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*Supplement of*

# Nighttime atmospheric chemistry of iodine

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Table 1. Iodine chemistry scheme in CAM-Chem: Bimolecular, thermal decomposition and termolecular reactions.

| **Reaction** | **k / cm$^3$ molecule$^{-1}$ s$^{-1}$** | **Notes** |
|---|---|---|
| $I + O_3 \rightarrow IO + O_2$ | $2.1 \times 10^{-11}\ e^{(-830\ /\ T)}$ | 1 |
| $IO + O_3 \rightarrow OIO + O_2$ | $3.6 \times 10^{-16}$ | 2 |
| $I + HO_2 \rightarrow HI + O_2$ | $1.5 \times 10^{-11}\ e^{(-1090\ /\ T)}$ | 3 |
| $IO + NO \rightarrow I + NO_2$ | $7.15 \times 10^{-12}\ e^{(300\ /\ T)}$ | 1 |
| $IO + HO_2 \rightarrow HOI + O_2$ | $1.4 \times 10^{-11}\ e^{(540\ /\ T)}$ | 1 |
| $IO + IO \rightarrow OIO + I$ | $2.13 \times 10^{-11}\ e^{(180/\ T)} \times [1 + e^{(-p\ /\ 191.42)}]$ | 1, 4 |
| $IO + IO \rightarrow I_2O_2$ | $3.27 \times 10^{-11}\ e^{(180\ /\ T)} \times [1 - 0.65\ e^{(-\ p\ /\ 191.42)}]$ | 1, 4 |
| $IO + OIO \rightarrow I_2O_3$ | $w_1 \cdot \exp(w_2 \cdot T)$ [a] | 4, 5, 6 [g] |
| $OIO + OIO \rightarrow I_2O_4$ | $w_1 \cdot \exp(w_2 \cdot T)$ [b] | 4, 5, 6 [g] |
| $I_2 + O \rightarrow IO + I$ | $1.25 \times 10^{-10}$ | 1 |
| $IO + O \rightarrow I + O_2$ | $1.4 \times 10^{-10}$ | 1 |
| $IO + OH \rightarrow HO_2 + I$ | $1.0 \times 10^{-10}$ | 7 |
| $I_2O_2 \rightarrow OIO + I$ | $w_1 \cdot \exp(w_2\ /\ T)$ [c] | 5, 6 , 8 [g] |
| $I_2O_2 \rightarrow IO + IO$ | $w_1 \cdot \exp(w_2\ /\ T)$ [d] | 5, 6 , 8 [g] |
| $I_2O_4 \rightarrow 2\ OIO$ | $w_1 \cdot \exp(w_2\ /\ T)$ [e] | 5, 8 [g] |
| $I_2 + OH \rightarrow HOI + I$ | $1.8 \times 10^{-10}$ | 3 |
| $I_2 + NO_3 \rightarrow I + IONO_2$ | $1.5 \times 10^{-12}$ | 9 |
| $I + NO_3 \rightarrow IO + NO_2$ | $1.0 \times 10^{-10}$ | 1 |
| $OH + HI \rightarrow I + H_2O$ | $1.6 \times 10^{-11}\ e^{(440\ /\ T)}$ | 1 |
| $I + IONO_2 \rightarrow I_2 + NO_3$ | $9.1 \times 10^{-11}\ e^{(-146\ /\ T)}$ | 5 |
| $HOI + OH \rightarrow IO + H_2O$ | $2.0 \times 10^{-13}$ | 10 |
| $IO + DMS \rightarrow DMSO + I$ | $3.2 \times 10^{-13}\ e^{(-925\ /\ T)}$ | 11 |
| $INO_2 \rightarrow I + NO_2$ | $1008 \times 10^{15}\ e^{(-13670\ /\ T)}$ | 12, 13, 14 |
| $IONO_2 \rightarrow IO + NO_2$ | $w_1 \cdot \exp(w_2\ /\ T)$ [f] | 5, 15 |
| $INO + INO \rightarrow I_2 + 2NO$ | $8.4 \times 10^{-11}\ e^{(-2620/T)}$ | 3 |
| $INO_2 + INO_2 \rightarrow I_2 + 2NO_2$ | $4.7 \times 10^{-13}\ e^{(-1670\ /\ T)}$ | 1 |
| $OIO + NO \rightarrow IO + NO_2$ | $1.1 \times 10^{-12}\ e^{(542\ /\ T)}$ | 14 |
| $HI + NO_3 \rightarrow I + HNO_3$ | $1.3 \times 10^{-12}\ e^{(-1830\ /\ T)}$ | 16 |
| $IO + BrO \rightarrow Br + I + O_2$ | $0.30 \times 10^{-11}\ e^{(510/T)}$ | 1 |
| $IO + BrO \rightarrow Br + OIO$ | $1.20 \times 10^{-11}\ e^{(510/T)}$ | 1 |
| $I + BrO \rightarrow IO + Br$ | $1.44 \times 10^{-11}$ | 17, 18, 19 |

