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The far-infrared spectrum of the ^{14}NH radical in its $X^3\Sigma^-$ state

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Abstract

Pure rotational transitions of the ^{14}NH radical in the $v = 0$ level of the $X^3\Sigma^-$ ground state have been detected using tunable far-infrared radiation generated by third-order mixing of radiation from two CO_2 lasers with that from a microwave source. The NH radical was formed in a cooled dc electric discharge through ammonia gas in helium. The rotational transitions from $N = 1$–0 up to 5–4 inclusive were detected. The nuclear hyperfine splittings become progressively less well resolved as N increases. These measurements have been combined with previous, more accurate measurements of the $N = 1$–0 transition [Astron. Astrophys. 322 (1997) L1] to determine an improved set of molecular parameters for ^{14}NH.
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1. Introduction

The NH free radical is of fundamental importance. It contains only eight electrons and so is susceptible to accurate ab initio calculations [1]. It plays a significant role in many chemical processes, including combustion [2]. It has also been identified in interstellar space through transitions in its electronic, vibration–rotation, and high-N rotational spectra [3,4]. More recently, the $N = 2$–1 transition of ^{14}NH has been detected in the direction of Sagittarius B2 as part of the Infrared Space Observatory (ISO) program [5] using an interferometer mounted on a satellite platform. A knowledge of the abundance of NH in dark clouds is of importance for the study of nitrogen chemistry because it is likely to be an intermediate in the formation of NH_3 by successive hydrogenation reactions [6,7].

For all these and other reasons, NH has been extensively studied by spectroscopy. Many measurements have been made of its electronic spectrum, dating back to 1893 [8]. In the recent era, the $A^3\Pi$–$X^3\Sigma^-$ transition at 336 nm has been investigated by Brazier et al. [9] with a high-resolution FT interferometer. The (0–0) band of this electronic transition has also been studied under molecular beam conditions by Ubachs et al. [10] to reveal the nuclear hyperfine structure. The fundamental band in the vibration–rotation spectrum of NH has been studied in absorption by Bernath and Amano [11] using a difference-frequency laser and in emission by Sakai et al. [12] using Fourier transform methods. Ram et al. [13] have recently recorded a more extensive emission spectrum of NH in the infrared. They observed all bands up to the (5–4) band and obtained improved molecular parameters. The rotational spectrum of NH falls in the far–infrared (FIR) region of the electromagnetic spectrum. The first studies of transitions in this region were made by Radford and co-workers [14,15] using the technique of laser magnetic resonance (LMR). These experiments provided the first measurements of the ^{14}N and ^{1}H hyperfine parameters for this molecule. They were followed by a

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study of the $N = 1$–0 transition at zero magnetic field using a tunable FIR source by van den Heuvel et al. [16]. A more extensive recording of the same spectral region has been reported recently by Klaus et al. [17]. These authors used a backward wave oscillator as the radiation source. Since it was capable of delivering much more power, their observations and measurements are of significantly higher quality.

The present paper reports the observation and measurement of higher rotational transitions of NH in the $v = 0$ level of the $X^3\Sigma^-$ state (up to $N = 5$–4) using tunable FIR radiation generated by third-order mixing of two CO_2 lasers with microwave radiation. The results are combined with those for the $N = 1$–0 transition from the Cologne group [17] to give an improved set of molecular parameters. While this paper was in preparation, we learned of a study of the $N = 2$–1 transition of NH by the Cologne group [18]. Their preliminary results are in good agreement with those reported here.

2. Experimental details

The initial observations of the rotational spectrum of NH were made at the Boulder laboratories of NIST; fuller, more careful measurements were made subsequently at the Department of Physics, Toyama University. The tunable far-infrared spectrometers in the two laboratories were essentially identical [19,20]. Far-infrared (FIR) radiation was generated by mixing mid-infrared radiation from two frequency-stabilized carbon dioxide lasers (of frequencies v_1 and v_2) and microwave radiation (of frequency v_M) on a metal–insulator–metal (MIM) diode consisting of a sharpened tungsten whisker in contact with a polished cobalt rod. The FIR radiation was collimated with a parabolic mirror, passed through an absorption cell and focussed onto a liquid-helium-cooled bolometer or photoconductor. Molecular spectra were acquired by modulating the frequency of the FIR radiation at about 1 kHz and detecting the absorption signal with a lock-in amplifier. Consequently, the spectra were displayed as the first derivatives of the absorption profile.

