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DETECTION OF INTERSTELLAR NH$_3$ IN THE FAR-INFRARED:
WARM AND DENSE GAS IN ORION-KL

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ABSTRACT

We report the detection of the $(J,K) = a(4,3) \to s(3,3)$ rotation-inversion transition of ammonia at 124.6 μm toward the center of the Orion-KL region. The line is in emission and has a FWHM $\geqslant 30$ km s^{-1}. The far-IR ammonia line emission probably comes mainly from the "hot core", a compact region of warm, very dense gas previously identified by the radio inversion lines of NH$_3$. The $a(4,3) \to s(3,3)$ line is very optically thick ($\tau \sim 10^3$), and since it is seen in emission, radiative excitation of the (4,3) NH$_3$ level by far-IR emission from dust within the source can be ruled out. Radiative excitation via the 10 μm ro-vibrational transitions of NH$_3$ also seems unlikely. Hence, the (4,3) level is probably collisionally excited and the gas in the hot core region is warmer than the dust. Since the far-IR line emission is highly trapped, densities of $\sim 10^7$ cm^{-3} are high enough to explain the observations. Shock heating by the mass outflow from IRc2 may account for the high gas temperatures in the hot core region.

Key words: infrared: sources - infrared: spectra - interstellar: molecules - nebulae: Orion Nebula
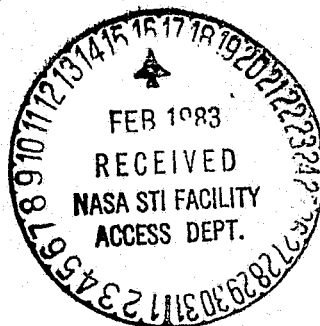
I. INTRODUCTION

Interstellar ammonia was first discovered by its inversion transitions at 1.3 cm (Cheung et al. 1968) and has become an important probe of the physical conditions in interstellar molecular clouds. Recent single dish observations of several of the 1.2 cm inversion transitions toward the center of the Orion-KL region have shown the existence of a component of "hot" ammonia gas in addition to the "spike" NH_3 emission from the quiescent molecular cloud (cf. Barrett et al. 1977; Wilson et al. 1979; Morris et al. 1980; Ziurys et al. 1981). High resolution mapping with the VLA has shown that the hot core NH_3 emission comes from a region of angular diameter about $10''$ (7×10^{16} cm) and temperature 150 to 200 K. The opacities of many of the inversion lines are large ($\tau \geqslant 10$), and peak NH_3 column densities reach 5×10^{18} cm^{-2} (Genzel et al. 1982; Pauls et al. 1983; Palmer et al. 1983). The NH_3 hot core component may come from both streaming gas within and turbulent, swept up gas in interaction with outflow from the luminous infrared source IRc2 (Downes et al. 1981). Morris et al. (1980) have shown that the radio data are consistent with pure collisional excitation of the NH_3 levels if densities are 10^9 cm^{-3}, or with a combination of far-IR radiative excitation and collisional excitation at densities $\sim 10^7$ cm^{-3} (assuming the NH_3 lines are optically thin). Intense emission at 3.5 mm from SO and SiO with characteristics similar to the NH_3 emission and from about the same region has been found by Plambeck et al. (1982) and Wright et al. (1983). Emission lines from vibrationally excited HC_3N, CH_3CN and torsionally excited CH_3OH have been detected in single dish observations of Orion-KL and probably also come from the hot core Orion-KL region (Clark et al. 1976; Loren et al. 1981; Goldsmith et al. 1982; Hollis et al. 1983). In the present paper, we report the first detection of a far-IR emission line of NH_3. The new data are inconsistent with radiative excitation of the (4,3) NH_3 level, and support a collisional model. A hydrogen density of $\sim 10^7$ cm^{-3} is all that is required, as the far-IR NH_3 lines are very optically thick. Collisional excitation at that density may also explain the emission of some of the other molecular lines from the hot core region.