| | | |
|---|---|---|
| $IO + ClO \rightarrow I + OClO$ | $2.585 \times 10^{-12} e^{(280/T)}$ | 1 |
| $IO + ClO \rightarrow I + Cl + O_2$ | $1.175 \times 10^{-12} e^{(280/T)}$ | 1 |
| $IO + ClO \rightarrow ICl + O_2$ | $0.940 \times 10^{-12} e^{(280/T)}$ | 1 |
| $IO + Br \rightarrow I + BrO$ | $2.49 \times 10^{-11}$ | 18, 19 |
| $IO + NO_3 \rightarrow OIO + NO_2$ | $9.0 \times 10^{-12}$ | 20 |
| $IO + CH_3O_2 \rightarrow CH_2O + I + HO_2$ | $2.0 \times 10^{-12}$ | 2[h] |
| $CH_3I + OH \rightarrow I + H_2O + HO_2$ | $2.90 \times 10^{-12} e^{(-1100/T)}$ | 3 |
| $I + NO_2 (+ M) \rightarrow INO_2 (+ M)$ | $k_0 = 3 \times 10^{-31} \times (T / 300)^{-1}$<br>$k_\infty = 6.6 \times 10^{-11}$ | 3[i] |
| $IO + NO_2 (+ M) \rightarrow IONO_2 (+ M)$ | $k_0 = 6.5 \times 10^{-31} \times (T / 300)^{-3.5}$<br>$k_\infty = 7.6 \times 10^{-12} \times (T / 300)^{-1.5}$ | 3[i] |
| $I + NO (+ M) \rightarrow INO (+ M)$ | $k_0 = 1.8 \times 10^{-32} \times (T / 300)^{-1}$<br>$k_\infty = 1.7 \times 10^{-11}$ | 3[i] |
| $OIO + OH (+ M) \rightarrow HOIO_2 (+ M)$ | $k_0 = 1.5 \times 10^{-27} \times (T / 300)^{-3.93}$<br>$k_\infty = 7.76 \times 10^{-10} \times (T / 300)^{-0.8}$ | 14[j] |
| $HOI + NO_3 \rightarrow IO + HNO_3$ | $2.7 \times 10^{-12} (300/T)^{2.66}$ | 21 |

[1] IUPAC-2008 (Atkinson et al., 2007) ; [2](Dillon et al., 2006b); [3] JPL-2010 (Sander et al., 2011); [4](Gómez Martín et al., 2007); [5](Kaltsoyannis and Plane, 2008); [6](Galvez et al., 2013); [7](Bösch et al., 2003); [8] (Gómez Martín and Plane, 2009); [9](Chambers et al., 1992); [10](Chameides and Davis, 1980); [11](Dillon et al., 2006a); [12](McFiggans et al., 2000); [13](Jenkin et al., 1985); [14](Plane et al., 2006); [15](Allan and Plane, 2002); [16] (Lancar et al., 1991); [17](Laszlo et al., 1997); [18](Bedjanian et al., 1997); [19](Gilles et al., 1997); [20](Dillon et al., 2008); [21]This work.

*a* $w1 = 4.687 \times 10^{-10} - 1.3855 \times 10^{-5} \times e^{(-0.75\,p / 1.62265)} + 5.51868 \times 10^{-10} \times e^{(-0.75\,p / 199.328)}$

$w2 = -0.00331 - 0.00514 \times e^{(-0.75\,p / 325.68711)} - 0.00444 \times e^{(-0.75\,p / 40.81609)}$

*b* $w1 = 1.1659 \times 10^{-9} - 7.79644 \times 10^{-10} e^{(-0.75\,p/22.09281)} + 1.03779 \times 10^{-9} \times e^{(-0.75\,p / 568.15381)}$

$w2 = -0.00813 - 0.00382 \times e^{(-0.75\,p / 45.57591)} - 0.00643 \times e^{(-0.75\,p / 417.95061)}$

