Absorption spectra of ammonia near 1 μm

Emma J. Barton, Oleg L. Polyansky, Sergei. N. Yurchenko, Jonathan Tennyson

Department of Physics and Astronomy, University College London,London, WC1E 6BT, UK

S. Civiš, M. Ferus

Academy of Science Czech Republic, J Heyrovsky Inst Phys Chem, Dolejskova 3, CZ-18223 Prague 8, Czech Republic

R. Hargreaves

Department of Chemistry and Biochemistry, Old Dominion University, Norfolk, VA 23529 USA

R.I. Ovsyannikov, A.A. Kyuberis, N. F. Zobov

Institute of Applied Physics, Russian Academy of Science, Uljanov Street 46, Nizny Novgorod, Russia, 603950

S. Béguier, A. Campargue

Université Grenoble Alpes, LIPhy, F-38000 Grenoble, France.

CNRS, LIPhy, F-38000 Grenoble, France

Abstract

An ammonia absorption spectrum recorded at room temperature in the region 8800 – 10 400 cm^{-1} is analysed using a variational line list, BYTe, and ground state energies determined using the MARVEL procedure. BYTe is used as a starting point to initialise assignments by combination differences and the method of branches. Assignments are presented for the region 9400 – 9850 cm^{-1}. 642 lines are assigned to 6 previously unobserved vibrational

bands, $(2v_1+2v_4^2)^\pm$, $(2v_1+v_3^1)^\pm$ and $(v_1+v_3^1+2v_4^2)^\pm$, leading to 428 new energy levels with 208 confirmed by combination differences. A recently calculated purely *ab initio* NH$_3$ PES is also used to calculate rovibrational energy levels. Comparison with assigned levels shows better agreement between observed and calculated levels than for BYTe for higher vibrational bands.

1. Introduction

Ammonia is an atmospheric trace species which is frequently the by-product of human activity [1]. Ammonia is present in a variety of astronomical environments, including the interstellar medium, gas giant planets [2] and brown dwarfs [3]; indeed NH$_3$ is thought to provide the signature of coolest brown dwarfs known as Y-dwarfs [4]. NH$_3$ is also used in a number of industrial processes, such as the reduction of NOx emissions in smoke stacks [5] and the manufacture of hydrogen cyanide by the Andrussow process [6]. This has motivated a large number of experimental studies of ammonia spectra; those reported up to late 2014 are reviewed in the MARVEL (measured active rotation-vibration energy levels) study of NH$_3$ performed by Al-Derzi *et al.* [7], which is discussed further below.

A number of new ammonia spectra have been reported in the last two years [8, 9, 10, 11, 12, 13, 14]. Of particular relevance to this work is the analysis by Barton *et al.* [12] of a near-infrared Fourier transform spectrum which was originally recorded by Dr Catherine de Bergh in 1980 at Kitt

Peak. Barton *et al.* used a combination of the BYTe variational line list of Yurchenko, Barber and Tennyson [15], energy levels from the MARVEL study, and the method of branches [16] to assign 2474 lines in the 7400 - 8600 cm^{-1} region; this is the first time any assignments had been made for ammonia spectra in this region.

The success of this work, and the availability of unassigned, shorter-wavelength ammonia spectra in the Kitt Peak archive and from elsewhere (see below) motivated us to attempt to extend the analysis techniques employed by Barton *et al.* [12] to higher wavenumbers. The results of this analysis are reported here. We note that the 2012 release of HITRAN contained no data on NH$_3$ above 7000 cm^{-1}.

One reason for extending the range of assigned NH$_3$ spectra is to help the construction of accurate potential energy surfaces (PES). Quite a number of PES are available for the ground states of NH$_3$. The majority of these are the products of *ab initio* electronic structure calculations [17, 18, 19, 20, 21, 22, 23], although surfaces that use experimental data to improve their accuracy are also available [24, 25, 26]. Recently, Polyansky *et al.* [23] computed an *ab initio* surface with which they were able to make, for the first time, vibrational assignments to the optical spectrum of ammonia recorded by Coy and Lehmann [27, 28]. We consider results obtained with this PES further below.

