A NEW UNIDENTIFIED FAR-INFRARED BAND IN NGC 7027

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ABSTRACT

We report on the detection of a molecular band centered at ~98 µm (~102 cm⁻¹), observed with the Infrared Space Observatory in the young planetary nebula NGC 7027. The band structure and intensity cannot be reproduced by atomic fine-structure lines, recombination lines, or the rotational emission of abundant molecules. We discuss the possible contribution of the low-energy bending modes of pure carbon chains to the unidentified far-IR bands observed in C-rich evolved objects. In particular, we speculate that the band emission could arise from the ν₀ and ν₇ bending modes of C₆ and C₅, for which wavenumbers of 90 ± 50 and 107 ± 5 cm⁻¹ have been estimated from photoelectron spectroscopy.

Subject headings: circumstellar matter — infrared: stars — ISM: molecules — line: identification — stars: individual (NGC 7027)

On-line material: color figures

1. INTRODUCTION

Carbon-chain molecules are of special interest for astrophysics since Douglas (1977) proposed them as possible carriers of the diffuse interstellar bands (DIBs). In the past, many polar carbon chains have been detected in the interstellar and circumstellar media (ISM and CSM, respectively) through their pure rotational spectrum at radio wavelengths. Major examples are the cyanopolyynes, HCₙ₊₁N with n = 1–5 (Turner 1971; Avery et al. 1976; Kroto et al. 1978; Broten et al. 1978; Bell et al. 1997), and hydrogenated carbon-chain radicals such as C₄H, C₅H, C₆H, and C₇H (Cernicharo et al. 1986; Guélin et al. 1987, 1997; Cernicharo & Guélin 1996).

On the other hand, larger carbon molecular complexes such as the polyacetylenic aromatic hydrocarbons (PAHs) are believed to dominate the ubiquitous mid-IR emission seen in the unidentified infrared bands (UIBs). However, only the single aromatic species benzene has so far been identified through its IR active modes (Cernicharo et al. 2001).

The diversity of these species suggests that the growth mechanisms producing complex carbon molecules such as the PAHs or the fullerenes are highly efficient. Nevertheless, the set of “building blocks” and possible chemical reactions still have to be identified and clarified. Among the possible species, the pure carbon chains, (Cₙ₊₀, van Orden & Saykally 1998), could be the skeletons from which larger organic molecules can be formed (see Cernicharo et al. 2000). Because of the lack of a permanent electric dipole, these species do not have rotational spectra observable from radio telescopes. The only way to detect them in the dense ISM and CSM is through their asymmetrical stretching modes around ~5 µm (2000 cm⁻¹) and/or through their low-energy bending modes around ~100 µm (~100 cm⁻¹). The former technique allowed the detection of C₃ (Hinkle et al. 1988) and C₄ (Bernath et al. 1989) in the circumstellar envelope of the bright IR-evolved star IRC +10216. However, few sources (especially in the ISM) have enough flux at ~5 µm to allow systematic studies of the Cₙ stretching modes, and the less-known far-IR bending modes are the only way to detect these species.

Before the launch of the Infrared Space Observatory (ISO; Kessler et al. 1996), we proposed to observe the bending modes of several polyatomic molecules in the far-IR. As a result, the ν₂ bending mode of C₄ has been observed in Sgr B2 and IRC +10216 (Cernicharo et al. 2000). In addition, we have detected several unidentified far-IR bands (UIFBs) in the ISO spectrum of many C-rich sources that may also be related to the bending modes of carbon-chain species. In particular, we have tentatively assigned a UFIB at ~57.5 µm (~174 cm⁻¹), observed in Sgr B2 and in C-rich evolved stars including the planetary nebula (PN) NGC 7027, to the ν₅ bending mode of C₄ (Cernicharo et al. 2002).

NGC 7027 is one of the most studied evolved objects in the Galaxy. It is a young PN, ~1000 years since it left the asymptotic giant branch (AGB) stage, and is characterized by a relatively compact ionized region (Volk & Kwok 1997), driven by the radiation that arises from a central source at ~200,000 K (Latter et al. 2000). In addition, a rich C chemistry is taking place in the larger molecular envelope (~40° in CO; Masson et al. 1985) that surrounds the inner photon-dominated regions. In fact, NGC 7027 was the first object to show UIB emission, later attributed to the PAH emission (Gillett et al. 1973), and is the only source where pure rotational lines of CH⁺ have been detected (Cernicharo et al. 1997).

