

## ***Interactive comment on “A theoretical study on UV-spectroscopy, electronic structure and reactivity properties of sesquiterpenes” by S.-X. Hu et al.***

**Anonymous Referee #1**

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This manuscript focuses on the prediction and assignment of vertical electronic transitions in a number of sesquiterpenes by different electronic structure methods (DFT, TDDFT, CIS, ZINDO). The vertical transition energies are calculated with Gaussian 03 and correlated to structures of the sesquiterpenes.

It is well known that alkenes have strong  $\pi$  to  $\pi^*$  transitions in the UV range (around 200 nm). According to Woodward's rules, the transition wavelengths can be shifted to the red by conjugation or by certain substituent groups. However, even for the sesquiterpenes containing conjugated double bonds, the  $\pi$  to  $\pi^*$  bands are expected to be below 250 nm. Therefore, sesquiterpenes, which never reach the stratosphere

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due to their exceptionally high reactivity, cannot be electronically excited under realistic atmospheric conditions.

The authors hope that results of their calculations will be useful for distinguishing different sesquiterpenes. I doubt it will be the case as the absorptions below 250 nm are not very specific; a number of different organic and inorganic atmospheric molecules absorb in this region.

I think the paper should be published, however, given that UV absorptions by sesquiterpenes are not going to be of much interest to atmospheric scientists, Atmospheric Chemistry and Physics is clearly not the best choice for this publication. The authors should consider submitting the manuscript to a more specialized journal focusing on theoretical calculations of electronic properties.

I also recommend that the authors re-write some of the sentences in their manuscript before the resubmission. In several instances they are using terminology that is not in wide use and likely to be misinterpreted by readers. Examples of phrases that are guaranteed to raise readers' eyebrows include: conceptual DFT; transit energies; sub-particles; formational mechanism; sub-volatile; isomeric changes; etc.

Finally, I want to stress that the authors do not calculate "absorption spectra". They calculate vertical transition energies. There is an important distinction between the two.

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