Hypervolatiles in a Jupiter-Family Comet: Observations of 45P/Honda–Mrkos–Pajdušáková Using iSHELL at the NASA-IRTF

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Abstract

We used the new high spectral resolution cross-dispersed facility spectrograph, iSHELL, at the NASA Infrared Telescope Facility on Maunakea, HI, to observe Jupiter-family comet (JFC) 45P/Honda–Mrkos–Pajdušáková. We report water production rates, as well as production rates and abundance ratios relative to H₂O, for eight trace parent molecules (native ices), CO, CH₄, H₂CO, CH₃OH, HCN, NH₃, C₂H₂, and C₂H₆, on 2 days spanning UT 2017 January 6/7 and 7/8, shortly following perihelion. Trace species were measured simultaneously with H₂O and/or OH prompt emission, a proxy for H₂O production, thereby providing a robust and consistent means of establishing the native ice composition of 45P. Its favorable geocentric radial velocity (approximately −35 km s⁻¹) permitted sensitive measures of the “hypervolatiles” CO and CH₄, which are substantially undercharacterized in JFCs. Our results represent the most precise ground-based measures of CO and CH₄ to date in a JFC, providing a foundation for building meaningful statistics regarding their abundances. The abundance ratio for CH₄ in 45P (0.79% ± 0.06% relative to H₂O) was consistent with its median value as measured among Oort Cloud comets, whereas CO (0.60% ± 0.04%) was strongly depleted. Compared with all measured comets, HCN (0.049% ± 0.012%) was strongly depleted, CH₃OH (3.6% ± 0.3%) was enriched, and the remaining species were consistent with their respective median abundances. The volatile composition measured for 45P could indicate processing of ices prior to their incorporation into its nucleus. Spatial analysis of emissions suggests enhanced release of more volatile species into the sunward-facing hemisphere of the coma.

Key words: comets: general – comets: individual (45P/Honda–Mrkos–Pajdušáková) – techniques: spectroscopic

1. Hypervolatiles in Jupiter-family Comets and the Recent Apparition of 45P/H-M-P

Jupiter-family comets (JFCs) represent the dynamical end state of “ecliptic” comets, which are fed primarily from the scattered Kuiper disk and typically have low orbital inclination with respect to the ecliptic plane. This distinguishes them from nearly isotropic (long-period, dynamically new, or nonreturning) comets that have random inclinations and are traced to the Oort Cloud; these will henceforth be referred to as Oort Cloud comets (OCCs).

Owing to their small size, comets lack significant gravitational heating of material in their nuclei. These volatile-rich small bodies are generally thought to contain a preserved compositional record of icy solar system material dating to the period of their formation (Bockelée-Morvan et al. 2004; Mumma & Charnley 2011). A key question in cometary science is whether systematic differences in composition exist between JFCs and OCCs.

Are comets primarily pristine relics versus being significantly chemically evolved, perhaps even collisional fragments of larger bodies (Schlichting et al. 2013; Morbidelli & Rickman 2015)? The recent Rosetta mission to JFC 67P/Churyumov–Gerasimenko provided high spatial resolution imaging that revealed substantial morphological diversity (El-Maarry et al. 2015), suggesting that previously posited collisional evolution scenarios (Davis & Farinella 1997) could be relevant, at least for some comets. Measuring the abundances of ices having low sublimation temperatures, for example, the “hypervolatiles” CO and CH₄ that are the central theme of our study, can test retention of a primitive record. These highly volatile species should be preferentially lost, unless trapped in less volatile species such as H₂O. No definitively high CO or CH₄ abundances have been found to date in a JFC (see, e.g., Dello Russo et al. 2016a, and references therein).

The initial relatively simplistic paradigm, in which OCCs formed between heliocentric distances Rₖ ~ 5 and 30 au while ecliptic comets formed at larger Rₖ, has been largely replaced by the notion of a more “mixed” formation region for comets. This evolution in thinking resulted from increasingly sophisticated dynamical models (Levison & Duncan 1997; Gomes et al. 2005; Morbidelli et al. 2005; Levison et al. 2011; Nesvorný et al. 2017) and also from the presence of crystalline silicates in comets. These were first seen in 1P/Halley (Bregman et al. 1987) and subsequently in JFCs 9P/Tempest 1, through remote sensing of material released as a result of the Deep Impact experiment (Harker et al. 2005), and also in 81P/Wild 2, through analysis of grains returned by the Stardust mission (Zolensky et al. 2009). The presence of crystalline
silicates in comets supports thermal processing of material at small $R_{\odot}$ and large-scale mixing in the early solar nebula, as suggested previously (Nuth et al. 2000).

There is unambiguous compositional diversity over the entire comet population; however, differences between dynamical classes appear more understated, albeit with some emerging trends (see below; also Bockelée-Morvan et al. 2004; DiSanti & Mumma 2008; Dello Russo et al. 2016a, and references therein). Disentangling natal from evolutionary effects is necessary for linking present-day cometary compositions to their birthplaces in the early solar nebula, and comparing the chemistry of JFCs and OCCs, comets with different dynamical histories, is key to addressing this goal.

The largest sample size for testing compositional differences among comets from both JFC and OCC dynamical populations is based on a compilation of product species abundances for more than 200 comets studied at optical wavelengths and spanning four decades (A’Hearn et al. 1995; Fink 2009; Cochran et al. 2012; Schleicher & Bair 2014). Compositional diversity is confirmed among comets, in that approximately one-third of those measured were depleted in $C_2$ and $C_3$ relative to CN and OH, suggesting carbon-chain depletion. Of these, about one-half of JFCs but only 10% of OCCs were carbon chain depleted, pointing to a systematic compositional difference (A’Hearn et al. 1995) that appears tied more to natal (i.e., formation) conditions than to evolutionary processing (Schleicher 2007; Dello Russo et al. 2009; Fink 2009).

Despite this relatively large database, a complete understanding of comet composition requires linking product species to potential progenitor (primary, or “parent”) molecules, released in the coma upon sublimation of ices contained in the nucleus (referred to as “native ices”). A suite of parent species emit through vibrational bands at infrared wavelengths and, where allowed, through rotational transitions at millimeter/submillimeter wavelengths and electronic transitions in the ultraviolet.

The taxonomy of comets based on the composition of native ices also supports diversity, both among individual comets and between dynamical classes. The most comprehensive review to date compiles results for 9 JFCs and 21 OCCs (Dello Russo et al. 2016a), summarizing abundance ratios for up to eight native trace ices relative to $H_2O$, the most abundant ice in comet nuclei. Comparing results among comets can test whether JFCs and OCCs experienced different processing histories; however, it is essential to bear in mind that taxonomic results are continually evolving as more comets are measured, and that for JFCs mean abundance ratios are generally less well established. For example, the four most volatile ices systematically measured in comets are $CO$, $CH_4$, $C_2H_2$, and $C_2H_6$—the last three of which lack a dipole moment and so can be measured only in the IR. Of these, $C_2H_2$ and $C_2H_6$ have systematically lower abundance ratios in JFCs; however, this is based on small numbers of measured comets (<10).

Measurements of CO and $CH_4$, which have the lowest sublimation temperatures among molecules systematically targeted in comets, are particularly sparse in JFCs. Lines of these two important hypervolatiles have highly opaque counterparts in the terrestrial atmosphere. Therefore, their measurement from the ground requires sufficient geocentric radial velocity ($\Delta_{geo}$) to Doppler-shift cometary emission lines into regions of sufficiently high atmospheric transmittance. The relative paucity of CO and $CH_4$ abundances in JFCs (see, e.g., Figure 2 and Table 4 in Dello Russo et al. 2016a) has traditionally resulted from a combined lack of sensitivity and/or unfavorable observing circumstances: because JFCs are generally less productive than OCCs, they are most easily measured when near closest approach to Earth, yet at this time they have near-zero $\Delta_{geo}$. Thus, CO and $CH_4$ are substantially underrepresented in studies of JFCs, yet their robust measure is essential for establishing statistically meaningful abundance ratios.

A highly favorable opportunity to more completely sample the chemistry in a JFC presented itself with comet 45P/Honda–Mrkos–Pajdušáková (hereafter 45P) shortly following its perihelion passage on UT 2016 December 31. Discovered in 1948 (Nakano Note NK673), subsequent analysis of its orbit revealed a close passage to Jupiter (0.08 au) in 1935 that decreased its perihelion distance ($q$) from 0.64 to 0.58 au. Another encounter with Jupiter in 1983 decreased $q$ to 0.54 au,10 close to its current value (0.5325 au). Results from optical observations place 45P in the “typical” range in terms of $C_2$ and $C_3$ abundance (A’Hearn et al. 1995); however, little is known of its native ice composition. Submillimeter wavelength observations detected HCN (Biver 1997), $H_2O$, $CH_3OH$, and $NH_3$ (Biver et al. 2014; N. Biver, personal communication).

