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Supplement of

Kinetics of the OH + NO_2 reaction: effect of water vapour and new parameterization for global modelling

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Supplementary information

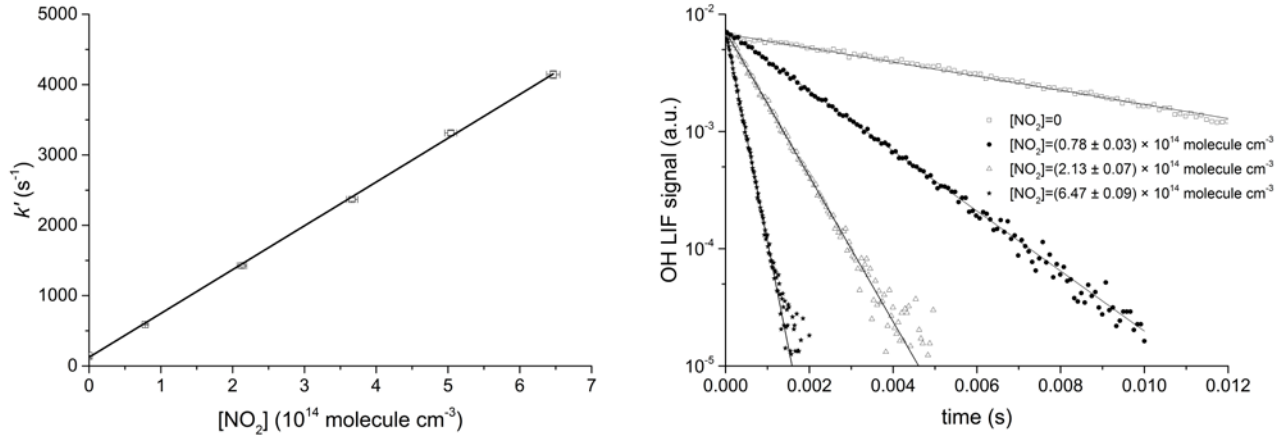

Figure S1. *Left panel*: Plots of k' versus $[NO_2]$ at 500 Torr He and 292 K. The lines are least-squares fits to the data using Eq. (2) (see main text). Error bars are 2σ statistical only. *Right panel*: Exponential decay of the OH LIF signal in 500 Torr He, at 292 K, and at four different NO_2 concentrations. The solid lines are fits to the datasets using Eq. (1) (see main text).

