

Revised molecular constants and term values for the $X^3\Sigma^-$ and $A^3\Pi$ states of NH

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ARTICLE INFO

Article history:

Received 28 December 2009

Available online 25 January 2010

Keywords:

Spectroscopy

Vibration–rotation spectra

Free radicals

Solar spectra

ABSTRACT

The vibration–rotation spectra of NH have been reinvestigated using laboratory spectra and infrared solar spectra recorded from orbit by the ACE and ATMOS instruments. In addition to identifying the previously unobserved 6–5 vibration–rotation band in the laboratory spectra, many additional high N rotational lines have been observed. By combining the new observations with the previously published data and recent far infrared data, an improved set of molecular constants and term values have been derived for the $X^3\Sigma^-$ and $A^3\Pi$ states.

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1. Introduction

NH is an important free radical in astronomy and has been extensively studied by both experimental and theoretical methods. A review of previous studies on the electronic spectra of NH can be found in our previous papers [1–3]. Work on NH includes our high resolution study of the $A^3\Pi-X^3\Sigma^-$ transition [2] and the $X^3\Sigma^-$ vibration–rotation bands using a Fourier transform spectrometer [3]. Morino and Kawaguchi [4] have made far infrared observations of the NH, NH₂, NHD and ND₂ radicals. Their NH measurements agree to ± 0.00062 cm⁻¹ with the values predicted based on our previous ground state constants. Several new measurements of the pure rotational transitions have been made recently in order to derive more precise rotational, distortion and hyperfine parameters for astronomical applications [5–7]. Lewen et al. [5] have measured the ¹⁴N nuclear hyperfine patterns accompanying the $N=2 \leftarrow 1$ rotational transition, while Brown and coworkers [6,7] have reported the observation of hyperfine structure associated with transitions up to $N=5 \leftarrow 4$ in the $v=0$ vibrational level and up to $N=4 \leftarrow 3$ for the $v=1$ and 2 vibrational levels, and have determined an improved set of spectroscopic and hyperfine parameters for the $v=0, 1$ and 2 vibrational levels. In addition to the triplet states, there are four low-lying singlet electronic states, $a^1\Delta$, $b^1\Sigma^+$, $c^1\Pi$ and $d^1\Sigma^+$. Although the singlet–triplet manifolds were connected by the observation of the $b^1\Sigma^+-X^3\Sigma^-$ transition

by Masanet et al. [8,9] and the $a^1\Delta-X^3\Sigma^-$ transition by Rohrer and Stuhl [10] in gas phase photolysis experiments of NH₃, the more recent observation of the completely resolved spectrum of the strongly forbidden $a^1\Delta-X^3\Sigma^-$ transition by Rinnenthal and Gericke [11] resulted in a more precise determination of the singlet–triplet separation. This study locates the $a^1\Delta$ state at 12,687.865 cm⁻¹ above the ground state of NH.

The vibration–rotation spectra of NH have been investigated in several laboratories. Boudjaadar et al. [12] observed the $\Delta v=1$ vibration–rotation bands up to 5–4. More recently we observed the infrared spectra of NH using a Fourier transform spectrometer and a cryogenic echelle spectrograph (the Phoenix spectrometer) at the National Solar observatory at Kitt Peak [3]. In that study, many additional rotational lines were observed in the bands reported by Boudjaadar et al. [12] and improved spectroscopic constants were determined for the ground state. It also demonstrated that Phoenix is much more sensitive than the Kitt Peak Fourier transform spectrometer.

There is great interest in NH since it has been observed in diffuse interstellar clouds [13–15], cool stars [15–19], comets [20,21] and solar spectra [22–24]. The vibration–rotation lines of NH were identified in the spectrum of the M supergiant α -Orionis by Lambert and Beer [16]. It has also been observed in the spectra of both oxygen-rich [17,18] and carbon-rich stars [19]. NH vibration–rotation lines have also been identified in the solar spectrum by Grevesse et al. [22] using the ATMOS (Atmospheric Trace Molecular Spectroscopy) Fourier transform spectrometer on the 1985 Spacelab-3 flight of the Space Shuttle [23]. Geller et al. [24] identified some pure rotational lines of NH in the ATMOS spectrum. Three pure rotational transitions ($N=3 \leftarrow 2$, $2 \leftarrow 1$, $1 \leftarrow 0$) of

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^{14}NH have recently been detected in Sgr B2 using the ISO LWS (Infrared Space Observatory, Long Wavelength Spectrometer) that yield a column density of $4 \times 10^{14} \text{ mol cm}^{-2}$ [25].

