# Discovery of far-IR pure rotational transitions of $CH^+$ in NGC 7027[1]

J. Cernicharo

CSIC, IEM, Dpto. Física Molecular, Serrano 123, E-28006 Madrid, Spain

X.-W. Liu

Department of Physics and Astronomy, University College London, Gower Street, London WC1E 6BT, UK

E. González-Alfonso

Universidad de Alcalá de Henares, Dpto. Física, Campus Universitario, E-28871 Alcalá de Henares, Spain

P. Cox

Institut d'Astrophysique Spatiale, Bât. 121, Université de Paris XI, F-91405 Orsay Cedex, France

M. J. Barlow

Department of Physics and Astronomy, University College London, Gower Street, London WC1E 6BT, UK

T. Lim

The LWS Instrument-Dedicated Team, ISO Science Operations Centre. PO Box 50727. E-28080 Madrid. Spain

B.M. Swinyard

Rutherford Appleton Lab., Chilton, Didcot, Oxon OX11 0QX. UK

**accepted for publication in the Astrophysical Journal Letters**

Received ________________; accepted ________________

## ABSTRACT

We report the discovery of the rotational spectrum of $CH^+$ in the ISO LWS spectrum of the planetary nebula NGC 7027. The identification relies on a reanalysis of the LWS spectrum published by Liu et al. (1996, L96 hereafter) and on new LWS data. The strong line at 179.62 $\mu$m (coinciding with the $2_{12}$-$1_{01}$ transition of water vapour) and the lines at 119.90 and 90.03 $\mu$m (reported as unidentified by L96), whose frequencies are in harmonic relation 2:3:4, are shown to arise from the J=2-1, 3-2, and 4-3 rotational transitions of $CH^+$. This identification is strengthened by the new LWS spectra of NGC 7027 which clearly show the next two rotational lines of $CH^+$, at 72.140 and 60.247 $\mu$m. This is the first time that the pure rotational spectrum of $CH^+$ has been observed. This discovery opens the possibility to probe the densest and warmest zones of photodissociation regions. We derive a rotational temperature for the $CH^+$ lines of 150$\pm$20 K and a $CH^+$/CO abundance ratio of 2-6 $10^{-4}$.

*Subject headings:* planetary nebulae: individual: (NGC 7027) — infrared lines: individual: molecular: circumstellar

---

[1]Based on observations with ISO, an ESA project with instruments funded by ESA Member States (especially the PI countries: France Germany, the Netherlands and the United Kingdom) and with the participation of ISAS and NASA.

## 1. Introduction

The spectrometers on board the Infrared Space Observatory (ISO) provide a unique opportunity to study important molecular species through transitions which are inaccessible from the ground or airborne platforms. This has been illustrated by the recent ISO results on the thermal lines of water vapour. Water vapour has been measured in high abundance ($x(H_2O)\simeq 10^{-5}$) in star forming regions and evolved stars using both the SWS and the LWS, e.g., van Dishoeck and Helmick (1996), Barlow et al. (1996), Cernicharo et al. (1997) and Cox et al. (1997). The detection of water vapour (together with OH) was also reported by L96 in the LWS spectrum of the planetary nebula (PN) NGC 7027. This was an unexpected result because NGC 7027 is a carbon-rich source.

In this Letter, we rediscuss the previous identification of the water vapour emission lines in the LWS spectrum of NGC 7027. The 179.53 $\mu$m line together with two lines at 119.89 $\mu$m (near the OH 119.3 $\mu$m doublet) and 90.07 $\mu$m, both unidentified in L96, are now shown to arise from the pure rotational spectrum of $CH^+$. We also present new ISO/LWS data which show two further rotational lines of $CH^+$ and confirm the previous detection of OH and probably also of $H_2O$.