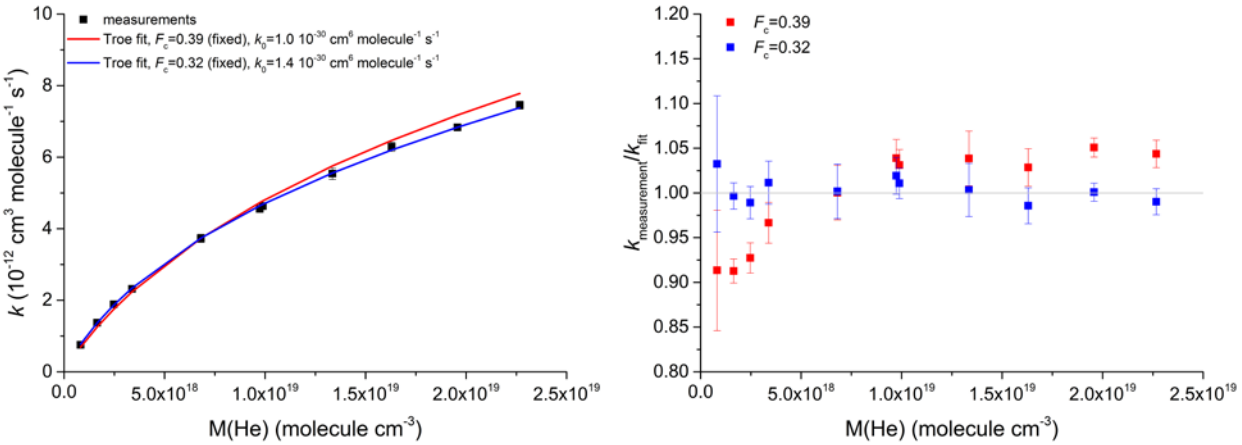

Figure S2. *Left panel*: Measurements of k_1 as a function of He density. The blue line corresponds to a fit using equation (2) whereby F_c was fixed to 0.32 leading to k_0^{He} =1.4 × 10^{-30} cm^6 molecule^{-2} s^{-1}. The red line corresponds to a fit using equation (2) whereby F_c was fixed to 0.39 leading to k_0^{He} =1.0 × 10^{-30} cm^6 molecule^{-2} s^{-1}. Other parameters were fixed to: m = 3.1, k_∞ = 6.3 × 10^{-11} cm^3 molecule^{-1} s^{-1} and n = 0. *Right panel*: Ratio of the measured rate constant vs. the parametrisation using F_c = 0.39 and F_c = 0.32

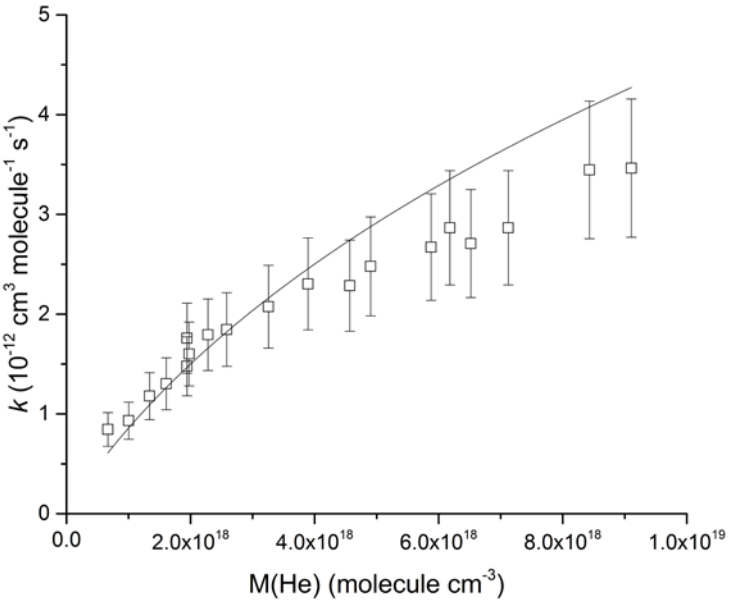

Figure S3. Comparison with previous experimental data. The data points are measurements by Morley and Smith (1972) at 300 K, the solid line represents our parametrisation at 300 K.

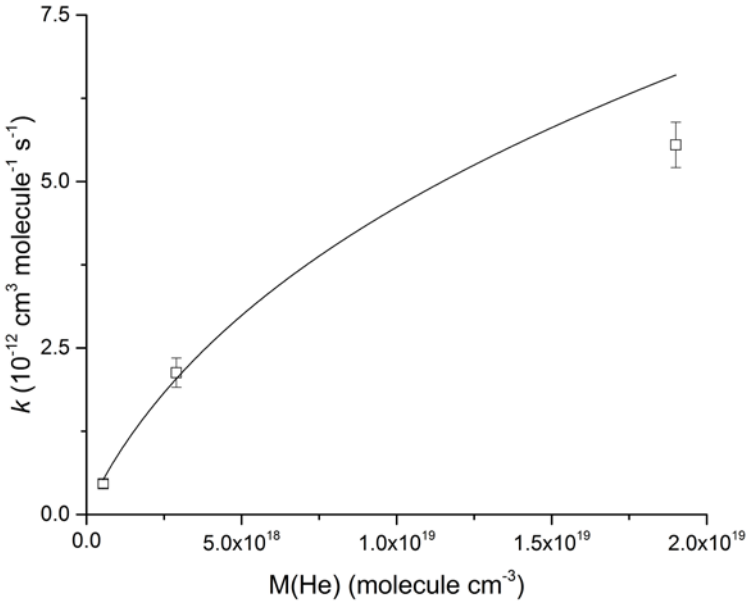

Figure S4. Comparison with previous experimental data. The data points are measurements by Wine et al. (1979) at 297 K, the solid line represents our parametrisation at 297 K.