2. Experimental Data

The Kitt Peak data center provides open access to laboratory Fourier Transform (FT) spectra recorded at the National Solar Observatory. The

room temperature laboratory absorption spectrum of NH_3 analysed here was recorded by Dr. Catherine de Bergh using a one meter FT spectrometer in 1980 and corresponds to FITS file 800407R0.003 in the Kitt Peak archive. The spectrometer in question was a permanent instrument on the McMath Solar Telescope and was used for both solar and laboratory analysis.

A summary of information provided by the header of the archive file is presented in Table 1 and an overview of the raw spectrum is given in Fig. 1. Absorption lines were detected between 8800 and 10400 cm^{-1}.

The wavenumber scale was calibrated using water lines which are clearly apparent between 8800 and 9000 cm^{-1}. A few additional water lines are also detected near the high energy limit at 10200 cm^{-1}. On the basis of the HITRAN list for water vapor, 113 lines were identified as water lines using an automatic search program taking into account both positions and line intensities. Their positions were used for frequency calibration of the spectrum. A correction factor of 0.99999625(4) was determined and applied to the frequency scale (the frequency correction is about -0.035 cm^{-1} at 9000 cm^{-1}).

Line centers and line intensities were systematically retrieved using a multiline fitting of the spectrum based on a homemade three step suite of programs written in Labview and C++. An effective Voigt profile, including the contribution of the apparatus function, was first determined from a small number of isolated lines and used as default profile. Then an automatic multiline fit was performed over the entire analysed region by adjusting only the line centre and integrated line absorbance, the shape of all the lines being fixed to the default Voigt profile. Finally, a manual adjustment was per-

Table 1: Key experimental information provided in the FITS header downloaded from the Kitt Peak Archive.

Archive Name	800407R0.003
Temperature	296 K
Pressure	5 Torr
Path length	25 m
Spectral Type	Absorption
Wavenumber Start	8978 cm^{-1}
Wavenumber Stop	10348 cm^{-1}

formed by further refining the profile parameters and adding/deleting weak lines (see more details in Ref. [12]). The quality with which the spectrum is reproduced is illustrated in Fig. 2.

Overall a list of more than 12900 lines was obtained. After exclusion of the lines due to water vapor and of the weak lines with intensities below 10^{-25} cm/molecule, a list of 12064 lines of ammonia lying between 8978 and 10348 cm^{-1} was considered for ro-vibrational assignment. This line list given in the supplementary data is presented in Fig. 3. Of importance for the search for combination differences is the fact that the accuracy of the line centers is believed to be better than 0.005 cm^{-1} for non-blended lines as the rms deviation of the position of the 113 water lines used for calibration is 0.0038 cm^{-1}. The average uncertainty on the retrieved line intensities is estimated to be about 15 % for isolated lines of intermediate intensity.

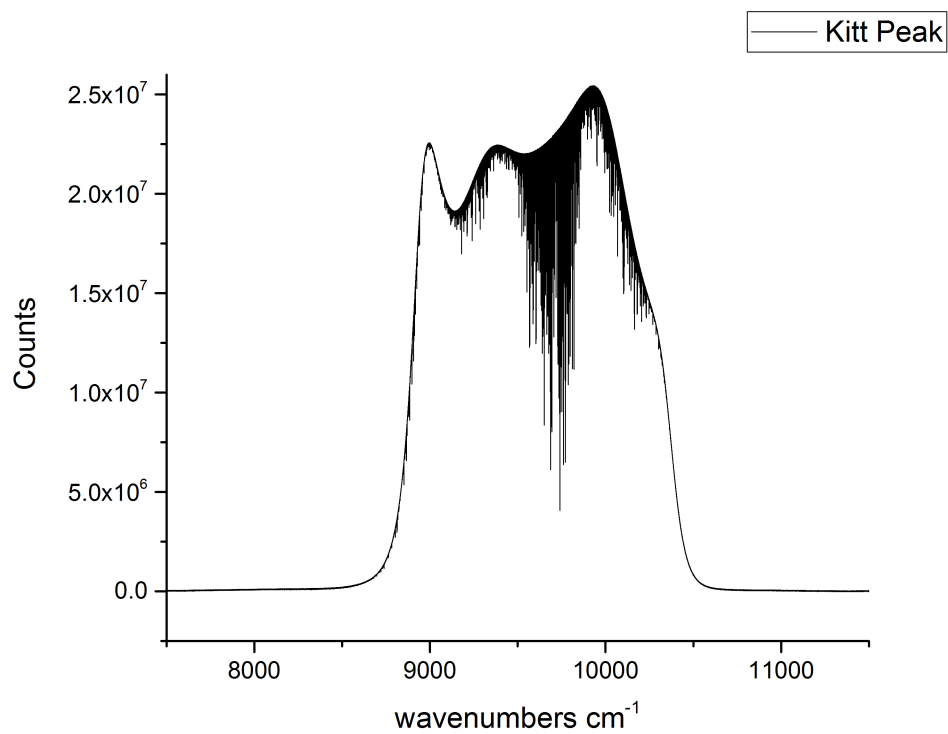In parallel, new spectra were recorded at the Academy of Science of the