## 2. Identification of $CH^+$

The identification of water vapour in NGC 7027 by L96 relies mainly on the observation of a strong line at 179.56 $\mu$m coinciding with the 179.53$\mu$m $H_2O$ rotational $2_{12}$-$1_{01}$ transition. Two other features quoted as possible water lines in L96 were flagged as "identification questionable". In addition to the $H_2O$ line, L96 also reported the detection of OH through the 119.3 $\mu$m fundamental transition. This line is blended with an equally strong feature at 119.89 $\mu$m which remained unidentified. Two other OH lines (at 79.2 and 84.5 $\mu$m) were tentatively reported.

L96 also reported a strong unidentified line at 90.07 $\mu$m. We note that the wavelengths of the lines at 179.56, 119.89 and 90.07 $\mu$m are nearly in the harmonic relation 2:3:4. Assuming that the 179.56 $\mu$m line does not arise from water vapour but instead that the three lines are arising from another molecular carrier, these lines could correspond to the rotational transitions J=2-1, 3-2, and 4-3 of a linear molecule. From the three lines we derive the following rotational constants for the carrier: B=13.95$\pm$0.03 cm$^{-1}$ and D=0.0017$\pm$0.0005 cm$^{-1}$ ($1\sigma$ errors). The observed frequencies and inferred rotational constants indicate that the carrier must be diatomic and should contain a hydrogen atom. The rotational constants are comparable to those of CH (B=14.19 cm$^{-1}$, D=0.0014 cm$^{-1}$) and show an excellent agreement with those of the $CH^+$ ion (B=13.9302 cm$^{-1}$ and D=0.0014 cm$^{-1}$; Carrington & Ramsay 1982).

Prompted by the observation of three lines in harmonic relation that are consistent with $CH^+$, we have processed all the ISO LWS01 grating spectra of NGC 7027 so far obtained up to ISO Revolution 377, in an effort to detect the J=5–4 and 6–5 transitions of $CH^+$, which are predicted at wavelengths of 72.15 and 60.26 $\mu$m and were not detected by L96. In total, there are 9 separate observations, each covering a wavelength range from 43–195$\mu$m, obtained during Revs. 27, 39, 342, 349, 356, 363 and 377. All the data were calibrated using Version 6 of the Off-line Processing package (OLP). The observation from Rev. 27 consists of 3 scans, with two 0.5 s integration ramps at each grating position, sampled at 1/4.5 of a spectral resolution element, the latter being 0.3$\mu$m for the SW1–SW5 detectors ($\lambda < 93\mu$m) and 0.6$\mu$m for the LW1–LW5 detectors ($\lambda > 84\mu$m). Each of the five observations obtained between Rev. 342 and 377 consists of six scans with one 0.5 s ramp at each grating position, sampled at 1/9 of a resolution element. Three observations were obtained in Rev. 39. Each consists of five scans with two 0.5 s ramps at each grating position, sampled at 1/15 of a resolution element. The total on-target integration time was 23930 s. The LWS has a circular aperture of diameter 85 arcsec, significantly larger than the ionized or neutral regions of NGC 7027. The analysis presented in L96 was based on the three observations carried in Rev. 39, processed with Version 5 of the OLP. Although the current data has a total on-target time only 65% larger than that analyzed by L96, the final co-added spectrum has a much better S/N, by more than a factor of two in some wavelength regions, thanks to the much-improved instrumental filter profiles derived from additional observations of Uranus, and the implementation of an algorithm which corrects for detector sensitivity drifts. The fluxes derived from the individual independent observations are in good agreement and we estimate an accuracy of better than 20% for the absolute flux calibration.

Fig. 1 shows the five $CH^+$ lines detected in our new spectra, including the two lines at 72.15 and 60.26$\mu$m which are clearly detected in the present data. These five lines definitely establish the presence of $CH^+$ in NGC 7027. This is the first time that $CH^+$ is seen through its pure rotational spectrum. $CH^+$, a common molecule in the diffuse interstellar medium, has been detected in the optical spectrum of only two evolved carbon-rich stars : in emission in the Red Rectangle and, in absorption, in HD 213985 (Balm & Jura 1992; Hall et al. 1992; Waelkens et al. 1992; Bakker et al. 1997). Given the carbon-rich nature of NGC 7027 and the strong radiation field in its inner regions it is thus not too surprising to find $CH^+$ in this prototypical PN. In fact, soon after the detection of $H_2$ in NGC 7027 (Treffers et al. 1978), Black (1978) predicted that $CH^+$, OH and $HeH^+$ might have detectable abundances in this nebula.

