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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.

Anonymous Referee #1

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It is a very interesting topic. The authors discussed the thermodynamics of cluster growth of gaseous hydrated O2- and O3-clusters using high levels of ab initio theory. They reported that anionic O−2 (H2O)n and O−3 5 (H2O)n clusters were thermally stabilized at typical atmospheric conditions for at least n = 5. The first 4 water molecules were strongly bound to the anion due to delocalization of the excess charge while stabilization of more than 4 H2O was due to normal hydrogen bonding. In all systems, the central ion was located at or near the surface of the hydrogen bonded network and the excess electron was in all clusters at least 80% localized at the O2 or O3 species. This signified that the central ion retained much of its reactivity despite hydration and was easily accessible to further chemical reactions. Overall, the manuscript is well written.

If I am supposed to give an advice to enhance the quality of the work with a more

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realistic environmental issue (even though the present work is already interesting), I think that the authors may discuss the distribution of the hydarated ozone anion clusters depening on temperature and pressure in the real environments. To do this, the authors may consult a paper published in Phys. Rev. A. 48, 3764, 1993. Otherwise, I have nothing to add.

The manuscript is recommended for publication either with or without revision.

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