Therefore, the detection of unidentified features in the IR spectrum of NGC 7027 has historically contributed to a better understanding of the interstellar carbon complexity. In this work, we report the detection of a new UFIB at ~98 µm (~102 cm⁻¹) in the far-IR spectrum of NGC 7027 and speculate about its possible origin.

2. OBSERVATIONS

The possible emission/absorption produced by the low-energy bending modes of C₅ species has been searched using the ISO Long-Wavelength Spectrometer (LWS; Clegg et al.
Fig. 1. — Top: Expected band shape for a $^1\Pi - ^1\Sigma$ transition (as the $v_7$ mode of C$_5$) and for a $^3\Pi - ^3\Sigma$ transition (as the $v_9$ mode of C$_6$) with $\Delta \nu_0 = 3.5 \text{ cm}^{-1}$. The excitation temperature for both transitions is 100 K. The intrinsic line width is 10 km s$^{-1}$ and the spectral resolution $\lambda/\Delta \lambda = 200$. Middle: Observed ISO LWS spectrum of NGC 7027 between $\approx 86$ and 110 $\mu$m (middle curve). The ordinate corresponds to the flux over the continuum flux and the abscissa to the wavelength in $\mu$m. The lower curve represents the large velocity gradient model for the pure rotational emission of CO, CH$^+$ and OH (Herpin et al. 2002), and the upper curve represents the total model for the bending modes of C$_5$ and C$_6$. The thick horizontal arrow represents the observational uncertainty for the $v_7$ C$_5$ band origin (from Kitsopoulos et al. 1991). The experimental uncertainty for the $v_9$ C$_6$ mode is $90 \pm 50$ cm$^{-1}$ (Xu et al. 1997; see text). Bottom: Observed ISO LWS spectrum of IRC +10216 between $\approx 86$ and 110 $\mu$m (upper curve). The ordinate corresponds to the continuum-subtracted flux and the abscissa to the wavelength in $\mu$m. The lower curve represents the large velocity gradient model for the pure rotational emission of CO $\nu = 0, 1$; $^{13}$CO $\nu = 0$; HCN and H$^{13}$CN $\nu = 0$; and HCN$_{vib}$ $\nu_2 = 1, 2$ and $\nu_1, 3 = 1$ (Cernicharo et al. 1996). The rotational transitions of CO, HCN in the ground state and HCN$_{vib}$ $\nu_2 = 1, 2$, and $\nu_1, 3 = 1$ are indicated. [See the electronic edition of the Journal for a color version of this figure.]
In the case of the NGC 7027 PN, we have used all of the LWS AOT L01 data taken by ISO (see Herpin et al. 2002). The LWS grating spectra of NGC 7027 taken during orbits 21, 342, 349, 356, 363, 377, 537, 552, 559, 566, 579, 587, 594, 601, 706, 713, 720, 727, 734, 741, 755, 762, 769, 776, and 783 have been averaged. The total on-source time was 53,409 s and the signal-to-noise ratio (S/N) is very high. Here we present part of the spectrum taken with the LWS between $\lambda/C_24^{86}$ and $110/C_22$ m ($\lambda/C_0^{116}$ to $91/C_0$ m at a resolution of $k/C_1^{200}$. The resulting spectrum is shown in Figure 1 (middle panel). We also present the same wavelength range in the LWS spectrum (TDT19800158) of IRC +10216 (see Fig. 1, lower panel). The full spectrum was shown and modeled by Cernicharo et al. (1996).

In addition, we present part of the ISO Short-Wavelength Spectrometer (SWS; de Graauw et al. 1996) spectrum of NGC 7027 between $\sim 4$ and 7 $\mu$m ($\sim 2500$ and 1430 cm$^{-1}$). The resolution of the SWS01 observation template in this interval is $\lambda/\Delta\lambda \approx 1500$. Many carbon chains (polar and nonpolar) possess prominent IR active stretching modes in this wavelength range. However, Figure 2 shows that the bulk of the emission in NGC 7027 arises from narrow ionic and recombination lines from the inner H$\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!$ region. Only the well-known UIB broad emission at $\sim 6.2/C_0$ m is detected. This band corresponds to the relaxation of excited vibrational states of aromatic species pumped by absorption of visible-UV photons from the hot central star. The full SWS spectrum has been presented by Bernard Salas et al. (2001).

