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An *ISO* Long Wavelength Spectrometer detection of CH in NGC 7027 and an HeH^+ upper limit

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ABSTRACT

We have detected an emission line at 149.18 ± 0.06 μm in the ISO Long Wavelength Spectrometer (LWS) grating spectrum of the planetary nebula NGC 7027. This line coincides in wavelength with both the HeH^+ $J=1$–0 fundamental pure rotational line at 149.14 μm and the CH $^2\Pi_{3/2}$ (F_2) $J=3/2$–$^2\Pi_{1/2}$ (F_2) $J=1/2$ fundamental pure rotational lines at 149.09 and 149.39 μm. Another feature of similar strength at 180.7 μm is well-fitted by the CH doublet $^2\Pi_{1/2}$ (F_1) $J=5/2$–$3/2$ at 180.48 and 180.93 μm. We therefore attribute both the 149.18- and 180.7-μm lines to CH, the first evidence of this molecule in NGC 7027 and the first detection anywhere of the far-infrared lines of CH in emission. We estimate a CH/CO abundance ratio of ~0.06 and a CH/CH^+ ratio of ~0.2, the latter being more than an order of magnitude lower than predicted for photodissociation regions. The contribution from the HeH^+ $J=1$–0 line to the 149.18-μm feature is at least a factor of three lower than the predictions of Cecchi-Pestellini & Dalgarno (1993).

Key words: atomic processes – ISM: molecules – planetary nebulae: general – planetary nebulae: individual: NGC 7027.

1 INTRODUCTION

The Long Wavelength Spectrometer (LWS; Clegg et al. 1996) on board the *Infrared Space Observatory* (*ISO*; Kessler et al. 1996) provides the opportunity to study molecular species by observations of pure rotational transitions which fall within its 43–197-μm spectral range. Many arise from key molecules, such as HD, OH, H_2O, CH, CH^+ and CH_2^+, which are expected to be abundant in the dense hot layers of photodissociation regions (PDRs). In particular, the C-rich planetary nebula (PN) NGC 7027 affords an interesting case for the study of the carbon chemistry in dense molecular material exposed to intense UV radiation fields (e.g. Cox 1997). A preliminary analysis of early LWS grating observations of NGC 7027 was presented by Liu et al. (1996, hereafter L96). Amongst the lines reported is a weak feature at 149.23 μm, which was tentatively assigned to CH. The feature coincides also in wavelength with the HeH^+ $J=1$–0 fundamental pure rotational line. With more observations and a better calibration, we have reanalysed all the LWS grating spectral observations of NGC 7027, in an effort to obtain better constraints on the assignment of this feature and its implications for the CH and HeH^+ chemistry.

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The possibility that HeH^+ may exist in astrophysical environments was introduced by Dabrowski & Herzberg (1978). As it is composed of the two most abundant elements in the Universe, HeH^+ is of fundamental astrophysical importance, particularly for the chemistry of the early Universe before the first generation of massive star formation, when the Universe was free of heavy elements (Hirasawa 1969; Dalgarno & Lepp 1987). Early predictions of HeH^+ abundances and emission line intensities in nebulae (Black 1978; Flower & Roueff 1979) suggested that HeH^+ would be difficult to detect. Detailed calculations of HeH^+ formation and destruction mechanisms in astrophysical plasmas (Roberge & Dalgarno 1982) showed that HeH^+ might be detectable in PN and in dense molecular clouds subject to X-ray and extreme UV ionization, via its $J=1$–0 pure rotational line at 149.14 μm and its $v=1$–0 $R(0)$ and $P(2)$ rovibrational lines at 3.364 and 3.608 μm. NGC 7027 has one of the hottest central stars known for a PN ($T_{\rm eff} \geq 140\,000$ K: Gruenwald & Péquignot 1989; Middlemass 1990), needed for an appreciable HeH^+ formation rate, while its very high nebular electron density (5–7×10^4 cm^{-3}) ensures that any HeH^+ that is created will be efficiently excited (we note that HeH^+ is predicted to be formed, and excited by electron collisions, entirely within the *ionized* zone of the nebula). These properties of NGC 7027 make it one of the most promising astronomical sites for detecting HeH^+ in space. An early ground-based search (Moorhead et al. 1988, hereafter M88) for the HeH^+ $v=1$–0 $R(0)$ and $P(2)$ lines from NGC 7027 yielded a flux upper limit of 3.7×10^{-14} erg cm^{-2} s^{-1} for the $R(0)$ line. Detailed predictions of the HeH^+ emission line intensities from NGC 7027 are made by Cecchi-Pestellini & Dalgarno (1993, hereafter CD93), using specific models of the nebula. Their predicted intensities should be reduced by a factor of four because of an error in the rate coefficient of the formation reaction $He^+ + H \rightarrow HeH^+ + \gamma$ (Stancil & Zygelman 1996). When the correction is made, the predicted intensities are consistent with the measured upper limit of M88.

