Testing Short-term Variability and Sampling of Primary Volatiles in Comet 46P/Wirtanen

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Abstract

The exceptionally favorable close approach of Jupiter-family comet 46P/Wirtanen in 2018 December enabled characterization of its primary volatile composition with exceptionally high spatial resolution and sensitivities using the iSHELL spectrograph at the NASA Infrared Telescope Facility on Maunakea, Hi. We sampled emissions from H$_2$O, HCN, C$_2$H$_2$, NH$_3$, C$_2$H$_6$, and CH$_3$OH on UT 2018 December 21 using two instrumental settings that spanned the 2.9–3.6 μm spectral region. We also obtained a sensitive 3σ upper limit for H$_2$CO and for the rarely studied molecule HC$_5$N. We report rotational temperatures, production rates, and mixing ratios (relative to H$_2$O as well as to C$_2$H$_6$). We place our results in context by comparing them with other comets observed at near-IR wavelengths. We also compare our results with those obtained using the NIRSPEC-2 spectrograph on Keck II on UT December 17 and 18 and with results obtained from iSHELL on other dates during the same apparition. Within 1–2σ uncertainty, production rates obtained for all molecules in this work were consistent with those obtained using NIRSPEC-2 except H$_2$O, indicating low-level variability on a timescale of days. Mixing ratios with respect to H$_2$O in 46P/Wirtanen were consistent with corresponding values from NIRSPEC-2 within the uncertainty with the exception of CH$_3$OH, which yielded a higher ratio on December 21. Our measurements afforded a high temporal resolution that spanned ~2/3 of the rotational period of 46P/Wirtanen, enabling us to test short-term variability in the production rates of H$_2$O and HCN due to rotational effects. Both H$_2$O and HCN production rates showed similar temporal variability, resulting in nearly constant HCN/H$_2$O.

Unified Astronomy Thesaurus concepts: Comet volatiles (2162); Near infrared astronomy (1093); Molecular spectroscopy (2095); Comets (280); High resolution spectroscopy (2096); Comae (271)

1. Introduction

Comets are relatively unprocessed remnants of the early solar system. As some of the first objects to have accreted in the cold regions (>5 au) of the solar nebula, comets may retain the compositional record of icy materials present in the solar nebula. Processes that can affect the properties of cometary nuclei generally alter a very thin layer near the surface, which is thought to be lost during a typical perihelion passage (Stern 2003; Gronoff et al. 2020), preserving the primitive nature of comets. Furthermore, because comets lack a known mechanism for internal heating owing to their small sizes, their present-day composition may reflect the chemistry and prevailing conditions in the early solar system where they formed ~4.5 billion years ago (Bockelée-Morvan et al. 2004; Mumma & Charnley 2011).

Initially, it was widely accepted that Oort Cloud comets (OCCs) formed at a heliocentric distance ($R_0$) of ~5–30 au, whereas Jupiter-family comets (JFCs) formed even farther out in the early solar nebula. However, the presence of crystalline silicates in comets from both dynamical classes, such as C/2001 Q4 (NEAT; Wooden et al. 2004), 1P/Halley (Bregman et al. 1987), 9P/Tempel 1 (Harker et al. 2005), and 81P/Wild 2 (Zolensky et al. 2006), and improved dynamical models (Levison & Duncan 1997; Gomes et al. 2005; Morbidelli et al. 2005; Levison et al. 2011; Nesvorný et al. 2017) suggest that comets may have formed in large but spatially overlapping regions in the solar nebula (A’Heaırn et al. 2012). Considering these distinct versus overlapping formation region scenarios, an important goal in cometary science is to ascertain whether systematic differences exist between the chemical compositions of these two dynamical classes of comets. If comets were formed in overlapping regions, their present-day composition may reflect the composition in those regions provided that evolutionary effects do not dominate. On the other hand, if post-formation thermal processing effects dominate in comets, these effects will be more pronounced in JFCs (owing to their frequent and repeated passages close to the Sun) as compared to OCCs (Combi et al. 2019).
Near-IR spectroscopy is a powerful tool to characterize the primary volatiles (i.e., gases subliming directly from the nucleus and thus indicative of its native composition) in comets by sampling the rovibrational transitions of a suite of molecules between $\sim 2.9 \text{–} 5 \mu m$. To date, roughly 40 comets have had their volatile composition characterized near-IR, but only $\sim 15$ of those have been JFCs. Emerging trends suggest that on average JFCs are depleted in some parent volatiles (especially in hypervolatiles) as compared to OCCs (Dello Russo et al. 2016). In contrast, more than 200 comets have been sampled at optical wavelengths, (A’Heam et al. 1995; Fink 2009; Cochran et al. 2012; Schleicher & Bair 2014) where nearly one-third exhibit depletion in carbon-chain species. Of these, about half are JFCs whereas only 10% are OCCs, suggesting that the compositional differences between the two dynamical classes may be natal rather than due to post-formation processing (Schleicher 2007; Dello Russo et al. 2009; Fink 2009).