In addition, five OH lines are present (Fig. 2) confirming the previous detection of OH by L96. The $CH^+$ and OH line fluxes are given in Table 1. Apart from the 179.6$\mu$m line, two marginal features at 174.6 and 180.5$\mu$m were tentatively assigned in L96 as possible

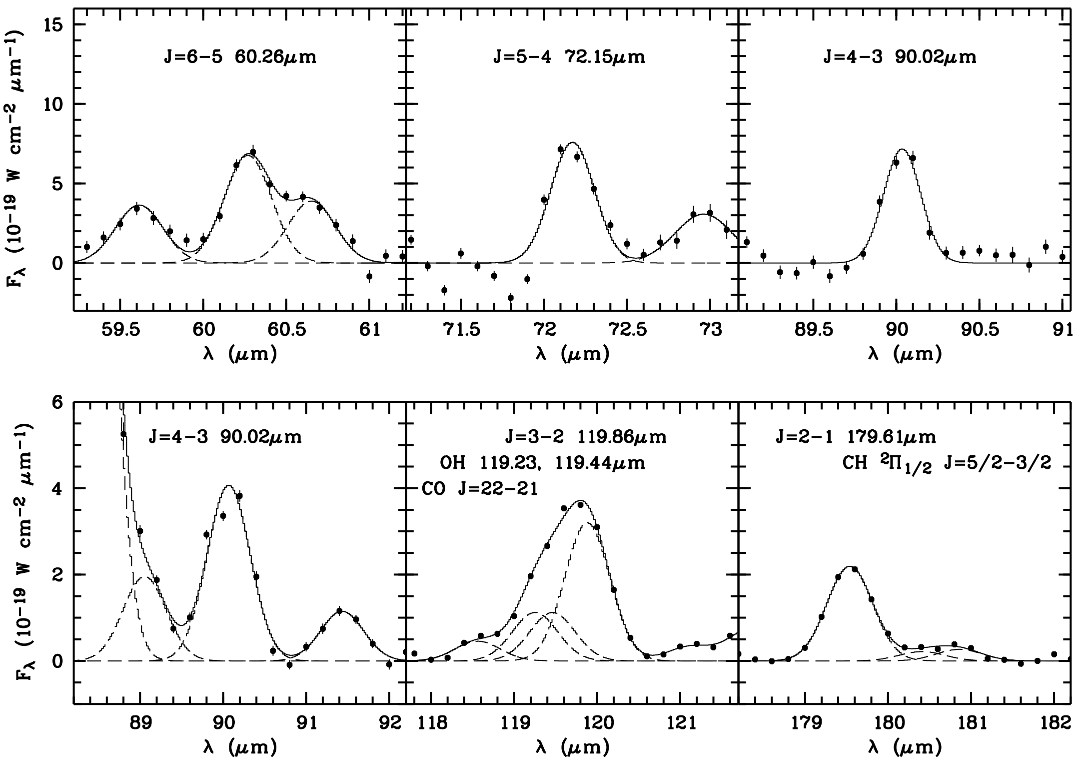


Fig. 1.— $CH^+$ lines observed in NGC7027 (the continuum has been subtracted from the data). The solid lines are gaussian line profile fits to the observed features (for blends, contributions from individual components are shown as dashed lines). The J=2-1 line at 179.62 $\mu$m was previously assigned to $H_2O$. For the J=4-3 line, spectra from two different detectors - LW1 (bottom panel) – the sharp rise at short wavelengths is due to the strong [O III] 88.36$\mu$m line – and SW5 (upper panel) are shown. The J=4-3 line is blended with the J=29-28 line of CO at 90.16 $\mu$m which could contribute with an intensity $<10^{-19}$ W cm$^{-2}$ - the J=27-26 and J=26-25 lines of CO can be seen in the bottom left panel of Fig. 2 with intensities of $\sim 10^{-19}$ W cm$^{-2}$. The lines at 59.5 and 60.7 $\mu$m in the top-left panel are unknown