The NH radicals were formed in a dc electric discharge through a flowing gas mixture of NH_3 in helium or occasionally through pure NH_3. Typical partial pressures were 20 Pa NH_3 and 10 Pa He. The discharge cell consisted of a pyrex tube of 1.7 m length and 26 mm inner diameter; the windows were made from polypropylene sheet of 60 μm thickness. It was pumped rapidly by either a rotary pump or a mechanical booster pump and its walls were cooled to dry ice temperatures. The electric discharge was struck between a pair of hollow cylinder electrodes. The typical voltage was 3 kV and the optimum current was 200 mA; the plasma was approximately 140 cm in length.

3. Results, line-shape fitting, and analysis

3.1. Results and line-shape fitting

Rotational transitions of NH in the $v = 0$ level of the $X^3\Sigma^-$ state have been recorded in the range $N = 1$–0 to 5–4 inclusive. The resulting measurements are given in Table 1. Two examples of experimental recordings are given in Figs. 1 and 2. The first shows the ^1H and ^{14}N nuclear hyperfine structure associated with the $J = 3$–2 spin component of the $N = 2$–1 transition at 1.955 THz. The observed spectrum consists of many hyperfine transitions which are only partially resolved with the experimental, Doppler-limited linewidths. The main line arises from the strong transitions with $\Delta F = \Delta F_1 = +1$ while the two weak features to lower frequency arise from $\Delta F = 0$, $\Delta F_1 = +1$ transitions.[3] The individual hyperfine transitions are shown below in the form of a stick diagram; these have been computed using the final set of molecular parameters. The second example shows the $J = 5$–4 spin component of the $N = 5$–4 transition at 4.874 THz. No hyperfine structure was observable for this transition. The reasons for this are: (i) the experimental linewidth at these higher frequencies is proportionally greater and (ii) the satellite hyperfine lines (with $\Delta F \neq \Delta F_1$) are weaker for these larger quantum numbers.

In order to extract the full value from the experimental observations, a calculated line-shape function has been fitted to each observed spectral feature. The line-shape is a Voigt profile, formed from a convolution of Gaussian (Doppler broadening) and Lorentzian (pressure broadening) line-shapes. Under the conditions of our experiments, the Doppler broadening makes a dominant contribution to the experimental linewidth.

In the commonly occurring situation where a single observed feature was composed of several hyperfine components, it was modelled by adjusting the frequency of one of the stronger transitions with all the others locked to it at fixed off-set frequencies. The frequencies and intensities of these subordinate transitions were fixed relative to those of the lead transition using values calculated with the parameters obtained from a fit of the hyperfine structure of the $N = 1$–0 transition by Klaus et al. [17]. It is the frequency of this lead hyperfine transition which is reported in Table 1, together with the estimated experimental uncertainty. The Doppler linewidths obtained in this fitting procedure depended linearly on the frequency as expected (see Fig. 3). From these measurements, the temperature of the discharge plasma can be estimated to be 393 ± 4 K.

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[3] The quantum numbers are labelled according to the following coupling scheme:

$$N + S = J; J + I_H = F_1; F_1 + I_N = F.$$

Table 1
Observed frequencies for the rotational transitions of ^{14}NH in the $v = 0$ level of the $X^3\Sigma^-$ state

