Examination of Fragment Species in the Comae of Several Comets Using an Integral Field Unit Spectrograph

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Abstract

Spectra of the comae of four comets were obtained with an integral field unit spectrograph on the Harlan J. Smith Telescope at McDonald Observatory. The passband of the spectrograph permitted the observation of C2, C3, CH, CN, and NH2 transitions for these comets. The classical Haser model was used to derive production rates for each observed species. The production rates obtained for the comets were also used to obtain mixing ratios relative to CN. The relative abundances with respect to CN obtained for these comets vary greatly, but are largely consistent with ranges established from prior comet chemistry surveys. The notable exception is 168P/Hergenrother, which the results suggest is extremely depleted in volatiles, even with respect to many other comets designated as volatile depleted in prior surveys. The results for comet Hergenrother add to a small, but growing, body of data suggesting that there may be a subgroup of carbon-chain-depleted Jupiter-family comets that are also depleted in ammonia.

Unified Astronomy Thesaurus concepts: Comets (280); Comae (271); Neutral coma gases (2158); Molecular spectroscopy (2095)

Supporting material: data behind figures

1. Introduction

Comets are widely considered to be important remnants from the time of the formation of the solar system. In particular, comet studies are valuable for learning more about the conditions of the outer solar system during the time of buildup of planetesimals, and for furthering our understanding of the formation of the giant planets. Comet nuclei are currently classified into families based on their orbit dynamical properties, giving indications as to whether they likely spent time in dynamical storage following their dispersion to either the scattered Kuiper disk or the Oort cloud. However, significant uncertainty remains as to the strength of the relationship between comets’ dynamical histories and their chemical properties.

Prior comet chemistry surveys of photolytic daughter species produced in the coma, such as the narrowband photometry study of 85 comets by A’Hearn et al. (1995), the spectroscopic study of 92 comets by Fink (2009), or the spectroscopic survey of 130 comets by Cochran et al. (2012), all reveal that fractions of Jupiter-family comets and Oort Cloud comets are depleted in C2 with respect to the population as a whole. However, this carbon depletion occurs in a higher fraction of the Jupiter-family comets than in the Oort Cloud comets. Reasons for these depletions, as well as the overlap with dynamical families, may include time and rate of formation, as well as location of formation, in the protoplanetary disk (Eistrupp et al. 2019).

In this study, the comae of four comets were observed with an integral field unit (IFU) spectrograph to learn more about their chemical properties. This spectrograph has been used previously to study the coma of comet 103P/Hartley 2 around the time of the EPOXI flyby encounter (Vaughan et al. 2017). The sample analyzed in this paper includes three Jupiter-family comets (10P/Temple 2, 168P/Hergenrother, 260P/McNaught) and one long-period comet (C/2009 P1 Garradd). The spectra were analyzed to look for signatures of C2, C3, CH, CN, and NH2, species with emission features that coincide with the wavelength range covered by the spectrograph. For species with sufficient signal, production rates and mixing ratios were derived to place these comets into broader context chemically. In the following sections, the observation details, the analysis, and the significance of the results are described.

2. Observations

The spectral data were obtained with the George and Cynthia Mitchell Spectrograph (Hill et al. 2008), a high-efficiency, low- to moderate-resolution spectrograph designed for use on the 2.7 m Harlan J. Smith Telescope. The spectrograph consists of 246 optical fibers, each with a diameter of 4′′, arranged in a 1′′ × 1′′ array. The spectrograph setup used for these observations samples the wavelength range from 3600 to 5800 Å with a spectral resolving power (λ/Δλ) of 850. The detector is a Fairchild CCD with 2048 × 2048 pixels used with no binning. We obtained more than one spectrum per night of each comet. This allows a check on the values for the column densities at each position that we measure. We also obtained separate sky observations, flux calibration stars, and solar analog stars. When observing the comets, we held the comet in one position on the array by tracking a star using a fiducial that moves opposite to the cometary motion. This occasionally allows a star to cross through the field of view but does not smear each comet position over more than one fiber. Interloper star spectra were removed during analysis.

