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Detection of interstellar NH towards ζ Ophiuchi by means of ultra-high-resolution spectroscopy

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ABSTRACT

We have obtained an ultra-high-resolution (0.38 km s^{-1} FWHM) spectrum of the $R_1(0)$ (3358.053 \AA) line of interstellar NH towards ζ Oph. These observations comprise the first detection of NH towards ζ Oph, and the third reported detection of this molecule by absorption-line spectroscopy towards any star. The equivalent width ($0.36 \pm 0.05 \text{ m\AA}$) corresponds to a column density of $8.8 \pm 1.2 \times 10^{11} \text{ cm}^{-2}$. This is more than an order of magnitude higher than that expected on the basis of equilibrium gas-phase models, but is consistent with models incorporating grain-surface chemistry. The line profile is fully resolved, and has an intrinsic velocity dispersion characterized by $b = 1.15 \pm 0.12 \text{ km s}^{-1}$. This is sufficiently narrow to exclude the possibility of hot NH formation through the endothermic reaction $\text{N} + \text{H}_2 \rightarrow \text{NH} + \text{H}$. There is evidence that the NH line is split into two velocity components (separation $1.26 \pm 0.17 \text{ km s}^{-1}$), with relative strengths mirroring those of the two CN components towards this star. We argue that this correlation also supports the case for grain surface reactions dominating the nitrogen chemistry of diffuse molecular clouds.

Key words: stars: individual: ζ Oph – ISM: molecules.

1 INTRODUCTION

The NH molecule is expected to play a central role in the nitrogen chemistry of diffuse molecular clouds (e.g. Pickles & Williams 1977). However, the strongest line accessible to ground-based optical spectroscopy [the $R_1(0)$ line of the $\text{A}^3\Pi\text{--X}^3\Sigma^-$ (0–0) band at 3358.053 \AA , Dixon 1959] is very weak ($W_\lambda \leq 1 \text{ m\AA}$, see below), and occurs at a wavelength where poor atmospheric transmission and detector sensitivities combine to make detection difficult. For these reasons, NH was not discovered in the diffuse interstellar medium until Meyer & Roth (1991) detected it towards ζ Per and HD 27778.

The column densities of NH towards these two stars ($\approx 10^{12} \text{ cm}^{-2}$) were found to be an order of magnitude larger than expected from models involving purely gas-phase chemistry (e.g. van Dishoeck & Black 1988), and this has renewed interest in the idea that NH might be formed on the surfaces of interstellar grains. Detailed models of the ζ Per cloud, incorporating both gas-phase and grain-surface reactions, have been produced by Wagenblast et al. (1993) and Wagenblast & Williams (1993, 1996). These calculations confirm that purely gas-phase models fail by a factor of 30 to account for the observed NH abundance, while models that include surface chemistry give NH abundances that lie within the observed range.

An alternative route to NH formation is at high temperature, via the reaction



which has an energy barrier equivalent to $16\,600 \text{ K}$, and a reaction rate (Millar, Farquhar & Willacy 1997) of

$$k_1 = 4.65 \times 10^{-10} \times (T/300 \text{ K})^{1/2} \times \exp[-16\,606 \text{ K}/T] \text{ cm}^3 \text{ s}^{-1}. \quad (2)$$

Thus, this reaction, perhaps taking place in a warm cloud interface [such as those suggested by Duley et al. (1992) to explain the comparable over-abundance of CH^+], might be able to produce the observed NH abundances. For example, at $T = 7000 \text{ K}$ we have $k_1 = 2.1 \times 10^{-10} \text{ cm}^3 \text{ s}^{-1}$, which would lead Reaction 1 to dominate NH formation.

In principle, this possibility could be checked if the line profiles were resolved by means of high-resolution spectroscopy, as NH formed at a temperature of several thousand K will have much broader absorption lines than NH formed at low temperature on grain surfaces. For example, $T = 7000 \text{ K}$ would result in an NH velocity dispersion (b -value) of 2.8 km s^{-1} , whereas $T = 100 \text{ K}$ would result in a velocity dispersion of only 0.3 km s^{-1} (assuming no turbulent broadening of the line profiles).

