H2O and O2 absorption in the coma of comet 67P/Churyumov–Gerasimenko measured by the Alice far-ultraviolet spectrograph on Rosetta

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ABSTRACT

We have detected H$_2$O and O$_2$ absorption against the far-UV continuum of stars located on lines of sight near the nucleus of Comet 67P/Churyumov–Gerasimenko using the Alice imaging spectrograph on Rosetta. These stellar appulses occurred at impact parameters of $\rho$ = 4–20 km, and heliocentric distances ranging from $R_h$ = −1.8 to 2.3 au (negative values indicate pre-perihelion observations). The measured H$_2$O column densities agree well with nearly contemporaneous values measured by VIRTIS-H. The clear detection of O$_2$ independently confirms the initial detection by the ROSINA mass spectrometer; however, the relative abundance of O$_2$/H$_2$O derived from the stellar spectra (11–68 per cent, with a median value of 25 per cent) is considerably larger than published values found by ROSINA. The cause of this difference is unclear, but potentially related to ROSINA measuring number density at the spacecraft position while Alice measures column density along a line of sight that passes near the nucleus.

Key words: comets: individual: 67P – ultraviolet: planetary systems.

1 INTRODUCTION

One of the most significant results from the Rosetta mission to Comet 67P/Churyumov–Gerasimenko (67P/C–G) has been the persistent detection of O$_2$ in the coma (Bieler et al. 2015; Fougere et al. 2016) by the double-focusing mass spectrometer (DFMS) of the Rosetta Orbiter Spectrometer for Ion and Neutral Analysis (ROSINA; Balsiger et al. 2007). The initial detection by Bieler et al. (2015) found that the relative number density of O$_2$ with respect to H$_2$O ranged from 1–10 per cent, with a mean of $n_{O2}/n_{H2O}$ = 3.85 ± 0.85 per cent for measurements taken between 2014 September and 2015 March. Further modelling by Fougere et al. (2016) found that the relative production rate of O$_2$ with respect to H$_2$O is ≈1–2 per cent for measurements taken prior to 2016 February. Both studies find that the number densities of O$_2$ and H$_2$O are highly correlated, with Pearson correlation coefficients $>0.8$.

Surprisingly, O$_2$ is the fourth most abundant species in the coma of 67P/C–G (behind H$_2$O, CO$_2$ and CO; Le Roy et al. 2015; Fougere et al. 2016), despite the fact that it had never been detected in a cometary coma before (Bieler et al. 2015). Subsequent reanalysis of mass spectrometer data from Giotto’s visit to Oort-Cloud Comet 1P/Halley has found that $n_{O2}/n_{H2O}$ = 3.7 ± 1.7 per cent is consistent with the measurements (Rubin et al. 2015), suggesting that O$_2$ may be a common constituent of all comets, not just Jupiter Family Comets such as 67P/C–G. New theories are being developed to explain these O$_2$ detections, such as trapping O$_2$ in clathrates prior to agglomeration during comet formation (Mousis et al. 2016), astrochemical production of O$_2$ in dark clouds or forming protoplanetary discs (Taquet et al. 2016) and formation of O$_2$ during the evaporation of H$_2$O ice via dismutation of H$_2$O$_2$ (Dulieu, Minissale & Bockelée-Morvan 2017).
In this Paper, we present H₂O and O₂ column densities measured along lines of sight to background stars projected near the nucleus of 67P/C-G by the Alice far-UV spectrograph (Stern et al. 2007). These stellar sight lines allow the coma of 67P/C-G to be studied in far-UV absorption, where column densities can be measured directly. Alice’s previous characterizations of the coma of 67P/C-G have primarily used emission lines from CO and atomic hydrogen, oxygen, carbon and sulphur (e.g. Feldman et al. 2015, 2016). While the strengths of these emission lines can only be used to derive molecular column densities under specific assumptions (i.e. pure resonance fluorescence), the ratios of strong, commonly observed lines can be diagnostic of physical conditions in the coma. Feldman et al. (2016) inferred that O₂ was the primary driver of certain gaseous outbursts that exhibit a sudden increase in the O:\n ratio in the sunward coma without any corresponding increase in dust production. Feldman et al. (2016) estimate that O₂/H₂O ≥ 50 per cent during these outbursts, substantially higher than the mean value of 3.85 ± 0.85 per cent found by Bieler et al. (2015).

Several of Rosetta’s instruments are capable of measuring the abundance of H₂O (as well as CO and CO₂) in the coma of 67P/C-G. Most notably, ROSINA measures the number density of water, \(N_{\text{H₂O}}\), at the spacecraft location using mass spectroscopy, while the Visible and Infrared Thermal Imaging Spectrometer (VIRTIS; Coradini et al. 2007) and the Microwave Instrument for the Rosetta Orbiter (Gulkis et al. 2007) measure the column density of water, \(N_{\text{H₂O}}\), along a specific line of sight using rotational and/or vibrational transitions. The UV-absorption spectra presented herein also allow Alice to directly measure \(N_{\text{H₂O}}\), and facilitate comparisons with nearly contemporaneous measurements from ROSINA (Fougere et al. 2016) and VIRTIS-H (the high spectral resolution channel of VIRTIS; Bockelée-Morvan et al. 2016).