3. RESULTS

After identified and modeled the molecular rotational lines of CO $J = 30$–$29$ to 25–$24$, CH$^+$ $J = 4$–$3$, and OH $^2\Pi_{1/2} J = 5/2$–$3/2$ (see Herpin et al. 2002 for details), a strong bandlike feature constituted by several lines was identified between 91 and 102 $\mu$m. Only the high-$J$ CO rotational emission produces a modest contribution in the band wavelengths. Figure 1 also shows the maximum contribution expected for the rotational...
$^2\Pi_{1/2}$ 5/2–3/2 line of OH at $\sim$98 $\mu$m, estimated from the clearer detections at $\sim$79 and $\sim$84 $\mu$m. Note that no water lines have been detected in the far-IR spectrum of NGC 7027 (Cernicharo et al. 1997), and thus, no other O-bearing species are contaminating the $\sim$86–110 $\mu$m window.

Because of the presence of an H ii region in the inner envelope, we have also searched for all of the possible atomic transitions that could arise from the nebular gas. The most likely atomic lines in a PNe such as NGC 7027 (i.e., fine-structure and recombination lines), taken from the Atomic Line List,$^3$ of Peter van Hoof have been analyzed. We note that lines from [V iv], [V iii] and [Ti iii] with transitions in the considered wavelength range have been previously detected in the optical spectrum of NGC 7027 (Baluteau et al. 1995), while several H i recombination lines are observed in the mid-IR (e.g., see Fig. 2).

To estimate the H i emission in the far-IR, we have considered a H ii region (2″–4″) of $\sim$0.022 $M_\odot$ (see the model of Volk & Kwok 1997) with $n_1 = n_2$ and assumed that the H i population is given by the Saha-Boltzmann equation. With these parameters, we can predict the H i recombination lines observed in the mid-IR by Bernard Salas et al. (2001) and estimate the opacity of the far-IR lines. We found that only the $H\alpha\beta\gamma$ series, with $n$ ranging from 10 to 15, may produce modest emission in the LWS range. However, none of these lines appear between 90 and 110 $\mu$m. In addition, we have analyzed the possible overlapping with fine-structure lines. In particular, the [Ti ii] 96.68, 106.27 $\mu$m and [V ii] 97.79 $\mu$m lines could produce some emission in the considered range. Even assuming a vanadium abundance 10 times larger than the solar abundance, the [V ii] 97.79 $\mu$m ($^3D_3–^3D_2$) line would be extremely weak. Note that the [V ii] 141.68 $\mu$m ($^3D_2–^3D_1$) line is also not detected in NGC 7027. Finally, the solar abundance of Ti is $\sim$10 times that of vanadium. We also computed that that is too low to produce significant emission in the [Ti ii] 96.68, 106.27 $\mu$m lines. Hence, the integrated band intensity and the different lines or subbands could not be fully assigned to any of these atomic lines or to the pure rotational lines with significant line strength arising from the light species in the circumstellar envelope.

We also note that after subtracting the emission of CO, HCN, and HCN(vib) (pure rotational lines in vibrational excited states) from the spectrum of IRC +10216, some of the remaining peaks also agreed with the unidentified peaks observed in NGC 7027 (see Fig. 1). However, the spectral resolution is too poor to distinguish unidentified features from the forest of HCN(vib) rotational lines that contaminate the far-IR spectrum of IRC +10216 but are missing in NGC 7027. The HCN abundance in IRC +10216 is very high, $\sim3 \times 10^5$, with HCN/CO = 1/10. In fact, HCN is the main coolant of this C-rich AGB star (Cernicharo et al. 1996). However, the molecule is photodissociated during the post-AGB evolution as the UV radiation field from the evolving star increases. From far-IR observations of HCN pure rotational lines, Herpin et al. (2002) found minimum abundances of HCN/CO = 1/100 and 1/1000 for the proto-PNe CRL 2688 and CRL 618, respectively. The extreme case is NGC 7027, where a great part of HCN molecules must have been photodissociated into CN and H. In fact, Bachiller et al. (1997) found CN/HCN $\sim$10 for this object. Thus, the low abundance of HCN for NGC 7027 compared to IRC +10216 is consistent with the nondetection of far-IR HCN lines (Herpin et al. 2002). Pure rotational lines of other cyanopolyne species such as HCN cannot produce emission in this range because of the high energy levels associated with its far-IR transitions.

