Line positions and intensities in the 7400–8600 cm⁻¹ region of the ammonia spectrum*

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ABSTRACT

The positions and intensities of 1936 lines observed in the range 7400–8600 cm⁻¹ of two absorption spectra of ammonia recorded at high resolution using Fourier transform spectroscopy are reported. The accuracy of these line positions is estimated to range from 0.001 to 0.002 cm⁻¹ from the lower to the upper limits of the spectral range considered, while the accuracy of the line intensities is estimated to be around 10% or better. Also reported are less-accurately measured positions and intensities of 1985 lines retrieved from these two spectra or from only one of them. These results are compared with the data measured recently in a spectrum recorded in 1980 at the Kitt Peak National Solar Observatory [Barton *et al.*, *J. Mol. Spectrosc.* **325**, 7 (2016)] and provided in HITRAN 2016, as well as line positions and intensities measured in this work in the same Kitt Peak spectrum.

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1. Introduction

Ammonia is observed in environments as diverse as the atmosphere of the Earth [1,2], the atmospheres of the giant planets of the solar system [3–5], cometary atmospheres [6] and molecular clouds [7]. Its complex infrared spectrum resulting from the excitation of its four modes of vibration has been extensively studied (see e.g. [8–11] and references therein). However, the spectral range above 7000 cm⁻¹ has received much less attention [12–16]. This was reflected by the lack of spectroscopic information for this range up to the 2012 edition of the HITRAN database [17], lack that is still effective in the current version of the GEISA database [18].

In their very recent study, Barton *et al.* [15] generated a list of 8466 experimental ammonia line positions

and intensities measured between 7400 and 8640 cm⁻¹ in a Fourier transform absorption spectrum recorded in 1980 by Dr Catherine de Bergh at the Kitt Peak National Solar Observatory (in the remainder of the article, this spectrum will be referred to as the ‘Kitt Peak spectrum’), and 2475 of these lines were assigned with the quantum numbers recommended by Down *et al.* [8]. This experimental linelist, from which three duplicate lines at 7724.99138, 7950.82966 and 7975.53377 cm⁻¹ were removed, was included in HITRAN 2016, the line positions and intensities being given uncertainties of 0.001–0.01 cm⁻¹ and 10–20 %, respectively [19]. These uncertainties are in line with the statement of Barton *et al.* [15] that the accuracy of the line positions and intensities reported for isolated lines of medium intensity are

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of the order of 0.003 cm^{-1} and 15%, respectively. However, Barton *et al.* [15] also stated that the uncertainty in the retrieved intensities may significantly exceed 15% for lines stronger than $1.0 \times 10^{-22} \text{ cm}^{-1}/(\text{molecule cm}^{-2})$.

The aim of the present study is to bring experimental information in the $7400\text{--}8600 \text{ cm}^{-1}$ region of the absorption spectrum of ammonia and compare it with the data reported by Barton *et al.* [15]. In view of discrepancies observed between line positions and intensities measured in this work and reported by Barton *et al.* [15], we also measured NH_3 line positions and intensities in the Kitt Peak spectrum. To help assess the uncertainties of measurement in the present work, NH_3 line positions and intensities were also measured in the $6800\text{--}7000 \text{ cm}^{-1}$ spectral range and compared with the information reported by Sung *et al.* [20], and H_2O line positions measured in the $8700\text{--}8950 \text{ cm}^{-1}$ region were compared with HITRAN 2016 data [19].

This article is structured as follows. The recording of high-resolution spectra of ammonia and the measurements of line positions and intensities therein are described in Section 2. Section 3 starts with the comparisons with the previous work [19,20] of NH_3 line positions and intensities measured in the $6800\text{--}7000 \text{ cm}^{-1}$ range and H_2O line positions measured in the $8700\text{--}8950 \text{ cm}^{-1}$ region. It then details the ammonia line positions and intensities measured in the spectra recorded in Brussels. Comparisons of the latter with the data reported by Barton *et al.* [15] as well as NH_3 line positions and intensities measured in this work in the Kitt Peak spectrum are described in Section 4. Section 5 concludes the article.

