LINE INTENSITY CORRECTIONS AND REASSIGNMENT OF THE SPECTRAL LINES OF WATER VAPOR IN THE HITRAN AND GEISA DATABASES IN THE SHORT-WAVE REGION

[*]L. P. Giver, [**]P. Varanasi, [*]C. Chackerian, Jr., [*]D. W. Schwenke,
[¶]R. S. Freedman, [¶]M. D. Di Rosa, and [¶¶]R. L. Sams
[*]NASA-Ames Research Center, Moffett Field, CA.
[**] State University of New York at Stony Brook, NY 11794-5000
[¶]Space Physics Research Institute, Sunnyvale, CA.
[¶¶]Pacific Northwest National Laboratory, Richland, WA

While measuring the weak water vapor lines in the wings of the 0.94 μm band on spectra obtained with the 25m base-path White cell and Bomem DA8 Fourier-transform spectrometer (FTS), we compared some of our measured intensity data to those listed in the *HITRAN*-96 (*HI*gh resolution *TRAN*smission molecular absorption) database [1] data and also with the prior measurements of Chevillard *et al.*[2] Our measurements were, on the average, about 20 % higher than the entries in *HITRAN*, but generally compatible with the intensities reported by Chevillard et al. This seemed strange, since *HITRAN* referred to the Chevillard publication as the source data for most of the lines listed in the 9500 to 11500 cm^{-1} region. We therefore selected over 50 of the best-measured lines from the tables of Chevillard et al. to compare with the *HITRAN* values. About half of these lines were previously measured by Giver *et al.* [3]; each of these prior line measurements agreed with the corresponding measurements by Chevillard et al within 6 %, which was their estimate for the uncertainty. After making this comparison and finding that the *HITRAN* intensities did not agree with Chevillard's published values, we made similar comparisons of the experimental data from four other articles reporting the line intensities in the visible and near-infrared that formed the basis for *HITRAN* lists in the respecive spectral regions. The four articles are by Camy-Peyret et al [4], Mandin et al [5], Mandin et al [6], and Toth [7]. The measured intensity data are all in the units of cm^{-1}/(cm-atm) at room temperature. All the measurements described in the five mentioned articles are based on FTS spectra obtained with the 6 meter base-path White cell at the Kitt Peak solar telescope and they all contain reports of intensities in the units of cm^{-2} atm^{-1}. The unit used in the *HITRAN* database for the line intensity is cm/molecule at 296. The corrections we refer to here point toward to several cases of oversight by the creators of the database during the process of converting the measured intensity data reported in the five source papers into the units adapted by the creators of the database. The corrections needed to bring the *HITRAN* intensities into agreement with the published measurements have been described by Giver et al. [8] . These corrections only apply to assigned lines of the main isotopomer of water reported in the above cited five publications of experimental data, but these lines account for over 97% of the absolute intensity in each of the wavenumber intervals of interest. The corrections are described in detail by Giver et al. [8]. The list of parameters for lines between8000 to 25200 cm^{-1}, with the proper intensity revisions, has been posted on the "database updates" page of the *HITRAN* internet site: http://www.hitran.com. These corrections affect the *GEISA* (*G*estion et *E*tude des *I*nformations *S*pectroscopiques *A*tmospheriques) databank[9] as well.

We have also investigated the absorption band at 1.38 μm (5750-7965 cm^{-1}) to determine if any similar systematic differences exist between the entries in the databases and published mesurements of intensities. While there are many substantial differences between the latest published measurements by Toth [10] and the *HITRAN* database values, there is no systematic correction that can be applied; the intensity data of the databases require improvements on a line-by-line basis, which is beyond the scope of the present work. This region is similar to the 11610 - 12861 cm^{-1} region, in that many lines on *HITRAN* were obtained from preliminary measurements by Toth, which were subsequently completed and published in 1994. However, in the 1.38 μm region, many strong lines on *HITRAN* '86 were not replaced by Toth's preliminary measurements; in fact, only about 35% of the total intensity of lines in this region are listed as coming from Toth's work. Therefore, when we ratioed Toth's [10] measured intensities to *HITRAN* '96 values, we did not find any systematic trends as was found in the higher wavenumber regions. We have now converted *HITRAN* intensities to measurement units, sorted the *HITRAN* lines out as 1986 hold-overs or Toth's preliminary entries, and ratioed Toth's published measurements to them. Toth's measured values are typically about 75% of the *HITRAN* intensities for the old 1986 hold-over lines, with some notable exceptions. Also, his final measured intensities are generally larger than the *HITRAN* values from his own preliminary measurements; some lines are about 40 % larger. This is very different from the comparison of Toth's published measurements [7] to *HITRAN* values in the 820 nm region, where Toth's published values were apparently very close to his preliminary values used by *HITRAN*. There is nothing systematic found in the ratios in the 1.38 μm region. New spectra have been obtained in the 7250 cm^{-1} region at the Pacific Northwest National Laboratory, using a Bruker FTS with spectral resolution better than 0.01 cm^{-1}. These spectra were obtained with a path-length of 20 cm, and pressures of pure H_2O vapor between 2 and 15 torr. Several lines in these observations were compared to simulations using *HITRAN* '96 line positions and intensities. Six of these lines were hold-overs from *HITRAN* '86. A comparison of these new spectra with *HITRAN* suggest the need for some improvement in the *HITRAN* hold-over values of both positions and intensities. But intensities and positions for the strong lines measured on these spectra at the Pacific Northwest National Laboratory are generally in good agreement with Toth's published values.[10] We have compared *HITRAN* intensities with the published measurements of Toth. We recommend that for the most part, the *HITRAN* and *GEISA* databases should be updated using Toth's finalized measurements of both positions and intensities