The resolving power employed by Meyer & Roth ($R \equiv \lambda/\Delta\lambda = 40\,000$, corresponding to a velocity resolution of 7.5 km s^{-1} FWHM) was not sufficient for them to determine the intrinsic widths of the NH lines. Here we report observations of the interstellar NH $R_1(0)$ line towards ζ Oph, obtained at much higher resolution ($R \approx 800\,000$) using the Ultra-High-Resolution Facility (UHRF) at the Anglo-Australian Telescope. These observations

constitute the first detection of interstellar NH towards this much-studied star, and the uniquely high resolution has enabled us to determine the intrinsic line width for the first time.

2 OBSERVATIONS

The UHRF is currently the highest resolution optical astronomical spectrograph in the world, and has been described in detail by Diego et al. (1995). As used here, the detector was a 1024×1024 Tektronix CCD (24- μm pixels), and the ‘extraslow’ readout speed was adopted so as to minimize the readout noise (2.3 e^- pixel $^{-1}$ rms). For these observations the instrument was used in conjunction with an image slicer (Diego 1993), and the CCD output was binned by a factor of 8 perpendicular to the dispersion direction in order to reduce further the readout noise associated with extracting the very broad spectrum produced by the image slicer. The dispersion was 0.075 \AA mm $^{-1}$, and the resolution, measured with the aid of a stabilized He–Ne laser, was 0.38 ± 0.01 km s $^{-1}$ FWHM (corresponding to a resolving power $R = 790\,000$).

The observations were made on three nights as follows: 1996 July 03 (6 × 1200-s exposures); 1997 June 19 (14 × 1200-s); and 1997 June 20 (15 × 1200-s). The total integration time was therefore 11 h 40 min, which resulted in a total recorded continuum flux of 6.4×10^4 counts (electrons). After every three or four exposures the grating angle was moved slightly (and a new wavelength calibration spectrum obtained) so as to minimize residual flat-fielding errors by ensuring that the NH line fell on a range of different CCD pixels. In addition, the 1997 data were obtained through a UG11 filter; although this reduced the overall throughput by about 15 per cent, it was found to reduce significantly the level of (non-UV) scattered light falling on the detector.

The individual spectra were extracted from the CCD images using the FIGARO data reduction package (Shortridge 1988). Each spectrum was divided by a flat-field, and scattered light was measured from the inter-order region and subtracted. Wavelength calibration was performed by means of a Th–Ar lamp (linear fits to four Th–Ar lines identified within the 1.8- \AA coverage of the detector yielded residuals of less than 3×10^{-4} \AA , or 0.027 km s $^{-1}$, rms). Before co-adding the individual spectra, each was converted to the heliocentric velocity frame so as to avoid degrading the resolution due to the changing component of the Earth’s velocity along the line of sight during the observations. The resulting spectrum (normalized by division of a linear least-squares fit to the adjacent continuum) is shown in Fig 1.

3 DISCUSSION

The line profile parameters (heliocentric velocity, equivalent width and velocity dispersion) were determined from a least-squares Gaussian fit to the observed profile. The column density was obtained from the equivalent width (assuming a linear curve of growth, and an oscillator strength of 0.0041: Meyer & Roth 1991). Two cases were considered: (a) a single-component fit which, given the signal-to-noise ratio, may be considered to be the conservative interpretation; and (b) a two-component fit, the justification for which is the slight asymmetry of the line profile, and the fact that two velocity components are known to be present in other molecular species towards this star (see below). The results are given in Table 1, and include 1σ errors on the derived parameters.

The total equivalent width of the $R_1(0)$ line, 0.36 ± 0.05 m \AA (Table 1), is an order of magnitude smaller than the upper limit of 3 m \AA obtained by Herbig (1968), and very similar to the value of

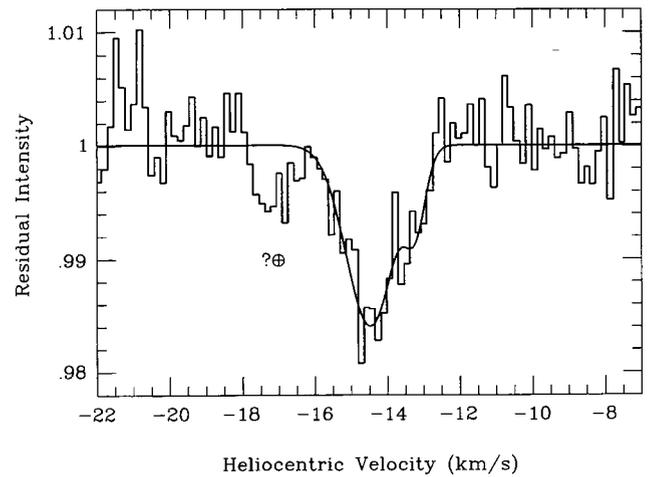


Figure 1. The interstellar $R_1(0)$ line of NH towards ζ Oph. The data points are plotted as histograms; the smooth curve is a two-component least-squares Gaussian fit with the parameters given in Table 1. The apparent feature near -17.5 km s $^{-1}$ does not correspond to any known interstellar absorption component towards this star, and was in any case present in only one night’s data (1997 June 19); it must therefore be either spurious, or possibly a weak transient telluric line.

