The Peculiar Volatile Composition of CO-dominated Comet C/2016 R2 (PanSTARRS)

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Received 2019 May 17; revised 2019 July 12; accepted 2019 July 15; published 2019 August 27

Abstract

Comet C/2016 R2 (PanSTARRS) has a peculiar volatile composition, with CO being the dominant volatile, as opposed to H2O, and one of the largest N2/CO ratios ever observed in a comet. Using observations obtained with the Spitzer Space Telescope, NASA’s Infrared Telescope Facility, the 3.5 m Astrophysical Research Consortium telescope at Apache Point Observatory, the Discovery Channel Telescope at Lowell Observatory, and the Arizona Radio Observatory 10 m Submillimeter Telescope, we quantified the abundances of 12 different species in the coma of R2 PanSTARRS: CO, CO2, H2O, CH4, C2H6, HCN, CH3OH, H2CO, OCS, C2H5, NH3, and N2. We confirm the high abundances of CO and N2 and heavy depletions of H2O, HCN, CH3OH, and H2CO compared to CO reported by previous studies. We provide the first measurements (or most sensitive measurements/constraints) on H2O, CO2, CH4, C2H6, OCS, C2H5, and NH3, all of which are depleted relative to CO by at least 1–2 orders of magnitude compared to values commonly observed in comets. The observed species also show strong enhancements relative to H2O and, even when compared to other species like CH4 or CH3OH, most species show deviations from typical comets by at least a factor of 2–3. The only mixing ratios found to be close to typical are CH3OH/CO2 and CH4/CH4. The CO2/CO ratio is within a factor of 2 of those observed for C/1995 O1 (Hale-Bopp) and C/2006 W3 (Christensen) at a similar heliocentric distance, though it is at least an order of magnitude lower than many other comet observed with AKARI. While R2 PanSTARRS was located at a heliocentric distance of 2.8 au at the time of our observations in 2018 January/February, we argue, using sublimation models and comparison to other comet observed at similar heliocentric distance, that this alone cannot account for the peculiar observed composition of this comet and therefore must reflect its intrinsic composition. We discuss possible implications for this clear outlier in compositional studies of comets obtained to date and encourage future dynamical and chemical modeling in order to better understand what the composition of R2 PanSTARRS tells us about the early solar system.

Key words: astrochemistry – comets: individual – planets and satellites: composition

1. Introduction

Comets are primitive, volatile-rich remnants from the formation of the solar system, and for this reason, their volatile composition is considered indicative of the physics and chemistry occurring in the protosolar disk during the planet formation stage. While there is diversity in compositions among the cometary population, comets consist primarily of H2O, followed by CO and CO at the 1%–30% level, with trace species such as HCN, CH3OH, and C2H6 being present at the few percent level or less (Mumma & Charnley 2011). The optical taxonomy of comets also shows diversity and evidence for modality (i.e., clumps of different compositional types), but in general, optical cometary spectra are dominated by OH (and therefore H2O), with CN, C2, C3, CH, NH, and NH3 present at the percent level or less (e.g., A’Hearn et al. 1995; Cochran et al. 2012).

However, a few comets do not fit neatly into the established taxonomies. Comet 96P/Machholz shows an extremely atypical coma composition at optical wavelengths (though OH is still the dominant species), with a C2/CN ratio an order of magnitude higher than that of other comets (Langland-Shula & Smith 2007; Schlatten 2008). Some comets, such as 29P/Schwassman-Wachmann 1, have observed CO/H2O ratios ≳1 (Ootsubo et al. 2012), though this is often at least partially explained by its heliocentric distance being beyond the water ice line where water ice does not readily sublimate, meaning that the observed coma composition is not necessarily indicative of the ice composition of the nucleus (Womack et al. 2017).
Comet C/2016 R2 (PanSTARRS) was observed to have a peculiar optical spectrum when it was at a heliocentric distance of 3.1 au, dominated by emission from CO$^+$ and N$_2^+$ with a lack of emission from other species, such as CN and C$_2$, typically observed at these wavelengths (Cochran & McKay 2018). From these observations, it was derived that N$_2$/CO $\sim$ 0.06, among the highest values observed in a comet. This result, coupled with the lack of many of the usual emissions observed in optical cometary spectra, suggested that this comet has a composition very different from any other comet observed to date. This was quickly communicated to the cometary science community for additional observations. Observations with the Arizona Radio Observatory 10 m Submillimeter Telescope (ARO SMT) confirmed a very high CO production rate and identified a low HCN abundance (Wierzchos & Womack 2017, 2018; de Val-Borro et al. 2018). Observations with the IRAM 30 m telescope and the Nancay radio telescope provided a more complete picture of the volatile composition of R2 PanSTARRS, confirming the high CO abundance and anomalously low abundances of other volatiles, such as HCN and H$_2$O, compared to CO (Biver et al. 2018). Additional high spectral resolution optical observations obtained with the UVES instrument on the Very Large Telescope (VLT) were reported by Optom et al. (2019), confirming the findings of Cochran & McKay (2018), as well as providing new insights, such as the first detection of [N I] emission in a cometary coma.

We present an analysis of IR measurements obtained with the Spitzer Space Telescope and iSHELL on the NASA Infrared Telescope Facility (IRTF) designed to quantify a suite of species observed in comets: H$_2$O, CO$_2$, CO, C$_2$H$_6$, CH$_3$OH, CH$_4$, H$_2$CO, and OCS. We also present optical measurements used to study HCN (through CN emission), NH$_3$ (through NH$_2$ emission), N$_2$ (through N$_2^+$), C$_2$H$_2$ (through C$_2$), and H$_2$O (through OH and [OI] 6300 Å emission), as well as new millimeter-wavelength observations of CO that are contemporaneous with our Spitzer observations. Section 2 presents our observations, and Section 3 presents our analysis procedures and results. Section 4 discusses this truly peculiar comet in the context of current compositional taxonomies and possible implications for the physics and chemistry of the comet-forming region during the protoplanetary disk phase. Section 5 concludes the paper and encourages future work to better understand what R2 PanSTARRS reveals about the early solar system.

2. Observations

We obtained observations in 2018 January/February with several facilities, both space-borne and ground-based. These observations are detailed in Table 1.

### Table 1

| UT Date       | $R_0$ (au) | $V_0$ (km s$^{-1}$) | $\Delta^a$ (au) | $\Delta^b$(km s$^{-1}$) | Solar Standard | Tell. Standard | Flux Standard  |
|---------------|------------|---------------------|----------------|--------------------------|----------------|---------------|---------------|
| NASA IRTF iSHELL |            |                     |                |                          |                |               |               |
| 2018 Jan 30   | 2.81       | −6.8                | 2.27           | +17.2                    | ...            | ...           | HR 1165       |
| 2018 Feb 13   | 2.76       | −6.0                | 2.41           | +19.5                    | ...            | Chopper Wheel | ...           |
| APO ARCES     |            |                     |                |                          |                |               |               |
| 2018 Jan 30   | 2.81       | −6.8                | 2.27           | +17.2                    | Hyades 64      | 55 Persei     | HR 1544       |
| 2018 Feb 13   | 2.76       | −6.0                | 2.41           | +19.5                    | ...            | ...           | ...           |

Notes.

$^a$ Values for $\Delta$ and $\Delta$ are the distance to the observer and velocity relative to the observer, respectively. Therefore, for Spitzer observations, these are relative to the Spitzer spacecraft, while for ground-based observations, these are relative to Earth.

$^b$ Spitzer astronomical observation request numbers 65280768, 65281280, 65281024, and 65281536.

2.1. NASA IRTF iSHELL

We obtained Director’s Discretionary Time to observe R2 PanSTARRS with the powerful iSHELL IR spectrograph on the NASA IRTF on Maunakea, Hawaii, on UT 2018 January 29 and 30. While poor weather precluded obtaining useful data on January 29, we obtained high-quality spectra on January 30. The iSHELL detector is a 2048 $\times$ 2048 pixel Hawaii H2RG array with sensitivity over a wavelength range of $\sim$1–5 $\mu$m. As a cross-dispersed instrument, iSHELL measures signal in many $(>10)$ consecutive echelle orders simultaneously with complete (for $\lambda \leq 4 \mu$m) or nearly complete (for $\lambda > 4 \mu$m) spectral coverage, a significant improvement over the previous IRTF high-resolution facility spectrograph, CSHELL (Tokunaga et al. 1990). More details on iSHELL can be found in Rayner et al. (2012, 2016).

For our observations of R2 PanSTARRS, we used the 0′′75 wide slit, which provides a spectral resolution of $R \equiv \lambda / \Delta \lambda \sim 38,000$ for a uniform monochromatic source. We also observed an early-type IR standard star with the 4″ wide slit to serve as a flux calibrator and telluric standard (see Section 3.1). This slit provides lower spectral resolution ($R \sim 20,000$) but minimizes slit losses and therefore systematic errors in flux calibration. Both the comet and standard star were observed using the classic ABBA nodding sequence, with a 7′5 telescope nod (half the slit length) along the slit between the A and B positions, located equidistant to either side of the slit midpoint. We employed two grating settings: M2 and Lp1. Setting M2 covers a wavelength range of $\sim$4.52–5.25 $\mu$m,
encompassing spectral lines of CO, H₂O, and OCS, and Lp1 covers the wavelength range ~3.28–3.65 μm and targets emission from CH₄, C₂H₂, CH₃OH, H₂CO, and OH prompt emission (a well-established proxy for H₂O production in comets; Bonev et al. 2006). Our comet observations resulted in 29.2 minutes on source in M2 and 59.8 minutes on source in Lp1. We obtained flats and darks at the end of each observing sequence for each grating setting.

Guiding was achieved through filter imaging with the slit viewer camera, performed in specific wavelength bands independent of the wavelength regime used to obtain spectra. The slit viewer allows active guiding on sufficiently bright targets while obtaining spectra. Short-timescale guiding is achieved through a boresight guiding technique, which utilizes “spillover” flux that falls outside the slit to keep the optocenter on the slit. However, while easily visible in the guider using a broadband J filter, R2 PanSTARRS was not bright enough for active guiding. We instead performed offset guiding using a reference (guide) star in the slit viewer field of view (FOV). Owing to the small nonsidereal rates of R2 PanSTARRS, this worked very well; we verified that the comet’s position with respect to the slit remained very stable over the course of our observations, with minimal adjustments needed to keep it in the slit. More details relevant to cometary observations using iSHELL are presented in DiSanti et al. (2017).

2.2. ARO SMT

Observations of the CO(2–1) line at 230.53799 GHz were performed with the ARO SMT on 2018 February 13 at 5:16 UT using the 1.3 mm dual polarization receiver with ALMA Band 6 sideband-separating mixers. The observations began 11 hr after the first Spitzer epoch. Data acquisition was done in beam-switching mode with a +2′ throw in azimuth, and standard 6 minute scans were acquired. System temperatures had peak values of 390 K but, on average, remained under 340 K. The chopper wheel method was used to determine the temperature scale for the SMT receiver systems with a beam efficiency of \( \eta = 0.74 \). The back-end configuration that provided the best velocity resolution (0.325 km s⁻¹ channel⁻¹) consisted of a 2048 channel 250 KHz channel⁻¹ filter bank in parallel mode. The accuracy of the pointing and tracking was checked against the JPL Horizons ephemeris position and found to be better than \(<1''\) rms. Due to high winds, only 12 scans were obtained, but the CO line was strong enough to be seen in single scans.

2.3. Spitzer IRAC

We obtained Director’s Discretionary Time to observe R2 PanSTARRS with Spitzer IRAC on 2018 February 12 at 18:22 UT and 2018 February 21 at 01:03 UT in order to measure the CO₂ production rate. As Spitzer is well into its post-cryogenic mission, IRAC presently observes in two passbands: one centered at 3.6 μm and the other at 4.5 μm. Both filters have broad wavelength coverage, with bandwidths of 0.8 and 1.0 μm, respectively. The 4.5 μm band has been used extensively in the past for measuring CO₂ production rates in comets, as this bandpass includes the ν₁ band of CO₂ at 4.26 μm (e.g., Reach et al. 2013; McKay et al. 2016). It also contains the ν(1–0) band of CO at 4.7 μm, but in many comets in the AKARI survey (Ootsubo et al. 2012), the CO₂ feature was at least 10 times brighter than the CO feature, and so CO₂ is typically assumed to be the dominant gas emission feature in the IRAC 4.5 μm band. This is due to the fluorescence efficiency of CO₂ being approximately an order of magnitude larger than that for CO, coupled with the fact that the CO₂ abundance in comets is often equal to or greater than the CO abundance. There are examples, however, such as C/2006 W3 (Christensen) and 29P/Schwassmann-Wachmann 1, where CO emission contributes significantly to the 4.5 μm band flux (Ootsubo et al. 2012; Reach et al. 2013). The high CO production rate found for R2 PanSTARRS (Biver et al. 2018; de Val-Borro et al. 2018; Wierzchos & Womack 2018) means that CO emission may not be negligible in the Spitzer imaging and may in fact dominate signal in the 4.5 μm channel. We discuss how we account for the CO contribution in the Spitzer imaging in Section 3.3.