Here we present $H_2O$ production rates and production rates and abundance ratios with respect to $H_2O$ for eight trace volatiles ($CO$, $CH_4$, $C_2H_2$, $C_2H_6$, $H_2CO$, $CH_3OH$, $HCN$, and $NH_3$) in 45P using iSHELL, the new high-resolution, cross-dispersed spectrograph at the NASA Infrared Telescope Facility (IRTF). Its daytime observing capability (unique among IR platforms), combined with the large $\Delta_{geo}$ of 45P, enabled the scope of our investigation (see Sections 2.2 and 3.4). In all cases trace volatiles were co-measured with $H_2O$ and/or OH prompt emission (denoted OH*). OH* is well established as a proxy for the production and spatial distribution of its parent, $H_2O$ (Mumma et al. 2001; Bonev 2005; Bonev et al. 2006). Obtaining robust measures of abundance ratios relative to $H_2O$ for native ices in 45P—especially CO and $CH_4$—was the principal objective of our study.

2. The Advantages of iSHELL at the IRTF

2.1. Basics of iSHELL

The recent commissioning of iSHELL (Rayner et al. 2012, 2016), which replaced the heritage CSHELL spectrograph and became available for use through proposal peer review beginning in 2016 October, has opened a new realm for the study of native ice abundances in comets. This powerful new instrument11 features both high-resolution long-slit spectroscopy and imaging/active guiding in the near-IR ($\lambda = 1.1–5.4 \mu m$), with eXecutable User Interfaces (XUIs) for each patterned after SpeX, the IRTF moderate-resolution spectrograph/imager.

The iSHELL long-slit echelle spectrograph incorporates a 2048 $\times$ 2048 pixel Hawaii 2RG array detector and delivers spectral resolving power ($\lambda/\Delta \lambda$) up to $\sim 7.5 \times 10^4$ with the narrowest (0′′375-wide) slit. This slit maps a spatially uniform monochromatic source (e.g., an arc lamp or sky emission line) onto 3 spectral pixels (FWHM), thus providing an effective

10 For historical highlights, see http://cometography.com/jpcomets/045p.html. 11 The latest iSHELL manual is available for download from the IRTF website: http://irftpweb.ifa.hawaii.edu/~ishell/.
0\textquoteleft 125 pixel\(^{-1}\) plate scale at the entrance slit. Additional slit widths are available, including 4\textquoteleft for minimizing slit losses and thereby achieving accurate absolute flux calibration. For our observations of 45P, we used a 0\textquoteleft 75 (6 pixel) wide slit. This delivers \(\lambda/\Delta \lambda \approx 3.8 \times 10^{3}\) for a uniform monochromatic source; our comet spectra were consistent with this or slightly higher values (see Section 3.2). Through its cross-dispersing capability, iSHELL simultaneously measures signal in many (>10) consecutive echelle orders (Figure 1). In the spatial dimension (i.e., along the slit), its cross-dispersing optics produce a (modestly) wavelength-dependent plate scale on the array of 0\textquoteleft 16–0\textquoteleft 17 pixel\(^{-1}\) for the orders included in our study. Multiple slit lengths are available; our observations were conducted at \(\lambda > 2.8 \mu m\), allowing use of a 15\textquoteleft slit. This permitted detailed spatial analysis of emission profiles (Section 5.5).

The free spectral range is matched to the array at \(\lambda \approx 4 \mu m\), meaning that iSHELL is spectrally continuous for shorter wavelengths (i.e., there are no interorder “gaps” in wavelength), making it unique among IR echelle spectrographs. A given L or L-prime instrument setting spans a total range of 10%–11% of the selected wavelength (e.g., as seen in Figure 1). At longer wavelengths (∼4.5–5.3 \mu m), two identical cross-dispersing gratings are required to achieve full spectral coverage. These gratings are tilted slightly relative to each other in the dispersion direction, such that one extends to the blue end of each encompassed order and the other to the red end, with approximately 85% overlap in their wavelength coverage.

The iSHELL imager has a 42\textquoteleft circular field of view and a pixel scale of approximately 0\textquoteleft 01. Filter imaging is performed in specific wavelength bands, independent of the wavelength regime being used to obtain spectra. The slit-viewing camera allows for guiding on targets while obtaining spectra. As with SpeX, active (or “auto”) guiding is achieved through periodic measurement of the photo-center for “spillover” light (i.e., that not passed through the entrance slit), provided that the target is sufficiently bright and the background sky is sufficiently stable. The centroid position is relayed to the Telescope Control System to correct pointing in real time as needed. Active guiding was not possible for our (daytime) observations of 45P (see Section 3.1).

2.2. Challenges with Measuring Cometary CO and CH\(_4\)

The hypervolatiles CO and CH\(_4\) are substantially under-represented in taxonomic studies of parent volatile composition in JFCs. The difficulty associated with these measurements is illustrated in Figure 2, in which histograms (panels (a) and (b)) show the very few measurements of CH\(_4\) and CO in JFCs (these panels are taken from Figure 2 of Dello Russo et al. 2016a). Panel (c) illustrates the high degree of accuracy required to separate lines of cometary CH\(_4\) from their (opaque) telluric counterparts, even for \(\Delta \text{dot} = 10–15 \text{ km s}^{-1}\) and in the case of a relatively bright comet having a substantial abundance ratio CH\(_4\)/H\(_2\)O; the example shown is C/2001 A2 LINEAR (CH\(_4\)/H\(_2\)O = 1.5 \times 10^{-2}), obtained with NIRSPEC at Keck II (\(\lambda/\Delta \lambda \approx 24,000\); Gibb et al. 2007). The higher spectral resolving power of iSHELL, together with the daytime observing capability of the IRTF, ameliorates this difficulty, although disentangling cometary emission from telluric absorption remains problematic for small Doppler shifts. Near perihelion, 45P had highly favorable \(\Delta \text{dot}\) (Table 1), displacing lines of CH\(_4\) and CO well away from their absorbing counterparts in the telluric atmosphere.

3. Observations of Comet 45P/H-M-P with iSHELL
3.1. Acquisition of Spectra

We targeted 45P shortly prior to (on UT 2016 December 30–31) and following (on UT 2017 January 6–8) its perihelion passage. On all dates 45P was located <30° from the Sun, and therefore all observations were conducted during daytime. The pre-perihelion dates were weathered out, but we obtained high-quality post-perihelion spectra. Here we report results from two days, bridging UT 2017 January 6/7 and 7/8 (Table 1). For convenience these will henceforth be referred to as (UT) January 7 and 8, respectively.

We first imaged Venus (to establish telescope pointing), then a bright star near our target, and finally 45P using a broadband K filter. Only this and shorter-wavelength filters were available at the time of our observations of 45P. Broadband and narrowband L and L-prime and narrowband M filters have since been added.

For the small solar elongation of 45P, the background sky level was relatively high. We found that short-term background fluctuations were comparable to or greater than the comet signal, and this precluded using the iSHELL auto-guider. Instead, we established nonsidereal telescope tracking rates that were adequate to maintain the comet at a constant location on the array—within the seeing disk, approximately 0\textquoteleft 9–1\textquoteleft and 1\textquoteleft 2–1\textquoteleft 5 on January 7 and 8, respectively—for the duration of a spectral observing sequence (amounting to 3–5 minutes of clock time). We acquired spectra using our standard ABBA sequence of telescope nodding, with approximately 30–40 s of integration time in each of the four scans, which were stored as individual frames. Both A and B beams were in the slit, spatially separated by half its length (7\textquoteleft 5) and positioned symmetrically with respect to its midpoint (see Figures 1 and 3 (a)). We oriented the slit along the projected Sun–comet direction on the dates of our observations (Table 1), which permitted comparing release of material into sunward- versus anti-sunward-facing hemispheres (see Figure 7, and discussion in Section 5.5).
At the end of each ABBA spectral sequence, we moved the telescope 10′ north (approximately perpendicular to the slit) and re-imaged the comet; this permitted assessing its position more clearly. We then repositioned it at the fiducial A-beam location and began the next spectral sequence. This process was repeated until adequate signal-to-noise ratio was accumulated in targeted cometary emissions, based on running stacks of raw difference frames (A – B) such as that shown in Figure 1. The comet was bright enough to recognize continuum and/or brighter emission lines in most individual A–B spectral difference frames, as displayed in the spectrometer data viewer XUI.