II. OBSERVATIONS AND RESULTS

The data were taken in February, 1982, with the 91.4 cm telescope on board the NASA Kuiper

Airborne Observatory. The spectrometer was a liquid helium cooled, tandem Fabry-Perot described by

Storey, Watson and Townes (1980), with a photoconductive detector. The angular resolution was 44″

(FWHM, or 55″ equivalent disk), and the chopper throw was 4′ at a chopping frequency of 29 Hz. The

total system NEP (noise equivalent power) was 3×10^{-14} W Hz$^{-\frac{1}{2}}$. The $J = 4 \rightarrow 3$, a $\rightarrow$ s * NH$_3$ rota-

tion inversion transitions at 125 μm in Orion-KL were observed at a resolving power $\lambda/\Delta\lambda = 3400$,

resulting in a Lorentzian instrumental profile of FWHM 90 km s^{-1}. Wavelength and velocity calibra-

tion was provided by the NH$_3$ $J = 4 \rightarrow 3$ lines in a gas cell, and an HDO line at 124.9547 μm

(McClatchey et al. 1973), with a precision of about $\pm$10 km s^{-1}. To calibrate the line intensities near

125 μ m, we used the line to continuum ratios and assumed a flux density of 6.0×10^4 Jy for the cen-

tral 60″ of the Orion-KL region at 125 μm (Werner et al. 1976). The $J = 5 \rightarrow 4$, a $\rightarrow$ s transition

region at 100 μm was observed at a resolving power of $\lambda/\Delta\lambda = 4000$, resulting in a velocity resolution

(FWHM) of 75 km s^{-1}. Absolute wavelength calibration was provided by the NH$_3$ lines in a gas cell,

and a telluric H$_2^{18}$O line at 100.2601 μm. The observed 125 μm spectrum of Orion-KL is shown in

Fig. 1, and the main results are as follows:

1) The $(J,K) = a(4,3) \rightarrow s(3,3)$ line (rest wavelength, 124.6474 μm, Urban et al. 1981) is present in

   emission with an LSR velocity centroid of 0 $\pm$10 km s^{-1}, in agreement with the velocity centroids

   of the radio inversion lines ($v_{LSR} = 5$ to 8 km s^{-1}). The observed line width (FWHM) is

   140$\pm$20 km s^{-1}, which is significantly wider than the instrumental resolution (90$\pm$10 km s^{-1}).

   Hence, the intrinsic velocity width of the line in Orion-KL has to be $\geq$30 km s^{-1} if the line

   profile is Lorentzian. For a Gaussian shape the width would be substantially larger than this, and

   may be due to high velocity gas with too small a column density to have been detected in the

   inversion spectrum. The peak line flux ($\sim$5 $\times 10^{-18}$ W cm^{-2} within the pass-band of the spec-

   trometer) is $\sim$6% the intensity of the continuum at the resolution used. The effective line

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*s,a refer to the symmetry of the rotation inversion wave function with respect to reflection about the plane
of the hydrogens. An a $\rightarrow$ s transition is between the upper inversion level in the upper rotational state to
the lower inversion level in the lower rotational state. Each inversion level is further split by hyperfine struc-
ture, which is not resolved in the present measurements.

brightness temperature is 25 to 30 K, assuming that the NH_3 sources fill the beam.

2) The neighboring $(J,K) = (4,2) \rightarrow (3,2)$ line at 124.7957 μm (Urban et al. 1981) is not evident. At $v_{LSR} = 5$ km s^{-1}, the 3 σ upper limit to the line intensity is 2×10^{-18} W cm^{-2}, that is, about 3 times weaker than the (4,3) line. There is a feature at $v_{LSR} = +70$ km s^{-1} which, however, is not interpreted as significant, as its width is less than the instrumental resolution.

3) The $(4,1) \rightarrow (3,1)$ and $(4,0) \rightarrow (3,0)$ transitions (rest wavelengths 124.8835 and 124.9125 μm, Urban et al. 1981) are close to the bottom of a telluric HDO absorption line. The offset to shorter wavelengths of the center of absorption in Fig. 1a from the HDO rest frequency, and what may be additional absorption at the wavelengths corresponding to $v_{LSR} \sim 5$ km s^{-1} is not inconsistent with nonlinearities in the sweep due to distortion of the piezoelectric element in the Fabry-Perot drive.