Taking into account the high S/N of the NGC 7027 spectrum and the absence of the band in sources such as Orion, Sgr A or O-rich evolved stars, we believe that the lines are real. Because of the chemistry of NGC 7027, the most probable carrier should be the low-energy bending mode of a polyatomic molecule containing carbon.

4. DISCUSSION

Both PAHs and pure carbon chains possess low-energy bending modes in the far-IR. Contrary to the UIB emission in the mid-IR, the far-IR skeletal modes of PAHs (vibrations associated with the bending of the skeletal structure) depends on the exact nature of the species. Hence, the vibrorational structure of the PAH skeletal mode has to be calculated for each specific PAH. For example, the lowest energy active mode of coronene (C24H12) lies at $\sim$127 cm$^{-1}$ (Joblin et al. 2002), while for ovalone (C32H14), two far-IR skeletal modes at $\sim$120 cm$^{-1}$ and $\sim$66 cm$^{-1}$ have been theoretically investigated (Mulas et al. 2003). The far-IR emission of a few PAHs have also been observed in gas-phase experiments (Zhang et al. 1996). However, if one of the observed UFIBs belongs to a specific PAH, other bands (generally stronger) should be observed in the IR spectrum. This is not the case of the new UFIB presented in this work, and we consider the low-energy modes of pure carbon chains as possible carriers of the observed UFIB.

The detection of several vibrorational lines of the $v_2$ bending mode of C3 (63 cm$^{-1}$) in Sgr B2 and IRC +10216 evidenced high abundances for this species and opened the possibility to detect more carbon chains in the ISM and CSM (Cernicharo et al. 2000). At the low resolution of the LWS/grating, the more intense C3 lines [$Q(2,4,6)]$ are blended with the strong [C ii] 158 $\mu$m line and no assignment could be made in NGC 7027. However, the tentative detection of the $v_5$ bending mode of C4 in many objects, including NGC 7027 ($\sim$174 cm$^{-1}$; Cernicharo et al. 2002), if confirmed, implies a C3/C4 $<$ 10 abundance ratio, which suggests that the abundance of C4 do not decrease drastically when $n$ increases.

In spite of their importance, the C6 bending modes are difficult to characterize spectroscopically in the laboratory or by ab initio computations. As expected, the main uncertainties complicating their astronomical detection are the band origin and the IR intensity. Moreover, the induced dipole moments and other spectroscopic constants are often known for the fundamental transition, but less or nothing is known about overtone transitions within the bending mode or transitions to other excited states, including the stretching modes.

The ground electronic state is different for the odd- and even-numbered cumulenic chains. This property determines the observed band shape of the bending mode. Odd-numbered linear Cn have a single $1\Sigma_g^+$ ground electronic state, which results in a perpendicular $^1\Pi_{\nu vib}–^1\Sigma_g^+$ vibronic spectrum with a strong $Q$ branch and weak $P$ and $R$ branches. On the other hand, even-numbered linear Cn have a triplet $3\Sigma_g^+$ ground electronic state. Hence, each rotational line is split in three components because of spin couplings. This splitting increases with the number of atoms but is particularly small for C4 and C6 (Giesen et al. 2001). The vibronic transition is now $^3\Pi_{\nu vib}–^3\Sigma_g^+$, and despite the null component of the electronic orbital momentum in the ground state, the spin-orbit constant

$^3$ The Atomic Line List (ver. 2.04) is available at http://www.pa.uky.edu/~peter/atomic.
(\(A_{SO}\)) could be large for even- \(C_n\). In such a case, the resulting band shape is notoriously affected by the value of \(A_{SO}\).