The $^3\Sigma^-$ ground state of NH has a large magnetic moment of $2\mu_B$ that allows magnetic trapping at low temperatures. NH has been cooled to less than 1 K by collisions with ^3He buffer gas and then trapped [26]. It has also been Stark-decelerated in the metastable $a^1\Delta$ state which has a linear Stark effect, and then trapped electrostatically [27]. The radiative lifetime of the $v=1, N=0$ level has been measured to be 37.0 ms using a magnetic trap [28], and the resulting revised infrared line strengths means that solar and stellar abundances based on NH vibration–rotation lines will need to be revised by nearly 30%. The trapping of NH is a very active topic with considerable theoretical work: for example, Wallis and Hutson [29] have recently proposed that magnetically-trapped NH can be cooled to much lower temperatures by collisions with ultra-cold Mg atoms (sympathetic cooling).

The presence of NH in the new high signal-to-noise ACE (Atmospheric Chemistry Experiment [30]) solar spectrum [31] recorded (like ATMOS) with a Fourier transform spectrometer in low earth orbit prompted us to re-examine the infrared spectrum. In addition

to the ACE spectrum, we had at our disposal the improved ATMOS solar spectrum recorded in 1994 during the Atlas-3 mission [32] and high quality laboratory spectra of NH recorded at Kitt Peak. A comparison of the laboratory spectra with the two solar spectra allowed us to find a number of additional high J R lines in the 1–0, 2–1, 3–2, 4–3 and 5–4 bands. A successful search was also made for the 6–5 band in the laboratory spectra using predictions based on the spectroscopic constants reported earlier [3]. A search for this weak band in the ATMOS 1994 [32] spectrum and the ACE [31] spectrum was not conclusive because of frequent overlapping from other much stronger features in the $2300\text{--}2500 \text{ cm}^{-1}$ region. In the end, we combined the new measurements with the older data available for NH in order to get an improved fit.

2. Observation and analysis

As mentioned above, Grevesse et al. [22] have identified 1–0, 2–1, 3–2 and 4–3 bands in the ATMOS 1985 [23] solar spectrum, and by using the measurements of the 1–0 and 2–1 vibration–rotation bands of NH along with available theoretical values of the transition probabilities they have determined the nitrogen abundance

