

## Appendix A

**Table A1.** Bimolecular reactions and parameters used for the modelling described in Sect. 2.5. Reactions follow the rate expression  $k(T) = A(T/298)^n e^{-E_a/R^T}$  (Burkholder et al., 2015).

| Reaction                                                                                  | A                        | n    | E <sub>a</sub> (kJ mol <sup>-1</sup> ) | Reference                    |
|-------------------------------------------------------------------------------------------|--------------------------|------|----------------------------------------|------------------------------|
| ClNO <sub>2</sub> + M ==> Cl + NO <sub>2</sub>                                            | 9.13 × 10 <sup>-11</sup> | 0    | 106                                    | Baulch et al. (1981)         |
| Cl + Cl ==> Cl <sub>2</sub>                                                               | 6.15 × 10 <sup>-34</sup> | 0    | -7.53                                  | Baulch et al. (1981)         |
| M + ClONO <sub>2</sub> ==> NO <sub>2</sub> + ClO                                          | 2.76 × 10 <sup>-5</sup>  | 0    | 94.78                                  | Anderson and Fahey (1990)    |
| CH <sub>4</sub> + Cl ==> CH <sub>3</sub> + HCl                                            | 8.24 × 10 <sup>-13</sup> | 2.49 | 5.06                                   | Bryukov et al. (2002)        |
| HCl + OH ==> H <sub>2</sub> O + Cl                                                        | 3.74 × 10 <sup>-12</sup> | 0    | 4.27                                   | Baulch et al. (1981)         |
| HCl + M ==> H + Cl                                                                        | 7.31 × 10 <sup>-11</sup> | 0    | 342                                    | Baulch et al. (1981)         |
| CH <sub>3</sub> + HCl ==> CH <sub>4</sub> + Cl                                            | 3.89 × 10 <sup>-13</sup> | 0    | 9.64                                   | Baulch et al. (1981)         |
| CH <sub>3</sub> + NO <sub>2</sub> ==> CH <sub>3</sub> O + NO                              | 3.44 × 10 <sup>-11</sup> | 0    | 0                                      | Srinivasan et al. (2005)     |
| O <sub>3</sub> + M ==> O + O <sub>2</sub>                                                 | 7.6 × 10 <sup>-10</sup>  | 0    | 93.12                                  | Heimerl and Coffee (1979)    |
| CH <sub>3</sub> + O ==> CH <sub>2</sub> O + H                                             | 2.26 × 10 <sup>-11</sup> | 0    | 0                                      | Baulch et al. (1992)         |
| HCl + O ==> OH + Cl                                                                       | 7.07 × 10 <sup>-14</sup> | 2.87 | 14.72                                  | Mahmud et al. (1990)         |
| OH + CH <sub>4</sub> ==> CH <sub>3</sub> + H <sub>2</sub> O                               | 4.16 × 10 <sup>-13</sup> | 2.18 | 10.24                                  | Srinivasan et al. (2005)     |
| Cl <sub>2</sub> + M ==> Cl + Cl                                                           | 3.85 × 10 <sup>-11</sup> | 0    | 196                                    | Baulch et al. (1981)         |
| Cl + Cl ==> Cl <sub>2</sub>                                                               | 6.15 × 10 <sup>-34</sup> | 0    | -7.53                                  | Baulch et al. (1981)         |
| Cl <sub>2</sub> + O ==> ClO + Cl                                                          | 4.17 × 10 <sup>-12</sup> | 0    | 11.39                                  | Baulch et al. (1981)         |
| Cl <sub>2</sub> + H ==> HCl + Cl                                                          | 1.43 × 10 <sup>-10</sup> | 0    | 4.91                                   | Baulch et al. (1981)         |
| Cl <sub>2</sub> + OH ==> HOCl + Cl                                                        | 3.60 × 10 <sup>-12</sup> | 0    | 9.98                                   | Atkinson et al. (2007)       |
| CH <sub>3</sub> + O <sub>2</sub> ==> CH <sub>3</sub> O + O                                | 2.19 × 10 <sup>-10</sup> | 0    | 131                                    | Baulch et al. (1992)         |
| ClO + O ==> O <sub>2</sub> + Cl                                                           | 2.50 × 10 <sup>-11</sup> | 0    | -0.91                                  | Atkinson et al. (2007)       |
| OH + ClO ==> HO <sub>2</sub> + Cl                                                         | 6.86 × 10 <sup>-12</sup> | 0    | -2.49                                  | Atkinson et al. (2007)       |
| OH + ClO ==> HCl + O <sub>2</sub>                                                         | 4.38 × 10 <sup>-13</sup> | 0    | -2.49                                  | Atkinson et al. (2007)       |
| CH <sub>3</sub> O + NO ==> CH <sub>2</sub> O + HNO                                        | 4.00 × 10 <sup>-12</sup> | -0.7 | 0                                      | Atkinson et al. (1992)       |
| CH <sub>3</sub> O + O <sub>2</sub> ==> CH <sub>2</sub> O + HO <sub>2</sub>                | 7.20 × 10 <sup>-14</sup> | 0    | 8.98                                   | Atkinson et al. (1992)       |
| HOCl + O ==> OH + ClO                                                                     | 1.70 × 10 <sup>-13</sup> | 0    | 0                                      | Atkinson et al. (2007)       |
| ClCO + M ==> CO + Cl                                                                      | 4.10 × 10 <sup>-10</sup> | 0    | 24.6                                   | Atkinson et al., (2007)      |