To prepare the raw data for analysis, the observed spectral fluxes had to be converted into column density values for each observed species. Upon subtraction of bias and flat-fields, the fiber output alignments were confirmed using master flats. Using these alignments, we extracted a spectrum corresponding to each fiber in the array, yielding 245 individual spectra (one
fiber was broken) at 245 individual positions in the coma. The fibers are fixed in position relative to one another with good metrology, so we know what position in the coma each fiber’s spectrum measures. A HgCd lamp was used as a calibration source to calculate the spectral dispersion for each fiber independently. Standard stars were observed for flux calibration. The atmospheric extinction was removed using mean extinction coefficients for McDonald Observatory. The spectrum of a comet is a mix of molecular emission bands from the gas in the coma superposed on a continuum formed from the reflection of the solar spectrum off the dust in the coma. To remove the continuum, we observed a solar analog star every night and removed its spectrum from each comet spectrum by matching the flux level and color of the solar analog star to the comet observations. These comets were extended and generally filled most or all of the fibers. Thus, to remove any sky spectrum, we observed separate sky fields well-removed from the comet but at comparable airmasses. Any fiber without a star was summed to increase the signal-to-noise ratio of the sky spectrum. The passband of the spectrograph covers the Swan Bands of C2 (d3Π_u^±→a3Π_g) (Phillips & Davis 1968), the Comet Head Group of C3 (A2Π_u–X1Σ_g^+) (Gausset et al. 1965; Merer 1967), the A2Δ_u–X2Π_u band of CH (Jørgensen et al. 1996), the Violet System of CN (B2Σ_g^+–X2Σ_g^−) (Kurucz 1995), and the A^2A_1→X^3B_1 band of NH2 (Cochran & Cochran 2002). The total band flux for each molecular band was measured by fitting a continuum on either side of the band and integrating the bandpass above the continuum. The locations of the bandpasses for each species are provided in one of the spectra obtained for comet 260P/McNaught as shown in Figure 1, and the wavelength ranges of the molecular bands and the continuum regions are provided in Table 1. Note that both of the continuum bands for NH2 are to the blue of the feature because the spectrum ends too soon to put a continuum on the red side. The night sky 5577 Å oxygen line is poorly removed, having an over-under that indicates there is a slight shift between the solar and comet spectra.

Figure 1. Spectrum of 260P/McNaught from 2012 August 23. The upper panel is scaled to the strong CN feature at ~3880 Å. The C3 and C2 features are easy to see in this panel. The lower panel is blown up in the flux axis so that it is possible to see some of the weaker features. NH2 is easily seen as two distinct band manifolds. The CN gDv = −1 band is clearly seen. CH is extremely weak and does not stand out. Under the spectrum is this panel, the bandpasses used for each molecule flux integration are denoted. The thick red line is the bandpass for the feature, while the thinner blue lines represent the bounds of the continuum used for each species, generally one on each side. Wavelength ranges of the molecular bands and continuum regions are provided in Table 1. Note that both of the continuum bands for NH2 are to the blue of the feature because the spectrum ends too soon to put a continuum on the red side. The night sky 5577 Å oxygen line is poorly removed, having an over-under that indicates there is a slight shift between the solar and comet spectra.

Table 1

| Species | Band Wavelengths (Å) | Blueward Continuum (Å) | Redward Continuum (Å) |
|---------|----------------------|------------------------|-----------------------|
| CN      | 3830–3905            | 3715–3770              | 4150–4175             |
| C3      | 3975–4150            | 3715–3770              | 4150–4175             |
| CH      | 4280–4340            | 4150–4175              | 4400–4460             |
| C2 Del v = 0 | 4860–5185 | 4770–4830              | 5220–5270             |
| NH2     | 5665–5760            | 5220–5270              | n/a*                 |

Note. * Two blueward bands were used due to the edge of wavelength coverage of the spectrograph.
The comets were selected for this study because they were sufficiently bright around the time they were relatively close to Earth, and they were easily viewable from McDonald Observatory. Table 2 provides the basic observation details for each of the four comets at their times of observation. The orbit information presented in Table 2 was obtained from the JPL

![Sample reduced spectra from the fibers corresponding to the optocenters of each of the four comets in our sample. Emission from major species, or the positions they are otherwise expected to be seen, are labeled in each spectrum. The tall spikes seen in all four spectra correspond to the violet band of CN.](image)