water vapour lines. The 180.5 $\mu$m line is now shown to arise from CH (see Liu et al. 1997). However, the new data confirm the 174.6 $\mu$m line ($F = (1.44 \pm 0.17) \times 10^{-20}$W cm$^{-2}$), and in addition show two lines at $108.05 \pm 0.1\mu$m ($F = (5.9 \pm 0.6) \times 10^{-20}$ W cm$^{-2}$), and $75.39 \pm 0.03\mu$m ($F = (6.6 \pm 2.5) \times 10^{-20}$ W cm$^{-2}$) coincident in wavelength with the $2_{21}$–$1_{10}$ (108.08$\mu$m) and the $3_{21}$–$2_{12}$ (75.38 $\mu$m) lines of o-$H_2O$. Taking into account the density of lines, and the lack of emission in the lines of para-water, the definitive assignment of these lines to water vapour will require high spectral resolution observations. No $^{13}CH^+$ lines were detected in current spectrum. Finally, Fig. 1 shows that the CH rotational line at 180.6 $\mu$m is much weaker than the nearby $CH^+$ J=2-1 line. A comparison of the observed intensities yields a $CH^+$/CH abundance ratio of $\simeq$ 5-10 (see also Liu et al. 1997).

## 3. Discussion

The line fluxes of Table 1 have been used to derive the rotational temperature, $T_{rot}$, of $CH^+$. From a standard rotational analysis, in which we assume a uniform rotational temperature for all the rotational levels of $CH^+$, we obtain $T_{rot} \simeq 150\pm20$ K (see Fig. 3), a $CH^+$ total column density of 2.5 $10^{47}$. It is worth noting that similar $CH^+$ rotational temperatures were derived from optical observations in the Red Rectangle and in HD213985 by Bakker et al (1997), i.e. 202 and 155 K, respectively. A similar rotational analysis for the CO line fluxes given by L96 yields a rotational temperature for CO of 240 K and a total number of CO molecules $\simeq 10^{51}$. Assuming that the molecular emission of both species arises from the same region we obtain a $CH^+$/CO abundance ratio of $2\,10^{-4}$. Assuming that the size of the photodissociation region (PDR) in NGC 7027 is about 6 arcsec, we derive a column density for $CH^+$ of $8\,10^{13}$ cm$^{-2}$.

In order to estimate the physical conditions needed to produce the observed $CH^+$ fluxes, we have made LVG calculations that allow us to estimate the $H_2$ volume density