The highly favorable apparition of 46P/Wirtanen (hereafter 46P) in 2018 was the focus of a worldwide observing campaign (http://wirtanen.astro.umd.edu). 46P reached its perihelion on UT 2018 December 12, with a heliocentric distance ($R_h$) of $\sim 1.05$ au. Shortly after its perihelion, it reached a minimum geocentric distance of 0.077 au ($\sim 30$ lunar distances) and its visual magnitude of $\sim 3$, resulting in exceptional observing circumstances for a JFC. It remained within a distance of 0.1 au from Earth for $\sim 20$ consecutive days, allowing for detailed observations by both professional and amateur astronomers.

46P was the original target of the Rosetta spacecraft mission; however, 67P/Churyumov–Gerasimenko was selected for the mission due to a delay in launch. We emphasize that knowledge of the overall activity and composition is often an important parameter in assessing the suitability of a comet as a mission target. It is also useful in placing mission data in context with the much larger database of remote-sensing observations of comets. The historic 2018 apparition of 46P thus provided a timely opportunity for sampling the primary volatile composition of a JFC that remains a favorable candidate for a future mission.

The importance of 46P as a JFC, coupled with the exceptional and rare observing conditions during its 2018 apparition, lends great significance to these observations, as well as to the scientific knowledge that will be extracted from them. Moreover, distinguishing between natal versus post-formation processing effects in OCCs and JFCs requires comparison of a sufficiently large sample of comets from each dynamical class. Sampling of the chemical composition of 46P using near-IR spectroscopy is a useful addition to the overall comet inventory as well as to the generally underrepresented JFCs.

An increasing number of comets measured to date have displayed variability in their coma composition within an apparition as well as across perihelion passages. This variability has been attributed to numerous effects, including seasonal effects on the nucleus, diurnal illumination effects, and chemically heterogeneous nuclei (Feaga et al. 2014; Hässig et al. 2015; Lupsay-Kuti et al. 2015; McKay et al. 2015; Bockelée-Morvan et al. 2016; Fink et al. 2016; Combi et al. 2020b). Surface regions of some comets were observed to have been covered by thermally processed fall-back material. For example, the north hemisphere of 67P/Churyumov–Gerasimenko (Keller et al. 2017) and the waist of 103P/Hartley 2 (A’Heam et al. 2011; Kelley et al. 2013) are covered by processed material. However, the coma activity was dominated by the fresh material emitted by the southern hemisphere of 67P/Churyumov–Gerasimenko and ends of the small lobe of 103P/Hartley 2. This mass transfer on comet nuclei due to fall-back material may affect their surface evolution and is an example of post-formation processing.

Remote-sensing observations do not resolve the nucleus, and time-resolved compositional measurements through a complete nucleus rotation are lacking at near-IR wavelengths. Jehin et al. (2018) reported a $\sim 9$ hr rotational period for 46P using a CN lightcurve measured from photometry obtained at the TRAPPIST telescopes on UT 2018 December 9–10. The relatively short rotational period of 46P provided us with an opportunity to sample $\sim 2/3$ of its period during a single observing night on UT 2018 December 21, and to test for rotational variability in HCN and H$_2$O on a timescale of a few hours.

In this work, we report production rates and mixing ratios (i.e., abundance ratios in percent) of H$_2$O, HCN, CH$_3$OH, C$_2$H$_4$, C$_2$H$_5$, and NH$_3$ with respect to H$_2$O and C$_2$H$_6$ and report stringent $3\sigma$ upper limits for H$_2$CO and HC$_3$N. We also discuss possible variability in the production rates of H$_2$O and HCN in comet 46P post-perihelion. In Section 2, we review our observations and data reduction. In Section 3, we present our results. In Section 4, we discuss our results and place them into context with comets observed to date.

