

## ***Interactive comment on “Ab initio studies of $O_{bf2}^-(H_2O)_n$ and $O_3^-(H_2O)_n$ anionic molecular clusters, $n \leq 12$ ” by N. Bork et al.***

**N. Bork et al.**

nbor@space.dtu.dk

Received and published: 22 June 2011

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  
C5262

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 →  $O_2^-(H_2O)_n$  clusters

$O_3$  clusters →  $O_3^-(H_2O)_n$  clusters

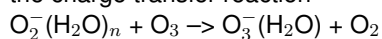
Reply: The corrections have been made.

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 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  $O_2^-(H_2O)$  cluster 13 kJ/mol more stable towards dissociation than the  $O_3^-(H_2O)_n$  cluster. Consequently, the charge transfer reaction



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

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.

C5264