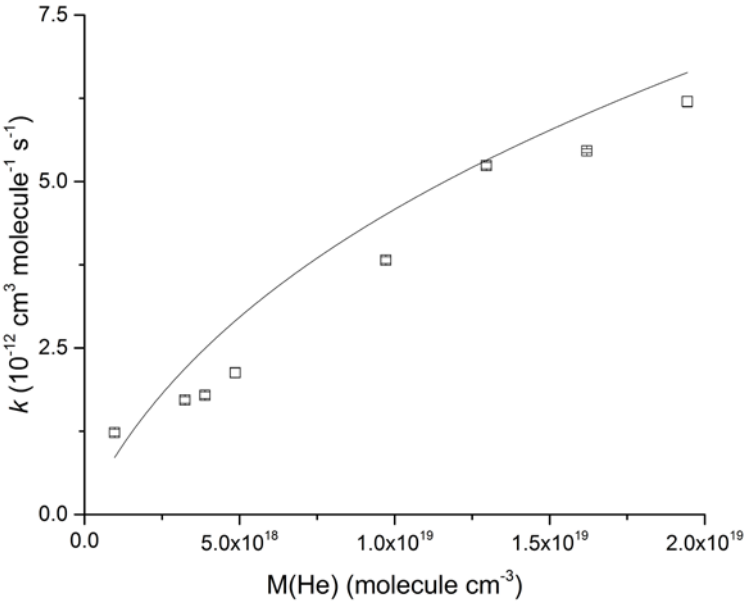

Figure S5. Comparison with previous experimental data. The data points are measurements by D'Ottone et al. (2001) at 298 K, the solid line represents our parametrisation at 298 K.

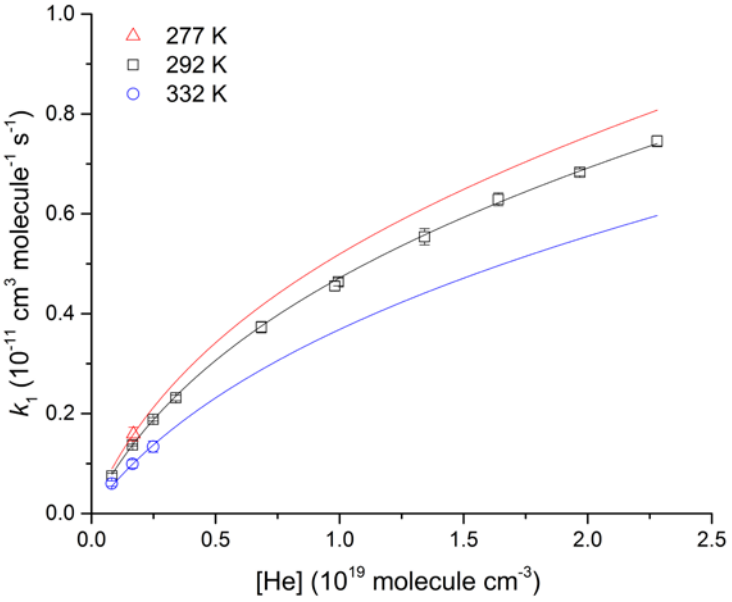

Figure S6. Measurements of k_1 in He bath gas at 277, 292 and 332 K. The solid line is a fit to our data using Eqn. (4) with k_0 = 1.4×10^{-30} cm^6 molecule^{-2} s^{-1}, k_∞ = 6.3×10^{-11} cm^3 molecule^{-1} s^{-1}, F_c = 0.32, m = 3.1 and n = 0.