We supply the details of our observations in Table 1. The IRAC array is a 256 × 256 pixel InSb array covering a 5/2 × 5/2 FOV with a spatial scale of 1''2 pixel⁻¹, which for our observations corresponds to a projected FOV of \(~500,000 \) km and a spatial scale of \(~1900 \) km pixel⁻¹. We employed a nine-position random dither pattern. Each bandpass is observed with independent arrays, such that when one array is observing the comet, the other is on an adjacent field. The sequence takes about 12 minutes to execute. For each epoch, we performed observations of the comet field several days after each cometary observation in order to image the field without the comet in it. These images are termed “shadow observations” and provide a measurement of the background to be subtracted from the cometary images. Our observations were obtained in high dynamic range (HDR) mode, which entailed obtaining exposures with both short (1.2 s) and long (30 s) exposure times in order to avoid saturation of the inner coma while still keeping a high signal-to-noise ratio (S/N) in the fainter outer coma. Observing in HDR mode also helps protect against saturation due to bright field stars. For these observations, no pixels were saturated; therefore, to optimize the S/N, we analyzed the longest exposure time images.

2.4. DCT LMI

We observed R2 PanSTARRS with the Large Monolithic Imager (LMI) on the 4.3 m Discovery Channel Telescope (DCT) at Lowell Observatory from 2:51 to 4:13 UT on 2018 February 21. The observations were a target-of-opportunity (ToO) request that interrupted normal observations and began within 2 hr of the Spitzer observations in order to provide a near-simultaneous constraint on the water production of R2 PanSTARRS. The DCT ToO requests are limited to 2 hr, which allowed us sufficient time to focus the instrument, observe high- and low-airmass standard stars (listed in Table 1), and obtain ~83 minutes on R2 PanSTARRS. Conditions were photometric, with seeing ~1''2. The comet was ~33'' from a 26% illuminated moon, although no stray light attributable to the moon was evident in any of our images. The comet’s airmass ranged from 1.06 to 1.23.

The LMI has a 12/3 × 12/3 FOV and 6.1 K × 6.1 K e2v CCD. On-chip 3 × 3 binning resulted in a pixel scale of 0''636 pixel⁻¹. We obtained images using a standard broadband SDSS r' filter and narrowband ion (CO⁺ central wavelength/bandpass width = 4266 Å/64 Å), gas (OH 3090/62, CN 3870/62), and dust continuum (UC 3448/84, BC 4450/67) filters that are all part of the comet Hale-Bopp set (Farnham et al. 2000). Single frames were acquired at the start and end of the sequence in the two filters with the highest S/N, r' (30 s)}
and CO$^+$ (300 s). In between, sets of exposures were acquired in OH (three exposures each of 600 s), UC (3 × 300 s), and BC (2 × 120 s), with the sets proceeding from shortest to longest wavelength in order to minimize the effects of atmospheric extinction as the airmass increased. A single CN exposure (180 s) was also acquired at the end of the sequence. The telescope followed the comet’s ephemeris rate for all comet images.

### 2.5. APO ARCES

We obtained Director’s Discretionary Time to observe R2 PanSTARRS with the ARCES instrument on the Astrophysical Research Consortium (ARC) 3.5 m telescope at Apache Point Observatory (APO) in Sunspot, New Mexico, on UT 2018 January 30, just hours before the iSHELL observations. ARCES provides a spectral resolving power of $R = 31,500$ and a spectral range of 3500–10000Å with no interorder gaps. More specifics for this instrument are discussed elsewhere (Wang et al. 2003).

Observational details are described in Table 1. For all observations, we centered the 1″6 × 3″2 slit on the optocenter of the comet. We obtained six spectra of 1800 s each over the course of the night. These spectra were averaged after extraction and calibration to increase S/N. We obtained an ephemeris generated from JPL Horizons for nonsidereal tracking of the optocenter. For short-timescale guiding, the guiding software employs a boresight technique to keep the optocenter centered in the slit. We observed a G2V star in order to remove the underlying solar continuum and Fraunhofer absorption lines, a fast-rotating ($v \sin(i) > 150$ km s$^{-1}$) B star to account for telluric features, and spectra of a flux standard to establish absolute intensities of cometary emission lines. The calibration stars used are given in Table 1. We obtained spectra of a quartz lamp for flat-fielding and a ThAr lamp for wavelength calibration.

### 3. Data Analysis and Results

#### 3.1. IRTF iSHELL

Figure 1 shows raw spectral-spatial difference frames (total A-beam minus B-beam exposures) of R2 PanSTARRS for our M2 (panel (a)) and Lp1 (panel (b)) observing sequences. We applied our general methodology for processing IR spectra (e.g., Dello Russo et al. 2006; Villanueva et al. 2011; DiSanti et al. 2014). New techniques specific to iSHELL are described in detail in DiSanti et al. (2017; see also Roth et al. 2018). We provide a brief summary of our reduction procedures below.

Processing of each iSHELL order produces a “rectified” spectral-spatial frame, meaning each column pertains to a unique wavelength and each row to a unique spatial location along the slit. An example is shown in Figure 1 for the region of Lp1 order 157 containing the cometary R0 and R1 lines of CH$_4$ (panel (e)). Such rectified orders consist of three parts: the bottom and top thirds show the comet signal obtained from A- and B-beam observations, respectively (in black), and the middle third shows the combined signal [(A+B)/2] (in white). Spectral extracts for the standard star and comet are obtained by summing the signal over a range of rows in the central (combined-beam) portion of their rectified frames.
To achieve absolute flux calibration and determine the column burdens of absorbing species in the terrestrial atmosphere, we fit a synthetic atmospheric transmittance model to the standard star spectrum for each processed order. We applied this optimized atmospheric transmittance model (calculated at the airmass of R2 PanSTARRS), convolved it to the spectral resolution of the cometary observations, and scaled it to the cometary continuum level (the continuum is virtually absent for our observations of R2 PanSTARRS). Subtracting the scaled model yields the net observed cometary emission spectrum, still multiplied by monochromatic atmospheric transmittance at the Doppler-shifted frequency of each cometary line. Correcting for transmittance and incorporating flux calibration factors from our standard star spectra allows establishing line fluxes incident at the top of the terrestrial atmosphere. Fully calibrated spectral extracts for R2 PanSTARRS showing emission lines of CO and CH4 are shown in Figure 2. All other species searched for were not detected.

We establish molecular column densities (or upper limits) by dividing these transmittance-corrected line fluxes by appropriate line-specific fluorescence g-factors, the values of which depend on rotational temperature \(T_{\text{rot}}\). For our study of R2 PanSTARRS with iSHELL, only CO presented enough lines with high S/N that spanned a sufficient range of rotational energy to obtain a measure of \(T_{\text{rot}}\). Because the solar spectrum contains CO absorption lines, an accurate treatment required using “reduced” CO g-factors that incorporate the Swings effect for the heliocentric velocity of the comet at the time of our observations (~6.8 km s\(^{-1}\); see Table 1). Our analysis of CO provided a best-fit value \(T_{\text{rot}} = 13 \pm 2\) K. We assume this temperature also applies to other species, as observations of brighter comets in which \(T_{\text{rot}}\) was measured for multiple species demonstrate that this is generally a valid assumption (e.g., Dello Russo et al. 2011; Mumma et al. 2011; Gibb et al. 2012; DiSanti et al. 2014).

We obtained molecular production rates as follows. We extracted a “nucleus-centered” spectrum by summing the signal over 15 rows (~225) centered on the peak emission, and each line is labeled with its rotational identification. We detected nine CO lines spanning two echelle orders and two CH4 lines within a single order.

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We obtained molecular production rates as follows. We extracted a “nucleus-centered” spectrum by summing the signal over 15 rows (~225) centered on the row containing the peak emission line intensity. Application of Swings-corrected g-factors and geometric parameters (\(R_h\), \(\Delta\), beam size at the comet) to transmittance-corrected line fluxes provides the nucleus-centered production rate, \(Q_{\text{nc}}\). However, owing primarily to seeing, \(Q_{\text{nc}}\) invariably underestimates the actual “total” (or “global”) production rate, \(Q_{\text{tot}}\). To obtain \(Q_{\text{tot}}\), we multiplied each \(Q_{\text{nc}}\) by an appropriate growth factor (GF), determined through the well-documented “Q-curve” method for analyzing spatial profiles of emissions (Dello Russo et al. 1998). For each spatial step, a “symmetrized” Q-curve was produced by averaging the signal at equal but diametrically opposed distances from the nucleus. For our observations, only CO and CH4 were detected. Each showed bright enough emissions to allow a reliable Q-curve analysis to be performed.
We present spatial profiles and symmetrized Q-curves for CO and CH$_4$ in Figure 3. For each Q-curve, the GF is depicted graphically as the level of the upper horizontal line (representing $Q_{\text{tot}}$) divided by that of the corresponding lower horizontal line (representing $Q_{\text{nc}}$). We refer to the region of the coma over which $Q_{\text{tot}}$ is measured as the “terminal region.”

Comparison of the profiles in Figure 3 reveals a relatively broad (and, in particular, “flat-topped”) spatial distribution for the observed CO emission. This is demonstrated by its much larger GF compared to CH$_4$, as well as that leveling its Q-curve required beginning two steps from the nucleus instead of one step, as was used for CH$_4$. This could indicate extended release of CO (e.g., from grains) in the inner coma and/or optical depth in the CO lines (particularly along lines of sight passing close to the nucleus). The high CO production rates reported from millimeter observations of R2 PanSTARRS with IRAM (Biver et al. 2018) and SMT (Wierzchos & Womack 2018), as well as from our iSHELL observations (see Table 3), suggest that the IR lines of CO are affected by optical depth.

Several previous CO-rich comets revealed optically thick emissions that in all cases were most pronounced for lines of sight passing through the innermost coma. For observations of C/1995 O1 (Hale-Bopp) and C/1996 B2 (Hyakutake) with CSHELL at the IRTF, observed column densities and Q-curves were corrected for opacity in the solar pump, assuming uniform gas outflow at constant speed (DiSanti et al. 2001, 2003). Observations of C/2006 W3 (Christensen) with CRIRES at the ESO/VLT (Bonev et al. 2017) at a similar observing geometry to our observations of R2 PanSTARRS also revealed optically thick CO for a production rate only slightly lower than what has been reported for R2 PanSTARRS. Bonev et al. (2017) developed a formalism for addressing optical depth effects in CO emission based on a curve-of-growth analysis, demonstrating through their Q-curve analysis that the effects of optical depth on retrieved production rates can be quantified (and thus corrected for).

Provided that the signal in the terminal region (i.e., the ends of the slit farthest from the comet optocenter) approximates

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**Figure 3.** Spatial profiles (left) and symmetrized Q-curves (right) from our iSHELL observations of R2 PanSTARRS, representing the sum of nine CO lines (top) and two CH$_4$ lines (bottom). For the spatial profiles, the sunward-facing hemisphere is to the left, as indicated. For CO (panels (a) and (b)), dashed lines represent observed emission, while solid lines represent emission after correcting line-by-line for optical depth in the solar pump, following the methodology of DiSanti et al. (2001). In all cases, the GF is given by the ratio of total $Q$ ($Q_{\text{tot}}$: upper horizontal line) to nucleus-centered $Q$ ($Q_{\text{nc}}$: corresponding lower horizontal line). The GF for CO prior to correcting for optical depth ($2.93 \pm 0.04$) is much larger than that measured for (optically thin) CH$_4$ ($1.70 \pm 0.19$). However, the opacity-corrected CO Q-curve has a much lower GF = $1.67 \pm 0.04$, consistent with that for CH$_4$. We note that for CO, our formalism for correcting optical depth increases $Q_{\text{nc}}$ by 91% but increases $Q_{\text{tot}}$ by only 5.6% (well within the 1σ uncertainty; see Table 3). This suggests that our approach for modeling optical depth, coupled with the Q-curve formalism, provides robust production rates for these two species in R2 PanSTARRS.
optically thin conditions, the $Q$-curve will level out, as was observed for these three previously observed CO-rich comets, and as we also observed for R2 PanSTARRS (Figure 3). Although in this case, for CO, the central region is optically thick, the GF still allows establishing a reliable approximation of the actual $Q_{\text{tot}}$ but with the GF for CO being significantly larger than the corresponding value for the optically thin CH$_4$ emission in R2 PanSTARRS (see Figure 3). For all of these comets (including R2 PanSTARRS), values of $Q_{\text{tot}}$(CO) as retrieved from optically thin and thick treatments are in formal agreement (i.e., they agree to within their respective 1$\sigma$ uncertainties); see Figure A4 of DiSanti et al. (2001), Figure 4 of DiSanti et al. (2003), and Figure 4 of Bonev et al. (2017). We demonstrate this by applying the methodology detailed in the Appendix of DiSanti et al. (2001) to the observed CO emission in R2 PanSTARRS. The presence of optically thick CO emission in R2 PanSTARRS is supported by the much larger GF for the observed CO profile (2.93 ± 0.04) versus that for (optically thin) CH$_4$ (1.70 ± 0.19), a discrepancy that is resolved by correcting for optical depth in the CO lines (resulting in 1.67 ± 0.04; see Figure 3(b)). Therefore, we conclude that our $Q$-curve analysis for CO mitigates the effects of optical depth on our measured CO production rate. It also reinforces our decision to apply its “corrected” GF (1.7) to obtain a realistic upper limit for comeasured OCS and, similarly, to constrain $Q_{\text{tot}}$ using the (identical within 1$\sigma$ uncertainty) GF from CH$_4$ for comeasured, undetected species included in the Lp1 setting (C$_2$H$_6$, CH$_3$OH, and H$_2$CO). Derived production rates and mixing ratios are shown in Table 3.