Figure 1: Overview of Kitt Peak FT spectrum of ammonia recorded with a pathlength of 25 m and a pressure of 5 Torr (Ref. 800407R0.003).
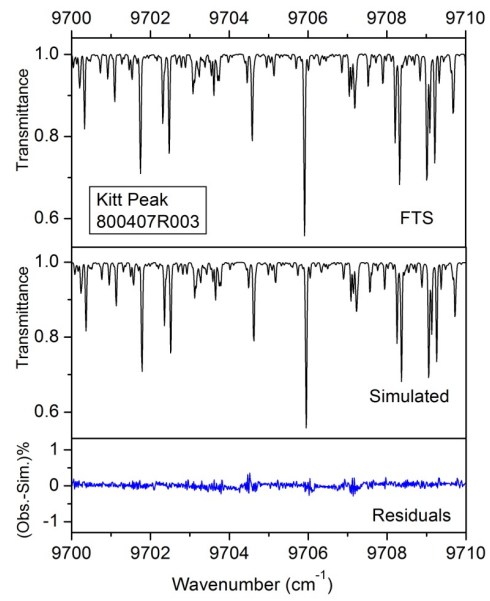
Figure 2: Illustration of the multiline fitting procedure adopted to retrieve the ammonia line parameters. The FTS spectrum (800407R0.003) was recorded by was recorded by C. de Bergh and corresponds to a 25 m pathlength and a 5 Torr pressure.
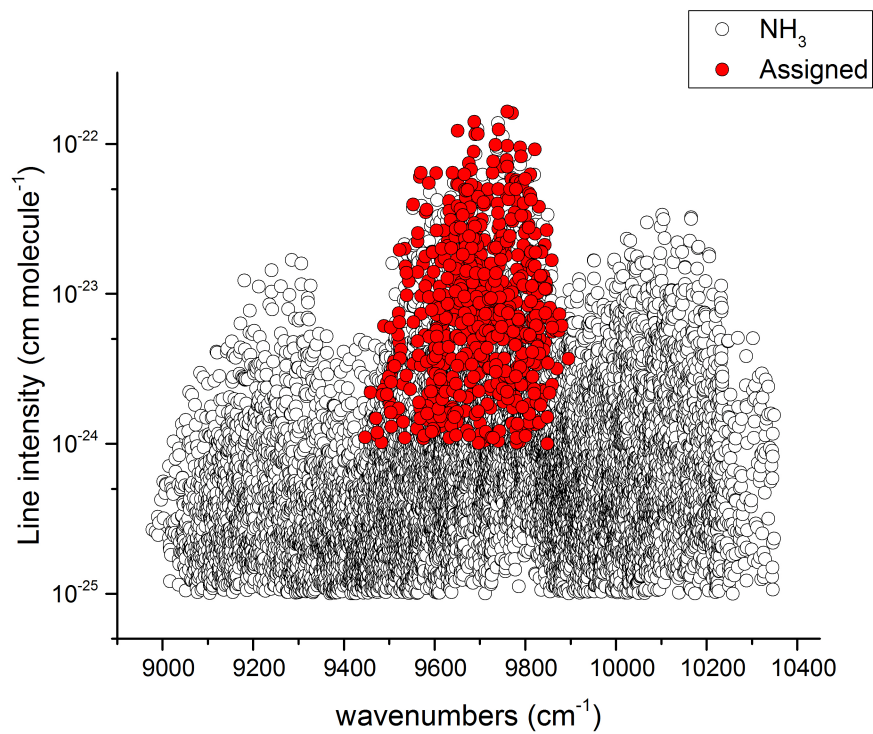
Figure 3: Overview of the NH$_3$ line list for the region 9000 – 10,000 cm^{-1} retrieved from the Kitt Peak archive. Fully assigned lines are highlighted in filled in red, unassigned lines are open black circles.

