

## OBSERVATIONS OF THE 4 MICRON FUNDAMENTAL BAND OF $\text{H}_3^+$ IN JUPITER

T. OKA

Department of Astronomy and Astrophysics and Department of Chemistry, University of Chicago

AND

T. R. GEBALLE

Joint Astronomy Centre, Hilo

Received 1989 October 24; accepted 1989 December 14

### ABSTRACT

Emission lines of the  $\nu_2$  fundamental vibration-rotation band of  $\text{H}_3^+$  have been detected in the northern and southern polar ionospheres of Jupiter. The recently discovered  $2\ \mu\text{m}$  overtone band of  $\text{H}_3^+$  is currently absent from the spectra of Jupiter's poles, as are lines of several other "hot bands" of  $\text{H}_3^+$  and  $2\ \mu\text{m}$  lines of  $\text{H}_2$ , implying that physical conditions in Jupiter's auroral regions have changed considerably within a period of  $\sim 1$  yr. The present observations provide added evidence for a large abundance of  $\text{H}_3^+$  in localized zones of the Jovian atmosphere.

*Subject headings:* infrared: spectra — line identifications — molecular processes — planets: Jupiter

### I. INTRODUCTION

The recent detection of the molecule  $\text{H}_3^+$  in the Jovian auroral regions (Maillard and Drossart 1989; Trafton, Lester, and Thompson 1989; Drossart *et al.* 1989), via its  $2\ \mu\text{m}$  overtone ( $\nu_2 = 2 \rightarrow 0$ ) band, is the first instance in which this hydrogenic species, which is thought to be basic to the production of many complex molecules in the interstellar medium, has been detected by astronomical observations. Previously, some searches for  $\text{H}_3^+$  in dense molecular clouds have been made (e.g., Geballe and Oka 1989). The above measurements of  $\text{H}_3^+$  have provided definitive evidence for high ion concentration, high temperature, and localization of the ionized regions near the poles of Jupiter.

In this *Letter* we report the detection of the  $4\ \mu\text{m}$  fundamental  $\nu_2$  band of  $\text{H}_3^+$  in Jupiter. The relation between the overtone band, the fundamental band, and some of the hot bands which are discussed in this *Letter* is shown in Figure 1. The detailed rotational structure of the fundamental  $\nu_2$  band has been well characterized in the laboratory (Oka 1980, 1981; Watson *et al.* 1984; Majewski *et al.* 1987), based on the *ab initio* calculations of Carney and Porter (1976, 1980). The rotational structure of the hot bands,  $2\nu_2(2) \rightarrow \nu_2$ ,  $2\nu_2(0) \rightarrow \nu_2$ ,  $\nu_1 + \nu_2 \rightarrow \nu_1$  (Bawendi, Rehffuss, and Oka 1989), and overtone band,  $2\nu_2 \rightarrow 0$  (Majewski *et al.* 1989; Xu, Gabrys, and Oka 1989) have been determined by recent laboratory spectroscopy aided by the first principle calculations of Miller and Tennyson (1987, 1988, 1989).

The vibrational Einstein spontaneous emission rates calculated by Carney and Porter (1976) are shown in Figure 1. These rates imply that if spontaneous emission of the overtone band is detectable, as it was in Jupiter during 1987–1988, then there are four vibrational transitions which should produce detectable and comparable numbers of photons in the  $4\ \mu\text{m}$  region.

### II. OBSERVATIONS

Spectra of Jupiter were obtained at the United Kingdom Infrared Telescope (UKIRT) on Mauna Kea in two sessions in 1989, during the mornings of September 6 and 9–10 and during September 14–19. UKIRT's cooled grating spectrometer