2. Experimental details and analysis

Two unapodised absorption spectra of a commercial sample of ammonia (Aldrich, stated purity $\geq 99.99\%$), in natural abundance and used without further purification, were recorded with a Bruker IFS120 (upgraded to IFS125) HR Fourier transform spectrometer. The instrument was fitted with a tungsten source, a quartz beam-splitter and an InSb detector cooled down to 77 K. The spectra were recorded in the range $2700\text{--}10500 \text{ cm}^{-1}$, at room temperature [293 (1) K] stabilised by an air-conditioning system, and at a resolution of 0.02 cm^{-1} corresponding to a maximum optical path difference of 45 cm. The sample was contained in a Pyrex White-type cell, set to provide an absorption path length of 27.62 (8) m and closed by CaF_2 windows. The two spectra correspond to average pressures of 3.44 (11) and 1.284 (46) hPa, measured with an MKS Baratron gauge model 690A of 10 torr full scale range. The numbers between parentheses provided for the pressures are the

uncertainties mainly arising from the slow decrease of the ammonia pressure from the beginning to the end of the recording of the interferograms, which respectively lasted 4.5 and 18 h. The rate of decrease of the pressure ranged from about 0.26 hPa/h during the first 15 min of the recording of the higher-pressure spectrum to about 0.044 hPa/h during the last 15 min of its recording, and was roughly constant ($\sim 0.009 \text{ hPa/h}$) for the lower pressure spectrum, recorded last. This evolution of the rate of decrease of the pressure may indicate that some ‘passivation’ of the cell occurred and, combined with the duration of the recordings, led to the same relative reduction of about 11–12% of the ammonia pressure for both spectra. The higher and lower pressure spectra are characterised by the RMS signal-to-noise ratios of about 700 and 1200, respectively. They were interpolated four times prior to their analysis. They are presented in Figure 1.

The positions and intensities of the absorption lines observed in the two spectra were measured by non-linear least-squares curve fitting using the program ‘WSpectra’ [21]. Each line in the lower pressure spectrum was given a Gaussian profile, while a Voigt profile was used for the higher pressure spectrum. The fitted line parameters were the position, intensity and full width at half maximum (FWHM), to which the so-called ‘damping’ parameter (ratio of the Lorentz to the Voigt FWHM) was added when using the Voigt profile. The instrumental effects arising from the truncation of the interferogram were included as fixed contributions. The measured positions $\tilde{\nu}_{\text{obs}}$ of 145 water vapour lines, observed in the ranges $5255\text{--}5536 \text{ cm}^{-1}$ and $7054\text{--}7398 \text{ cm}^{-1}$ in the lower pressure spectrum, were matched to reference positions $\tilde{\nu}_{\text{HITRAN}}$ available in HITRAN [19], originating from a linelist generated by Toth [22] and characterised by uncertainties ranging from 0.00001 to 0.0001 cm^{-1} . The differences $\tilde{\nu}_{\text{HITRAN}} - \tilde{\nu}_{\text{obs}}$ were fitted to the following expression:

$$\tilde{\nu}_{\text{HITRAN}} - \tilde{\nu}_{\text{obs}} = a + b\tilde{\nu}_{\text{obs}}, \quad (1)$$

where a and b were adjusted parameters. An RMS deviation of $1.0 \times 10^{-4} \text{ cm}^{-1}$ was obtained. The spectra and positions of ammonia lines were calibrated using this expression and the values of the coefficients thus determined.

3. Results

Figure 2 compares the calibrated positions of ammonia lines measured in the $6800\text{--}7000 \text{ cm}^{-1}$ range of the lower pressure spectrum with the corresponding line positions reported by Sung *et al.* [20]. The average of the differences presented in Figure 2, equal to $0.0001 (4) \text{ cm}^{-1}$, is in agreement with the accuracy of 0.0001 cm^{-1} (or

Figure 1. Region considered in the two high-resolution spectra of ammonia recorded in this work [27.62 (8) m, 293 (1) K, 1.284 (46) hPa (black trace) and 3.44 (11) hPa (grey trace)].