In contrast to the situation with H₂O, only Alice and ROSINA are capable of directly measuring O₂. This makes the observations reported herein an important and unique confirmation of the initial O₂ detections (Bieler et al. 2015). However, direct comparisons between ROSINA’s \textit{in situ} measurements and Alice’s measurements along specific lines of sight are not straightforward. The remainder of this Paper is organized as follows: the Alice spectrograph and stellar spectra are described in Section 2; H₂O and O₂ column densities are derived in Section 2; our values are compared with ROSINA and VIRTIS-H measurements in Section 3; and our conclusions are presented in Section 4.

2 STELLAR APPULSE OBSERVATIONS

Alice is a low-power, lightweight far-UV imaging spectrograph funded by NASA for inclusion on the ESA Rosetta orbiter (Stern et al. 2007). It covers the wavelength range 750–2050 Å with a spectral resolution of 8–12 Å, and has a slit that is 6° long, and narrower in the centre (0.05 wide) than the edges (0.1 wide; Stern et al. 2007). Over the course of Rosetta’s orbital escort mission, Alice probed the sunward coma of 67P/C-G in absorption 30 times using UV-bright stars located along lines of sight near the nucleus as background sources. Here we report on the 29 observations (‘appulses’) that were not occulted by the nucleus; we will report the details of our single stellar occultation separately (B. Keeney et al., in prep).

Quantifying the nature of the cometary coma required re-observing, or ‘revisiting’, these stars when they were far from the nucleus to characterize their intrinsic stellar spectra. This allowed us to isolate the coma absorption signature from the combined background effects of the stellar continuum and interstellar absorption. Further, there are two varieties of appulse observations, which we term ‘targeted’ and ‘archival’ appulses.

For the targeted appulses, we actively searched during operations planning for upcoming opportunities where a known bright star would be located within a few degrees of the nucleus. Inertial pointings were designed that facilitated long stares at these stars during the appulses, at the expense of a time-varying distance to the nucleus over the course of each observation. These targeted appulses were observed between 2015 December 25 and 2016 February 1 at heliocentric distances of \(R_h = 1.97–2.26\) au, and are characterized by long exposure times (typically 12 Alice spectral images with exposure times of 10–20 min each were obtained per appulse), large off-nadir angles (\(\theta \approx 5–10°\)), and large \(R_h\) compared to their archival counterparts.

To complement the targeted appulses, we also searched the extensive Alice archive (~40 000 exposures include the nucleus in the field of view) for instances where we serendipitously observed a UV-bright star near the nucleus as part of normal operations. This search returned hundreds of candidates that were prioritized by the star’s brightness and proximity to the nucleus, as well as the duration of the appulse and its proximity to the comet’s perihelion passage on 2015 August 12, when coma activity was near its peak (Fougere et al. 2016). Since our typical pointing during normal operations was fixed with respect to the nucleus (i.e. not an inertial reference frame), we do not know the exact duration of the archival appulses because the star is moving with respect to the slit; however, we can estimate their durations with uncertainties of ~10 per cent using Navigation and Ancillary Information Facility SPICE (Acton 1996). The archival appulses were observed between 2015 April 29 and 2015 December 26 at \(R_h = 1.24–1.98\) au, and typically have shorter durations (10–20 min), smaller off-nadir angles (\(\theta < 5°\)), and smaller \(R_h\) than their targeted counterparts. However, the smaller off-nadir angles for the archival appulses are somewhat counteracted by the large spacecraft-comet distance, \(\Delta\), near perihelion, which led to similar impact parameters (\(\rho = \Delta \sin \theta \approx 5–20\) km) for all appulses.

Tables 1 and 2 list the properties of the seven targeted and 22 archival appulses, respectively. The following information is listed by column: (1) the name of the star; (2) the stellar type and luminosity class as listed by SIMBAD (Wenger et al. 2000); (3) the observation type (either ‘appulse’ or ‘revisit’); (4) the date of observation; (5) the total exposure time, in minutes; (6) the heliocentric distance, \(R_h\), in au, where negative values indicate that the observation occurred prior to perihelion on 2015 August 12; (7) the phase angle, \(\phi\), in degrees; (8) the off-nadir angle, \(\theta\), in degrees; and (9) the impact parameter, \(\rho\), in km. The impact parameter is only listed for appulse observations, not revisits, and the entries are ordered by appulse date.

Appulse observations have small off-nadir angles by construction (\(\theta = 0°\) implies we are looking straight at the nucleus), and revisits were constrained to have \(\theta > 30°\), although most were acquired when \(\theta > 90°\). Most of the appulses and revisits were observed at ~90° phase, with occasional deviations up to ±30° from this value. Note that one of the targeted stars, HD 40111, has two distinct appulses separated by ~2 weeks (see Table 1).

All exposures for a given appulse or revisit were flux-calibrated using spectrophotometric standard stars. Stellar spectra were then extracted from the spectral images and background subtracted. Spectra extracted from individual exposures were combined to improve the signal-to-noise ratio after first being normalized to have the same median flux from 1800–1900 Å. This range was chosen...
because both H2O and O2 have very small absorption cross-sections in this region (Chung et al. 2001; Yoshino et al. 2005), but the stellar spectra still have sufficient signal to noise to allow a robust flux measurement (the effective area of Alice decreases rapidly for wavelengths >1800 Å; Stern et al. 2007).

Next, the co-added revisit spectrum was scaled to have the same median flux from 1800–1900 Å as the co-added appulse spectrum. Finally, the appulse spectrum was divided by the scaled revisit (i.e. unocculted) spectrum to create a normalized spectrum in which the intrinsic stellar flux and interstellar absorption have been removed and only the differences in foreground coma absorption between the appulse and revisit spectra remain. By normalizing the spectra in this manner we also make ourselves insensitive to the uncertainty in the amount of time the star was in the slit.

