An infrared L- and M-band spectral survey, performed toward the young planetary nebula NGC 7027 with the iSHELL instrument on NASA’s Infrared Telescope Facility (IRTF), has revealed more than 20 vibrational lines of the molecules HeH$^+$, H$_2$, and CH$^+$ and more than 50 spectral lines of atoms and atomic ions. The present paper focuses on the atomic line emissions, the molecular lines having been discussed in two previous publications. The atomic lines detected with high confidence in the 2.951–5.24 μm region covered (incompletely) by this survey comprise (1) six collisionally excited lines of metal ions that had previously been identified in astrophysical nebulae but for which the present observations provide the most accurate wavelength determinations obtained to date; (2) a spectral line at 4.6895 μm, not previously reported, for which the probable identification is the $^2P_{7/2}{-}^4P_{9/2}$ fine-structure transition of [Zn VI]; (3) 39 recombination lines of H and He$^+$, with upper states of principal quantum number up to 38 (H) or 24 (He$^+$); (4) 10 recombination lines of the multielectron species He, C$^{2+}$, and C$^{3+}$.

Unified Astronomy Thesaurus concepts: Planetary nebulae (1249); Interstellar line emission (844); Infrared astronomy (786); Atomic spectroscopy (2099)

1. Introduction

Planetary nebulae are heated, photoionized, and photodissociated by the continuum emission from a hot central star with an effective temperature that may exceed 200,000 K. They are characterized by line emission from a multitude of species that include neutral atoms, atomic ions (some—such as Ne$^{4+}$—with appearance potentials in excess of 100 eV), diatomic and polyatomic molecules, and molecular ions. The latter include the HeH$^+$ cation, the astrophysical discovery of which was reported recently toward the young, carbon-rich planetary nebula NGC 7027 (Güsten et al. 2019). This detection of HeH$^+$, obtained through SOFIA/GREAT observations of its fundamental rotational transition in the far-IR spectral region, was followed by the detection of two HeH$^+$ rovibrational lines using the infrared spectrograph, iSHELL, on the Infrared Telescope Facility (IRTF) on Maunakea (Neufeld et al. 2020, hereafter Paper I). The iSHELL observations reported in Paper I also led to the serendipitous discovery of rovibrational emissions from the CH$^+$ molecular ion, motivating a more extensive L- and M-band survey discussed in Neufeld et al. (2021, hereafter Paper II).

While the previous papers in this series have focused on the infrared molecular emissions observed from NGC 7027, the present paper discusses the many spectral lines of atoms and atomic ions that have also been detected. A recent discussion of the source has been presented in Papers I and II and will not repeated here. In Section 2 below, I discuss the iSHELL observations performed toward NGC 7027 and the methods used to reduce the resulting data. The results are presented in Section 3, and the key findings are discussed in Section 4: these include the most accurate wavelength determinations yet obtained for several fine-structure transitions, the likely discovery of a fine-structure line of [Zn VI], and a comparison of the relative strengths of the observed hydrogen and helium recombination lines with theoretical predictions. A summary follows in Section 5.

2. Observations and Data Reduction

The observations reported in Paper I were performed at the IRTF on 2019 July 19 and September 6 UT with the iSHELL spectrograph (Rayner et al. 2016) in its Lp1 and Lp2 modes respectively. These were followed on 2020 July 8, 13, 14, and 15 UT by observations with the Lp3, L2, L1, M1, and M2 settings. Unfortunately, the night of 15 July UT was mainly cloudy and no usable data could be acquired with the M2 setting. Because the free spectral range of the spectrograph cannot be covered fully by the M-band detector, two settings (M1 and M2) are needed to obtain a full M-band spectrum; without usable data from the M2 setting, the M-band spectrum obtained from these observations therefore shows small wavelength gaps between the spectrograph orders. These gaps account for roughly 8% of the M-band (4.517–5.239 μm) spectral coverage. Moreover, in the region of spectral overlap between the L1 and L2 settings, the L2 observations performed on 2020 July 13 yielded data of considerably higher quality than the L1 observations; moreover, the spectral region shortward of 2.951 μm that is covered by L1 but not L2 was severely affected by telluric lines. The L1 data obtained on 2020 July 14 were therefore of little utility and were also excluded from the analysis. The resultant survey therefore provides complete coverage of the L-band spectral region from 2.951 to 4.155 μm. The observing and data reduction procedures were similar for all observations and were described in detail in Paper I and summarized in Paper II. The observations involved the use of a narrow slit—of width 0″375 and length 15″—that was oriented along the minor axis of the nebula at position angle 59° east of north. The spectral resolving power achieved with this 0″375 slit is $\lambda/\Delta\lambda = 80,000$. The wavelength calibration
procedure made use of telluric lines (along with lines from a thorium–argon arc lamp in the case of the L1 mode); the accuracy of the wavelength measurements it enabled for the spectral lines observed from NGC 7027 is discussed in Section 4.1 below.