(CGS2) was used to obtain medium-resolution spectra in the  $1.95\text{--}2.55\ \mu\text{m}$  ( $600 < R < 900$ ) and  $2.85\text{--}4.15\ \mu\text{m}$  ( $350 < R < 550$ ) intervals during the first session. During the second session, CGS2 was employed in series with Fabry-Perot interferometers to obtain spectra of resolving power  $\sim 12,000$  near  $2,093\ \mu\text{m}$  and  $2.31\ \mu\text{m}$  and  $\sim 8000$  in various spectral intervals near  $4\ \mu\text{m}$ . The field of view was a  $5''$  circular aperture, used with a chopper throw and nods of  $45''$  EW. On each morning the seeing was better than  $1''$  until about 8:00 A.M., when it degraded to several arcseconds; pointing was accurate to  $\pm 1''$  until that time and  $2''\text{--}3''$  thereafter. Flux calibration was achieved through observations of BS 2088, BS 1708, and BS 1713. Wavelength calibration was obtained from absorption lines of telluric  $\text{N}_2\text{O}$  and lines of Ar in a discharge lamp.

As far as the spectrum of  $\text{H}_3^+$  is concerned, all meaningful detections were obtained from the higher resolution spectroscopy used in the second session. In addition to providing some significant upper limits to  $2\ \mu\text{m}$  lines of  $\text{H}_3^+$  and  $\text{H}_2$ , the lower resolution spectroscopy has produced interesting overview  $2\text{--}4\ \mu\text{m}$  spectra of Jupiter in various locations. These will be reported in a separate paper.

### III. RESULTS

The frequencies, intensities, and identifications of 10  $\text{H}_3^+$  lines from the  $\nu_2$  fundamental band, which were detected in Jupiter, are listed in Table 1. All of these lines have been measured in the laboratory. Examples of observed lines are shown in Figures 2–4; note that the Jovian spectrum near  $4\ \mu\text{m}$  was Doppler-shifted by  $+0.25\ \text{cm}^{-1}$  during these observations. In Jupiter the  $\text{H}_3^+$  emission spectrum near  $4\ \mu\text{m}$  is superposed on a continuum with strong and broad absorption features. The  $(1, 0, -1) \rightarrow (1, 0)$  transition shown in Figure 2 is the strongest line of  $\text{H}_3^+$  that we detected and is very useful for mapping. The continuum from Jupiter near this line is totally absorbed, except at  $\sim 2533\ \text{cm}^{-1}$ , clearly demonstrating that the emitting  $\text{H}_3^+$  exists at high altitude. Figure 3 shows a quartet of  $\text{H}_3^+$  lines corresponding to the  $(5, K, -1) \rightarrow (5, K)$  transitions with  $K = 0, 1, 2, 3$ . The greater intensities of the  $K = 0$  and  $K = 3$  lines reflect the ratio of ortho ( $I = 3/2$ ) to para ( $I = 1/2$ ) spin

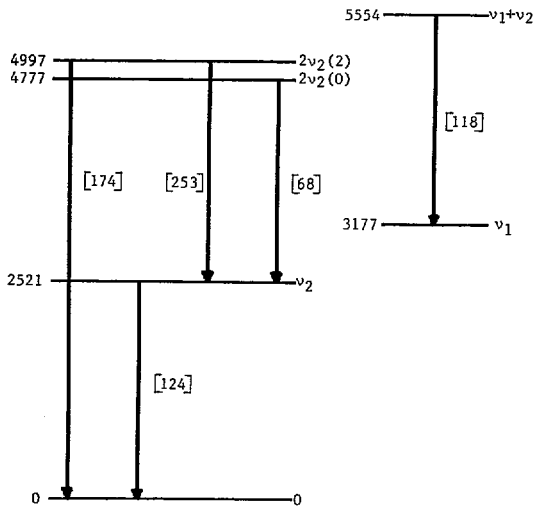


FIG. 1.—Diagram of the lower vibrational levels of  $H_3^+$  showing allowed vibrational transitions. Energies of levels are in  $cm^{-1}$ ; numbers in brackets are Einstein  $A$ -coefficients in  $s^{-1}$ .

statistical weights of 4 to 2. The weak feature at  $2468.0\text{ cm}^{-1}$  coincides with  $H_3^+(5, 4, -1) \rightarrow (5, 4)$ ; however, the Doppler-shifted position of  $H\text{ I Br}\alpha$  (rest frequency of  $2467.76\text{ cm}^{-1}$ ) also is close. The somewhat larger width of this feature may be due to a blend of these two lines; further spectroscopy at higher resolution is required to settle this question. Figure 4 shows the doublet  $(3, K, -1) \rightarrow (3, K)$  with  $K = 0, 1$ , which is superposed on the shoulder of a strong absorption feature.