Our spatial profiles also permit testing for asymmetric gas outflow in the coma. This is very pronounced for CH$_4$ (Figure 3(c)), indicating a large enhancement in the anti-sunward-facing hemisphere, particularly considering the relatively small solar phase angle of R2 PanSTARRS at the time of our observations (~19°) and thus the potential high degree of projection onto the sky plane. The column density of CH$_4$ averaged between ~2000 and 8000 km from the nucleus (projected on the sky) is a factor of 2.65 ± 0.55 larger in the anti-sunward direction compared to the solar direction, while the CO profile is much more symmetric, its corresponding ratio being only 1.03 ± 0.02.

It is possible that the asymmetry observed for CH$_4$ is associated with rotation of the nucleus. However, for the measured gas speed $v_{\text{exp}}$ of 0.52 km s$^{-1}$ (from our SMT observations; see Section 3.2), the time required to exit the iSHELL terminal region (extending to 4°9 from the nucleus) is approximately 4.3 hr, longer than the clock times encompassed by our M2 and Lp1 sequences (obtained consecutively and together spanning 2.65 hr of elapsed clock time). This suggests that gas in the iSHELL slit was not replenished (at least significantly) between M2 and Lp1 sequences, and thus the large differences in the degrees of asymmetry observed for CO and CH$_4$ cannot be explained by temporally variable outgassing. Nonetheless, these results indicate that the abundance ratio CH$_4$/CO was higher in the anti-sunward-facing hemisphere than in the sunward-facing hemisphere by a factor of ~2.5; therefore, assuming little to no replenishment of coma gas between M2 and Lp1 sequences, this implies a significantly higher CH$_4$/CO abundance ratio in the anti-sunward direction at the time of our iSHELL observations.

Figure 4 shows the spectrum resulting from coadding all 12 scans on UT February 13. We calculated the column density assuming optically thin gas (appropriate for the relatively large beam diameter of 32") with $T_{\text{rot}}$ = 23 K (Biver et al. 2018; see Section 4 for discussion of differences with iSHELL), and we calculated the production rate assuming a simple symmetric outflow expansion model with $V_{\text{exp}}$ = 0.52 km s$^{-1}$ consistent with our spectra and other detailed modeling of the spectral line profiles (Biver et al. 2018; Wierzchos & Womack 2018). We adopt this expansion velocity for all analysis in this work. The CO production rate is (5.5 ± 0.89) × 10$^{28}$ mol s$^{-1}$ (see Table 3).

### 3.2. ARO SMT

We combined all images of the same exposure time using the MOPEX software (Makovoz & Khan 2005). This process creates a mosaic in the rest frame of the comet from the individual images, averaging overlapping data together but ignoring cosmic rays and bad pixels. Two mosaics are created: one for the comet data, the other for the sky (background) data. We subtracted the sky mosaic from the comet mosaic to remove the background. This includes zodiacal light and celestial sources. While this removes background stars and most of the sky background, it may not completely remove the sky background (for instance, zodiacal light for a given R.A. and decl. varies with time). We used the sky value from the adjacent image of blank sky to remove any residual background that remained after shadow subtraction. The resulting images are shown in the first two columns of Figure 5.

After the mosaic images were created and the sky background was subtracted, we removed the dust contribution from the 4.5 μm band flux, isolating the gas emission. As the level of dust contamination is minimal, as inferred from the 3.6 μm image being much fainter than the 4.5 μm image (see Figure 5), we simply applied a scaling factor of 0.9 to the 3.6 μm image and subtracted it from the 4.5 μm image to remove the dust contribution from the 4.5 μm image. The scale factor of 0.9 was derived from a model for cometary dust accounting for the expected contributions of reflected light and thermal emission.
at the heliocentric distance of R2 PanSTARRS, based on the empirical coma dust model of Kelley et al. (2016) and the dust color of comet 67P/Churyumov-Gerasimenko at 2.8 au (Snodgrass et al. 2017). The resulting dust-subtracted images are shown in the third column of Figure 5. The fourth column of Figure 5 shows the dust-subtracted images normalized by a $1/\rho$ surface brightness distribution, where $\rho$ is the projected distance to the peak brightness, which enhances coma asymmetries. The enhanced images show strong spiral structures, as well as an ion tail that we attribute to CO$^+$ (see Section 4). A more detailed analysis of the coma morphology is beyond the scope of this paper.

As mentioned in Section 2.3, CO likely contributes significant flux to the Spitzer 4.5 $\mu$m channel, especially considering the large CO production rates measured for R2 PanSTARRS at millimeter wavelengths (Biver et al. 2018; Wierzchos & Womack 2018) and in the IR with iSHELL (Figure 3(b)). Also, CO$_2$ is observed with strong emission at this wavelength in many comets (Ootsubo et al. 2012), with few other likely contributors (see Section 4 for a discussion of other possible contaminating species). Therefore, we assume that the gas emission at 4.5 $\mu$m predominantly arises from CO and CO$_2$, and we separate their contributions with a three-step process: (1) we initially assume that 100% of the gas emission flux comes from CO molecules and derive a CO production rate; (2) we subtract the contemporaneous ground-based measured CO production rate, taking care to match the projected photometric aperture used for the Spitzer observations, which leaves a residual amount; and (3) we then recharacterize this residual as a CO$_2$ production rate.

From the dust-subtracted image of gas emission, we measured the flux for apertures ranging from 10 to 100 pixels (12\\degree–120\\degree) in radius. We converted the broadband photometry to CO line fluxes in photons following the IRAC data handbook (Laine 2015). The line fluxes were then used to calculate the total number of CO molecules inside the photometric aperture ($N_{CO,100\%}$) using

$$N_{CO,100\%} = 4\pi\Delta^2 F R_h^2 g_{CO},$$

where $\Delta$ is the Spitzer–comet distance, $F$ is the observed photon flux, $R_h$ is the heliocentric distance of the comet, and $g_{CO}$ is the $g$-factor for excitation of the CO $1 \rightarrow 0$ fundamental vibrational band, which is $2.5 \times 10^{-4}$ photons s$^{-1}$ (Debout et al. 2016). Then, the production rate $Q_{CO,100\%}$ is given by

$$Q_{CO,100\%} = \frac{2v}{\pi\rho} N_{CO,100\%},$$

where $N_{CO,100\%}$ is the total number of CO molecules in the photometric aperture, $v$ is the expansion velocity, and $\rho$ is the projected radius of the photometric aperture. We assume an expansion velocity of the coma of 0.52 km s$^{-1}$, consistent with CO line widths from our SMT observations (see Section 3.2) and expansion velocities reported for R2 PanSTARRS by Biver et al. (2018) and Wierzchos & Womack (2018). This approach assumes a negligible effect of photodissociation on the spatial profile in the photometric aperture, which is justified, as our photometric apertures are $<$10% of both the CO$_2$ and CO photodissociation scale lengths. We calculated production rates

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**Figure 5.** Shadow-subtracted images of C/2016 R2 (PanSTARRS) obtained with Spitzer IRAC at 3.6 $\mu$m (first column) and 4.5 $\mu$m (second column), as well as the dust-subtracted images (third column) on UT 2018 February 12 (top row) and UT 2018 February 21 (bottom row). These images are for the longer exposure time (30 s) in our HDR mode observations. The solar direction is downward in all images. The spherical coma geometry observed in the 4.5 $\mu$m channel, as well as the large flux ratio between the two filters, is indicative of a large gas contribution to the observed flux due to CO$_2$ and CO. The last column shows the dust-subtracted images normalized by a $1/\rho$ surface brightness distribution, where $\rho$ is the projected distance to the peak brightness, which enhances coma asymmetries. There is clear evidence for a strong ion tail, which we attribute to CO$^+$ (see Section 4). There is also a clear spiral structure in the innermost coma indicative of a rotating jet and a large circular arc that is present on February 21 but not February 12, possibly indicative of an impulsive outgassing event between the two observation epochs. On both dates, there is broad sunward enhancement, indicative of preferential outgassing from the sunward hemisphere, which is consistent with results from CO spectral line profiles and spatial mapping measured at millimeter wavelengths (Biver et al. 2018; Wierzchos & Womack 2018). A more detailed analysis of the coma morphology is beyond the scope of this paper and will be deferred to a future publication.
for a variety of aperture sizes to quantify any trends in derived production rates with aperture size. Since we found the deviations between derived production rates for different aperture sizes to be minimal (<5%), for the rest of this paper, we quote production rates derived using a photometric aperture that matches the projected distance at the comet of the ARO SMT observation beam (see Section 2.2). This is a 14 pixel radius on UT February 12 and a 15 pixel radius on UT February 21. This choice minimizes systematic errors when subtracting the expected CO flux from the Spitzer images (see below).

If we assume that all of the gas flux in the Spitzer 4.5 μm image is due to CO and calculate its corresponding production rate using Equations (1) and (2), we find \( Q_{\text{CO,100\%}} \sim 1.6 \times 10^{29} \text{ mol s}^{-1} \), higher than the values derived from ground-based CO observations (Biver et al. 2018; de Val-Borro et al. 2018; Wierzchos & Womack 2018; this work).

Therefore, we conclude that CO is probably not the sole contributor to the observed flux. However, it is a major contributor, and accounting for it does have a strong influence on the derived CO2 production rate. While CO contributes significantly to the observed Spitzer fluxes, the excess we attribute to CO2 is still >50% of the observed flux, so the detection of CO2 is robust.

To calculate \( Q_{\text{CO}} \), and account for the CO contribution to the Spitzer 4.5 μm images, we employ our contemporaneous observations of CO at millimeter wavelengths obtained with the ARO SMT (Section 2.2). We favor using the contemporaneous SMT results over the IRTF CO measurements from several weeks earlier for subtraction of the CO contribution from the Spitzer imaging in order to minimize effects due to possible comet variability. Moreover, the production rates from SMT and Spitzer data were obtained using the same-sized photometric aperture, whereas the iSHELL observations cover a much smaller projected region of the coma, making it more sensitive to short-timescale changes in gas production such as rotational variation. This approach minimizes systematic uncertainties introduced by possible variability in the comet’s activity.

We subtracted the millimeter wavelength–derived CO production rate, \( Q_{\text{CO,mm}} \) (see Section 3.2), from the derived \( Q_{\text{CO,100\%}} \) value, which leaves a residual production rate: \( Q_{\text{residual}} = Q_{\text{CO,100\%}} - Q_{\text{CO,mm}} \). We attribute the residual gas production to CO2 (see Section 4 for a discussion of other possible contaminating species). This residual production rate is then converted to \( Q_{\text{CO2}} \) by taking advantage of the scaling relationship between production rates and fluorescence efficiencies,

\[
Q_{\text{CO2}} = Q_{\text{residual}} \frac{g_{\text{CO2}}}{g_{\text{CO}}},
\]

where \( g_{\text{CO}} = 2.69 \times 10^{-3} \text{ photons s}^{-1} \) (Debout et al. 2016). Using the SMT CO production rate, we derive \( Q_{\text{CO2}} = (1.0 \pm 0.1) \times 10^{28} \text{ mol s}^{-1} \) (Table 3). As a demonstration of the sensitivity of our derived CO2 production rate to the assumed value for CO, if \( Q_{\text{CO}} = 0 \), then \( Q_{\text{CO2}} \sim 1.5 \times 10^{28} \text{ mol s}^{-1} \), while \( Q_{\text{CO}} = 1.0 \times 10^{29} \text{ mol s}^{-1} \) (closer to the iSHELL value) results in \( Q_{\text{CO2}} \sim 6.0 \times 10^{27} \text{ mol s}^{-1} \).