4.1. Tentative Detection of \(C_6\) and \(C_5\)

With the exception of the \(v_2\) mode of \(C_7\), the band origins of other \(C_n\) bending modes are not accurately constrained. Hence, their assignment as carriers of the UFIBs is not obvious. Although the low-lying bending modes of \(C_5\) and \(C_6\) have not been directly observed in gas phase, different studies suggest wavenumbers around \(\sim 100\) cm\(^{-1}\) (see below). The observed new UFIB around \(\sim 98\) \(\mu\)m is composed of several peaks at \(\sim 91.8, 92.8, 93.9, 95.2, 97.6, 98.9, 100.5,\) and \(101.7\) \(\mu\)m. In the following, we consider the possibility that any of these peaks is related to the \(v_\nu\) and \(v_\gamma\) bending modes of \(C_6\) and \(C_5\), respectively.

\(C_5\) was first detected in the gas phase by Heath et al. (1989), who observed the \(v_\nu\) stretching mode at \(\sim 2169\) cm\(^{-1}\) (\(\sim 4.6\) \(\mu\)m). The same mode was observed in IRC +10216 by Bernath et al. (1989). Actually, \(C_5\) is the largest \(C\) species detected in the CSM. On the other hand, \(C_6\) was first identified in the laboratory by its electronic spin-resonance spectrum in an Ar matrix (van Zee et al. 1987) and later observed in gas phase through its \(v_\nu\) stretching mode at \(\sim 1960\) cm\(^{-1}\) (\(\sim 5.1\) \(\mu\)m) by Hwang et al. (1993). Moazzen-Ahmadi et al. (1989) observed the \((v_3 + v_\nu) - v_\gamma\) and \((v_3 + 2v_\nu) - 2v_\gamma\) hot bands arising from the \(v_\gamma\) bending mode of \(C_5\). From the \(\nu\)-doubling constant \(g_\nu\), they estimated a frequency of \(v_\gamma = 118 \pm 3\) cm\(^{-1}\). More recently, \(C_5\) has been observed in photolysis spectra. In particular, Arnold et al. (1991) measured the \(2v_\nu\) transition and estimated \(v_\gamma = 101 \pm 45\) cm\(^{-1}\), while Kissopoulos et al. (1991) obtained \(v_\gamma = 107 \pm 5\) cm\(^{-1}\). Ab initio calculations predict an infrared intensity around \(36\) km mol\(^{-1}\) \([A(v_\nu = 1-0) \approx 0.06\) s\(^{-1}\); Hutter & Lüthi 1994; Martin et al. 1995]. Figure 1 shows the expected band shape for a \(\Pi_{\nu\text{vib}}\rightarrow\Sigma_{\nu\text{vib}}\) transition with this intensity and the molecular constants for the \(v_\gamma\) mode (Moazzen-Ahmadi et al. 1989) centered at 104.8 cm\(^{-1}\) (95.4 \(\mu\)m). As noted before, any of the band peaks observed in NGC 7027 around \(\sim 98\) \(\mu\)m (\(\sim 102\) cm\(^{-1}\)) could well be responsible of the \(v_\nu\) mode. However, only the best fit to the band including the \(C_6\) model is shown in Figure 1. If the carrier of the 95.5 \(\mu\)m feature is finally \(C_5\) at \(v_\nu = 104.8\) cm\(^{-1}\), the estimated column density, assuming an excitation temperature of 100 K (typical of a PN envelope), is \(N(C_5) = 1.8 \times 10^{14}\) cm\(^{-2}\). Assuming 1.5–4.0 mag of visual extinction in the neutral envelope (Hasegawa et al. 2000), the typical abundance of \(C_5\) in NGC 7027 would be (0.5–1.0) \(\times 10^{-7}\), similar to that derived by Bernath et al. (1989) for IRC +10216.

Figure 2 shows that, for the same column densities required to reproduce the bending modes, the \(v_\nu\) and \(v_\gamma\) stretching modes of \(C_6\) and \(C_5\) are not detected in NGC 7027. Different excitation conditions of the stretching and bending modes and geometrical effects may explain this conjecture. Although carbon clusters have a moderate size, we could also expect an efficient pumping of the stretching and bending modes through UV photons. Mid-IR photons could also contribute to the excitation of the high \(\nu\)-bending excited states and the stretching modes, as well. Finally, the low-energy bending modes could be pumped solely by the absorption of far-IR dust photons (see the case of the \(C_3\) excitation in Cernicharo et al. 2000). However, the smaller volume of the photon-dominated regions relative to the far-IR dusty envelope in NGC 7027 and the larger mid-IR flux of IRC +10216 (where the \(C_3\) and \(C_5\) stretching modes were detected) compared to NGC 7027 (a factor \(\sim 10^3\) at 5 \(\mu\)m but only a factor \(\sim 4\) at 100 \(\mu\)m) can favor the observation of the \(C_n\) bending modes within the large ISO beam. Under these conditions, the detection of the bending modes and the nondetection of the stretching modes in NGC 7027 is plausible.

