5600 | 0.0126 | 0.88 | Bräuer et al. (2013) |

(a) in M \text{atm}^{-1}; (b) in K; (c) in m$^2$ s$^{-1}$
Table S9  Implemented aqueous-phase reactions in the CAPRAM-HM3.0red

| Reaction | Reaction | $k_{298}$ | $E_A/R$ | Comment |
|----------|----------|-----------|---------|---------|
| H223 ̈  | Cl\(^{+}\) + H\(_2\)O\(_2\) \rightarrow 2 Cl\(^+\) + H\(^+\) + HO\(_2\) | 6.20 \times 10^5 | 3340 | Jacobi et al. (1999) |
| H224 ̈  | Cl\(^{+}\) + H\(_2\)O \rightarrow H\(^+\) + Cl\(^+\) + ClOH\(^-\) | 2.34 \times 10^4 | | Buxton et al. (1998) |
| H225 ̈  | HOC\(_1\) + HO\(_2\) \rightarrow Cl\(^+\) + H\(_2\)O + O\(_2\) | 7.50 \times 10^6 | | Bräuer et al. (2013) |
| H226 ̈  | HOCl + OH \rightarrow ClO + H\(_2\)O | 2.00 \times 10^9 | | Bräuer et al. (2013) |
| H227 ̈  | Cl\(^{+}\) + HSO\(_3\) \rightarrow 2 Cl\(^+\) + H\(^+\) + SO\(_3\) | 1.70 \times 10^8 | 400 | Jacobi (1996) |
| H228 ̈  | HOCl + HSO\(_3\) \rightarrow Cl\(^+\) + H\(^+\) + SO\(_3\) | 7.60 \times 10^6 | | Herrmann (2003) |
| H229 ̈  | Cl\(^+\) + HSO\(_3\) \rightarrow HOCl + SO\(_2\)\(^2\)\(^-\) | 1.80 \times 10^7 | 7352 | Fortnum et al. (1960) |
| H230 ̈  | Cl\(^{+}\) + Fe\(_2\)\(^+\) \rightarrow 2 Cl\(^+\) + Fe\(_2\)\(^+\) | 1.00 \times 10^7 | 3030 | Thornton and Laurence (1973) |
| H231 ̈  | Cl\(^{+}\) + Fe\(_2\)\(^+\) + Fe\(_2\)\(^+\) + ClOH\(^-\) + OH\(^-\) - H\(_2\)O | 1.00 \times 10^7 | | Jacobsen et al. (1998) |
| H232 ̈  | Cl\(^{+}\) + Mn\(_2\)\(^+\) \rightarrow MnCl\(_2\) | 2.00 \times 10^7 | 4090 | Laurence and Thornton (1973) |
| H233 ̈  | MnCl\(_2\) + 0.588 Cl\(^{+}\) + 0.588 Mn\(_2\)\(^+\) + 0.824 Cl\(^{+}\) + 0.412 Mn\(_2\)\(^+\) | 5.10 \times 10^3 | | Deguillaume et al. (2010); Laurence and Thornton (1973) |
| H234 ̈  | 2 ClO \rightarrow Cl\(^+\) + ClO\(_2\) + 2 H\(^+\) | 2.50 \times 10^9 | | Klanning and Wolff (1985) |
| H235 ̈  | OH + ClO\(_2\) \rightarrow ClO + O\(_2\) + OH\(^-\) | 1.00 \times 10^6 | | Buxton and Subhani (1972) |
| H236 ̈  | Cl\(_2\) + H\(_2\)O \rightarrow 2 H\(^+\) + 2 Cl\(^+\) + O\(_2\) | 1.83 \times 10^7 | 5387 | Connick (1947) |
| H237 ̈  | Cl\(_2\) + SO\(_3\) \rightarrow HOC\(_1\) + Cl\(_2\)O\(_3\) | 1.62 \times 10^6 | 2800 | Shi et al. (2001) |
| H238 ̈  | Cl\(_2\) + HC\(_2\)O\(_2\) \rightarrow 2 Cl\(^+\) + H\(^+\) + C\(_2\)O\(_4\) | 1.30 \times 10^6 | | Bräuer et al. (2013) |
| H239 ̈  | Cl\(_2\) + C\(_2\)O\(_2\) \rightarrow 2 Cl\(^+\) + C\(_2\)O\(_4\) | 4.00 \times 10^6 | | Bräuer et al. (2013) |
| H240 ̈  | ClCHO \rightarrow CO + H\(^+\) + Cl\(^-\) | 1.00 \times 10^4 | | Prager et al. (2001) |
| H241 ̈  | Br + H\(_2\)O \rightarrow H\(^+\) + Br\(^-\) + HO\(_2\) | 4.00 \times 10^6 | | Sutton et al. (1965) |