3. Results

Figure 1, covering the 4.0–4.1 μm region, shows an example of the full-slit spectra that are obtained by summing the signal over all 15 extraction regions. Ten emission lines are readily identified in this small fraction (∼6%) of the available spectral coverage. For the same example spectral region, Figure 2 provides information about the spatial variation of the intensity along the slit. Here, the vertical axis represents the distance along the slit, and the intensity is color-coded on a logarithmic scale as a function of position and wavelength. For an isolated spectral line, Figure 2 shows a position–velocity (PV) diagram of the type presented in Paper II (their Figures 2–4). The ring-like morphology typically exhibited here is precisely that expected for an expanding shell when long-slit spectroscopy is performed with the slit positioned along the diameter.

To implement a uniform criterion for line detection, I have developed a template-fitting algorithm. Here, the PV diagrams

Figure 1. Sample spectrum covering the 4.0–4.1 μm range, summed over the full slit length. The wavelength scale is for an assumed LSR velocity of 25 km s\(^{-1}\) for the source. This value is the mean LSR velocity of the ionized nebula as determined (Paper I) from a Gaussian fit to the H\(\text{I}\) 19–6 line.
for five spectral lines are adopted as templates. The template transitions are all unblended, detected at a high signal-to-noise ratio, and have rest wavelengths that are known to high accuracy. They are the He II 7–6, He I 53F0–43D, H I 14–6, CH+ v = 1–0 P(5), and H2 ν = 1–0 O(5) transitions, each of which shows a slightly different morphology in the PV diagram. These templates are then shifted in wavelength, and the linear correlation coefficient between these templates and the observed position–wavelength diagram (e.g., Figure 2) is computed as a function of wavelength. Figure 3 shows the resultant correlation coefficients, plotted in red, green, blue, magenta, and black respectively for the five transitions listed above. Local maxima appear at the rest wavelengths of possible lines that are detected. Moreover, a possible line identification may be suggested by observing which of the five templates yields the largest correlation coefficient. Vertical lines in Figure 3 indicate the locations of the local maxima and are labeled with the rest wavelength in microns. These lines and labels are color-coded with the same colors as the plotted curves. For all nine of the spectral lines attributable to species in the template set (i.e., to H, He, He+), this methodology yields the correct line identification, revealing two lines of CH+, three lines of

Figure 2. Sample position–wavelength diagram covering the 4.0–4.1 μm range, showing the variation of the intensity along the slit. The color bar shows—which a logarithmic scale—the intensity relative to the maximum intensity achieved within the 4.0–4.1 μm wavelength range.
He I, two lines of He II, and two lines of H I. The tenth line shown in Figure 3, at a wavelength of 4.0862 μm, is a fine-structure transition of [Ca VII].

As expected, given the highly ionized nature of this species, its PV diagram is most similar to that of the He II 7–6 template.

For clarity, the wavelength region close to the He I 53 F0–43 D transition is shown on an expanded scale in Figure 4. Because this line is itself a template line, the correlation coefficient plotted in green reaches unity at the precise wavelength of the transition. For the different templates, there are small shifts in the location of the peaks; these reflect small differences in the velocity centroids for the different template lines.

This algorithm yields the line lists given in Table 1 for H I recombination lines and Table 2 for He I and He II recombination lines. To be included in these tables, the maximum correlation coefficient had to exceed a threshold that was set at 0.7; with that threshold, every line but one was correctly identified by the algorithm. That exception was the H I 33–6 transition, for which the best-correlated template (second column from right) was the He II 7–6 transition instead of H I 14–6.

Tables 1 and 2 show the observed rest wavelength of each line λ0, as determined with the template-fitting algorithm, along with the laboratory or theoretical determination of the line wavelength, λ0. The values of λ0 are those appearing in the Atomic Line List v3.00b4 (hereafter AtLL) compiled by van

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1 A secondary local maximum appearing slightly redward of the strong feature at 4.0523 μm (H I 5–4; Brackett-α) lacks any obvious identification as a distinct line and may originate from redshifted ionized gas; it is also apparent as a red wing on the Brackett-α line in the full-slit spectra plotted in Figure 1.

2 This was a case in which the correlation coefficients with the two template transitions were very nearly equal: 0.809 and 0.804, respectively, for the He II 7–6 and H I 14–6 transitions.
Hoof (2018). The rms fractional discrepancy between $\lambda_{\text{obs}}$ and $\lambda_0$ was $7.4 \times 10^{-6}$ for the lines listed in Tables 1 and 2, corresponding to a Doppler velocity of $2.2 \text{ km s}^{-1}$ at the wavelengths of relevance. This is somewhat smaller than the velocity resolution of the spectrograph ($3.75 \text{ km s}^{-1}$). The maximum fractional discrepancy was $2.3 \times 10^{-5}$. Although small, these discrepancies greatly exceed the uncertainties in the laboratory or theoretical determinations of the line wavelengths. Thus they provide a measure of the accuracy to which line wavelengths may be determined when the template-fitting algorithm is applied to the NGC 7027 data.

Table 1 and 2 also show the peak correlation coefficients achieved at wavelength $\lambda_{\text{obs}}$ and the template that yields the maximum correlation. The rightmost column lists the line fluxes, determined by the method that was described in Paper II and is discussed briefly below.