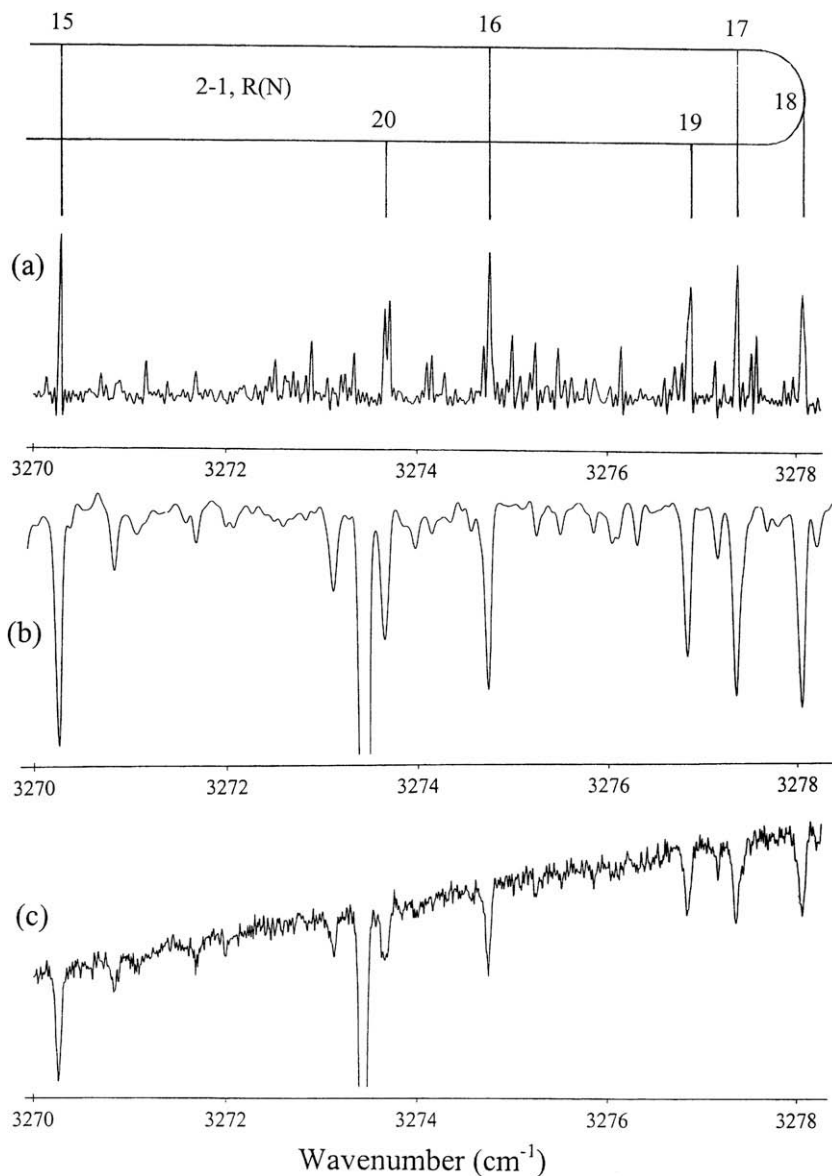


Fig. 1. A comparison of a portion of the 2–1 band from the laboratory (a), ACE (b) and ATMOS (c) spectra.

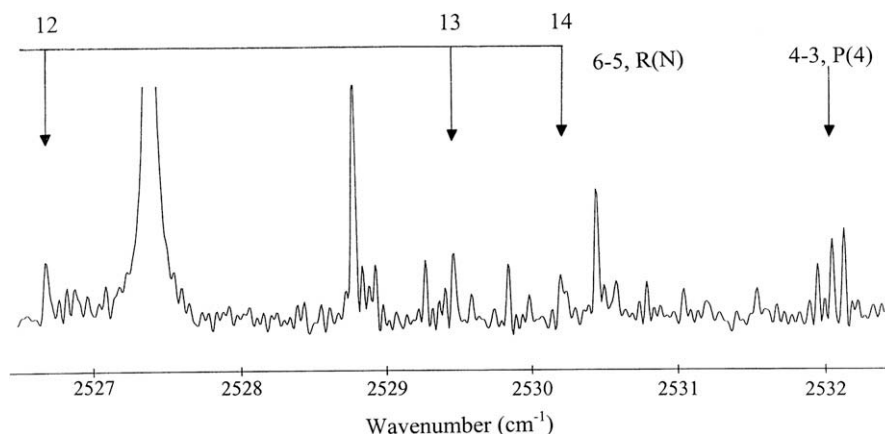


Fig. 2. A portion of the 6–5 vibration–rotation band of NH near the R head. Some R lines of this band as well as the P(4) line of the 4–3 band have been marked.

in the sun (which needs to be re-evaluated in the light of the new work by Campbell et al. [28]). The ACE solar spectrum [31] has NH lines with a higher signal-to-noise ratio compared to the ATMOS spectra [23,32]. In the vibration–rotation bands of NH in the solar spectra, the three spin components of each line are generally not resolved, and the lines are much broader than in the laboratory

spectra. This prompted us to search for higher J lines in the previously observed bands and also to look for new bands by comparing laboratory and solar spectra.

We have observed many new high J lines in the 1–0, 2–1, 3–2, 4–3 and 5–4 bands. The P branch lines are generally much weaker in intensity than the R lines due to Herman–Wallis effects [33], and

Table 1

Observed rotational line positions in cm^{-1} for the 6–5 vibration–rotation band of NH.

J	$R_1(J)$	O–C	$P_1(J)$	O–C	$R_2(J)$	O–C	$P_2(J)$	O–C	$R_3(J)$	O–C	$P_3(J)$	O–C
4	2454.619	26	2184.331	15								
5	2470.189	20	2151.850	15	2454.557	–2	2184.391	–7				
6	2484.048	–19			2470.136	–9	2151.903	–9	2454.557	15	2184.468	–6
7	2496.236	–4			2484.048	–1			2470.136	3	2151.984	–2
8	2506.632	–6			2496.236	9			2484.048	6		
9	2515.209	–3			2506.632	3			2496.236	13		
10	2521.902	–8			2515.209	3			2506.632	4		
11	2526.682	3			2521.902	–5			2515.209	1		
12	2529.462	1			2526.682	5			2521.902	–8		
13	2530.198	1			2529.462	2			2526.682	0		
14					2530.198	3			2529.462	–3		
15									2530.198	–2		

Note: O–C are observed minus calculated wavenumbers in units of 10^{-3}cm^{-1} .

Table 2

Spectroscopic constants (in cm^{-1}) for the $X^3\Sigma^-$ state of NH.

