THE COMET CIPHER: UNDERSTANDING THE ULTRAVIOLET EMISSIONS OF COMETARY COMAE

by

John William Noonan

Copyright © John William Noonan 2022

A Dissertation Submitted to the Faculty of the
DEPARTMENT OF PLANETARY SCIENCES

In Partial Fulfillment of the Requirements
For the Degree of

DOCTOR OF PHILOSOPHY

In the Graduate College

THE UNIVERSITY OF ARIZONA

2022
THE UNIVERSITY OF ARIZONA
GRADUATE COLLEGE

As members of the Dissertation Committee, we certify that we have read the dissertation prepared by John William Noonan entitled The Comet Cipher: Understanding the Ultraviolet Emissions of Cometary Comae and recommend that it be accepted as fulfilling the dissertation requirement for the Degree of Doctor of Philosophy.

Walter M. Harris
Date: 7 January 2022

Vishnu Reddy
Date: 7 January 2022

Erik Asphaug
Date: 7 January 2022

Kathryn Volk
Date: 7 January 2022

Dennis Bodewits
Date: 7 January 2022

Final approval and acceptance of this dissertation is contingent upon the candidate’s submission of the final copies of the dissertation to the Graduate College. I hereby certify that I have read this dissertation prepared under my direction and recommend that it be accepted as fulfilling the dissertation requirement.

Dissertation Director: Walter M. Harris
Date: 7 January 2022
ACKNOWLEDGEMENTS

At the very beginning of this entire graduate school process I anticipated that writing an acknowledgement section of this Dissertation would feel like something I would do to find closure with the process. As I sit here on a rainy December day, with the vast majority of the work done and a blank acknowledgments section in front of me, it’s hard not to feel that closure setting in.

The University of Arizona, as a public land grant institution, sits on lands that are ancestral to the Hohokam, Tohono O’odham, and the Pascua Yaqui peoples. The ability to live and work on these lands during my time was truly an honor and I am grateful for the opportunity. Part of this work was also carried out on lands of the Wabanaki, and my stay in the verdant rolling hills of what is now known as the Upper Valley of the Connecticut has been most enjoyable.

The work in this Dissertation would not have been done had it not been for colleagues around the world willing to entertain my frequent curiosities. In particular I’d like to acknowledge the Rosetta Alice team for bringing me on as an undergrad and fostering my interest in studying comets in the UV. Without their assistance and patience with my unbridled excitement about working on a spacecraft mission I’m not sure I would have been in this position today. For that, Alan Stern, Joel Parker, Paul Feldman, Mike A’Hearn, Lori Feaga, Matthew Knight, Hal Weaver, Andrew Steffl, Jean-Loup Bertaux, Brian Keeney, Rebecca Schindhelm, Jon Pineau, and Ron Vervack have my deepest thanks.

A large part of my enjoyment of graduate school derives from the people that were around me. The students, faculty, post-docs, research scientists, laboratory techs, business office, and custodial staff were all instrumental in my development of this thesis, whether it was via discussions at journal club, assistance in the lab, or with grant submissions. In particular I’m incredibly grateful for the best roommates/neighbor partners in crime/science that I could have wished for, Patrick O’Brien, Ben Sharkey, and Teddy Kareta. My time in Tucson was enriched beyond measure thanks to their willingness to stare at plots, eat gyros and pho, go out for beers at the drop of a hat, and doodle on whiteboards. In truth they have all shaped my approach to this thesis in different ways, ways that I will forever use to improve the quality of my work.

My time at the Lunar and Planetary Laboratory was made most enjoyable in large part to my LPL advisors and mentors, Walt Harris, Vishnu Reddy, Kat Volk, and Erik Asphaug. I’ve worked with each of them on a varying number of projects ranging from UV observations with Hubble to dynamical simulations of asteroids to impact simulations on the asteroid Ryugu. In each case, it’s been something out of my wheelhouse and new, daunting on its face but made enjoyable by the easy-going
and incredibly helpful nature of each of them.

Without the incredible assistance of the remaining committee member, Dennis Bodewits, who I first met as an undergrad, I’m not sure that I ever would have tried to use the Hubble Space Telescope at all. Our research history together has produced an incredible range of proposals and projects thus far, and I’m eager to see what intersection of atomic physics and observational astronomy our sights land on in the future.

