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Atmospheric chemistry of iodine anions: elementary reactions of I^-, IO^-, and IO_2^- with ozone studied at 300 K in an ion trap

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1 Supplementary information

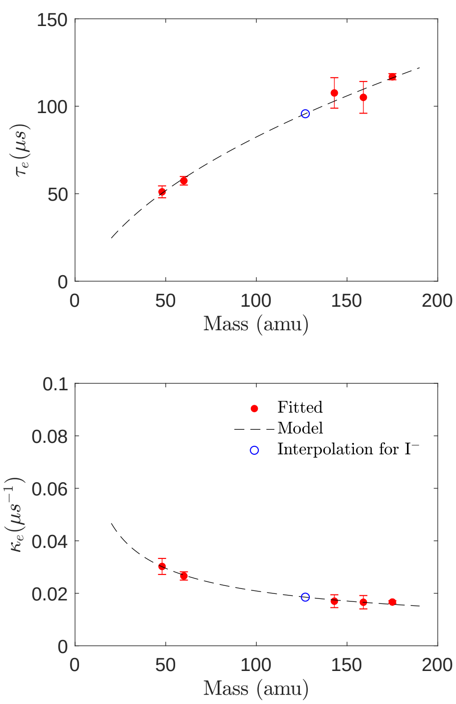

Fig. S1 Representation of the time-of-flight spectra (see Fig. 2) by the formula in Eq. (1). (a) Fitted parameters (red points) of the minimum time τ_e. The dashed black line shows a fit with a model function $\tau_e = a \times \sqrt{m_p} + b$, where a and b are determined by the fit. The blue circle represents the interpolated value for I^-. (b) Fitted parameters (red points) of the decay rate κ_e. The dashed black line shows a fit with a model function $\kappa_e = a/\sqrt{b \times m_p}$, where a and b are determined by the fit. The blue circle represents the interpolated value for I^-.

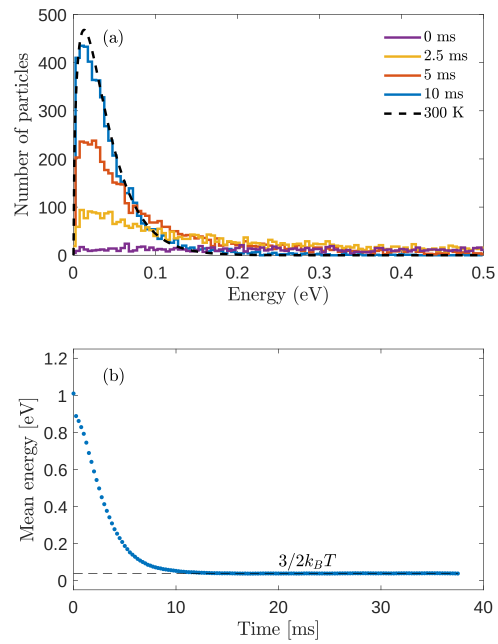

Fig. S2 Results of the Monte Carlo simulation on the thermalization of I^- ions in trap through elastic collisions with O_2 and O_3 at 300 K, a total pressure of $p_T = p_{O_2} + p_{O_3} = 5 \times 10^{-5}$ mbar, and an ozone fraction of $p_{O_3}/p_T = 5\,\%$. For the simulation, 5000 ions were initiated with a flat distribution of energies in the range 0 - 2 eV. Only elastic collisions were considered with rates $k_L = 5.8 \times 10^{-10}$ cm^3/s for the $I^- + O_2$ and $k_L = 6.7 \times 10^{-10}$ cm^3/s for the $I^- + O_3$ system. The effect of reactive collisions were not considered in the shown simulation. (a) Energy distributions at four different different times after the start of the simulation as well as the Maxwell-Boltzmann distribution at 300 K (dashed black line). (b) Evolution of the mean energy of I^- as a function of trapping time. The horizontal line corresponds to the mean value for a thermal distribution at 300 K.

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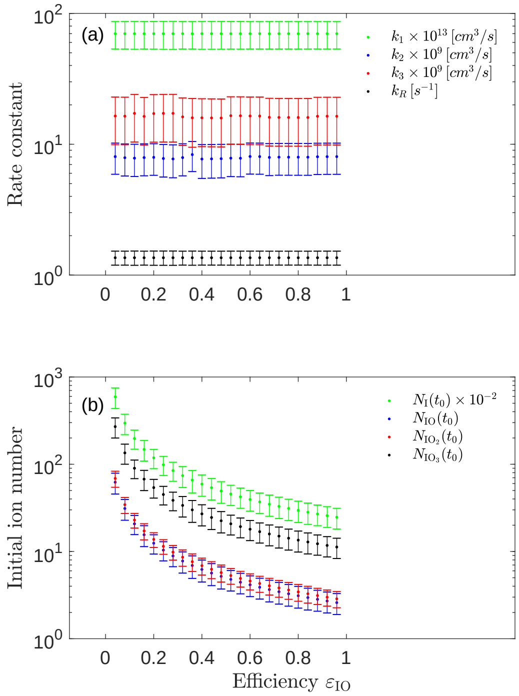

Fig. S3 Illustration of the robustness of the least squares fitting used to determine the experimental reaction rate constants k_{1-3}. The figure shows the determined values of (a) reaction rate constants k_{1-3} and background rate k_R and (b) the initial ion numbers $N_P(t_0)$ as a function of a fixed value of the detection efficiency $\varepsilon_{\mathrm{IO}} = \varepsilon_{\mathrm{IO_2}} = \varepsilon_{\mathrm{IO_3}}$ and with $\varepsilon_{\mathrm{I}} = 0.11 \times \varepsilon_{\mathrm{IO}}$.

Table S1 Reaction rate constants for the reaction R1-R3 obtained from fits to eight different data sets obtained with different ozone concentrations and trap settings. These data are displayed graphically in Fig. 6(b).

n_{O_3} (cm^{-3})	V_{RF} (V)	k_1 (cm^3/s)	k_2 (cm^3/s)	k_3 (cm^3/s)
4.2×10^{10}	120	$(12.6\pm3.1)\times10^{-12}$	$(11.8\pm5.6)\times10^{-9}$	$(20.5\pm9.7)\times10^{-9}$
7.7×10^{10}	120	$(6.6\pm3.1)\times10^{-12}$	$(7.6\pm4.1)\times10^{-9}$	$(14.6\pm9.6)\times10^{-9}$
5.2×10^{10}	120	$(5.6\pm3.1)\times10^{-12}$	$(8.6\pm3.9)\times10^{-9}$	$(15.2\pm7.7)\times10^{-9}$
2.5×10^{10}	120	$(6.3\pm3.1)\times10^{-12}$	$(11.6\pm4.0)\times10^{-9}$	$(16.1\pm6.4)\times10^{-9}$
5.2×10^{10}	120	$(6.0\pm3.1)\times10^{-12}$	$(8.9\pm7.1)\times10^{-9}$	$(15.5\pm12.6)\times10^{-9}$
4.6×10^{10}	120	$(11.0\pm3.1)\times10^{-12}$	$(10.5\pm4.7)\times10^{-9}$	$(16.5\pm7.7)\times10^{-9}$
4.8×10^{10}	60	$(10.8\pm3.1)\times10^{-12}$	$(9.4\pm3.8)\times10^{-9}$	$(15.3\pm6.5)\times10^{-9}$
1.6×10^{10}	60	$(8.6\pm3.1)\times10^{-12}$	$(13.7\pm4.6)\times10^{-9}$	$(17.7\pm6.5)\times10^{-9}$