Figure 5 shows the PV diagrams for a selection of H I recombination lines. Each pixel covers 1″ in the spatial dimension and 5 km s$^{-1}$ in the velocity dimension. Here, unlike in Figure 2, the intensities are normalized to the maximum value individually in each panel, and the color bar applies to the intensity on a linear, not logarithmic, scale. The yellow rectangle in the panel for H I $n = 14 - 6$ shows the region over which the intensity was integrated to obtain the flux of that line in Table 1. White circles indicate the brightest $N_{\text{pix}}$ pixels, where $N_{\text{pix}}$ (47 in this case) is chosen to optimize the signal-to-noise ratio for the total flux in this subset of pixels. As described in Paper I and discussed briefly below, the fluxes for other H I lines are obtained by computing their strengths, relative to the H I $14 - 6$ line, in this subset of pixels. This method—which assumes an identical intensity distribution (in position and velocity) for all H I lines—improves the accuracy of the flux estimates for weak lines.

The H I recombination lines with PV diagrams shown in Figure 5 have fluxes that range over three orders of magnitude from the Br$\alpha$ line ($n = 5 - 4$) to the 38–6 line. The smaller signal-to-noise ratios for the weaker lines are readily apparent in the plots. For the 18–6 line, a vertical stripe centered near an LSR velocity of $5 \text{ km s}^{-1}$ is also apparent. This arises at the position of a terrestrial atmospheric feature, where the imperfect subtraction of a sky emission line leaves a residual that is independent of slit position. The affected velocity range

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**Figure 4.** Enlarged version of Figure 3, covering the 4.034–4.040 μm range. The feature detected here is the He I $5^{3}P_{0} - 4^{3}D$ line.
Table 1
Hydrogen Recombination Lines Observed toward NGC 7027

| iSHELL mode | Line | \( \lambda_{\text{obs}} \) (\( \mu \)m) | \( \lambda_0 \) (\( \mu \)m) | \( \lambda_{\text{obs}} - \lambda_0 \) (10^{-5} \( \mu \)m) | Correl. Coeff. | Best Template | Flux \(^a\) |
|-------------|------|-----------------|-----------------|-----------------|--------------|---------------|------|
| L2          | H I  | 10–5            | 3.039193        | 3.039202        | −0.9         | 0.980         | H I 146.3 |
| Lp1         | H I  | 9–5             | 3.296994        | 3.296992        | 0.2          | 0.984         | H I 301.6 |
| Lp1         | H I  | 38–6            | 3.366233        | 3.366265        | −3.2         | 0.780         | H I 2.5   |
| Lp1         | H I  | 34–6            | 3.387807        | 3.387845        | −3.8         | 0.831         | H I 3.7   |
| Lp1         | H I  | 33–6            | 3.394593        | 3.394558        | 3.5          | 0.809         | He II 6.1 |
| Lp1         | H I  | 32–6            | 3.401878        | 3.401940        | −6.2         | 0.880         | H I 4.4   |
| Lp1         | H I  | 31–6            | 3.410077        | 3.410086        | −1.0         | 0.868         | H I 4.3   |
| Lp1         | H I  | 30–6            | 3.419025        | 3.419105        | −8.0         | 0.941         | H I 6.9   |
| Lp1         | H I  | 27–6            | 3.452850        | 3.452852        | −0.2         | 0.789         | H I 7.3   |
| Lp1         | H I  | 26–6            | 3.466059        | 3.466973        | −1.4         | 0.903         | H I 8.0   |
| Lp1         | H I  | 25–6            | 3.482948        | 3.482959        | −1.1         | 0.929         | H I 8.2   |
| Lp1         | H I  | 24–6            | 3.501149        | 3.501164        | −1.5         | 0.946         | H I 9.5   |
| Lp1         | H I  | 23–6            | 3.522025        | 3.522025        | −0.0         | 0.974         | H I 11.6  |
| Lp1         | H I  | 22–6            | 3.546100        | 3.546101        | −0.1         | 0.966         | H I 13.1  |
| Lp1         | H I  | 21–6            | 3.574152        | 3.574105        | 4.8          | 0.926         | H I 15.3  |
| Lp1         | H I  | 20–6            | 3.606973        | 3.606968        | 0.5          | 0.967         | H I 17.8  |
| Lp1         | H I  | 19–6            | 3.645923        | 3.645923        | 0.0          | 0.972         | H I 21.7  |
| Lp2         | H I  | 18–6            | 3.692635        | 3.692633        | 0.1          | 0.973         | H I 22.2  |
| Lp2         | H I  | 8–5             | 3.740568        | 3.740556        | 1.2          | 0.992         | H I 394.0 |
| Lp2         | H I  | 17–6            | 3.749388        | 3.749393        | −0.5         | 0.977         | H I 24.7  |
| Lp3         | H I  | 16–6            | 3.819447        | 3.819451        | −0.4         | 0.988         | H I 23.4  |
| Lp3         | H I  | 15–6            | 3.907571        | 3.907549        | 2.2          | 0.974         | H I 34.2  |
| Lp3         | H I  | 14–6            | 4.020869        | 4.020867        | 0.1          | 1.000         | H I 36.3  |
| Lp3         | H I  | 5–4             | 4.052277        | 4.052262        | 1.5          | 0.994         | H I 247.0 |
| M1          | H I  | 11–6            | 4.672512        | 4.672509        | 0.3          | 0.984         | H I 73.2  |

Note.