Figure 2. Differences between the calibrated $^{14}\text{NH}_3$ line positions measured in this work (TW) in the lower pressure spectrum [1.284 (46) hPa] and reported by Sung *et al.* [20]. Note: The error bars represent the uncertainties reported by Sung *et al.* [20].

better) stated for the line positions by Sung *et al.* [20]. A similar comparison of the intensities of the same lines is presented in Figure 3. It shows that the line intensities reported by Sung *et al.* [20] are on average about 4% stronger than measured in the present work. Note that examination of the spectrum shows that the larger positive discrepancies observed can generally be

attributed to weak lines blended with the lines of interest. The larger negative discrepancies correspond to weak lines in the present work, and most probably reflect the precision of measurement of their intensities. The good agreement between the line intensities measured in both studies somewhat confirms the expectation of Sung *et al.* [20] that the absolute accuracy of their line intensities

Figure 3. Comparison between line intensities measured in this work (TW) in the $6800\text{--}7000\text{ cm}^{-1}$ range of the lower pressure spectrum [1.284 (46) hPa, 293 K] and reported by Sung *et al.* [20] at 296 K. Notes: The error bars represent the uncertainties reported by Sung *et al.* [20]. In the present work, line intensities equal to 10^{-22} and $4 \times 10^{-23}\text{ cm}^{-1}/(\text{molecule cm}^{-2})$ correspond to peak transmittances of about 0.75 and 0.9, respectively.

Figure 4. Comparison of H_2^{16}O line positions measured and calibrated in this work (TW) with the corresponding information available in HITRAN [19], characterised by uncertainties in the range $0.0001\text{--}0.001\text{ cm}^{-1}$ (see text for details on the meaning of the filled and open symbols).

is better than 10%. Figure 4 compares the calibrated positions of a few water vapour lines observed between 8675 and 8926 cm^{-1} with the corresponding information available in HITRAN [19] (note that these lines were too weak to be used for calibration purposes). The average of the differences involving the calibrated line positions (neglecting the three outliers identified with open symbols) is equal to 0.00055 (88) cm^{-1} , which is within the uncertainty range of 0.0001–0.001 cm^{-1} stated for these line positions in HITRAN [19].

The parameters of a total of 3499 and 3606 lines were measured in the 7400–8600 cm^{-1} range of the lower and higher pressure spectra, respectively. These lines have an intensity larger than $3 \times 10^{-24} \text{ cm}^{-1}/(\text{molecule cm}^{-2})$ at 293 K, which corresponds to peak transmittances of about 0.99 and 0.98 at the lower and higher pressures, respectively. These transmittance limits correspond to about five times the peak-to-peak noise level in the spectra. The two lists of line parameters were then merged, averaging the positions and intensities of the same lines measured in the two spectra (two positions were considered to correspond to the same line when

their difference was smaller than half of the spectral resolution). The resulting list contains the positions and intensities of 3921 lines, average values being provided for 3182 of them and the parameters of 315 and 424 lines only originating from the lower and higher pressure spectra, respectively.

The differences between the positions and intensities of the 3182 lines measured in the higher and lower pressure spectra are presented in Figure 5. Because ‘WSpectra’ always fits the line widths without any constraints, some filtering of the results needed to be applied. In Figure 5, the filled symbols highlight differences associated with lines having a measured FWHM bounded by the calculated Doppler broadening and the width of the Voigt profile assuming a self-broadening coefficient of 0.676 $\text{cm}^{-1} \text{ atm}^{-1}$, i.e. the largest value found in the HITRAN database [19]. The contribution of the FWHM of the instrument line shape (i.e. the sinc function) was taken into account in both limiting line widths. From now on, the 1936 lines the widths of which match this criterion are identified as *primary lines*. The *secondary lines* are the remaining lines as well as the 315 + 424 lines