**Table 2**

| Comet                | Obs. Date (UT) | $r_H$ (au) | $\Delta_b$ (au) | Num. Spectra $\times$ Exposure (s) | Airmass Range | Pre/Post Perihelion |
|----------------------|----------------|------------|-----------------|------------------------------------|---------------|---------------------|
| 10P/Tempel 2         | 2010 Jul 15    | 1.43       | 0.72            | 1 $\times$ 300                     | 1.34–1.95     | Post                |
|                      | 2010 Sep 13    | 1.60       | 0.67            | 2 $\times$ 600                     | 1.51–1.94     | Post                |
|                      |                |            |                 | 3 $\times$ 900                     |               |                     |
| 168P/Hergenrother    | 2012 Oct 6     | 1.42       | 0.44            | 5 $\times$ 1200                    | 1.01–1.06     | Post                |
|                      | 2012 Oct 8     | 1.42       | 0.44            | 14 $\times$ 1200                   | 1.01–1.38     | Post                |
|                      | 2012 Oct 9     | 1.42       | 0.44            | 18 $\times$ 1200                   | 1.01–1.41     | Post                |
| 260P/McNaught        | 2012 Aug 23    | 1.51       | 0.71            | 1 $\times$ 45                      | 1.11–1.83     | Pre                 |
|                      |                |            |                 | 1 $\times$ 600                     |               |                     |
|                      |                |            |                 | 6 $\times$ 1200                    |               |                     |
|                      |                |            |                 | 1 $\times$ 1200                    |               |                     |
|                      |                |            |                 | 4 $\times$ 1800                    |               |                     |
|                      | 2012 Oct 8     | 1.52       | 0.59            | 3 $\times$ 1800                    | 1.13–1.33     | Post                |
|                      |                |            |                 |                                   |               |                     |
|                      | 2012 Oct 9     | 1.52       | 0.59            |                                   |               |                     |
| C/2009 P1 (Garradd)  | 2011 Aug 20    | 2.28       | 1.40            | 1 $\times$ 300                     | 1.03–2.25     | Pre                 |
|                      |                |            |                 | 9 $\times$ 600                     |               |                     |
|                      |                |            |                 | 2 $\times$ 900                     |               |                     |
|                      | 2011 Aug 21    | 2.27       | 1.39            | 13 $\times$ 600                    | 1.03–1.62     | Pre                 |
|                      | 2011 Aug 22    | 2.26       | 1.39            | 9 $\times$ 600                     | 1.03–2.13     | Pre                 |

**Notes.**

$^a$ Heliocentric distance.

$^b$ Distance from the earth.
HORIZONS system. The fiber array also allows all position angles on the sky to be sampled simultaneously for each comet, thus permitting the spatial distributions of the observed species to be visualized. Representative coma maps of CN for each comet are presented in Figure 3.

3. Obtaining Production Rates Using the Haser Model

The observed species are not released from the nucleus, but are likely the photochemical products of one or more native species released from the nucleus. The native and daughter species each have a scale length, a product of their velocity and photochemical lifetime, that dictates their spatial distribution in the coma. The classic Haser model (Haser 1957), which requires parent and daughter species scale lengths as input parameters, was used to model the radial profiles of the line-of-sight column densities derived from the emissions of the

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**Table 3**

Adopted Haser Model Scale Lengths at 1 au (10^4 km)

| Species | Parent | Daughter | Reference                  |
|---------|--------|----------|----------------------------|
| C2      | 2.5    | 12       | Cochran (1985)             |
| C1      | 0.31   | 15       | Cochran (1985)             |
| CH      | 7.8    | 0.48     | Cochran & Cochran (1990)   |
| CN      | 1.7    | 30       | Cochran (1985)             |
| NH2     | 0.41   | 6.2      | Cochran et al. (1992)      |

