

ADDITIONS AND CORRECTIONS

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William S. Barney, Lisa M. Wingen, Matthew J. Lakin, Theo Brauers, Jochen Stutz, and Barbara J. Finlayson-Pitts*: Infrared Absorption Cross-Section Measurements for Nitrous Acid (HONO) at Room Temperature

Pages 1692–1699. In a recent paper¹ we published FTIR absorbance cross-sections for three mid-infrared bands of nitrous acid (HONO). In that analysis, we curve fit the three individual bands centered at 790 (trans- ν_4), 852 (cis- ν_4), and 1263 cm^{-1} (trans- ν_3), respectively, using software which was limited to a 128 cm^{-1} spectral segment applied to each band separately. There was a curved baseline that was particularly difficult to subtract out from the trans- ν_4 band at 790 cm^{-1} using the 128 cm^{-1} spectral width. In response to an inquiry (J. Kleffmann, personal communication) regarding the relative intensities of these three bands, we have refit our spectra using new software (Igor Pro, Wavemetrics, Inc.) that allows us to fit all three bands simultaneously using the entire spectrum from 650 to 1400 cm^{-1} . This allows better baseline subtraction. However, because of the higher uncertainty in the baseline from 650 to 750 cm^{-1} , the error bars have been increased for the 790 cm^{-1} band. Other than the size of the spectral segment used, the techniques used

in the new analysis were identical to those described in our previous paper.¹

Tables 2, 3, and 5 give the revised analysis using the much larger spectral region for fitting the three bands simultaneously. As expected, because of the baseline, the largest changes are in the cross sections for the trans- ν_4 band at 790 cm^{-1} . For the integrated band intensities, these revised values now give relative band intensities that are in good agreement with those of Kagann and Maki² and several unpublished studies.^{3,4}

Acknowledgment.

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References and Notes

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- (3) Wallington, T.; Hurley, M. Private communication.
- (4) Kleffmann, J. Private communication.
- (5) Chan, W. H.; Nordstrom, R. J.; Calvert, J. G.; Shaw, J. H. *Environ. Sci. Technol.* **1976**, *10*, 674.
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TABLE 2: (Revised) Infrared Absorption Cross-Sections: Q-Branch Intensity at Given Wavenumber

	effective ^a cross section σ ($10^{-19} \text{ cm}^2 \text{ molecule}^{-1}$, base 10)			trans/cis ratio used	absolute ^b cross section σ ($10^{-19} \text{ cm}^2 \text{ molecule}^{-1}$, base 10)			Q_{1263}/Q_{852}
	790 cm^{-1}	852 cm^{-1}	1263 cm^{-1}		790 cm^{-1}	852 cm^{-1}	1263 cm^{-1}	
this work ^c	2.8 ± 0.6	2.7 ± 0.3	3.7 ± 0.4	2.30	4.0 ± 0.8	9.0 ± 0.9	5.2 ± 0.5	0.58
Chan et al. ⁵		3.79 ± 0.38	4.82 ± 0.48	2.29		12.5 ± 1.3	6.93 ± 0.70	0.56
Sakamaki et al. ⁶		2.86	2.78	2.27		9.34	4.00	0.43

^a Calculated from $\sigma = (1/C_{\text{HONO}}) \log_{10}(I_0/I)$, where C_{HONO} is the total HONO concentration (trans plus cis). ^b Corrected for the trans/cis ratio. ^c Our error bars are 1 standard deviation. Those of Chan et al.⁵ are not stated, and Sakamaki et al.⁶ do not give error bars for their cross-sections.

TABLE 3: (Revised) Infrared Absorption Cross-Sections: Integrated Band

	integrated effective ^a cross sections S ($10^{-18} \text{ cm molecule}^{-1}$, base 10)			trans/cis ratio used	integrated absolute ^b cross sections S ($10^{-18} \text{ cm molecule}^{-1}$, base 10)		
	740–820 cm^{-1}	820–900 cm^{-1}	1220–1300 cm^{-1}		740–820 cm^{-1}	820–900 cm^{-1}	1220–1300 cm^{-1}
this work	7.0 ± 1.4^c	6.3 ± 0.6^c	8.2 ± 0.8	2.3	10.0 ± 2.0	21 ± 2.1	11.7 ± 1.2
Kagann and Maki ²			8.1 ± 1.0	2.0			12.2 ± 1.5

^a Calculated from $S = (1/C_{\text{HONO}}) \int_{\text{band}} \log_{10}(I_0(\bar{\nu})/I(\bar{\nu})) d\bar{\nu}$, where C_{HONO} is the total HONO concentration (trans plus cis). ^b Corrected for the trans/cis ratio. ^c The cutoff between the trans- ν_4 band at 790 cm^{-1} and the cis- ν_4 band at 852 cm^{-1} was taken to be 820 cm^{-1} . Kagann and Maki reported values for the cross-sections² for the 790 and 852 cm^{-1} bands of $(6.5 \pm 1.0) \times 10^{-18} \text{ cm molecule}^{-1}$ and $(5.6 \pm 0.8) \times 10^{-18} \text{ cm molecule}^{-1}$, respectively. However, our values may not be directly comparable to theirs because the wavenumber region used for each band was not stated in that work.

TABLE 5: (Revised) Parameters Used to Generate Model Reference Spectra^a

m	852 cm^{-1}			1263 cm^{-1}		
	α_m ($10^{-19} \text{ cm}^2 \text{ molecule}^{-1}$)	β_m (cm^2)	γ_m (cm^{-1})	α_m ($10^{-19} \text{ cm}^2 \text{ molecule}^{-1}$)	β_m (cm^2)	γ_m (cm^{-1})
1	1.40 ± 0.01^b	0.007 ± 0.0001	866.94 ± 0.08	1.76 ± 0.01	0.0062 ± 0.0001	1278.0 ± 0.1
2	0.59 ± 0.05	0.032 ± 0.003	840.9 ± 0.1	1.1 ± 0.2	0.012 ± 0.002	1249.8 ± 0.1
3	1.31 ± 0.06	2.3 ± 0.2	852.25 ± 0.02	1.1 ± 0.1	0.87 ± 0.29	1264.5 ± 0.2
4	0.98 ± 0.01	0.0043 ± 0.0003	830.7 ± 0.5	0.71 ± 0.1	0.0037 ± 0.0007	1239.8 ± 3.1
5	1.16 ± 0.05	0.35 ± 0.02	852.92 ± 0.04	2.6 ± 0.3	2.4 ± 0.3	1263.52 ± 0.03

^a These parameters are used in conjunction with eq IX to produce model references. References can be used to analyze spectra with any software which can perform a linear least-squares fit between two sets of data. ^b Error bars are 1 standard deviation and reflect only the uncertainty associated with the nonlinear fit. See Table 2 for the error bars of the actual measured cross-sections.

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