

Interactive comment on “Hydration increases the lifetime of HSO_5 and enhances its ability to act as a nucleation precursor – a computational study” by T. Kurtén et al.

Anonymous Referee #1

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General comments:

The manuscript presented (Hydration increases the lifetime of HSO_5 and enhances its ability to act as a nucleation precursor - a computational study) by Theo Kurten and co-workers present an interesting study on the possibility of radicals formed during the oxidation of SO_2 to contribute or be responsible for the formation of clusters which could act as first step in the nucleation process. The authors used advanced quantum chemical methods to estimate the effect of hydration on increasing the lifetime of HSO_5 . In my opinion this manuscript will fit complete in the frame of the journal ACP and contributes very interesting aspects to the still hot topic of atmospheric nucleation. The

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Interactive Discussion

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manuscript is written in very good English and is well structured; it should be published after minor consideration

I would advise the authors to change the statement in the beginning of the abstract (first sentence) in a more optional way. The findings in the manuscripts the authors mention are not showing any direct proofs that HSO₅ radicals are involved in the nucleation process but only that the possibility of a path parallel to the oxidation of SO₂ could be involved in the nucleation. However, there are still other possibilities like e.g. the photo oxidation of organic molecules (which are always present in such chamber experiments) and the contribution of the reaction product. No manuscript at least up to my knowledge has shown any indications that HSO₅ radicals can play a key role in the nucleation of atmospheric SO₂ oxidation products.

The title of chapter 4.1 should be changed to kinetic modeling of chamber experiments and exclude the atmospheric implications. Using a kinetic model to simulate chamber experiments in very simplified way with only 11 reactions could not be representative under atmospheric conditions.

In the same chapter the authors use the kinetic model to estimate the possible role of the achieved hydration rates in the chamber experiments performed at IFT. The results discussed in the end of this chapter stated that the rate at which the reaction products are produced is slightly larger than the formation rate of detected particles measured. I believe it would be very interesting for the community when the authors include the expected lifetimes of none-, single and double hydrated radicals.

Interactive comment on Atmos. Chem. Phys. Discuss., 9, 2823, 2009.

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