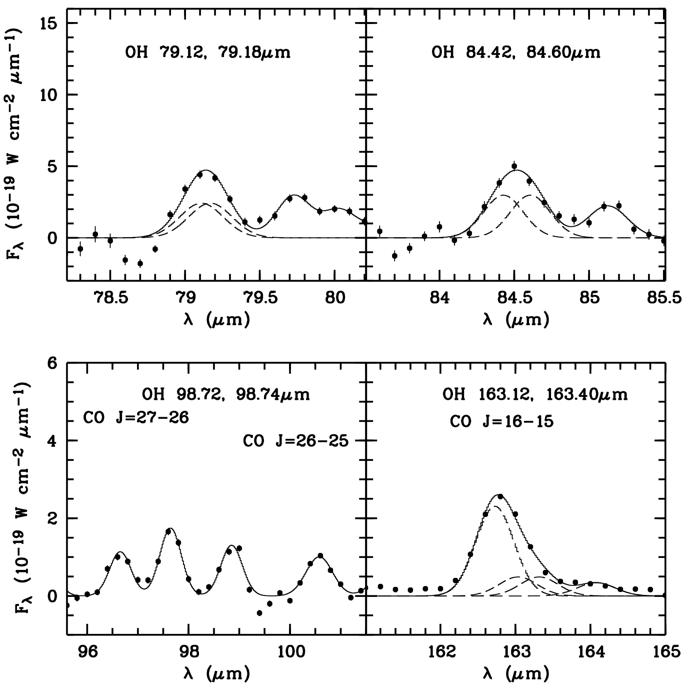


Fig. 2.— OH lines observed in NGC7027 (after subtraction of the continuum). The OH 119.23, 119.44$\mu$m lines, blending with the $CH^+$ 119.86$\mu$m line, are shown in the lower middle panel of Fig. 1. Due to the $\Lambda$-doubling, each of the OH transition consists of two components, and two gaussians of equal line width and intensity, having a central wavelength difference given by their laboratory values, were used to fit the line profiles, except for the 98.73 $\mu$m transition which has a negligeable wavelength splitting. Two lines in the bottom left panel correspond to the J=27-26 and J=26-25 transitions of CO (at 96.77 and 100.46 $\mu$m, respectively), while the line at 97.6 $\mu$m in the same panel is unknown

Table 1. $CH^+$ and OH line fluxes from NGC 7027

| $\lambda_{obs}$ ($\mu$m) | Flux ($^{a)}$) | $\lambda_{vac}$ ($\mu$m) | Transition |
|---|---|---|---|
| | | $CH^+$ | |
| 179.60±0.04 | 1.51±0.05 | 179.61 | J=2-1 |
| 119.88±0.06 | 2.18±0.17 | 119.86 | J=3-2 |
| 90.09±0.06 | 2.64±0.28 | 90.02 | J=4-3$^{b)}$ |
| 90.02±0.03 | 2.00±0.22 | 90.02 | J=4-3$^{c)}$ |
| 72.17±0.03 | 2.50±0.41 | 72.15 | J=5-4 |
| 60.27±0.03 | 2.41±0.33 | 60.26 | J=6-5 |
| | | OH | |
| 119.36±0.06 | 1.53±0.11 | 119.34 | $^2\Pi_{3/2}$ J=5/2-3/2$^{d)}$ |
| 84.50±0.02 | 1.98±0.15 | 84.51 | $^2\Pi_{3/2}$ J=7/2-5/2 |
| | <2.4 (3$\sigma$) | 65.20 | $^2\Pi_{3/2}$ J=9/2-7/2 |
| 163.23±0.08 | 0.62±0.07 | 163.26 | $^2\Pi_{1/2}$ J=3/2-1/2$^{e)}$ |
| 98.85±0.10 | 0.69±0.12 | 98.73 | $^2\Pi_{1/2}$ J=5/2-3/2 |
| 79.12±0.04 | 1.76±0.23 | 79.15 | $^2\Pi_{1/2-3/2}$ J=1/2-3/2 |

[a] in $10^{-19}$ W cm$^{-2}$ [b] LW1 detector [c] SW5 detector [d] blended with $CH^+$ J=3-2 [e] blended with CO J=16-15