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Figure 3. Representative maps showing the spatial distribution of CN in the comae of the four comets in the sample: (a) 10P/Tempel 2, (b) 168P/Hergenrother, (c) 260P/McNaught, and (d) C/2009 P1 (Garradd). Lighter colors indicate higher column densities (the column density scale is shown in the vertical bar to the immediate right of each map in log(cm⁻²)). The crosses in each figure correspond to the nucleus locations and are the positions at which the spectra presented in Figure 2 were measured.
observed species to obtain production rates and mixing ratios relative to CN. The Haser equation for the line-of-sight column density was fit to the average observed column density profiles for each species:

\[
N_d(\rho) = \frac{Q}{2\pi \rho v} \frac{\gamma_d}{\gamma_p - \gamma_d} \left[ \int_0^{\rho_p/v} K_0(y)dy - \int_0^{\rho/v} K_0(y)dy \right],
\]

where \( Q \) is the production rate, \( \rho \) is the projected distance of a given line of sight from the nucleus, \( v \) is the radial outflow speed, \( K_0 \) is the modified Bessel function of the first kind, and \( \gamma_p \) and \( \gamma_d \) are the scale lengths of the parent and daughter species, respectively.

Although the Haser model relies on basic assumptions of pure radial outflow and spherical coma symmetry, which do not apply to all comets, it still yields reasonable values for production rates in cases where it cannot fit the exact shape of the radial profile (Cochran et al. 2012). Because the production rates obtained in prior comet chemistry surveys of radical species were obtained with the Haser model, the Haser model was used here to facilitate comparison with known values for other comets to place the results of this study into a larger context. The parent and daughter scale lengths used for this study are provided in Table 3. These scale lengths are based on results of prior surveys and are strictly empirical—they do not carry assumptions regarding the parent molecules of the observed fragment species. The scale lengths were also adjusted to account for different heliocentric distances using the 0.85 \( r_h^{-0.5} \) km s\(^{-1}\) velocity scaling relation of Delsemme (1982) and the \( r_h^{-2} \) relationship for photodestruction lifetimes (\( r_h^{-2.5} \) was used for \( C_2 \)) (Cochran et al. 2012).

4. Results

Table 4 lists the production rates obtained from the best-fit Haser model profile to the average observed radial profile of each species, with error bars based on radial profiles driven by the standard deviations of the spreads in the column density data. In some cases, particularly with CH, the signals were insufficient to obtain a robust Haser model fit, thus no production rates are provided for these cases. In some cases, the weaker signals, coupled with large scatter in the data for the CH and NH\(_2\) profiles, yield large error bars on the production rates and thus render the results more as upper limits rather than robust values. The observed radial profiles, along with the best-fit Haser model profiles, are shown in Figures 4–7. The observed radial profiles include all data for their respective nights, which in nearly all cases, includes data from multiple spectral images. Given that some prior comet chemistry surveys have used slightly different parent and daughter species scale lengths, it is appropriate to question the robustness of the derived production rates from the Haser model results presented here. Scale lengths used in the study by A’Hearn et al. (1995) were also tested. The fit quality and the derived production rates were found to be consistent with these results within the error bars provided in Table 4.

In Table 5, the mixing ratios of the various observed species with respect to CN, derived from the Haser model production rates, are presented for each comet on each night of observation. A comet is considered depleted in a particular species if its mixing ratio is low, based on parameters defined in prior surveys. The results presented here suggest that Garradd is typical in terms of carbon-bearing species, and our results for Tempel 2 confirm its status as a typical comet. Furthermore, the results for comet McNaught suggest that it is among the population of Jupiter-family comets that are \( C_2 \) depleted. Comet Hergenrother, another Jupiter-family comet, is not only found to be depleted in carbon-chain species, but it is depleted in ammonia-related species as well. This likely explains the large scatter in the data, due to decreasing signal to noise, at large distances from the nucleus as seen in Figure 5.

5. Discussion

Little data exist in the literature currently on comets Hergenrother and McNaught. However, the production rates we obtained for \( C_2\), \( C_3\) and CN are nearly identical to those reported by Schleicher for comet Hergenrother at the same heliocentric distance (IAUC 9255). On the other hand, comets Tempel 2 and Garradd have been studied through a variety of means, and Tempel 2 has been studied extensively over multiple apparitions. The production rates for Tempel 2 that were derived in this study are consistent with narrowband photometry results obtained by Knight et al. (2012) when the
**Figure 4.** Haser model profiles for the observed species in the coma of comet Tempel 2. Plots in the left-hand column are from the 2010 July 15 observation, and plots in the right-hand column are from the 2010 September 13 observation. In all cases, the derived column densities from the spectra are indicated by the gray stars (each gray star represents the derived value from one of the IFU fibers). The observed radial profiles include data from multiple spectral images. Vertical spreads in the data points are due to asymmetries in the coma about the optocenter. The black curve in each plot is the best-fit Haser model result. The derived column densities from the spectra are available as data behind the Figure.