3.2. Processing of Spectral Data

Our methodology for processing spectra is detailed in the refereed literature (Bonev 2005; DiSanti et al. 2006, 2014; Villanueva et al. 2009; Radeva et al. 2010) and so will not be repeated here, except for aspects pertaining uniquely to the layout of iSHELL orders on the array. In contrast to the tilting (or slanting) of orders in long-slit spectral data obtained with other high-resolution infrared spectrometers (specifically, NIRSPEC/Keck II, CSHELL/IRTF, CRRES/VLT, and IRCs/Subaru), the curvature (“bowing”) of iSHELL orders required isolating these and spatially resampling (i.e., straightening) through use of a second-order polynomial (a parabolic function). Once accomplished, the subsequent steps of (1) spectral resampling through registration of observed sky emission lines along the slit, (2) obtaining the approximate spectral calibration through comparison of sky line positions with a modeled telluric radiation spectrum, and (3) improving spectral calibration and establishing spectral resolving power and column burdens of terrestrial atmospheric absorbers were accomplished as discussed previously. All spectra of 45P shown in Figures 3–5 represent the signal contained in 15 spatial pixels (amounting to a 0.′75 × 2.′5 aperture) centered on the peak comet signal, taken to be the approximate line of sight to the nucleus. These 15-row spectral extracts were performed on processed orders, using the combined A- and B-beam signal. Figure 4(c) shows a two-dimensional (spatial-spectral) representation of the combined signal from order 155, separate beams of which are shown in raw form in Figure 1.

For all comet settings, we also obtained spectra of the bright IR flux standard star BS 8709 using the 4″-wide slit (Table 1). Comparisons between observed stellar spectra and modeled atmospheric transmittance were performed (step 3 above). We used active guiding on BS 8709; thus, its spectral resolving power depended primarily on the stellar point-spread function and hence on atmospheric seeing. Our values for BS 8709 consistently clustered around $\lambda/\Delta \lambda = 2 \times 10^4$, considerably larger than that expected for uniform monochromatic illumination of the 4″ slit ($\sim (6–8) \times 10^3$).

Contributions from continuum and gaseous emissions in the comet spectra were established as described previously (e.g., DiSanti et al. 2016); the procedure is illustrated in Figures 3–5. The fully resolved transmittance function was convolved to the spectral resolving power of the data (approximately $4.0 \times 10^6$) and scaled to the observed comet spectrum. Cometary emission lines were isolated by subtracting the modeled continuum, and this difference, representing the observed net emission spectrum, was compared with molecular fluorescence models.

In practice, all models (continuum and molecular) were fit simultaneously to each observed comet spectrum so as to minimize rms deviations in the overall residuals (corresponding
Table 1
Log of IR Spectral Observations of Comet 45P/H-M-P with iSHELL.a

<table>
<thead>
<tr>
<th>2017 January UT Date</th>
<th>Setting ID</th>
<th>(\Delta \nu ) (cm(^{-1}))</th>
<th>UT Start–End</th>
<th>(R_h) (au)</th>
<th>(\Delta) (au)</th>
<th>(\Delta)w (km s(^{-1}))</th>
<th>Molecule(s) (orders)(^b)</th>
<th>(T_{int}) (s)</th>
<th>Slit PA (deg)</th>
</tr>
</thead>
<tbody>
<tr>
<td>06/07</td>
<td>M2</td>
<td>2159.6–2141.5, 2140.2–2122.2</td>
<td>23:04–00:37</td>
<td>0.552</td>
<td>0.567</td>
<td>−35.56</td>
<td>CO, H(_2)O (111, 110)</td>
<td>1051</td>
<td>74.5</td>
</tr>
<tr>
<td></td>
<td>Lp1</td>
<td>3043.5–3019.1, 3005.1–2980.6</td>
<td>00:56–01:48</td>
<td>0.552</td>
<td>0.565</td>
<td>−35.36</td>
<td>CH(_3), OH(^<em>) (157, 155) C(_2)H(_6), CH(_3)OH, CH(_4), OH(^</em>) (155, 147) H(_2)CO, OH(^*) (147, 144)</td>
<td>1186</td>
<td>74.5</td>
</tr>
<tr>
<td>07</td>
<td>L1</td>
<td>3465.8–3438.0</td>
<td>02:28–02:58</td>
<td>0.552</td>
<td>0.564</td>
<td>−35.19</td>
<td>H(_2)O (179)</td>
<td>830</td>
<td>74.5</td>
</tr>
<tr>
<td>BS 8709(^g)</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>07/08</td>
<td>L2</td>
<td>3389.0–3361.8, 3312.4–3285.6, 3389.0–3361.8</td>
<td>22:35–00:18</td>
<td>0.558</td>
<td>0.546</td>
<td>−34.98</td>
<td>H(_2)O (175) HCN, NH(_3), C(_2)H(_2) (171) NH(_3) (175, 171)</td>
<td>1779</td>
<td>74.0</td>
</tr>
<tr>
<td>08</td>
<td>M2</td>
<td>2159.6–2141.5, 2140.2–2122.2</td>
<td>00:37–01:28</td>
<td>0.558</td>
<td>0.545</td>
<td>−34.86</td>
<td>CO, H(_2)O (111, 110)</td>
<td>1751</td>
<td>74.0</td>
</tr>
<tr>
<td></td>
<td>Lp2</td>
<td>2793.1–2770.6</td>
<td>02:09–02:54</td>
<td>0.558</td>
<td>0.544</td>
<td>−34.70</td>
<td>H(_2)CO, OH(^*) (144)</td>
<td>1186</td>
<td>74.0</td>
</tr>
<tr>
<td>BS 8709(^g)</td>
<td></td>
<td></td>
<td></td>
<td></td>
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</tr>
</tbody>
</table>

Notes.

- The slit dimensions used for 45P were 0\(^\prime\)75 \times 15\(^\prime\). The spatial scale on the spectrometer array is approximately 0\(^\prime\)16–0\(^\prime\)17 pixel\(^{-1}\) in the orders analyzed for our study. Our results are not sensitive to the exact value used; we adopted the value 0\(^\prime\)16 pixel\(^{-1}\) in calculating production rates and abundance ratios (Table 2).
- Spectral settings were chosen to optimize the sampling of molecular composition in comet 45P.
- Approximate frequency range covered within each targeted order.
- Encompassed molecules/radicals (OH\(^*\)) that are addressed in this paper. Echelle order(s) in which emissions occur are listed in parentheses.
- Total on-source integration times, by setting.
- Slit position angle on the sky, measured clockwise from north as usual. On both dates this corresponds to the extended heliocentric radius vector (i.e., the projected Sun–comet direction).
- IR flux standard star observed on each date, measured in all settings used for 45P. BS 8709 is spectral type A3 V, L/Lp-magnitude 3.05, and M-magnitude 3.06. The slit dimensions used for BS 8709 were 4\(^\prime\)0 \times 15\(^\prime\), chosen to maximize the fraction of stellar flux transmitted through the slit.
Figure 3. Panel (a): section of the M-band echellogram showing simultaneous measurement of CO and H₂O in 45P on 2017 January 8 (29.2 minutes on source). Lines of H₂O in two orders are marked (circles); these and others are apparent, superimposed on the comet continuum in both A (white) and B (black) beams. CO lines are labeled with rotational designations, and horizontal gold ticks indicate displacements from corresponding telluric absorptions due to the favorable geocentric Doppler shift of 45P that permitted robust measurement of CO (and also CH₄; Figure 4). Panels (b) and (c): extracted spectra, with traces and labels as described in Section 3.4.1. Note the gap in encompassed frequency/wavelength between the right edge of order 111 and the left edge of order 110, amounting to about 6.4% of the spectral coverage within either order.
power, our results remained constant to well within 1σ uncertainty. For this reason all production rates and abundance ratios reported here are based on $\lambda/\Delta \lambda = 4.0 \times 10^4$.

### 3.3. Molecular Production Rates

We obtained "nucleus-centered" production rates ($Q_{\text{nu}}$) using a well-established formalism (Dello Russo et al. 1998; DiSanti et al. 2001; Bonev 2005; Villanueva et al. 2011a). This relates observed emission line flux to (modeled) fluorescence efficiency (g-factor) multiplied by atmospheric transmittance at each Doppler-shifted line frequency and includes molecular photodissociation lifetime together with geometric parameters. Additional details are found in Section 3.2.2 of DiSanti et al. (2016), and papers detailing the fluorescence models used in our analysis are cited by molecule in Section 3.2 of Paganini et al. (2014). Individual line g-factors depend on rotational temperature ($T_{\text{rot}}$), which for our present study is consistent with 90 K, as determined from measurement of H$_2$O lines (see Figure 5(a), and Section 3.5.1 in a spectral region first identified from spectral analysis of comet 153P/Ikeya–Zhang (Dello Russo et al. 2004).