2. Observations and Data Reduction

iSHELL at the NASA Infrared Telescope Facility (IRTF) became available for cometary observations in 2016 (Rayner et al. 2012, 2016). This instrument is capable of both high-resolution long-slit spectroscopy and imaging in the 1.1–5 $\mu$m range, with a spectral resolving power ($\lambda/\Delta\lambda$) of up to $7.5 \times 10^4$ using its narrowest slit (0''375). Extra slit widths are available for minimizing slit losses and accurate flux calibration. Owing to its cross-dispersed capability, iSHELL can measure a signal in more than ten consecutive echelle orders simultaneously, whereas its daytime observing capability allows for observations of objects best observed during daylight hours, namely comets close to the Sun. These features make iSHELL unique among contemporary spectrographs operating in the near-IR wavelength regime.

We observed 46P post-perihelion on UT 2018 December 21 at $R_h \sim 1.06$ au and geocentric distance ($\Delta$) $\sim 0.082$ au (see Table 1 for observing details). We used the iSHELL Lp1 and a custom L setting (hereafter L-custom) to sample emissions from the primary volatiles H$_2$O, HCN, CH$_3$OH, C$_2$H$_6$, C$_2$H$_5$, NH$_3$, H$_2$CO, and HC$_3$N. Flux calibration was achieved using a bright nearby IR flux standard star (BS8781) using the 4'' wide slit. We acquired comet data with the 0''755 (6 pixel) wide slit using an ABBA nod sequence, with the A and B beams placed symmetrically about the midpoint along the 15'' long slit and separated by half its length. To cancel continuum emissions from the thermal background, instrumental biases, and sky emission (lines and continuum), the spectra were combined as A–B–B–A. The dark subtracted flats were applied to the data, which were subsequently cleaned of cosmic-ray hits and hot pixels. We alternated between two slit orientations while using the L-Custom setting: one along the Sun–comet line (position angle, PA 134°) and the other orthogonal to the Sun–comet line (PA 44°), with each slit orientation sampling a unique projection of the coma into the sky plane. Our observations spanned $\sim 2/3$ of a complete rotation for 46P. In this way we obtained a total of four separate observations, with two sets
each corresponding to the mutually perpendicular slit orientations (see Table 1).

The data-reduction procedures have been rigorously tested and are well-documented in the literature (see Bonev 2005; DiSanti et al. 2006, 2014; Villanueva et al. 2009; Radeva et al. 2010). For their applications to unique aspects of iSHELL spectra, see Section 3.2 of DiSanti et al. (2017).

Contributions from continuum and gaseous emissions in our spectra were determined as previously described by DiSanti et al. (2016). We illustrate the procedure in Figure 1, which shows a sample spectrum of H$_2$O fluorescent emissions in order 179 of the third PA set of the L-Custom setting spanning ~3437.8–3465.8 cm$^{-1}$. We used the Planetary Spectrum Generator (https://psg.gsfc.nasa.gov/; Villanueva et al. 2018) to generate telluric transmittance models, to perform wavelength calibration of the spectra, and to determine column burdens of the absorbing molecules in the terrestrial atmosphere. The fully resolved transmittance function was convolved to the resolving power (~4.5 × 10$^{5}$) of the instrument and scaled to the continuum level of the comet. The telluric model was then subtracted from the observed spectrum to isolate cometary emission lines. Intensities of these emission lines were compared to fluorescent emission models after correcting each modeled line intensity for the monochromatic atmospheric transmittance at its Doppler-shifted wavelength based on the geocentric velocity (~3.4–3.9 km s$^{-1}$) of the comet at the time of the observation.

### 3. Results

#### 3.1. Spatial Profiles

A comparison between spatial profiles of co-measured coma volatiles can indicate whether these species sublimated directly from the comet nucleus, from one or more extended outgassing sources within the coma, or a combination of both. In general, ices sublimating directly from the nucleus exhibit a spatial profile that peaks in intensity at or near the nucleus and then falls off as $r^{-2}$, where $r$ is the projected nucleocentric distance. On the other hand, spatial profiles of molecules produced by photolysis or extended sources in the coma fall off more slowly with a flatter distribution. Figure 2 shows spatial profiles of co-measured HCN and H$_2$O along with the dust continuum in each PA set of the L-Custom setting. In each of these sets, the gas profiles track each other somewhat closely whereas the dust profile is narrower. The gas profiles are also asymmetric and are extended in the projected anti-sunward direction. These asymmetries are more pronounced in the first two PA sets (Figures 2(A) and (B)). Figure 3 shows spatial profiles of co-measured CH$_3$OH and C$_2$H$_6$ overplotted with the dust profile. The relatively noisy CH$_3$OH spatial profile is broader than both the co-measured C$_2$H$_6$ as well as dust profile, whereas both of the gas profiles are broader than the dust profile. An anti-sunward extension in gas profiles is also evident. We note that spatial profiles of all of these gases appear to be consistent with their growth factors (GFs; defined as $Q/Q_{NC}$ where $Q$ and $Q_{NC}$ are the global and nucleus-centered production rates, respectively); i.e., H$_2$O and HCN GFs are relatively similar whereas the CH$_3$OH GF is significantly larger than that of C$_2$H$_6$ (see Table 2).