The most remarkable outcome of these observations is the complete absence of emission lines starting from excited vibrational states above  $v_2 = 1$ . In particular, we did not detect the strongest overtone emission line,  $(7, 9, +2) \rightarrow (6, 6)$  at  $4777.226$

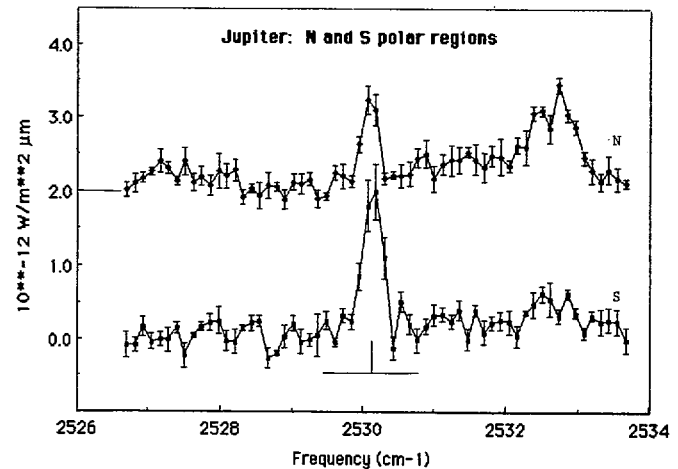


FIG. 2.—Spectra of the  $1, 0, -1 \rightarrow 1, 0$  line of  $H_3^+$  at  $2530\text{ cm}^{-1}$  in the polar regions of Jupiter, observed at longitudes of  $160^\circ$  and  $181^\circ$ . Refer to Table 1 for details. The bump at  $2533\text{ cm}^{-1}$  is believed to be continuum radiation in a gap between strong Jovian absorption lines.

$cm^{-1}$ , seen by Trafton, Lester, and Thompson (1989) and Drossart *et al.* (1989). We estimate that the surface brightness in this line was at least 10 times lower than at the times of the above observations. Other overtone lines detected by the above observers were also not detected in the present observations. The absence of lines from highly excited vibrational states is further confirmed by the failure to detect hot band spectral lines in the  $4\text{ }\mu\text{m}$  region. In addition, the  $H_2\text{ S}(1)$  line at  $2.12\text{ }\mu\text{m}$  was also searched for at a number of locations and not detected; our limiting surface brightnesses for this line are typically 3 times less than those seen by Trafton, Lester, and Thompson (1989) and Drossart *et al.* (1989). Thus, the present

TABLE 1  
OBSERVED  $v_2 \rightarrow 0$  LINES OF  $H_3^+$  DURING 1989 SEPTEMBER 17–19