Fig. 1 displays co-added revisit spectra for three main sequence stars that span the range of stellar types observed. All three stars have sufficient flux at λ > 1400 Å to create normalized spectra with reasonable signal to noise, but the early- and mid-type B stars have considerably more flux at shorter wavelengths than the late-type B stars do. Thus, normalized spectra for late-type appulse stars are inherently noisier at bluer wavelengths than normalized spectra for earlier-type stars.

We note that in a few cases we normalized the spectra from 1400–1450 Å when normalization from 1800–1900 Å was problematic. While 1400–1450 Å has small H2O absorption cross-sections (Chung et al. 2001), it is the region where O2 absorption cross-sections are largest (Yoshino et al. 2005). The 1400–1450 Å region is therefore not ideal for spectral normalization, since using it reduces our sensitivity for O2 absorption. Fits to spectra where we had to use this normalization region are not used for detailed analyses.

We have searched for optically-thin absorption from H2O and O2 in the normalized stellar spectra as described above. For a given molecule, i, we model the optical depth, τi, as a function of wavelength, λ, as

\[ \tau_i(\lambda) = N_i \sigma_i(\lambda), \]

where \( N_i \) is the column density of species i and \( \sigma_i(\lambda) \) is the absorption cross-section of species i as a function of wavelength. Combining absorption from several different species yields an expected (normalized) model flux of

\[ F(\lambda) = e^{-\sum \tau_i(\lambda)}. \]

This model spectrum can then be compared to the normalized stellar spectrum to constrain the column densities of interest.

Table 3 lists the ten species that we model in our analysis. While we are primarily interested in H2O and O2, other abundant species must be included to robustly constrain the range of permissible H2O and O2 column densities. All species with >0.5 per cent abundance relative to H2O in the coma of 67P/C-G in Le Roy et al. (2015) with available far-UV absorption cross-sections are tabulated. Table 3 lists the following information by column: (1) species; (2) wavelength range; (3) measurement temperature; and (4) measurement reference. The adopted cross-sections were downloaded from the PHoto Ionization/Dissociation RATES website1 (Huebner & Mukherjee 2015); for most species, they are composites of several different measurements covering the wavelength range 900–2000 Å. The molecular cross-sections in Table 3 are displayed in Fig. 2.

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1 http://phidrates.space.swri.edu

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Table 1. Journal of Targeted Stellar Appulse observations.

| Star     | Sp. type | Obs. type | Date             | UTC       | Duration (min) | Rb (au) | φ (°) | ρ (km) |
|----------|----------|-----------|------------------|-----------|----------------|---------|-------|--------|
| HD 140008 | B5 V     | Appulse   | 2015 December 25 | 14:27:11  | 57             | 1.97    | 89.8  | 4.8–5.3 | 6.4–7.2 |
| –        | –        | Revisit 1  | 2016 February 29 | –         | 37             | 2.47    | 92.9  | 88.3–88.9 | –       |
| –        | –        | Revisit 2  | 2016 March 12    | –         | 39             | 2.56    | 91.9–92.0 | 87.0–88.0 | –       |
| HD 144294 | B2.5 V   | Appulse   | 2015 December 25 | 15:37:11  | 111            | 1.97    | 89.8  | 9.9–10.8 | 13.3–14.6 |
| –        | –        | Revisit 1  | 2016 March 4     | –         | 127            | 2.51    | 91.8  | 120.0–123.8 | –       |
| HD 42933  | B1/2 III | Appulse   | 2016 January 10  | 07:19:29  | 164            | 2.09    | 89.6  | 5.1–6.5  | 7.0–8.9 |
| –        | –        | Revisit 1  | 2016 February 29 | –         | 51             | 2.47    | 92.9  | 171.1–171.8 | –       |
| –        | –        | Revisit 2  | 2016 March 12    | –         | 77             | 2.48    | 92.6  | 172.9–173.8 | –       |
| HD 89890  | B5 II    | Appulse   | 2016 January 18  | 13:28:59  | 169            | 2.16    | 60.4–60.5 | 12.1–12.9 | 17.1–18.2 |
| –        | –        | Revisit 1  | 2016 March 15    | –         | 84             | 2.59    | 89.1  | 145.3–148.4 | –       |
| HD 40111  | B0/1 II/III | Appulse | 2016 January 25  | 17:32:33  | 222            | 2.21    | 60.2–60.4 | 11.4–12.5 | 14.0–15.4 |
| –        | –        | Appulse 2  | 2016 February 9  | 19:38:27  | 170            | 2.33    | 64.9–65.6 | 8.8–9.8  | 7.8–8.6  |
| –        | –        | Revisit 1  | 2016 February 23 | –         | 131            | 2.43    | 89.2–90.1 | 120.4–122.3 | –       |
| –        | –        | Revisit 2  | 2016 February 26 | –         | 88             | 2.45    | 94.8  | 171.2–172.0 | –       |
| HD 42933  | B1/2 III | Appulse   | 2016 February 1  | 13:28:59  | 170            | 2.26    | 60.2–60.4 | 9.8–9.9  | 10.0–10.1 |
| –        | –        | Revisit 2  | 2016 April 1    | –         | 62             | 2.71    | 112.1–112.9 | 177.8–178.7 | –       |