#### 3.2. Molecular Fluorescence Analysis

The g-factors used in this work were generated with quantum mechanical models developed for H$_2$O (Villanueva et al. 2012b), C$_2$H$_6$ (Villanueva et al. 2011b), CH$_3$OH (Villanueva et al. 2012a; DiSanti et al. 2013), H$_2$CO (DiSanti et al. 2006), C$_3$H$_2$ (Villanueva et al. 2011a), NH$_3$ (Villanueva et al. 2013), and HCN (Lippi et al. 2013). HC$_3$N is a simple

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**Table 1**

| iSHELL Setting | Slit PA (deg) | Wavelength Range (cm$^{-1}$) | Time (UT) | $R_0$ (au) | $\Delta$ (au) | $\Delta$-dot (km s$^{-1}$) | $T_{int}$ (minute) |
|----------------|--------------|-------------------------------|-----------|------------|--------------|--------------------------|-------------------|
| Lp1            | 134          | 2750–3060                     | 5:45–6:02 | 1.061      | 0.082 5      | 3.379                    | 16                |
| L-Custom       | 134          | 3210–3580                     | 6:10–7:29 | 1.061      | 0.082 5      | 3.379                    | 72                |
| L-Custom       | 44           | *                             | 7:43–8:52 | 1.061      | 0.082 6      | 3.561                    | 64                |
| L-Custom       | 134          | *                             | 8:57–10:07| 1.061      | 0.082 7      | 3.713                    | 64                |
| L-Custom       | 44           | *                             | 10:21–11:55| 1.061      | 0.082 8      | 3.867                    | 84                |

**Note.** Slit PA, $R_0$, $\Delta$, $\Delta$-dot, and $T_{int}$ are the slit position angle, heliocentric distance, geocentric distance, geocentric velocity, and total on-source integration time, respectively.
linear molecule, and its g-factors were obtained using a rotational constant of 0.15174 cm$^{-1}$ (Creswell et al. 1977). To fit fluorescent emissions from all molecules simultaneously in each echelle order, a Levenberg–Marquardt nonlinear minimization technique (Villanueva et al. 2008) was used. This technique allows for results with high precision even in spectrally crowded regions having many lines within a single resolution element of the instrument. Production rates for each targeted primary volatile were then determined from the corresponding synthetic model at a well-constrained rotational temperature (T$_{\text{rot}}$).

### 3.3. Determination of Rotational Temperature (T$_{\text{rot}}$)

Calculating a robust rotational temperature (T$_{\text{rot}}$) is crucial for an accurate calculation of molecular production rates and, hence, mixing ratios. We determined T$_{\text{rot}}$ using correlation and excitation analyses (Bonev 2005; Bonev et al. 2008; DiSanti et al. 2006). In general, a well-constrained T$_{\text{rot}}$ can be derived for molecules with strong lines that span a broad range of excitation energies. For this work, these conditions were satisfied by combining lines from different orders to obtain T$_{\text{rot}}$ for H$_2$O in each PA set of the L-Custom setting (see Table 2). These values were similar to the H$_2$O T$_{\text{rot}}$ obtained on UT December 14 (84 ± 3) (Saki et al. 2020), UT December 17 (89 ± 2) and UT December 18 (87 ± 1) with NIRSPEC-2 (Bonev et al. 2021), and (94 ± 5) on December 18 with iSHELL (Roth et al. 2021). We also obtained a relatively well-constrained T$_{\text{rot}}$ for HCN in each PA set by combining lines from different orders. In general, rotational temperatures calculated for different molecules using IR observations are consistent, and small variations in T$_{\text{rot}}$ result