| O <sub>3</sub> + NO ==> O <sub>2</sub> + NO <sub>2</sub>                                  | 1.40 × 10 <sup>-12</sup> | 0    | 10.9                                   | Atkinson et al. (2004)       |
| CH <sub>3</sub> O <sub>2</sub> + NO ==> CH <sub>3</sub> O + NO <sub>2</sub>               | 2.30 × 10 <sup>-12</sup> | 0    | -2.99                                  | Atkinson et al. (2006b)      |
| HO <sub>2</sub> + NO ==> NO <sub>2</sub> + OH                                             | 3.6 × 10 <sup>-12</sup>  | 0    | -2.24                                  | Atkinson et al. (2004)       |
| CH <sub>2</sub> O + Cl ==> HCl + HCO                                                      | 8.20 × 10 <sup>-11</sup> | 0    | 0.28                                   | Atkinson et al. (1992)       |
| CH <sub>2</sub> O + OH ==> HCO + H <sub>2</sub> O                                         | 4.73 × 10 <sup>-12</sup> | 1.18 | -1.87                                  | Baulch et al. (1992)         |
| CH <sub>3</sub> O <sub>2</sub> + HO <sub>2</sub> ==> CH <sub>3</sub> OOH + O <sub>2</sub> | 3.80 × 10 <sup>-13</sup> | 0    | -6.49                                  | Atkinson et al. (1992)       |
| CH <sub>3</sub> OOH ==> CH <sub>3</sub> O + OH                                            | 6.00 × 10 <sup>-14</sup> | 0    | 177                                    | Baulch et al. (1994)         |
| HCO + O <sub>2</sub> ==> CO + HO <sub>2</sub>                                             | 5.20 × 10 <sup>-12</sup> | 0    | 0                                      | Atkinson et al. (2006b)      |
| CO + OH ==> CO <sub>2</sub> + H                                                           | 5.40 × 10 <sup>-14</sup> | 1.5  | -2.08                                  | Baulch et al. (1992)         |
| Cl + HO <sub>2</sub> ==> HCl + O <sub>2</sub>                                             | 1.80 × 10 <sup>-11</sup> | 0    | -1.41                                  | Atkinson et al. (1992)       |
| Cl + HO <sub>2</sub> ==> ClO + OH                                                         | 6.30 × 10 <sup>-11</sup> | 0    | 4.74                                   | Atkinson et al. (2007)       |
| Cl + O <sub>3</sub> ==> ClO + O <sub>2</sub>                                              | 2.80 × 10 <sup>-11</sup> | 0    | 2.08                                   | Atkinson et al. (2007)       |
| CO + Cl ==> ClCO                                                                          | 1.33 × 10 <sup>-33</sup> | -3.8 | 0.00                                   | Atkinson et al. (2007)       |
| OH + HOCl ==> H <sub>2</sub> O + ClO                                                      | 5.00 × 10 <sup>-13</sup> | 0    | 0                                      | Atkinson et al. (2007)       |
| ClO + HO <sub>2</sub> ==> HOCl + O <sub>2</sub>                                           | 2.20 × 10 <sup>-12</sup> | 0    | -2.8                                   | Atkinson et al. (2007)       |
| ClO + ClO ==> Cl <sub>2</sub> + O <sub>2</sub>                                            | 1.00 × 10 <sup>-12</sup> | 0    | 13.22                                  | Atkinson et al. (2007)       |
| ClO + ClO ==> OClO + Cl                                                                   | 3.50 × 10 <sup>-13</sup> | 0    | 11.39                                  | Atkinson et al. (2007)       |
| ClO + ClO ==> ClOO + Cl                                                                   | 3.00 × 10 <sup>-11</sup> | 0    | 20.37                                  | Atkinson et al. (2007)       |
| ClO + NO ==> Cl + NO <sub>2</sub>                                                         | 6.20 × 10 <sup>-12</sup> | 0    | -2.45                                  | Atkinson et al. (2007)       |
| CH <sub>2</sub> O + O ==> HCO + OH                                                        | 1.78 × 10 <sup>-11</sup> | 0.57 | 11.56                                  | Baulch et al. (1992)         |
| OH + NO <sub>2</sub> ==> HNO <sub>3</sub>                                                 | 2.70 × 10 <sup>-11</sup> | 0    | 0                                      | Troe (2012)                  |
| CH <sub>3</sub> Cl + OH ==> CH <sub>2</sub> Cl + H <sub>2</sub> O                         | 1.40 × 10 <sup>-12</sup> | 1.6  | 8.65                                   | Cohen and Westberg (1991)    |
| CH <sub>3</sub> Cl + H ==> CH <sub>3</sub> + HCl                                          | 6.14 × 10 <sup>-11</sup> | 0    | 38.9                                   | Westenberg and deHaas (1975) |
| CH <sub>3</sub> Cl + CH <sub>3</sub> ==> CH <sub>4</sub> + CH <sub>2</sub> Cl             | 2.09 × 10 <sup>-12</sup> | 0    | 48.6                                   | Macken and Sidebottom (1979) |
| CH <sub>3</sub> Cl + Cl ==> CH <sub>2</sub> Cl + HCl                                      | 3.30 × 10 <sup>-11</sup> | 0    | 10.39                                  | Atkinson et al. (2008)       |
| CHCl <sub>3</sub> + Cl ==> CCl <sub>3</sub> + HCl                                         | 4.90 × 10 <sup>-12</sup> | 0    | 10.31                                  | Atkinson et al. (2008)       |
| Cl + C <sub>3</sub> H <sub>6</sub> ==> Products                                           | 2.70 × 10 <sup>-10</sup> | 0    | 0                                      | Atkinson et al. (2006b)      |
| Cl + C <sub>5</sub> H <sub>8</sub> ==> Products                                           | 4.30 × 10 <sup>-10</sup> | 0    | 0                                      | Orlando et al. (2003)        |
| ClNO + M ==> Cl + NO                                                                      | 2.16 × 10 <sup>-9</sup>  | 0    | 134                                    | Baulch et al. (1981)         |