4) None of the observed $J = 5 \rightarrow 4$ transitions falling within observed wavelengths (K = 3, 100.1046 μm; K = 2, 100.2129 μm; K = 1, 100.2772 μm, Urban et al. 1981) are present to a 3 σ limit greater than 5×10^{-18} W cm^{-2} (in absorption or emission). Only the $(5,3) \rightarrow (4,3)$ transition is not confused by telluric absorption. The $(5,4) \rightarrow (4,4)$ line wavelength was not observed since this line was known to be almost coincident with a strong telluric H_2O line.

It may not be surprising that the $(4,3) \rightarrow (3,3)$ line is stronger than the other transitions, since it is the only observed transition whose upper level has K = J-1. Non-metastable levels with K $\leqslant$ J-2 are expected to require substantially higher densities or a more intense radiation field to be populated equivalently to the K = J - 1 levels.

III. DISCUSSION

In the following, we discuss possible excitation mechanisms for the NH_3 gas and investigate which of the known gas components at the center of Orion-KL may account for the far-IR emission. Table 1 lists the characteristics of the different components. In addition to the hot core and spike seen in the NH_3 inversion lines, there are also the "plateau" and "shocked gas" components in other molecular lines which probably come from gas within and in interaction with the "high velocity" outflow (e.g., Scoville

1981; Beckwith 1981). The spike feature has a linewidth of only a few km s^{-1}, and almost certainly cannot contribute significantly to the far-IR line (apart from lack of excitation, see below).

1. Radiative Excitation

The detection of an emission line immediately rules out that far-IR continuum radiation by dust mixed with the gas or by a far-IR source embedded in the line emitting region can <u>alone</u> account for the excitation of the (4,3) level. Far-infrared radiation by an <u>internal</u> source can only result in an absorption line or in a redistribution of the continuum radiation, but not in a <u>net</u> emission line. Resonant scattering by NH_3 molecules behind or beside a continuum source could conceivably produce the emission line, but there is no observational evidence for a strong far-IR continuum source <u>external</u> to the center of the region (Wynn-Williams et al. 1983). Radiative excitation is also possible via the ro-vibrational bands of NH_3, particularly the ν_2 bands at 10 μm. Radiation from the luminous, compact source IRc2, for example, could be efficiently pumping the 10 μm transitions, since its spectrum peaks at about 8μm. However, detailed considerations, based on present knowledge of the structure of this region, rule out such excitation. To pump the far-IR transitions, the total number of 10 μm photons in a given ro-vibrational line should be greater than or equal to the observed number of photons in the far-IR line ((4,3) -> (3,3): $N_{FIR} = 1.5 \pm 0.5 \times 10^{47}$ s^{-1}). The number of 10 μm photons emitted by IRc2 per ro-vibrational transition is about $N_{IRc2} \approx 5 \times 10^{46} \Delta v_{10}$ (s^{-1}), where Δv_{10} is the FWHM of a ro-vibrational line in units of 10 km s^{-1}. This value is an upper limit for the number of photons available for pumping the 10 μm NH_3 transitions in gas in the emitting region. For such a value, one must assume that the luminosity of IRc2 is $10^5 L_\odot$, that is, equal to the luminosity of the whole Orion-KL region. Furthermore, the number of 10 μm photons coming from IRc2 has to be corrected for emission and absorption of dust along the path to the far-IR emitting region. Recent infrared observations suggest that there is a cavity of low dust density out to a radius of $\sim$4 $\times$ 10^{16} cm from IRc2, which is surrounded by the dense, clumpy hot core region and a region which contains most of the quiescent and the high velocity gas (Werner et al. 1983; Wynn-Williams et al. 1983). The 10μm dust opacities through these regions are substantial ($\tau \sim$3 to >10). Because of the presence of the large cavity

around IRc2, the dust grains in the hot core, spike, plateau and shocked regions absorb near infrared radiation from IRc2, but are too far from that source to reach temperatures so that they significantly emit at 10 μm. The dust in the far-IR emitting region, therefore, cannot contribute significantly to 10 μm pumping. Since the far-infrared NH_3 lines are optically thick, the emission must come from the outer surface of the region, where the 10μm radiation of IRc2 is attenuated by 1 to 4 orders of magnitude. Therefore, the number of 10 μm photons available in the far-IR emitting region, $N_{IRc2} \times e^{-\tau}$, is probably much smaller than N_{FIR}. This probably rules out 10μm radiative pumping.