Thanks to the guidance from Dr. Bodewits, some data in this thesis is from observations made by the NASA/ESA/CSA Hubble Space Telescope and obtained at the Space Telescope Science Institute, which is operated by the Association of Universities for Research in Astronomy. While the more typical acknowledgement can be found in the relevant chapter, I’d like to extend my sincere thanks to Alison Vick, Tom Brown, Tony Sohn, and William Fischer for helping schedule and execute these challenging observations. I’m grateful to be able to work with such an incredible telescope and instrument suite.

I’d like to acknowledge my family, Rossi and Noonan alike. Their unwavering support throughout this nearly three decades long education has meant so much to me, and I’m thrilled to bring it to a conclusion. For my aunts and uncles who requested printed copies of this Dissertation, I sure hope I was able to get them printed. To my parents, the complete lack of pressure you placed on me allowed me to define my own boundaries and find my own way, and for that I am incredibly grateful. To Kaia, the most driven sister I could ever hope for, thanks for pushing me to find my own path as I watched you forge your own. Finally, to Allie, my best friend and partner in life, who helped me fine tune papers, proposals, presentations, and plots, who has been an absolute pillar of strength in this 10 year process while simultaneously pursuing her own doctorate, thanks for your brilliance and wisdom.
DEDICATION

For my family.
# Table of Contents

LIST OF FIGURES ........................................................................... 10

LIST OF TABLES ........................................................................ 22

ABSTRACT .................................................................................. 24

CHAPTER 1 Introduction ................................................................. 26
  1.1 The Comet Cipher ............................................................... 26
  1.2 Comets in Context ............................................................... 28
    1.2.1 Early Solar System Formation ...................................... 29
    1.2.2 Forming the Modern Solar System ............................. 33
    1.2.3 The Planetesimals ...................................................... 38
  1.3 The Physics of Comet Activity ............................................. 49
    1.3.1 Orbital Evolution and Thermal Processing of Jupiter Family Comets ................................................................. 50
    1.3.2 Tools for Characterizing Cometary Activity ................. 57
    1.3.3 Emission Physics in Cometary Atmospheres ............... 62
  1.4 UV Comet Observations ....................................................... 70
    1.4.1 UV Comet Observations in History ............................ 72
    1.4.2 UV Comet Observations At Large and Small Scales: Goals of the Alice UVS ...................................................... 76
  1.5 Motivation and Organization of this dissertation ................. 78

CHAPTER 2 Analysis of Hybrid Gas-Dust Outbursts Observed at 67P/Churyumov-Gerasimenko ......................................................... 81
  2.1 Introduction ........................................................................ 81
  2.2 Observations ...................................................................... 85
    2.2.1 Geometry and Spacecraft Pointing ............................ 85
    2.2.2 Alice Instrument Description .................................... 85
    2.2.3 Alice Dataset .......................................................... 86
    2.2.4 VIRTIS-M Instrument Description ........................... 86
  2.3 ALICE Results: Gas properties ............................................ 91
    2.3.1 Spectra ................................................................. 91
    2.3.2 Light Curves .......................................................... 94
    2.3.3 Spatial Profiles ....................................................... 96
  2.4 VIRTIS Results: Dust properties ......................................... 97
TABLE OF CONTENTS — Continued

2.4.1 Outburst morphology and light curves ........................................... 100
2.4.2 Color .......................................................................................... 103
2.5 Additional Datasets ............................................................................ 104
  2.5.1 OSIRIS Images ................................................................. 104
  2.5.2 NAVCAM Images .......................................................... 109
2.6 Discussion ......................................................................................... 109
  2.6.1 Excitation Mechanisms .......................................................... 109
  2.6.2 Gas Composition ................................................................. 113
  2.6.3 Outburst Location ................................................................. 117
  2.6.4 Comparing Alice and VIRTIS-M ............................................. 118
2.7 Summary ............................................................................................ 123
2.8 Acknowledgements ............................................................................. 125