Czech Republic in Prague. FTIR spectra were measured in a 50 m long optical White cell equipped with CaF_2 windows. The cell was interfaced to a sealable glass-tube joint for the transfer of the ammonia gas from a side ampule. The optical cell was further equipped with a second vacuum valve (ACE glass, USA) for the gas handling and connection to the vacuum line. The pressure in the measuring cell was 2 Torr, measured with a MKS Baratron pressure gauge (0 – 10 Torr pressure range). The spectral measurement was performed using the Bruker IFS 125 HR spectrometer (CaF_2 beam splitter, InSb detector) in a spectral range of $1800 – 10\,000$ cm^{-1}. The spectra were measured in the gas phase with a resolution of 0.01 cm^{-1} with 100 scans using the Blackmann-Harris apodization function. This spectrum was helpful for confirming calibration but yielded few lines above 9000 cm^{-1} so is not considered further here.

3. Data Analysis

Our procedure for making line assignments followed closely our previous analysis of a near infrared Kitt Peak spectrum [12]. Data analysis relied on the use of MARVEL data and the BYTe variational line list [15]. There are a number of variational line lists are available for NH_3 [15, 29, 30] but BYTe, which was designed to be used up to 12 000 cm^{-1}, is the only one which really extends above 9000 cm^{-1}.

The MARVEL algorithm [31, 32] is designed to invert all available assigned and labelled experimental lines, to give accurate empirical energy levels. Although the recent NH_3 MARVEL analysis of Al-Derzi *et al.* [7] included transitions up to 17 000 cm^{-1}, there was a gap between 7000 – 15,000

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cm^{-1} due to absence of any assigned NH$_3$ lines in this region.

A list of observable BYTe lines for the experimental conditions was generated. This list included all lines with an absorption intensity greater that 1×10^{-25} cm/molecule at 296 K. In the 9400 – 9850 cm^{-1} region, this list contains 11 251 lines of which 151 are stronger than 3×10^{-23} cm/molecule which can be compared to the observations which contain 5776 and 150 lines, respectively, in this region for the given intensity cut-offs.

BYTe is expected to be fairly complete in the region of interest but not particularly accurate as BYTe is known to be less accurate for higher wavenumber transitions [25, 30, 33, 12]. In particular our previous study of the 7400 – 8600 cm^{-1} region found that BYTe predictions differed by between -2 and $+3$ cm^{-1} from the observed transition wavenumbers. In this work we only considered transitions which lay within 5 cm^{-1} of the BYTe predictions. Given that the BYTe predictions are expected to deteriorate to higher wavenumbers, this limit may well have precluded some matches.

Figure 4 compares the Kitt Peak spectrum with the predictions of the BYTe line list. The overview comparison given in the upper part of the figure shows very good overall agreement between the two spectra, albeit with some variation between the observed and computed intensities. However, the more detailed comparison given below shows that there are significant shifts between the line position predicted by BYTe and the observed ones.

