THE ASTROPHYSICAL JOURNAL, 177:514–545, 1972 October 15

VIBRATION-ROTATION BANDS OF NH IN THE SPECTRUM OF ALPHA ORIONIS

D. L. LAMBERT
McDonald Observatory and Department of Astronomy, University of Texas, Austin

AND

R. BEER
Space Sciences Division, Jet Propulsion Laboratory, California Institute of Technology
Received 1972 March 20; revised 1972 May 10

ABSTRACT

Several lines of the 1–0 and 2–1 fundamental vibration-rotation bands of the NH radical are identified on a high-resolution spectrum of the supergiant α Orionis.

I. INTRODUCTION

A high-resolution spectrum of the supergiant α Ori in the atmospheric window between 3 and 4 μ was obtained recently, and it showed strong absorption lines which were identified with the fundamental vibration-rotation bands of the hydroxyl (OH) radical (Beer *et al.* 1972). Since all molecules composed of the abundant light elements (H, C, N, O) possess fundamental vibration-rotation bands in or near this window, a thorough search promises to provide identifications for the unidentified stellar lines listed by Beer *et al.* A search for the vibration-rotation bands of the imidyl radical NH is described here.

An electronic transition of the NH radical has prominent compact bandheads in the ultraviolet—λ3360 0–0 and λ3370 1–1—which have been detected in K and M stars (Schmitt 1969). Although a specific identification for α Ori could not be traced, these NH bands are predicted to be recognizable in the ultraviolet spectrum. Unfortunately, the spectrum is so rich in absorption features that an accurate estimate of the NH abundance will not be possible.

II. THE NH VIBRATION-ROTATION SPECTRUM

A laboratory analysis of the fundamental bands is not available. Hence, line frequencies must be derived from studies of the ultraviolet ($A\,^3\Pi_i$–$X\,^3\Sigma^-$) electronic transition for which measurements on the vibrational bands 0–0, 1–1, 1–0, 0–1, 2–1, and 1–2 were variously analyzed by Funke (1935, 1936), Dixon (1959), Murai and Shimauchi (1966) and Malicet, Brion, and Guenebaut (1970). The vibration-rotation spectrum may be calculated from the derived molecular constants for $X\,^3\Sigma^-$ or from combination relations; for example, the *R*-branch of the 1–0 band is given by the relation

$$R(J) = Q_\alpha(J) - P_\beta(J+1) + \Delta(v', J)\,,$$

where α and β denote the bands v'–0 and v'–1, respectively, in the A–X system. The energy difference $\Delta(v', J)$ between the Λ-doublet states in $A\,^3\Pi_i$ may be calculated from the A–X observations by a standard combination relation (see, for example, Dixon 1959). The pairs of bands 0–0, 1–0 and 1–1, 1–2 may be used to provide the 1–0 and 2–1 vibration rotation bands in the $X\,^3\Sigma^-$ ground state.

Unfortunately, close examination of the A–X analyses reveals a discrepancy between the 1–0 band observations reported by Dixon and Malicet *et al.*; the mean difference is $\Delta\bar{\nu} = \bar{\nu}(D) - \bar{\nu}(\mathrm{MBG}) = 0.25\ \mathrm{cm}^{-1}$ from 45 lines common to their lists. This discrepancy is not remarked upon by Malicet *et al.* Since Dixon states that the ground-state combination relations for the 1–0 and 0–0 bands coincide to within the experimental error of $\pm 0.03\ \mathrm{cm}^{-1}$, the source of the discrepancy is presumably in the analysis by Malicet *et al.* No direct evidence is available on possible errors affecting their measurements for other bands but they must be considered suspect. Hence, the use of combination relations to calculate the vibration-rotation spectrum is restricted to the 1–0 band from the 1–1 and 1–0 A–X bands. These predictions were in good agreement with predictions obtained directly from the molecular constants for $X\,^3\Sigma^-$ given by Murai and Shimauchi. The latter results were adopted for the search.