N	J	F_1	F	$\nu_{obs.}$ (MHz)	o − c (kHz)
$1 \leftarrow 0^a$	$0 \leftarrow 1$	$1/2 \leftarrow 1/2$	$1/2 \leftarrow 3/2$	946380.724(50)^b	−8
		$1/2 \leftarrow 1/2$	$3/2 \leftarrow 1/2$	946419.975(50)	30
		$1/2 \leftarrow 3/2$	$3/2 \leftarrow 5/2$	946475.820(50)	−38
		$1/2 \leftarrow 3/2$	$3/2 \leftarrow 3/2$	946509.310(50)	−9
		$1/2 \leftarrow 3/2$	$1/2 \leftarrow 1/2$	946527.481(100)	59
	$2 \leftarrow 1$	$3/2 \leftarrow 1/2$	$3/2 \leftarrow 3/2$	974436.266(200)	−98
		$5/2 \leftarrow 3/2$	$3/2 \leftarrow 3/2$	974444.044(50)	20
		$3/2 \leftarrow 1/2$	$1/2 \leftarrow 1/2$	974450.438(50)	−12
		$5/2 \leftarrow 3/2$	$3/2 \leftarrow 1/2$	974462.216(100)	−59
		$5/2 \leftarrow 3/2$	$5/2 \leftarrow 3/2$	974470.832(300)	−186
		$5/2 \leftarrow 3/2$	$7/2 \leftarrow 5/2$	974478.714(500)	295
		$3/2 \leftarrow 3/2$	$5/2 \leftarrow 5/2$	974574.428(100)	62
	$1 \leftarrow 1$	$3/2 \leftarrow 1/2$	$5/2 \leftarrow 3/2$	999878.056(500)	−356
		$1/2 \leftarrow 1/2$	$3/2 \leftarrow 3/2$	999882.089(50)	−12
		$3/2 \leftarrow 1/2$	$1/2 \leftarrow 3/2$	999907.929(50)	33
		$1/2 \leftarrow 1/2$	$3/2 \leftarrow 1/2$	999921.020(200)	−145
		$3/2 \leftarrow 1/2$	$3/2 \leftarrow 1/2$	999945.056(50)	−26
		$1/2 \leftarrow 1/2$	$1/2 \leftarrow 1/2$	999958.242(50)	−6
		$3/2 \leftarrow 3/2$	$5/2 \leftarrow 5/2$	999973.385(50)	−5
		$3/2 \leftarrow 3/2$	$3/2 \leftarrow 5/2$	1000001.018(50)	25
		$3/2 \leftarrow 3/2$	$5/2 \leftarrow 3/2$	1000006.822(100)	−31
		$1/2 \leftarrow 3/2$	$3/2 \leftarrow 3/2$	1000010.521(100)	−20
		$3/2 \leftarrow 3/2$	$3/2 \leftarrow 3/2$	1000034.490(50)	34
		$1/2 \leftarrow 3/2$	$1/2 \leftarrow 3/2$	1000047.436(200)	−183
		$3/2 \leftarrow 3/2$	$1/2 \leftarrow 1/2$	1000054.515(300)	−66
$2 \leftarrow 1$	$3 \leftarrow 2$	$5/2 \leftarrow 3/2$	$5/2 \leftarrow 5/2$	1954986.168(203)	49
		$5/2 \leftarrow 3/2$	$3/2 \leftarrow 3/2$	1954999.303(299)	−61
		$7/2 \leftarrow 5/2$	$9/2 \leftarrow 7/2$	1955029.520(18)	−1
	$2 \leftarrow 1$	$5/2 \leftarrow 3/2$	$5/2 \leftarrow 3/2$	1958191.921(31)	28
		$5/2 \leftarrow 3/2$	$7/2 \leftarrow 5/2$	1958206.834(120)	−56
		$5/2 \leftarrow 3/2$	$5/2 \leftarrow 5/2$	1958219.227(273)	−268
	$1 \leftarrow 0$	$1/2 \leftarrow 1/2$	$3/2 \leftarrow 1/2$	1978369.372(59)	36
		$1/2 \leftarrow 1/2$	$1/2 \leftarrow 3/2$	1978434.952(170)	−220
		$3/2 \leftarrow 1/2$	$5/2 \leftarrow 3/2$	1978457.618(54)	−37
		$3/2 \leftarrow 1/2$	$3/2 \leftarrow 3/2$	1978514.785(79)	−38
		$3/2 \leftarrow 1/2$	$1/2 \leftarrow 1/2$	1978546.018(155)	56
$3 \leftarrow 2$	$4 \leftarrow 3$	$9/2 \leftarrow 7/2$	$11/2 \leftarrow 9/2$	2931761.678(31)	−9
	$3 \leftarrow 2$	$7/2 \leftarrow 5/2$	$9/2 \leftarrow 7/2$	2934246.555(40)	−9
	$2 \leftarrow 1$	$5/2 \leftarrow 3/2$	$7/2 \leftarrow 5/2$	2939474.959(87)	105
$4 \leftarrow 3$	$5 \leftarrow 4$	$11/2 \leftarrow 9/2$	$13/2 \leftarrow 11/2$	3904460.874(31)	4
	$4 \leftarrow 3$	$9/2 \leftarrow 7/2$	$11/2 \leftarrow 9/2$	3906624.968(50)	−17
	$3 \leftarrow 2$	$7/2 \leftarrow 5/2$	$9/2 \leftarrow 7/2$	3909784.835(263)	217
$5 \leftarrow 4$	$6 \leftarrow 5$	$13/2 \leftarrow 11/2$	$15/2 \leftarrow 13/2$	4872148.336(36)	4
	$5 \leftarrow 4$	$11/2 \leftarrow 9/2$	$13/2 \leftarrow 11/2$	4874132.623(54)	−0
	$4 \leftarrow 3$	$9/2 \leftarrow 7/2$	$11/2 \leftarrow 9/2$	4876597.238(33)	−9