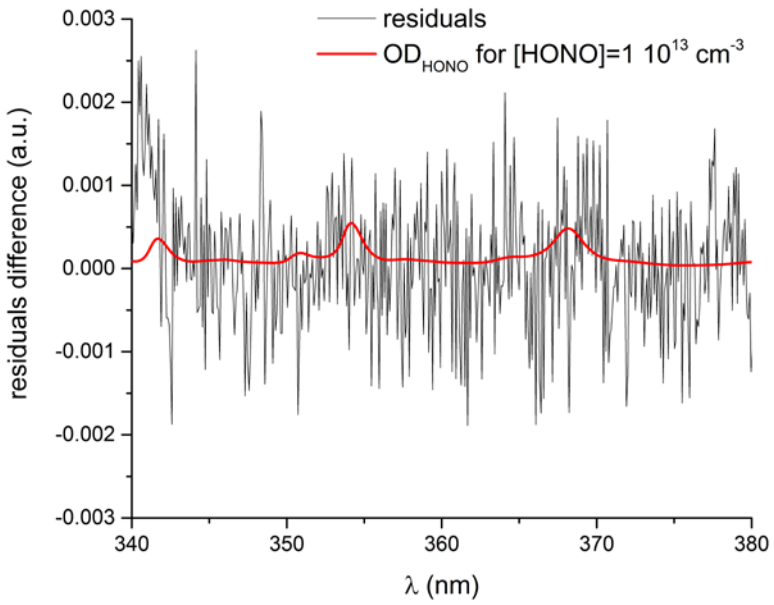

Figure S7. Spectrum of the difference between the residuals of NO_2 spectra with and without H_2O ($[H_2O] = 4.5 \times 10^{17}$ molecule cm^{-3}, $[NO_2] = 1.7 \times 10^{15}$ molecule cm^{-3}) recorded at 50 Torr He, at room temperature. The red line corresponds to absorption by HONO at a concentration of 1×10^{13} molecule cm^{-3}.

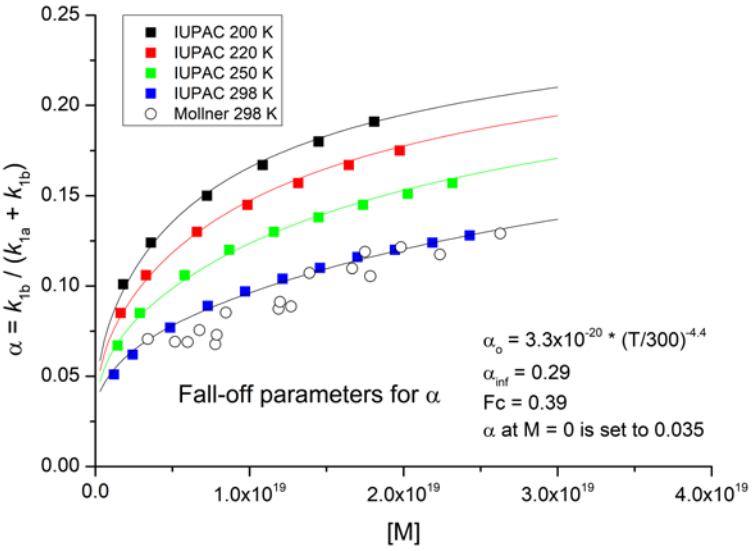

Figure S8. Parameterisation of the temperature and pressure dependent yield of HOONO in the reaction between OH and NO_2.