\(^a\) In a 0.375° × 15° slit (units of 10^{-18} W m^{-2}). The flux measurement uncertainties are dominated by systematic errors that may be estimated (Section 4.3) as ±20% (68% confidence limit).

Table 2
Helium Recombination Lines Observed toward NGC 7027

| iSHELL Mode | Line | \( \lambda_{\text{obs}} \) (\( \mu \)m) | \( \lambda_0 \) (\( \mu \)m) | \( \lambda_{\text{obs}} - \lambda_0 \) (10^{-5} \( \mu \)m) | Correl. Coeff. | Best Template | Flux \(^a\) |
|-------------|------|-----------------|-----------------|-----------------|--------------|---------------|------|
| L2          | He II | 7–6             | 3.091693        | 3.091693        | −0.0         | 1.000         | He II 720.5 |
| L2          | He II | 14–9            | 3.145466        | 3.145477        | −1.1         | 0.992         | He II 29.4 |
| L2          | He II | 19–10           | 3.151436        | 3.151448        | −1.2         | 0.976         | He II 9.4  |
| Lp1         | He II | 17–10           | 3.484007        | 3.484011        | −0.4         | 0.976         | He II 14.0 |
| Lp1         | He II | 24–11           | 3.490132        | 3.490119        | 1.3          | 0.856         | He II 4.6   |
| Lp1         | He II | 13–9            | 3.544310        | 3.544315        | −0.5         | 0.989         | He II 58.8 |
| Lp1         | He II | 23–11           | 3.574516        | 3.574577        | −6.0         | 0.905         | He II 6.7   |
| Lp2         | He II | 16–10           | 3.738962        | 3.739029        | −6.7         | 0.877         | He II 20.3 |
| Lp2         | He II | 21–11           | 3.799406        | 3.799424        | −1.8         | 0.890         | He II 6.4   |
| Lp3         | He II | 20–11           | 3.952601        | 3.952618        | −1.7         | 0.904         | He II 6.0   |
| Lp3         | He II | 10–8            | 4.050576        | 4.050609        | −3.3         | 0.850         | He II 115.4 |
| Lp3         | He II | 15–10           | 4.101234        | 4.101248        | −1.4         | 0.962         | He II 20.3 |
| Lp3         | He II | 19–11           | 4.146888        | 4.146914        | −2.6         | 0.776         | He II 7.0   |
| M1          | He II | 17–11           | 4.742625        | 4.742613        | 1.2          | 0.814         | He II 8.6   |

Note.

\(^a\) In a 0.375° × 15° slit (units of 10^{-18} W m^{-2}). The flux measurement uncertainties are dominated by systematic errors that may be estimated (Section 4.3) as ±20% (68% confidence limit).

was excluded when the flux relative to the 14–6 line was computed, as indicated by the absence of white dots at velocities below 25 km s\(^{-1}\). Figure 6 shows analogous PV diagrams for a selection of He I and He II lines. The relative spatial extents observed for these different sets of recombination lines will be discussed quantitatively at the end of Section 3.
In Table 3, the fluxes of several metal lines are listed. These may be divided into collisionally excited metal lines (first seven listed, of which six are fine-structure transitions within the ground-state term) and dipole-allowed lines, populated by recombination (next six lines). As in Tables 1 and 2, the rest frequencies of the lines, $\lambda_{\text{obs}}$, were measured using the template-fitting method; these are listed, along with the wavelength estimates, $\lambda_0$, appearing in the A'LL (van Hoof 2018). In the case of these metal lines, the previous wavelength estimates are typically far more uncertain than the current measurements. In addition to showing the difference $\lambda_{\text{obs}} - \lambda_0$, I have therefore also shown the stated uncertainties for $\lambda_0$ (here denoted $\sigma(\lambda_0)$ and obtained from the A'LL). In all cases, $|\lambda_{\text{obs}} - \lambda_0| \leq \sigma(\lambda_0)$, providing support for the line identification. Figure 7 shows the PV diagrams for a selection of the metal lines listed in Table 3.

Of the six fine-structure lines listed in Table 3, all except the [Zn VI] line have been identified previously in planetary nebulae (e.g., Beintema & Pottasch 1999; Dinerstein & Geballe 2001). Indeed, for the [K VII], [Ar VI], and [K III] transitions the recommended values of $\lambda_0$ appearing in the A'LL are astronomical determinations (Feuchtgruber et al. 1997). As far as I am aware, the line near 4.689497 $\mu$m has not been reported previously. My proposed identification of this line as the \(^{4}F_{7/2} - ^{4}F_{9/2}\) transition within the ground-state term of Zn\(^{5+}\) will be discussed below in Section 4.2.

