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Comment

Interactive comment on “Ab initio studies of $\text{O}_{bf2}^-(\text{H}_2\text{O})_{\vec{n}}$ and $\text{O}_3^-(\text{H}_2\text{O})_{\vec{n}}$ anionic molecular clusters, $n \leq 12$ ” by N. Bork et al.

N. Bork et al.

nbor@space.dtu.dk

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We thank the reviewer for the positive review of our manuscript.

The reviewer has the following points:

1) typo: page 13958, line 18: HOMO orbita → HOMO orbital.

Reply: The typo has been corrected

2) page 13959, if possible, can you provide the table for (R4-R7) as a summary?

Reply: We agree that is unsatisfying to list these reactions but not present any data to

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validate the conclusions made. However, since we reject the atmospheric relevance for reaction R3, we argue that such a table does not belong in the main article. A table with the thermodynamic of reactions (R3-R7) has therefore been attached, intended as supplementary information for the article.

3) page 3959, line 23. please check the following correction:

O_2 clusters $\rightarrow \text{O}_2^-(\text{H}_2\text{O})_n$ clusters

O_3 clusters $\rightarrow \text{O}_3^-(\text{H}_2\text{O})_n$ clusters

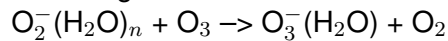
Reply: The corrections have been made.

4) Personally, Section 3.4 Simple chemistry is understandable, but it seems to me that they discussed the charge transfer will be occurred from $\text{O}_2^-(\text{H}_2\text{O})_n$ to O_3 without the strong computational data.

Reply: It is known that O_3 is much more electron affinitive than O_2 and hence, upon collision the charge will transfer with high energy gain. However, since many of the $\text{O}_2^-(\text{H}_2\text{O})_n$ clusters are more stable towards dissociation than the corresponding $\text{O}_3^-(\text{H}_2\text{O})_n$ clusters the charge transfer reaction will be less exothermic. For assessing this, the computational data is used.

To clarify the arguments, the section could be rephrased accordingly:

"From Figs. 1 and 2 it is however apparent that several of the O_2 clusters are significantly more stable than the corresponding O_3 clusters and that the charge transfer process will become correspondingly less exothermic. E.g. is the $\text{O}_2^-(\text{H}_2\text{O})$ cluster 13 kJ/mol more stable towards dissociation than the $\text{O}_3-(\text{H}_2\text{O})_n$ cluster. Consequently, the charge transfer reaction



is only ca. 147 kJ/mol exothermic. However, ..."

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We trust that with these adjustments and corrections, the manuscript will be suitable for publication.

Please also note the supplement to this comment:

<http://www.atmos-chem-phys-discuss.net/11/C5262/2011/acpd-11-C5262-2011-supplement.pdf>

Interactive comment on Atmos. Chem. Phys. Discuss., 11, 13947, 2011.

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