Notes. The phase angle is denoted by φ and the off-nadir angle by θ. The last column lists the impact parameter, ρ.
All of the cross-section measurements were performed near room temperature and laboratory measurements are not consistently available for all species in Table 3 at any other temperature; however, the gas kinetic temperature in the coma of 67P/C–G varies considerably. Barucci et al. (2016) found that exposed water ice on the nucleus has $T \approx 160–220$ K, while Lee et al. (2015) found that the temperature of the coma decreases as $T \propto \rho^{-1}$ until it reaches a terminal temperature of $T \approx 50–75$ K. The discrepancy between the temperature of the gas whose cross-section was measured and the temperature of the absorbing coma gas introduces a systematic uncertainty in our model column densities that is not quantified by our modelling procedure. The peak $O_2$ cross-section decreases by $\sim 0.1$ dex as the temperature decreases from 295 to 78 K (Yoshino et al. 2005); thus, by assuming room-temperature cross-sections we are systematically under-estimating the $O_2$ column density required to match the observed absorption. Unfortunately, no $H_2O$ cross-sections are available at $T < 250$ K, so we are unable to estimate the magnitude of the systematic variation in $O_2/H_2O$.

We estimate the molecular column densities using non-linear least-squares regression of equation (2) with MPFIT2 (Markwardt 2009). The free parameters of the fit are the logarithm of the $H_2O$ column density, in units of cm$^{-2}$, and the relative column densities of $O_2, CO, CO_2$ etc. with respect to water ($e.g., O_2/H_2O \equiv N_{O_2}/N_{H_2O}$). The $O_2, CO$ and $CO_2$ columns are constrained to lie in the range of 0–100 per cent relative to $H_2O$, and all other species are
Table 3. Molecular cross-sections.

| Species | \( \lambda \) (Å) | \( T \) (K) | Reference |
|---------|-----------------|-------------|-----------|
| H\(_2\)O | 1400–1898 | 250 | Chung et al. (2001) |
| – | 1148–1939 | 298 | Mota et al. (2005) |
| – | 850–1110 | 298 | Watanabe & Jursa (1964) |
| – | 1060–1860 | 295 | Yoshino et al. (2005) |
| – | 1163–2000 | 298 | Ackerman, Baume & Kockarts (1970) |
| O\(_2\) | 584–1038 | 298 | Cairns & Samson (1965) |
| – | 1061–1187 | 295 | Stark et al. (2007) |
| – | 1167–1755 | 295 | Hitchcock, Brion & van der Wiel (1980) |
| CO | 1380–1600 | 295 | Mount & Moos (1978) |
| – | 952–1306 | 295 | Sun & Weissler (1955) |
| – | 773–1370 | 298 | Ditchburn (1955) |
| CO\(_2\) | 1050–2011 | 298 | Nakayama & Watanabe (1964) |
| – | 600–1000 | 298 | Metzger & Cook (1964) |
| – | 1380–1600 | 295 | Okabe & Becker (1963) |
| – | 1160–1200 | 298 | Koch & Skibowski (1971) |
| C\(_2\)H\(_2\) | 500–1200 | 296 | Schoen (1962) |
| – | 1065–1960 | 298 | Zelikoff & Watanabe (1953) |
| – | 1210–1730 | 296 | Okabe (1981) |
| – | 1600–2600 | 295 | Fahr & Nayak (1994) |
| H\(_2\)CO | 600–1760 | 296 | Mentall et al. (1971) |
| – | 1760–1850 | 298 | Gentieu & Mentall (1970) |

Figure 2. Molecular absorption cross-sections used in this work.

Figure 3. Fits to the appulse absorption of HD 26912 (FQ = 2). Top: the normalized stellar flux (black) with best-fitting ensemble absorption (brown) overlaid. Individual absorption from H\(_2\)O (blue), O\(_2\) (green), and other species (purple; ensemble sum of CO, CO\(_2\), C\(_2\)H\(_2\), and other species from Table 3) are also shown. Bottom: the residual of the ensemble fit, with 1σ flux uncertainty (orange) overlaid. Masked regions are shown in lighter hues in both panels; these regions are not used to constrain the fits. Absorption fits for all targeted and archival stellar appulses are shown in Appendix A.
CO2 absorption with a column density relative to water uniformly which we superimposed H2O absorption with a column density ranges that were used in the fits to the appulse observations. However, Bieler et al. (2015) find no evidence of systematically not overlap with the dates of the Bieler et al. (2015) measurements. account for some of this difference since the dates of our appulses do stars with FQ

\begin{align*}
\text{FQ} & = 4 \text{ to the appulse of HD 89890, whose fit preferred } N_{O_2} > N_{H_2O} \\
\text{and had systematic discrepancies throughout the fitting range. Only} \text{ stars with FQ} \leq 3 \text{ are used in subsequent analyses.}
\end{align*}

There are two notable features of the best-fitting column densities in Table 4. The first is that the formal fitting uncertainties are very small. The second is that the O2/H2O values are considerably higher than those in Bieler et al. (2015), who found a mean value of 3.85 ± 0.85 per cent over an approximately seven month period when R0 = −3.4 to −2 au. It is possible that seasonal variations can account for some of this difference since the dates of our appulses do not overlap with the dates of the Bieler et al. (2015) measurements. However, Bieler et al. (2015) find no evidence of systematically increasing O2/H2O in their measurements, almost all of which have O2/H2O < 0.1, and several of the best-fitting values in Table 4 have O2/H2O > 0.5.

