

Interactive comment on “Thermodynamics of reactions of ClHg and BrHg radicals with atmospherically abundant free radicals” by T. S. Dibble et al.

M.E. Goodsite (Referee)

michaelg@hih.au.dk

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The authors are to be congratulated on this paper, which makes available quantum calculations and analysis that advance the state of understanding of this field. The scientific significance is absolutely within the scope of this journal, the scientific approach and methods valid. The results are discussed in an appropriate and balanced way, with excellent consideration of previous work, though as with all manuscripts, there are probably additional articles that might also be taken into consideration in the introduction and/or discussion. The presentation quality is also excellent. This paper could be published as is without further revision, but a more in depth discussion, though not

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absolutely necessary for this article, would add value to the paper.

Individual scientific questions/issues:

As a minor correction, I recommend that the authors cite: P.A. Ariya, H. Skov, MML Grage and M. E. Goodsite, "Gaseous elemental mercury in the ambient atmosphere: Review of the application of theoretical calculations and experimental studies for determination of reaction coefficients and mechanisms with halogens and other reactants", *Advances in Quantum Chemistry*, 55: 43-55 (2008) ([http://dx.doi.org/10.1016/S0065-3276\(07\)00204-3](http://dx.doi.org/10.1016/S0065-3276(07)00204-3)). The review adds credence to the need for the type of calculations performed by the authors. Though not a stringent requirement to cite absolutely all literature in the field, I think that the reader would be excellently served with the type of information available in the review, and the authors could refer to it in the introduction. Other reviews also might be relevant in the introduction or discussion: such as: Parisa A. Ariya, Kirk Peterson, Graydon Snider and Marc Amyot, *Mercury Chemical transformation in the gas, aqueous and heterogeneous phases: State-of-the art science and uncertainties*, book chapter 15, *Mercury fate and transport in the global atmosphere*, Pirrone and Mason editors, Springer, pp, 459-501, ISBN: 987-0-387-93957-5 (2009); however a review from Subir et. al., (2011) is cited and probably is sufficient for the purpose of discussion in this paper.

The authors might also develop their discussion more, as to what exactly their calculations could mean for the fate of mercury. The authors do an excellent job of discussing what follow up studies should be conducted in the field and in the laboratory to address new scientific issues arising from their studies, so this could be the subject of another short review, rather than lengthen this paper; though I feel that a more in depth discussion would add additional value to the paper.

I have no technical corrections to suggest. The paper with all of its figures, tables etc. are publishable as is.

In conclusion, aside from adding one reference to the introduction and/or discussion,

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it is my conclusion that this manuscript can and should be published as is. The discussion may be lengthened to add greater value to the paper, but this is not at all a necessity.

Interactive comment on Atmos. Chem. Phys. Discuss., 12, 17887, 2012.

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