Lastly, we derived the \( \alpha_f \) value as a proxy for the dust production based on the 3.6 μm flux levels using the same photometric aperture as for the gas photometry and assuming all of the flux is solar continuum reflected off of dust particles in the coma (i.e., negligible emissions from gaseous species and no thermal emission). We follow the methodology of A’Hearn et al. (1984) to calculate \( \alpha_f \). We derive \( \alpha_f \) values of 896 ± 27 cm on February 12 and 884 ± 27 cm on February 21, very low for a comet of this activity level and heliocentric distance. We derive log[\( \alpha_f / \rho(H_2O) \)] = −23.54 ± 0.03, log[\( \alpha_f / \rho(CO) \)] = −25.79 ± 0.04, and log[\( \alpha_f / \rho(CO_2) \)] = −25.05 ± 0.04. For similar reasons discussed above, we compare \( \alpha_f \) to the CO production rate measured by SMT rather than IRTF.

Due to the high quality of our Spitzer data, uncertainties in the photometry are dominated by the absolute calibration uncertainty of Spitzer IRAC, which is approximately 3% (Reach et al. 2005).

### 3.4. DCT LMI

The images were bias subtracted and flat-field corrected following standard practices, and all images for a given set (OH, UC, or BC) were median combined to improve S/N and mitigate background (stellar) contamination. Absolute calibrations and gas/dust decontamination for the narrowband filters were performed using extinction coefficients determined from the two standard stars and following the procedures outlined in Farnham et al. (2000), with sky values determined from regions near the corners of the CCD that appeared to be visually free of gas/dust/ions. The CN and UC images exhibited extended filamentary structures similar to those seen with the CO+ filter. Although the filters were designed to isolate gas (CN) or to be a nearly emission-free continuum area (UC), the CN bandpass includes N2− emission (Cochran & McKay 2018; Optiom et al. 2019), and both bandpasses contain emission from CO− ions (Pearse & Gaydon 1976, and references therein). For most comets, these ions are much fainter than the intended gas and/or continuum and can be safely ignored, but this is not the case for R2 PanSTARRS. We thus conclude that the features we observed are ions and that UC and CN cannot be interpreted in their normal fashion. As a result, absolute calibrations of the OH images were performed using only the BC filter to define continuum, with solar color assumed. Flux-calibrated and decontaminated images are shown in Figure 6.

Our normal procedure for determining gas production rates from fully calibrated images (e.g., Knight & Schleicher 2015) is to measure the flux in a circular aperture centered on the central condensation and convert to a production rate using a Haser model and standard assumptions about the appropriate lifetimes and scale lengths (A’Hearn et al. 1995). However, we elected to perform a more complex analysis, detailed below, due to several factors. First, the low S/N of our “pure” OH image meant that trailed stars or their negative residuals from the continuum image that was removed could significantly impact our inferred OH signal. Second, the aforementioned difficulties in decontaminating the image may have potentially led to over- or underremoval of the sky background and/or underlying dust continuum. Finally, we identified four lines of CO+ from the \( A^2\Pi-X^2\Sigma^+ \) “comet-tail system” (Pearse & Gaydon 1976, and references therein) that fall in the OH filter bandpass. While no ion tail structure is evident by eye in our OH image, we were nonetheless concerned about possible ion contamination that was not accounted for in the standard comet filter reduction procedures.
In order to understand the extent to which our “pure” OH image might be contaminated by improperly removed continuum and/or ions, we extracted radial profiles from the uncalibrated CO+, BC, and OH images after removing the background. The radial profiles were binned in distance from the nucleus, \( \rho \), and in azimuthal angle, with a resistant mean used to screen out anomalously high or low pixel values. The dust and ion tails were oriented nearly due east, at a position angle (PA) of \( \sim 90^\circ \), slightly offset from the anti-sunward direction of PA = \( 79^\circ \), so we determined radial profiles for the sunward and tailward hemispheres, as well as 90\(^\circ\) wedges centered at 0\(^\circ\), 90\(^\circ\), 180\(^\circ\), and 270\(^\circ\). We then fit slopes to the profiles from \( \rho = 4000–60,000 \) km (the inner radius was set to be about twice the seeing disk). The exact slopes retrieved are very sensitive to the background level, but the behavior of the slopes with azimuth is not. The OH slope was the flattest, falling off as roughly \( \rho^{-0.7} \) in all four quadrants. The BC slope was steeper, falling as roughly \( \rho^{-1.1} \) in all four quadrants. The CO+ exhibited the steepest slope and was the only one that varied significantly with PA, falling as \( \rho^{-1.4} \) in the sunward quadrant and \( \rho^{-1.0} \) in the other quadrants. The CO+ slopes are consistent with the expected behavior of ions whose sunward extent is minimal, while the consistency of the OH and BC slopes at all PAs suggests that each is relatively free of ion contamination. Furthermore, the more rapid falloff of BC and CO+ compared to OH suggests that, even if there were problems with improper decontamination of the OH image, the flux should increasingly approach the true OH signal at larger distances, with the sunward direction providing the least-contaminated OH signal.

This exercise also demonstrated that despite our previous concern about the low S/N of individual pixels in the OH image, with appropriate binning, a clear signal could be detected to at least \( \rho = 1.2 \times 10^5 \) km. Thus, we measured a radial profile in the sunward quadrant for the “pure” OH image and used this to determine the \( \mathrm{H}_2\mathrm{O} \) production rate on the assumption that the coma was spherically symmetric as follows. We created a synthetic OH profile using J. Parker and M. Festou’s online version\(^\text{12} \) of the vectorial model (Festou 1981) using the standard parameters given in Table 2 and scaling for the geometry of R2 PanSTARRS during our observations. We then interpolated the model to the midpoints of our radial profile \( \rho \) bins and scaled it up or down to minimize \( \chi^2 \) from \( \rho = (4000–1.2) \times 10^5 \) km. We repeated the process but added a second parameter, a fixed background offset that was allowed to be positive or negative, to minimize \( \chi^2 \) again. We continued to add complexity by including the BC and CO+ profiles, first individually and then together, ultimately testing all combinations of vectorial model, fixed background, BC profile, and CO+ profile. We repeated the fitting using an OH image that was flux calibrated with the continuum component set to zero as a further test of the reduction process.

The DCT images of OH (left, after dust and ion removal), BC (middle), and CO+ (right, after dust removal). The OH image has been rebinned 8 \times 8 to improve S/N. Background stars are visible as trailed streaks in all images, while the negative of background stars (the continuum image) are also visible in the OH and CO+ images as black trailed streaks. Artifacts from a bad column on the CCD are faintly seen as vertical lines in the BC and CO+ panels. A scale bar and arrows indicating north, east, and the directions to the Sun and the heliocentric velocity vector are given on the CO+ panel.

| Molecule | Parent Life-time (s)\(^a\) | Daughter Life-time (s)\(^a\) | g-factor (erg s\(^{-1}\) molecule\(^{-1}\))\(^b\) |
|----------|-----------------------------|-----------------------------|-----------------------------|
| CN       | 1.3 \times 10^4            | 2.1 \times 10^5            | 2.6 \times 10^{-13}         |
| C2       | 2.2 \times 10^4            | 6.6 \times 10^4            | 4.5 \times 10^{-13}         |
| NH\(_2\) | 4.1 \times 10^3            | 6.2 \times 10^4            | 6.40 \times 10^{-15}        |
| \(\mathrm{O}\)\(_{\alpha}\) | 8.3 \times 10^4            | ...                        | ...                        |
| \(\mathrm{O}\)\(_{\beta}\) | 1.3 \times 10^4            | ...                        | ...                        |
| OH       | 8.3 \times 10^4            | 1.3 \times 10^5            | 1.54 \times 10^{-15}        |

\(^a\) Given for \( r = 1 \) au. For CN and OH, given for \( r = 0 \) km s\(^{-1}\) but varies with \( r \).

\(^b\) For [O II] from dissociation of \( \mathrm{H}_2\mathrm{O} \) into \( \mathrm{H}_2 \) and O; the branching ratio employed is 0.07 (Bhardwaj & Raghuram 2012).

\(^\text{12}\) http://www.boulder.swri.edu/wvm-2011/
largest variations occurring for fits using only background fluxes (e.g., no continuum or ion component). We tested reasonable deviations from the standard vectorial model assumptions, such as varying lifetimes and velocities, but these only changed $Q(\text{H}_2\text{O})$ at the $\sim20\%$ level or less. The fits consistently show that the OH signal is much stronger than the CO$^+$ and dust continuum beyond $\sim20,000$ km. Figure 7 shows a “pure” OH image using our best-fit parameters (top left panel), the residual flux after removing the modeled OH component from the “pure” OH image (bottom left), and the radial profiles in our best-fit model (right).

The residual OH image has been highly stretched to emphasize subtle features but shows a hint of overremoval in the tailward direction and slight underremoval of the inner core. Despite the large number of uncertainties and assumptions needed to deal with this unusual comet, we are confident that we have constrained $Q(\text{H}_2\text{O})$ to less than $10^{27}$ mol s$^{-1}$, with a most likely value of $\sim(3.1 \pm 0.2) \times 10^{26}$ mol s$^{-1}$ (Table 3). The uncertainty quoted is strictly for our modeled assumptions and does not include systematic uncertainties that are difficult to quantify but could be larger.

Using the observed flux in the BC image, we calculated Af$\rho$ as described in Section 3.3, although for the DCT data, we used a smaller photometric aperture projected at the comet of 10,000 km, in line with the typical apertures employed by other optical dust photometry observations. We obtain Af$\rho = 561 \pm 6$ cm (Table 3).

3.5. APO ARCES

Spectra were extracted and calibrated using IRAF scripts that perform bias subtraction, cosmic-ray removal, flat-fielding, and wavelength calibration. We removed telluric absorption features and the reflected solar continuum from the dust coma and flux calibrated the spectra, employing our standard star observations. We assumed an exponential extinction law and extinction coefficients for APO when flux calibrating the coma spectra (Hogg et al. 2001). More details of our reduction procedures can be found in McKay et al. (2012) and Cochran & Cochran (2002). We determined slit losses for the flux standard star observations by performing aperture photometry on the slit viewer images as described in McKay et al. (2014). Slit losses introduce a systematic error in the flux calibration of $\sim10\%$.

In our optical spectra, we report an analysis of five molecular species ($\text{N}_2^+$, CO$^+$, CN, NH$_2$, and C$_2$) and one atomic species (O1). Our analysis of CN, C$_2$, and NH$_2$ employs the same empirical fitting model employed by McKay et al. (2014), which utilizes a molecular line list from Cochran & Cochran (2002) to fit Gaussian profiles to observed emission features. For $\text{N}_2^+$ and CO$^+$, we adapt the model from McKay et al. (2014) to include CO$^+$ by adding line positions from Kuo et al. (1986) and Haridass et al. (1992, 2000) and $\text{N}_2^+$ line positions from Dick (1978). We integrate over the fits to measure the observed flux. While we detect multiple bands of CO$^+$, we use the (2, 0) band for analysis, as it has the highest S/N.
For CN, C_2, and NH_2, these fluxes are converted to production rates using a Haser model in which the input scale lengths are modified to emulate the vectorial model and \( g \)-factors from the literature. The molecular lifetimes and \( g \)-factors employed are given in Table 2. For [O I], we employ the observed [O I] 6300 Å emission as a proxy for \( \text{H}_2\text{O} \) production using a similar Haser model (see McKay et al. 2012, 2014 for more details about the Haser models employed). While [O I] 6300 Å emission is often used as a proxy for \( \text{H}_2\text{O} \) production in comets (e.g., Morgenstaller et al. 2001; Fink 2009; McKay et al. 2018), it assumes that \( \text{H}_2\text{O} \) is the dominant oxygen-bearing species in the coma, which is not the case for R2 PanSTARRS (see Table 3).

Ions do not follow a Haser profile. Therefore, we do not calculate production rates from derived fluxes for N_2^+ and CO^+, only the relative ratio of N_2^+ / CO^+ using

\[
\frac{N_{N_2^+}}{N_{\text{CO}^+}} = \frac{F_{N_2^+} g_{\text{CO}^+}}{F_{\text{CO}^+} g_{N_2^+}},
\]

where \( N_x \) denotes the column density of species \( x \), \( F_x \) is the observed flux of species \( x \), and \( g_x \) is the \( g \)-factor for the observed transition of species \( x \). The \( g \)-factors employed are \( g_{\text{CO}^+} = 3.55 \times 10^{-3} \) photons s\(^{-1}\) mol\(^{-1}\) (Magnani & A'Hearn 1986) and \( g_{N_2^+} = 7.00 \times 10^{-2} \) photons s\(^{-1}\) mol\(^{-1}\) (Lutz et al. 1993).

For the ARCES observations, we show our detections of N_2^+ and CO^+ in Figure 8 and the detection of [O I] 5577 Å emission in Figure 9. We do not detect CN or NH_2 emission and have a tentative detection of the C_2 bandhead at 5165 Å, all of which we show in Figure 10.