### 2.1 Adopted Values of $N_{H_2O}$ and $O_2/H_2O$

We tested our fitting procedure by forward modelling simulated data with pre-defined, ‘true’, values of S/N, $N_{H_2O}$ and $O_2/H_2O$. We began with a flat-spectrum source ($F(\lambda) = 1$ at all wavelengths) upon which we superimposed H2O absorption with a column density uniformly drawn from the range $15 < \log N_{H_2O} < 17.5$, O2, CO and CO2 absorption with a column density relative to water uniformly drawn from the range 0–100 per cent, and CH4, C2H2, C3H2, C2H6, C3H2, C2H4 and H2CO absorption with a column density relative to H2O uniformly drawn from the range 0–1 per cent. These are the same ranges that were used in the fits to the appulse observations.

Next, we added to the spectrum Poisson noise that had a median S/N in the 1250–2000 Å range chosen uniformly from 0.7 < log S/N < 2.3, bracketing the observed values. A template for the S/N as a function of wavelength was derived from the revisit (i.e. unocculted) spectra of our appulse targets by normalizing each spectrum to have the same median S/N from 1250–2000 Å. Then at each wavelength we chose the median ‘normalized S/N’ value from all of the spectra to form the S/N profile of a ‘typical’ appulse star. This template achieves peak S/N at ~1350 Å and varies by a factor of ~10 over the wavelength range 950–2000 Å.

This noisy, simulated spectrum was then treated just like the stellar appulse observations; i.e. it was normalized to have $F(\lambda) = 1$ from 1800–1900 Å and then fit with the same procedure described above. The best-fitting column densities and uncertainties were then saved along with the true values used to generate the simulated spectrum, and the process was repeated 500 000 times to thoroughly sample the full range of parameter space.

The best-fitting and true values of $N_{H_2O}$ and $O_2/H_2O$ are compared as a function of S/N in Fig. 4. These images are two-dimensional histograms, where the colour bars display the mean offset between the best-fitting and true values in a given bin. Systematic offsets are present in both $N_{H_2O}$ and $O_2/H_2O$ when S/N < 10, but are quite modest at the higher S/N values typical of our appulse observations (see Table 4). Fig. 5 is similar to Fig. 4, except its colour bars display the RMS deviations between the best-fitting and true values in a given bin after correcting for the systematic offsets in Fig. 4. These deviations quantify the spread in true values that are associated with a particular best-fitting value.
Figure 4. Average offsets between the true and best-fitting values of log \(N_{\text{H}_2\text{O}}\) (top) and \(O_2/H_2\text{O}\) (bottom) as a function of log S/N. When S/N > 10, the magnitude of the log \(N_{\text{H}_2\text{O}}\) offset is typically \(\lesssim 0.05\) dex, and the magnitude of the \(O_2/H_2\text{O}\) offset is \(\lesssim 0.02\).

The ‘adopted’ values of \(N_{\text{H}_2\text{O}}\) and \(O_2/H_2\text{O}\) are derived from our Monte Carlo simulations by identifying the 1000 simulated spectra with S/N and best-fitting values closest to those measured for a given observation, and fitting a Gaussian to the distribution of true values. We treat the mean of this Gaussian as the adopted value and its standard deviation as the 1σ uncertainty. Since our fits constrain the allowable range of \(O_2/H_2\text{O}\), we quote limits whenever the adopted value is <3σ from these boundaries.

The last two columns of Table 4 list the adopted values of log \(N_{\text{H}_2\text{O}}\) and \(O_2/H_2\text{O}\), respectively, for our stellar appulse observations. Fig. 6 shows absorption profiles of \(\text{H}_2\text{O}\) and \(O_2\) and their associated 95 per cent (2σ) confidence bands using the adopted values for the appulse of HD 26912. These profiles are overlaid on the normalized stellar spectrum as in Fig. 3, along with confidence bands for the sum of all other modelled species and the total absorption from all species. These profiles clearly show that the adopted values of log \(N_{\text{H}_2\text{O}}\) and \(O_2/H_2\text{O}\) are consistent with the data. Absorption profiles derived from the adopted values for all targeted and serendipitous appulses are presented in Appendix B.

3 DISCUSSION

3.1 H2O Column Densities

The Monte Carlo simulations presented in Section 2.1 are one way to gain confidence in the validity of our absorption fits. Another is to compare our \(\text{H}_2\text{O}\) column densities with values measured by

Figure 5. RMS deviations between the true and best-fitting values of log \(N_{\text{H}_2\text{O}}\) (top) and \(O_2/H_2\text{O}\) (bottom) as a function of log S/N, after correcting for the systematic offsets in Fig. 4. When S/N > 10, the RMS of log \(N_{\text{H}_2\text{O}}\) is typically 0.05–0.10 dex and the RMS of \(O_2/H_2\text{O}\) is \(\sim 0.05\).

Figure 6. Adopted column densities for the appulse of HD 26912 (FQ = 2), with 95 per cent (2σ) confidence bands. Top: the normalized stellar flux with ensemble fit (brown) and individual-species absorption overlaid using the adopted column densities of \(\text{H}_2\text{O}\) and \(O_2\) from Table 4. Bottom: the residual of the ensemble fit with 1σ flux uncertainty (orange) overlaid. Masked regions are shown in lighter hues in both panels; these regions are not used to constrain the fits. Adopted column densities for all targeted and archival stellar appulses are shown in Appendix B.
other instruments on Rosetta at similar times. Fig. 7 shows the adopted values of $N_{\text{H}_2\text{O}}$ for our stellar appulse observations as a function of $R_h$, compared to the VIRTIS-H measurements of Bockelée-Morvan et al. (2016). Despite the large scatter in the column densities for a given value of $R_h$, the adopted values for our appulse observations are reassuringly similar to the measured values from VIRTIS. One reason for the differences that do exist is the fact that the VIRTIS measurements were taken at systematically lower impact parameters than the appulses, as shown in the top panel of Fig. 7.