CHAPTER 3 Spatial Distribution of Ultraviolet Emission from Cometary Activity at 67P/Churyumov-Gerasimenko ................................................................. 127
  3.1 Introduction .................................................................................... 127
  3.2 Observations .................................................................................... 130
    3.2.1 Instrument Description ........................................................... 130
    3.2.2 Geometry and Spacecraft Pointing .......................................... 130
  3.3 Mapping Methods ............................................................................ 133
    3.3.1 NAVCAM Correlation ........................................................... 134
  3.4 Results ............................................................................................ 138
    3.4.1 Spectra .................................................................................... 138
    3.4.2 Light Curves ............................................................................ 141
    3.4.3 Emission Mapping ................................................................. 143
    3.4.4 Correlation to VIRTIS and MIRO ............................................. 145
  3.5 Discussion ........................................................................................ 152
    3.5.1 Morphology ............................................................................ 157
    3.5.2 Composition ............................................................................ 159
    3.5.3 Excitation Processes ............................................................... 163
  3.6 Summary ........................................................................................... 165
  3.7 Acknowledgements ........................................................................... 166

CHAPTER 4 Ultraviolet observations of Coronal Mass Ejection impact on comet 67P/Churyumov-Gerasimenko by Rosetta Alice ..................................................... 167
  4.1 Introduction ....................................................................................... 167
  4.2 The Alice Spectrograph .................................................................... 169
  4.3 Observations and Analysis ................................................................. 169
    4.3.1 Alice Observations ................................................................. 171
TABLE OF CONTENTS – Continued

4.3.2 Geometry and Spacecraft Pointing ........................................ 174
4.3.3 Complementary Observations ............................................. 176
4.3.4 Dissociative Electron Impact Analysis ................................. 177
4.4 Results .................................................................................. 181
  4.4.1 Concurrent Electron Density Measurements ......................... 181
  4.4.2 Spectra ........................................................................... 186
4.5 Discussion ............................................................................. 189
  4.5.1 Electron Impact Emission ................................................... 189
  4.5.2 $O_2$ in the Coma ............................................................... 194
4.6 Summary .............................................................................. 195
4.7 Acknowledgements ................................................................. 196

CHAPTER 5 FUV Observations of the Inner Coma of 46P/Wirtanen ...... 197
  5.1 Introduction ........................................................................... 197
  5.2 Observations ....................................................................... 200
    5.2.1 Data Reduction ................................................................. 203
  5.3 Results .................................................................................. 204
    5.3.1 Spectra ........................................................................... 204
    5.3.2 Coma Emission Modeling ................................................. 206
  5.4 Discussion ............................................................................. 215
    5.4.1 Upper limits on CO Abundance ...................................... 216
    5.4.2 Upper limits on dissociative electron impact emission ....... 217
    5.4.3 Atomic emission ............................................................... 218
  5.5 Summary .............................................................................. 226

CHAPTER 6 Conclusions and Evaluations ...................................... 228
  6.1 Connecting Emissions to Cometary Compositions and Formation .. 228
    6.1.1 Outburst Influences on FUV Cometary Spectra ................. 229
    6.1.2 $O_2$ in the Cometary Coma ............................................. 231
    6.1.3 The HST Bottleneck .......................................................... 232
  6.2 Future Studies with New and Existing FUV Comet Data ............ 234
    6.2.1 Comparison to UV Protoplanetary Disk Observations ......... 235
    6.2.2 The Cometary Sulfur Question ........................................ 237
    6.2.3 The Solar Flashlight .......................................................... 238
  6.3 More Questions than Answers ................................................. 240

APPENDIX A Calculating Photo-fluorescence Efficiencies .................. 242
TABLE OF CONTENTS – Continued

APPENDIX B  Calculating Plasma Dependent Emission Efficiencies . . . . . . 245
  B.1 Dissociative Electron Impact Emissions . . . . . . . . . . . . . . . . . . 245
  B.2 Recombination Emission . . . . . . . . . . . . . . . . . . . . . . . . . . 246
  B.3 Determining Relative Neutral Abundances for Noonan et al. (2018) . 247