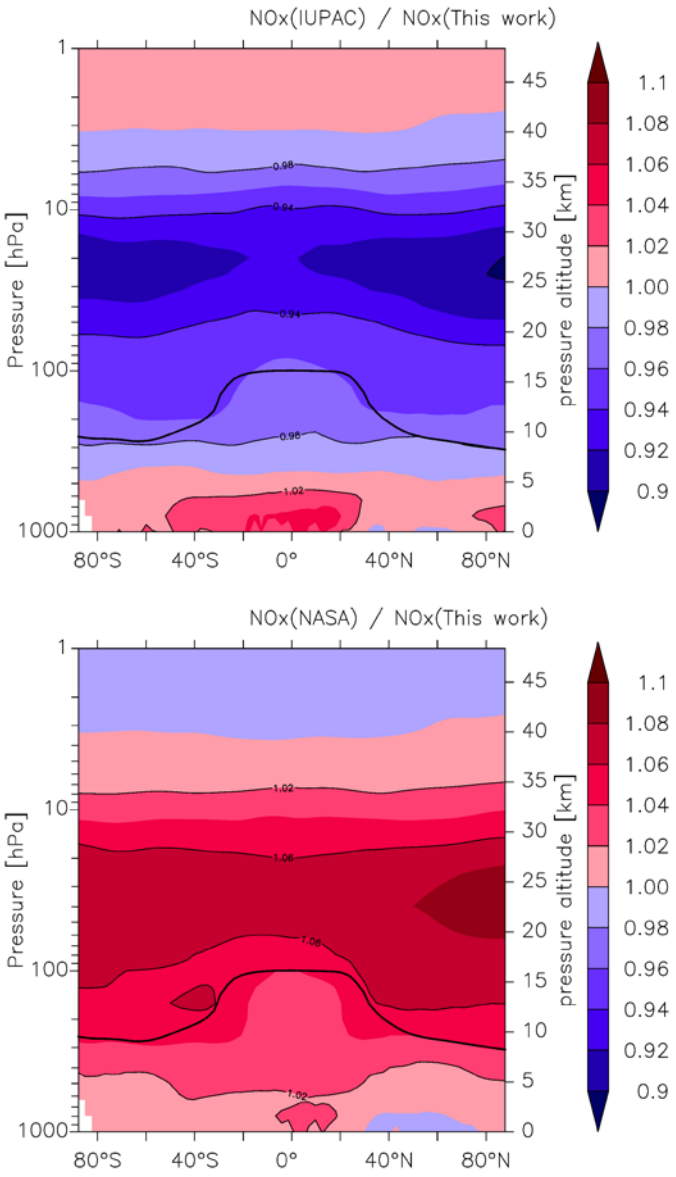

Figure S9. Effect of different parameterisations of k_1 on the global (zonal and yearly averaged) concentration of NO_X. The upper panel plots $[NOx]_{IUPAC}$ / $[NOx]_{this\ work}$, the lower panel plots $[NOx]_{NASA}$ / $[NOx]_{this\ work}$. The black line represents the model tropopause.

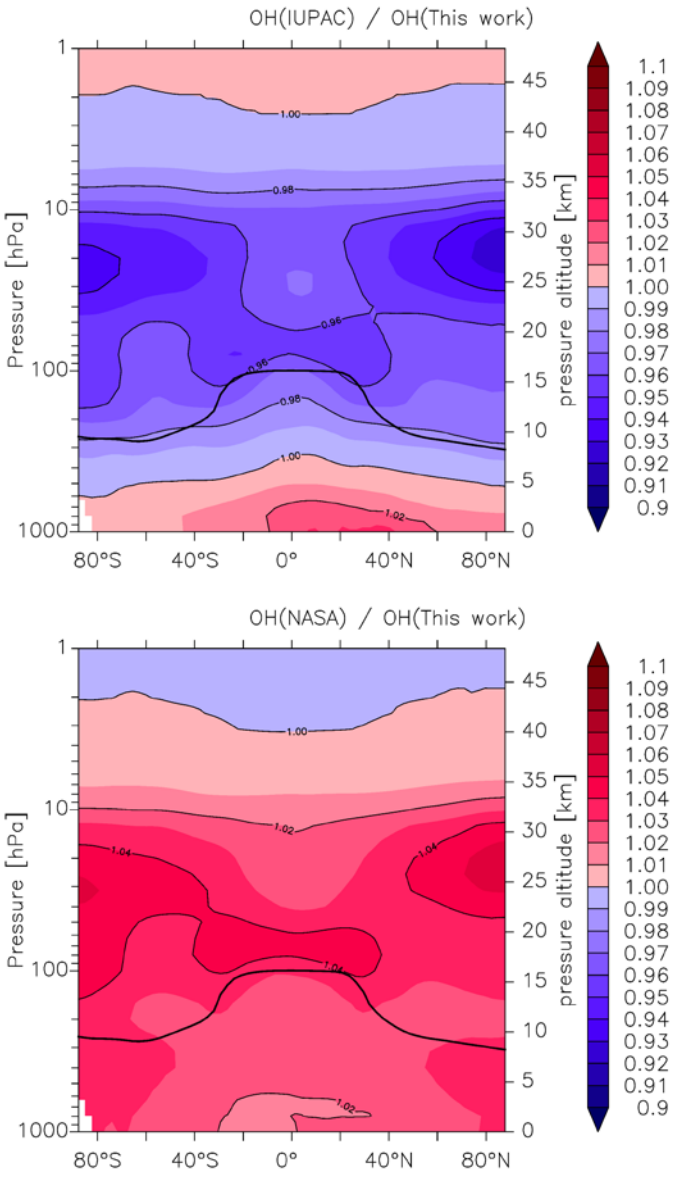

Figure S10. Effect of different parameterisations of k_1 on the global (zonal and yearly averaged) concentration of the hydroxyl radical, [OH]. The upper panel plots $[OH]_{IUPAC}$ / $[OH]_{this\ work}$, the lower panel plots $[OH]_{NASA}$ / $[OH]_{this\ work}$. The black line represents the model tropopause.

References

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