The $Q_{\text{nu}}$ were then multiplied by an appropriate growth factor (GF), determined through the well-documented "Q-curve" method for analyzing spatial profiles of emissions and dating to our study of carbonyl sulfide in C/1995 O1 (Hale-Bopp; Dello Russo et al. 1998). This primarily corrects for atmospheric seeing—which invariably suppresses signal along lines of sight passing close to the nucleus—while also accounting for potential slight drift of the comet during the course of the ABBA spectral sequences. The product $Q_{\text{nu}} \times$ GF is taken to be the "total" (or "global") molecular production rate, denoted $Q_{\text{tot}}$. Our results for 45P are summarized in Table 2.

#### 3.3.1. Dependence on Gas Outflow Speed

We assumed the canonical outflow speed $v_{\text{gas}} = 800 \text{ m s}^{-1} \times R_8^{0.5}$ in determining our production rates. We note that GBT 18 cm OH spectra of 45P spanning 2016 December 16 to 2017 January 22 measured a constant value from the line velocity profile ($750 \pm 80 \text{ m s}^{-1}$; Harris et al. 2017). Assuming $v_{\text{gas}} = 800 \text{ m s}^{-1}$ for our observations, as opposed to $\approx 1080 \text{ m s}^{-1}$ based on the above power law for $R_8 \approx 0.55 a$, would decrease our production rates by approximately 35%. However, this would not significantly change our abundance ratios relative to H$_2$O (the focus of our study), and therefore our production rates in Table 2 are based on the power-law-based value for $v_{\text{gas}}$.

#### 3.4. Secure Detection of Hypervolatiles in Comet 45P

The highly favorable geocentric radial velocity of 45P near perihelion ($\Delta_{\text{ret}} \approx -35 \text{ km s}^{-1}$) combined with the sensitivity and high spectral resolution of iSHELL, permitted robust measurements of both CO and CH$_4$ (Table 2). We expect our results for 45P, together with similar measurements of future targets, to establish meaningful statistics for abundance ratios of these two substantially underrepresented hypervolatiles, particularly in JFCs as illustrated unequivocally in Figures 2(a)/(b) (also see Figures 6(a)/(b) and discussion in Section 5.1).

#### 3.4.1. CO

We obtained secure detections of CO measured simultaneously with H$_2$O (Figure 3), on both January 7 and 8. In
Figure 3(a), lines of H$_2$O are marked (circles) in the two orders (110 and 111) containing the strongest observed lines of CO, with additional H$_2$O apparent in the two other orders shown. Many more H$_2$O lines are covered in this setting (M2), which in total encompasses (most of) orders 99–114.

Extracted spectra reveal emissions from both CO and H$_2$O superimposed on the cometary continuum (Figures 3(b), (c)). The modeled continuum is represented by the gold trace overlaying each spectrum. Below these are fluorescence models (color-coded and labeled by molecule), shifted in frequency according to the $\Delta_{\text{rot}}$ of 45P, multiplied by the modeled monochromatic atmospheric transmittance at each Doppler-shifted line frequency, and scaled to the observed emission line intensity in excess of the continuum. The red trace is the overall modeled spectrum (continuum + molecular), and the bottom trace (labeled “residuals”) is observed spectrum minus overall modeled spectrum. Figures 4 and 5 show analogous representations for other instrument settings/orders.

Abundances of CO in JFCs (plus 2P/Encke) previously obtained by remote sensing number only five. Of these, one is a (3$\sigma$) upper limit (in 2P/Encke; Radeva et al. 2013) and one represents a range of values observed with the Hubble Space Telescope (in 103P/Hartley 2; Weaver et al. 2011). The remaining three measurements have $\pm$1$\sigma$ uncertainties that are very large compared with our measurement of CO in 45P (see Figure 6(a), and Section 5.1).

3.4.2. CH$_4$

Having a large geocentric Doppler shift is even more beneficial in the case of methane. We measured CH$_4$ in two orders within the Lp1 setting (Figure 4). As is the case with CO, the large geocentric velocity of 45P ($\Delta_{\text{rot}} \approx -35$ km s$^{-1}$) displaced each cometary emission line of CH$_4$ well away from its absorbing counterpart in the terrestrial atmosphere, seen to the right of each comet line.

Previously reported abundances of CH$_4$ among JFCs through remote sensing number only four, fewer than in the case of CO. Two of these (73P/Schwassmann–Wachmann 3 and 103P/Hartley 2) are upper limits (Villanueva et al. 2006; Kawakita et al. 2013), and as with CO, the other two have much larger associated uncertainties compared with our measurement of CH$_4$ in 45P (Figure 6(b)).

3.5. Additional Measurements in 45P with iSHELL

Our study emphasizes measurement of the hypervolatiles CO and CH$_4$; however, only by characterizing a suite of native volatiles can the chemistry of 45P be framed in a more complete context. Robust measurement of molecular production rates requires knowledge of rotational temperature ($T_{\text{rot}}$) in the coma. We accomplished this through targeting water near 2.9 $\mu$m.
Table 2
Molecular Production Rates and Abundances in 45P/H-M-P

<table>
<thead>
<tr>
<th>2017 UT Date</th>
<th>Setting/Order</th>
<th>Species</th>
<th>(10^{-26} \text{ mol s}^{-1})</th>
<th>(Q_{\text{tot}})</th>
<th>(Q_{\text{tot}}/Q_{\text{H2O}})</th>
</tr>
</thead>
<tbody>
<tr>
<td>Jan 6/7</td>
<td>M2/111</td>
<td>(\text{H}_2\text{O})</td>
<td>6.06</td>
<td>172 ± 9.0</td>
<td>(1.62 ± 0.09)</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(\text{CO})</td>
<td>1.04 ± 0.09</td>
<td>1.69 ± 0.16</td>
<td>0.61 ± 0.05</td>
</tr>
<tr>
<td></td>
<td>M2/110</td>
<td>(\text{H}_2\text{O})</td>
<td>5.57</td>
<td>162 ± 11</td>
<td>(1.63 ± 0.10)</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(\text{CO})</td>
<td>0.96 ± 0.11</td>
<td>1.56 ± 0.18</td>
<td>0.56 ± 0.06</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(\text{H}_2\text{O})</td>
<td>171 ± 8.9(^f)</td>
<td>1.62 ± 0.07</td>
<td>0.59 ± 0.04(^g)</td>
</tr>
<tr>
<td>Jan 7</td>
<td>Lp1/157</td>
<td>(\text{OH}^+)</td>
<td>8.80</td>
<td>110 ± 31</td>
<td>(2.16 ± 0.54)</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(\text{CH}_4)</td>
<td>0.80 ± 0.06</td>
<td>1.49 ± 0.13</td>
<td>0.77 ± 0.07</td>
</tr>
<tr>
<td>Jan 7/8</td>
<td>Lp2/175</td>
<td>(\text{H}_2\text{O})</td>
<td>16.0</td>
<td>165 ± 9.5</td>
<td>(1.94 ± 0.24)</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(\text{OH}^+)</td>
<td>173 ± 13</td>
<td>337 ± 49</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Lp2/171</td>
<td>(\text{OH}^+)</td>
<td>15.1</td>
<td>130 ± 21</td>
<td>257 ± 48</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(\text{H}_2\text{O})</td>
<td>0.080 ± 0.020</td>
<td>0.156 ± 0.042</td>
<td>0.049 ± 0.012</td>
</tr>
<tr>
<td></td>
<td>Lp2/144</td>
<td>(\text{OH}^+)</td>
<td>7.85</td>
<td>118 ± 21</td>
<td>(1.96 ± 0.27)</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(\text{CH}_4)</td>
<td>0.30 ± 0.06</td>
<td>0.55 ± 0.11</td>
<td>0.28 ± 0.06</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(\text{CH}_3\text{OH})</td>
<td>104 ± 9(^f)</td>
<td>1.85 ± 0.06(^b)</td>
<td>192 ± 18</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(\text{H}_2\text{CO})</td>
<td>115 ± 15</td>
<td>(1.87 ± 0.16)</td>
<td>213 ± 28</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(\text{H}_2\text{CO})</td>
<td>3.48 ± 0.22</td>
<td>6.44 ± 0.45</td>
<td>3.35 ± 0.28</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(\text{CH}_3\text{OH})</td>
<td>0.48 ± 0.08</td>
<td>0.88 ± 0.15</td>
<td>0.46 ± 0.08</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(\text{H}_2\text{O})</td>
<td>0.080 ± 0.020</td>
<td>0.156 ± 0.042</td>
<td>0.049 ± 0.012</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(\text{CH}_3\text{OH})</td>
<td>0.126 ± 0.043</td>
<td>0.245 ± 0.088</td>
<td>0.076 ± 0.026</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(\text{H}_2\text{O})</td>
<td>0.106 ± 0.39</td>
<td>2.06 ± 0.80</td>
<td>0.64 ± 0.24</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(\text{H}_2\text{CO})</td>
<td>165 ± 9.2(^e)</td>
<td>1.94 ± 0.24</td>
<td>325 ± 34</td>
</tr>
<tr>
<td>Jan 8</td>
<td>M2/111</td>
<td>(\text{H}_2\text{O})</td>
<td>6.80</td>
<td>143 ± 7.8</td>
<td>(2.36 ± 0.11)</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(\text{CO})</td>
<td>1.09 ± 0.12</td>
<td>2.35 ± 0.32</td>
<td>0.72 ± 0.07</td>
</tr>
<tr>
<td></td>
<td>M2/110</td>
<td>(\text{H}_2\text{O})</td>
<td>6.51</td>
<td>172 ± 10</td>
<td>(2.00 ± 0.13)</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(\text{CO})</td>
<td>0.86 ± 0.07</td>
<td>1.87 ± 0.21</td>
<td>0.57 ± 0.04</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(\text{H}_2\text{O})</td>
<td>150 ± 7.9(^f)</td>
<td>2.17 ± 0.18</td>
<td>0.61 ± 0.09(^b)</td>
</tr>
<tr>
<td>Jan 8</td>
<td>Lp2/144</td>
<td>(\text{OH}^+)</td>
<td>7.88</td>
<td>183 ± 18(^a)</td>
<td>2.77 ± 0.40</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(\text{H}_2\text{CO})</td>
<td>0.669 ± 0.055</td>
<td>1.86 ± 0.31</td>
<td>0.37 ± 0.04</td>
</tr>
</tbody>
</table>