0.37 ± 0.08 m \AA found for the ζ Per sightline by Meyer & Roth (1991). The corresponding NH column density towards ζ Oph ($8.8 \pm 1.2 \times 10^{11}$ cm $^{-2}$) is a factor of 40 larger than that predicted by the equilibrium gas-phase models of van Dishoeck & Black (1988). This discrepancy supports the conclusion, already drawn from Meyer & Roth’s (1991) results for ζ Per and HD 27778, that there must be an additional route to NH formation in diffuse molecular clouds that has not been included in the gas-phase equilibrium models. However, we note that the observed column density is very similar to that predicted for the ζ Oph sightline on the basis of grain-surface chemistry by Wagenblast & Williams (1996).

We are now in a position to address directly the question as to whether Reaction 1 contributes significantly to NH formation in the ζ Oph molecular cloud(s). The last column of Table 1 gives the rigorous upper limits to the NH kinetic temperature, T_k^{ul} , determined from the observed line widths. On the assumption of a single velocity component, we find $T_k^{\text{ul}} = 1200$ K. Equation (2) then gives $k_1 = 9 \times 10^{-16}$ cm 3 s $^{-1}$, which is negligible compared with other relevant reaction rates. Moreover, the temperature must, in reality, be substantially less than 1200 K, both because some turbulent contribution must be present, and because the total observed line width is almost certainly shared between two discrete absorption components (Table 1). This observation is therefore sufficient to rule out any significant contribution of Reaction 1 to the observed ζ Oph NH column density.

In addition to Reaction 1, other suggestions have been made for the gas-phase production of interstellar NH (cf. the discussion by Meyer & Roth 1991). Assuming that dissociative recombination of NH_2^+ is fast and leads to NH, one possibility is



for which Scott et al. (1997) have recently reported a room temperature measurement of $k_3 = (4.5 \pm 1.8) \times 10^{-10}$ cm 3 s $^{-1}$. However, using the estimated H_3^+ abundance for the ζ Oph sightline (Wagenblast & Williams 1996), it can be shown that Reaction 3 still fails by between one and two orders of magnitude to account for the observed NH column density.

Table 1. Line profile parameters (1σ errors) for the interstellar NH $R_1(0)$ line towards ζ Oph determined from least-squares Gaussian fits under the assumptions of (a) a single velocity component and (b) two velocity components (see text for details). v_{helio} is the heliocentric radial velocity; W_λ is the equivalent width, and N the corresponding column density [for the reasons outlined in section 3.4 of Barlow et al. (1995), these errors include the effect of a 10 per cent zero-level error in addition to the statistical scatter about the fit]; b is the velocity dispersion parameter (after deconvolution of the instrumental resolution); and T_k^{ul} is the upper limit to the kinetic temperature determined from the observed line width (i.e. assuming there is no turbulent contribution to the line profile).

Components	v_{helio} (km s^{-1})	W_λ ($\text{m}\text{\AA}$)	N (cm^{-2})	b (km s^{-1})	T_k^{ul} (K)
(a) One-component fit:	-14.35 ± 0.08	0.36 ± 0.05	$(8.8 \pm 1.2) \times 10^{11}$	1.15 ± 0.12	1200_{-240}^{+260}
(b) Two-component fit:	-14.48 ± 0.09 -13.22 ± 0.15	0.30 ± 0.05 0.05 ± 0.03	$(7.3 \pm 1.2) \times 10^{11}$ $(1.2 \pm 0.7) \times 10^{11}$	0.91 ± 0.15 0.33 ± 0.13	750_{-230}^{+270} 100_{-60}^{+90}

