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Atmospheric Chemistry and Physics Discussions

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 #2

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This is a very nice paper on a highly relevant subject. The role of possible new pathways for atmospheric aerosol formation via different hydrated oxidized sulfur species is examined in terms of quantum chemical calculations and elementary kinetic considerations. Because the energies of such weakly bound complexes are still difficult to predict, quite a number of different quantum chemical methods was applied. The results are carefully compared and discussed. Even though the conclusions regarding possible precursors and reaction pathways to nucleation have to remain semi-quantitative in character, the paper opens up interesting perspectives for further, more detailed studies of a probably important sub-mechanism of atmospheric aerosol formation.

The manuscript is very well written and should be published after some minor, mainly technical corrections. I recommend the following points to be addressed:

1. For the sake of consistence, reaction R5 should be written in the form HSO5 + M -> SO3 + HO2 + M; the same applies for reactions (R2c) - (R2f).

2. The equations R2d and R2e do not correspond to real reactions since a transition state is involved. It is physically unreasonable to formulate reactions with a transition state as a reactant or product. Since I realize the intention of this representation for later discussions, I recommend at least a corresponding note.

3. Page 2827, line 19: "... via path (4) or (2f)." should better read as "... via path (4) and (2f), respectively." (reaction R2f is in fact the way reaction R4 proceeds).

4. Page 2828, lines 3/4: "Reaction (2d)" should read as "Reaction (2d) + (2e)" (see my comment No. 2).

5. Page 2836, line 11: "(2c)+(2d)" should read as "(2d)+(2e)".

6. Page 2837, line 1: "mechanism 1" should read as "mechanism 3" (?).

7. Page 2837, line 3: "mechanism 2" should read as "mechanism 1" (?).

8. Page 2837, line 6: "mechanism 1" should read as "mechanism 3" (?).

It would be useful for the scientific community if the frequencies for all species could be included in the Electronic Supplement.

The numbering of the sections is inappropriate: a section 3.1 normally requires a section 3.2; the same applies for section 4.1. In my opinion, the numbering of the primary manuscript was more appropriate.

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

ACPD

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Interactive Comment