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Atmospheric Measurement Techniques Discussions

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

Anonymous Referee #1

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The PNNL quantitative spectral database (Sharpe et al. 2004, Johnson et al. 2010) his a high quality library of quantitative infrared absorption spectra of small to medium sized molecules. This paper describes the quantitative measurements (with errors) of the spectrum of isoprene, 2-methyl-1,3-butadiene, for addition to the PNNL library. This is a very valuable addition because of isoprene's great importance to atmospheric chemistry. The quantitative measurements are fully described, vibrational assignments made or revised, and estimates of detectability with infrared measurement techniques are given. This paper is well suited to AMT, complete and thorough, and should be published subject to the following minor and technical revisions.

Minor revisions:

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.

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 Table4 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

Technical revisions:

P4164 Abstract. The second sentence is ungrammatical, suggest rephrase as "Isoprene is produced by vegetation as well as anthrogogenic sources, and its OH- and O3-inititaed oxidations are a major source. . ..."

P4164 L7: "standoff" I am not accustomed to this term, please clarify (also later)

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

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

P4165 L5: ppbv – please spell out and define abbraviations at first use. Ppbv = nmol mol-1. 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.

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

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

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.

P4168 L16: Baratron singular.

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.

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

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.

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.

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

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.

P4174 L8: sensitivity is an imprecise word. Perhaps replace by . . .an optical system with a noise level of less than 1.2x10-3 (log10). . ..

P4174 L16: remove "seminal"

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

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