^{a} Data for the $N = 1$–0 transition taken from [17].
^{b} The figures in parentheses give the experimental uncertainty, determined as described in the text.

3.2. Determination of molecular parameters

The experimental frequencies listed in Table 1 have been used to determine values for the parameters of an effective Hamiltonian for a molecule in a $^3\Sigma$ state with two non-zero nuclear spins. The effective Hamiltonian contains all significant contributions:

$$H = H_{rot} + H_{cd} + H_{ss} + H_{sr} + H_{hfs}(^1H) + H_{hfs}(^{14}N). \quad (1)$$

The various operators on the right-hand side are completely standard; their detailed forms have been given in many places in the literature, e.g. [15,21] as have the matrix elements in appropriate representations [22–24]. The calculations of the eigenvalues of this effective Hamiltonian were performed using a complete basis set for a given value of F ($\Delta N = \pm 4$). The data set used in the least-squares fit to determine the molecular parameters is given in Table 1; it consists of our
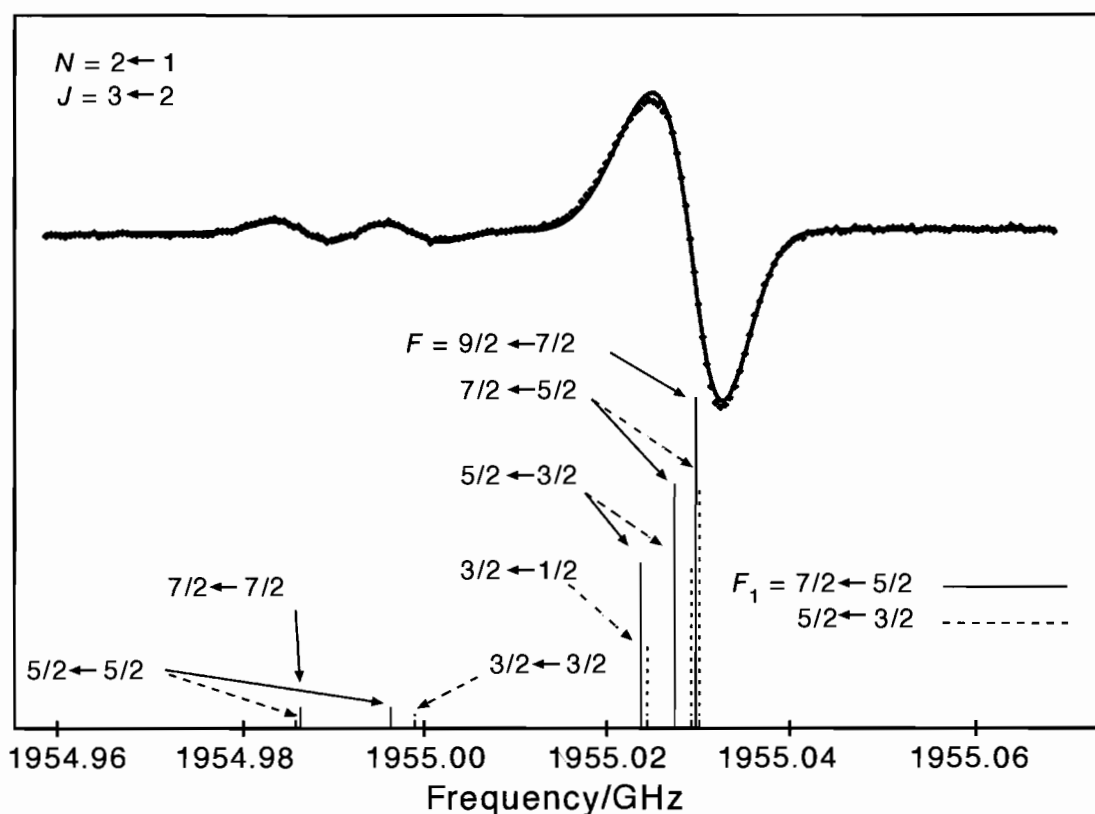
Fig. 1. The observed hyperfine structure associated with the $J = 3$–2 spin component of the $N = 2$–1 rotational transition of the ^{14}NH radical in the $v = 0$ level of the $X^3\Sigma^-$ state. The signal was recorded through frequency modulation; consequently, the lineshape is that of the first derivative of the absorption profile. The individual data points are represented by dots while the smooth curve through them is the best fit to these points using the line-fitting procedure described in the text. The detailed hyperfine structure associated with this part of the spectrum is shown in the lower part of the figure in the form of a stick diagram. All the transitions obey the selection rule $\Delta F_1 = +1$; the stronger group are $\Delta F = +1$ transitions while the weaker ones are $\Delta F = 0$.

