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## Interactive comment on "A upper limit for water dimer absorption in the 750 nm spectral region and a revised water line list" by A. J. L. Shillings et al.

## A. Campargue (Referee)

alain.campargue@ujf-grenoble.fr

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This paper is a very interesting contribution to an issue of importance for atmospheric science. It is well written and very pleasant to read in particular the Introduction which includes a nice review on the subject. Nevertheless I have several comments which are of importance and should be considered in the revised version:

1- a great part of the results and conclusion relies on the quality of the monomer database near 740 nm. It leads to the UCL08 line list which is a mixture of experimental and calculated data. My major concern is that the most relevant experimental source in the region was missed by the authors. This source is "ICLAS of water in the

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770 nm transparency window (12746-13558 cm-1). Comparison with FTS databases.J. Quant. Spectrosc. Radiat. Transfer 109 (2008) 2832-2845.by A. Campargue, S. N. Mikhailenko, and A. W. Liu. In this paper, we compared the different theoretical and experimental databases in the spectral region of interest, in particular HITRAN, Tolchenov and Tennyson 2008 and BT2!! The sensitivity of the ICLAS technique allowed detecting more than two times the number of transitions in Tolchenov and Tennyson 2008, now adopted in the HITRAN database. This paper following Kassi 2005 was motivated by the same goal: improving the monomer database in the region where Pfeilsticker et al claimed the detection of the WD signature and our conclusion was:" Considering these results and the fact that WD signature at 750 nm could not be confirmed by subsequent measurements, "the first evidence for atmospheric WD detection as reported in Ref. [1] had to be revoked" [5]. The Fig. 6 of our paper shows low resolution simulations very similar to those presented in the paper under review. The ICLAS experimental line list should have been used by Shillings et al or at least they should have compared to low resolution simulations obtained with ICLAS and UCL08 line lists to evaluate the "missing" absorption of the ICLAS data in the region of interest.

- 2- I have now some questions about the UCL08 line list: It is always a responsibility to release such database for water. It extends much further than the spectral region of interest and the reader (and potential user) would like to have some more information about the construction of this database: The UCL08 line list includes minor isotopologues, how were obtained line parameters of the isotopologues which may contribute significantly to the absorption in the considered transparency window. The authors give only the BT2 line list as reference for the calculated data but BT2 is limited to the main isotopologue... How were "mixed " the experimental line list and the calculated line list? It is a very difficult task as the rovibrational labelling of the calculated line list are not always reliable...
- 3- the discussion about the width of the dimer signature considers that the amplitude of the residuals between the UCL08 simulation and the BBCRDS spectra is a good es-

timation of the maximum values of the dimer absorption. Nevertheless the uncertainty on the BBCRDS and UCL08 simulations themselves may add additional contribution which should be evaluated and discussed. For instance, as mentioned above UCL08 line list can be compared to ICLAS line list. What is the noise level on the BBCRDS spectra? What is the error which may be induced by the procedure used to linearise the absorption cross sections?

- 4- Several comparisons (see for instance Fig. 5) present the BBCRDS spectra of water in air (at 1atm?) compared to a simulation from UCL08 linelist. No information is provided about the way that the UCL08 stick spectrum was convoluted with the BBCRDS apparatus function. This is of major impact for the strong lines. Also, was the pressure broadening taken into account in the UCL08 simulation? Which air broadening coefficients?
- 5- Fig.4 looks very strange with a intensity weighted average strongly different than the average intensity values. Does it means that the problem on the HITRAN values affects mostly the strongest lines? A plot of the ratio versus the intensities in the 8000-9500 cm-1 region would be instructive.

6-finally, as far as I understand, the present title is not the most appropriate: instead of "A upper limit for water dimer absorption  $\dots$ ", I will propose "A upper limit on the band width of water dimer absorption  $\dots$ 

No doubt that this paper should be published as it confirms the conclusions of Kassi et al 2005 and adds significant information about the expected dimer signature around 750 nm. In particular, the discussion on the temperature dependence of the rate constant and the band strength in relation with the BBCRDS results obtained at high temperature is instructive.

Interactive comment on Atmos. Chem. Phys. Discuss., 10, 23345, 2010.

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