REFERENCES . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . 250
<table>
<thead>
<tr>
<th>Figure</th>
<th>Description</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.1</td>
<td>Diagram detailing the components of a typical 1 M☉ T Tauri disk as a function of radius from star and height above the disk midplane adapted from Dutrey et al. (2014). The photon dominated region, where the volume density is approximately 200-300 cm⁻³ is labeled. Two solid black lines represent isotherms at 17 and 20 K, respectively. Note in particular the high temperatures and low densities where cosmic ray and UV radiation is dominant along the hot “atmosphere” of the disk that is exposed, while the cooler molecular layer and mid-plane of the disk have densities between 5 and 7 orders of magnitude higher, depending on the radius. respectively.</td>
<td>34</td>
</tr>
<tr>
<td>1.2</td>
<td>Semi-major axis and perihelion distribution of known comets, Centaurs, and KBOs as queried from the Minor Planet Center in November of 2021. The intensity color bar shows the Tisserand parameter for each object, as calculated in Equation 1.2. Note the clustering of T_J ≤3 at low semi-major axes and moderate perihelion.</td>
<td>47</td>
</tr>
<tr>
<td>1.3</td>
<td>Semi-major axis and inclination distribution of known comets, Centaurs, and KBOs as queried from the Minor Planet Center in November of 2021. The intensity color bar shows the Tisserand parameter for each object, as calculated in Equation 1.2. Note the clustering of T_J ≤3 at low semi-major axes and low inclinations.</td>
<td>48</td>
</tr>
<tr>
<td>1.4</td>
<td>Plots detailing the sublimation rate of H₂O,CO₂,CO for an idealized comet with Bond albedo of 0.04 and emissivity of of 0.9. Parameters are taken from Prialnik et al. (2004), plot styled after Delsemme (1982) and Meech and Svoren (2004).</td>
<td>54</td>
</tr>
<tr>
<td>1.5</td>
<td>Results of a simple Rebound simulation (Rein and Liu, 2012) showing the semi-major axis (black), perihelion (magenta), and eccentricity of a sample of 100 comets placed into near circular orbits just beyond Jupiter (i.e. Centaurs) allowed to evolve dynamically with the Sun, Jupiter, Saturn, Uranus, and Neptune perturbing their orbits for 10,000 years. Comets are scattered both inward and outward from these orbits, evolving into JFCs and back into Centaurs. Note in particular that the perihelion of this population is never raised beyond the initial value on this timescale.</td>
<td>55</td>
</tr>
</tbody>
</table>
1.6 Idealized production rates for four Centaurs from the Rebound simulation shown in Figure 1.5 transitioning between the Centaur and JFC populations. A radius of 5000 meters, a Bond albedo of 0.04, an emissivity of 0.9, and an active area that is 5% of the total surface area for H$_2$O, CO, CO$_2$ is assumed. The semi-major axis is plotted with a faint blue line for context. Rotation rate and solar incidence angle effects are ignored for simplicity. 56

1.7 Comparison of a 2-component Haser model and a vectorial model for the distribution of OH from a H$_2$O parent for a comet with a $Q_{H_2O}$ of $10^{28}$ mol s$^{-1}$ at 0.87 au, as is the test case described in Festou (1981). 61

1.8 An example set of modeled resonance fluorescence and dissociative electron impact spectra overlaid on a typical FUV comet coma spectrum from 67P/Churyumov-Gerasimenko by the R-Alice spectrograph. The plot on the left shows modeled contributions from individual sources (dissociative electron impact and resonance fluorescence), and the plot on the right shows only the model added to a solar continuum spectrum vs. the observed cometary spectrum. Note that the line shape of the hydrogen Lyman-α feature at 1216 Å is substantially lower than predicted. This is due to gain sag of the R-Alice detector, and renders that area of the detector less sensitive to incoming Lyman-α photons. 71

2.1 NAVCAM images from November 7 at 15:11, 17:15, and 19:18 UTC with nucleus pixels masked to highlight faint activity. The Alice slit is overlaid in white. The Sun is to the right in all three images. With the exception of faint jets emanating from the neck in image c) there is no evidence of significant background activity. 87