Figure 5. PV diagrams for a selection of hydrogen recombination lines.
The observed value (from Tables 1 and 3) is 1.88 \times 10^{-3}, in reasonable agreement with the expected value. Six additional spectral lines are plausibly identified as C III and C IV recombination lines. For the C III transitions, the configurations of the upper and lower states are 1s^22snl and thus the total spins are 0 or 1. However, because the energy differences between the singlet and triplet states are very small, and because only one electron has nonzero orbital angular momentum, specifying nl suffices to identify the upper and lower states. Recombination lines of C III and C IV have been previously detected toward NGC 7027 at optical wavelengths (Baluteau et al. 1995; Zhang et al. 2005).

Table 3, like Tables 1 and 2, indicates which of the five line templates yields the best correlation with the PV diagram. For three of the fine-structure transitions, the maximum correlation coefficient did not exceed the threshold of 0.7 that I adopted in compiling the list of recombination lines. These three lines comprise the weakest two lines, [Fe VII] and [Ca VII], and the [Ar VI] line that is very strong but suffers interference from a nearby telluric feature.

As expected, the more highly ionized species typically resemble the He I template more than any other template, while the lower ionization species (Zn^{3+} and K^{2+}) resemble He I most closely. Spatial moments provide an alternative method of quantifying the distribution of the observed emission for each spectral line. In particular, we may consider the quantity

$$\theta_{\text{rms}} = \sqrt{\frac{\int I(\theta)(\theta - \theta_c)^2 \, d\theta}{\int I(\theta) \, d\theta}}$$

Figure 6. PV diagrams for a selection of helium recombination lines.
where $I(\theta)$ is the velocity-integrated intensity at angular position $\theta$ along the slit, and $\theta_c$ is the centroid position:

$$
\theta_c = \int I(\theta) \theta \, d\theta.
$$

The quantity $\theta_{rms}$, which represents the rms angular displacement of the observed emission from its centroid, is plotted in Figure 8 for a selection of spectral lines (which include the CH$^+$ and H$_2$ emissions reported in Paper II). The error bars shown here represent 68.3% confidence limits. These were obtained by computing $\theta_{rms}$ in a set of 1000 simulations in which Gaussian random noise was added to the data with an amplitude equal to the noise observed in line-free spectral regions. Vertical dashed lines show the weighted means of $\theta_{rms}$ for lines of a given species.

The results shown in Figure 8 indicate that the molecular emissions are significantly more extended than the emissions from atoms and atomic ions, as expected because the molecular gas lies outside the photoionized nebula. The He II lines have a smaller $\theta_{rms}$ than the H I lines, consistent with expectation that the He$^{2+}$ zone is smaller than the H$^+$ zone. On the other hand, the He I lines have a larger $\theta_{rms}$ than the H I lines. This behavior is also expected: while the outer edge of the He$^+$ zone is roughly cospatial with that of the H$^+$ zone, the He$^+$ zone also has an inner edge within which He$^+$ is absent (having been ionized to form He$^{2+}$).

For the metal lines in Figure 8, shown in black, two key energies are listed in parentheses with the notation $I_1-I_2$. Here, $I_1$ eV is the appearance potential (i.e., the minimum photon energy needed to produce the relevant ion by photoionization), and $I_2$ eV is the ionization potential for that ion. In this context, the “relevant ion” is the emitting ion for the collisional excited lines (e.g., K$^+$ for [K III], Ar$^{5+}$ for [Ar VI]). For recombination lines, however, the relevant ion is the recombining ion (e.g., H$^+$ for H I, C$^{4+}$ for C IV). The results shown in Figure 8 show the expected trend that higher ionization species show emission with a smaller spatial extent.
4. Discussion

4.1. Improved Wavelength Determinations for Infrared Metal Lines

The wavelengths of many infrared fine-structure transitions are poorly known from laboratory experiments. In many cases, they must be estimated by analyzing differences in the measured wavelengths of dipole-allowed ultraviolet transitions at much higher frequencies. The fractional accuracy of the derived infrared wavelengths can therefore be worse than that of the measured ultraviolet wavelengths by two orders of magnitude or more. In the case of \([\text{Zn} \, \text{VI}] \, ^{4}F_{7/2} - ^{4}F_{9/2}\) for example, which has the...

Figure 8. Spatial extent of selected lines, \(\theta_{\text{rms}}\) (see the text for the definition).
Table 3
Metal Lines Observed toward NGC 7027