| H242 ̈  | Br\(_2\) + HO\(_2\) \rightarrow Br\(^+\) + Br\(^-\) + 0.5 Br\(_2\) + 0.5 H\(_2\)O\(_2\) + 0.5 O\(_2\) | 8.80 \times 10^4 | | Sutton and Downes (1972) |
| H243 ̈  | BrO + BrO \rightarrow BrO\(_2\) + HOB\(_r\) + H\(^+\) | 2.80 \times 10^6 | | Klanning and Wolff (1985) |
| H244 ̈  | HOB\(_r\) + OH \rightarrow BrO + H\(_2\)O | 2.00 \times 10^6 | | Klanning and Wolff (1985) |
| H245 ̈  | HOB\(_r\) + HO\(_2\) \rightarrow Br + H\(_2\)O + O\(_2\) | 1.00 \times 10^6 | | Bräuer et al. (2013) |
| H246 ̈  | HOB\(_r\) + H\(_2\)O \rightarrow H\(^+\) + Br\(^-\) + H\(_2\)O + O\(_2\) | 3.50 \times 10^6 | | Young (1950) |
| H247 ̈  | HOB\(_r\) + HSO\(_3\) \rightarrow H\(^+\) + Br\(^-\) + HSO\(_3\) | 5.00 \times 10^6 | | Bräuer et al. (2013) |
| H248 ̈  | Br + HSO\(_3\) \rightarrow HOB\(_r\) + SO\(_2\)\(^2\)\(^-\) | 1.00 \times 10^6 | 5338 | Fortnum et al. (1960) |
| Reaction | $k_{298}^{(a)}$ | $E_a/R^{(b)}$ | Comment |
|----------|----------------|---------------|---------|
| H249     | Br' + NO₃ → Br + NO₂⁻ | 3.80×10⁹ | Zellner et al. (1996) |
| H250     | Br⁺ + Fe²⁺ → 2 Br⁺ + Fe³⁺ | 3.60×10⁶ | 3330 Thornton and Laurence (1973) |
| H251     | Br⁺ + Mn²⁺ → MnBr₂⁺ | 6.30×10⁶ | 4330 Thornton and Laurence (1973) |
| H252     | MnBr₂⁺ → 0.577 Br₂⁻ + 0.577 Mn²⁺ + 0.846 Br⁺ + 0.423 Mn³⁺ | 5.20×10⁶ | Thornton and Laurence (1973); Deguillaume et al. (2010) |
| H253     | BrO₂⁻ + SO₄²⁻ → BrO + O₂ + SO₄²⁻ | 1.40×10⁶ | Zuo and Katsumura (1998) |
| H254     | Br + O₁ → BrO + O₂ | 1.50×10⁸ | Von Gunten and Oliveras (1998) |
| H255     | BrO⁻ + HSO₃⁻ → BrO₂⁻ + SO₂⁻ + H⁺ | 2.70×10⁻² | Szirovicz and Boga (1998) |
| H256     | BrO⁻ + OH → BrO + O₂ + OH⁻ | 5.00×10⁶ | Amichai et al. (1969) |
| H257     | BrNO₁ → HOBr + HNO₂ | 1.00×10⁹ | Hanson et al. (1996) |
| H258     | BrO₂⁻ + HC₂O₄⁻ → BrO₂⁻ + 2 CO₂ + H₂O | 7.47×10⁻⁴ | Pelle et al. (2004) |
| H259     | BrCHO → CO + H⁺ + Br⁻ | 1.00×10⁴ | Bräuer et al. (2013) |
| H260     | CH₂BrCO₂⁻ + H₂O → CH₂BrCOOH + HO₂ | 3.55×10⁵ | Bräuer et al. (2013) |
| H261     | Br⁻ + HCOO⁻ → 2 Br⁻ + COOH | 4.90×10³ | Jacobi et al. (1996) |
| H262     | Br⁻ + HOCl → BrCl + H₂O – H⁺ | 1.30×10⁶ | Kumar and Margerum (1987) |
| H263     | BrO₂⁻ + HOCl → 0.85 ClO₂⁻ + 0.93 HOBr + 0.08 ClO⁻ + 0.07 BrO₃⁻ + 0.92 Cl⁻ + 0.92 H⁺ - 0.85 HOC₁ | 1.60×10⁵ | Nicson et al. (2003) |
| H264     | I⁻ + O₁ → HOI + O₂ | 2.17×10⁹ | 8790 Magi et al. (1997) |
| H265     | IO + IO → HOI + HIO + H⁺ - H₂O - H₂O₂ | 1.50×10⁹ | Buxton et al. (1986) |
| H266     | HOI + HSO₄⁻ → H⁺ + I⁻ + HSO₄⁻ | 5.00×10⁹ | Pechtl and von Glasow (2007) |