2.2 The figure shows the configuration of the nucleus of the comet and outburst with respect to the VIRTIS-M slit (horizontal red line) and its scan direction (red arrow). The VIRTIS-M data cubes are acquired with a scan in which each line corresponds to a given time (white arrows). The orange thick line shows the Sun direction. The spacecraft is approximately in a terminator orbit with a phase angle of 90°, so that one side of the comet is illuminated by the Sun and the other side is in darkness. 88
2.3 VIRTIS-M images taken between 15:04 and 18:49 UTC on November 7. The maps are composite images where the comet nucleus image (taken as an average in the wavelength range between 0.45 and 0.55 μm) is superimposed on the maps of the dust continuum at 0.55 μm to highlight activity and the Sun is always at the top of each image. The images on the top of each VIRTIS-M image show the configuration of the nucleus with respect to the VIRTIS-M frames (green rectangles) and the Alice slit in red from the Rosetta 3D tool. Frames 2 and 4 correspond to outbursts A and B, respectively, with both notable extensions and intensities of dust relative to the other frames. The radiance has units of W m⁻² sr⁻¹ μm⁻¹. The cube details are listed in Table 2.1.

2.4 Spectra derived from rows 15-18 taken during a quiescent period, the VIRTIS-M outburst detections, and near-alignment of a cometary jet with the Alice slit on November 7. Of particular interest is the O I] 1356 and O II304 ratio, indicative of dissociative electron impact. Spectra are offset by 2.5 photons cm⁻² s⁻¹ Å⁻¹. There is also faint CO Fourth Positive emission in the 1400 Å to 1600 Å region mixed with emission from dissociative electron impact excitation of CO₂, discussed further in Section 2.6. Errorbars are plotted but are largely smaller than the line-width at wavelengths less than 1800 Å.

2.5 Difference spectra resulting from the subtraction of the 15:04 UTC spectrum from the 16:07 and 17:32 UTC spectra on November 7. Spectra are offset by 2.5 photons cm⁻² s⁻¹ Å⁻¹. Notice the substantial difference in O I] 1356/O II304 Å emission between VIRTIS-M outbursts A and B.

2.6 Light curves for dominant atomic emission features between 12:00 and 20:00 UTC on November 7, integrated over rows 15-18 on the Alice detector. Errorbars on each point are driven by variation between rows, which is amplified by the odd-even detector effect. The observation used for quiescent subtraction is marked with a black dot-and-dashed line, observations coinciding with VIRTIS-M outburst detections are marked with blue lines for outbursts A and B at 16:07 and 17:32 UTC, respectively. The observation of the nearly in-slit jet is marked with a red dashed line.
LIST OF FIGURES – Continued

2.7 Spatial profiles of dominant emission features in Alice spectra at 15:04, 16:07, 17:32, and 19:18 UTC. The sunward direction is in the $+X$ direction. Each detector row subtends approximately 1.2 km. Of particular note is the change in slope for O I] 1356 Å between quiescent, initial activity at 17:32 UTC, and the parallel jet observation at 19:18 UTC between 0 and 12 km. 98

2.8 Light curves of the outbursts A (left) and B (right) acquired on November 7. The multicolor curves are the VM radiance at 0.55 μm multiplied by the distance from the comet center. The images on the top show the VM image frame for the observations A and B, and the yellow lines show where the lightcurve profiles have been extracted. The colorbar used for the VM light curves refer to the distance from the comet center and not the intensity displayed in the upper plots. For reference, a flatter curve represents a more linear relationship between radiances and distance from comet center. The deviations present at 16:13 UTC and 17:33 UTC are interpreted as the start of the outbursts. 101

2.9 Images of the outburst of November 7 in the VIS at 0.55 μm (upper plots) and the VIS spatial distribution of the color (lower plots) calculated in the yellow square of the dust image. The colorbar used for the VM color maps refer to $\% (100 \text{ nm})^{-1}$ for the cometary dust in the lower plots and not the intensity displayed in the upper plots. The location of maximum radiances, assumed to be the outburst source, has been marked with a red star. Ejecta from outburst A or B do not display any evident color gradient, unlike other outbursts observed by VM (Rinaldi et al., 2018). 102