Figure 5. Differences between the positions (top) and intensities (bottom) of lines measured in the higher and lower pressure spectra between 7400 and 8600 cm^{-1} as a function of the average intensity of the lines. A line intensity of 1×10^{-22} (resp. 8×10^{-24}) $\text{cm}^{-1}/(\text{molecule cm}^{-2})$ corresponds to peak transmittances of about 0.4 and 0.7 (resp. 0.94 and 0.98) in the higher and lower pressure spectra, respectively. The filled and open symbols identify differences obtained for the primary and secondary lines, respectively (see text for details).

measured in only one spectrum. The differences obtained for the primary lines in Figure 5 show that the line positions measured in the higher pressure spectrum are on average about 0.0002 cm^{-1} lower than measured at the lower pressure. If it is attributed solely to self-shifting of the lines, this difference leads to a self-shift coefficient of about $-0.09\text{ cm}^{-1}\text{ atm}^{-1}$, significantly different from the crude estimate of $-0.06\text{ cm}^{-1}\text{ atm}^{-1}$ of Sung *et al.* [20] although self-shift coefficients have been measured for ammonia ([23,24], for example), they are limited to lower energies to the best of our knowledge]. The intensity differences show that the lines measured at the higher pressure are stronger than measured at the lower pressure, the discrepancy being negligible for weak lines and increasing with increasing intensity to reach about 5–10% for the strongest lines measured in this work. Additionally, many intensity differences are positive and most probably result from a large number of medium to very weak lines blended with the lines of interest. The largest absolute differences are observed for the positions and intensities of the very weak lines [intensity smaller than $8 \times 10^{-24}\text{ cm}^{-1}/(\text{molecule cm}^{-2})$]. In this respect, the intensities of these lines should be regarded as estimates.

The positions and intensities of the 3921 lines generated as described above are provided as supplementary material with this article. The uncertainties on the average positions and intensities of the primary lines provided therein are the precision of measurement, estimated as the square root of the sum of the squares of half of the differences presented in Figure 5 and the uncertainties of measurement estimated by ‘WSpectra’. We did not attempt to estimate the uncertainties of measurement of the positions and intensities of the secondary lines. Relying on the comparisons of Figures 2, 4 and 5, we conservatively estimated that the accuracy of the calibrated line positions ranges from 0.001 to 0.002 cm^{-1} from the lower to the upper limits of the spectral range considered. Similarly, relying on the comparisons of Figures 3 and 5, we estimated that the accuracy of the intensities of the primary lines is around 10% or better.

4. Comparison with HITRAN 2016 and the Kitt Peak spectrum

Figures 6 and 7 compare the positions and intensities of the primary lines with the corresponding information available in HITRAN [19] (open red symbols). Figure 6 shows that discrepancies between the two sets of line positions are observed, increasing linearly with the line positions from about 0.001 cm^{-1} to about 0.003 cm^{-1} . These discrepancies are within the uncertainty stated

for the line positions provided in HITRAN (ranging from 0.001 to 0.01 cm^{-1}), but the differences at higher energies are larger than the estimated accuracy of the positions of the primary lines. Figure 7 shows that the line intensities obtained in this work agree with HITRAN data within estimated uncertainties (better than 20% and 10% for HITRAN and this work, respectively) up to about $10^{-22}\text{ cm}^{-1}/(\text{molecule cm}^{-2})$. Note, however, that the weakest lines are on average 10% stronger in HITRAN than measured in the present work. Above $10^{-22}\text{ cm}^{-1}/(\text{molecule cm}^{-2})$, the HITRAN line intensities are increasingly larger than the present results as the line intensities get larger, leading to discrepancies as large as 70% around $2.5 \times 10^{-22}\text{ cm}^{-1}/(\text{molecule cm}^{-2})$. These discrepancies are larger than the uncertainties quoted in HITRAN and estimated in the present work. However, they are in line with the statement of Barton *et al.* [15] that the uncertainty in the retrieved intensities may significantly exceed 15% for lines stronger than $1.0 \times 10^{-22}\text{ cm}^{-1}/(\text{molecule cm}^{-2})$.