Notes.

\(^a\) Values assume a rotational temperature of 90 K, based on relative intensities among \(\text{H}_2\text{O}\) lines in a “nucleus-centered” extract (see Figure 5(a) and related text in Section 3.5.1). All uncertainties represent 1\(\sigma\), and the upper limit for \(\text{NH}_3\) in order 175 of the L2 setting represents 3\(\sigma\).

\(^b\) Calibration factor \([10^{-18} \text{ W m}^{-2} \text{ (cm}^{-1})^{-1}/(\text{ADU s}^{-1})]\), from IR flux standard BS 8709 (Table 1).

\(^c\) Production rate based on a nucleus-centered aperture having angular extent 0\(^\circ\)75 x 2\(^\circ\)5 (Section 3.2). The weighted mean \(Q_{\text{tot}}\) for \(\text{H}_2\text{O}\) within each iSHELL setting is in italics, in the last line of entries (see Section 4).

\(^d\) Slit-loss factor, for converting \(Q_{\text{tot}}\) to total (i.e., global) production rate \((Q_{\text{tot}}/Q_{\text{H2O}})\) see note “e”). Within each iSHELL setting, GF was measured for one or more simultaneously observed emission lines having high signal-to-noise ratio. Italicized values in parentheses are those measured for specific molecules; their weighted mean value (listed with the corresponding mean \(Q_{\text{tot}}\) for \(\text{H}_2\text{O}\)) is assumed to apply to all co-measured species.

\(^e\) Total production rate. Uncertainties in \(Q_{\text{tot}}\) incorporate those in GF and \(Q_{\text{tot}}\), and also an assumed uncertainty of ±5% in \(\Gamma\).

\(^f\) Molecular abundance relative to \(\text{H}_2\text{O} = 100\). For all species, this is expressed as the ratio of \(Q_{\text{tot}}\) to the mean \(Q_{\text{tot}}\) for simultaneously measured water (\(\text{H}_2\text{O}\) and/or \(\text{OH}^+\)), listed in italics (note “c”). Entries in bold italics represent weighted mean abundances for molecules measured in multiple echelle orders.

\(^g\) Abundances in bold italics are weighted mean values, for species falling in multiple orders. These are \(\text{CO, CH}_4, \text{CH}_3\text{OH}, \) and \(\text{H}_2\text{CO}\) on January 7 and \(\text{CO}\) on January 8.

\(^h\) For Lp1 on January 7, the mean GF for \(\text{OH}^+\) in the four orders is listed (1.82±0.12). The overall GF for this setting (1.85±0.06) incorporates this plus those measured for \(\text{CH}_4, \text{CH}_3\text{OH}, \) and \(\text{CH}_3\text{OH}.\)
Figure 6. (a and b) Abundance ratios of hypervolatiles in 45P (with ±1σ error bars), together with results for previously measured JFCs (upper limits are 3σ) and median values among OCCs (in brown). Given the paucity of previous measurements in JFCs, no meaningful statistics exist; our measurements in 45P lay the foundation for this. (c) Abundances for additional trace volatiles in 45P, and median values among JFCs (in green) and OCCs (in brown). Also shown are in situ post-perihelion abundance measurements of the inner coma of 67P obtained with the ROSINA mass spectrometer aboard Rosetta (Gasc et al. 2017; see discussion in Section 5.2.3). Due to the very high precision of the in situ measurements, no error bars are shown for them.

3.5.1. Measurement of Rotational Temperature in Comet 45P

We sampled a spectral region encompassing H2O lines (Figure 5(a)) that together span a large range of rotational energies (approximately 50–550 cm⁻¹) and provide a robust measure of rotational temperature for realistic values found in cometary comae (values of T旋转 among comets range from ~30 to 150 K). This region was first identified in studies of Halley-family comet 153P/Ikeya–Zhang, using a single CSHELL setting that encompassed nearly the same spectral extent as that shown in Figure 5(a) (Dello Russo et al. 2004). The value of T旋转 we measured for 45P is consistent with 90 K.

We adopt this value of T旋转 for all molecules reported here. To validate this assumption, we also measured T旋转 for CH3OH (Villanueva et al. 2012; DiSanti et al. 2013), isolating the net signal in its ν5 band (in order 147 of the Lp1 setting) by subtracting (modeled) contributions from continuum, H2CO, and OH⁺ emissions (see Section 3.5.2 and Figure 5(c)). This provided a value (86⁺11/⁻9 K) consistent with the T旋转 we measured for H2O (89 ± 3 K), albeit less well constrained owing primarily to the smaller range of energies sampled (~10–200 cm⁻¹) and also to the high density of lines for CH3OH leading to spectral confusion (see, e.g., discussion in Section 3.1 of Gibb et al. 2012). Similarly, from C2H6 ν7 emission (Villanueva et al. 2011b) in Lp1 order 155 (Figure 4(b)) we measured T旋转 = 98⁺18/⁻15 K, even less well constrained than T旋转 for CH3OH but still consistent with our value for H2O.

We were unable to obtain meaningful values of T旋转 for other species, because their emissions were too weak and/or because their lines did not sample a sufficient range of rotational energies to obtain an accurate determination. Nonetheless, as an additional validation to our approach we note that in most cases rotational temperatures among species derived from IR observations of a given comet are in agreement, and that slight changes in T旋转 result in only very small differences in production rates and hence abundance ratios relative to H2O (Gibb et al. 2012). For these reasons, we take 90 K to be the most probable value for T旋转 in 45P and base our results for all molecules on this temperature.

3.5.2. Additional Molecules

We measured emissions near 3.0 μm from the nitrogen-bearing molecules HCN and NH3 and from C2H2 (Figure 5(b)). Compared to most other molecules systematically measured at infrared wavelengths in comets, emissions from these species tend to be weak, particularly when abundance ratios are relatively low. Nonetheless, we achieved secure detections of these three trace volatiles in 45P (see Section 4).

In addition to C2H2 ν7 band emission and CH3OH ν5 band emission in the order containing P-branch lines of CH4 (Figure 4(b)), we also co-measured CH3OH ν1 and ν3 band emission together with lines of (primarily) the ν5 band of H2CO (Figure 5(c)) and H2CO lines in both ν1 and ν3 bands (Figure 5(d)). These four molecules (CH4, C2H2, CH3OH, and H2CO) were co-measured, with OH⁺ included in each of the four orders highlighted in Figure 1. Corresponding spectra are shown in Figures 4, 5(c), and 5(d). We obtained measures of water production from OH⁺ in each of these four orders in the Lp1 setting (Table 2).