2) Collisional Excitation: The Far-Infrared Emission Comes from the "Hot Core"

We have used the values of temperature, hydrogen density and total mass within the field of view listed in Table 1, to derive the maximum number of photons from (4,3) -> (3,3) transitions, for the different components of molecular gas in Orion-KL. For the hot core and spike, the column density of NH_3 can be directly estimated from the radio opacities. In other regions, the total number of NH_3 molecules is assumed to be approximately 10^{-7} that of H_2. Table 1 shows that only the hot core gas has sufficient density and numbers of NH_3 molecules to produce the observed (4,3)$\rightarrow$(3,3) emission intensity. The spike region does not produce quite enough photons, and furthermore, its doppler velocity width is much too small to provide the width found in the (4,3)$\rightarrow$(3,3) transition. Other regions would produce far too few collisional excitations. We propose, therefore, that the NH_3 far-IR emission comes from the hot core region, and that the (4,3) level is collisionally excited. As a consequence of the high opacity expected for the (4,3)$-$(3,3) transition from the hot core ($\tau_{FIR} \sim 600$), the far-IR line also has to be broader than the 1.3 cm inversion lines, since amounts of gas at high velocity which are almost transparent at the inversion frequency can be observed in the rotational transition. This is consistent with the observed broadening of the 125 μm line. If it is assumed that all of the 125 μm continuum comes from a source 10" in diameter, the radiation temperature would be about 200 K. An extrapolation of the 10 μm opacity, with opacity proportional to $\alpha \lambda^{-\alpha}$ and $\alpha = 1$ or 2, gives a 125 μm opacity of 1 to 5, so this temperature should also be about equal to that of the dust. However, estimates based on the total luminosity and on the dust emission at 8 to 30 μm give a dust temperature of $\leqslant 140$ K for this 10" region. Some of the continuum radiation almost certainly comes from the

surrounding region and explains this discrepancy. The observed increase in emission at the (4,3)→(3,3) transition of about 6% above the continuum intensity would be due to an effective temperature for the transition of 210 K if the entire emission comes from the 10" region. In any case, for the line to be in emission the rotational temperature must be higher than that of the dust; the above estimates show that the temperature difference is probably a few tens of degrees.

The apparent absence of the (4,2)−(3,2) and (5,3)−(4,3) lines suggests that densities are not high enough to populate the (4,2) and (5,3) levels to the equivalent excitation temperature of the (4,3) transition. Microwave observations indicate that indeed the population of the (4,2) level is less than its thermal equilibrium value. The observed opacity of the (4,3) inversion line averaged over the source is consistent with thermal equilibrium at about 200 K (Genzel et al. 1982, Table 2). However, the observed opacity of the inversion line of (4,2) is between 0.5 and 0.9, about half that expected for LTE. While this is an indication that the (4,2) level is not in LTE, it is the population ratio between (4,2) and (3,2) states to which the far-IR is sensitive, rather than the population itself, since the gas is optically thick at 125 μm. For the (4,2) - (3,2) transition to show no emission at all, or perhaps an absorption of the dust continuum, its effective temperature must be reduced at least to 200 K and possibly as low as 140 K. The latter, more stringent requirement implies that relative populations are $(n_{4,2} - n_{3,2})/ (n_{4,3} - n_{3,3}) \leq 0.77$. Thus, a 23% change in relative populations between upper and lower states due to a smaller ratio between the collisional and radiative rates would explain the nondetection of emission from the (4,2)-(3,2) transition. This smaller ratio would have such an effect, of course, only if the excitation and radiative rates are comparable. For an optically thin medium, the radiative transition rates for the (4,3) and (4,2) states are proportional to $(J^2 - K^2)$ through the rotational matrix elements. This gives a ratio for the two radiative rates of 0.58, with the (4,3)−(3,3) transition more easily brought into temperature equilibrium by collisions than (4,2)−(3,2). Since the medium in fact has substantial optical depth, the smaller optical depth of the (4,2)−(3,2) transition further enhances the difference in excitation between it and the (4,3)−(3,3) transition. Table 2 gives parameters for several non-metastable NH_3 levels. The values of τ_{FIR} and $\beta (\tau_{FIR})$ are derived from the observed opacities of the 1.3 cm inversion lines. Values for collisional cross sections between He