In view of the discrepancies reported here above, we decided to remeasure line positions and intensities in the original Kitt Peak spectrum [file named ‘800407R0.004’, in FITS format (<https://fits.gsfc.nasa.gov>)], which we downloaded from the Kitt Peak repository located at ftp://nispdata.nso.edu/FTS_cdrom/FTS03/. This spectrum (presented in Figure 1 of the Barton *et al.* paper [15]) was recorded at a resolution of $0.01109469\text{ cm}^{-1}$, a temperature of 21.5° C , an absorption pathlength of 25 m and an ammonia pressure of 5 torr. We measured the line positions and intensities using the program ‘WSpectra’ [21], giving each line a Voigt profile and including as fixed contributions instrumental effects arising from the truncation of the interferogram at a maximum optical difference of 54.4 cm (determined assuming that the spectral resolution given is the FWHM of the sinc function). The possible use of an apodisation function not being mentioned, we assumed that none was used. Following the procedure described in Section 2, we matched the measured positions $\tilde{\nu}_{\text{obs}}$ of 139 water vapour lines, observed in the ranges $7006\text{--}7416\text{ cm}^{-1}$ and $8738\text{--}8942\text{ cm}^{-1}$, to reference positions $\tilde{\nu}_{\text{HITRAN}}$ available in HITRAN [19] and originating from linelists generated by Toth [22], Tennyson *et al.* [25] and Mikhailenko *et al.* [26]. The differences $\tilde{\nu}_{\text{HITRAN}} - \tilde{\nu}_{\text{obs}}$ were fitted to Equation(1) with an RMS deviation of $2.5 \times 10^{-4}\text{ cm}^{-1}$. The Kitt Peak spectrum and positions of ammonia lines measured therein were calibrated using Equation 1 and the values of the a and b parameters thus determined. 6588 lines with intensities larger than $3.0 \times 10^{-25}\text{ cm}^{-1}/(\text{molecule cm}^{-2})$ were identified in the Kitt Peak spectrum. They were filtered according to their measured FWHM following the procedure that led to the primary lines (see

Figure 6. Differences between the positions of the primary lines of this work (TW) with the $^{14}\text{NH}_3$ line positions provided in HITRAN [19] (open symbols) and measured in this work in the Kitt Peak spectrum (filled symbols) (OW = other work). Four points are off-scale (the full Y scale is -0.0049 ; to $+0.0072 \text{ cm}^{-1}$).

Figure 7. Differences between $^{14}\text{NH}_3$ line intensities provided in HITRAN [19] (open symbols) and measured in this work in the Kitt Peak spectrum (filled symbols) (OW = other work) with the intensities of the primary lines of this work, plotted versus the intensities of the primary lines of this work (TW). The difference associated with the largest intensity in HITRAN [$2.1 \times 10^{-21} \text{ cm}^{-1}/(\text{molecule cm}^{-2})$ for the line at $7707.0006 \text{ cm}^{-1}$] is off-scale.

Section 3), leading to 6331 lines. As the aim of the analysis of the Kitt Peak spectrum carried out in this work was not to redo the analysis of Barton *et al.* [15] but rather to try and understand the origin of the discrepancies

observed for the larger line intensities, only the lines having an intensity larger than $3.0 \times 10^{-24} \text{ cm}^{-1}/(\text{molecule cm}^{-2})$, i.e. the intensity cut-off applied to the lines measured in the spectra recorded in this work, were

Figure 8. Part of the lower pressure spectrum of ammonia recorded in this work [27.62 (8) m, 293 (1) K, 1.284 (46) hPa (red trace (appearing grey in the printed version))] and corresponding spectrum calculated using the positions and intensities of the primary and secondary lines (upper panel); residuals corresponding to the spectra calculated with the primary and secondary lines (black trace) and the line positions and intensities measured in this work in the Kitt Peak spectrum (red trace (appearing grey in the printed version); middle panel) (TW = this work); residuals obtained using the data in HITRAN [19] (lower panel). Note the change of scales for the residuals presented in the middle and lower panels.