4. Measured Production Rates and Abundances in Comet 45P

Table 2 includes both nucleus-centered and total production rates. All abundance ratios compare Qnc to the mean value for simultaneously measured H2O, i.e., the weighted mean Qnc from H2O and/or OH⁺ contained within the same setting. This guards against potential temporally variable gas production and also against uncertainties in GF among settings (Section 5.5.1). Mean values for Qnc(H2O) are italicized in Table 2, in the last line of
Table 3
Abundance Ratios in 45P at $R_h = 0.55–0.56$ au Post-perihelion (Percent Relative to H$_2$O)$^a$

<table>
<thead>
<tr>
<th>Source</th>
<th>CO (24)</th>
<th>CH$_4$ (31)</th>
<th>C$_2$H$_6$ (44)</th>
<th>C$_2$H$_2$ (54)</th>
<th>H$_2$CO (64)</th>
<th>NH$_3$ (78)</th>
<th>HCN (95)</th>
<th>CH$_3$OH (99)</th>
</tr>
</thead>
<tbody>
<tr>
<td>45P</td>
<td>0.60 ± 0.04</td>
<td>0.79 ± 0.06</td>
<td>0.52 ± 0.04</td>
<td>0.076 ± 0.026</td>
<td>0.36 ± 0.04</td>
<td>0.64 ± 0.24</td>
<td>0.049 ± 0.012</td>
<td>3.59 ± 0.31</td>
</tr>
<tr>
<td>JFCs</td>
<td>...$^b$</td>
<td>...$^b$</td>
<td>0.34 ± 0.07(8)</td>
<td>0.07 ± 0.02(7)</td>
<td>0.26 ± 0.10(7)</td>
<td>0.59 ± 0.11(6)</td>
<td>0.17 ± 0.03(8)</td>
<td>1.73 ± 0.33(8)</td>
</tr>
<tr>
<td>OOCs</td>
<td>4.0 ± 0.9(21)</td>
<td>0.88 ± 0.10(19)</td>
<td>0.63 ± 0.10(19)</td>
<td>0.16 ± 0.03(18)</td>
<td>0.33 ± 0.08(17)</td>
<td>0.91 ± 0.30(11)</td>
<td>0.22 ± 0.03(19)</td>
<td>2.21 ± 0.24(17)</td>
</tr>
</tbody>
</table>

Notes.
$^a$ Molecules are listed in order of increasing vacuum sublimation temperature (K, in parentheses; taken from Crovisier & Encrenaz 2000; also see Crovisier 2007; Yamamoto 1985). Uncertainties represent 1σ. For JFCs and OCCs, the number in parentheses indicates the sample size of comets for which each species has been measured.
$^b$ No values are listed for CO or CH$_4$ in JFCs, due to the extreme paucity of measurements (see Figures 2(g) and (h) and Table 3 in Dello Russo et al. 2016a). Accordingly, in Figures 6(a) and (b), respectively, we show individual JFC values for CO and CH$_4$, together with our values for 45P.
entries for each setting on both days. Also listed in Table 2 are mean abundance ratios for species having emissions in more than one (simultaneously observed) echelle order. These are CO in M2 orders 110 and 111 on both January 7 and 8, CH₄ in Lp1 orders 157 and 155 on January 7, CH₃OH in Lp1 orders 155 and 147 on January 7, and H₂CO in Lp1 orders 147 and 144 on January 7. (NH₃ was targeted on January 8 in L2 orders 175 and 171 but was detected only in order 171; Figure 5(d)).

Table 3 summarizes our measured molecular abundances in 45P. For species measured on both January 7 and 8 (CO and H₂CO), 2-day-mean values are given. Our abundances for 45P are also compared with median values in OCCs and, other than for CO and CH₄, in JFCs. Because so few measurements of the two hypervolatile CO and CH₄ exist for JFCs, meaningful statistics do not yet exist, and therefore no values are listed in Table 3. We instead show (in Figures 6(a) and (b)) individual measurements together with our measured abundances for 45P. Some JFC values are merely upper limits, or a broad range of measured values (i.e., 0.15%–0.45% for CO in 103P/Hartley 2; Weaver et al. 2011). Inspection shows that even for values with ±1σ error bars, the uncertainties associated with previous JFC hypervolatile measurements are considerably larger than those associated with our measurements of 45P. For the six additional trace ices we show (Figure 6(c)) our measurements along with median values for JFCs (in green) and OCCs (in brown), even though for these molecules fewer JFCs than OCCs are measured to date as noted in Table 3.

In addition to abundances obtained through remote sensing observations, Figure 6 shows in situ abundance measurements of the inner coma (within 100 km of the nucleus) of JFC 67P/Churyumov-Gerasimenko by the Rosetta Orbiter Spectrometer for Ion and Neutral Analysis (ROSINA) mass spectrometer (Balasger et al. 1998). These were averaged over Rₖ = 2.0–2.7 au post-perihelion, which straddled the outbound (vernix) equinox at 2.63 au (Gasc et al. 2017). Comparisons with our results for 45P are presented in Section 5.2.3.

5. Discussion

Our measured abundance ratios for trace volatiles in 45P are expressed relative to simultaneously measured H₂O (and/or OH); see Figure 6 and also the rightmost column in Table 2. This provides more consistent measures than comparing with the daily mean Q(H₂O). For example, the respective abundance ratios agree on January 7 and 8 for CO (0.59% ± 0.04% and 0.61% ± 0.09%) and H₂CO (0.34% ± 0.08% and 0.37% ± 0.04%), even though the water production rate was considerably higher on the latter day (and varied over the course of each day; Section 5.6). Therefore, our approach also guards against possible temporal changes in gas production.

5.1. The Significance of CO and CH₄ Abundances in 45P

Our secure detections of CO and CH₄ in 45P do not simply augment statistics regarding their abundances in JFCs. Rather, they are critical for establishing statistically meaningful abundances for these hypervolatiles in this significantly underrepresented population of comets, as illustrated by the very few previous measurements in JFCs obtained by remote sensing (five for CO, and four for CH₄; Figures 6(a) and (b)). CO was depleted relative to its median value measured among OCCs and seemingly enriched in 45P compared to the few JFCs measured to date. Although the abundance ratios of CO and CH₄ are fairly similar in 45P (0.6%–0.8%), the emerging (and evolving) overall compositional taxonomy among all measured comets (primarily OCCs) suggests they are not correlated (as opposed to anticorrelated). This was first demonstrated by Gibb et al. (2003) based on a sample of eight OCCs, and more recently in a compilation of 19 OCCs, for which the formal Pearson product–moment correlation coefficient (r) was <0.5 (Dello Russo et al. 2016a). Too few JFCs have been measured to assess a meaningful comparison between their CO and CH₄ abundances. The noncorrelated nature of CO and CH₄ abundance ratios in OCCs suggests that thermal processing may not be the dominant factor in determining hypervolatile abundances.

This may also be true for 45P. Its substantial abundance of CH₄ demonstrates that this low sublimation temperature (Tₘₐₓ) species can be preserved in a JFC, perhaps even trapped in less volatile ice to survive the thermal effects of repeated (and frequent) passages to well within 1 au of the Sun. This supports retention of a significant primitive record. The depleted abundance of CO (relative to its median value among OCCs; Figure 6(a)) may indicate its loss through evolutionary processing or, given its similarly low Tₘₐₓ to that of CH₄ (see Table 3, note a), its efficient conversion to CH₃OH through H-atom addition reactions on grain surfaces during the formative epoch (Section 5.2.2), demonstrated through irradiation of laboratory ices at very low temperatures (<25 K; Watanabe et al. 2004; Oba et al. 2010).

5.2. Abundance Comparisons with Other Comets

5.2.1. Hypervolatiles: CO, CH₄, and C₂H₆

Among the species available for systematic study in comets using IR spectroscopy, CO, CH₄, and C₂H₆ have the lowest vacuum sublimation temperatures (see Table 3). Assessing the abundance ratios CO/CH₄ and C₂H₆/CH₄ in 45P for the first time allows a robust comparison of values in a JFC with those measured in a number of OCCs. In 45P, we find CO/CH₄ = 0.76 ± 0.08 and C₂H₆/CH₄ = 0.66 ± 0.07. Figure 7 in Bovey et al. (2017) shows these ratios against each other for 18 OCCs, plus JFC 67P/Churyumov-Gerasimenko from in situ (Rosetta) measurements (LeRoy et al. 2015). Our value for CO/CH₄ in 45P falls near the low end, and for C₂H₆/CH₄ near the middle of the distribution, between the points for 8P/Tuttle and C/2006 M4 (SWAN). As with 45P, both of these comets had depleted CO abundance ratios relative to H₂O (Boehnhardt et al. 2008; DiSanti et al. 2009). In terms of its abundance ratio CH₄/CO, this places 45P near the high end among measured comets.

5.2.2. Additional Species

Figure 6(c) shows that for C₂H₂, H₂CO, NH₃, and C₃H₆, the abundances we measured in 45P were either consistent with their median value among JFCs (for C₂H₂) or between their respective median values among JFCs and OCCs. Notable is strongly depleted HCN in 45P. Although C₂H₂ and HCN appear to be highly correlated among comets (r ~ 0.8; see Table 5 in Dello Russo et al. 2016a), this is apparently not the case with 45P near perihelion. In fact, its abundance ratio C₂H₂/HCN (10.6 ± 2.7) is the highest measured among comets, similar only to that found for JFC 6P/d’Arrest, which had stronger depletions of both C₂H₂ and HCN relative to H₂O (see Figure 3 of Dello Russo et al. 2009).
Also notable is methanol enrichment in 45P relative to its median value, among both JFCs and OCCs (see Table 3 and Figure 6(c)). As the least volatile “trace” ice systematically measured in comets, CH$_3$OH may present a unique challenge to the taxonomy of parent volatiles, in that it has shown abundance ratios relative to H$_2$O that are higher than expected in several observed comets, when compared to other species (e.g., C$_2$H$_6$). Examples are OCCs 8P/Tuttle (Boehnhardt et al. 2008; Bonev et al. 2008), C/2006 M4 (SWAN; DiSanti et al. 2009), and C/2007 N3 (Lulin; Gibb et al. 2012), JFC 21P/Giacobini–Zinner (DiSanti et al. 2013), plus 2P/Encke (Radeva et al. 2013).