| H267     | HOI + OH → IO + H₂O | 7.00×10⁹ | Buxton and Mulazzani (2007) |
| H268     | INO₁ → HOI + HNO₂ | 1.62×10⁶ | 2800 Hoffmann et al. (2019b) |
| H269     | IO₂ + H⁺ → HIO₂ + HOI + H⁺ | 3.20×10⁴ | Valkai and Horvath (2016) |
| H270     | IO⁻ + OH → IO + O₂ + OH⁻ | 1.08×10⁵ | Mezyk (1996) |

(a) $k_{298}^{2nd}$ in l¹ mol⁻¹ s⁻¹; $k_{298}^{1st}$ in s⁻¹; (b) in K
Table S10  Implemented aqueous-phase equilibrium reactions in the CAPRAM-HM3.0red

- reactions that run in the cloud mode ‘sub#1’, ○ reactions that run in the aerosol mode ‘sub#2’, ● already included in CAPRAM3.0red

| Reaction                          | K(a)   | k_o,298(b) | E_A/R(c) | k_o,298(b) | E_A/R(c) | References                      |
|-----------------------------------|--------|------------|----------|------------|----------|---------------------------------|
| H271○•                            | Cl + Cl‘ ⇌ Cl^− | 1.4×10^4 | 8.5×10^9 | 6.0×10^4 | 6.0×10^4 | Buxton et al. (1998)            |
| H272○•                            | Cl_2 + H_2O ⇌ H^+ + Cl^− + HOC1 | 1.9×10^0^e^−4500/T | 4.0×10^4 | 8000 | 2.1×10^4 | 3500 | Wang and Margerum (1994) |
| H273○•                            | HCl ⇌ H^+ + Cl^− | 1.72×10^0^e^−6900/T | 5.0×10^11 | -6890 | 2.9×10^4 | Marsh and McElroy (1985); Graedel and Weschler (1981) |
| H274○•                            | Cl^− + OH ⇌ ClOH | 7.0×10^4 | 4.3×10^9 | 6.1×10^9 | 6.1×10^9 | Jayson et al. (1973)           |
| H275○•                            | Cl + OH' ⇌ ClOH' | 7.8×10^4 | 1.8×10^10 | 2.3×10^10 | 2.3×10^10 | Klining and Wolff (1985)       |
| H276○•                            | ClOH' + H' ⇌ Cl + H_2O | 5.1×10^4 | 2.1×10^10 | 4.1×10^10 | 4.1×10^10 | Jayson et al. (1973)           |
| H277○•                            | ClOH' + Cl' ⇌ Cl^− + OH' | 2.2×10^4 | 1.0×10^4 | 4.5×10^7 | 4.5×10^7 | Grigor'ev et al. (1987)        |
| H278○•                            | Cl^− + SO_4^2− ⇌ Cl + SO_4^2− | 1.2×10^6 | 2.5×10^8 | 2.1×10^8 | 2.1×10^8 | Buxton et al. (1999b)          |
| H279○•                            | Cl^− + NO_3^− ⇌ Cl + NO_3^− | 3.4×10^0^e^−4300/T | 3.4×10^8 | 4300 | 1.0×10^8 | Buxton et al. (1999a)          |
| H280                              | HOCl + NO_2 ⇌ ClNO_2 + OH' | 3.9×10^4 | 1.9×10^7 | 5.0×10^7 | 5.0×10^7 | Lahoutifard et al. (2002)      |
| H281○•                            | Cl^− + SO_4^2− ⇌ Cl^− + HOC1 + HSO_4^− | 1.1×10^4 | 3.2×10^10 | 2.8×10^10 | 2.8×10^10 | Wang and Margerum (1994)       |
| H282○•                            | Cl^− + NO_3^− ⇌ ClO_2 + NO_2 | 1.4×10^4 | 3.9×10^10 | 2.7×10^10 | 2.7×10^10 | Behnke et al. (1997)           |