While the $N_{\text{H}_2\text{O}}$ values from Alice and VIRTIS are in good agreement, there may be discrepancies with the ROSINA measurements. Fougere et al. (2016) present a sophisticated Direct Simulation Monte Carlo (DSMC) model of the major species ($\text{H}_2\text{O}$, $\text{CO}_2$, $\text{CO}$ and $\text{O}_2$) in the coma of 67P/C–G, which derives molecular production rates from a non-uniform surface activity distribution. The DSMC model does a remarkable job of reproducing the in situ ROSINA measurements of the number density of these species for all data taken before 2016 March (Fougere et al. 2016). However, when the model production rates are used to predict the $N_{\text{H}_2\text{O}}$ values along the lines of sight probed by Bockelée-Morvan et al. (2016), it finds model column densities that are four times higher than those measured by VIRTIS (Fougere et al. 2016). The cause of this discrepancy is unclear, which illustrates the difficulty of directly comparing measurements from in situ instruments such as ROSINA to those from remote-sensing instruments such as VIRTIS and Alice.

### 3.2 $\text{O}_2/\text{H}_2\text{O}$

Fig. 8 shows the relative abundance of $\text{O}_2$ with respect to $\text{H}_2\text{O}$ (top panel) and the column density of $\text{O}_2$ (bottom panel) as a function of $R_h$. Fig. 9 shows the same quantities as a function of impact parameter. The relative $\text{O}_2/\text{H}_2\text{O}$ abundance tends to increase with increasing heliocentric distance and increasing impact parameter. These correlations (3.9σ and 2.5σ significance, respectively, according to Kendall’s τ test) cause the distributions of $N_{\text{O}_2}$ as a function of $R_h$ and $\rho$ to be flatter than the corresponding distributions of $N_{\text{H}_2\text{O}}$ shown in Fig. 7.

The relatively flat distribution of $N_{\text{O}_2}$ as a function of $\rho$ is particularly interesting, as it suggests a distributed source of $\text{O}_2$. This would seem to argue against the variety of mechanisms that Mousis et al. (2016) suggest for trapping $\text{O}_2$ in the icy $\text{H}_2\text{O}$ matrix of 67P/C–G. Formation of $\text{O}_2$ through the dismutation of $\text{H}_2\text{O}_2$ during the evaporation of $\text{H}_2\text{O}$ ice, as suggested by Dulieu et al. (2017), might be able to explain the shape of the $\text{O}_2/\text{H}_2\text{O}$ distribution as a function of $\rho$. Interestingly, ROSINA detects $\text{H}_2\text{O}$ in the coma of 67P/C–G (see Fig. 4 of Le Roy et al. 2015 and Fig. 4 of Bieler et al. 2015), but with a relative abundance of $\text{H}_2\text{O}/\text{O}_2 < 0.1$ per cent (Bieler et al. 2015), far less than the ratio of $\text{H}_2\text{O}_2/\text{O}_2 = 2$ predicted by the dismutation reaction (Dulieu et al. 2017).

Feldman et al. (2016) used Alice to study gaseous outbursts in the coma of 67P/C–G. These outbursts exhibit no increase in long-wavelength solar reflected light that would indicate an increase in dust production, and are characterized by a sudden increase in the brightness ratio of $\text{O}_1\lambda 1356/\lambda 1304$ in the sunward coma. Feldman et al. (2016) infer that these outbursts are driven by $\text{O}_2$ release, and estimate that $\text{O}_2/\text{H}_2\text{O} \geq 50$ per cent during the outbursts.

Coincidentally, our earliest archival appulse (HD 26912; see Fig. 3 and Fig. 6) occurred during the onset of one of the Feldman et al. (2016) outbursts (see their section 2.5). We adopt $\text{O}_2/\text{H}_2\text{O} = 31.5 \pm 5.6$ per cent for this appulse (see Table 4), which is somewhat lower than the Feldman et al. (2016) estimate. This apparent discrepancy is likely a result of timing differences; i.e. the adopted value from the appulse measures the ambient $\text{O}_2/\text{H}_2\text{O}$ in the coma just prior to outburst, whereas the Feldman et al. (2016)
Figure 8. $O_2/H_2O$ (top) and $N_O2$ (bottom) as a function of $R_h$. Symbol sizes are the same as in Fig. 7. Heliocentric distances in the beige hatched region are smaller than the perihelion distance of 1.24 au. The grey hatched region in the top panel indicates typical values of $O_2/H_2O$ measured by ROSINA (Bieler et al. 2015; Fougere et al. 2016). The value measures the peak $O_2/H_2O$ over the ~30-minute duration of the outburst.

As mentioned in Section 2, the $O_2/H_2O$ values in Table 4 are generally higher, and have considerably larger scatter, than the values found by ROSINA–DFMS. Bieler et al. (2015) found $n_{O2}/n_{H2O} = 3.85 \pm 0.85$ per cent in data taken between 2014 August and 2015 March, and Fougere et al. (2016) found $Q_{O2}/Q_{H2O} \approx 2$ per cent throughout the time frame of our appulse observations. Notably, neither Bieler et al. (2015) nor Fougere et al. (2016) list a single observation where $O_2/H_2O > 15$ per cent, but we find a median value of 25 per cent.