Given its small perihelion distance and 3.3 yr orbital period, 2P/Encke may represent a special case in that its enriched CH$_3$OH could be evolutionary in nature, resulting from low volatility relative to other trace volatiles, making it less susceptible to repeated heating. However, HCN is only slightly more volatile than CH$_3$OH, yet it was strongly depleted in 2P near $R_h$ = 1.2 au pre-perihelion during its 2003 apparition (Radeva et al. 2013). This may indicate that, as with enriched CH$_3$OH produced through efficient conversion of CO, depleted HCN could result from radiative processing of pre-cometary ices, and this may also be the case for 45P. Regardless of the interpretation—primordial, for example, through production of CH$_3$OH and destruction of HCN, versus evolutionary through depletion of ices due to episodic heating of the nucleus—it is of fundamental importance to establish how common higher methanol abundances (and also lower HCN abundances) are among comets, both OCCs and JFCs. Our measurements of 45P add another piece toward interpreting cometary compositions.

5.2.3. Comparisons with Rosetta Measurements of JFC 67P/Churyumov-Gerasimenko

For 67P, pre-perihelion densities were measured 10 km over (primarily) southern (winter) and northern (summer) hemispheres by the ROSINA mass spectrometer on successive dates in 2014 October, when the comet was at $R_h$ ≈ 3.15 au. Large north–south asymmetries were observed (LeRoy et al. 2015), reinforcing reported compositional heterogeneity (Luspay-Kuti et al. 2015). The abundance ratios CO/CH$_4$ and C$_2$H$_6$/CH$_4$ measured by ROSINA on these dates (respectively 21 and 2.5 for the summer hemisphere, 36 and 5.9 for the winter hemisphere; LeRoy et al. 2015) are much higher than we obtained for 45P.

However, the 67P measurements may not reflect the bulk coma composition, and this, together with the large difference in heliocentric distance between those observations and ours of 45P, makes direct comparisons difficult. ROSINA measured localized molecular densities, whereas our measurements of 45P (and all other measurements in Figure 6) refer to the bulk coma composition. Additionally, 67P was observed pre-perihelion beyond 3 au, where water sublimation was likely not yet fully developed. This could lead to overestimated abundance ratios relative to H$_2$O.

A better comparison with our results may be presented by post-perihelion ROSINA measurements. Mean abundances relative to H$_2$O were obtained for the period 2016 January–April ($R_h$ = 2.0–2.7 au; Gasc et al. 2017), straddling the “outbound” (vernal) equinox at $R_h$ = 2.63 au. Results are shown in Figure 6 for the four molecules that are common to our study of 45P (CO, CH$_4$, HCN, and NH$_3$). The 67P value for CH$_4$ (0.71% ± 0.04%) is consistent with that in 45P (0.79% ± 0.06%); however those for CO and HCN are an order of magnitude larger and NH$_3$ an order of magnitude smaller than their respective values in 45P. Nonetheless, as with the pre-perihelion ROSINA measurements, direct comparison with our results—or with other remote sensing measurements of comets—assumes that the in situ results are representative of the bulk coma chemistry.

5.3. Parent-photodissociation Product Relationships in 45P

A primary means of addressing sources of radical species in cometary comae is comparing measured abundances from optical and IR observations. Comet 45P was classified as “typical” in terms of its abundance ratios C$_2$/OH and C$_3$/OH, and also its CN/OH and NH/OH (A’Hearn et al. 1995). Comparing these to our measured abundance ratios is useful for assessing potential “parent–daughter” relationships, for example, C$_2$ from C$_2$H$_2$, CN from HCN, and NH from NH$_3$. Our value for NH$_3$/H$_2$O in 45P is consistent with those measured among both JFCs and OCCs, whereas C$_2$H$_2$/H$_2$O is consistent with that among JFCs but below that among OCCs. Based on this (admittedly) somewhat simplistic reasoning, it is therefore plausible that the abundance we measured for NH$_3$/H$_2$O (0.64% ± 0.24%) can account for the NH/OH measured by A’Hearn et al. (1995); 0.59% ± 0.34%), notwithstanding the large uncertainties associated with both measurements. Nonetheless, in contrast, both C$_2$/OH (0.21% ± 0.04%) and CN/OH (0.13% ± 0.03%) are considerably higher than the respective 45P values for C$_2$H$_2$/H$_2$O (0.076% ± 0.026%) and HCN/H$_2$O (0.049% ± 0.012%), suggesting the need for one or more additional sources of both C$_2$ and CN.

5.4. The Importance of Compositional Measurements at Small Heliocentric Distances

Our results for 45P also contribute information on the volatile composition of comets at small heliocentric distance. This makes 45P the first JFC for which such a broad suite of parent volatiles have been measured at $R_h$ < 0.8 au. Such measurements are rare for both JFCs and OCCs, due largely to a combination of sensitivity limits and observational circumstances. In late 2013, an opportunity afforded itself with the dynamically new Sun-grazing OCC C/2012 S1 (ISON), for which compositional measurements extended inward to $R_h$ < 0.5 au. HCN, H$_2$CO, NH$_3$, and C$_2$H$_2$ in ISON exhibited increased abundance ratios within $R_h$ ∼ 0.8 au (Dello Russo et al. 2016b; DiSanti et al. 2016). In contrast, 45P had mixing ratios for H$_2$CO and NH$_3$ with respect to H$_2$O that were consistent with their respective median values among OCCs and JFCs, C$_2$H$_2$ was consistent with its median JFC value, and HCN was depleted (Figure 6(c)). The mixing ratios we measure for HCN, H$_2$CO, NH$_3$, and C$_2$H$_2$ in 45P are smaller than the few measurements obtained for OCCs within 0.8 au of the Sun. Our measurements of 45P near perihelion represent an important data point; however, more measurements are needed at small $R_h$ (for both JFCs and OCCs) to test potential abundance variations with $R_h$.

5.5. Spatial Profiles of Emissions in 45P

Figure 7 compares emission profiles from two settings on January 7, the day on which our observations sampled the largest number of molecules having strong emissions. For all spectral observations we oriented the slit along the projected Sun–comet direction (PA 74°5). It is important to note that
both the M2 and Lp1 settings represent independent snapshots of cometary activity, averaged over the time intervals specified in Figure 7(a) (and in Table 1). Over the approximately 1.5 hr interval between the (mid-sequence) times of the M2 and Lp1 observations, the dust continuum changed considerably: the M2 continuum was relatively symmetric about the nucleus (taken to be the zero-point on the x-axis), whereas the Lp1 continuum was clearly enhanced in the anti-sunward-facing hemisphere. The difference in dust coma morphology between M2 and Lp1 may be related to rotation of the nucleus, for which a period of ~7.5 hr was estimated from radar observations (Lejoly & Howell 2017, CBET 4357(2)).

This justifies comparison of spatial profiles measured simultaneously, because these are affected identically, irrespective of changes resulting from potential differences in slit-loss correction factor among settings, or from nucleus rotation. We therefore focus on comparing the distribution of parent volatiles within each iSHELL setting.

Because of the low CO abundance in 45P, we combined the five brightest lines in the M2 setting (R1 and R2 in order 111, and P3–P5 in order 110), and then binned (smoothed) the resulting profile by 2 in the spatial dimension to improve signal-to-noise ratio (Figure 7(b)). Similarly, in the Lp1 setting (Figure 7(c)) we combined nine lines of OH* spanning the four orders analyzed and smoothed the resulting profile by 2. The profile of OH* emission is critically important in that it faithfully tracks the distribution of parent H2O molecules in the coma (for details, see Bonev et al. 2006, and references therein).

Figure 7(b) shows that during the M2 observations H2O tracked the continuum fairly closely, whereas CO was significantly asymmetric in the sunward-facing hemisphere and its “secondary” peak (near 500–600 km sunward) was much stronger than the enhancement seen for co-measured H2O at a similar projected position. In the Lp1 setting, H2O and CH3OH tracked the continuum, whereas C2H6 and (more so) CH4 showed sunward asymmetry. These results may be indicative of an activated region that preferentially released more highly volatile species into the sunward-facing hemisphere, and if so, that the degree of asymmetry increased with decreasing native ice sublimation temperature. It also appears to have persisted for at least the nearly 3 hr interval encompassed by the combined measurements in the two settings. Alternatively, the secondary source may have been more pronounced during the M2 observations, and that this was responsible for the highly prominent emission profile intensity for CO offset sunward from the nucleus.