CH was first detected in the interstellar medium via observations of its optical absorption lines from the ground state (Adams 1941; McKellar 1941) and its radio ground-state Λ-doubling 3.3-GHz transitions (Rydbeck, Elldér & Irvine 1973; Turner & Zuckerman 1974). The 700-MHz Λ-doubling transitions from its $^2\Pi_{1/2}$ (F_1) $J=3/2$ first excited rotational level have also been detected (Ziurys & Turner 1985). The first detection of the fundamental pure rotational lines of CH at 149.09 and 149.39 μm, in absorption, was reported by Stacey, Lugten & Ganzel (1987) for the line of sight towards the bright far-infrared source Sgr B2. Observations of these far-infrared lines in emission had, however, not been reported at that time.

2 OBSERVATIONS

The results presented here are based on an analysis of all the LWS full grating scan observations of NGC 7027, carried out up to *ISO* revolution (Rev.) 377. In total, there are nine separate observations, each covering a wavelength range from 43–195 μm, 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 (Swinyard et al. 1996). The observation from Rev. 27 consists of three 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 μm from the SW1–SW5 detectors ($\lambda < 93$ μm) and 0.6 μm from the LW1–LW5 detectors ($\lambda > 84$ μm). Each of the five observations obtained between Revs. 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 23 930 s. The LWS has a circular aperture of full width at half maximum (FWHM) diameter 70 arcsec, significantly larger than the ionized or neutral regions of NGC 7027. The fluxes derived from the individual independent observations are in good agreement and we estimate an accuracy of better than 20 per cent for the absolute flux calibration.

3 RESULTS

The rotational constants of Purder et al. (1992) yield wavelengths of 149.1371 and 74.7850 μm for the HeH^+ $J=1$–0 and $j=2$–1 transitions, respectively. They agree to within six parts in a million with the recent experimental results of Liu & Davies (in preparation) for the HeH^+ rovibrational lines. The $J=1$–0 and $J=2$–1 lines have now been directly observed in the laboratory using a high-precision far-infrared spectrometer, yielding accurate wavelengths of 149.13685(1) and 74.784849(4) μm (Matsushima, Oka & Takagi 1997). We take the wavelengths of CH lines from Brown & Evenson (1983).

Fig. 1 shows the 142–161-μm spectrum of NGC 7027. A line with an observed wavelength of 149.18 ± 0.06 μm and a flux of $(4.2 \pm 0.6) \times 10^{-13}$ erg cm^{-2} s^{-1} is clearly present. The derived wavelength and flux of the 149.18-μm feature agree well with the earlier measurements by L96. The current spectrum has a better signal-to-noise (S/N) ratio and reveals new features that were previously unseen. The measured wavelength of 149.18 ± 0.06 μm agrees within the errors with the laboratory wavelength of 149.14 μm for the $J=1$–0 line of HeH^+ and the average wavelength of the CH $^2\Pi_{3/2}$ (F_2) $J=3/2$–$^2\Pi_{1/2}$ (F_2) $J=1/2$ fundamental pure rotational doublet at 149.09 and 149.39 μm, which have a wavelength split of only half the current spectral resolution element. The feature was tentatively assigned to CH by L96. To test this assignment, we have made a careful search for other CH lines that fall within the LWS window. These include the $^2\Pi_{1/2}$ (F_2) $J=5/2$–3/2 lines at 180.48 and 180.93 μm, the $^2\Pi_{1/2}$ (F_1) $J=7/2$–5/2 lines at 118.40 and 118.70 μm, and the $^2\Pi_{3/2}$ (F_2) $J=5/2$–3/2 lines at 115.60 and 115.93 μm. A broad feature at 180.7 μm, partially blending with the strong CH^+ $J=2$–1 line at 179.61 μm (Cernicharo et al. 1997), is clearly detected and can be well-fitted by the CH doublet at 180.48 and 180.93 μm, giving a total flux of $(3.3 \times 0.4) \times 10^{-13}$ erg cm^{-2} s^{-1} (Fig. 2). The red component of the doublet is 20 per cent brighter than the blue one, though the difference is within the measurement errors. Other possible carriers for this weak feature include the $J=2$–1 line of $^{13}CH^+$ at 180.68 μm and the 2_{21}–2_{12} line of ortho-H_2O (o-H_2O) at 180.49 μm. The possibility of a significant contribution from $^{13}CH^+$ can be ruled out on the basis