(The data used to create this figure are available.)
comet was at similar heliocentric distances during the 1983, 1988, 1999, and 2010 apparitions. Similarly, the abundance ratios of C2 and C3 with respect to CN that were derived here are identical to the ratios obtained from long-slit spectra by Cochran et al. (2012). This consistency suggests that there has not been selective devolatilization of Tempel 2 over the last several apparitions.

Comet Garradd was discovered in 2009 and is considered dynamically new (Bodewits et al. 2014). Therefore, the only observations with which to compare results also come from the same apparition. Our detections of C2, C3, CH, CN, and NH2 for comet Garradd were all strong, which is fully consistent with the observations of the same species by Shubina et al. (2014) and Ivanova et al. (2017).

The species observed in the four comets are all fragment species thought to come from larger species released from the nucleus. One of the ongoing efforts in comet studies is to link...
these fragment species with the native species in the nucleus and look for consistencies in observed abundances. However, this is particularly challenging given that some fragment species seen frequently in comets have unknown precursors, such as C$_3$ (Hoelscher 2015), and that others may have more than one precursor, such as CN (Cochran 1982; Schloerb et al. 1987).

Figure 6. Haser model profiles for the observed species in the coma of comet McNaught. Plots in the left-hand column are from the 2012 August 23 observation, plots in the middle column are from the 2012 October 8 observation, and plots in the right-hand column are from the 2012 October 9 observation. In all cases, the derived column densities from the spectra are indicated by the gray stars (each gray star represents the derived value from one of the IFU fibers). The observed radial profiles include data from multiple spectral images. Vertical spreads in the data points are due to asymmetries in the coma about the optocenter. The black curve in each plot is the best-fit Haser model result. The derived column densities from the spectra are available as data behind the Figure. (The data used to create this figure are available.)
Figure 7. Haser model profiles for the observed species in the coma of comet Garradd. Plots in the left-hand column are from the 2011 August 20 observation, plots in the middle column are from the 2011 August 21 observation, and plots in the right-hand column are from the 2011 August 22 observation. In all cases, the derived column densities from the spectra are indicated by the gray stars (each gray star represents the derived value from one of the IFU fibers). The observed radial profiles include data from multiple spectral images. Vertical spreads in the data points are due to asymmetries in the coma about the optocenter. The black curve in each plot is the best-fit Haser model result. The derived column densities from the spectra are available as data behind the Figure. (The data used to create this figure are available.)
Assuming the precursors are known, low abundances of fragment species imply depletion of the associated precursor species in the nucleus. Comet Tempel 2 was studied in near-IR wavelengths with NIRSPEC on Keck II by Paganini et al. (2012) around the same time as the July IFU observation presented here. A comparison of production rates derived from the NIRSPEC data with the IFU-derived production rates for Tempel 2 suggest that HCN is the likely precursor of CN, and C2H2 is likely a precursor of C2, but given that Paganini et al. report only an upper limit for C2H2, another precursor for C2 cannot be ruled out entirely. Additionally, the IFU production rate of NH2 is significantly less than the NIRSPEC production rate of NH3, which is frequently implicated as the parent of NH2.