*c* $w1 = 3.54288 \times 10^{10} + 1.8523 \times 10^{11} \times 0.75\,p - 1.45435 \times 10^{8} \times (0.75p)^2 + 60799.4344 \times (0.75p)^3$

$w2 = -9681.65989 + 346.95538 \times e^{(-0.75\,p / 343.25322)} + 251.78032 \times e^{(-0.75\,p / 44.1466)}$

*d* $w1 = 255335000000 - 4418880000 \times 0.75\,p + 85618600 \times (0.75\,p)^2 + 14218.81 \times (0.75\,p)^3$

$w2 = -11466.82304 + 597.01334 \times e^{(-0.75\,p / 1382.62325)} - 167.3391 \times e^{(-0.75\,p / 43.75089)}$

*e* $w1 = -1.92626 \times 10^{14} + 4.67414 \times 10^{13} \times 0.75\,p - 3.68651 \times 10^{8} \times (0.75\,p)^2 - 3.09109 \times 10^{6} \times (0.75\,p)^3$

$w2 = -12302.15294 + 252.78367 \times e^{(-0.75\,p / 46.12733)} + 437.62868 \times e^{(-0.75\,p / 428.4413)}$

*f* $w1 = -2.63544 \times 10^{13} + 4.32845 \times 10^{12} \times (0.75\ p) + 3.73758 \times 10^{8} \times (0.75\ p)^{2} - 628468.76313 \times (0.75\ p)^{3}$

$w2 = -13847.85015 + 240.34465 \times e^{(-0.75\ p\ /\ 49.27141)} + 451.35864 \times e^{(-0.75\ p\ /\ 436.87605)}$

*g* The empirical expressions of the form $w_1 \cdot \exp(w_2 \cdot T)$ were obtained by non-linear least squares fitting of *Rice–Ramsperger–Kassel–Marcus* (RRKM) theoretical results for the indicated reaction rate constants and thermal dissociation rates in the (27 – 1013) hPa pressure range. RRKM calculations were carried out using the MESMER algorithm (Glowacki et al., 2012) as indicated in the corresponding references (e.g. (Galvez et al., 2013). Expression *a* produces negative values outside the range of modelled rate constants ($p < 20$ hPa), and therefore a fixed rate constant of $3 \times 10^{-11}$ $cm^3$ $molecule^{-1}$ $s^{-1}$ was assumed. Expressions *e* and *f* generate negligible dissociation rates below ~500 hPa which become negative at ~8 hPa – in this case they are set to zero below that pressure.

*h* Updated heats of formation for IO, OIO, and $CH_3O_2$ (Dooley et al., 2008; Gómez Martín and Plane, 2009; Knyazev and Slagle, 1998) show that the only accessible exothermic product channel of $CH_3O_2 + IO$ (Drougas and Kosmas, 2007) is $CH_2O + I + O_2$ ($\Delta H_r = -5 \pm 6$ kJ $mol^{-1}$), consistent with the high yield of I and low yield of OIO found experimentally (Bale et al., 2005; Enami et al., 2006). Sensitivity studies have been carried out (Saiz-Lopez et al., 2014) using the preferred rate constant for this reaction of $2 \times 10^{-12}$ $cm^3$ $molecule^{-1}$ $s^{-1}$ (Dillon et al., 2006b), resulting in an enhancement of the ozone loss of 0.5% in the MBL and of less than 0.1% integrated throughout the troposphere in the $J_{IxOy}$ scenario, and similarly negligible enhancements in the Base scenario. Impacts in the $I_y$ partitioning are also very minor.

*i* The temperature and pressure dependent rate constant (k) is computed based on the low pressure ($k_0$) and the high-pressure ($k_\infty$) rate coefficients following JPL-2010 (Sander et al., 2011).

*j* The Fast rate constants and a thermally stable product $HOIO_2$ have been predicted theoretically (Plane et al., 2006), but no experimental studies reporting observation of $HOIO_2$ and its photochemical properties in the gas phase are available. Since the level of uncertainty is even larger than for the $I_xO_y$, it has not been included in the mechanism.