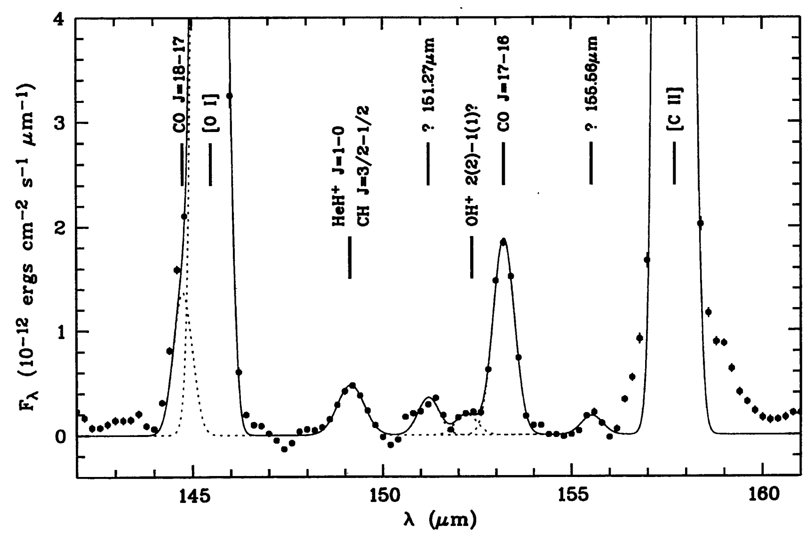

Figure 1. The *ISO* LWS grating spectrum of NGC 7027 from 142–161 μm, after subtraction of the nebular dust continuum. The solid line is the sum of Gaussian fits to the observed line profiles. Contributions from individual components of a blending feature are shown as dotted lines. The [C II] 157.74-μm and [O I] 145.52-μm lines are respectively 32 and 16 times stronger than the CO $J=17$–16 line. A feature with an observed wavelength of 149.18 ± 0.06 μm is clearly present, coinciding in wavelength with the $J=1-0$ fundamental pure rotational line of HeH^+ at 149.14 μm and with the $^2\Pi_{3/2}$ (F_2) $J=3/2$–$^2\Pi_{1/2}$ (F_2) $J=1/2$ fundamental pure rotational lines of CH at 149.09 and 149.39 μm. The weak feature at 152.28 μm is possibly due to the OH^+ 2(2)–1(1) line at 152.37 μm, whereas the features at 151.27 and 155.56 μm are unknown. Unidentified weak features can also be seen in the red wing and possibly also in the blue wing of the [C II] line.