| iSHELL mode | Line          | $\lambda_{obs}$ (\(\mu m\)) | $\lambda_0$ (\(\mu m\)) | $\sigma(\lambda_0)$ (10^{-3} \(\mu m\)) | $\lambda_{obs} - \lambda_0$ (10^{-5} \(\mu m\)) | Correl. Coeff. | Best Template | Flux $^a$ |
|-------------|---------------|-------------------------------|--------------------------|------------------------------------------|-----------------------------------------------|---------------|---------------|-----------|
| L2          | [K III] \(^2 P_{3/2} - ^2 P_{1/2}\) | 3.190414                      | 3.19053                  | 15                                       | -12                                           | 0.887          | He II         | 20.8      |
| Lp1         | [Fe VII] \(^3 P_{1} - ^1 D_2\)        | 3.384102                      | 3.3846                   | 100                                      | 50                                            | 0.657          | He II         | 4.8       |
| Lp1         | [Zn IV] \(^2 D_{3/2} - ^2 D_{5/2}\)    | 3.624956                      | 3.6244                   | 120                                      | 56                                            | 0.979          | He I          | 45.7      |
| Lp3         | [Ca VII] \(^3 P_{1} - ^3 P_{1}\)        | 4.086196                      | 4.0875                   | 150                                      | -130                                          | 0.576          | He II         | 4.4       |
| M1          | [Ar VII] \(^2 P_{3/2} - ^2 P_{1/2}\)   | 4.529302                      | 4.5295                   | 31                                       | -20                                           | 0.501          | He II         | 7170      |
| M1          | [K III] \(^2 P_{1/2} - ^2 P_{3/2}\)    | 4.617788                      | 4.61802                  | 47                                       | -23                                           | 0.896          | He I          | 126       |
| M1          | [Zn VI] \(^4 F_{5/2} - ^4 F_{7/2}\)     | 4.689497                      | 4.69                     | 2000                                     | -50                                           | 0.965          | He II         | 38        |
| L2          | C III 9i–8j  | 3.076921                      | 3.0772                   | 130                                      | -28                                           | 0.805          | He II         | 2.3       |
| L2          | C III 9k–8l  | 3.083853                      | 3.0838                   | 130                                      | 5                                             | 0.919          | He II         | 4.6       |
| L2          | C IV 14f–12d | 3.086660                      | 3.0868                   | 210                                      | -14                                           | 0.905          | He I          | 5.2       |
| Lp1         | C IV 11k–10i | 3.281740                      | 3.2817                   | 150                                      | 4                                             | 0.951          | He II         | 15.8      |
| Lp1         | C IV 17k–14i | 3.469021                      | 3.4691                   | 170                                      | -8                                            | 0.751          | He II         | 2.3       |
| Lp3         | C IV 15k–13i | 3.867415                      | 3.8674                   | 210                                      | 2                                             | 0.777          | He II         | 3.5       |

Note.

$^a$ In a 0.375" × 15" slit (units of 10^{-18} W m^{-2}). The flux measurement uncertainties are dominated by systematic errors that may be estimated (Section 4.3) as ±20% (68% confidence limit).
wavelength that is least well known, the estimate of \( \lambda_0 \) in Table 3 was derived from spectroscopic measurements of the \( 3d^44p−3d^2 \) system in the 209–284 Å region (van Het Hof et al. 1994). The wavelength accuracy was 0.004 Å, which is equivalent to a wavenumber accuracy of 5–9 cm\(^{-1}\). At the frequency of the \(^4F_{7/2}−^4F_{9/2} \) transition (~2132 cm\(^{-1}\)), this corresponds to a fractional accuracy of 0.2%–0.4%. Theoretical calculations of spin–orbit coupling generally fare no better, with state-of-the-art techniques providing typical accuracies no better than \( \sim 0.4 \) cm\(^{-1}\) (Lan Cheng, personal communication).

For fine-structure transitions that are observed from gaseous nebulae, astronomical observations sometimes provide the best wavelengths currently available. Such is the case for the \([\text{K} \, \text{VII}], \,[\text{Ar} \, \text{VI}], \) and \([\text{K} \, \text{III}]\) transitions listed in Table 3, for which the wavelength estimates \( \lambda_0 \) were obtained from Infrared Space Observatory (ISO) observations of the planetary nebulae NGC 7027 and NGC 6302 (Feuchtgruber et al. 1997). These observations were performed with the SWS grating spectrometer, which had a spectral resolving power \( R = \lambda/\Delta \lambda \sim 1000–2000 \). The observations reported here, performed at considerable higher resolution \( (R = 80,000) \) with the iSHELL spectrometer, yield substantial accuracy improvements for the three transitions that were considered by Feuchtgruber et al. (1997); for the other transitions, the gains in accuracy are even larger. The values of \( \lambda_{\text{obs}} \) given in Table 3 are therefore the most accurate values obtained to date. The integrated spectra for a selection of metal ions are shown in Figure 9.

There are two sources of uncertainty in the values of \( \lambda_{\text{obs}} \) that are obtained. The first relates to the fundamental accuracy of the wavelength measurements obtained from the new observational data and may be evaluated by considering the results shown in Tables 1 and 2. Because these involve lines for which the wavelengths \( \lambda_0 \) have negligible uncertainties, we may adopt the rms value of \( (\lambda_{\text{obs}} − \lambda_0)/\lambda_0 \), or 7.4 \( \times 10^{-6} \), as an estimate of the fractional accuracy of the wavelength measurements. The second source of uncertainty arises from the possibility that the metal line emissions may have a systematic Doppler shifts relative to the best-fit templates (He I or He II). This possibility is suggested by a careful examination of Figure 4, in which the five curves peak at slightly different wavelengths. Considering only the templates for atomic recombination lines, the maximum fractional variation is 6 \( \times 10^{-5} \), which may be taken as a reasonable estimate of the fractional accuracy of the improved metal line wavelengths reported here. This represents a factor 5–15 improvement over the previous astronomical wavelength estimates, and a factor 30–400 improvement over the laboratory measurements.