Predictions for the 2–1 band from the 1–1 and 1–2 bands in the A–X system are subject to an unknown error arising from the discovery of the $0.25\ \mathrm{cm}^{-1}$ error in the 1–0 band wavenumbers reported by Malicet *et al.* Unfortunately, Malicet *et al.* are the only authors to report observations of the 1–2 band. On the assumption that the error is a constant affecting equally all lines in a band,[1] the rotational constants are probably derived without error. Therefore, a compromise was adopted; the 2–1 vibration-rotation transitions were predicted from the molecular constants for $v = 2$ given by Malicet *et al.* and for $v = 1$ from Murai and Shimauchi. The results for quantum numbers $N \leq 10$ are consistent with the combination relation predictions and an error of about $0.3\ \mathrm{cm}^{-1}$ in the 1–2 A–X band positions. Beyond $N = 11$, the two methods give more widely differing results, and therefore the search for NH lines was restricted to $N \leq 10$.

III. A SEARCH FOR NH IN ALPHA ORIONIS

The 1–0 and 2–1 bands have origins near 3125 and $2970\ \mathrm{cm}^{-1}$, respectively. In α Ori, the most intense absorption lines are expected to occur at $N \approx 10$. The 1–0 R-branch to $N = 12$ lies within the region of the α Ori spectrum. The head is at $3461\ \mathrm{cm}^{-1}$ and beyond the short-wavelength limit of the spectrum. Returning R-branch lines with $N \geq 26$ may appear in the spectrum. The entire R-branch of the 2–1 band is accessible with a band head near $3281\ \mathrm{cm}^{-1}$ obscured by strong telluric absorption. The P-branches are on the long-wavelength side of the origins and in regions with a lower density of telluric absorption lines, but the signal-to-noise ratio in the α Ori spectrum is unfortunately less than for the region of the R-branches.

All stellar absorption features considered coincident with NH predicted line frequencies are presented in table 1. NH lines not listed there are either masked by stronger telluric or stellar OH lines or located in a region where the position of the continuum level is uncertain to such an extent that an NH line with an equivalent width $W_{\bar{\nu}} < 0.05\ \mathrm{cm}^{-1}$ cannot be excluded. Three of the newly identified stellar lines (see fig. 1) are listed in the table of unidentified lines given by Beer *et al.* (1972). The identification of NH is considered to be most probable, but confirmation should be sought when spectra with improved signal-to-noise ratio are available for $\bar{\nu} < 2700\ \mathrm{cm}^{-1}$. An effective search for P-branch lines will then be possible.

IV. OBSERVED AND PREDICTED NH INTENSITIES FOR ALPHA ORIONIS

A detailed interpretation of the NH equivalent widths is withheld pending a laboratory or an astrophysical determination of the vibration-rotation line strengths. An approximate analysis is presented here.

[1] Examination of the 1–0 band shows that the discrepancy between Dixon and Malicet *et al.* is systematically smaller for the stronger Q-branch lines: $\Delta\nu = +0.15\ \mathrm{cm}^{-1}$ and $\Delta\nu = +0.25$ for all lines in the band. Hence, the error is possibly intensity dependent.

TABLE 1

NH LINES IN THE SPECTRUM OF α ORIONIS

Band	Line	$\tilde{\nu}$* pred (cm^{-1})	$\tilde{\nu}_\alpha$† (cm^{-1})	$W\tilde{\nu}$ (cm^{-1})	Comments
1–0..............	$R_1(4)$	3268.76			Blended with OH
	R_2	3268.81	8.53	0.07	1–0 $P_{12}(6)$.
	R_3	3268.84			
	$R_1(6)$	3315.93			‡
	R_2	3315.96	5.85	0.05	
	R_3	3315.96			
	$R_1(11)$	3405.87			‡. Possibly blended with
	R_2	3405.87	5.74	0.06	$R(26)$ at a mean posi-
	R_3	3405.83			tion of 3405.53.
	$P_1(6)$	2911.52			Superposed on a weak
	P_2	2911.44	11.50:	0.03:	telluric line.
	P_3	2911.32			
2–1..............	$R_1(9)$	3205.02			‡
	R_2	3205.05	05.08	0.05	
	R_3	3205.06			

NOTE.—A colon following a number denotes an uncertain value.

* See text.

† Includes a 0.18 cm^{-1} correction for the stellar radial velocity.

‡ This line was included in a list of unidentified lines given by Beer *et al.* (1972).