| H283○•                            | Br + Br' ⇌ Br_2^{-} | 6.3×10^5 | 1.2×10^10 | 1.9×10^10 | 1.9×10^10 | Merenyi and Lind (1994)         |
| H284○•                            | Br_2 + H_2O ⇌ H^+ + Br + HBr | 1.0×10^4^e^−7500/T | 1.7×10^9 | 7500 | 1.6×10^10 | Beckwith et al. (1996)         |
| H285○•                            | HBr + H' ⇌ Br' + Br | 1.0×10^5 | 5.0×10^11 | 5.0×10^11 | 5.0×10^11 | Lax (1969)                     |
| H286○•                            | Br + OH ⇌ BrOH' | 3.3×10^2 | 1.1×10^10 | 3.3×10^10 | 3.3×10^10 | Zehavi and Rabani (1972)       |
| H287○•                            | Br + OH' ⇌ BrOH' | 3.1×10^3 | 1.3×10^10 | 4.2×10^6 | 4.2×10^6 | Zehavi and Rabani (1972); Klining and Wolff (1985) |
| H288○•                            | BrOH' + H' ⇌ Br + H_2O | 1.8×10^12 | 4.4×10^10 | 2.4×10^12 | 2.4×10^12 | Zehavi and Rabani (1972); Klining and Wolff (1985) |
| H289○•                            | BrOH' + Br ⇌ Br_2^{-} + OH' | 7.0×10^4 | 1.9×10^8 | 2.7×10^6 | 2.7×10^6 | Zehavi and Rabani (1972); de Violet (1981) |
| H290                              | HBr + HOBr ⇌ H^+ + Br + BrO_2^{-} | 6.7×10^12 | 2.0×10^5 | 3.0×10^6 | 3.0×10^6 | Field and Foersterling (1986) |
| H291                              | HBr + BrO_2^{-} ⇌ H^+ + Br + BrO_3^{-} | 1.7×10^9 | 3.2×10^0 | 2.0×10^0 | 2.0×10^0 | Field and Foersterling (1986) |
| H292○•                            | CH_3BrCOOH ⇌ CH_3BrCOO^- + H^+ | 1.75×10^5^e^6/T | 8.75×10^5 | -46 | 5.0×10^10 | Bräuer et al. (2013) |
| H293○•                            | Br_2 + SO_4^2- + H_2O ⇌ HBr + Br + HSO_4^- | 6.15×10^6 | 2.28×10^4 | 3.7×10^4 | 3.7×10^4 | Beckwith et al. (1996)         |
| H294○•                            | BrCl ⇌ HOBr + H^+ + Cl^- - H_2O | 1.8×10^5 | 1.0×10^5 | 5.6×10^9 | 5.6×10^9 | Wang et al. (1994)             |
| H295○•                            | BrCl‘ ⇌ Br’ + Cl^- | 1.6×10^7 | 1.9×10^3 | 1.2×10^10 | 1.2×10^10 | Donati (2002)                  |
| Reaction | K(a) | $k_{298}^{(b)}$ | $E_A/R^{(c)}$ | $k_{298}^{(b)}$ | $E_A/R^{(c)}$ | References |
|----------|------|----------------|----------------|----------------|----------------|------------|
| H296◎ | BrCl $\rightleftharpoons$ Br + Cl$^-$ | $6.10 \cdot 10^4$ | $6.10 \cdot 10^4$ | $1.00 \cdot 10^8$ | Donati (2002) |
| H297◎ | BrCl$^+$ + Br $\rightleftharpoons$ Br$_2$ + Cl$^-$ | $1.86 \cdot 10^9$ | $8.00 \cdot 10^9$ | $4.30 \cdot 10^6$ | Ershov (2004) |
| H298◎ | BrCl$^+$ + Cl$^-$ $\rightleftharpoons$ Br$^+$ + Cl$_2$ | $2.75 \cdot 10^8$ | $1.10 \cdot 10^2$ | $4.00 \cdot 10^6$ | Ershov (2004) |