**Figure 2.** Spatial profiles of co-measured H$_2$O (pink solid line), HCN (blue solid line), and the continuum from dust (red dashed line) on UT 2018 December 21. Panels (A)–(D) correspond to PA 134°, 44°, 134°, and 44°, respectively. The horizontal bar indicating 1" corresponds to a projected distance of ~60 km at the geocentric distance of 46P. The Sun–comet–Earth angle (phase angle, β) of 19° is also shown.
in only minor differences in production rates (Gibb et al. 2012). For this reason, we assumed a \( T_{\text{rot}} \) of 80 K (consistent with the \( H_2O \) and HCN \( T_{\text{rot}} \) across all PA sets) for molecules where a rotational temperature could not be derived (i.e., \( C_2H_6, CH_3OH, H_2CO, C_2H_2, NH_3, \) and \( HC_3N \)).

**3.4. Determination of Molecular Production Rates**

Nucleus-centered production rates \((Q_{NC})\) and global production rates \((Qs)\) were determined using the well-established \( Q \)-curve method described in Xie & Mumma (1996), Dello Russo et al. (1998), DiSanti et al. (2001, 2016), Bonev (2005), Bonev et al. (2006, 2017), Villanueva et al. (2011a), and Gibb et al. (2012). This method provides a GF that corrects for atmospheric seeing, which suppresses the signal along lines of sight passing close to the nucleus due to the use of a narrow slit, as well as potential perpendicular drift of the comet during an exposure sequence. We assumed a canonical spherically symmetric outflow velocity \((v_{\text{gas}} = 800 \ R_6^{-0.5} \text{ m s}^{-1})\) in determining production rates. This velocity is based on velocity-resolved observations of several moderately bright comets at radio wavelengths (Biver et al. 2006; Cordiner et al. 2014; also see Bonev 2005 supporting this assumption). We note that our assumed outflow velocity \((\sim 780 \text{ m s}^{-1})\) is in good agreement with the sunward hemisphere and with mean expansion speeds \((\sim 800 \text{ and } \sim 700 \text{ m s}^{-1})\), respectively, measured through velocity-resolved Atacama Large Millimeter/submillimeter Array (M. A. Cordiner et al. 2021, in preparation) and the Institut de Radioastronomie Millimétrique (N. Biver 2020, private communication) observations. Reasonably contemporaneous to our observations, Wang et al. (2020) and Coulson et al. (2020) reported outflow velocities of 500 and 600 m s\(^{-1}\), respectively. Assuming these lower outflow velocities will decrease the overall production rates by \( \sim 20\% \), but does not significantly change the mixing ratios. We obtained GFs for \( H_2O \) and HCN in each PA set of the L-Custom setting and used them to calculate co-measured \( H_2O \) and HCN production rates in each PA set. We could not obtain well-constrained GFs for the weaker species \( C_2H_2, NH_3, \) and \( HC_3N \); therefore, we used a GF of 2.2 (consistent with the \( H_2O \) GFs across all PA sets) for these species. Similarly, we obtained GFs for \( CH_3OH \) and \( C_2H_6 \) and used the \( CH_3OH \) GF to get an upper limit on co-measured \( H_2CO \). GFs, Qs, and mixing ratios with respect to \( H_2O \) and to \( C_2H_6 \) corresponding to all primary volatiles targeted in this work are listed in Table 2. We note that Qs for all molecules were obtained by adding lines from multiple orders. For deriving HCN mixing ratios in each PA set, we used the co-measured \( H_2O \) production rate. For mixing ratios of all other molecules, we used the \( H_2O \) production rate obtained by adding lines from multiple orders within a PA set and then coadding all of those L-Custom sets.

**3.5. Potential Variability in the Production Rates of \( H_2O \) and HCN**

Figure 4 shows variation in the production rates of \( H_2O \) and HCN during observations spanning \( \sim 6 \text{ hr.} \) We obtained four sets using the L-Custom setting by varying the slit PA by \( 90^\circ \) after each individual set (see Section 2). Both species are color coded and the corresponding error bars are also shown, along with range of UT time corresponding to each set. For clarity, HCN production rates have been vertically offset. \( H_2O \) and HCN production rates obtained in each PA set of the L-Custom setting are shown in Table 2.