Constants	$v = 0$	$v = 1$	$v = 2$	$v = 3$
T_v	0.0	3125.572486(102)	6094.874867(176)	8907.595251(364)
B_v	16.343275263(395)	15.696418284(664)	15.050471062(651)	14.40201424(872)
$D_v \times 10^3$	1.7028445(106)	1.67936108(900)	1.6612632(121)	1.6506064(553)
$H_v \times 10^7$	1.238065(286)	1.171315(181)	1.104920(276)	1.02953(113)
$L_v \times 10^{11}$	–1.45460(273)	–1.428646(964)	–1.66709(162)	–2.10970(687)
$M_v \times 10^{16}$	6.9165(804)	0.0	0.0	0.0
$\gamma_v \times 10^2$	–5.485506(133)	–5.197386(357)	–4.908779(335)	–4.61922(304)
$\gamma D_v \times 10^5$	1.51582(371)	1.47892(518)	1.38427(403)	1.33190(894)
$\gamma H_v \times 10^9$	–1.2744(612)	–1.0255(757)	0.0	0.0
λ_v	0.91989675(238)	0.91947092(823)	0.91790688(952)	0.915473(332)
$\lambda D_v \times 10^7$	3.436 ^a	0.0	0.0	0.0
	$v = 4$	$v = 5$	$v = 6$	
T_v	11562.315232(660)	14056.152740(954)	16384.34774(310)	
B_v	13.7459245(174)	13.0763110(320)	12.3840839(548)	
$D_v \times 10^3$	1.644947(113)	1.654057(265)	1.678250(208)	
$H_v \times 10^7$	0.72193(199)	0.46183(583)	0.0	
$\gamma_v \times 10^2$	–4.29585(553)	–3.99959(932)	–3.5477(115)	
$\gamma D_v \times 10^5$	0.9914(240)	0.8641(563)	0.0	
λ_v	0.911010(617)	0.904573(855)	0.90305(207)	

Note: Numbers quoted in parentheses are one standard deviation error in the last digits.

^a Fixed value, see text for details.

Table 3
Spectroscopic constants (in cm^{-1}) for the $A^3\Pi$ state of NH.

Constants	$\nu = 0$	$\nu = 1$	$\nu = 2$
T_ν	29761.182869(158)	32795.927980(208)	35633.719638(491)
B_ν	16.32147263(525)	15.57624983(662)	14.7989200(236)
$D_\nu \times 10^3$	1.7897015(437)	1.8029819(548)	1.837037(275)
$H_\nu \times 10^7$	1.07610(136)	0.93315(157)	0.43450(851)
$L_\nu \times 10^{11}$	-1.6904(177)	-3.0096(145)	0.0
$M_\nu \times 10^{15}$	-2.5322(823)	0.0	0.0
A_ν	-34.619342(287)	-34.650210(370)	-34.682905(740)
$AD_\nu \times 10^5$	-8.14 ^a	-8.14 ^a	-8.14 ^a
λ_ν	-0.201511(173)	-0.199128(216)	-0.196763(554)
$\gamma_\nu \times 10^2$	2.97879(173)	2.87425(276)	2.77926(460)
$\gamma D_\nu \times 10^6$	-5.2496(537)	-4.6176(922)	0.0
$p_\nu \times 10^2$	5.52344(364)	5.15700(437)	4.7514(131)
$pD_\nu \times 10^5$	-1.7785(186)	-1.8431(149)	-2.499(108)
$pH_\nu \times 10^9$	2.107(208)	0.0	0.0
$q_\nu \times 10^2$	-3.159263(505)	-2.956795(495)	-2.73765(150)
$qD_\nu \times 10^5$	1.38538(362)	1.38897(297)	1.5182(102)
$qH_\nu \times 10^9$	-1.9159(799)	-1.0355(421)	0.0
$qL_\nu \times 10^{13}$	2.275(543)	0.0	0.0
o_ν	1.284246(268)	1.225808(305)	1.150774(723)
$oD_\nu \times 10^4$	-1.3100(253)	-1.8524(155)	-2.1913(978)
$oH_\nu \times 10^8$	-3.777(377)	0.0	0.0

Note: Numbers quoted in parentheses are one standard deviation error in the last digits.

^a Fixed value, see text for details.

therefore the measurements were generally extended only in the R branches of these bands. We now have observations up to R(35), R(33), R(30), R(20) and R(17) in the these five bands compared to our previous measurements up to R(26), R(25), R(23), R(18) and R(12), respectively. In addition, we have also identified rotational lines of the 6–5 vibration–rotation band. We have also measured a few additional pure rotational lines in the $\nu = 0$ and 1 vibrational levels of the ground state, although a search for pure rotational transitions in the $\nu = 2$ vibrational level was unsuccessful.