retained. The positions and intensities of the resulting 3717 lines are also provided as supplementary material with this article. Figures 6 and 7 also compare the positions and intensities of the primary lines of this work with the positions and intensities of the 3717 lines reported in this work for the Kitt Peak spectrum (filled black symbols). These Kitt Peak line positions are systematically larger than those measured in the Brussels spectra by about 0.001 to 0.0005 cm^{-1} from the lower to the upper limits of the spectral range considered, and the discrepancies between the line intensities are at most about 15–20%. Note that the differences between the line intensities measured in this work in the Kitt Peak spectrum and the intensities of the primary lines exhibit a dependence for the strong lines that matches the dependence observed for the same intensities in the differences shown in the lower panel of Figure 5. This may indicate that the line intensities retrieved from the higher pressure Brussels spectra are overestimated. Nevertheless, the discrepancies between the line positions and intensities measured in this work in the Kitt Peak spectrum with the positions and intensities of the primary lines are within the estimated accuracies and do not exhibit the dependences observed with the results reported by Barton *et al.* [15]. As far as we can tell, the main difference between the two studies is the inclusion of the contribution of the instrument function in the present work and its neglect in the analysis performed by Barton *et al.* [15], followed

by the application of some correction on the measured line intensities to compensate for that. As the inclusion or neglect of the instrument function is not expected to have a significant impact on the line positions, the most obvious reason for the discrepancies observed for the line positions is the application of different wavenumber calibrations.

Figure 8 compares the lower pressure spectrum of ammonia recorded in this work with spectra calculated using the positions and intensities of the primary and secondary lines of this work, the positions and intensities measured in this work in the Kitt Peak spectrum, and the spectroscopic information available in HITRAN. This comparison shows that the first two sets of line positions and intensities are in reasonable agreement note that the signature observed near 7651 cm^{-1} in the residuals obtained with the parameters retrieved from the Kitt Peak spectrum (red trace (appearing grey in the printed version) in the middle panel of Figure 8) has a minimum of -0.08 . The large intensities in HITRAN for the strong lines are clearly apparent (note the change of scales for the residuals presented in the middle and lower panels).

5. Conclusion

In this work, the positions and intensities of 1936 lines observed in the range $7400\text{--}8600\text{ cm}^{-1}$ of two absorption spectra of ammonia recorded at high resolution using

Fourier transform spectroscopy are reported. The accuracy of these line positions was estimated to range from 0.001 to 0.002 cm^{-1} from the lower to the upper limits of the spectral range considered, while the accuracy of the line intensities was estimated to be around 10% or better. Also reported are less-accurately measured positions and intensities of 1985 lines retrieved from the two spectra analysed in this work or from only one of them.

Comparison of the positions and intensities of the 1936 (primary) lines with the information retrieved from a spectrum recorded in 1980 at the Kitt Peak National Solar Observatory [15] and provided in HITRAN [19] show discrepancies within the uncertainties estimated by Barton *et al.* [15] but larger than estimated in the present work. If these discrepancies are within the uncertainties stated in HITRAN [19] for the line positions, they are (significantly) larger for line intensities larger than $10^{-22} \text{ cm}^{-1}/(\text{molecule cm}^{-2})$. The line positions and intensities measured in this work in the same Kitt Peak spectrum agree within estimated uncertainties with the positions and intensities of the 1936 lines reported. In view of these agreements, a simultaneous analysis of the spectra recorded in this work and at Kitt Peak could have been carried out. It was not undertaken as we believe that it would not bring much because the pressure–pathlength (PL) product of the Kitt Peak spectrum (167 hPa m) is close to the PL product of one of the spectra recorded in this work (95 hPa m). The data retrieved from the spectra recorded in this work and at Kitt Peak are provided as separate supplementary materials, leaving to the user the decision of merging them if worthwhile.

Figure 8 shows that there is room for improvement. Indeed, the very limited set of experimental information used in the present work imposed the use of the standard Gaussian and Voigt line shape models, the measurement of line parameters one spectrum at a time, and did not allow determination of line shape parameters such as pressure broadening coefficients. Further work should involve the analysis of several spectra recorded in a rather large range of ammonia pressures using multi-spectrum fitting techniques and a more appropriate modelling of the spectra [23].

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Disclosure statement

No potential conflict of interest was reported by the authors.

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