To derive upper limits on production rates, we employ empirical spectral fits of comet C/2009 P1 (Garradd) at a similar heliocentric distance using the spectral fitting model of McKay et al. (2014) and scale these models so that the strongest lines would be present at the 3σ level (for C_2, we scaled the model so that it corresponded to the candidate bandhead feature). We then integrated over this model to obtain an upper limit on the observed flux and convert to the production rate using our Haser model as described above. We present the production rate upper limits for CN, NH_2, and C_2 in Table 3. Regardless of whether the inferred flux for C_2 is interpreted as an upper limit or a detection, the upper limit inferred for C_2H_2 is unchanged, since C_2 has multiple sources in cometary comae (Combi & Fink 1997). For ARCES observations, we compare to the iSHELL observations of CO because the data were taken contemporaneously and both are narrow-slit spectrometers sampling similar portions of the coma.

From the ARCES spectra, we measure an N_2^+ / CO^+ ratio of 0.05 ± 0.01. We follow the arguments of Cochran & McKay (2018) and assume that N_2^+ / CO^+ = N_2 / CO (see Section 4 for discussion of the validity of this assumption). Therefore, we infer an N_2 / CO ratio of 0.05 ± 0.01. Using the CO production rate derived from our iSHELL observations, we derive an N_2 production rate of 4.8 \times 10^{27} \text{mol s}^{-1} (see Table 3).

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### Table 3

Production Rates and Abundances

| Instrument   | Species | \( Q \left( 10^{27} \text{mol s}^{-1} \right) \) | \( X / \text{H}_2\text{O}^+ \) (%) | \( X / \text{CO}^+ \) (%) |
|--------------|---------|---------------------------------|---------------------------------|-------------------|
| IRTF iSHELL  | CO      | 95.4 ± 9.1                      | (3.08 ± 0.35) \times 10^4      | ...               |
|              | CH_4    | 0.56 ± 0.07                     | 181 ± 25                        | 0.59 ± 0.09       |
|              | OCS     | <0.23                           | <74                             | <0.24             |
|              | C_2H_2  | <0.085                          | <27                             | <0.089            |
|              | CH_3OH  | <0.36                           | <116                            | <0.38             |
|              | H_2CO   | <0.49                           | <158                            | <0.51             |
|              | H_2O^+  | <78.4                           | ...                             | <82               |
|              | H_2O^2  | <72.9                           | ...                             | <76               |
| Spitzer IRAC | CO_2^+  | 10.0 ± 1.0                      | 3230 ± 380                      | 18.2 ± 3.5        |
|              | AF_r    | 890 ± 19 cm                     | −23.54 ± 0.03^f                 | −25.79 ± 0.04^f   |
| APO ARCES    | N_2     | 4.8 ± 1.1^b                      | 1550 ± 370                      | 5.0 ± 1.0         |
|              | CN      | <0.02                           | <6.5                            | <0.021            |
|              | NH_2    | <0.01                           | <3.2                            | <0.010            |
|              | C_2     | <0.021                          | <6.8                            | <0.011            |
|              | H_2O (via [O I]) | 10.5 ± 0.5 | ... | ... |
| DCT LMI      | H_2O (via OH) | 0.31 ± 0.02 | −23.74 ± 0.03^f | −25.99 ± 0.04^f |
|              | AF_r    | 561 ± 6 cm                      | ...                             | ...               |

Notes.

^a^ Compared to the measured value from OH observations with the DCT, as this is the most robust measure of the \( \text{H}_2\text{O} \) production rate.

^b^ Compared to the iSHELL CO production rate except for CO_2 and AF_r, which are compared to the SMT CO value, as this value was measured contemporaneously and used to correct the Spitzer observations for the expected CO contribution. The N_2 / CO is calculated from the optical observations of N_2^+ and CO^+ as described in the text.

^c^ Derived from H_2O lines in the M2 setting.

^d^ Derived from OH prompt emission in the Lp1 setting.

^e^ Derived accounting for the expected CO contribution based on the SMT observations using the methodology detailed in Section 3.3.

^f^ \( \log(\text{AF}_r / \text{Q}_{\text{CO}}) \).

^g^ \( \log(\text{AF}_r / \text{Q}_{\text{CO}}) \).

^h^ Calculated using the N_2 / CO ratio derived from optical observations multiplied by the iSHELL CO production rate.
We present the \( \text{H}_2\text{O} \) production rates derived from the \([\text{O I}] 6300 \, \text{Å}\) emission measured by ARCES and OH emission from DCT in Table 3. There is a clear discrepancy (factor of \( \sim 30 \)) between the \( \text{H}_2\text{O} \) production rate derived from the \([\text{O I}] 6300 \, \text{Å}\) emission and the value derived from our OH narrow-band observations. However, the methodology for deriving water production rates from \([\text{O I}] 6300 \, \text{Å}\) emission assumes that \( \text{H}_2\text{O} \) photodissociation is the dominant source of \( \text{O I} \) in the coma. While this is a valid assumption for most comets and has been used in the past to derive reliable \( \text{H}_2\text{O} \) production rates (e.g., Morgenthaler et al. 2001; Fink 2009; McKay et al. 2018), the large \( \text{CO} \) and \( \text{CO}_2 \) production rates found by both ourselves and other authors compared to our derived water production rate suggest that this is not a valid assumption for R2 PanSTARRS. Not accounting for contributions from the photodissociation of other oxygen-bearing species such as \( \text{CO} \) and \( \text{CO}_2 \) when they are more abundant than \( \text{H}_2\text{O} \) results in a large overestimate of the \( \text{H}_2\text{O} \) production rate. The \( \text{O I} \) photochemistry in comets has been of interest for some time (e.g., Festou & Feldman 1981; Cochran 2008; Decock et al. 2013, 2015; McKay et al. 2013, 2015), and the study of both the \([\text{O I}] 6300 \, \text{Å}\) line and the \([\text{O I}] 5577 \, \text{Å}\) line (which we also detect in our ARCES spectra; see Figure 9) in such a \( \text{CO}^- \) and \( \text{CO}_2^- \)-rich comet could provide new insights into \( \text{O I} \) photochemistry in comets. We measure the flux ratio of the \([\text{O I}] 5577 \, \text{Å}\) line to the sum of the \([\text{O I}] 6300 \, \text{Å}\) and \([\text{O I}] 6364 \, \text{Å}\) lines (the oxygen line ratio) to be \( 0.20 \pm 0.03 \), in agreement with the value of \( 0.23 \pm 0.03 \) measured by Opitom et al. (2019). This ratio is higher than typically observed but similar to other comets observed at heliocentric distances near 3 au (McKay et al. 2012, 2015; Decock et al. 2013). This is consistent with the large \( \text{CO}_2/\text{H}_2\text{O} \) and \( \text{CO}/\text{H}_2\text{O} \) ratios observed. However, a detailed study of the \( \text{O I} \) photochemistry in R2 PanSTARRS is beyond the scope of this paper and will be pursued in a future publication.

### 3.6. Summary of Production Rates and Relative Abundances

A summary of our resulting production rates and abundances is presented in Table 3. We pursued several methods for determining the water production rate: \( \text{H}_2\text{O} \) and OH prompt emission from iSHELL, OH emission from DCT, and \([\text{O I}] 6300 \, \text{Å}\) emission from APO ARCES. The OH data from DCT provided the best measure of \( \text{H}_2\text{O} \) production; therefore, all mixing ratios compared to \( \text{H}_2\text{O} \) use the DCT-derived \( Q(\text{H}_2\text{O}) \) as the reference. While we detected \([\text{O I}] 6300 \, \text{Å}\) emission, there
is significant evidence that this emission is actually dominated by contributions from CO₂ and/or CO photodissociation rather than H₂O, so for R2 PanSTARRS, it does not serve as a reliable proxy for H₂O (see Section 3.5).

3.7. Active Areas

We employ our CO₂, H₂O, and CO production rates to calculate the active areas of the cometary surface using the sublimation model of Cowan & A’Hearn (1979); these are given in Table 4. Following arguments given in Bodewits et al. (2014) and McKay et al. (2017, 2018), we adopt the slow rotator model, for which every facet of the nucleus surface is in equilibrium with the solar radiation incident upon it. While the size of the nucleus of R2 PanSTARRS is not known, we convert these active areas to active fractions for a 1 and 10 km radius nucleus, which encompasses the range of most cometary nuclei for which measurements are available, including an upper limit of \( R < 15 \) km determined for R2 PanSTARRS from Wierzchos & Womack (2018).

4. Discussion

4.1. Other Potential Molecular Emissions in Spitzer Imaging

As our CO₂ abundance is dependent on an analysis of broadband imaging, not spectroscopy, it is possible that there are other emission features in our bandpass besides CO₂ and CO, the species commonly assumed to dominate the flux. This would lead to an overestimate of the CO₂ production rate. The leading neutral candidates are OCS and N₂O. Hot bands of water in the 4.5–5.0 \( \mu \)m region would normally be important (Ootsubo et al. 2012), but the extremely low H₂O/CO and H₂O/CO₂ ratios for R2 PanSTARRS mean they can be neglected.

At \( \sim 4.9 \) \( \mu \)m, OCS has a strong band and has been observed in comets at an abundance of approximately 0.1%–0.4% with respect to H₂O (Bockelée-Morvan et al. 2004; Mumma & Charnley 2011; Dello Russo et al. 2016b, and references therein). It is covered by the M2 grating setting in our iSHELL observations (Figure 1) and was not detected, placing an upper limit on its abundance ratio compared to CO of 0.24%. At this level, OCS is not a significant contributor to the 4.5 \( \mu \)m band flux.

The other neutral molecule with strong emission in the 4.5 \( \mu \)m bandpass is N₂O. To date, N₂O has never been detected.
in a comet, despite Infrared Space Observatory and AKARI observations that cover this wavelength range (Crovisier et al. 1997; Ootsubo et al. 2012). As of this writing, we are not aware of any reported detection of N$_2$O by the Rosetta instruments around 67P/Churyumov-Gerasimenko. However, the large N$_2$ abundance and the presence of an intrinsically strong N$_2$O band at $\sim$4.5 $\mu$m could perhaps indicate a strong contribution of this molecule to our Spitzer photometry. The N$_2$O emission is too far to the blue to be covered by our iSHELL observations in the M2 grating, and the region around the N$_2$O emission band is heavily affected by telluric CO$_2$ absorption. Therefore, we cannot definitively rule out the presence of N$_2$O emission in our Spitzer images. The g-factor for the relevant N$_2$O transition is $1.5 \times 10^{-3}$ photons s$^{-1}$ mol$^{-1}$, meaning that an N$_2$O production rate of $\sim 1.8 \times 10^{28}$ mol s$^{-1}$ could account for the residual flux we attribute to CO$_2$. This suggests that even at

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**Figure 10.** Spectral regions around C$_2$ (top), CN (middle), and NH$_2$ (bottom) emission features. The number above the top left corner of each plot (e.g., “1e-15” for C$_2$) denotes the multiplier for the units of the y-axis. Here CN and NH$_2$ are not detected, while there is a candidate feature corresponding to the C$_2$ bandhead. Overplotted are empirical fits to a spectrum of C/2009 P1 (Garradd) at a similar heliocentric distance scaled to the flux levels of the observed R2 PanSTARRS spectra, which serve as 3$\sigma$ upper limits on the observed flux. For C$_2$, the model matches the peak flux of the candidate bandhead at 5165 Å. Although we interpret this as a tentative detection of C$_2$, for this work, we are employing C$_2$ as a constraint on the C$_2$H$_2$ abundance, so even a detection of C$_2$ only provides an upper limit on C$_2$H$_2$ due to multiple sources of the C$_2$ molecule in comets. These upper limits then provide us with an upper limit on the production rate.
Notes.

a iSHELL-derived CO production rate.

b SMT-derived CO production rate.

\(\sim 1.8 \times 10^{-27} \text{ mol s}^{-1}\). \(\text{N}_2\text{O}\) could account for 10% of the flux we attribute to \(\text{CO}_2\). However, \(\text{N}_2\text{O}\) is also very efficient at releasing \(\text{O}^+\text{(S)}\) into the coma (Huebner et al. 1992), and at these high production rates, we may expect it to dominate the \(\text{O}1\) photochemistry and drive the oxygen line ratio to be \(\sim 1\).

However, we measure an oxygen line ratio of 0.20 (Section 3.5), suggesting that \(\text{N}_2\text{O}\) is not a dominant source of \(\text{O}1\) in the coma. While \(\text{O}1\) photochemistry in comets is not well understood, this, combined with a lack of previous detections in comets, likely implies that \(\text{N}_2\text{O}\) is not contributing much more than 10% to the residual flux we attribute to \(\text{CO}_2\).