measurements for the transitions $N = 2$–1 to $N = 5$–4 together with those of Klaus et al. [17] for the $N = 1$–0 transitions. The latter are judged to be more accurate than our measurements because the backward wave oscillator source used in their experiments was significantly more powerful than our difference frequency source. Each datum in the fit was weighted inversely as the square of its experimental uncertainty, also given in Table 1.

The results of the fit are given in Table 1 (residuals) and Table 2 (parameter values determined). It can be seen from Table 2 that it has been necessary to include up to sextic centrifugal corrections to the rotational energy (H) and the quadratic corrections to the spin–spin and spin–rotation parameters (λ_D and γ_D, respectively). The octic centrifugal distortion parameter L is marginally significant; it makes a contribution of -0.272 MHz to the $N = 5$–4 transition frequency. This parameter has therefore been constrained to the value determined by Ram and co-workers [13] from the vibration–rotation spectrum. The standard deviation of the fit relative to the experimental uncertainty (0.6774) is entirely satisfactory.

4. Discussion

Measurements of the rotational (far-infrared) spectrum of the ^{14}NH radical in the $v = 0$ level of its $X^3\Sigma^-$ state have been extended to the $N = 5$–4 transition. As a result, the molecular parameters have been refined, particularly those associated with centrifugal distortion effects. The values obtained can be compared with those from other studies as shown in Table 2. The nuclear hyperfine parameters are determined primarily (but not completely) by the measurements of Klaus et al. [17] on the $N = 1$–0 transition. They are therefore little changed by the present work although it is gratifying that the estimated uncertainties are somewhat reduced. Our analysis differs from that of Klaus et al. in one respect; we have been able to determine the value for an additional nuclear spin–rotation parameter, $C_I(H)$. The interpretation of the hyperfine parameters is well-established by the excellent ab initio calculations of Kristiansen and Veseth [1] who obtained the following values (in MHz):