**3.6. Coma Volatile Composition of 46P**

Figures 5(A)–(C) shows spectra of HCN, \( C_2H_2, NH_3, CH_3OH, \) and \( C_2H_6 \). Fully leveraging the large spectral grasp of iSHELL, we combined lines for weaker species that were sampled in multiple orders simultaneously in each individual slit orientation set, followed by coadding all of the L-custom sets. In this way, we were able to increase the signal-to-noise and detect the generally weaker species \( C_2H_2 \) and \( NH_3 \), which are offset vertically in the figure.

Being the dominant volatile in most comet nuclei, \( H_2O \) is used as a baseline for calculating mixing ratios of primary volatiles in comets (the exception being C/2016 R2, Pan-STARRS; McKay et al. 2019). In addition to its dominance of the volatile content of most comets, strong lines of \( H_2O \) (or its proxy, \( OH^+ \), prompt emission; Bonev et al. 2006) are available throughout the 2–5 \( \mu m \) region and can be sampled simultaneously with the lines of trace species, minimizing the effects of potential production rate variability when calculating mixing ratios.

Alternate compositional baselines utilizing other species satisfying these conditions can provide complementary insights into the volatile content of comets. In addition to \( H_2O \), we therefore calculated mixing ratios of primary volatiles with respect to \( C_2H_6 \). These measurements will help motivate the development of taxonomies based on alternative compositional baselines in future work. \( C_2H_6 \) generally tends to exhibit a
distinct outgassing behavior compared to $\text{H}_2\text{O}$, its sublimation temperature is among the lowest, and it is relatively easy to detect in the near-IR wavelength range. These characteristics make $\text{C}_2\text{H}_6$ one of the suitable molecules that can be used as an alternative compositional baseline (for a comprehensive discussion on the value of alternative baseline compositional studies and the case for $\text{C}_2\text{H}_6$, see Sections 4.4 and 5.4.2 of Bonev et al. (2021)).

4. Discussion

4.1. Testing Possible Variability in Production Rates

Ground-based remote-sensing observations do not resolve the nucleus of a comet (and thus do not permit identifying individual active regions on the surface), and the limited observation time available generally inhibits sampling of the full surface of a comet during a rotation cycle. There are only a few comets for which the nucleus has been resolved—those visited by spacecraft. As a comet rotates on its axis, different regions of its surface are exposed to solar irradiation, resulting in the activation of distinct sublimation regions on the nucleus. If the nucleus is heterogeneous, this may lead to variability in the composition of coma primary volatiles (e.g., in comet 67P/Churyumov–Gerasimenko; Hässig et al. 2015; Luspay-Kuti et al. 2015).

During our observations, the nucleus of 46P rotated by ∼225°, which is about two-thirds of its rotational period. During this time, the sub-solar point changed its position on the surface by ∼195° (Knight et al. 2020), and the illumination switched from one hemisphere to the other, emphasizing the significance of our time series of measurements. Production rates of $\text{H}_2\text{O}$ and HCN during this period showed a similar trend across the four PA sets: the second PA set showed relatively higher production rates for both species indicating a closer alignment to the nucleus during this period.
low-level variability, whereas the production rates corresponding to all other PA sets were consistent with each other within the uncertainty. The mixing ratio of HCN with respect to H$_2$O, however, remained nearly constant across all of the PA sets. (see Table 2 and Figure 4). We note that the spatial profiles (Figure 2) are similar in each PA set, and the enhancement in production rates is only in one, suggesting that the differences are due to time variability rather than due to nonuniform spatial distributions, for example. Wang et al. (2020) reported moderate time variability in the HCN production rate in 46P on December 14 and 15 using radio observations of the HCN ($J=1–0$) transition. They also reported asymmetric HCN outgassing, although they found that the asymmetric enhancement was in the sunward direction. Due to time constraints, we were not able to sample a full rotation period ($\sim$9 hr) of 46P; therefore, searches for variability on timescales greater than or equal to a single rotation period must be addressed in future perihelion passages of 46P.

4.2. Composition of 46P in the Context of JFCs, OCCs, and the Comet Population Measured at Near-IR Wavelengths

The classification of comets based on their volatile composition (both primary and product species) is an important but complex task in cometary science. Over the past few decades, extensive work at optical wavelengths has resulted in a taxonomic classification of comets based on abundances of their product species. According to this scheme, comets can be classified as “typical” or “carbon-chain depleted” (A’Hearn et al. 1995; Cochran et al. 2012 and references therein); however, tying product species abundances directly to those of their parents is a complex endeavor given their potentially complicated lineage (i.e., multiple potential volatile parents as well as dust for a given product species). More recent work based on the composition of product species in comets (Schleicher & Bair 2014; Cochran et al. 2015) suggested that there can be as many as seven taxonomic groups owing to the complex chemical diversity in comets. Observations of comets using radio techniques have shown no evidence of clear taxonomic groupings (Crovisier et al. 2009;
value of the CH$_3$OH mixing ratio (2.8 ± 0.3%) in 46P on December 18. Based on observations from different dates in 2019 January, McKay et al. (2021) reported an average CH$_3$OH mixing ratio of 2.99 ± 0.23.

