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Atmospheric Chemistry and Physics Discussions

Interactive comment on "Ab initio studies of $O^{-}_{bf2}(H_2O)_{\vec{n}}$ and $O^{-}_{3}(H_2O)_{\vec{n}}$ 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

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 $\rightarrow$ $O_2^-(H_2O)_n$ clusters
O_3 clusters $\rightarrow$ $O_3^-(H_2O)_n$ 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 $O_2^-(H_2O)_n$ 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 $O_2^-(H_2O)_n$ clusters are more stable towards dissociation than the corresponding $O_3^-(H_2O)_n$ clusters the charge transfer reaction will be less exothermic. For assessing this, the computational data is used.

To clarify the arguments, the section could been 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 $O_2^-(H_2O)$ cluster 13 kJ/mol more stable towards dissociation than the O3-(H2O)n cluster. Consequently, the charge transfer reaction
$O_2^-(H_2O)_n$ + O_3 –> $O_3^-(H_2O)$ + O_2
is only ca. 147 kJ/mol exothermic. However, ..."

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11, C5262–C5264, 2011

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

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