| H299◎ | Br$_2$Cl $\rightleftharpoons$ BrCl + Br$^-$ | $5.60 \cdot 10^5$ | $4.30 \cdot 10^5$ | $7.70 \cdot 10^6$ | Wang et al. (1994) |
| H300◎ | BrCl$^+$ $\rightleftharpoons$ Br$_2$ + Cl$^-$ | $7.60 \cdot 10^4$ | $3.80 \cdot 10^4$ | $5.00 \cdot 10^4$ | Wang et al. (1994); Matthew and Anastasio (2006) |
| H301◎ | BrCl$_2$ $\rightleftharpoons$ BrCl + Cl$^-$ | $1.70 \cdot 10^4$ | $1.70 \cdot 10^5$ | $1.00 \cdot 10^4$ | Ershov (2004) |
| H302◎ | BrCl$^+$ $\rightleftharpoons$ Br$^+$ + Cl$_2$ | $1.50 \cdot 10^4$ | $9.00 \cdot 10^4$ | $6.00 \cdot 10^9$ | Ershov (2004) |
| H303 | I$_2$ + OH$^-$ $\rightleftharpoons$ I$_2$OH$^-$ | $5.00 \cdot 10^8$ | $1.00 \cdot 10^4$ | $2.00 \cdot 10^9$ | Buxton and Mulazzani (2007) |
| H304 | I$_2$OH$^-$ $\rightleftharpoons$ HOI + I$^-$ | $8.30 \cdot 10^6$ | $2.49 \cdot 10^9$ | $3.00 \cdot 10^8$ | Buxton and Mulazzani (2007) |
| H305 | HOI + H$^+$ + I$^-$ $\rightleftharpoons$ I$_2$ + H$_2$O | $1.47 \cdot 10^{12}$ | $4.40 \cdot 10^{12}$ | $3.00 \cdot 10^8$ | Eigen and Kustin (1962) |
| H306◎ | HIO$_3$ $\rightleftharpoons$ H$^+$ + IO$_4^-$ | $1.70 \cdot 10^4$ | $8.50 \cdot 10^9$ | $5.00 \cdot 10^4$ | Lide et al. (1995) |
| H307◎ | HOI + H$^+$ + Cl$^-$ $\rightleftharpoons$ ICl | $1.20 \cdot 10^4$ | $2.90 \cdot 10^{10}$ | $2.40 \cdot 10^6$ | Wang et al. (1989) |
| H308◎ | HOI + H$^+$ + Br$^-$ $\rightleftharpoons$ IBr | $5.10 \cdot 10^9$ | $4.10 \cdot 10^{12}$ | $8.00 \cdot 10^9$ | De Barros Faria et al. (1993) |
| H309◎ | ICl + Br$^-$ $\rightleftharpoons$ IBr + Cl$^-$ | $3.30 \cdot 10^4$ | $1.65 \cdot 10^{14}$ | $5.00 \cdot 10^4$ | Wagman et al. (1982) |

(a) in $M^{m-n}$, n order of reaction of forward reaction, m order of reaction of backward reaction; (b) $k_{298}^{2nd}$ in $l^1$ mol$^{-1}$ s$^{-1}$, $k_{298}^{1st}$ in s$^{-1}$; (c) in K
| HCl | BrO* | Location | Comment | Reference |
|-----|------|----------|---------|-----------|
| daily average: 133 – 675 ppt | | | | Keene and Savoie (1999) |
| range: 30–250 ppt | | | | Pszenny et al. (2004) |
| median: 351 ppt | | | | Keene et al. (2007) |
| daily median: 82–682 ppt | | | | Keene et al. (2009) |
| median: 206 ppt | | | | |
| max. 1–3.6 ppt | | | | Sander et al. (2013) |
| average 2.3 ppt | | | | Leser et al. (2003) |
| average max. 2.5 ± 1.1 ppt | | | | Saiz-Lopez et al. (2004) |
| < 0.5 ppt | | | | Read et al. (2008) |
| 0.03 ± 0.26 ppt | | | | Volkamer et al. (2015) |
| 0.17–1.64 ppt | | | | Chen et al. (2016) |
| DL – Detection Limit; * for a more detailed overview on measurements before 2003 see Sander et al. (2003) |

Table S11  Measured values of HCl and BrO in marine environments.
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