

Interactive comment on “Kinetics of the OH + NO₂ reaction: Effect of water vapour and new parameterisation for global modelling” by Damien Amedro et al.

Anonymous Referee #3

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See attached

Please also note the supplement to this comment:

<https://www.atmos-chem-phys-discuss.net/acp-2019-1103/acp-2019-1103-RC3-supplement.pdf>

Interactive comment on Atmos. Chem. Phys. Discuss., <https://doi.org/10.5194/acp-2019-1103>,
2019.

C1

Review of Amedro et al

This manuscript presents the first study of the effectiveness of H₂O as a third body on the recombination of OH with NO₂. This careful experimental study shows that water vapor is much more effective than N₂ or O₂ in causing recombination. It also presents a global modeling study of a new parameterization of the OH + NO₂ reaction as compared to the IUPAC and JPL recommendations; this parameterization uses the results of a previous study showing that O₂ and N₂ have different efficiencies in quenching the products of OH + NO₂. The modeling suggests that HOONO could be a non-negligible reservoir of NO_x in some parts of the atmosphere. This is a very important paper that is clearly in the scope of ACP. There are no major problems with the manuscript, but a few of points should be clarification or emphasized more strongly before publication in ACP.

My major concern about this manuscript is actually rather minor: In the global modeling, it is not clear how much of the effects of the new parameterization, occurs due to water vapor and how much due to the use of the results of the author's previous paper on N₂ vs O₂ as colliders. This should be made clear.

The enhancement of the quenching of the energized HNO₂ intermediate (HNO₂*) due to H₂O vapor is presumably due to the strong hydrogen bonding between the two (stronger than OH-H₂O or NO₂-H₂O). It would be good to make this explicit and add some references to the literature on the HONO₂-HOH complex.

There must be previous field work measuring [NO₂]/[HONO₂] and corresponding modeling work that did or did not find discrepancies. It seems that the authors should refer discuss a few of these, at least briefly.

Minor Issues:

Line 12: “molecule” is missing an “i”

Line 45: “being” should be “is”

Line 50-52. The sentence beginning “Theoretical calculations...” might better appear immediately after the discussion of the chaperone mechanism, rather than after the introduction of enhanced collider gases.

line 68 “prevented” should be “preventing”

line 75: “in Tables 1 and 2.” might better be phrased as “in the notes to Tables 1 and 2.”

It might help orient readers if the manuscript provided some idea of the conditions under which the OH + NO₂ → HONO₂ is nearly in the low-pressure limit and high-pressure limit.

Line 102: The manuscript states that the low vapor pressure of water prevents it from being used as a bath gas by itself, but 5 Torr of water vapor is roughly equivalent of 50 Torr of He. So I

Fig. 1.

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