5.5.1. Possible Effects of Spatial Profiles on Molecular Abundance Ratios

Distinct spatial profiles (Figure 7) suggest nonhomogeneous outgassing, which can affect relative coma-integrated abundances of parent volatiles. We therefore investigated the extent to which differences in observed spatial profiles influence molecular abundance ratios for 45P. Measuring GFs (Section 3.3) through spatial analysis for various species provides a quantitative means of assessing the influence of nonhomogeneous outgassing in the coma.

We measured a GF of 1.93 ± 0.14 for the summed CO profile shown in Figure 7(b), which is larger than that for co-measured H2O by a factor of 1.17 ± 0.10. Applying this GF to CO therefore increases its production rate and abundance ratio by 17% on January 6/7, leading to CO/H2O = 0.69% ± 0.07%. However, this is within 1σ of the value listed in Table 2 based on the ratio of Q_{inc} for CO and H2O (0.59 ± 0.04). Even applying its
larger, independently measured GF still implies substantially depleted CO in 45P relative to its median value among OCCs. Our measured GFs in the Lp1 setting were based on stronger emissions from CH₄, C₂H₆, CH₃OH, and OH⁺ (Table 2). Although the spatial distributions of these species differ (Figure 7(c)), their independently determined GFs (listed in parentheses in Table 2) agree within their respective 1σ uncertainties. The GF we used in calculating Q tot for all species in the Lp1 setting (1.85 ± 0.06) is the weighted mean from all co-measured profiles. This implies that (total) production rates for all species are well within 1σ of those obtained by using their respective individual GFs, and also justifies using the ratios of Q nc in calculating molecular abundance ratios.

All production rates (both Q nc and Q tot) measured for 45P include an estimated 5% uncertainty in absolute flux calibration (Γ; see Table 2, notes b and e), arising, for example, from uncertainties in stellar magnitude for the flux standard. However, this uncertainty is not incorporated into molecular abundance ratios relative to (simultaneously measured) water within each setting because it affects all production rates equally. It is also not included in the increased abundance ratio for CO on January 7 based on applying independently measured GFs for CO and H₂O (as discussed above), since again Q(CO) and Q(H₂O) are affected equally.

5.6. Evidence for Temporally Variable Gas Production in 45P

Our (global) water production rates in Table 2, using emissions from H₂O and/or OH⁺ measured within each iSHELL setting, generally agree (to within their respective 1σ uncertainties). However, measured GFs increased with time on both days, consistent with degradation in atmospheric seeing arising from direct sunlight warming the telescope environment and structure over the course of each day. This makes it necessary to compare global production rates (Q tot) for H₂O measured in different settings, when assessing the evolution in gas production in 45P.

On the first day (bridging UT January 6/7), the value of global Q(H₂O) from the M2 observations (2.77 ± 0.18 × 10⁻⁴ molecules s⁻¹) was higher than the mean of those from Lp1 and L1 (order 179 only), (2.19 ± 0.07) × 10⁻⁵ s⁻¹. This suggests a decrease in gas production by 26% ± 9% over approximately a 3 hr period. On the second day (bridging UT January 7/8), global values of Q(H₂O) increased by a factor of 1.56 ± 0.29 between the interval UT22:35–01:28 (based on the mean from L2 and M2 settings, 3.25 ± 0.23 × 10⁻⁴ s⁻¹) and UT02:09–02:54 (from the Lp2 setting, 5.08 ± 0.89 × 10⁻⁴ s⁻¹; Table 1). These Lp2 observations had the largest GF measured for any setting on either day; however, we note that Lp2 also had the largest nucleus-centered water production rate for any setting on either day. Given the rotation period estimated from radar measurements of 45P (~7.5 hr; Lejoly & Howell 2017, CBET 4357(2)), it is conceivable that its activity varied on timescales of hours; however, a more rigorous study than our observations permit is necessary to test such variations.

Overall, the mean water production was larger by 46% ± 11% on January 7/8 than on January 6/7. Whatever the cause of these variations in measured water production (both on each day and day to day), this argues strongly for assessing volatile abundance ratios relative to simultaneously measured water production, as was done for our study and which, as stated previously, provided consistent values for species measured on both days (CO and H₂CO; Section 4).

6. Summary of Results on 45P with iSHELL

We used the cross-dispersed high-resolution spectrograph, iSHELL, at the NASA Infrared Telescope Facility to measure H₂O and the eight trace native ices CO, CH₄, H₂CO, CH₃OH, HCN, NH₃, C₂H₆, and C₂H₅ in JFC 45P/Honda–Mrkos–Pajdušáková on 2 consecutive days, bridging UT 2017 January 6/7 and 7/8, shortly following its perihelion passage on UT 2016 December 31. Our observations provided the first detections of cometary parent volatiles with this powerful new instrument. Most notably, the highly favorable geocentric velocity of 45P, together with the sensitivity of iSHELL and daytime observing capability at the IRTF, resulted in secure retrievals of CO and CH₄, the two most highly volatile ices systematically measured in comets. These hypervolatiles are substantially undercharacterized in JFCs; thus, statistics on their abundances are severely lacking. Our measurements of 45P represent the most precise ground-based measures of CO and CH₄ to date in a JFC, and therefore provide a foundation for building meaningful statistics for their abundances.

Compared with the ensemble of 30-plus comets measured to date using IR spectroscopy, our study revealed depleted abundance ratios (relative to H₂O) for CO and HCN, enriched CH₃OH, and abundance ratios for the other molecules that were consistent with their respective median values among OCCs and/or JFCs. Our results may indicate efficient conversion of CO to CH₃OH through H-atom addition on surfaces of grains, and possibly also radiative processing of HCN prior to incorporation into the nucleus. Relative to other comets, 45P exhibited one of the highest abundance ratios CH₅/CO. Comparison with optical observations of 45P suggests sufficient NH₃ to provide NH, whereas one or more additional sources other than C₂H₂ and HCN are required to account for observed abundances of C₂ and CN, respectively.

Spatial analysis of emissions contained in the Lp1 setting on January 7 revealed asymmetries for C₂H₆ and especially CH₄ in the sunward-facing hemisphere. CH₃OH and H₂O (as revealed by OH prompt emission) closely tracked the continuum emission from simultaneously measured dust and overall showed asymmetry in the anti-sunward-facing hemisphere. In the M2 setting, which immediately preceded the Lp1 observations, H₂O also closely tracked the co-measured continuum, whereas CO showed an even more pronounced sunward asymmetry than did CH₄ in Lp1. This could indicate preferential release of more highly volatile species into the sunward-facing hemisphere at the time of our observations, arising, for example, from activation of a region of the nucleus enriched in hypervolatiles.

7. Recent Observations and Prospects for Future Studies of JFCs with iSHELL

The recent perihelion passage of 45P represents the first in a series of long-awaited favorable opportunities for short-period comets. The availability of iSHELL, coupled with the daytime observing capability of the IRTF, has opened a unique and powerful window for studying comets in general and for short-period comets in particular. It allows optimizing the science returned from compositional measurements of this highly important yet traditionally underrepresented dynamical class of
comets. The current ∼2 yr period features the most highly concentrated succession of favorable apparitions for short-period comets (JFCs, plus 2P/Encke) to take place in recent decades.

In addition to 45P, we obtained high-quality post-perihelion spectra of 2P/Encke and pre- and post-perihelion spectra of 41P/Tuttle-Giacobini-Kresak with iSHELL in the 2017 February–April time frame. These measurements, as well as those presented here for 45P, are important for building a statistically meaningful compositional taxonomy for short-period comets. They also are excellent test beds for JFCs 21P/Giacobini–Zinner in 2018 and 46P/Wirtanen in late 2018/early 2019.

Comet 21P has higher gas production than most JFCs, and in 2018 it will become the first comet for which compositional studies using high-resolution IR spectroscopy will have spanned three separate orbital epochs (perihelion passages), the two previous ones being 1998 (with IRTF/CSHELL; Weaver et al. 1999; Mumma et al. 2000) and 2005 (with Keck/NIRSPEC: DiSanti et al. 2013). Comet 46P was the original target of the European Space Agency’s Rosetta mission, which recently completed its successful rendezvous with 67P/Giacobini–Tunamyov–Gerasimenko. In 2018 December, 46P will remain close to Earth (within Δ = 0.1 au) for several weeks, and a coordinated worldwide observing campaign is being organized to study its activity. Comets 21P and 46P have perihelia near 1 au, and serial measurements spanning ranges in heliocentric distance are planned for both. The IRTF and iSHELL are expected to play a critical role.

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