and NH_3 were taken from Green (1982), and were multiplied by 2.5 to account for the faster thermal speed of H_2 over He and for enhanced collisional cross sections of H_2 molecules which are in rotational states $J > 0$. The quantities $n_{0.5}^{crit}$ and $\beta \times n_{0.5}^{crit}$ listed in Table 2 are the densities at which the population is half of that at LTE without and with trapping corrections. $\beta \times n_{0.9}^{crit}$ is the density at which the population is 0.9 that at LTE, with trapping included. Table 2 shows that because of the large trapping corrections, densities of $\sim 10^7 \, cm^{-3}$ are sufficient to account for the population of the (4,3) and (4,2) levels. Higher densities may be necessary to also account for the observed radio brightness temperatures of higher excitation lines, such as (7,6) and (10,9). Such high densities, however, may be inconsistent with the weakness of the (4,2) radio and infrared lines. A possible solution might be a mixture of radiative and collisional excitation. At hydrogen densities of $\sim 10^7 \, cm^{-3}$, the NH_3 abundance in the hot core is $\sim 10^{-6}$ to 10^{-5}. A possible mechanism to heat the 1 to 10 $M_\odot$ of gas in the hot core region above the dust temperature may be the mechanical (shock) heating by the mass outflow from IRc2. The mechanical luminosity of this source is estimated to lie between 10 and 1000 $L_\odot$, which is sufficient to account for the total line cooling from ammonia and other molecules.

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Figure Captions

Fig. 1. 125 μm spectrum toward the core of the Orion-KL region, with a 44" beam FWHM. The spectral resolution is a Lorentzian of FWHM 90±10 km s^{-1}.

Lower (a): Observed spectrum, with arrows marking the positions of the a(4,K)→s(3,K) rotational inversion transitions of NH$_3$ toward Orion (v_{LSR} = + 5 km s^{-1}). Also marked is a telluric HDO line on the left side of the spectrum. The K = 0 and K = 1 NH$_3$ lines are close to the bottom of this absorption feature. There is a second HDO absorption line at 124.3008 μm which causes the downward slope on the right side of the spectrum.

Upper (b): The same spectrum, but smoothed and with Lorentzians fitted to the HDO lines and then divided out. The positions of the K = 2 and K = 3 NH$_3$ lines are indicated, together with the appropriate velocity scales. A Lorentzian fit to the (4,3)→(3,3) transition (thin line) gives an LSR velocity centroid of 0±10 km s^{-1}, and a FWHM of 140±20 km s^{-1}, that is, significantly wider than the resolution. The K = 2 line is at least three times weaker than the K = 3 line. The positive bump at LSR + 70 km s^{-1} is probably narrower than our resolution, and therefore is not interpreted as real.

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TABLE 1

Far-Infrared NH_3 Line Emission/Absorption and the Kinematic Components in Orion-KL

	"spike"	"hot core"	"plateau"	"shocked gas"
Size of Region (arc sec)	$\geq 1'$	10"	40"	1'
Velocity Width (km s^{-1})	2.5 (FWHM)	10 (FWHM)* / 30 to 40	60 (FWHM) / 150*	60 (FWHM) / 120*
Temperature (K)	70	200 ± 50	100	1000
Hydrogen Density (cm^{-3})	10^6	$\geq 10^7$	10^5 to 10^6	1 to 3×10^6
Hydrogen Column Density (cm^{-2})	5×10^{23}	5 to 20 10^{23}	1 to 5×10^{22}	3 to 10×10^{21}
Total Mass ($M_\odot$)	100 to 200	1 to 10	1 to 10	0.5 to 3
RADIO τ_{NH_3} (4,3)	0.1	8 ± 2	-	-
FIR τ_{NH_3} (4,3)	2	600	$\sim 1*(\frac{N_{H_2}}{3 \times 10^{22}})*(\frac{\chi NH_3}{10^{-7}})$	$\sim 0.1*(\frac{N_{H_2}}{5 \times 10^{21}})*(\frac{\chi NH_3}{10^{-7}})$
Max. FIR photons/sec †	$10^{46.5}$	$10^{48.3}$	$10^{44.7}$	10^{46}