Transition $J', G', U' \rightarrow J, K$	Frequency ( $cm^{-1}$ laboratory)	Intensity ( $10^{-16}\text{ W m}^{-2}, 5''\text{ beam}$ )	Location	Longitude (System III)
$5, 4, -1 \rightarrow 5, 4 (+\text{ Br}\alpha?)$	2467.553	$3.0 \pm 1.0$	$3^\circ\text{N}$ of S limb	$338^\circ$
$5, 0, -1 \rightarrow 5, 0$	2471.923	$14. \pm 2.$	$3^\circ\text{S}$ of N limb	12
		$9.1 \pm 1.5$	S limb	35
$5, 1, -1 \rightarrow 5, 1$	2472.325	$5.5 \pm 1.5$	$3^\circ\text{S}$ of N limb	12
		$4.0 \pm 1.5$	S limb	35
$5, 3, -1 \rightarrow 5, 3$	2472.846	$12. \pm 2.$	$3^\circ\text{S}$ of N limb	12
		$8.0 \pm 1.5$	S limb	35
$5, 2, -1 \rightarrow 5, 2$	2473.238	$6.5 \pm 1.5$	$3^\circ\text{S}$ of N limb	12
		$4.0 \pm 1.5$	S limb	35
$3, 1, -1 \rightarrow 3, 1$	2508.131	$4.2 \pm 1.0$	$3^\circ\text{N}$ of S limb	15
		$3.2 \pm 1.0$	$3^\circ\text{N}$ of S limb	118
$3, 0, -1 \rightarrow 3, 0$	2509.075	$6.0 \pm 1.0$	$3^\circ\text{N}$ of S limb	15
		$4.8 \pm 1.0$	$3^\circ\text{N}$ of S limb	118
$2, 1, -1 \rightarrow 2, 1$	2518.207	$3.5 \pm 1.0$	$3^\circ\text{N}$ of S limb	118
		$3.8 \pm 1.0$	$3^\circ\text{N}$ of S limb	136
$1, 0, -1 \rightarrow 1, 0$	2529.724	$9.3 \pm 1.0$	$3^\circ\text{N}$ of S limb	160
		$4.7 \pm 1.0$	$3^\circ\text{S}$ of N limb	181
		$18. \pm 2.$	S limb	283
		$22. \pm 2.$	S limb	299
		$8.1 \pm 1.$	$3^\circ\text{S}$ of S limb	303
		$6.0 \pm 1.$	$3^\circ\text{N}$ of S limb	305
		$3.5 \pm 1.$	$6^\circ\text{N}$ of S limb	308
		$6.5 \pm 1.$	N limb	312
		$40. \pm 4.$	$3^\circ\text{S}$ of N limb	314
		$6.1 \pm 1.$	$6^\circ\text{S}$ of N limb	317
		$4.0 \pm 1.0$	S limb	339
$1, 1, +1 \rightarrow 1, 1$	2545.418	$9.3 \pm 1.0$	$3^\circ\text{S}$ of N limb	342

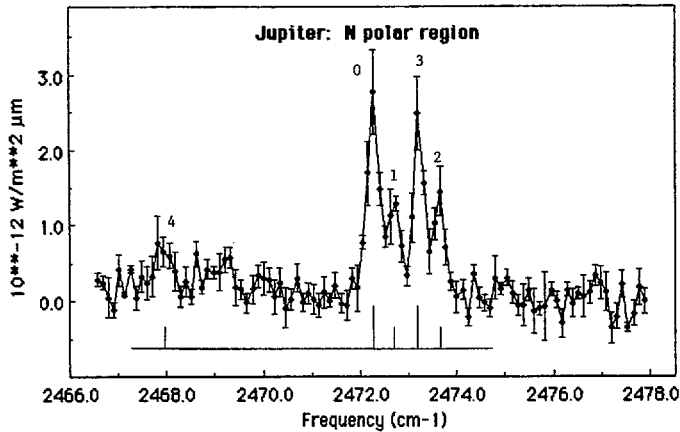


FIG. 3.—A quartet of lines in Jupiter connecting  $J = 5$  levels in the  $\nu_2$  band of H<sub>3</sub><sup>+</sup>. See Table 1 for identifications. The weak feature at 2468 cm<sup>-1</sup> may be a blend of an H<sub>3</sub><sup>+</sup> line with H 1 Br $\alpha$ .

data provide convincing evidence for large time variations of the physical conditions in Jupiter's auroral plasma. Our negative results are summarized in Table 2. Note that lines of HeH<sup>+</sup> (Bernath and Amano 1982) and H<sub>2</sub>D<sup>+</sup> (Foster *et al.* 1986) fell in some of the observed spectral intervals near 4  $\mu$ m and were absent.