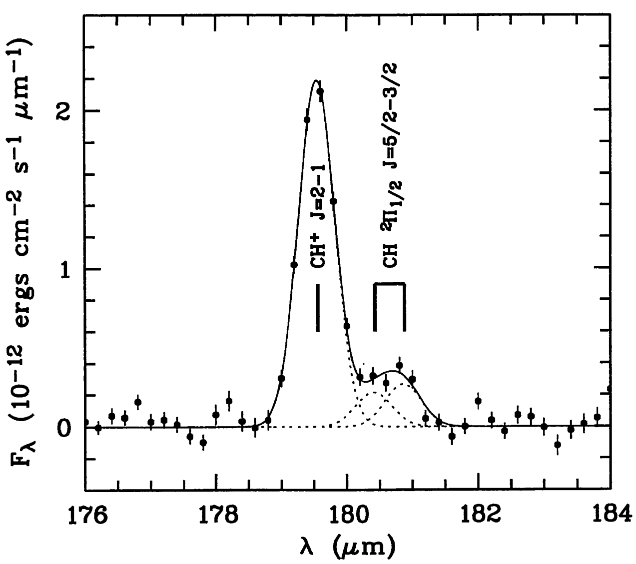

Figure 2. The LWS spectrum of NGC 7027 from 176–184 μm, after subtraction of the nebular dust continuum. The broad feature redwards of the CH^+ 179.61-μm line is attributed to the CH doublet at 180.48 and 180.93 μm. The sum of three Gaussians (solid line) of equal line width was used to fit the whole blend, with the differences between the central wavelengths of individual components fixed to those given by the laboratory values for CH^+ and CH. The dotted lines show contributions from the individual components.

of the very large $^{12}C/^{13}C$ isotope ratio (≥ 65) measured by Kahane et al. (1992) for NGC 7027 and the measured flux of the $^{12}CH^+$ line at 179.61 μm, which is at most only moderately optically thick ($\tau\sim1$; Cernicharo et al. 1997). Similarly, from the weakness of the probable o-H_2O 2_{21}–1_{10} line at 108.07 μm (Cernicharo et al. 1997), which has the same upper level as the o-H_2O 180.49-μm line, we estimate any contamination to the observed feature at 180.7 μm from the o-H_2O 180.49μm line to be less than 15 per cent of the measured flux. A weak feature at 115.71 ± 0.10 μm, with a flux of $(2.0\pm0.5)\times10^{-13}$ erg cm^{-2} s^{-1}, is possibly due to the CH doublet at 115.60 and 115.93 μm. The CH 118.40, 118.70 μm doublet is blended with the CO $J=22$–21 118.58-μm line. From the fluxes of the adjacent CO lines, we estimate the contribution of the CH 118.40, 118.70-μm doublet to the feature to be less than 1×10^{-13} erg cm^{-2} s^{-1}. We conclude that the above line identifications strengthen the case for the presence of CH in NGC 7027 and rule out a significant contribution of HeH^+ to the line detected at 149.18 μm. This is the first time that CH has been detected in emission in the far-infrared (far-IR). The implications of these findings are discussed below.

4 DISCUSSION

4.1 CH lines

Detailed calculations of the chemistry in dense photodissociation regions (Sternberg & Dalgarno 1995) show that a significant amount of CH can be formed via the dissociative recombination of CH_2^+ and CH_3^+. The latter two species are formed in a sequence of reactions initiated by the rapid formation of CH^+, resulting from the elevated temperatures in dense PDRs exposed to strong UV radiation fields. This scenario is supported by the recent detection of CH^+ in the LWS spectrum of NGC 7027 (Cernicharo et al. 1997). In the models of Sternberg & Dalgarno (1995), most of the CH forms in the warm PDR, peaking at a temperature of 800 K.

The observed CH lines are excited by collisions with atomic and molecular hydrogen. Only restricted information on the collisional excitation rates of CH by H and H_2 impacts is available (Bouloy, Nguyen-Q-Rieu & Field 1984) and we have used the $OH+H_2$ collisional de-excitation rates calculated by Dewangan, Flower & Alexander (1987), who used the close-coupling method but with the modified potential surface of Kochanski & Flower (1981). With a dipole moment of 1.46 Debye (Phelps & Dalby 1966), the $^2\Pi_{1/2}$ (F_2) $J=3/2$ first excited rotational level of CH has a critical density of $\sim 4\times10^6$ cm^{-3}, while all the other excited levels have a critical density in excess of 10^8 cm^{-3}. Analysis of the far-infrared CO lines suggests that the warm PDR of NGC 7027 has a density of $n(H_2)\sim10^5$–10^6 cm^{-3} (L96). At such densities, only the lowest two rotational levels of CH, $^2\Pi_{1/2}$ (F_2) $J=1/2$ and $^2\Pi_{1/2}$ (F_1) $J=3/2$, will be significantly populated. For $n(H_2)=10^5$ cm^{-3}, the fractional population of CH in the $^2\Pi_{1/2}$ (F_1) $J=3/2$ level is a few per cent, which increases to nearly 30 per cent for $n(H_2)=10^6$ cm^{-3}. The fractional population could be higher if the $^2\Pi_{1/2}$ (F_1) $J=3/2$–$^2\Pi_{1/2}$ (F_2) $J=1/2$ line at 560 μm is optically thick. Collisional excitation from both the $^2\Pi_{1/2}$ (F_2) $J=1/2$ and $^2\Pi_{1/2}$ (F_1) $J=3/2$ states may thus contribute to the emission in the 149.2- and 180.7-μm lines. For $n(H_2)=10^5$ cm^{-3}, the CH doublets at 180.7 and 149.2 μm have an intensity ratio of ~0.8, i.e. identical to the observed value of 0.8 ± 0.2, if we assume that the observed line at 149.18 μm is entirely due to CH.