and the $CH^+$ column density. Collisional cross sections for $CH^+$ with $H_2$ are not available and we have used those of $N_2H^+$ (Green 1975). The values of the collisional cross sections for high kinetic temperatures were obtained from the $N_2H^+$ data available for 10-40 K by extrapolating the rate coefficients as the root square of the kinetic temperature. Typical estimates for the excitation rate coefficients are $\sim 10^{-10}$ $\mathrm{cm^3\,s^{-1}}$. With a dipole moment of 1.68 D (e.g. Follmeg, Rosmus & Werner 1987), the relevant critical $H_2$ densities for the $CH^+$ J=1 level are of the order of $\sim 10^7\,\mathrm{cm^{-3}}$. Larger densities could be even necessary to pump by collisions the high J levels (the J=6-5 rotational transition has an Einstein coefficient for spontaneous emission of 1.9 $\mathrm{s^{-1}}$). For a distance of 700 pc (Hajian et al. 1993) and adopting a line width of 30 $\mathrm{kms^{-1}}$, the observed $CH^+$ fluxes can be roughly explained with the following parameters: n($H_2$)=$2-5\,10^7$ $\mathrm{cm^{-3}}$, $T_K$=300-500 K and a $CH^+$ column density of $2.5\,10^{14}$ $\mathrm{cm^{-2}}$ which implies a $CH^+$/CO abundance ratio of $\simeq 6\,10^{-4}$. The dashed line in Figure 3 shows the computed $CH^+$ line intensity fluxes for n($H_2$)=$5\,10^7$ $\mathrm{cm^{-3}}$ and $T_K$=300 K. An improved fit to the data could be obtained with a model where the low J transitions are excited in a region of moderate kinetic temperature and the high J levels in a region with temperatures around 1000 K. But in any case, the density must be very high in order to explain the population of the J=4, 5, and 6 rotational levels of $CH^+$. The rotational lines of $CH^+$ could also be collisionally excited by impact of H and $e^-$. For collisions with $e^-$, $\gamma[\mathrm{J}+1 \rightarrow \mathrm{J}] \sim$ a few $\times 10^{-7}$ $\mathrm{cm^3\,s^{-1}}$ for $T_e$ between 100 and 1000 K (Dickinson & Flower 1981). Hence, electrons may compete with $H_2$ in populating the $CH^+$ rotational levels if $n_e/n(\mathrm{H}) \sim 10^{-3}$, a condition reached only in the warm PDR where all the carbon is in form of $C^+$. In this region, the $H_2$ densities quoted above could be lowered by a factor 2-3 if collisions with $e^-$ are taking into account. In addition, we must consider the possibility of excitation of the $CH^+$ rotational levels through absorption of photons in the $^1\Pi -^1\Sigma$ transition, followed by decay back to the ground state (in the Red Rectangle, the $CH^+$ $^1\Pi -^1\Sigma$ lines are observed in emission). Observations at optical wavelenghts of

$CH^+$ in NGC 7027 might provide important insights into the excitation mechanism of $CH^+$. If such pumping mechanism plays a role in the excitation of the rotational levels of $CH^+$ then the densities necessary to explain the emission would be considerably lower.

The discrepancy between the $CH^+$/CO abundance ratio derived from the LVG calculations and that derived from the rotational analysis of the $CH^+$ lines arises from two facts. First, the assumptions in the rotational analysis that the $CH^+$ lines are optically thin (from the LVG calculations, the opacities are estimated to be $\simeq$ 1-5) and have a uniform rotational temperature. Second, from the uncertainties in the collisional cross-sections used in the LVG models.

The formation of $CH^+$ via the reaction $C^+ + H_2 \rightarrow CH^+ + H$, which has an activation energy of $\sim$ 4000K, requires a gas at high kinetic temperature ($\simeq$1000 K). However, the present observations suggest that, in NGC 7027, the temperature of the region where $CH^+$ is emitting is much lower. In the interface region between the cold neutral gas and the fully ionized zone, a significant fraction of the $H_2$ population will be vibrationally excited carrying an important part of the energy needed to activate the above reaction (Sternberg & Dalgarno 1995). A similar situation has been proposed by Jura et al. (1997) to explain the $CH^+$ emission in the Red Rectangle. For densities $10^6 < n(H_2) < 10^7$ cm$^{-3}$, the formation rate of $CH^+$ could be high enough to produce column densities similar to those derived in this work, i.e., 0.8-2 $10^{14}$ cm$^{-2}$, as predicted in the models of Sternberg & Dalgarno (1995). However, if the density becomes too high, $CH^+$ might not survive because it will be rapidly destroyed by the reaction $CH^+ + H_2 \rightarrow CH_2^+ + H$. Like in the diffuse interstellar medium, $CH^+$ could be formed efficiently in a region of moderate temperature in the presence of shocks with velocities of a few km s$^{-1}$. Low velocity shocks have been observed in NGC 7027 (Jaminet et al. 1991) and should thus be taken into consideration in any detailed study of the formation and excitation of $CH^+$ in this planetary nebula.

