

Interactive comment on “Quantitative infrared absorption cross-sections of isoprene for atmospheric measurements” by C. S. Brauer et al.

C. S. Brauer et al.

carolyn.brauer@pnnl.gov

Received and published: 19 August 2014

We thank you for the time you have invested in reviewing this paper and appreciate your insightful comments. The following is our detailed response to your comments and how we propose to address them in the updated manuscript.

Comment 1: P4169 L1-5. Please make a quantitative statement about linearity of the abs coeff vs concentration plots, as this is crucial to the method in which the quantitative data are produced. If covered in the previous papers from Sharpe and Johnson, a reference would be sufficient.

C2255

Response: *Thank you for pointing this out. The following has been inserted into the paragraph: “The nonlinearity correction removes most of the effects due to deviations from Beer’s Law, but the magnitude of the deviation can still be extracted from statistical uncertainty of the fit of the slope for the absorption coefficient at each wavelength bin. The uncertainties arise from baseline drift, contaminant features etc. but still tend to be larger for larger absorption coefficient and in general such errors are on the order of 2%-3% (2σ). [S.W. Sharpe, T.J. Johnson, P.M. Chu, J. Kleimyer and B. Rowland, ‘Quantitative infrared spectra of vapor phase chemical agents,’ Proc. SPIE 5085, 19-27, (2003)].”*

Comment 2: Table 4, Figure 1. Numbering system. Isoprene’s unambiguous systematic name is 2-methyl-1,3-butadiene, as stated in the abstract line 1. The numbering system in Fig 1 and Table 4 is different, presumably driven by the modelling calculations. The numbering in Fig 1 and Table 4 and anywhere else in the text should be changed to reflect the correct systematic numbering: C4 → C1 C2 → C2 C3 → C5 C1 → C3 C5 → C4

Response: *We agree that the numbering system should be changed to reflect the systematic numbering. Figure 1 has been corrected and the manuscript has been updated with the correct numbering system.*

Comment 3: P4164 Abstract. The second sentence is ungrammatical, suggest rephrase as “Isoprene is produced by vegetation as well as anthropogenic sources, and its OH- and O3-initiated oxidations are a major source. . . .”

Response: *Thank you for the suggestion. We have incorporated your phrasing into the manuscript.*

Comment 4: P4164 L7. “standoff” I am not accustomed to this term, please clarify (also later)

C2256

Response: The term “standoff” is used to describe detection from a distance, in contrast to “point” or “in situ” detection, which describes detection at the source or in the laboratory. Although we are not aware of a formal distinction, standoff is generally understood to be at distances of tens to hundreds of meters, whereas “remote detection” refers to greater distances.

Comment 5: P4164 L10: Bruker 66V FTIR spectrometer. (add spectrometer)

Response: Thank you for pointing this out. It has been corrected.

Comment 6: P4164 L14-18: Please invert the order of description of isoprene sources – first the major one, 99.9% from plants, then the minor sources.

Response: We agree that a “top-down” approach makes more sense. This section has been revised.

Comment 7: P4165 L5: ppbv – please spell out and define abbreviations at first use. Ppbv = nmol mol⁻¹.

Response: Thank you. The correction has been made.

Comment 8: P4167 L6: I suggest replacing the full stop with semi-colon so that the sentence “using the quantitative. . .” is logically attached to the preceding sentence which connects to it.

Response: Thank you. The correction has been made.

Comment 9: P4167 L23: globar rather than glow bar (also in Table 1)

Response: The authors believe that the use of “glow bar” is, in fact, correct. Global[®] is the registered trademark of one source manufacturer, but this is not the manufacturer
C2257

that Bruker uses.

Comment 10: P4167 L25. (instrument resolution is defined here as 0.9/OPD) add “here”, this is a definition used only by Bruker.

Response: This is an important distinction. Thank you for bringing this to our attention. The word “here” has been added.

Comment 11: P4168 L3. The spectra are not actually 2x zero filled, that is again Bruker’s setting. For resolution 0.12 cm⁻¹, the point spacing without zerofilling would be 0.06 cm⁻¹.

Response: Thank you for bringing this to our attention. This sentence can be rewritten as: “A zerofill factor of 2x (per Bruker definition) was used such that the raw single beam spectra recorded at 0.112 cm⁻¹ had a point spacing of 0.06 cm⁻¹.”

Comment 12: P4168 L16. Baratron singular.

Response: Thank you. The correction has been made.

Comment 13: P4169 Eq 2 and 3. It would be good to stress here that “ppm” refers to ppm at 1 atm and 296K. It is said elsewhere, but could also well be stated here in context of the equations.

Response: Thank you. The correction has been made.

Comment 14: P4170 L25. Please include the conversion to the more preferred SI unit kJ mol⁻¹.

Response: Thank you. The SI conversion has been added.

Comment 15: P4171 L 4-10. Please add a sentence for the uninitiated to describe the qualitative difference between A, B and C type bands. Perhaps use nu9 and nu23 as examples.

Response: *We agree that providing a statement regarding the band types would be beneficial to the reader. It has been added to the manuscript.*

Comment 16: P4172 L18. How well do the integrated bands strengths agree when they DO agree? Give a percentage, so we can compare to those below that do not.

Response: *The integrated band strengths agree to within the stated 3% error. This has been added to the manuscript.*

Comment 17: P4172 L21 . . . higher in THE 323K spectrum. . .

Response: *Thank you for noticing this omission. The manuscript has been corrected.*

Comment 18: P4172 L25. The meaning of this sentence and the next needs clarification. I think you want to say it may be temperature dependence, is probably not due to an additional conformer, and probably is due to the baseline fitting.

Response: *Yes, that is exactly what is meant by the sentence. It has been clarified in the revised manuscript.*

Comment 19: P4174 L8: sensitivity is an imprecise word. Perhaps replace by . . .an optical system with a noise level of less than 1.2×10^{-3} (log10). . .

Response: *Thank you for the suggestion. We will replace the imprecise wording in the revised manuscript.*

Comment 20: P4174 L16. remove "seminal"

C2259

Response: *This word has been removed.*

Comment 21: Table 1. Clarify resolution 0.112 (0.9/L) and zerofilling x1 (Bruker setting x2)

Response: *For FT instruments, there are several different working definitions of spectral resolution. We have used the Bruker specification of 0.9/OPD, where the OPD is the optical path difference in cm, as measured by zero-crossings of the fringe pattern of the interferometer HeNe laser. Zerofilling defined as per comment 11.*

Interactive comment on Atmos. Meas. Tech. Discuss., 7, 4163, 2014.