A second interesting difference with some of the previous observations is the presence of H<sub>3</sub><sup>+</sup> lines from the  $\nu_2$  fundamental band at much wider variety of longitudes than that reported for the overtone band by Drossart *et al.* (1989). During 1989 September 17–19 we detected the (1, 0, -1)  $\rightarrow$  (1, 0) line over widely spaced longitudes, within a few arcseconds of both poles. Taken as a whole, our data set suggests that emission in the fundamental band was present at all longitudes within several arcseconds of each pole. The difference between our result and that of Drossart *et al.*, who found that overtone line emission near the south pole occurred only within a limited range of longitudes, may be related to the heightened sensitivity of the  $\nu_2 = 2$  level to excitation conditions. The latitude dependence that we found for the  $\nu_2 = 1 \rightarrow 0$  band, on the other hand, is quite similar to that reported by Trafton, Lester,

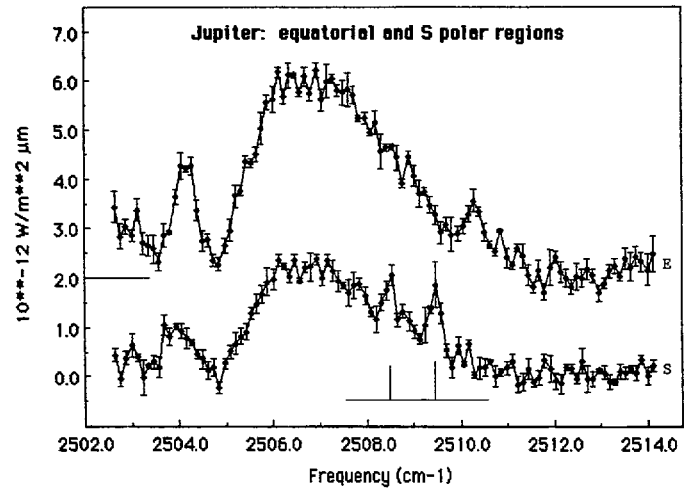


FIG. 4.—Two spectra of Jupiter, on the equator and near the south pole; the latter contains an H<sub>3</sub><sup>+</sup>  $J = 3$  doublet near 2509 cm<sup>-1</sup>, superposed on continuum emission with strong absorption lines.

and Thompson (1989); we found no H<sub>3</sub><sup>+</sup> line emission further than  $\sim 6''$  from either pole. The brightest  $\nu_2 = 1 \rightarrow 0$  lines we found were at the south limb at a System III longitude of  $\sim 299^\circ$  and 3" south of the north limb at a longitude of  $\sim 314^\circ$ ; however, we emphasize that complete coverage of either polar region was not achieved on any single morning.

#### IV. DISCUSSION

The detection of the 4  $\mu$ m band of H<sub>3</sub><sup>+</sup>, together with measurements of the 2  $\mu$ m band reported earlier, provide a number of significant pieces of information concerning the auroral regions of Jupiter. The present observations of the fundamental band confirm and extend the evidence that H<sub>3</sub><sup>+</sup> is abundant in the auroral regions (McConnell and Majeed 1987). Using the observed line intensities, we estimate rotational temperatures generally to be within 100 K of 670 K and derive column densities in the range 0.1–1.0  $\times 10^{11}$  cm<sup>-2</sup> in the  $\nu_2 = 1$  level near the poles. These column densities are factors of 7–70 times larger than that estimated by Drossart *et al.* (1989)