Table 5
Log Mixing Ratios

| Comet            | Obs. Date | C2/CN  | C3/CN  | CH/CN | NH2/CN       | Remarks                  |
|------------------|-----------|--------|--------|-------|--------------|--------------------------|
| 10P/Tempel 2     | Jul 15    | 0.075 ± 0.118 | −0.568 ± 0.136 | ...   | −0.05 ± 0.13 | Typical                  |
|                  | Sep 13    | 0.071 ± 0.142 | −0.589 ± 0.135 | ...   | −0.02 ± 0.15 | Typical                  |
| 168P/Hergenrother| Oct 6     | −0.907 ± 0.158 | −1.32 ± 0.140 | ...   | −1.32 ± 0.46 | C2, C3, NH2 Depleted     |
|                  | Oct 8     | −0.840 ± 0.174 | −1.70 ± 0.383 | ...   | −1.26 ± 0.40 | C2, C3, NH2 Depleted     |
|                  | Oct 9     | −0.814 ± 0.123 | −1.70 ± 0.315 | ...   | −1.18 ± 0.39 | C2, C3, NH2 Depleted     |
| 260P/McNaught    | Aug 23    | −0.574 ± 0.248 | −0.477 ± 0.289 | ...   | 0.222 ± 0.39 | C2 Depleted              |
|                  | Oct 8     | −0.553 ± 0.315 | ...   | 0.602 ± 0.168 | −0.097 ± 0.32 | C2 Depleted              |
|                  | Oct 9     | −0.269 ± 0.119 | ...   | 1.29 ± 0.113 | −0.114 ± 0.39 | C2 Depleted              |
| C/2009 P1 (Garradd) | Aug 20  | 0.018 ± 0.125 | −0.602 ± 0.094 | 0.097 ± 0.168 | −0.135 ± 0.210 | Typical                  |
|                  | Aug 21    | 0.073 ± 0.062 | −0.580 ± 0.050 | 0.022 ± 0.104 | −0.200 ± 0.136 | Typical                  |
|                  | Aug 22    | 0.087 ± 0.044 | −0.556 ± 0.040 | 0.046 ± 0.147 | −0.255 ± 0.132 | Typical                  |
| Typical Range    |           | 0.15 ± 0.2   | −0.68 ± 0.2 | 0.25 ± 0.19 | −0.09 ± 0.27 | Cochran et al. (2012)    |

Note. All error bars are 1σ.
due to its short photodissociation lifetime to form NH$_3$ at 95% efficiency (Cochran 1986; Meier et al. 1998; Rubin et al. 2020). Paganini et al. (2012) also found a significant difference between NH$_2$ and NH$_3$ abundances for Tempel 2 and suggested that NH$_3$ may not be driving the NH$_2$ production.

As shown in Table 5, the mixing ratios with respect to CN obtained for Hergenrother are extremely low. The derived mixing ratios for C$_2$ and C$_3$ are approximately a factor of 10 lower than what is considered typical in prior surveys. More curious, however, is the mixing ratio for NH$_2$, which is a factor of 20 below prior survey averages. These results suggest that Hergenrother is depleted in the likely precursor species of the observed fragments: HCN, C$_2$H$_2$, and NH$_3$. These results are also consistent with the optocenter spectrum of Hergenrother that is presented in Figure 2. Of the comets for which fragment species have been observed in prior studies, those that come closest to matching these conditions are 2IP/Giacobini-Zinner (Konno & Wyckoff 1989; Beaver et al. 1990; Cochran et al. 2020), 32P/Comas Solá (Cochran et al. 2012), 43P/Wolf-Harrington (Schleicher et al. 1993; Fink 2009), and 73P/Schwassmann–Wachmann 3 (Fink 2009; Schleicher & Bair 2011). These results suggest that there may be a subgroup of carbon-chain-depleted Jupiter-family comets that are also depleted in ammonia. This subclass of comets has been suggested before by Fink (2009), who called this group the “Giacobini-Zinner Type.” For perspective, representative short-period comets of three compositional families (typical, carbon-chain depleted but normal NH$_2$, and both carbon-chain and NH$_2$ depleted) are shown in Figure 8. This potential emerging subgroup of comets demonstrates the need for continued observations of fragment species in comet comae to place newer comet observations into context with historical observations and improve sample sizes for identifying comet chemical families.

6. Summary and Conclusions

Data of the spatial distribution of radical species in the comae of comets Tempel 2, Hergenrother, McNaught, and Garradd were obtained with an IFU spectograph. For each observed radical species in each comet coma, the Haser model was used to derive production rates and mixing ratios relative to CN. The results confirm the designation of Tempel 2 as a typical Jupiter-family comet in terms of carbon-chain species abundances as reported in multiple prior surveys, and our results suggest that Garradd is also typical in terms of carbon-chain abundances. Comets Hergenrother and McNaught are likely carbon-chain-depleted Jupiter-family comets. Hergenrother is also notable for its extremely low NH$_2$/CN mixing ratio, which has only been reported for a small number of other Jupiter-family comets.

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