We used the confirmed combination differences of the assigned levels to assess the BYTe predictions via the observed minus calculated (Obs. - Calc.) differences provided by the lines assigned using combination differences. For a given vibrational band, these (Obs. - Calc.) differences are normally sys-
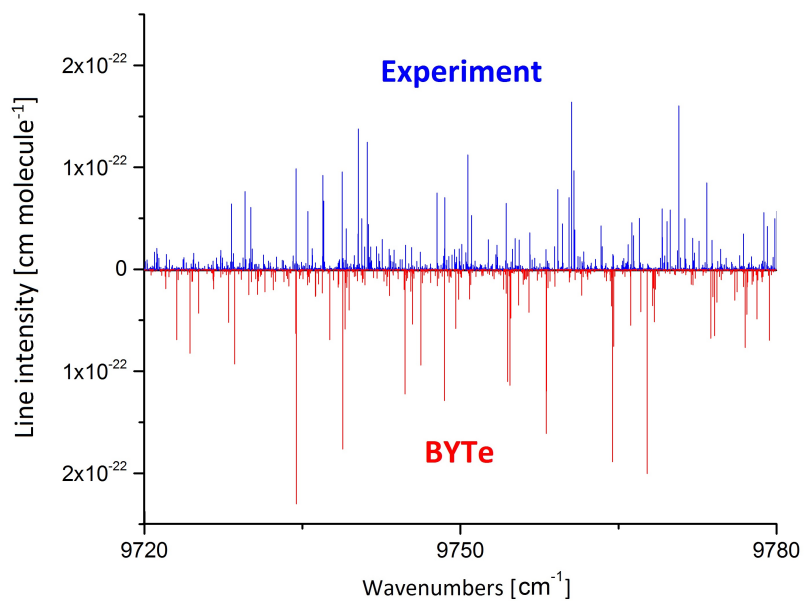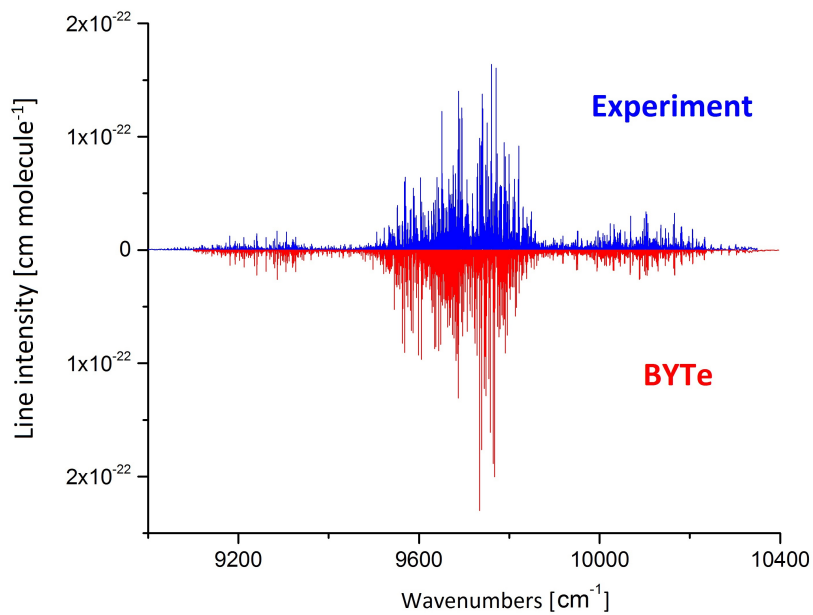
Figure 4: Comparison of the NH$_3$ spectrum between the Kitt Peak measurements (Experiment) and the predictions of the BYTe line list. The upper panel gives an overview of the entire $9000 - 10000$ cm^{-1} spectral region while the lower panel gives a more detailed comparison.

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tematic within a given vibrational band enabling us to use the method of branches [16], which exploits the systematic shifts of variational predictions within any one vibration band, to make further assignments. Lines assigned by this method are generally not confirmed by combination differences because the other transitions associated with the upper level either lie outside the spectral range considered or are too weak to be included in experimental line list. However, the ratio between observed and calculated intensities was used as additional check on these assignments. If these intensities differed by more than a factor of two then the tentative assigment was rejected.

4. Results and Discussion

A full list of lines obtained from the Kitt Peak spectrum is given in the supplementary information. The line assignements given use the full recommended quantum number set of Down *et al.* [34] and are labelled according to whether the assignments are based on combination differences or branch assignments. Table 2 and Table 3 gives a sample set of each type of assignment.

The final assignment list is a compilation of all combination difference (CD) and branch (Br) assignments. Our assignments are confined to the $9400 - 9850$ cm^{-1} region which contains the strongest bands. We did obtain some potential matches outside this region but, due to the inaccuracy of BYTe at these frequencies and lower intensity of the observed spectra leading to fewer combination differences, we could not be confident that our tentative assignments are correct. Analysis of transitions outside this region is therefore left for future work.

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Table 2: A sample of the assigned transitions confirmed by combination differences. Abbreviated $(v_1 v_2 v_3^{L_3} v_4^{L_4})^i$ vibrational labels followed by rotational quantum numbers J and K are given below, full quantum assignments are provided in the supplementary data.