TABLE 2  
NEGATIVE RESULTS FOR NORTH AND SOUTH POLAR REGIONS

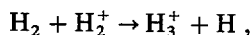
Species	Transition	Frequency (cm <sup>-1</sup> laboratory)	2 $\sigma$ Limit (10 <sup>-16</sup> W m <sup>-2</sup> , 5" beam)	Pole, Longitude (System III)
H <sub>3</sub> <sup>+</sup>	$2\nu_2 \rightarrow 0$ (6, 3, 2) $\rightarrow$ (7, 0)	4319.0 <sup>a</sup>	0.4	S 65°, N 80°
	$2\nu_2 \rightarrow 0$ (3, 1, 2) $\rightarrow$ (4, 4)	4325.893	0.4	S 65, N 80
	$2\nu_2 \rightarrow 0$ (7, 9, 2) $\rightarrow$ (6, 6)	4777.226	0.4	S 30–90, 220–280
	$2\nu_2 \rightarrow 0$ (7, 9, 2) $\rightarrow$ (6, 6)	4777.226	0.4	N 0–90, 220–280
	$2\nu_2(2) \rightarrow \nu_2$ (2, 0, -2) $\rightarrow$ (2, 0, -1)	2474.054	1.5	N 12, S 35
	$2\nu_2(2) \rightarrow \nu_2$ (4, 1, 2) $\rightarrow$ (4, 1, 1)	2508.757	2.0	S 15, S 118
	$2\nu_2(2) \rightarrow \nu_2$ (3, 1, 2) $\rightarrow$ (3, 1, 1)	2510.291	2.0	S 15, S 118
	$2\nu_2(2) \rightarrow \nu_2$ (1, 1, 2) $\rightarrow$ (1, 1, 1)	2515.755	2.0	S 118, S 136
	$2\nu_2(0) \rightarrow \nu_2$ (4, 4, 0) $\rightarrow$ (3, 4, 1)	2532.253	2.0	S 160, N 180
	H <sub>2</sub>	$\nu = 1 \rightarrow 0, J = 3 \rightarrow 1$	4712.91	0.7
$\nu = 1 \rightarrow 0, J = 3 \rightarrow 1$		4712.91	0.7	N 0–90, 220–280
HeH <sup>+</sup>	$\nu = 1 \rightarrow 0, J = 4 \rightarrow 5$	2529.134	2.0	S 160, N 180
H <sub>2</sub> D <sup>+</sup>	$\nu_3 \rightarrow 0, 4_{13} \rightarrow 3_{22}$	2505.693	2.0	S 15, S 118
	$\nu_3 \rightarrow 0, 2_{20} \rightarrow 1_{11}$	2509.541	2.0	S 15, S 118
	$\nu_2 \rightarrow 0, 3_{31} \rightarrow 2_{12}$	2512.598	2.0	S 15, S 118

<sup>a</sup> Theoretical value by Miller and Tennyson 1989.

to be present in the  $v_2 = 2$  level when the  $2 \mu\text{m}$  lines were detected.

A time variation in the excitation conditions for  $\text{H}_3^+$  is apparent from the present rotational temperature, which is much lower than the value of  $1100 \pm 100 \text{ K}$  found by Drossart in 1988 September. Assuming that the vibrational temperature is also  $\sim 670 \text{ K}$  (see below) and the above  $v_2 = 1$  column densities, we estimate the current polar column densities in  $v_2 = 2$  are 3–30 times less than in 1988 September, which is consistent with our upper limits to lines from that level.

The  $\text{H}_3^+$  ions are produced through the well-known ion-molecule reaction,



which has an exothermicity of  $1.8 \text{ eV}$  (see Oka 1983). Some of the excess energy is translational, but most remains within  $\text{H}_3^+$  as internal excitation (Bowers, Chesnavich, and Huntress 1973). Thus newly formed  $\text{H}_3^+$  must contain several quanta of vibrational energy. The observed absence of doubly excited states indicates that the observed line emission is not from freshly formed  $\text{H}_3^+$ , but from the mass of  $\text{H}_3^+$  which was in the ground vibrational state, but was excited to  $v_2 = 1$  by collisions with  $\text{H}_2$  or  $\text{He}$  (all other prominent Jovian gases, such as  $\text{CH}_4$ ,  $\text{NH}_3$ , and  $\text{H}_2\text{O}$ , have higher proton affinity than  $\text{H}_2$  and

destroy  $\text{H}_3^+$ ). Excitation by  $\text{H}_2$  is more efficient than by  $\text{He}$ , because it is a proton-hopping process with a Langevin rate.