The results of incorporating the major corrections to the intensities listed in the database are 14.4% and 8.7% increases in the 9500-11500 cm^{-1} and the 11500-13000 cm^{-1} spectral regions, respectively. The important 0.82 μm and 0.94 μm bands of water vapor are in these regions. The respective intensity corrections to the databases are sufficiently large as to warrant re-analyses of some atmospheric measurements made in these bands. For example, Nedoluha, *et al.*[11] have shown that correcting the 0.94 μm water band measurements by the *POAM* (Polar Ozone Atmospheric Measurements) satellite mission results in better agreement for *POAM III* and *HALOE* (*HAL*ogen *O*cculation *E*xperiment) water vapor abundances in the Antarctic lower stratosphere.

REFERENCES

1. Rothman, L. S., The HITRAN molecular spectroscopic database and HAWKS (HITRAN Atmospheric Workstation): 1996 edition, *J. Quant. Spectrosc. Radiat. Transfer,* Vol. 60, pp. 665-711, 1998

2. Chevillard, J.P., Mandin, J.-Y., Flaud, J.-M., and Camy-Peyret, C., $H_2{}^{16}O$: Line Positions and Intensities between 9500 and 11500 cm^{-1}." *Can. J. Physics* Vol. 66, pp. 997-1012, 1988.

3. Giver, L.P., Gentry, B., Schwemmer, G. and T.D. Wilkerson, T. D.,Water Absorption Lines, 931-961 nm; Selected Intensities, N_2-Collision-Broadening Coefficients and Pressure Shifts in Air, *J. Quant. Spectrosc. Radiat. Transfer,*.Vol. 27, pp. 423-436, 1982.

4. Camy-Peyret, C., Flaud, J.-M., Mandin, J.- Y., Chevillard, J. P., Brault, J., Ramsay, D. A., Vervloet, M., and Chauville, J., High-Resolution Spectrum of Water Vapor between 16500 and 25250 cm^{-1}, *J. Molec. Spectr*. Vol. 113, 208-228, 1986.

5. Mandin, J.-Y., J.P. Chevillard, C. Camy-Peyret, and J.-M. Flaud, High-Resolution Spectrum of Water Vapor; 13200 and 16500 cm^{-1}, *J. Molec. Spectr*. Vol. 116, pp.167-190, 1986.

6. Mandin, J.-Y., J.P. Chevillard, J.-M. Flaud, and C. Camy-Peyret, $H_2{}^{16}O$: Line positions and intensities between 8000 and 9500 cm^{-1}, *Can. J. Phys*. Vol. 66, pp. 997-1011, 1988.

7. Toth, R.A., Measurements of $H_2{}^{16}O$ Line Positions and Strengths: 11610 to 12861 cm^{-1}, *J. Molec. Spectr*. Vol. 166, pp. 176-183, 1994.

8. Giver, L.P., Chackerian, C. Jr., and Varanasi, P.,Visible and near-infrared $H_2{}^{16}O$ line intensity corrections for HITRAN-96, *J. Quant. Spectrosc. Radiat. Transfer.,* Vol. 66, pp. 101-105, 2000.

9. Jacquinet-Husson, N. et al., The 1997 Spectroscopic GEISA Databank, *J. Quant. Spectrosc. Radiat. Transfer,* Vo. 62, pp. 205-254, 1999.

10. Toth, R.A., Extensive Measurements of $H_2{}^{16}O$ Line Frequencies and Strengths: 5750 to 7965 cm^{-1}, *Appl. Opt*. Vol. 33, pp. 4851-67, 1994.

11. Nedoluha, G.E., Bevilacqua, R. M., Hoppel, K. W., Dachler, M., Shettle, E. P., Hornstein, J. H., Fromm, M. D., Lumpe, J. D., Rosenfeld, J. E., POAM III measurements of dehydration in the Antarctic lower stratosphere, Geophys. Research Letters, Vol. 27, pp. 1683-1686, 2000.