Lastly, the \(\Delta v = \sim 0\) band of \(\text{CO}^+\) is located at \(\sim 4.6 \mu\text{m}\). We do indeed observe a faint tail feature with structures reminiscent of an ion tail in both \textit{Spitzer} epochs (Figure 5). We attribute this to the \(\text{CO}^+\) band based on the large \(\text{CO}\) production rate and the strong \(\text{CO}^+\) tails observed in the optical for R2 PanSTARRS. However, this tail is much fainter than the neutral emission and only appears obvious in Figure 5 due to the image enhancement process. Additionally, this band is covered by our iSHELL observations, yet it is not detected. Therefore, we conclude that \(\text{CO}^+\) cannot account for the observed excess emission that we attribute to \(\text{CO}_2\). While we cannot unequivocally rule out \(\text{N}_2\text{O}\) emission, we conclude that our \textit{Spitzer} 4.5 \(\mu\text{m}\) band imaging is most likely dominated by a combination of \(\text{CO}_2\) and \(\text{CO}\) emission. After accounting for the expected \(\text{CO}\) contribution based on independent observations with other facilities, we think that our analysis provides an accurate measure of the \(\text{CO}_2\) abundance in R2 PanSTARRS.

### 4.2. Comparison to Other Observations of R2 PanSTARRS

Our \(\text{N}_2/\text{CO}\) ratio agrees well with the measurements made by Cochran & McKay (2018) in 2017 December, almost 2 months before our observations, as well as measurements by Biver et al. (2018) made about a week before our observations and Opitom et al. (2019) about 2 weeks after our observations. This suggests that there was little evolution in the \(\text{N}_2/\text{CO}\) ratio over the 2017 December–2018 February time frame.

Our iSHELL CO production rate agrees well with values determined by de Val-Borro et al. (2018) and Biver et al. (2018), whose observations were 1–2 weeks before ours (although these works used an asymmetric outgassing model, while we assume symmetric outflow). Our value is higher than that found by Wierzchos & Womack (2018) using the SMT in 2017 late December and 2018 mid-January, as well as the value we measure from our SMT observations. This could be due to a different FOV or the narrow nature of our slit. There is evidence from the millimeter observations of Biver et al. (2018) and Wierzchos & Womack (2018) that there is a significant sunward outgassing component, an enhancement also observed in our \textit{Spitzer} imaging (see Figure 5). As the iSHELL slit was oriented along the Sun–comet line, we may have sampled this enhancement, which, coupled with our application of a symmetric outgassing model, may result in an overestimate of the CO production rate, but we do not observe a strong asymmetry in the CO line profile (see Section 3.1, Figure 3), meaning that the iSHELL observations were not sensitive to the asymmetry inferred from the millimeter and \textit{Spitzer} observations. One reason for this discrepancy could be the limited spatial coverage of the iSHELL slit (slit width 0″75 × length \(\sim 6\)″) compared to the much larger circular beams in the submillimeter (10″–30″) and the arcminute spatial scale covered by the \textit{Spitzer} imaging. A narrow feature that is only slightly offset from the solar direction could be missed by the narrow iSHELL slit while still revealing an asymmetry that would be evident only on larger spatial scales. There is evidence from the coma morphology in the \textit{Spitzer} images that the asymmetry manifests as a large fan-shaped feature (Figure 5, fourth column), perhaps implying that the asymmetry would not be as pronounced in the inner coma sampled by iSHELL.

In analyzing our iSHELL spectra, we adopt the gas expansion velocity \(v_{\text{exp}}\) measured by SMT (0.52 km s\(^{-1}\)), but as the iSHELL slit samples the very inner coma, it is possible that the gas may not have been fully accelerated to the speed observed at larger nucleocentric distances. An \(\sim 30\%\) smaller assumed \(v_{\text{exp}}\) (i.e., from 0.52 to 0.35–0.40 km s\(^{-1}\)) would bring the iSHELL and SMT results for \(Q_{\text{CO}}\) into agreement within their respective 1σ uncertainties. As the resolving power of our iSHELL spectra (\(\lambda/\Delta\lambda \sim 4 \times 10^4\)) is insufficient to resolve the cometary lines, we obtain no information regarding \(v_{\text{exp}}\); therefore, we cannot confirm or refute the possibility of a lower expansion velocity in the inner coma. However, the rotational temperature we measured for \(\text{CH}_3\text{OH}\) from IRAM of 23 K (Biver et al. 2018) is significantly lower than that obtained for \(\text{CH}_3\text{OH}\) from IRAM of 23 K (Biver et al. 2018). This discrepancy may be due to photolytic heating of the coma as the gas expands. Based on this result, we might expect a smaller expansion velocity to be more relevant to the iSHELL observations, since the terminal region spanned lines of sight offset only \(\sim 1″–5″\) from the nucleus, in contrast to the much larger SMT/IRAM beam sizes (\(\sim 10″–30″\)). In any case, while absolute production rates are proportional to \(v_{\text{exp}}\) (assuming the beam size is small compared to the photodissociation scale length, which is the case for all species reported here), relative abundances (i.e., mixing ratios) are relatively insensitive to the adopted value of \(v_{\text{exp}}\) as long as a common \(v_{\text{exp}}\) is assumed for all species, which is the case in this work. Therefore, we would
expect negligible changes in abundance ratios for the other species included in the M2 and Lp1 settings (e.g., Table 3).

The different rotational temperature measured from our isHHELL observations versus the IRAM observations of Biver et al. (2018) and adopted for our SMT analysis could affect our results. For the isHHELL observations, adopting \( T_{\text{rot}} = 23 \) K results in an \(~\sim\)10% higher CO production rate, while adopting \( T_{\text{rot}} = 13 \) K for the SMT observations results in a CO production rate \(~\sim\)30% higher than the value for \( T_{\text{rot}} = 23 \) K. Adopting the higher \( T_{\text{rot}} \) for the isHHELL data results in an \(~\sim\)70% larger CH4 production rate, 15%–20% less sensitive upper limits on \( \text{CH}_2\text{OH} \) and \( \text{C}_2\text{H}_6 \), and a 10% more sensitive upper limit on OCS. In terms of mixing ratios compared to CO, the \( \text{CH}_4/\text{CO} \) ratio is most affected, having a value 50% higher for \( T_{\text{rot}} = 23 \) K than for \( T_{\text{rot}} = 13 \) K. The upper limits on \( \text{C}_2\text{H}_4/\text{CO} \) and \( \text{CH}_3\text{OH}/\text{CO} \) change minimally (\(~\sim\)5%) for the different values of \( T_{\text{rot}} \), while the upper limits on \( \text{H}_2\text{CO}/\text{CO} \) and OCS/CO are approximately 20% more sensitive for \( T_{\text{rot}} = 23 \) K. Analysis for the other instruments does not depend on \( T_{\text{rot}} \), though the slightly higher CO production rates determined from both isHHELL and SMT data using the alternate rotational temperature would result in proportionately lower values of the mixing ratios compared to CO.

Our upper limit for \( \text{CH}_3\text{OH} \) is a factor of 3 lower than the detection by Biver et al. (2018); this is independent of the value of \( T_{\text{rot}} \), as are all of the comparisons in this paragraph), which could be due to temporal and/or spatial variability in \( \text{CH}_3\text{OH} \) outgassing. The different projected areas observed for the IRAM and isHHELL observations could account for this discrepancy if a fraction of \( \text{CH}_3\text{OH} \) is released from icy grains in the coma. At the same time, our \( \text{H}_2\text{CO} \) upper limit is consistent with the detection of Biver et al. (2018). Our HCN upper limit (inferred from CN) is consistent with both the upper limit found by Wierzchos & Womack (2018) and the detection reported by Biver et al. (2018). Our \( \text{H}_2\text{O} \) production rate inferred from the OH DCT data is consistent with the upper limits reported by Biver et al. (2018) from observations of the OH 18 cm line at Nancay and by Opitom et al. (2019) using narrowband photometry from the TRAPPIST telescope.

At the time of this writing, our results are the first reported detections or upper limits on \( \text{CO}_2, \text{CH}_4, \text{C}_2\text{H}_6, \text{C}_2\text{H}_2, \text{OCS}, \) and \( \text{NH}_3 \) in R2 PanSTARRS. While Opitom et al. (2019) reported a lower limit on the \( N_{\text{2}}/N_{\text{H}} \) ratio (a proxy for \( N_{\text{2}}/N_{\text{H}} \)), this is a lower limit on the column density ratio in the slit, and because of the different spatial distributions of ions and neutrals, interpreting the column density ratio as an actual abundance ratio is complicated. Assuming \( N_{\text{2}}/\text{CO}^+ = N_{\text{2}}/\text{CO} \), we have used our neutral CO measurements to convert the \( N_{\text{2}}/\text{CO}^+ \) to an equivalent \( N_{\text{2}}/\text{CO} \) production rate, which can then be compared to the production rates derived for other neutrals such as \( \text{NH}_3 \) and HCN, as was also done by Wierzchos & Womack (2018). With those caveats aside, the lower limit on \( N_{\text{2}}/N_{\text{H}} \) provided by Opitom et al. (2019) is consistent with our constraints.

Opitom et al. (2019) also detected \( \text{CO}_2 \) emission and derived a \( \text{CO}_2/\text{CO}^+ \) ratio of 1.1 ± 0.3. They did not interpret this as the \( \text{CO}_2/\text{CO}^+ \) ratio, as \( \text{CO}_2 \) can also contribute to observed \( \text{CO}^+ \) emission. For this reason, Opitom et al. (2019) also expressed caution when interpreting the \( N_{\text{2}}/\text{CO}^+ \) ratio as a direct measurement of \( N_{\text{2}}/\text{CO} \), as \( \text{CO}_2 \) photodissociation could contribute to the observed \( \text{CO}^+ \) emission, and therefore the measured \( N_{\text{2}}/\text{CO}^+ \) ratio actually only provides a lower limit on \( N_{\text{2}}/\text{CO} \). However, from our Spitzer observations of neutral \( \text{CO}_2 \), we derive \( \text{CO}_2/\text{CO} \sim 18\% \), and at this low abundance, \( \text{CO} \) photodissociation should be the dominant source of \( \text{CO}^+ \) ions (Huebner et al. 1992). This appears to disagree with the large \( \text{CO}_2^+/\text{CO}^+ \) ratio observed by Opitom et al. (2019). The reason for the discrepancy between ion and neutral observations is unknown but may be related to our understanding of \( \text{CO}_2 \) and \( \text{CO} \) photochemistry.

The \( \text{Af}_\rho \) value we find for R2 PanSTARRS from our DCT BC imaging is lower than other measurements by Opitom et al. (2019), as well as from the cometary database developed by T. Noel13 quoted by Biver et al. (2018). There is some evidence for temporal variability in the observations of Opitom et al. (2019), so that may explain some of the discrepancy. Variable gas contamination by strong \( \text{CO}^+ \) emission could also be present, especially for the broadband photometry quoted by Biver et al. (2018). The \( \text{Af}_\rho \) value derived from our Spitzer imaging is higher than all values reported in the optical, including our DCT observations, which were contemporaneous with the Spitzer epoch on UT February 21. However, the different wavelength regimes for the IR and optical data make it unclear how comparable the \( \text{Af}_\rho \) values actually are. For the Spitzer data, we employed a larger photometric aperture than the optical studies (28,000 km versus 10,000 km); using a smaller aperture in line with other studies yields \( \text{Af}_\rho \sim 1000 \) cm, larger than what is found for the original aperture. While \( \text{Af}_\rho \) is independent of aperture size for ideal comae, the presence of a dust tail and acceleration of the dust can account for the decreasing trend with aperture size we observe for \( \text{Af}_\rho \). Spectral reddening of light scattered by comae can vary with wavelength, especially over such a large spectral range (Jewitt & Meech 1986). Nevertheless, we calculate the effective BC (0.45 \( \mu \)m) to 3.6 \( \mu \)m spectral slope as \(~\sim\)1.8% per 100 nm, similar to other comets observed in the NIR by Jewitt & Meech (1986).

4.3. Comparison to Other Comets

In this section, we compare R2 PanSTARRS to other comets. We first compare to the cometary population as a whole, then specifically to other comets observed at similar heliocentric distances.

4.3.1. Cometary Population

Table 5 summarizes the derived production rates (or upper limits) for R2 PanSTARRS, along with mixing ratios relative to \( \text{H}_2\text{O} \) and \( \text{CO} \), for 12 species. For comparison, the average values of these mixing ratios for the sample of Oort Cloud comets observed to date are also presented. Most values for R2 PanSTARRS are from this work, though for \( \text{CH}_3\text{OH} \), HCN, and \( \text{H}_2\text{CO} \), our observations only provide upper limits, while Biver et al. (2018) secured detections, so in Table 5, we present the detected production rates for these species from Biver et al. (2018).