Obs. cm^{-1}	Calc. [15] cm^{-1}	Upper Quanta	Lower Quanta	Type P/Q/R	Upper State Energy cm^{-1}
9537.9367	9536.2206	$(2v_1 + 2v_4^2)^-$ 5 0	0^- 6 1	P	9951.1746
9656.5442	9654.8310	$(2v_1 + 2v_4^2)^-$ 5 0	0^- 5 1	Q	9951.1743
9668.2356	9666.5237	$(2v_1 + 2v_4^2)^-$ 5 0	0^+ 5 2	Q	9951.1728
9755.5655	9753.8517	$(2v_1 + 2v_4^2)^-$ 5 0	0^- 4 1	R	9951.1769
9767.3398	9765.6336	$(2v_1 + 2v_4^2)^-$ 5 0	0^+ 4 2	R	9951.1688
7710.9095	7708.0570	$(2v_1 + 2v_4^2)^-$ 4 0	0^- 5 1	P	9848.2471
7837.5170	7834.6673	$(2v_1 + 2v_4^2)^-$ 4 0	0^- 4 1	Q	9848.2487
7849.1070	7846.2574	$(2v_1 + 2v_4^2)^-$ 4 0	0^- 3 1	R	9848.2476
7967.8183	7964.9705	$(2v_1 + 2v_4^2)^-$ 4 0	0^+ 3 2	R	9848.2467
7519.4722	7517.1594	$(2v_1 + 2v_4^2)^-$ 3 1	0^- 4 2	P	9764.0544
7537.0004	7534.6874	$(2v_1 + 2v_4^2)^-$ 3 1	0^- 3 2	Q	9764.0557
7655.9330	7653.6210	$(2v_1 + 2v_4^2)^-$ 3 1	0^- 2 2	R	9764.0558

Table 3: A sample of assignments made to vibrational band $(2v_1 + 2v_4^2)^-$ using the method of branches. The expected Obs. - Calc. of 0.9 cm^{-1} was determined by averaging the residuals from 24 combination difference pairs and 6 combination difference triplets.

Obs. cm^{-1}	Calc. [15] cm^{-1}	J'	K'	J''	K''	Type P/Q/R	Obs. - Calc. cm^{-1}
9596.1812	9595.3556	1	1	2	0	P	0.8255
9538.1258	9537.3414	7	6	8	7	P	0.7845
9672.8854	9671.8565	7	2	7	3	Q	1.0289
9646.7631	9645.9809	1	0	1	1	Q	0.7822
9811.3176	9810.0738	9	1	8	0	R	1.2439
9729.9545	9729.2452	7	5	6	4	R	0.7093

Table 4 summarizes the number of lines assigned for each of six bands analyzed and gives a breakdown between combination difference and branch assignments. A total of 642 lines are assigned, the majority of these are confirmed by combination differences. All assigned transitions are for overtone bands, i.e. involve absorption by the $0^{\pm}$ lower vibrational state.

Table 5 gives statistics for the energy levels obtained for each band. A full set of the 428 new energy levels obtained here, of which 208 are confirmed by combination differences, are given in the supplementary information. In addition a table with our new assignment arranged by vibrational band with increasing J is also provided so the trends in the (Obs. – Calc.) residues can readily be assessd.

Table 5 compares the band origins for the six new bands identified here

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Table 4: Summary of fully assigned observed bands in order of vibrational band origins (VBO) with abbreviated $(v_1 v_2 v_3^{L_3} v_4^{L_4})^i$ vibrational labels. N_{lines} is the total number of lines assigned to the band. CD and Br are the number of lines assigned using combination differences and the method of branches respectively. The VBO is derived from the observed P(1) transitions.

Band	VBO / cm^{-1}	N_{lines}	CD	Br
$(2v_1 + 2v_4^2)^+$	9641.060	117	76	41
$(2v_1 + 2v_4^2)^-$	9642.708	108	71	37
$(2v_1 + v_3^1)^+$	9690.260	98	61	37
$(2v_1 + v_3^1)^-$	9695.504	105	69	36
$(v_1 + v_3^1 + 2v_4^2)^+$	9724.073	100	63	37
$(v_1 + v_3^1 + 2v_4^2)^-$	9726.646	114	88	26

Table 5: Summary of fully assigned new NH_3 experimental energies above 9000 cm^{-1} with abbreviated $(v_1 v_2 v_3^{L_3} v_4^{L_4})^i$ vibrational labels and maximum rotational quantum numbers J_{max} and K_{max}. N_E is the total number of experimentally derived energies for the upper vibrational state. Obs. - Calc. gives the average experimental minus BYTe or *ab initio* energy difference for each band in cm^{-1}.