### 4.2. Probable Detection of the [Zn VI] \(^4F_{7/2}−^4F_{9/2} \) Fine-structure Transition

A spectral line is detected with high confidence with a rest wavelength of 4.689497 \( \pm 0.000047 \) \( \mu m \): the PV diagram is shown in Figure 6 (middle row, right column). Its probable identity is the \(^4F_{7/2}−^4F_{9/2} \) fine-structure transition within the (inverted) ground-state \(^4F\) term of [Zn VI], which has the configuration \([\text{Ar}]3d^9\). This identification is supported by a number of arguments: (1) this is the only plausible identification among the lines cataloged in the ALL; (2) the spatial extent, \( \theta_{\text{proj}} \), of the 4.6895 \( \mu m \) line (Figure 8) is in excellent agreement with that of the \(^2P_{3/2}−^2P_{1/2} \) line of \([\text{K} \, \text{VII}]\), which is emitted by an ion with ionization and appearance potentials similar to those of \( \text{Zn}^{2+} \); (3) another zinc ion has previously been identified in NGC 7027 by Dinerstein & Geballe (2001) (and detected again in the observations reported here): the \( \text{Zn}^{2+} \) ion, with its \(^2D_{3/2}−^2D_{5/2} \) transition near 3.62496 \( \mu m \). Although there is no evidence for the higher-lying \([\text{Zn} \, \text{VI}]^4F_{5/2}−^4F_{7/2} \) transition near 4.03 \( \mu m \), electron impact excitation from the \(^2F_{9/2} \) ground state to the upper \(^4F_{5/2} \) state for that transition is probably disfavored because collision strengths typically decline with \( \Delta \ell \).

To further evaluate the plausibility of this identification, I have obtained predictions for the ionization state of Zn using the CLOUDY photoionization model v17.02 (Ferland et al. 2017). Full details of the model parameters have been described in Paper I, where CLOUDY was used to model the HeH\(^+\) cation: the central star, with a photospheric temperature of 1.9 \( \times 10^5 \) K is assumed to irradiate a constant-pressure shell. The lower panel in Figure 10 shows how the ionization state of zinc varies with distance from the central star, for an adopted distance of 980 pc (see Paper I); the upper panel shows the variation of the electron temperature, \( T \), the electron density, \( n_e \), and the density of H nuclei, \( n_H \).

Based upon the ionization structure shown in Figure 10, I have computed the line emissivities for the \([\text{Zn IV}]\) and \([\text{Zn VI}]\) transitions listed in Table 3. As Smith et al. (2014) pointed out for the case of the \([\text{Zn IV}]\) transition, the estimated density of the nebula lies comfortably below the critical density above which collisional deexcitation becomes dominant. Thus, almost all \( \text{Zn}^{2+} \) ions will be in the ground \(^2D_{5/2} \) fine-structure state, and every excitation will be followed by the emission of a 3.62496 \( \mu m \) photon. Because the radiative decay rates for the \([\text{Zn VI}]\) and \([\text{Zn IV}]\) transitions are very similar, the same argument will apply to the \([\text{Zn VI}]\) transition. With these
assumptions, the emissivities are simply proportional to the elemental abundance ratio, $n_{Zn}/n_{H}$, and the dimensionless collision strength, $\Upsilon$.

Integrating the emissivity over the region enclosed by the iSHELL slit, the model yields a flux of $2.5 \times 10^{-17} \Upsilon_{3,6250} (10^6 n_{Zn}/n_{H})$ W m$^{-2}$ for the [Zn IV] $^2D_{3/2} - ^2D_{5/2}$ transition. Given the observed flux listed in Table 3 and an estimated collision strength $\Upsilon_{3,6250} = 1.4$ (Smith et al. 2014, citing a private communication by Butler), the zinc abundance is found to be $1.3 \times 10^{-8}$, in perfect agreement with the estimate of Smith et al. (2014). This amounts to roughly one-third of the solar abundance of Zn (Asplund et al. 2005).

For the [Zn VI] $^4F_{7/2} - ^2F_{9/2}$ transition, the predicted flux is $4.9 \times 10^{-18} \Upsilon_{4,6895} (10^5 n_{Zn}/n_{H})$ W m$^{-2}$, which would require $\Upsilon_{4,6895} (10^5 n_{Zn}/n_{H}) = 7.8$. I am not aware of any theoretical estimates for the collision strength $\Upsilon_{4,6895}$; given the zinc abundance determined above from the [Zn IV] transition, the required value is 6.0. This value is fairly large, but by no means outside the typical range (1 to 10; e.g., Draine 2011). To summarize, although my analysis of the 4.6895 $\mu$m line flux is limited by the absence of available collision strengths, it does indicate that the [Zn VI] $^4F_{7/2} - ^2F_{9/2}$ transition can very plausibly account for the observed flux of the 4.6895 $\mu$m line.

