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Atmospheric
Chemistry
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Discussions

Interactive comment on "Ultraviolet absorption cross sections of carbonyl sulfide isotopologues $OC^{32}S$, $OC^{33}S$, $OC^{34}S$ and $O^{13}CS$: isotopic fractionation in photolysis and atmospheric implications" *by* S. Hattori et al.

Anonymous Referee #1

Received and published: 5 August 2011

The authors present detailed absorption cross section measurements for OCS, an important molecule in atmospheric chemistry. The main part of the manuscript presents absorption cross sections for four isotopologues obtained with high resolution. There are several aspects which are of high interest for the community. First, the weak vibrational structures show systematic isotope shifts which are not correctly described by calculations based on a simple model. Second, the isotopic fractionation constants measured by the authors are quite well reproduced by the same simple model, but not by dynamics calculations based on supposedly accurate potential energy surfaces.

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As far as I know the literature concerning the dissociation of OCS there are several other aspects which require a state-of-the-art theoretical treatment: explanation of the vibrational structures, the partitioning of the excess energy, the angular dependence. Calculations of the type recently performed for N2O, which is isoelectronic to OCS, are required. The present investigation adds detailed data which are mandatory for a future comparison between theory and experiment.

Since I am not part of the atmospheric chemistry community, I am not able to comment on the atmospheric implications.

The manuscript is well organized and written in a transparent manner. I have only a few minor technical comments which the authors should consider before publication:

1) Page 20497, beginning of Section 3.4: The first two sentences are a bit puzzling to me: " The positions of the vibrational peaks .... were red-shifted ... in Fig. 3. The peak shifts change from negative (red-shift) to positive (blue-shift) at ..."

2) The quantities Q and d in eq(5) should be defined.

3) Eq(9): "Deviation from mass-dependent fractionation is often described using .." A reference or, even better, a short explanation would be helpful here.

Interactive comment on Atmos. Chem. Phys. Discuss., 11, 20487, 2011.

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