Depending on the N^+ abundance, another possible route to NH may be initiated by the reaction



for which Millar et al. (1997) list a reaction rate of $k_4 = 1.0 \times 10^{-9} \times \exp(-85 \text{ K}/T) \text{ cm}^3 \text{ s}^{-1}$. Although the slight endothermicity of Reaction 4 means that it is unlikely to contribute much to NH formation in the cold ($T_k \approx 30 \text{ K}$: van Dishoeck & Black 1986; Crawford 1997) core(s) of the ζ Oph clouds, a significant contribution from somewhat warmer regions ($T \approx 100 \text{ K}$) cannot be excluded by the present observations. There is some evidence (discussed below) to suggest that the NH probably is located in the cooler, central regions, which would tend to argue against a significant contribution from Reaction 4. Nevertheless, we accept that a full analysis of this reaction (including the effects of H_2 rotational and N^+ fine structure excitation) needs to be performed before it can be definitely excluded.

As is now well-known (e.g. Le Boulton, Gérin & Pérault 1989; Lambert, Sheffer & Crane 1990; Crawford et al. 1994; Sembach, Danks & Lambert 1996; Liszt 1997), the molecular lines forming the ‘main’ (-14 km s^{-1}) velocity component towards ζ Oph are in fact split into two discrete components separated by $1.1 \pm 0.1 \text{ km s}^{-1}$. This velocity structure is observed in the CH, CN, C_2 and CO lines, so it is natural to expect the NH line to be similarly split. Inspection of the observed data does reveal a slight asymmetry in the line profile, and a two-component Gaussian fit yields the parameters given in Table 1. The velocity separation of the two components ($1.26 \pm 0.17 \text{ km s}^{-1}$; 1σ errors) is consistent with that found for the other molecular species towards this star. Of course, each of these components have b -values less than that obtained for the whole absorption feature on the assumption of a single velocity component, and this further undermines the possible contribution of Reaction 1 to the NH column density (for $T = 750 \text{ K}$, the maximum value possible for the broader of the two lines, we find that $k_1 = 1.8 \times 10^{-19} \text{ cm}^3 \text{ s}^{-1}$, which is completely negligible). We should perhaps also note that while the -13.2 km s^{-1} NH component ($b = 0.33 \pm 0.13 \text{ km s}^{-1}$) appears to be somewhat narrower than found for other molecules, consideration of the 1σ errors suggests that this is probably not significant [for example, Crawford et al. (1994) obtained $b = 0.45 \pm 0.10 \text{ km s}^{-1}$ for the corresponding CN component, so the NH and CN velocity dispersion error bars overlap].

It is especially notable that this two-component fit reveals that the least blueshifted component (i.e. that at -13.2 km s^{-1}) is the weaker of the two, just as is found for the CN lines [compare the two-component fit shown in Fig. 1 with the CN $R(0)$ and $R(1)$ lines

shown in fig. 1 of Crawford et al. (1994)]. This apparent correlation of NH with CN further supports the role of grain-surface chemistry in the formation of the former. Indeed, van Dishoeck & Black (1988) have noted that ‘grain surface formation of NH_3 followed by reactions with C^+ could enhance the production of CN in diffuse clouds’, and Wagenblast & Williams (1996) have found that the observed CN column densities towards ζ Oph cannot be reproduced if grain-surface processes leading to the formation of the nitrogen hydrides are neglected.

4 CONCLUSION

We have detected the $R_1(0)$ line of interstellar NH towards ζ Oph for the first time, making this the third interstellar sightline for which this molecule has been detected. The NH column density ($8.8 \pm 1.2 \times 10^{11} \text{ cm}^{-2}$) is more than an order of magnitude higher than that expected on the basis of equilibrium gas-phase models, but is consistent with that expected on the basis of grain-surface chemistry for this line of sight (Wagenblast & Williams 1996).

Our instrumental resolution (0.38 km s^{-1} FWHM) was sufficient for us to resolve the line profile fully, and we found that the line is sufficiently narrow ($b < 1.2 \text{ km s}^{-1}$) to exclude the possibility that the NH has been formed in a hot gas by means of Reaction 1. The observed line profile is consistent with there being two NH velocity components towards ζ Oph (separated by $1.26 \pm 0.17 \text{ km s}^{-1}$), which is consistent with the velocity structure found for other molecules towards this star. The relative strengths of these components mirror those found previously for CN (e.g. Crawford et al. 1994). Both the high NH column density and the apparent correlation with CN support the conclusion that grain-surface reactions dominate the nitrogen chemistry in the ζ Oph molecular clouds.

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