The \(\nu_\nu\) low-energy bending mode of \(C_6\) is even less known. Ab initio calculations predict a \(\nu_\nu \sim 108\) cm\(^{-1}\) frequency and an infrared intensity of \(\sim 25\) km mol\(^{-1}\) \([A(\nu_\nu = 1-0) \approx 0.035\) s\(^{-1}\); Martin et al. 1990, 1995], while photoelectron spectroscopy experiments estimate \(\nu_\nu = 97 \pm 45\) cm\(^{-1}\) (Arnold et al. 1991) and \(\nu_\nu = 90 \pm 50\) cm\(^{-1}\) (Xu et al. 1997). Theoretical predictions have to be taken into account with caution, since they rely on the harmonic approximation, which can be in error for large amplitude benders such as radicals with low-lying electronic states. In particular, the infrared intensity has to be considered as a lower limit (and column densities as upper limits). Ab initio calculations do predict a low-energy bending band for \(C_6\) for open-shell species such as \(C_4\) or \(C_6\).

The term value for the \(1\Delta_\lambda\) lowest energy excited state of \(C_6\) has been recently determined by Xu et al. (1997) only at \(\sim 1400\) cm\(^{-1}\) from the ground. Hence, \(A_{SO}\) can effectively be larger even in the ground state (\(\lambda = 0\)). For example, the \(A_{SO}\) constant of \(C_4\) \((2\Sigma\) ground state\) is very large, \(\approx 3\) cm\(^{-1}\) (Yamamoto et al. 1987), because its \(2\Sigma\) electronic excited state is only \(\sim 468\) cm\(^{-1}\) above the ground. In the case of even-numbered \(C_n\) chains, \(A_{SO}\) can easily be larger because of the higher spin multiplicity of the ground state and the larger A value of the lowest lying electronic excited state. Figure 1 also shows the expected band shape for a \(\Pi_{\nu\text{vib}}\rightarrow\Sigma_{\nu\text{vib}}\) transition with \(A_{SO} = 3.5\) cm\(^{-1}\) (we estimated \(A_{SO} \approx 4\) cm\(^{-1}\) for \(C_4\)). The \(C_6\) molecular constants from Hwang et al. (1993) and van Zee et al. (1987, 1988), and the \(\nu_\nu\) band origin at 98.3 cm\(^{-1}\) (101.7 \(\mu\)m). Assuming the same excitation temperature as for \(C_5\), we derive \(N(C_6) = 0.8 \times 10^{14}\) cm\(^{-2}\). Hence, the \(C_6\) abundance will be a factor 2 smaller than that of \(C_5\).

Much more work has to be done to fully understand and characterize the low-energy vibrations of \(C_n\) chains in order to assign the UFIBs observed by ISO. The cyclic \(C_4n\) isomers could also produce spectral features in the far-IR; however, their active modes are even less known. While waiting for progress in this direction, space observations offer the unique opportunity to obtain spectra in the far-IR domain in which the bending modes appear and to motivate further laboratory and theoretical studies. The presence of small \(C_n\) chains in space, as well as their high reactivity suggest that these species may be involved in the formation of more complex organic molecules. In fact, for cumulenic clusters with \(n = 10\) to 20, linear structures are thought to close into rings, while for \(n > 30\), these species are thought to be more stable in aromatic and fullerene-like structures (O’Brien et al. 1988).

Future space heterodyne telescopes such as the Herschel Space Observatory, with much better sensitivity and spectral resolution in the far-IR, should allow the detection of longer \(C_n\) chains through their low-energy bending modes. This will be the fingerprint needed to understand the formation and the nature of the UIB and UFIB carriers.

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