Band	VBO / cm^{-1}	N_E	J_{max}	K_{max}	Obs.-Calc.	
					BYTe	ai
$(2v_1 + 2v_4^2)^+$	9641.060	75	10	9	5.90	-1.04
$(2v_1 + 2v_4^2)^-$	9642.708	68	11	11	0.23	-2.58
$(2v_1 + v_3^1)^+$	9690.260	64	13	13	4.40	-1.79
$(2v_1 + v_3^1)^-$	9695.504	66	13	13	3.16	2.51
$(v_1 + v_3^1 + 2v_4^2)^+$	9724.073	66	13	13	-1.36	2.14
$(v_1 + v_3^1 + 2v_4^2)^-$	9726.646	67	11	11	-3.23	2.58

for the first time with the predicted values from the BYTe line list [15] and obtained as part of an *ab initio* study of the spectrum of NH_3 [23]. The predictions reproduce the observed band origins with a standard deviation of 3.6 cm^{-1} (BYTe) and 2.2 cm^{-1} (*ab initio*). Given that the PES used in the BYTe calculations was determined using a considerable number of spectroscopic data it is interesting to note that the *ab initio* predictions are somewhat closer to the observations for the region studied here. We note that other bands, such as $(v_1 + 2v_2 + 2v_4^2)^-$, $(2v_2 + 2v_4^0)^\pm$ and $(v_1 + v_3^1 + 2v_4^2)^\pm$ are predicted to lie in the region studied. However, according to BYTe transitions in these bands are weaker than the ones listed in the table.

Table 6 gives a fuller comparison between the two calculations which cov-

ers all the vibrational band origins (VBOs) determined from Kitt Peak data both in the work and our previous study [12]; band origins for $(v_1 + v_2 + v_3^1)^-$ and $(2v_1 v_4^1)^\pm$ are not given since they were not determined experimentally, *i.e.* there no assignment to the P(1) transition in these bands, in our previous study. BYTe performs better than the *ab initio* study for VBOs in the lower energy region up to 8500 cm^{-1}. This observation is line with the general finding that spectroscopically determined PESs only extrapolate reliably over a short range whereas a well-constructed *ab initio* PES can be used to make useful predictions for a wide range of VBOs.

Figure 5 shows our assigned transitions classified according to whether $\Delta(K - \ell) = 0$ or 3. Usually strong transitions in ammonia have $\Delta(K - \ell) = 0$ and 'forbidden' transtions with $\Delta(K - l) > 0$ are much weaker. While there the strongest lines do indeed obey $\Delta(K - \ell) = 0$, a significant proportion of the transitions obey $\Delta(K - \ell) = 3$. We note that all approximate quantum numbers, *i.e.* vibrational labels, K and ℓ, were all taken directly from BYTe and cannot be considered to be definitive. It is therefore unclear if $\Delta(K - \ell) = 3$ transitions are indeed stronger than might be expected or if this an artefact of the way BYTe assigns quantum numbers.

5. Conclusions

We have assigned 624 NH_3 lines from a near 1 μm spectrum recorded in 1980 and obtained from the Kitt Peak archive. The whole spectrum contains 12 063 lines in the range 8978 – 10 349 cm^{-1}. Although some of these lines are not due to NH_3, indeed we removed 134 lines due to water, there are clearly many NH_3 lines that remain to be assigned. An updated version

Table 6: Comparison of observed vibrational band origins (VBO) from this work and Ref. [12] with the predicitons of BYTe [15] and the *ab initio* (ai) calculations of Polyansky *et al.* [23].