Table 2. Iodine chemistry scheme in CAM-Chem: Photochemical reactions.

| **Reaction** |
|---|
| $CH_3I + h\nu \rightarrow CH_3O_2 + I$ |
| $CH_2I_2 + h\nu \rightarrow 2I$ [a] |
| $CH_2IBr + h\nu \rightarrow Br + I$ [a] |
| $CH_2ICl + h\nu \rightarrow Cl + I$ [a] |
| $I_2 + h\nu \rightarrow 2I$ |
| $IO + h\nu \rightarrow I + O$ |
| $OIO + h\nu \rightarrow I + O_2$ |
| $INO + h\nu \rightarrow I + NO$ |
| $INO_2 + h\nu \rightarrow I + NO_2$ [b] |
| $IONO_2 + h\nu \rightarrow I + NO_3$ |
| $HOI + h\nu \rightarrow I + OH$ |
| $IBr + h\nu \rightarrow I + Br$ |
| $ICl + h\nu \rightarrow I + Cl$ |
| $I_2O_2 + h\nu \rightarrow I + OIO$ [c] |
| $I_2O_3 + h\nu \rightarrow IO + OIO$ [c] |
| $I_2O_4 + h\nu \rightarrow OIO + OIO$ [c] |

Photolysis rates are computed online considering the actinic flux calculation in CAM-Chem. The absorption cross-sections and quantum yields for all species besides the $I_xO_y$ have been taken from IUPAC-2008 (Atkinson et al., 2007; Atkinson et al., 2008) and JPL-2010 (Sander et al., 2011).

[a] radical organic products are not considered.
[b] only the reaction channel reported in JPL 06-02 (Sander et al., 2006) is considered.
[c] photolysis reactions only considered in the $J_{IxOy}$ scheme (Saiz-Lopez et al., 2014).

Table 3. Iodine chemistry scheme in CAM-Chem: Heterogeneous reactions.

| **Sea-salt aerosol reactions** | **Reactive uptake** |
|---|---|
| $IONO_2 \rightarrow 0.5$ IBr + 0.5 ICl | $\gamma = 0.01$ |
| $INO_2 \rightarrow 0.5$ IBr + 0.5 ICl | $\gamma = 0.02$ |
| HOI $\rightarrow 0.5$ IBr + 0.5 ICl | $\gamma = 0.06$ |
| $I_2O_2 \rightarrow$ | $\gamma = 0.01$[§] |
| $I_2O_3 \rightarrow$ | $\gamma = 0.01$[§] |
| $I_2O_4 \rightarrow$ | $\gamma = 0.01$[§] |

Values based on the THAMO model (Saiz-Lopez et al., 2008) and implemented in CAM-Chem following (Ordóñez et al., 2012).

[§] Deposition of $I_xO_y$ species on sea-salt aerosols has been included following the free regime approximation.

Table 4. Iodine chemistry scheme in CAM-Chem: Henry's Law constants and dry deposition velocities.

| **Species** | **$k_0$ (M atm$^{-1}$)** | **Deposition velocity[§] (cm s$^{-1}$)** | **Reference** |
|---|---|---|---|
| IBr $^{ice}$ | $2.4 \times 10^{1}$ | – | 1 |
| ICl $^{ice}$ | $1.1 \times 10^{2}$ | – | 1 |
| HI | $7.8 \times 10^{-1}$ | 1.0 | 1 $^{a}$ |
| HOI – ($J_{IxOy}$ / *Base*) | $1.9 \times 10^{3}$ / $4.5 \times 10^{3}$ | 0.75 | 1 $^{b}$ |
| $IONO_2$ $^{ice}$ | $1.0 \times 10^{6}$ | 0.75 | 2 $^{c}$ |
| $INO_2$ $^{ice}$ | $3.0 \times 10^{-1}$ | 0.75 | 1 $^{d}$ |
| IO | $4.5 \times 10^{2}$ | – | 2 |
| OIO | $1.0 \times 10^{4}$ | – | 2 |
| $I_2O_2$ | $1.0 \times 10^{4}$ | 1.0 | 2 |
| $I_2O_3$ | $1.0 \times 10^{4}$ | 1.0 | 2 |
| $I_2O_4$ | $1.0 \times 10^{4}$ | 1.0 | 2 |

[§] Dry deposition velocities are based on the THAMO model (Saiz-Lopez et al., 2008).
[1] Values reported in (Sander, 1999).
[2] Values based on the THAMO model (Saiz-Lopez et al., 2008).
[a] Considering a dissociation constant $K_a = 3.2 \times 10^9$ and a temperature dependent coefficient c = 9800 K
[b] Within the range of values given in the corresponding reference.
[c] Virtually infinite solubility is represented by using a very large arbitrary number.
[d] Value assumed to be equal to those of $BrNO_2$.
[ice] Species for which ice-uptake is considered following (Neu and Prather, 2012).

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