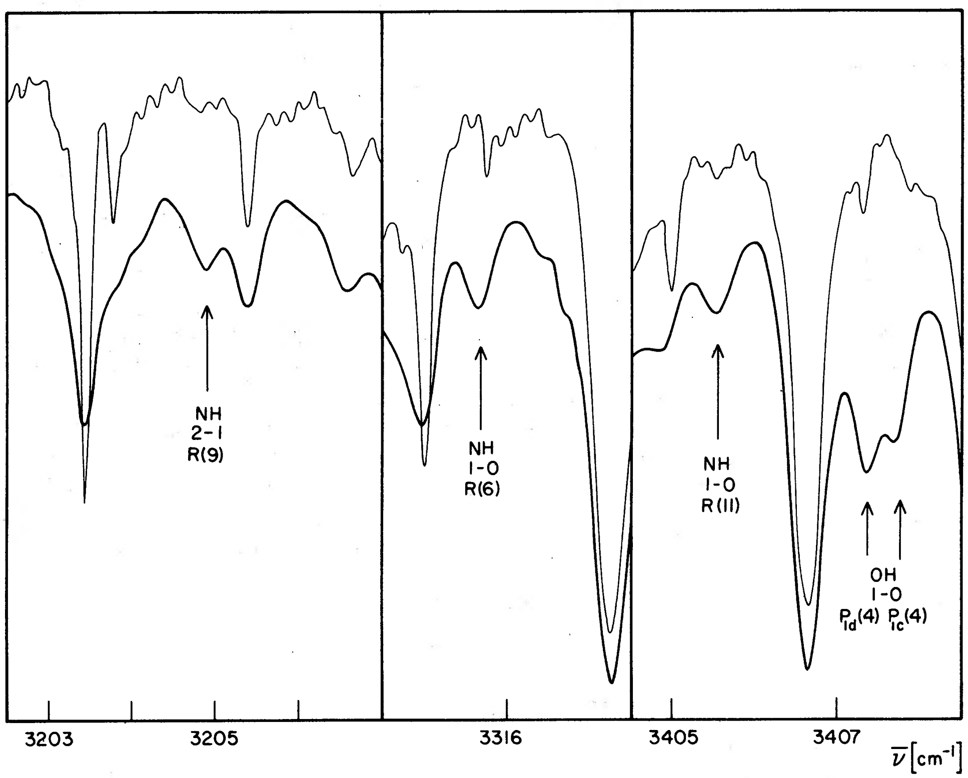

FIG. 1.—Portions of the spectra of α Orionis (*thick solid line*, resolution 0.29 cm^{-1}) and the Sun (*thin solid line*, resolution 0.07 cm^{-1}). The solar spectrum has been displaced upward relative to the stellar spectrum. Three NH lines and one OH doublet are identified.

The observed ratio $W_{\tilde{\nu}}(OH)/W_{\tilde{\nu}}(NH) = 4$ for lines near the intensity maximum. The NH lines are unresolved triplets, but the OH line intensity refers to a resolved component of a Λ-doublet. If this is taken into account and if the small differences in the molecular partition functions, etc., are ignored, the observed ratio converts to a column density ratio

$$(NL)_{NH}/(NL)_{OH} \approx 0.08 A_{OH}{}^{1-0}/A_{NH}{}^{1-0} ,$$

where A^{1-0} is the transition probability for the 1–0 vibration-rotation band.

Laboratory measurements of the NH vibration-rotation band transition probabilities or intensities have not been reported in the literature. A comparison of theoretical calculations for the ground states of NH (Kouba and Öhrn 1970) and OH (Cade 1967) indicates that the gradient of electric dipole moment is similar for the two molecules; the transition probability is proportional to the square of the dipole-moment gradient. High accuracy is not anticipated for these theoretical calculations, so a detailed analysis is unwarranted. On the assumption that the NH and OH transition probabilities are approximately equal, the observed column density ratio is $(NL)_{NH}/(NL)_{OH} \approx 0.08$.

Column densities for molecules in cool stellar atmospheres were predicted by Goon and Auman (1970). Solar abundances were assumed: $C/H = 5.3 \times 10^{-4}$, $N/H = 9.6 \times 10^{-5}$, and $O/H = 9.1 \times 10^{-4}$. The ratios estimated from their results are given in table 2 for three supergiant models (surface gravity: $\log g = 0.0$).

Beer *et al.* (1972) suggest that the effective temperature T_{eff} is unlikely to be less than about 3500° K because the predicted H_2O absorption lines are not seen in the observed spectrum. Faÿ (1972) proposes that the observed flux distribution may be explained by a model with effective temperature $T_{eff} = 3800°$ K and a surface gravity $\log g = 0.0$. This corresponds to $(NL)_{NH}/(NL)_{OH} \approx 0.016$. The temperature dependence of the ratio is marked. The ratio increases with decreasing surface gravity.

