

Interactive comment on “H-migration in peroxy radicals under atmospheric conditions” by Luc Vereecken and Barbara Nozière

Anonymous Referee #1

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This paper reports the structure-activity relationship (SAR) for the rate coefficients for the isomerization reactions of organic peroxy radicals (RO₂) to QOOH based on the experimental and theoretical investigations. It adds new class of knowledge on the atmospheric chemistry. I request the authors to address the following comment on the assumption in the analysis of experiments.

[1] In the analysis of experimental data, authors simple one-way reaction (R1). RO₂ → HOOQO₂ (R1) However, this should be actually the two-step reactions. RO₂ → QOOH (R2) QOOH → RO₂ (R-2) QOOH + O₂ → HOOQO₂ (R3) The assumption of simple one-way reaction (R1) is only valid when $k_3[\text{O}_2] \gg k_2$. My rough calculation shows that k_2 may be as large as 10^7 to 10^8 s⁻¹, which is comparable order with $k_3[\text{O}_2]$ at the authors experimental condition, (0.9 atm, 298 K, synthetic air), $k_3[\text{O}_2] =$

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$3 \cdot 10^7 \sim 1 \cdot 10^8$. Authors should properly discuss the effects of the backward reactions (R-2).

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