As discussed in Section 3.1, comparisons between the in situ measurements of ROSINA and the line-of-sight measurements of Alice and VIRTIS are not straightforward, even with a sophisticated coma model (Fougere et al. 2016). None the less, the large values of $O_2/H_2O$ derived from the Alice data are surprising. While we have included several minor species in our absorption fits (see Section 2), there are many species detected in the coma of 67P/C–G by ROSINA for which we were unable to find absorption cross-sections (e.g. HS, S$_2$, CH$_3$O; Le Roy et al. 2015). Some of these ‘missing’ species could have cross-sections large enough to cause measurable far-UV absorption, even for very small column densities, causing the current $O_2/H_2O$ values to be over-estimated. Quantifying the magnitude of these systematic uncertainties is exceedingly difficult without additional laboratory data for far-UV molecular absorption cross-sections.

Figure 9. $O_2/H_2O$ (top) and $N_O2$ (bottom) as a function of impact parameter. Symbol sizes are the same as in Fig. 7. The dashed vertical line is the effective radius of the nucleus and the dotted vertical lines indicate its minimum and maximum radii.

Further, even if our fits currently include all of the relevant species, the absorption cross-sections we use were all measured at $T \approx 300$ K (see Table 3). Since the absorbing coma gas is expected to be at lower temperature, variations in the absorption cross-sections with temperature could lead us to infer incorrect values of the column density with our current procedure. However, the scant existing data suggest that our procedure under-estimates the amount of low-temperature $O_2$ present by assuming room-temperature cross-sections (see discussion in Section 2; Yoshino et al. 2005), which would serve to increase the discrepancy between our results and those of ROSINA.

4 CONCLUSIONS

Using the Alice far-UV imaging spectrograph aboard Rosetta, we have independently verified the presence of $O_2$ in the coma of Comet 67P/C–G. $O_2$ was detected for the first time in the coma of a comet by Rosetta’s ROSINA mass spectrometer (Bieler et al. 2015; Fougere et al. 2016). In the present study, both $O_2$ and $H_2O$ were detected in far-UV absorption against the continuum of stars located near the nucleus of 67P/C–G, at impact parameters of 4–20 km. These stellar appulses occurred at heliocentric distances of $-1.8$ to $2.3$ au, where negative distances indicate pre-perihelion observations. The main results of our analysis are as follows:

(i) the $H_2O$ column densities derived from the stellar spectra are in good agreement with VIRTIS-H measurements from the same
time period taken at similar impact parameters (Bockelée-Morvan et al. 2016); and
(ii) the median value for the relative abundance of O$_2$ with respect to H$_2$O derived from the stellar spectra is O$_2$/H$_2$O = 25 per cent. This value is considerably higher than those reported by ROSINA; Bieler et al. (2015) and Fougere et al. (2016) found mean values of O$_2$/H$_2$O < 5 per cent.

We see no simple explanation for the difference in O$_2$/H$_2$O measured by Alice and ROSINA, unless it is related to the unmodelled species and T = 300 K cross-sections discussed at the end of Section 3.2. The Alice H$_2$O measurements are consistent with the values published by other remote-sensing instruments on Rosetta; and while this does not guarantee that our O$_2$ values are correct, it does suggest that our measurements are reasonably robust. The ROSINA measurements, on the other hand, are performed in situ at the spacecraft location, and the sophisticated coma model of Bockelée-Morvan et al. (2016), which were measured very close to perihelion (Fougere et al. 2016), clearly shows much future work to be done to reconcile these differences.

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APPENDIX A: BEST-FITTING ABSORPTION PROFILES

Figs A1–A29 present best-fitting absorption profiles for all targeted and archival stellar appulses, arranged chronologically. The top panel of each figure displays the normalized stellar flux, with best-fitting ensemble absorption (solid brown line) overlaid. Absorption from H$_2$O, O$_2$, and other species are also shown. The bottom panel of each figure displays the residual of the ensemble fit and the 1σ uncertainty of the normalized spectrum.

Figure A1. Fits to the appulse absorption of HD 26912 (FQ = 2).
Figure A2. Fits to the appulse absorption of HD 3901 (FQ = 4).

Figure A3. Fits to the appulse absorption of HD 29589 (FQ = 2).

Figure A4. Fits to the appulse absorption of HD 174585 (FQ = 3).

Figure A5. Fits to the appulse absorption of HD 180554 (FQ = 4).

Figure A6. Fits to the appulse absorption of HD 191692 (FQ = 2).

Figure A7. Fits to the appulse absorption of HD 195810 (FQ = 2).
Figure A8. Fits to the appulse absorption of HD 192685 (FQ = 1).

Figure A9. Fits to the appulse absorption of HD 68324 (FQ = 2).

Figure A10. Fits to the appulse absorption of HD 66006 (FQ = 1).

Figure A11. Fits to the appulse absorption of HD 64722 (FQ = 2).

Figure A12. Fits to the appulse absorption of HD 39844 (FQ = 2).

Figure A13. Fits to the appulse absorption of HD 207330 (FQ = 2).
Figure A14. Fits to the appulse absorption of HD 109387 (FQ = 1).