4.3. Relative Line Fluxes for Recombination Lines of H and He$^+$

The availability of reliable flux measurements for 39 infrared recombination lines of H I and He II enables a test of model predictions for their relative strengths. In Figure 11, the H I line fluxes are shown relative to the H I $n = 14-6$ line, on a logarithmic scale and as a function of the principal quantum number of the upper state, $n_{H}$. As indicated in the legend in the upper right, different colors denote different principal quantum numbers for the lower state, $n_{L}$; the H I lines observed in this spectral region include one Brackett line (Br$\alpha$, with $n_{L} = 4$), two lines from the Pfund series ($n_{L} = 5$), and 22 lines from the Humphreys series ($n_{L} = 6$, with $n_{U}$ covering the wide range from 10 to 38). Solid lines show the model predictions presented by Storey & Hummer (1995, hereafter SH95), for an assumed electron temperature of $1.5 \times 10^4$ K and electron density of $10^5$ cm$^{-3}$. The predictions were obtained for “Case B” recombination (i.e., under the assumption that the Lyman lines are optically-thick).

The rms deviation of $\log_{10}$ (line flux/$n = 14-6$ flux) from the model prediction is 0.078, corresponding to a fractional rms deviation of 20%. This then provides a validation of the SH95 model predictions over a wide range of $n_{L}$. Barring some conspiracy between the flux measurement errors and errors in the model predictions, it suggests a limit of 20% on the typical systematic errors for flux ratio measurements. It also confirms that the effects of differential dust extinction are negligible over the 3.0–4.7 $\mu$m range, as expected.\footnote{Given a reddening of 3.4 mag inferred by Zhang et al. (2005) at the H$\beta$ wavelength and the infrared extinction curve presented by Mathis (1990, his Table 1), the extinction is expected to be only 0.15 mag at 3.4 $\mu$m and 0.08 mag at 5 $\mu$m.}

The SH95 model predictions have been obtained over a range of electron temperatures $T$ from 3000 to 20,000 K and a
Figure 13. He II recombination line ratios. The line fluxes are presented as a ratio to the He II 16–10 line, as a function of the principal quantum number of the upper state, \( n_U \). Solid curves show the theoretical predictions (SH95) for “Case B” recombination with an assumed electron temperature of \( 1.5 \times 10^4 \) K and electron density of \( 10^5 \) cm\(^{-3}\). The observational data points and theoretical predictions are color-coded according the the principal quantum number of the lower state (see inset legend).

Figure 12. Goodness of fit for HI recombination line ratios in the \( T_e-n_e \) plane. Red, green, and blue contours show the 68%, 95%, and 99.7% confidence limits. The black locus shows the run of \( n_e \) with \( T_e \) in the ionized gas (from the CLOUDY model prediction shown in Figure 10, upper panel).
range of electron densities $n_e$ from $10^2$ to $10^{14}$ cm$^{-3}$. Figure 12 shows the goodness of fit in the $T-n_e$ plane for models with a constant temperature and density; here red, green, and blue contours represent the 68%, 95%, and 99.7% confidence limits. The black line indicates the locus of temperature and density that is predicted by the CLOUDY model (Section 4.2) within the region where hydrogen is mainly ionized. Because the predicted line ratios are only weakly dependent on $T$ and $n_e$, the recombination line ratios are not strongly constraining: only unrealistically high or low electron densities—or unrealistically low electron temperatures—are excluded at the 95% confidence level. Figure 13 shows the line fluxes observed for recombination lines of He II, compared with the corresponding SH95 predictions. Here the measured line fluxes are shown relative to the $n = 16–10$ line flux, and the rms deviation of log($f_{\text{line flux}}/n = 16–10$ flux) from the model prediction is 0.116. The set of observed lines has $n_U$ ranging from 7 to 23 and $n_L$ ranging from 6 to 11.

5. Summary

(1) An infrared $L$- and $M$-band spectral survey has been performed toward the young planetary nebula NGC 7027 with the iSHELL instrument on NASA’s Infrared Telescope Facility. It covers the 2.951–5.24 μm spectral region (incompletely) at a spectral resolving power of 80,000 and provides spatial information along a 15″ slit.

(2) When the spectral and spatial information from this survey is analyzed with the template-fitting algorithm described in Section 3, 56 transitions of atoms or atomic ions are detected with high confidence.

(3) A spectral line at 4.6895 μm is most probably the $^2F_{1/2} - ^2F_{9/2}$ fine-structure transition of Zn$^{5+}$, an ion that has not previously been detected in gaseous nebulae. An ionization model for NGC 7027, obtained with the CLOUDY photoionization code, predicts Zn$^{5+}$ to be the dominant ionization stage of zinc in the middle part of the irradiated shell. This model can simultaneously fit the 4.6895 μm line together with a [Zn IV] fine-structure line that has also been detected, given an assumed collisional strength of 6 for the electron impact excitation of Zn$^{5+}$ from the ground $^2F_{9/2}$ state to the $^2F_{7/2}$ state.

(4) The rest wavelengths of 13 metal lines—including six infrared fine-structure transitions—are determined to an unprecedented fractional accuracy of $1 \times 10^{-5}$. They are presented in Table 3.

(5) The relative strengths of 39 recombination lines of H and He$^+$, with upper states of principal quantum number up to 38 (H) or 24 (He$^+$), agree well with predictions obtained for Case B recombination (SH95).

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