| Band	VBO / cm^{-1}	Obs.-Calc. /cm^{-1}	
		BYTe	ai
$(v_1 + v_2 + 2v_4^2)^+$	7572.9549	2.3	2.5
$(v_1 + v_2 + 2v_4^2)^-$	7603.1713	2.9	3.5
$(v_1 + v_2 + v_3^1)^+$	7656.8700	0.6	-2.0
$(v_2 + 2v_3^2)^+$	7854.3892	2.9	-1.8
$(v_2 + 2v_3^2)^-$	7864.0831	2.4	-1.7
$(2v_1 + v_4^1)^+$	8086.5926	1.2	-6.0
$(v_1 + v_3^1 + v_4^1)^+$	8174.7017	-1.8	-2.4
$(v_1 + v_3^1 + v_4^1)^-$	8177.4358	-0.6	-1.4
$(v_1 + 3v_4^1)^+$	8253.7494	2.3	1.4
$(v_1 + 3v_4^1)^-$	8257.5341	2.2	4.3
$(v_1 + 2v_2 + 2v_4^2)^+$	8266.3284	1.4	1.5
$(2v_3^2 + v_4^1)^+$	8463.2901	2.4	4.4
$(2v_3^2 + v_4^1)^-$	8463.8719	2.2	4.9
$(2v_1 + 2v_4^2)^+$	9641.0599	5.9	-1.0
$(2v_1 + 2v_4^2)^-$	9642.7083	0.2	-2.6
$(2v_1 + v_3^1)^+$	9690.2596	4.4	-1.8
$(2v_1 + v_3^1)^-$	9695.5038	3.2	2.5
$(v_1 + v_3^1 + 2v_4^2)^+$	9724.0733	-1.4	2.1
$(v_1 + v_3^1 + 2v_4^2)^-$	9726.6462	-3.2	2.6
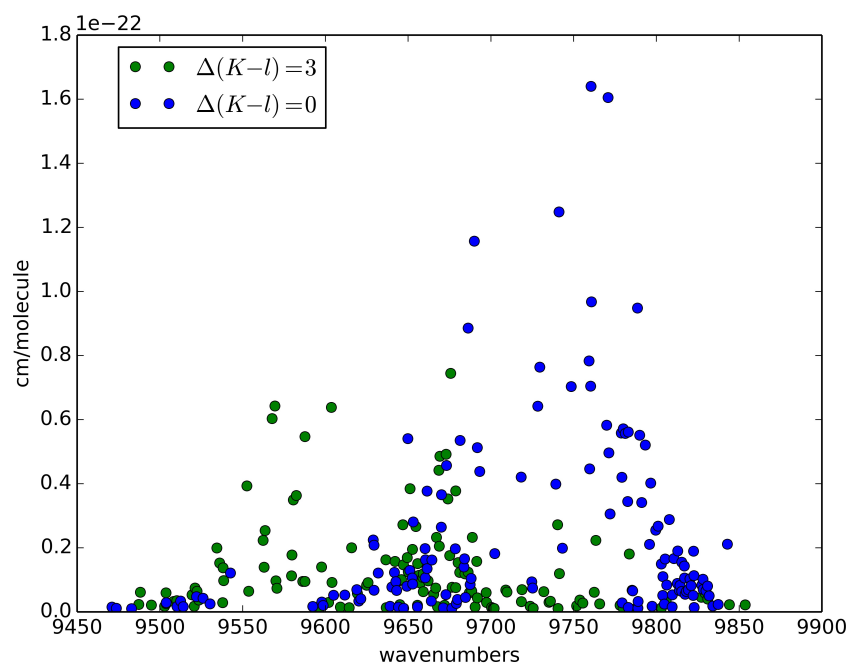
Figure 5: Line assignments labelled by $\Delta(K - \ell)$.

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of the NH_3 MARVEL dataset is under construction [35] based on both the newly assigned Kitt Peak spectra. Finally, the Prague FTIR spectrum has been extended to higher frequency; we are currently analyzing the lines in this new spectra.

The line assignments presented here are the first made for NH_3 in this spectral region. Comparisons are made with the predictions of the BYTe line list [15] and a recent, high accuracy *ab initio* calculation [23]. While both reproduce the overall structure of the spectrum it is clear that further improvements are required for the spectrum to be reproduced accurately by variational nuclear motion calculations. Work has started using the MARVEL energy levels plus the new data from the Kitt Peak spectra presented here and previously [12] as the inputs to a fit for the NH_3 potential energy surface (PES). The *ab initio* PES of Polyansky *et al.* [23] provides a good starting point for this undertaking.

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