Another significant factor has to be taken into account. The spectrum strongly suggests that the atmosphere has been processed through or contaminated with the products of the CNO thermonuclear cycle; the evidence is the low $^{12}C/^{13}C$ (Spinrad *et al.* 1971) and C/O (Beer *et al.* 1972) abundance ratios. A probable effect of the CNO cycle is the conversion of the initial supply of carbon into nitrogen via the CN bi-cycle. If the temperature is sufficiently high, some oxygen may also be processed to nitrogen. With the assumption that the CN bi-cycle has operated to near completion, the abundances should be $C/H \leq 10^{-4}$, $N/H \approx 6 \times 10^{-4}$, and $O/H \approx 9.1 \times 10^{-4}$. Then, the model $T_{eff} = 3800°$ K and $\log g = 0.0$ provides a ratio $(NL)_{NH}/(NL)_{OH} \approx 0.025$. This is within a factor of 3 of the observed ratio. An additional increase in this ratio would result from a partial processing of the initial oxygen supply to nitrogen. Abundance studies of young hot stars show that their N abundance probably exceeds the solar value (Scholz 1972). Since the initial composition of α Ori may have been similar, an additional increase in the predicted NH/OH ratio could be anticipated.

In conclusion, comparison with the predicted column density ratio suggests that the observations may be understood in terms of an atmosphere with $T_{eff} = 3800°$ K and $\log g = 0.0$ and a composition reflecting the operation of the CN bi-cycle. A more

TABLE 2

PREDICTED COLUMN DENSITIES FOR SUPERGIANT ATMOSPHERES OF SOLAR COMPOSITION

T_{eff}(°K)	$\log g$	$(NL)_{NH}/(NL)_{OH}$
3000.........	0.0	0.00013
3500.........	0.0	0.004
4000.........	0.0	0.05

detailed analysis including an improved determination of the effective temperature will be needed to establish whether the NH/OH ratio requires that the initial oxygen supply be partly processed to nitrogen. In particular, a measurement of the transition probabilities A_{NH}^{1-0} and A_{NH}^{2-1} will be required. This measurement of the NH transition probabilities may be possible from observation of the fundamental bands in sunspot spectra; calculations (Lambert and Mallia 1972) suggest that the NH lines should be detectable provided that the NH and OH transition probabilities are of similar magnitude. The calculations show that the NH lines are undetectable in the photospheric spectrum.

This research has been supported in part by the National Science Foundation under grant GP-32322X. This paper presents in part the results of one phase of research carried out at the Jet Propulsion Laboratory, California Institute of Technology, under contract NAS 7-100, sponsored by the National Aeronautics and Space Administration.

REFERENCES

Beer, R., Hutchison, R., Norton, R. B., and Lambert, D. L. 1972, *Ap. J.*, **172**, 89.
Cade, P. E. 1967, *J. Chem. Phys.*, **47**, 2390.
Dixon, R. N. 1959, *Canadian J. Phys.*, **37**, 1171.
Faÿ, T. D. 1972, *Bull. A.A.S.* (in press).
Funke, G. 1935, *Zs. f. Phys.* **96**, 787.
———. 1936, *ibid.*, **101**, 104.
Goon, G., and Auman, J. R. 1970, *Ap. J.*, **161**, 533.
Kouba, J., and Öhrn, Y. 1970, *J. Chem. Phys.*, **52**, 5387.
Lambert, D. L., and Mallia, E. A. 1972, in preparation.
Malicet, J., Brion, J., and Guenebaut, H. 1970, *J. Chem. Phys.*, **67**, 25.
Murai, T., and Shimauchi, M. 1966, *Science of Light*, **15**, 48.
Schmitt, J. L. 1969, *Pub. A.S.P.*, **81**, 657.
Scholz, M. 1972, *Vistas Astr.*, in press.
Spinrad, H., Kaplan, L. D., Connes, P., Connes, J., Kunde, V. G., and Maillard, J. P. 1971, *Proceedings of the Conference on Late-Type Stars*, ed. G. W. Lockwood and H. M. Dyck (Tucson: Kitt Peak National Observatory; Contribution No. 54).