The $CH^+$ J=2-1 line can contaminate the LWS observations of water vapour at 179.5 $\mu$m. The water line is seen in absorption towards several molecular clouds (Cernicharo et al. 1997, Cox et al. 1997) and arises from the ground level while the possible absorption by $CH^+$ will arise from the J=1 level which is 40 K above the ground. Contamination of the the $H_2O$ 179.5 $\mu$m absorption line by $CH^+$ absorption is thus unlikely. However, the interpretation of the 179.6 $\mu$m line in emission in PDRs will require high spectral resolution data or the study of other transitions to disentangle the contributions of the $H_2O$ and $CH^+$ lines.

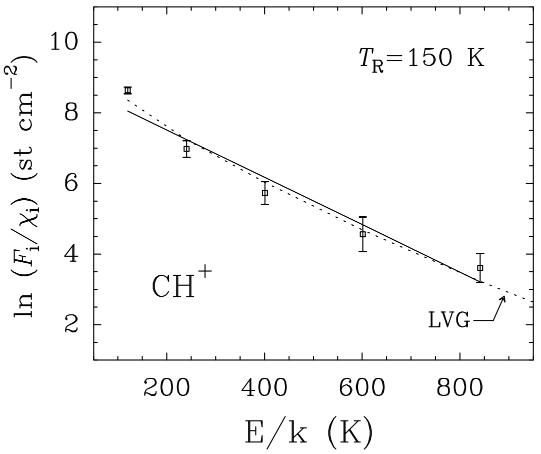


Fig. 3.— Rotational temperature analysis for CH$^+$ in NGC 7027. The ordinates represent the natural logarithm of the observed fluxes (in W cm$^{-2}$) divided by $\chi_i \equiv (16\,10^{-7}\pi^3\nu^4\mu^2 J_{up})/(3c^3)$, where the symbols have the usual meaning and are in c.g.s units. The abscissa corresponds to the energy of the upper level of each rotational transition. The solid line represents the fit to the data assuming an uniform rotational temperature, while the dashed line shows to the fluxes derived from the LVG models quoted in the text.

## REFERENCES


Bakker, E.J., van Dishoeck, E.F., Waters L.B.F.M., & Schoenmaker T. 1997, A&A, in press

Balm, S.P., & Jura, M. 1992, A&A, 261, L25

Barlow, M.J. et al. 1996, A&A, 315, L241

Black, J.H., 1978, ApJ, 222, 125

Carrington, A., & Ramsay, D.A. 1982, Physica Scripta, 25, 272

Cernicharo, J. et al. 1997, A&A, in press

Cox, P. et al. 1997, A&A, in press

Dickinson, A.S., & Flower, D.R. 1981, MNRAS, 196, 297

Follmeg, B., Rosmus, P., & Werner, H.-J. 1987, Chem. Phys. Letters, 136, 562

Green, S. 1975, ApJ, 201, 366

Hajian, A.R., Terzian, Y., & Bignell, C. 1993, AJ, 106, 1965

Hall, D.I., Miles, J.R., Sarre, P.J., & Fossey, S.J. 1992, Nature 358, 629

Jaminet, P.A., Danchi, W.C., Sutton, E.C., Russell, A.P.G., Sandell, G., Bieging, J.H., & Wilner, D. 1991, ApJ, 380, 461

Jura, M., Turner, J., & Balm, S.P. 1997, ApJ, 474, 741

Liu, X.-W. et al. 1996, A&A, 315, L257 (L96)

Liu X.-W., Barlow M. J., Dalgarno A., Tennyson J., Lim T., Swinyard B. M., Cernicharo J., Cox P., J.-P. Baluteau, Pequignot D., Nguyen-Q-Rieu, Emery R. J., Clegg P. E., 1997, ApJ, submitted

Sternberg, A., & Dalgarno, A. 1995, ApJSS, 99, 565

van Dishoeck, E.F., & Helmich, F.P. 1996, A&A, 315, L177

Treffers, R.R., Fink, U., Larson, H.P., & Gautier, T.N. III 1976, ApJ, 209, 793

Waelkens, C., van Winckel, H., Trams, N.R., & Waters L.B.F.M. 1992, A&A, 256, L15

This manuscript was prepared with the AAS LaTeX macros v4.0.