Figure A15. Fits to the appulse absorption of HD 124771 (FQ = 1).

Figure A16. Fits to the appulse absorption of HD 21428 (FQ = 4).

Figure A17. Fits to the appulse absorption of HD 32249 (FQ = 2).

Figure A18. Fits to the appulse absorption of HD 33328 (FQ = 2).

Figure A19. Fits to the appulse absorption of HD 106625 (FQ = 1).
Figure A20. Fits to the appulse absorption of HD 27376 (FQ = 3).

Figure A21. Fits to the appulse absorption of HD 23466 (FQ = 4).

Figure A22. Fits to the appulse absorption of HD 140008 (FQ = 2).

Figure A23. Fits to the appulse absorption of HD 144294 (FQ = 3).

Figure A24. Fits to the appulse absorption of HD 144217 (FQ = 3).

Figure A25. Fits to the appulse absorption of HD 42933 (FQ = 3).
APPENDIX B: ADOPTED ABSORPTION PROFILES

Figs B1–B29 present the adopted column densities for all targeted and archival stellar appulses, with 95 per cent (2\(\sigma\)) confidence bands. The top panel of each figure displays the normalized stellar flux and associated 95 per cent confidence band (grey), with ensemble fit (brown) and individual-species absorption overlaid using the adopted column densities of H\(_2\)O and O\(_2\) from Table 4. The bottom panel of each figure displays the residual of the ensemble fit and the 1\(\sigma\) uncertainty of the normalized spectrum.

Figure A26. Fits to the appulse absorption of HD 89890 (FQ = 4).

Figure A27. Fits to the first appulse absorption of HD 40111 (FQ = 3).

Figure A28. Fits to the appulse absorption of HD 144206 (FQ = 2).

Figure A29. Fits to the second appulse absorption of HD 40111 (FQ = 3).
Figure B2. Adopted column densities for the appulse of HD 3901 (FQ = 4), with 95 per cent (2σ) confidence bands.

Figure B3. Adopted column densities for the appulse of HD 29589 (FQ = 2), with 95 per cent (2σ) confidence bands.

Figure B4. Adopted column densities for the appulse of HD 174585 (FQ = 3), with 95 per cent (2σ) confidence bands.

Figure B5. Adopted column densities for the appulse of HD 180554 (FQ = 4), with 95 per cent (2σ) confidence bands.

Figure B6. Adopted column densities for the appulse of HD 191692 (FQ = 2), with 95 per cent (2σ) confidence bands.

Figure B7. Adopted column densities for the appulse of HD 195810 (FQ = 2), with 95 per cent (2σ) confidence bands.
Figure B8. Adopted column densities for the appulse of HD 192685 (FQ = 1), with 95 per cent (2σ) confidence bands.

Figure B9. Adopted column densities for the appulse of HD 68324 (FQ = 2), with 95 per cent (2σ) confidence bands.

Figure B10. Adopted column densities for the appulse of HD 66006 (FQ = 1), with 95 per cent (2σ) confidence bands.

Figure B11. Adopted column densities for the appulse of HD 64722 (FQ = 2), with 95 per cent (2σ) confidence bands.

Figure B12. Adopted column densities for the appulse of HD 39844 (FQ = 2), with 95 per cent (2σ) confidence bands.

Figure B13. Adopted column densities for the appulse of HD 207330 (FQ = 2), with 95 per cent (2σ) confidence bands.
Figure B14. Adopted column densities for the appulse of HD 109387 (FQ = 1), with 95 per cent (2σ) confidence bands.

Figure B15. Adopted column densities for the appulse of HD 124771 (FQ = 1), with 95 per cent (2σ) confidence bands.

Figure B16. Adopted column densities for the appulse of HD 21428 (FQ = 4), with 95 per cent (2σ) confidence bands.

Figure B17. Adopted column densities for the appulse of HD 32249 (FQ = 2), with 95 per cent (2σ) confidence bands.

Figure B18. Adopted column densities for the appulse of HD 33328 (FQ = 2), with 95 per cent (2σ) confidence bands.

Figure B19. Adopted column densities for the appulse of HD 106625 (FQ = 1), with 95 per cent (2σ) confidence bands.
Figure B20. Adopted column densities for the appulse of HD 27376 (FQ = 3), with 95 per cent (2σ) confidence bands.

Figure B21. Adopted column densities for the appulse of HD 23466 (FQ = 4), with 95 per cent (2σ) confidence bands.

Figure B22. Adopted column densities for the appulse of HD 140008 (FQ = 2), with 95 per cent (2σ) confidence bands.

Figure B23. Adopted column densities for the appulse of HD 144294 (FQ = 3), with 95 per cent (2σ) confidence bands.

Figure B24. Adopted column densities for the appulse of HD 144217 (FQ = 3), with 95 per cent (2σ) confidence bands.

Figure B25. Adopted column densities for the appulse of HD 42933 (FQ = 3), with 95 per cent (2σ) confidence bands.
**Figure B26.** Adopted column densities for the appulse of HD 89890 (FQ = 4), with 95 per cent (2σ) confidence bands.

**Figure B27.** Adopted column densities for the first appulse of HD 40111 (FQ = 3), with 95 per cent (2σ) confidence bands.

**Figure B28.** Adopted column densities for the appulse of HD 144206 (FQ = 2), with 95 per cent (2σ) confidence bands.

**Figure B29.** Adopted column densities for the second appulse of HD 40111 (FQ = 3), with 95 per cent (2σ) confidence bands.

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