4. The 3σ upper limit for H$_2$CO (<0.13σ) suggests that its value in 46P was depleted compared with the mean values among JFCs and OCCs.

5. Compared to the mean values among the overall comet population, 46P showed enrichment in the mixing ratios of CH$_3$OH and depletion in C$_2$H$_2$ and H$_2$CO (based on the 3σ upper limit), whereas C$_2$H$_6$, HCN, and NH$_3$ were consistent within the uncertainty with the mean value. We note that the CH$_3$OH/H$_2$CO ratio of >33 obtained for 46P is among the highest in comets (Dello Russo et al. 2016).

This comparison suggests that 46P is not adequately described as being enriched, depleted, or average in its volatile content, reinforcing the need for a greater sampling of comets in order to develop a more complete taxonomy of comets. Abundances from the 2018 apparition of 46P are an important addition to the ever-evolving repository of comets sampled at near-IR wavelengths and to the continually evolving compositional taxonomy based on these measurements.

4.3. Sensitive Upper Limit for Cyanocetylene (HC$_3$N)

Obtaining a stringent upper limit for molecules such as HC$_3$N is challenging because of its low abundance in comets, the presence of emission lines from many other species that can potentially cause blending, and atmospheric extinction of some lines. The continuous spectral grasp of iSHELL in the L-Custom setting allows for the simultaneous sampling of many lines of HC$_3$N. Combining multiple orders (spanning a frequency range of ~3316–3338 cm$^{-1}$) and all L-Custom observations on that night (a total of 4.715 hr of on-source integration time), coupled with the improved sensitivity of iSHELL, enabled us to derive a sensitive 3σ upper limit of HC$_3$N/H$_2$O of <0.007σ. Obtaining a sensitive upper limit for an underrepresented molecule such as HC$_3$N in a JFC (which are generally fainter and less productive than their Oort cloud counterparts) is important for discerning the lineage of the CN radical in comets. In some comets, the production rates, scale lengths, and spatial distributions of HCN and CN are not consistent (Fray et al. 2005, and references therein), implying that CN might be produced as a result of HC$_3$N photolysis (Bockelée-Morvan & Crovisier 1985; Krasnopolsky et al. 1991). Similar 3σ upper limits (of the order of 10$^{-3}$) for HC$_3$N were reported by Bockelée-Morvan et al. (1987) and Swade et al. (1987) in comet P/Halley observed at radio wavelengths. Croisier et al. (1993) reported a 3σ upper limit of <0.00019 in radio observations of comet Levy 1990 XX.

HC$_3$N was first identified with radio observations of comet C/1995 O1 (Hale–Bopp; Bockelée-Morvan et al. 2000) with an abundance ratio (relative to H$_2$O) of 0.02σ. HC$_3$N has since been detected in multiple comets at millimeter/submillimeter wavelengths through its pure rotational transitions, with abundances ranging from 0.002σ to 0.068σ (Bockelée-Morvan & Biver 2017). At near-IR wavelengths, HC$_3$N has been sampled in comets that include C/2009 P1 (Garradd; Villanueva et al. 2012c) with a 3σ upper limit of <0.03σ and comet 103P/Hartley 2 (Dello Russo et al. 2011) with a 3σ upper limit of <0.024σ. Our 3σ upper limit (<0.007σ) is
lower than these values, and it represents the most stringent measure of HC$_3$N at near-IR wavelengths to date. E. Jehin (2020, private communication) reported a Q(CN) of $(1.27 \pm 0.032) \times 10^{23}$ mol s$^{-1}$ on UT 2018 December 16 and $(1.14 \pm 0.021) \times 10^{23}$ mol s$^{-1}$ on December 23 in 46P using the robotic TRAPPIST-South and -North telescopes narrowband photometry. These values are relatively close to our HCN Qs in all PA sets (except for the second PA set, which resulted in a higher number), suggesting that HCN might be the predominant precursor of CN in 46P.