All detected species in R2 PanSTARRS are heavily enriched compared to \( \text{H}_2\text{O} \). Here \( \text{CO} \) is enriched by 4 orders of magnitude, with \( \text{N}_2 \) enriched by a similar amount (though the small sample size of \( \text{N}_2 \) measurements in comets makes this difficult to quantify), while \( \text{CH}_4, \text{CH}_3\text{OH}, \) and \( \text{CO}_2 \) are enriched by a factor of \(~\sim\)160–200. The \( \text{H}_2\text{CO} \) and HCN have

13 http://www.lesia.obspm.fr/comets/
Table 5

| Instrument | Species | $Q$ (10^19 mol s^(-1)) | Mean $X$/H$_2$O (%) | X/H$_2$O (%) | X/CO (%) | Mean X/CO (%) |
|------------|---------|------------------------|----------------------|-------------|-----------|---------------|
| Spitzer    | CO$_2$  | 10.0 ± 1.0             | 3230 ± 380           | 17.0 ± 6.0  | 18.2 ± 3.5 | 425 ± 178     |
| IRTF iSHELL| CO      | 95.4 ± 9.1             | (3.08 ± 0.35) × 10^4 | 4.0 ± 0.9   | ...       | ...           |
|            | CH$_4$  | 0.56 ± 0.07            | 181 ± 25             | 0.88 ± 0.10 | 0.59 ± 0.09 | 22.0 ± 5.5    |
|            | C$_2$H$_6$ | <0.085            | <27                  | 0.63 ± 0.10 | <0.089    | 15.8 ± 4.4    |
|            | OCS     | <0.23                 | <74                  | ~0.25       | <0.24     | ~6.3          |
| APO ARCES  | N$_2$   | 4.8 ± 1.1             | 1550 ± 370           | <17^d       | 5.0 ± 1.0  | <17^d         |
|            | NH$_3$  | <0.01                | <3.2                 | 0.91 ± 0.30 | <0.010    | 22.8 ± 9.1    |
|            | C$_2$H$_4$ | <0.021            | <6.8                 | 0.16 ± 0.03 | <0.022    | 4.0 ± 1.2     |
| DCT LMI    | H$_2$O  | 0.31 ± 0.02           | ...                 | ...         | 0.32 ± 0.04 | 2500 ± 560    |
| IRAM       | CH$_3$OH| 1.12 ± 0.07           | 360 ± 32             | 2.21 ± 0.24 | 1.04 ± 0.08 | 55.3 ± 13.8   |
|            | H$_2$CO | 0.045 ± 0.007         | 14.5 ± 2.4           | 0.33 ± 0.08 | 0.043 ± 0.006 | 8.0 ± 2.6    |
|            | HCN     | (4.0 ± 1.0) × 10^3    | 1.3 ± 0.3            | 0.22 ± 0.03 | (3.8 ± 1.0) × 10^3 | 5.5 ± 1.4 |

Notes:

a Mean mixing ratio compared to H$_2$O in the sample of Oort Cloud comets observed to date. The uncertainties reflect the standard deviation in measured values. All values except for N$_2$ and CO$_2$ are from Dello Russo et al. (2016a). The CO$_2$ value is from Otsu et al. (2012).

b Mean mixing ratio compared to CO in the sample of Oort Cloud comets observed to date. The uncertainties reflect the standard deviation in measured values. References for abundances are the same as for H$_2$O detailed in footnote a.

c Derived by multiplying the derived N$_2$/CO ratio from our ARCES observations by the CO production rate determined from our iSHELL observations.

d Due to the lack of observations of N$_2$ in comets, the mean mixing ratios compared to H$_2$O and CO are not meaningful to calculate. Therefore, the number included is based on past observations discussed in Cochran & McKay (2018) and has a very large uncertainty (indicated by “?”).

e Derived from our NH$_3$ upper limit assuming all NH$_3$ is released via NH$_3$ photodissociation (i.e., $Q_{NH3} = Q_{NH3}$).

f Derived from our C$_2$ upper limit assuming all C$_2$ is released via C$_2$ photodissociation (i.e., $Q_{C2} = Q_{C2H}$).

g Derived from our OH narrowband observations.

h Production rates from Biver et al. (2018). Mixing ratios compared to CO are taken directly from Biver et al. (2018), and mixing ratios for H$_2$O are calculated using our derived H$_2$O production rate.

less drastic enrichments of ∼40 and 6, respectively, though these are still extraordinary enhancements never before observed in a comet. We cannot draw any conclusions regarding the abundances of C$_2$H$_6$, NH$_3$, C$_2$H$_2$, or OCS compared to H$_2$O, though our results imply that while they could be heavily enriched compared to H$_2$O, this enrichment is not as drastic as that inferred for species such as CO and may be more in line with that observed for species such as H$_2$CO or HCN.

While a definitive comparison to H$_2$O is not possible for all species, the strong CO detection allows a comparison of all species to CO. We find that all species searched for are heavily depleted compared to CO, except for N$_2$, which is enhanced. Even for species that are not detected, the upper limits are sensitive enough to demonstrate heavy depletions. All depleted species are underabundant by at least 1–3 orders of magnitude compared to other comets.

A glimpse into a rarely observed (alternative) compositional taxonomy has been provided by R2 PanSTARRS, with CO replacing H$_2$O as the dominant gas in the coma. The measured abundance ratio CH$_4$/CO (∼0.6%; Table 3) approaches the mean CH$_4$/H$_2$O and C$_2$H$_6$/H$_2$O ratios among comets from the Oort Cloud (Bockelée-Morvan et al. 2004; Dello Russo et al. 2016b). In contrast, C$_2$H$_6$ is strongly depleted (by a factor of at least 6.6 relative to CH$_4$), with C$_2$H$_6$/CO riving or surpassing the level of depletion of C$_2$H$_6$ (relative to H$_2$O) measured for disrupted comet C/1999 S4 (LINEAR), a current “end member” in terms of its severe depletion in all reported volatiles with the exception of HCN (Mumma et al. 2001). Another peculiarity of R2 PanSTARRS is the large N$_2$ abundance, with N$_2$ being the dominant reservoir of volatile nitrogen, more abundant than even H$_2$O (only CO$_2$ and CO are more abundant than N$_2$). Typically, NH$_3$ and, to a lesser extent, HCN are the most abundant nitrogen-bearing volatiles in comets. However, in R2 PanSTARRS, NH$_3$/N$_2$ < 0.21% and HCN/N$_2$ = 0.08 ± 0.03%. So unless another, more complicated form of volatile nitrogen that is not constrained by our observations (e.g., N$_2$O, C$_2$N$_2$, CH$_3$CN) is present at significant levels, more than 99% of the volatile nitrogen in R2 PanSTARRS is contained in N$_2$. There are not many measurements of the NH$_3$/N$_2$ value in comets; however, this limit for R2 PanSTARRS is much lower than that measured for comet Halley (∼1000%) and closer to the derived values for several dense molecular clouds in star-forming regions (∼0.6%; Womack et al. 1992). The very low derived relative abundance of NH$_3$/N$_2$ is consistent with the suggestion by Wierzchos & Womack (2018) that R2 PanSTARRS formed in an environment with decreased photodissociation of N$_2$, leading to preserving or shielding of N$_2$ and inhibited production pathways of hydrogen-rich species, such as HCN and NH$_3$ (Hily-Blant et al. 2017).

We show additional mixing ratios compared to CO$_2$, CH$_4$, CH$_3$OH, H$_2$CO, and HCN in Table 6, with the mean ratio observed among comets listed in parentheses. A subset of this compilation is shown visually as histograms in Figure 11. For mixing ratios compared to CO$_2$, we employ the average CO$_2$/H$_2$O ratio in the AKARI sample (Otsu et al. 2012), while other species like CH$_3$OH have their average abundance compared to H$_2$O derived from ground-based IR studies (Dello Russo et al. 2016b). This means that CO$_2$ and the other species were not observed contemporaneously, and, in most cases, the sample of AKARI and ground-based IR observations sampled different comets. This means that interpretation of the average CO$_2$ abundance in Table 6 is limited by the degree to which the
AKARI and ground-based IR studies provide a random sample of the cometary population.

Almost all mixing ratios in R2 PanSTARRS deviate from typical values by at least a factor of 3, although for some species that were not detected, we do not have sufficient sensitivity to rule out a normal abundance (e.g., C₂H₆/HCN). The HCN is universally depleted by at least an order of magnitude compared to all detected species except H₂O. Interestingly, CH₃OH/CO₂ and CH₃OH/CH₄ are the only mixing ratios that are similar (within a factor of 2) to the average values observed among comets. Perhaps this commonality between the peculiar R2 PanSTARRS and other comets can shed light on its origin. In any case, the almost universal peculiarity of the observed abundances in R2 PanSTARRS compared to other comets implies that this is not a case of one or two species being anomalous (e.g., CO being heavily enriched and H₂O being heavily depleted), but rather a complete composition fundamentally different from the ensemble of comets observed to date.

This strong deviation from a “typical” cometary composition is also illustrated in Figure 12. Over 80% of the volatile composition of R2 PanSTARRS is CO, while H₂O is relegated to the status of a trace volatile. Also, N₂ is much more abundant than in typical comets and more abundant than the other typical trace species (i.e., other than CO, H₂O, and CO₂) combined. As a fraction of the volatile inventory of R2 PanSTARRS, CO₂ is actually fairly close to typical comets.

The Afₚ of R2 PanSTARRS is much lower than that of other comets with such high gas production observed at similar heliocentric distances, though concluding whether R2 PanSTARRS is dust- or gas-rich depends on which volatile is used as the reference. The value of log[Afₚ/Q(H₂O)] determined for R2 PanSTARRS is larger by a factor of 5–10 than most comets observed at Rₚ₁₉ > 3 au in the survey by A’Hearn et al. (1995), meaning that when H₂O is the comparison gas, R2 PanSTARRS is considered quite dusty. However, log[Afₚ/Q(CO₂)] is at the low end of comets observed with Spitzer and NEOWISE (Bauer et al. 2015; M. S. P. Kelley et al. 2019, in preparation) and approximately a factor of 10 lower than any Oort Cloud comet in those samples. So compared to CO₂, R2 PanSTARRS is considered a gas-rich comet. While no systematic study comparing Afₚ to CO has been done, the extremely high CO production rate suggests that if CO is the reference gas, R2 PanSTARRS is incredibly gas-rich, possibly the most gas-rich comet ever observed. Even in terms of the total gas production (typically dominated by H₂O but dominated by CO in the case of R2 PanSTARRS) compared to Afₚ, R2 PanSTARRS is very gas-rich.

### 4.3.2. Comets at Large Heliocentric Distance

A caveat to consider when interpreting observations of R2 PanSTARRS is the fairly large heliocentric distance of the observations, ∼2.8 au. We compare to other comets observed at large heliocentric distances (approaching or beyond 3 au) in Table 7. While these comets do show depletions compared to CO, R2 PanSTARRS shows heavier depletions by at least a factor of 2 for all species reported in Table 7. No comet in Table 7 shows an H₂O/CO ratio <20%, a limit 2 orders of magnitude higher than the observed value in R2 PanSTARRS, and most have H₂O/CO ≥ 100%. It should also be noted that there is a tendency for comets observed at large heliocentric distances to be highly active, which is potentially attributed to being CO-rich. Therefore, the general overabundance of CO compared to other volatiles for comets observed at large heliocentric distances could simply be due to this observational bias. Showing the most similarities with R2 PanSTARRS is 29P/Schwassman-Wachmann 1, with an H₂O/CO ratio of ∼20%, low abundances of CH₄ and C₂H₆ compared to CO, and a reported N₂/CO ratio of ∼1% (Ivanova et al. 2016). However, at 6.2 au, the CO sublimation rate is expected to be ∼10,000 times faster than the H₂O sublimation rate (Cowan & A’Hearn 1979), so accounting for this sublimation effect implies that the intrinsic H₂O/CO ratio in the nucleus of 29P may be more in line with that typically observed in comets (H₂O/CO > 300%; Womack et al. 2017). The upper limits on species such as CH₄/CO and HCN/CO are not sensitive enough to show whether 29P is similar to R2 PanSTARRS, as these upper limits are at least 1 order of magnitude larger than the observed abundances in R2 PanSTARRS.

Probably the best-studied comet at large heliocentric distances is 67P/Churyumov-Gerasimenko, for which in situ measurements with the OSIRIS mass spectrometer on board Rosetta are available (Le Roy et al. 2015; Rubin et al. 2015a). Values for the winter and summer hemispheres at 3.14 au perihelion are presented in Table 7. Similar to the other comets in Table 7, both hemispheres exhibit abundances different from R2 PanSTARRS by at least a factor of 3, with H₂O, CO₂, HCN, and C₂H₆ exhibiting the most striking differences. The N₂/CO ratio for 67P is approximately a factor of 10 smaller than the value for R2 PanSTARRS (Rubin et al. 2015a), which, combined with the CO/H₂O ratios given in Table 7, implies an N₂/H₂O ratio for R2 PanSTARRS 4–5 orders of magnitude larger than that for 67P.

Moderate enhancements in CO compared to H₂O are expected based on the sublimation model of Cowan & A’Hearn (1979), which predicts that the different volatilities of CO and H₂O can account for a factor of 2 at a heliocentric distance of 2.8 au, similar to the enhancement observed in other comets near 3 au but not the factor of ∼10,000 observed for R2
PanSTARRS. Therefore, the anomalous mixing ratios cannot be ascribed to the heliocentric distance alone and must reflect the intrinsic composition of the nucleus.