The total number of emitting CH molecules derived from the observed fluxes of the CH 149.2- and 180.7-μm lines is insensitive to the relative populations of these two lowest rotational levels, but is inversely proportional to the adopted density. For $n(H_2)=10^5$ cm^{-3}, we find the total number of CH molecules to be $\sim1\times10^{50}$, yielding a CH/CO ratio of 0.06, if we adopt L96's value of the total number of *warm* (~1000 K) CO molecules derived from the far-IR pure rotational lines.

Assuming a local thermodynamic equilibrium (LTE) level population for CH^+, Cernicharo et al. (1997) find a total number of CH^+ ions for NGC 7027 of $\sim2.5\times10^{47}$. The LTE assumption requires the gas density to be significantly higher than the critical densities of CH^+ lines, which are similar to those of CH, i.e. $\gtrsim10^8$ cm^{-3}. Cernicharo et al. also provide a second estimate of the CH^+ abundance based on large velocity gradient (LVG) calculations. They found that the observed CH^+ fluxes can be roughly explained by a density of $\sim5\times10^7$ cm^{-3} and CH^+ column density of 2.5×10^{14} cm^{-2}. For an assumed size of about 6 arcsec of the PDR in NGC 7027 at a distance of 700 pc, the latter corresponds to a total number of CH^+ ions of $\sim1.5\times10^{48}$. For a gas density of $\sim5\times10^7$ cm^{-3}, the total number of CH molecules required to explain the observed CH 149.2- and 180.7-μm line fluxes is approximately 2×10^{47}, yielding a CH/CH^+ abundance ratio of ~0.1. LVG excitation calculations for CH, assuming similar parameters for the density and size of the PDR and nebular distance as in Cernicharo et al., yield a CH column density of $\sim10^{14}$ cm^{-2}, implying a CH/CH^+ abundance ratio of ~0.4. The CH/CH^+ abundance ratio of less than unity derived here is significantly lower than the predictions of Sternberg & Dalgarno (1995), by nearly an order of magnitude. We stress that although the total number of CH and CH^+ molecules deduced from the observed CH and CH^+ line fluxes depend on the assumed density of the PDR, which is not well constrained by the observations, the CH/CH^+ abundance ratio is largely independent of the adopted density, provided it is lower than the CH and CH^+ critical densities of a few $\times10^8$ cm^{-3}, an assumption which is likely to be valid. However, the derived CH/CH^+ abundance ratio is inversely proportional to the ratio of the collisional excitation rates of CH and CH^+, which are both unknown. A more reliable CH/CH^+ abundance ratio therefore requires accurate collisional excitation rate coefficients to become available. In addition, electron impacts may be important in exciting the CH^+ lines. Inclusion of this process in the excitation analysis of CH^+, ignored in Cernicharo et al. because of a lack of relevant data, would lower the derived CH^+ abundance, yielding a CH/CH^+ abundance ratio in better agreement with the theoretical predictions. Alternatively, it is also possible that the branching of the dissociative recombination of CH_2^+ to form CH is smaller than assumed in the PDR chemistry models.