$b_F(^1H) = -67.43, \quad t(^1H) = 30.00,$
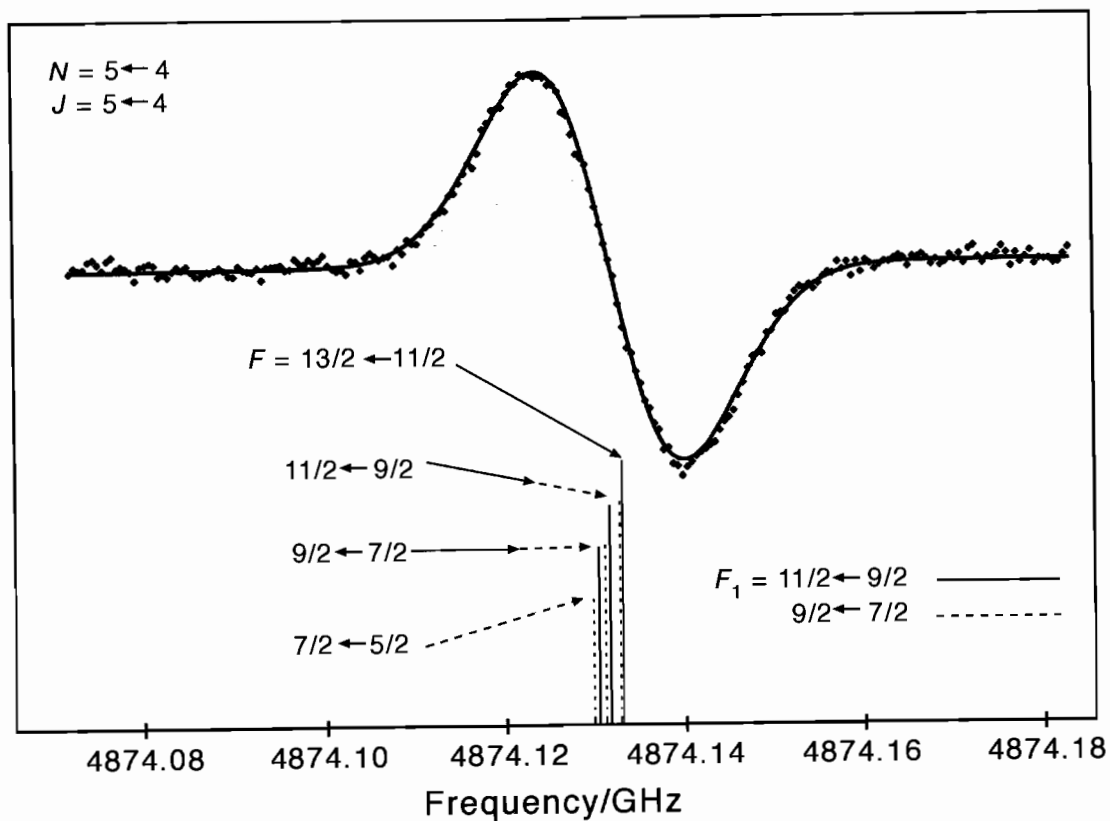
$b_F(^{14}N) = 18.79, \quad t(^{14}N) = -22.29.$