Regarding the ortho to para ratio of  $\text{H}_3^+$ , we note that the value of  $\sim 2$  found for Jupiter indicates that the abundances are thermalized at a relatively high temperature. This is not surprising given the likelihood of proton-hopping collisions for a rotational (kinetic) temperature of  $\sim 700 \text{ K}$ . Since the proton-hopping rate is comparable to the rotational relaxation rate, it is probably reasonable to assume a vibrational temperature of  $\sim 670 \text{ K}$ . We then obtain total  $\text{H}_3^+$  column densities of  $0.11\text{--}1.1 \times 10^{13} \text{ cm}^{-2}$ , comparable to the estimate of McConnell and Majeed (1987).

#### V. CONCLUSION

It is likely that the  $4 \mu\text{m}$  bands of  $\text{H}_3^+$  are uniquely suitable monitors of Jovian auroral activity. The present observations demonstrate the temporal nature of Jupiter's aurorae and point out the need for frequent monitoring in order to better correlate Jovian polar phenomena with solar and other activity.

We wish to thank the staff of UKIRT for its support. We also thank L. Kao for assistance with some of the observations. T. O. is supported by NSF grant PHY 87-07025 and Air Force contract FO4611-86-K0069.

#### REFERENCES

- Bawendi, M., Rehfuss, B. D., and Oka, T. 1989, unpublished.  
 Bernath, P., and Amano, T. 1982, *Phys. Rev. Letters*, **43**, 20.  
 Bowers, M. T., Chesnavich, W. J., and Huntress, W. T., Jr. 1973, *Internat. J. Mass Spectrometry Ion. Phys.*, **12**, 357.  
 Carney, G. D., and Porter, R. N. 1976, *J. Chem. Phys.*, **65**, 3547.  
 ———. 1980, *Phys. Rev. Letters*, **45**, 537.  
 Drossart, P., et al. 1989, *Nature*, **340**, 539.  
 Foster, S. C., McKellar, A. R. W., Peterkis, I. R., Watson, J. K. G., Pan, F. S., Crofton, M. W., Altman, R. S., and Oka, T. 1986, *J. Chem. Phys.*, **84**, 91.  
 Geballe, T. R., and Oka, T. 1989, *Ap. J.*, **342**, 855.  
 Maillard, J.-P., and Drossart, P. 1989, *California-France-Hawaii Telescope Bull.*, **20**, 13.  
 Majewski, W. A., Feldman, P. A., Watson, J. K. G., Miller, S., and Tennyson, J. 1989, *Ap. J. (Letters)*, **347**, L51.  
 Majewski, W. A., Marshall, M. D., McKellar, A. R. W., Johns, J. W. C., and Watson, J. K. G. 1987, *J. Molec. Spectrosc.*, **122**, 341.  
 McConnell, J. C., and Majeed, T. 1987, *J. Geophys. Res.*, **92**, 8570.  
 Miller, S., and Tennyson, J. 1987, *J. Molec. Spectrosc.*, **216**, 183.  
 ———. 1988, *J. Molec. Spectrosc.*, **128**, 530.  
 ———. 1989, private communication.  
 Oka, T. 1980, *Phys. Rev. Letters*, **45**, 531.  
 ———. 1981, *Phil. Trans. Roy. Soc. London*, **A303**, 543.  
 ———. 1983, in *Molecular Ions: Spectroscopy, Structure, and Chemistry*, ed. T. A. Miller and V. E. Bondybey (Amsterdam: North-Holland), p. 73.  
 Trafton, L., Lester, D. F., and Thompson, K. L. 1989, *Ap. J. (Letters)*, **343**, L73.  
 Watson, J. K. G., et al. 1984, *Canadian J. Phys.*, **62**, 1875.  
 Xu, L.-W., Gabrys, C., and Oka, T. 1989, unpublished.

T. R. GEBALLE: Joint Astronomy Centre, 665 Komohana Street, Hilo, HI 96720

T. OKA: Department of Chemistry, The University of Chicago, 5735 South Ellis Avenue, Chicago, IL 60637