

Addendum to: The Infrared Spectrum of CS₂ in the ν_3 Band Region

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In a recent paper by Wells et al. [1] the band origins of ν_3 of $^{12}\text{C}^{32}\text{S}_2$ and $^{13}\text{C}^{32}\text{S}_2$ have been determined with high accuracy from heterodyne frequency measurements. As mentioned in our paper on these bands [2] our spectra were calibrated with water vapour lines from [3]. This limited the accuracy of all band centers in the paper to $\pm 3 \cdot 10^{-4} \text{ cm}^{-1}$ (one standard error) – not allowing for any systematic error of the calibration lines, however.

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In a paper by Brown and Toth [4] it has been indicated that the frequencies of these calibration lines are $3.63 \cdot 10^{-4} \text{ cm}^{-1}$ too high (mean value for 71 lines). It should be noted that a corresponding correction has not been applied to the same frequencies in “Handbook of Infrared Standards” [5].

Indeed, a comparison of the band origins of [1] and [2] shows that our frequencies are 2.9(8) and $5.2(8) \cdot 10^{-4} \text{ cm}^{-1}$ too high for $^{12}\text{C}^{32}\text{S}_2$ and $^{13}\text{C}^{32}\text{S}_2$, respectively. This confirms the statement of [4] above about the water line frequencies.

In our spectra $^{13}\text{C}^{32}\text{S}_2$ was recorded in natural abundance so that the differences from the heterodyne measurements refer to the strongest and one of the weakest line series. There may have been a slight asymmetry in our line profiles (which we did not check), which would account for the incomplete numerical agreement for the two bands. However, a mean correction of $4 \cdot 10^{-4} \text{ cm}^{-1}$ should be subtracted from all band center frequencies given in our paper [2]. Their absolute accuracies should then all be about 10^{-4} cm^{-1} .

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