Fig. 2. The observed hyperfine structure associated with the $J = 5\text{-}4$ spin component of the $N = 5\text{-}4$ rotational transition of the ^{14}NH radical in the $v = 0$ level of the $X^3\Sigma^-$ state. The individual data points are represented by dots while the smooth curve through them is the best fit to these points using the line-fitting procedure described in the text. The detailed hyperfine structure associated with this part of the spectrum is shown in the lower part of the figure in the form of a stick diagram. All the transitions obey the selection rule $\Delta F = \Delta F_1 = +1$.
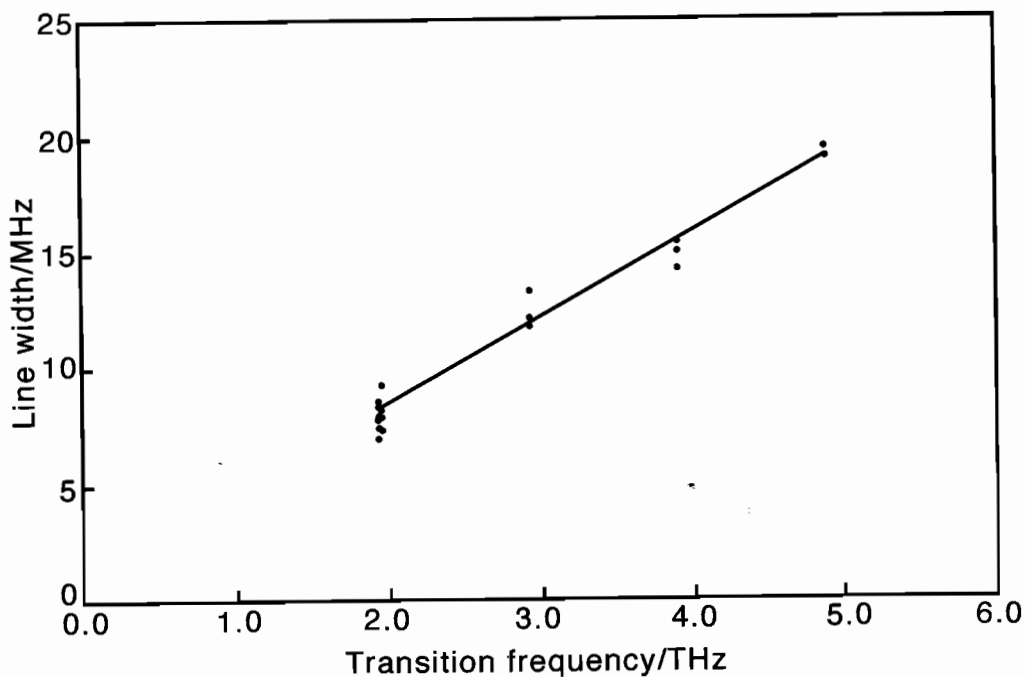
Fig. 3. Diagram showing the linear relationship between the experimental linewidth (FWHM), determined by fitting a Doppler lineshape to the experimental data, and the transition frequency for the rotational spectrum of the ^{14}NH radical in the $v = 0$ level of the $X^3\Sigma^-$ state. The best straight line through these points implies a translational temperature of $393 \pm 4\,K$ in the discharge plasma.

Table 2
Molecular parameters for ^{14}NH in the $v = 0$ level of the $X^3\Sigma^-$ state[a]

Parameters	This work	Brünken et al. [18]	Brazier et al. [9]
B_0	489959.0768(40)[b]	489959.068(22)	489959.16(13)
D_0	51.05111(33)	51.0344(59)	51.0482(10)
$H_0 \times 10^3$	3.7376(72)		3.7007(34)
$L_0 \times 10^7$	-4.376[c]		$-4.189(49)$
$M_0 \times 10^{11}$			1.25(24)
λ_0	27577.848(11)	27577.856(19)	27582.8(44)
λ_{D_0}	0.0103(24)		$-0.273(43)$
γ_0	$-1644.4860(72)$	$-1644.430(42)$	$-1644.18(66)$
γ_{D_0}	0.45181(30)	0.433(16)	0.4526(22)
$\gamma_{H_0} \times 10^5$			4.10(27)
b_F (N)	18.830(10)	18.829(14)	
t (N)[d]	$-22.6408(96)$	$-22.659(21)$	
eQq (N)	$-2.883(62)$	$-3.00(14)$	
C_I (N)	0.1455(89)	0.176(34)	
b_F (H)	$-66.131(15)$	$-66.120(21)$	
t (H)	30.097(28)	30.087(44)	
C_I (H)	$-0.061(23)$		

[a] The values of the parameters are given in MHz.

[b] The figures in parenthesis represent 1 standard deviation of the least-squares fit, in units of the last quoted decimal place.

[c] Parameter constrained to this value from [13] in the least-squares fit.

[d] The hyperfine parameter t is related to Frosch and Foley's c by $t = c/3$ [24].

The spin–rotation parameters (γ and γ_D) are in good agreement with those of Brazier et al. [9], Ram et al. [13], and Brünken et al. [18] and are again better determined. The spin–spin parameters (λ and λ_D) however differ considerably from the values determined by Brazier et al. [9]. In particular, the smaller value obtained for the parameter λ_D makes a significant improvement to the quality of our fit. The present values are to be preferred because they are not contaminated by correlation with the parameters for the excited $^3\Pi$ electronic state of NH as they are in the optical spectrum. In their study of the infrared spectrum, Ram et al. [13] obtained a value for λ close to ours (27577.70(74) MHz) but λ_D was too small to be determined which is also consistent with our result.