4.4. Active Fractions

Our derived active areas and fractions for H$_2$O, CO$_2$, and CO are given in Table 4. While the nucleus size of R2 PanSTARRS is not known, the very large active area required for CO would require the nucleus to be quite large (>5 km) for all the CO to come from surface sublimation. There is also the possibility of an extended source of CO, which adds additional available surface area for CO to sublimate from. However, our Spitzer data (which are sensitive to both CO and CO$_2$, as discussed earlier) do not show evidence for increasing production rate with photometric aperture size, as would be expected for an extended source (Combi et al. 2013; Bodewits et al. 2014; McKay et al. 2015), arguing against an extended source larger than ~10,000 km in radius (corresponding to ~5 pixels in our Spitzer images, the smallest photometric aperture for which reliable photometry can be performed) for these molecules. We cannot definitively rule out the possibility of an extended source of smaller spatial extent than our Spitzer photometric apertures, though our modeling of the CO spatial profile in our iSHELL observations using only optical depth effects (see Section 3.1) provides some evidence against a smaller extended source.

The derived H$_2$O active fraction is consistent with other comets if the nucleus is fairly small (<3 km), but this would contradict the large active area needed to explain the CO production. For a large nucleus (>10 km), this would imply a very low active fraction for H$_2$O sublimation, much lower than other comets (Sosa & Fernández 2011; Lis et al. 2019). This is additional evidence that the low water production is not simply an artifact of the large heliocentric distance of R2 PanSTARRS at the time of observation but rather is part of the inherent composition of this comet.

4.5. Implications

Compared to other comets observed to date, R2 PanSTARRS has an extremely anomalous composition. In the previous sections, we have demonstrated that the large heliocentric distance can only explain a small portion of the observed composition. Additionally, the depletion of highly volatile species like CO$_2$ and CH$_4$ compared to CO cannot be explained by the heliocentric distance either. Therefore, the observed anomalous abundances are not solely a consequence of the heliocentric distance. It is not likely due to thermal evolution from repeated solar passages, as this would work to deplete the most volatile species, like CO, N$_2$, CH$_4$, and CO$_2$, not enhance them as observed. Therefore, the composition of R2 PanSTARRS likely reflects its composition when it was formed.

The most primitive molecular forms of carbon and nitrogen in the universe are CO and N$_2$, respectively. They are often the starting point of chemical pathways that result in the formation of more complex molecules, such as CH$_3$OH, NH$_3$, and HCN.
Therefore, the large abundance of CO and N$_2$ in R2 PanSTARRS compared to these more complex molecules suggests that the region of the disk where R2 PanSTARRS formed was chemically inactive and shielded from photodestruction, leaving the volatile carbon and nitrogen in their simplest forms. Both CO and N$_2$ are also extremely volatile, as are CH$_4$ and CO$_2$. The presence of these molecules suggests that R2 PanSTARRS must have formed in the farthest reaches of the protosolar disk in order to retain these hypervolatiles. The presence of these hypervolatiles also suggests little depletion of these ices from repeated solar passages, despite R2 PanSTARRS likely not being dynamically new and therefore having likely experienced at least several passages through the planetary region. (A dynamical analysis by Opitom et al. 2019 found that 100% of their 1000 R2 clones experienced at least three perihelion passages of less than 3 au.) Wierzchos & Womack (2018) proposed that the CO, N$_2$, and HCN relative abundances in the coma may be explained by the comet forming in an environment of $\sim$50 K (though other models suggest that N$_2$ requires colder temperatures, around 20 K, to condense out of the gas phase; Drozdovskaya et al. 2016) with significant shielding for N$_2$. Our observations showing very high N$_2$ with very low NH$_3$ abundances may provide additional support for this model, and thus the comet may more closely resemble the composition of the nitrogen-bearing volatiles of dense molecular clouds (Womack et al. 1992) and young stellar objects (Gibb et al. 2004). The large abundance of CO and CO$_2$ in R2 PanSTARRS is typical of interstellar apolar ice mantles, and high N$_2$ abundances are also expected in these ice mantles (Gibb et al. 2004). However, interstellar ice grains also have an abundant polar component that has a large water ice abundance, resulting in H$_2$O ice being the dominant component of interstellar medium (ISM) ice grains (Gibb et al. 2004), unlike what we observe for R2 PanSTARRS.

Of the observed species, our measurements suggest that the dominant carbon-bearing molecules are CO and CO$_2$, while the dominant nitrogen-bearing molecule is N$_2$. While CO and CO$_2$ are the main reservoirs of volatile carbon in comets, NH$_3$ and, to a lesser extent, HCN are typically the dominant reservoirs of volatile nitrogen in comets. Assuming that CO and CO$_2$ contain the majority of the volatile carbon and N$_2$ the volatile nitrogen in R2 PanSTARRS implies a C/N ratio of $\sim$1, while most comets, for which NH$_3$ is the main volatile nitrogen carrier, have a higher C/N ratio of $\sim$20. The solar value for C/N is $\sim$3.4 (Lodders 2010), so while R2 PanSTARRS has a C/N ratio closer to solar than most comets observed to date, its coma is still deficient in nitrogen compared to the Sun.

Our results show that most of the volatile oxygen in R2 PanSTARRS is locked in CO and CO$_2$, not H$_2$O, as is typically the case. This may suggest that R2 PanSTARRS formed in a region of the protosolar nebula where the C/O ratio is $>1$, as chemical models predict that when carbon is more abundant than oxygen in the gas phase, most oxygen will be locked into CO and CO$_2$, leaving little to form H$_2$O. However, there is also evidence from both comets and protosolar disk models that most of the water in the solar system was inherited from the presolar cloud rather than formed in the protosolar disk (Cleeves et al. 2014; Altwegg et al. 2017). If accurate, then the lack of H$_2$O in R2 PanSTARRS could reveal details of how inherited H$_2$O was distributed throughout the protosolar disk, i.e., whether H$_2$O was distributed heterogeneously throughout the disk. Another possible reservoir for volatile oxygen is O$_2$, which was detected with a surprisingly large abundance by the Rosetta spacecraft at comet 67P/Churyumov-Gerasimenko (Bieler et al. 2015; Keeney et al. 2017) and also in archival data from the Giotto spacecraft at 1P/Halley (Rubin et al. 2015b). It is extremely difficult to detect O$_2$ remotely, and none of our observations are sensitive to O$_2$, so we cannot rule out the presence of a large amount of O$_2$ in R2 PanSTARRS. Production of O$_2$ at 67P was found to correlate well with H$_2$O production (Bieler et al. 2015; Fougere et al. 2016), and because of this, some theories for the origin of O$_2$ in comets invoke a strong tie to H$_2$O through either radiolysis or trapping in clathrates (e.g., Mousis et al. 2016; Dulieu et al. 2017; Laufer et al. 2017). Given the very low H$_2$O abundance in R2 PanSTARRS, this would suggest that the O$_2$ abundance should also be very low. However, given the very peculiar chemistry
of R2 PanSTARRS and our limited understanding of O2 incorporation into cometary nuclei, we do not consider this argument definitive proof against a substantial O2 abundance in R2 PanSTARRS.

All of these implications only apply to the volatile component of R2 PanSTARRS. There are no constraints on the composition of the refractory component (i.e., dust), so we cannot make any conclusions about atomic abundances in the bulk (i.e., dust and ice) composition of R2 PanSTARRS.

Biver et al. (2018) suggested that R2 PanSTARRS may be a fragment of a differentiated Kuiper Belt body in order to explain the large observed hypervolatile abundances. The relative abundances of CO, CH4, and N2 we observe for R2 PanSTARRS do not match the surface spectra of Pluto (Protopapa et al. 2008), though the relationship between the surface composition and the interior of large Kuiper Belt objects (KBOs) like Pluto is unclear. A detailed analysis of the dynamics of creating collisional fragments in the Kuiper Belt after differentiation and then dynamically transporting these fragments to the Oort Cloud (as well as the expected volatile composition of such fragments) must be further investigated.

Such an anomalous composition brings up the possibility that R2 PanSTARRS has an interstellar origin. While the current orbit of R2 PanSTARRS does not suggest an interstellar origin, R2 PanSTARRS could be a comet captured from another Oort Cloud in the Sun’s birth cluster (or a more distant planetary system, though this is less likely) during the solar system’s earliest stages. Interstellar origins have also been suggested for other comets with peculiar compositions, such as 96P/Machholz (Schleicher 2008) and C/1988 Y1 (Yanaka; Fink 1992). It has been shown that there could have been an exchange of comets between Oort Clouds in the Sun’s birth cluster (Levison et al. 2010). However, it is not clear whether these comets would be expected to be significantly different compositionally from “solar” comets, as both they and their host stars would have formed from the same nebular gas.

5. Conclusion

We present IR-, optical-, and millimeter-wavelength observations of comet C/2016 R2 (PanSTARRS) and show that it has a very peculiar composition compared to typical comets, with strong enhancements in species such as CO and N2 and strong depletions in species such as H2O and HCN, as revealed by previous studies. We determined through observations of a suite of 12 species that the anomalous composition of R2 PanSTARRS is not reserved for one or two species but exhibits strong deviations from typical comets for most species and reference points (i.e., comparing to H2O, CO, CH4, CH3OH, etc.). The lone exceptions are CH4OH/CO2 and CH3OH/CH4, which are considered typical. We also show that the peculiar composition of R2 PanSTARRS is not due solely to the large heliocentric distance at the time of observation and is intrinsic to the comet. What implications R2 PanSTARRS has for our knowledge of the early solar system are still unclear. We suggest some future lines of research that could shed light on this issue.

(1) Dynamical modeling of R2 PanSTARRS. This includes both its recent history, as investigated by Opitom et al. (2019),
and dynamical simulation of the Scattered Disk to evaluate the suggestion of Biver et al. (2018) that R2 PanSTARRS could be a collisional fragment from a differentiated KBO. Models would need to evaluate the likelihood of forming a differentiated KBO, collisionally fragmenting this KBO, then dynamically transporting this fragment to the Oort Cloud.

(2) Chemical modeling of protosolar disks. We believe that if R2 PanSTARRS is not a collisional fragment of a differentiated KBO, it provides a new constraint on the chemical models of protosolar disks. In the early solar system, H2O was likely inherited from the parent molecular cloud (Cleeves et al. 2014). Could this create a depletion mechanism for H2O in certain regions of the protosolar disk where R2 PanSTARRS formed? Is there a region of the protosolar disk where CO and N2 are not efficiently processed into more complex species in order to account for the strong enhancement of these species in R2 PanSTARRS? These are only a couple of the questions that chemical modeling of protoplanetary disks and observations of other protoplanetary disks can help answer.

(3) Continued compositional studies of comets. The comet R2 PanSTARRS is a case in point for the importance of remote-sensing observations to measure the composition of as many comets as possible. It was a not particularly bright comet and was at a large heliocentric distance, meaning that it could have easily been missed by compositional studies. More observations of comets are needed to determine how common comets like R2 PanSTARRS are. As pointed out by Biver et al. (2018), the closest comparisons in the historical literature are C/1908 R1 (Morehouse) and C/1961 R1 (Humason), but neither of these were studied with modern capabilities; therefore, very little is known about their overall composition. With current sky surveys like PanSTARRS and LSST coming on line in the coming years, the prospect for discovering more comets like R2 PanSTARRS grows. The frequency of objects like R2 PanSTARRS will provide meaningful constraints on its history and the formation of our solar system.

We are grateful to the anonymous reviewer for helpful comments that improved the quality of this manuscript. We thank Spitzer, IRTF, Apache Point Observatory, and the Discovery Channel Telescope for granting us DDT or ToO time to conduct the observations described in this paper. We thank Svetlana Jorstad for graciously allowing us to interrupt her program with our DCT ToO observations. These results made use of the Discovery Channel Telescope at Lowell Observatory. Lowell is a private, nonprofit institution dedicated to astrophysical research and public appreciation of astronomy and history and the formation of our solar system.

Postdoctoral Program, administered by the Universities Space Research Association. M.D. acknowledges support through NASA grant 15-S015-2-0028. M.M.K. acknowledges support from NASA Solar System Observations Program grant 80NSSC18K0856. M.W. and K.W. acknowledge support from NSF grant AST-1615917. O.H.P. acknowledges support from the USF Gentsh Family Doctoral Fellowship. B.P.B. acknowledges support from NSF grant AST-1616306. B.P., N.D.R., and R.J.V. acknowledge support from NASA Solar System Observations grant 80NSSC17K0705. N.R. acknowledges support from the NASA Earth and Space Science Fellowship Program (grant NNX16AP49H). A.L.C. acknowledges support from the NASA Solar System Observations Program (NNX17A186G).

Facilities: Spitzer IRAC, NASA IRTF iSHELL, ARC 3.5m, Discovery Channel Telescope, Arizona Radio Observatory (SMT).

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