As mentioned earlier, the ACE spectrum has much better signal-to-noise ratio than the spectra obtained in the ATMOS experiments. A comparison of a part of the spectrum of the 2–1 band near the R-head obtained in laboratory with the corresponding spectrum from the ATMOS 1994 [23] and ACE [31] is provided in Fig. 1. The lines in the solar spectrum are much broader because of the higher temperature and unresolved splitting of the three spin components. Therefore the lines from the ACE spectrum were given lower weights.

The strongest NH vibration–rotation lines were observed in the laboratory spectra recorded during a search for the CoN molecule from the reaction of Co atoms with N_2 in a hollow cathode lamp. The experimental conditions for obtaining the NH bands are provided in our previous paper [3]. We have used the same spectrum for the search for the very weak 6–5 vibration–rotation band. A part of the spectrum of the R branch near the head of the 6–5 band is presented in Fig. 2.

The spectroscopic constants for the different vibrational levels were determined by fitting the observed line positions using the customary $^3\Sigma^-$ Hamiltonian. An explicit listing of the $^3\Sigma^-$ Hamiltonian matrix elements was provided in our previous paper on NH [2]. The current set of measurements of the observed lines from the laboratory spectra have been combined with the lines of the $A^3\Pi$ – $X^3\Sigma^-$ transition [2] and other previously reported vibration–rotation lines [34], zero field pure rotational lines [5–7,35] and solar pure rotational lines [24] of the ground state using suitable weights.

3. Results and discussion

The observed rotational lines of the 6–5 band are listed in Table 1 while the spectroscopic constants for the $X^3\Sigma^-$ and $A^3\Pi$

states obtained from the combined fit are provided in Tables 2 and 3, respectively. The inclusion of pure rotational transitions from the LMR study of Brown and coworkers [6,7] as well as the observation of high N transitions in most of the vibration–rotation bands has enabled us to determine much improved spectroscopic constants for the different vibrational levels of the ground state. In the LMR study, Brown and coworkers obtained a small value of 0.0103(24) MHz ($3.436 \times 10^{-7} \text{ cm}^{-1}$) for the λ_D constant. Since the LMR value is unaffected by any correlation with the $A^3\Pi$ state, we have fixed this constant to the LMR value in our fit. This λ_D constant was not determined in our previous vibration–rotation study [3]. The A_D constant of the $A^3\Pi$ state was fixed at a value of $-8.14 \times 10^{-5} \text{ cm}^{-1}$ as explained in our previous paper on NH [2]. This value was determined using a formula provided by Veseth [36] which relates A_D to other spectroscopic constants. The term values for the observed vibrational levels of the $X^3\Sigma^-$ and $A^3\Pi$ states were calculated using the spectroscopic constants obtained in the final fit and are available on ScienceDirect (www.sciencedirect.com) and as part of the Ohio State University Molecular Spectroscopy Archives (http://msa.lib.ohio-state.edu/jmsa_hp.htm). The term values have been extrapolated to a few higher N rotational levels for each vibrational level. A list of all of the measurements used in the determination of the spectroscopic constants along with the obs.–calc. residuals is also available.

In addition to NH, the ATMOS and ACE spectra both show the presence of other free radicals such as OH and CH. A reinvestigation of the OH radical has been published recently using solar spectra [37]. These observations extend the vibration–rotation and pure rotational bands to higher J values, and pure rotational transitions were observed in the $\nu = 4$ vibrational level of the ground state for the first time. A similar reinvestigation of CH is in progress using solar and laboratory spectra.

4. Conclusion

The vibration–rotation bands of NH have been reinvestigated using a laboratory spectrum, the ATMOS 1994 [32] solar atlas and the new ACE [31] solar spectrum. It has been noted that the ACE spectrum has a better signal-to-noise ratio than the ATMOS spectrum and a comparative study of the three spectra has helped us extend the lines to higher J values. In addition we were able to

identify lines in the 6–5 vibration–rotation band. The observation of this new band plus additional lines in the previously reported bands [3] has enabled us to determine an improved set of spectroscopic constants for the ground state of NH.

Acknowledgments

The research described here was partially supported by funds from the NASA laboratory astrophysics program. Some support was also provided by the UK Engineering and Physical Sciences Research Council (EPSRC). The ACE mission is primarily funded by the Canadian Space Agency.

Appendix A. Supplementary data

Supplementary data for this article are available on ScienceDirect (www.sciencedirect.com) and as part of the Ohio State University Molecular Spectroscopy Archives (http://library.osu.edu/sites/msa/jmsa_hp.htm). Supplementary data associated with this article can be found, in the online version, at [doi:10.1016/j.jms.2010.01.006](https://doi.org/10.1016/j.jms.2010.01.006).

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