Despite the familiarity of the NH radical, further measurements of its rotational spectrum remain to be made. In particular, it is desirable to obtain accurate measurements of the transition frequencies in excited vibrational levels. Almost certainly, there is sufficient population of NH in the $v = 1$ level in the electric discharge used in our experiments for these transitions to be detectable. In addition, measurements on the ^{15}NH isotopomer would be much appreciated by astronomers attempting to detect this species in astrophysical sources such as the diffuse interstellar clouds [5]. Measurement of the relative abundances of different isotopic forms can provide valuable information on star formation processes. The only measurement reported on ^{15}NH to date is the one by Wayne and Radford [15] and even that is confined to a single spin component of the $N = 1$–0 transition.

Acknowledgments

References

[1] P. Kristiansen, L. Veseth, J. Chem. Phys. 84 (1986) 6336–6344.

[2] W. Hack, NH radical reactions, review article, in: Z.B. Alfassi (Ed.), N-Centered Radicals, Wiley, Chichester, 1998, pp. 413–466.

[3] D.L. Lambert, J.A. Brown, K.H. Hinkle, H.R. Johnson, Astrophys. J. 284 (1984) 223–237.

[4] D.M. Meyer, K.C. Roth, Astrophys. J. Lett. 376 (1991) L49–L52.

[5] J. Cernicharo, J.R. Goioechea, E. Caux, Astrophys. J. Lett. 534 (2000) L199–L202.

[6] A.P.C. Mann, D.A. Williams, Month. Not. R. Astron. Soc. 209 (1984) 33–49.

[7] R. Wagenblast, D.A. Williams, T.J. Millar, L.A.M. Nejad, Month. Not. R. Astron. Soc. 260 (1993) 420–424.

[8] K.-P. Huber, G. Herzberg, Constants of Diatomic Molecules, Van Nostrand Reinhold, New York, 1979.

[9] C.R. Brazier, R.S. Ram, P.F. Bernath, J. Mol. Spectrosc. 120 (1986) 381–402.

[10] W. Ubachs, J.J. ter Meulen, A. Dymanus, Can. J. Phys. 62 (1984) 1374–1391.

[11] P.F. Bernath, T. Amano, J. Mol. Spectrosc. 95 (1982) 359–364.

[12] H. Sakai, P. Hansen, M. Esplin, R. Johansson, M. Peltola, J. Strong, Appl. Opt. 21 (1982) 228–235.

[13] R.S. Ram, P.F. Bernath, K.H. Hinkle, J. Chem. Phys. 110 (1999) 5557–5563.

[14] H.E. Radford, M.M. Litvak, Chem. Phys. Lett. 34 (1975) 561–564.

[15] F.D. Wayne, H.E. Radford, Mol. Phys. 32 (1976) 1407–1422.

[16] F.C. van den Heuvel, W.L. Meerts, A. Dymanus, Chem. Phys. Lett. 92 (1982) 215–218.

[17] T. Klaus, S. Takano, G. Winnewisser, Astron. Astrophys. 322 (1997) L1–L4.

[18] S. Brünken, F. Lewen, G. Winnewisser, M. Simeckova, S. Urban, Eighteenth Colloquium on High Resolution Molecular Spectroscopy, Dijon, France, 2003, Poster M36.

[19] T.D. Varberg, K.M. Evenson, Astrophys. J. 385 (1992) 763–765.

[20] F. Matsushima, H. Odashima, D. Wang, S. Tsunekawa, K. Takagi, Jpn. J. Appl. Phys. 33 (1994) 315–318.

[21] J.M. Brown, E.A. Colbourn, J.K.G. Watson, F.D. Wayne, J. Mol. Spectrosc. 74 (1983) 294–318.

[22] T. Klaus, S.P. Belov, A.H. Salek, G. Winnewisser, E. Herbst, J. Mol. Spectrosc. 168 (1994) 235–247.

[23] T. Klaus, A.H. Salek, S.P. Belov, G. Winnewisser, Y. Hirahara, M. Hayashi, E. Kagi, K. Kawaguchi, J. Mol. Spectrosc. 180 (1996) 197–206.

[24] J.M. Brown, A. Carrington, Rotational Spectroscopy of Diatomic Molecules, Cambridge University Press, Cambridge, England, 2003.