

Interactive comment on “Exploring the chemical fate of the sulfate radical anion by reaction with sulfur dioxide in the gas phase” by N. T. Tsona et al.

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The manuscript is dedicated to the sulfur cycle relevant to the formation of H_2SO_4 , the key atmospheric nucleation precursor in the Earth's atmosphere. The topic is important and relevant directly to the atmospheric physics and chemistry.

The paper is nicely written, easy to follow, interesting and probably deserves publication.

However, there exist a few issues to be addressed prior to publication.

Specific comments.

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1. The authors have mentioned that "PW91 and B3LYP are two of the most popular functionals, but for anionic systems the CAM B3LYP functional is superior to B3LYP by the inclusion of long-range correction (Yanai et al., 2004)" and choose the CAM-B3LYP as the primary method for the geometry optimization and thermal correction. The authors provide a more detailed explanation of the importance of the "long-range correction" in the case, when strongly bonded ionic clusters are studied, and a clearer justification for the selection of the CAM B3LYP as the primary computational method. In particular, additional tests/benchmarks of PW91, B3LYP and CAM B3LYP methods on $\text{SO}_4^- + \text{H}_2\text{O} = \text{SO}_4 \cdot (\text{H}_2\text{O})$ and $\text{SO}_4^- + \text{SO}_2 = \text{SO}_4 \cdot (\text{SO}_2)$ reactions (Table 1) should be included in the revised manuscript. Based on the results presented in Table 1 showing clearly that CAM B3LYP significantly underestimates the reaction free energies, one could probably conclude that PW91 typically predicting stronger bonding may be a better choice than both B3LYP and CAM B3LYP.

2. Based on the data shown in Table 1 one can conclude that in most cases the single point CCSD(T) and CCSD(T)-F12 energy corrections do not seem to systematically improve the quality of the DFT results. The authors should briefly comment on this issue.

3. The hydration range ($n=0-2$) considered in the present paper does not seem to be wide enough to represent the real atmospheric conditions, at which higher hydrates may exist in significant concentrations. Please, explain your choice and comment on the impact of possible uncertainties related to hydration on conclusions made in the present paper.

Technical corrections.

Page 12864, last line, ",," should be replaced with ".".

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