4.2 Non-detection of HeH^+

CD93 predict the column emission intensities of the $J=1$–0 HeH^+ pure rotational line at 149.14 μm, and of the $v=1$–0 $R(0)$ 3.364-μm and $P(2)$ 3.608-μm rovibrational lines, for two detailed nebular models for the ionized region of NGC 7027, constructed by Gruenwald & Péquignot (1989) and by Middlemass (1990). Both nebular models yielded satisfactory descriptions of the UV, optical and the then-available infrared line and dust continuum emission of NGC 7027. For both models, CD93 predicted a similar intensity ratio for the 149.14- and 3.364-μm lines, $I(\lambda149.14$ μm$)/I(\lambda3.364$ μm$)=10.6$. Thus the flux upper limit of 3.7×10^{-14} erg cm^{-2} s^{-1} for the $R(0)$ line obtained by M88 should correspond to an upper limit of 3.9×10^{-13} erg cm^{-2} s^{-1} for the 149.14-μm line, which is compatible with our measured flux of $(4.2\pm0.6)\times10^{-13}$ erg cm^{-2} s^{-1} for the line at 149.18 ± 0.06 μm. The measured flux is consistent, within a factor of two, with the predicted fluxes for the HeH^+ $J=1$–0 line for either of the two models of CD93, when corrected for the revised rate coefficient. No line is detected in the current spectrum at the wavelength of the HeH^+ $J=2$–1 74.78-μm line, with a 3σ flux upper limit of 5×10^{-13} erg cm^{-2} s^{-1}. In the models of CD93, no HeH^+ rotational line other than the $J=1$–0 line has a detectable intensity, due to almost all of the HeH^+ population being in the ground state and the dipolar electron collisions solely selecting upward excitations with $\Delta J=1$.

Despite the close agreement found between the measured flux of the 149.18-μm line detected in our LWS spectrum of NGC 7027 and the theoretical predictions for the HeH^+ $J=1$–0 149.14-μm line, the detection of the feature at 180.7 μm, which currently has no obvious carrier other than the CH 180.48-, 180.93-μm doublet, and the fact that the intensity ratio of the 149.2- and 180.7-μm features is consistent with what is expected for the two CH doublets for a density of $n(H_2)=10^5$ cm^{-3}, strongly suggests that both the 149.2- and the 180.7-μm features actually arise from CH. We can thus use the observed flux of the CH 180.7-μm doublet and the predicted CH $I(180.7$ μm$)/I(149.2$ μm$)$ intensity ratio to estimate the contribution to the observed feature at 149.2 μm from the HeH^+ $J=1$–0 149.14-μm line. For $n(H_2)=10^5$ cm^{-3}, we thus find the maximum contribution from the HeH$^+$ $J=1-0$ line to the 149.18-μm line to be less than $\sim 8 \times 10^{-14}$ erg cm^{-2} s^{-1}, which is a factor of 6–9 lower than the (corrected) predictions of CD93. On the other hand, the predicted CH I(180.7 μm)/I(149.2 μm) ratio increases with density, approaching an asymptotic value of 1.6 at high densities when the two lowest CH rotational levels become thermalized. At $n(H_2)=10^6$ cm^{-3}, I(180.7 μm)/I(149.2 μm) $\sim$1.1. For this case, the observed flux of the CH 180.7-μm doublet corresponds to a predicted flux of $(3.0 \pm 0.4) \times 10^{-13}$ erg cm^{-2} s^{-1} for the CH 149.2-μm doublet, yielding a possible contribution of the HeH$^+$ $J=1-0$ line of $(1.2 \pm 0.7) \times 10^{-13}$ erg cm^{-2} s^{-1} to the feature at 149.18 μm, a factor of 3–6 smaller than the (corrected) predictions of CD93. Usage of the OH + H_2 collisional de-excitation rates calculated by Offer & van Dishoeck (1992) in coupled-states formulation but with the original potential surface of Kochanski & Flower (1981) predicts a slightly smaller CH I(180.7 μm)/I(149.2 μm) intensity ratio at a given density, yielding an even smaller estimate of any contribution from HeH$^+$ to the observed 149.2-μm feature.

The near-coincidence in wavelengths of the CH and HeH$^+$ lines makes the detection of HeH$^+$ by observation of its rotational emission at 149.14 μm unlikely. A search for the $v=1-0$ $R(0)$ and $P(2)$ lines, at 3.364 and 3.608 μm respectively, may be more productive. The expected fluxes for NGC 7027, based on a value of 1×10^{-13} erg cm^{-2} s^{-1} for the rotational line at 149.14 μm and the theoretical models of CD93, are 3×10^{-14} erg cm^{-2} s^{-1} for the $P(2)$ line and 1×10^{-14} erg cm^{-2} s^{-1} for the $R(0)$ line.

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