† The maximum FIR photons/sec which can be emitted or absorbed is taken to be $N_{NH_3} n_H \sigma v \exp(-h\nu/kT)$ where N_{NH_3} is the number of NH_3 molecules in the J = 3, K = 3 state if $\chi NH_3 = 10^{-7}$, σv is assumed to be 10^{-10} cm^3 s^{-1}, and $h\nu$ corresponds to the rotational energy difference. This is an upper limit to the number of photons emitted if the line has substantial opacity.

* Full width at zero power.

TABLE 2

Collisional Excitation of the NH_3 Levels

Upper Level	τ^{RAD} [a]	b_u [b]	τ^{FIR}	$\beta(\tau^{FIR})$ [c]	$n_{0.5}^{crit}$ [d]	$\beta \times n_{0.5}^{crit}$ [e]	$\beta \times n_{0.9}^{crit}$ [f]
$(J,K)=(4,3)$	8 ± 2	0.9 ± 0.2	600	6×10^{-4}	10^9	6×10^5	10^7
$(4,2)$	0.7 ± 0.2	0.4 ± 0.3	100	3×10^{-3}	2×10^9	6×10^6	6×10^7
$(7,6)$	0.7 ± 0.2	0.3 ± 0.2	30	10^{-2}	5×10^9	5×10^7	5×10^8
$(10,9)$	0.15 ± 0.08	0.4 ± 0.1	3	10^{-1}	10^{10}	10^9	10^{10}

[a] The opacities of the 1.3 cm inversion lines are estimated from the single dish observations by Morris et al. 1980, Zuckerman et al. 1981, Ziurys et al. 1981, and represent an average value across the source. For the (4,2), (7,6) and (10,9) lines, the opacities are obtained by comparing to the line temperature of the optically thick (4,3) line.

[b] The departure coefficients $b = n_{upper} / n_{upper}$ (LTE) are estimated from the observed opacities and the opacities extrapolated from $\tau(3,3) = 20$ at $T = 200$ K.

[c] The escape probability for far-infrared line radiation: $\beta(\tau) = \dfrac{1 - e^{-3\tau}}{3\tau}$. The value used is a compromise between an expanding source and Gaussian turbulence (de Jong et al. 1975, 1980).

[d] $n_{0.5}^{crit}$ is the density where $b = \frac{1}{2}$ without trapping of FIR radiation: $(b = n_{upper} / n_{upper(LTE)} = (1 + A_{u1} \beta (\tau^{FIR}) / C_{ul})^{-1}$, where A_{u1} is the Einstein coefficient and C_{ul} the collisional rate between upper and lower level).

[e] $\beta \times n_{0.5}^{crit}$ is the density where $b = \frac{1}{2}$ if trapping is taken into account.

[f] $\beta \times n_{0.9}^{crit}$ is the density where $b = 0.9$ if trapping is taken into account.

Orion - KL
44″ beam

NH$_3$ J = 4 → 3 a → s

Telluric line removed
(HDO J$_{K^-K^+}$ = 5$_{3,3}$ ← 5$_{2,4}$)

K = 3

K = 2

v$_{LSR}$ (km s^{-1})

+100   0   -100   +100   0   -100

Flux   (10^{-17} W cm^{-2} per resolution element)

K = 0

K = 1

K = 2

K = 3

Resolution

90 km s^{-1}

(10^{-17} W cm^{-2} per resolution element)

Wavelength (μm)

125.0   124.9   124.8   124.7   124.6