### 4.4. Comparison with iSHELL and NIRSPEC-2 Observations during the Same Perihelion Passage

Table 4 summarizes H$_2$O production rates in 46P in 2018 December. These results suggest that H$_2$O production rates obtained from iSHELL across other post-perihelion dates are consistent with our December 21 results, whereas those measured with NIRSPEC-2 on December 17 and 18 (Bonev et al. 2021) and with iSHELL on December 18 (Roth et al. 2021) are higher, despite only a marginal change in the geocentric and heliocentric distances of 46P between December 17 and 21 ($R_g$ varied from 1.057 to 1.061 au between these dates; $\Delta$ varied from 0.078 to 0.082 au). This might be an indication of variability in H$_2$O production rates on a timescale of days (addressing possible variability in 46P during its 2018 apparition is the subject of future work). Using measurements from SOHO/SWAN, Combi et al. (2020a) reported that the overall H$_2$O production rate in 46P decreased significantly throughout its 1997, 2002, 2008, and 2018 apparitions along with a large steepening of the change in H$_2$O production rate with $R_g$. While these measurements do not cover the dates listed in Table 4, the H$_2$O production rate measured on December 22, 976 ($\sim 1.6 \times 10^{28}$ mol s$^{-1}$) was significantly higher than our December 21 values of $\sim 6 \times 10^{27}$ mol s$^{-1}$ with the caveat that the SOHO/SWAN measurements may be more sensitive to an extended source of water in the coma than our near-IR measurements. With the exception of H$_2$O, the production rates of all molecules we measured agree within 1–2$\sigma$ uncertainty with values obtained from NIRSPEC-2 on UT December 17 and 18, whereas the mixing ratios we obtained agree with within 1$\sigma$ with values from NIRSPEC-2 with the exception that our CH$_3$OH mixing ratio is higher.

### 5. Summary and Future Outlook

We utilized the exceptional observing conditions offered by 46P/Wirtanen’s historical 2018 apparition to characterize its primary volatile content and to determine the spatial associations of species in the coma. Through our measurements we obtained the following results:

1. We obtained mixing ratios with respect to H$_2$O (and C$_2$H$_6$) of the primary volatiles H$_2$O, HCN, C$_2$H$_2$, NH$_3$, C$_3$H$_6$, and CH$_3$OH on UT 2018 December 21 using the iSHELL spectrograph at the NASA IRTF. We obtained stringent 3$\sigma$ upper limits for H$_2$CO and also HC$_3$N, a molecule that has been rarely studied in comets to date.

2. We placed the chemical composition of 46P/Wirtanen in the context of comets observed at near-IR wavelengths and found that the comet does not follow the simple three-tiered taxonomic scheme, i.e., it is not systematically enriched, depleted, or averaged in the mixing ratios of its volatiles.

3. We were able to extract spatial profiles for co-measured HCN and H$_2$O in multiple, independent slit orientations of the L-Custom setting. We also obtained spatial profiles for co-measured CH$_3$OH and C$_2$H$_6$. Both gases exhibited broader profiles compared to the profile from dust, whereas the CH$_3$OH profile was broader as compared to co-measured C$_2$H$_6$. Spatial profiles of all of the gases were asymmetric and extended in the projected antisunward direction.

4. We compared production rates of HCN and H$_2$O obtained from mutually perpendicular slit orientations to search for potential short-term variability and found that both of these species follow a similar trend and exhibit a low-level, short-term variability.

5. Our H$_2$O production rates generally agreed with those obtained on other dates post-perihelion except for measurements with iSHELL on December 18 and those obtained with NIRSPEC-2 on December 17 and 18, which yielded higher Q(H$_2$O), suggesting variability in the H$_2$O production rate over a time span of a few days.

Additional observations obtained using iSHELL and NIRSPEC during the exceptional 2018 apparition of 46P will enable future work testing for long-term variability in the comet, thus addressing the “snapshot” bias associated with cometary observations taken over a limited range of dates and/ or heliocentric distances. Comparisons between dates pre-perihelion, near-perihelion, and post-perihelion will test for potential seasonal effects in 46P (e.g., Hässig et al. 2015; McKay et al. 2015; Roth et al. 2018). Observations taken with sufficient geocentric velocity will enable the study of hypervolatiles CO and CH$_4$ by shifting their lines away from their telluric counterparts, increasing the sample size of these underrepresented molecules in studies of JFCs (e.g., DiSanti et al. 2017; McKay et al. 2021).

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