2.10 Three OSIRIS NAC images with 0.675 s exposure times taken between 15:05 and 16:15 UTC on November 7. The overexposed nucleus has been masked in the images to highlight activity and the Sun is to the right in these images. Both the top and middle image are taken during periods of typical cometary activity. The top corresponds with the Alice spectrum taken at 15:04 UTC in Figure 2.4, which is used for Alice quiescent subtraction. The image in the middle was taken 15 minutes prior to the Alice outburst detected in the 16:07 UTC Alice spectrum and the outburst imaged at 16:15 by OSIRIS, which is displayed in the bottom image. The Alice slit is overlaid in white with the approximate location of row 15 identified. 106
2.11 Image displaying the change in irradiance between OSIRIS NAC observations at 16:04 and 16:13 UTC on November 7. The Sun is to the right in the image. The exposure taken at 16:04 UTC has been subtracted from the 16:14 UTC exposure to show the change in activity levels. Between the two images the comet nucleus rotated approximately 5°, leading to some artifacts in the difference image on the masked surface.

2.12 Image showing a close-up of the change in limb activity in Figure 2.11 with a shifted color scheme to highlight the outburst’s fine structure. Note that four distinct areas are all active at 16:14 that were not at 16:04 UTC. The area integrated for outburst brightness as described in Vincent et al. (2016) is shown by a white trapezoid.

2.13 NAVCAM image from November 7 at 19:18 UTC, with Alice slit overlay in red. Subfigures b) and c) have been stretched to show cometary activity in the southern hemisphere. The slit was aligned with the activity at that time. The spectrum is shown in Figure 2.4. This geometry is representative of the stable pointing scheme. For this period the Alice slit subtends 22 km at the nucleus distance, approximately 1.2 km per pixel. The white vector in the image denotes the rotational axis of 67P. The Sun is to the right in all three images.

2.14 Alice quiescent-subtracted spectra showing the spectrum near outburst A (a), outburst B (b), and the outburst and/or jet (c). The spectrum from 15:04 UTC shown in Figure 2.4 is used as the quiescent spectrum. The modeled relative molecular abundances are reported in Table 2.4.

2.15 Source regions of the outbursts detected by VIRTIS-M. The red and yellow rectangles correspond to the outbursts A and B, respectively. The map is centered on the small lobe, the big lobe covers the left-hand and right-hand side of the map, and the contact area between the two lobes covers mainly the top of the map (regions Hapi and Seth). The boundary regions, shown in the map, have been defined by El-Maarry et al. (2015); El-Maarry et al. (2016).
2.16 Brightness in Rayleighs for row 16 of the Alice detector, integrated between 1850 and 1950 Å. Vertical lines represent quiescent (black dot-dash), outburst (blue solid), and jet (red dashed) observations. For this period of stable pointing row 16 was just off of the nucleus limb and only contains solar continuum emission reflected off dust. Of particular note are the $\sim\!36\%$ and $\sim\!22\%$ increases in brightnesses over the previous continuum measurements for outbursts A and B, respectively. Error bars on each measurement are smaller than the size of the points.

3.1 NAVCAM image from November 7 at 19:18 UTC with nucleus pixels masked to highlight faint activity. The rotation axis of 67P is marked with a white arrow. The Alice slit is overlaid in red and the Sun is to the right. With the exception of faint jets emanating from the neck there is no evidence of background activity.

3.2 Series of plots depicting the mapping method described in Section 3.3. The top figure depicts the average location of each row of the Alice detector for each observation in block 1 from Table 3.1, with the color scheme detailing the row number (row 5 is dark purple, on the left, row 23 is yellow, on the right). The figure second from the top shows the interpolation of the rows to a grid with a pixel size defined by the pixel size of each row and the scan rate of the Alice detector. The figure third from the top details the initial map that is generated by the program before any correction is applied to shift the measured reflected solar signal to center on the nucleus. The bottom figure shows the solar reflectance map for block 1 after the weighted barycenter shift has been applied. The Sun is to the right (+X) in this and all maps presented.
3.3 Stable pointing spectra from rows 18-23 taken during a quiescent period (black), a jet observation (magenta), and just following a large activity increase on November 7 (cyan). Flux error is plotted but is smaller than the plotted line width. Of particular interest is the O I] 1356 and O II]304 ratio, indicative of dissociative electron impact. Spectra are offset by 3 photons cm\(^{-2}\) s\(^{-1}\) Å\(^{-1}\). Rows 18-23 are between 5 and 11 km in the sunward direction from the nucleus center for these times. There is also faint CO Fourth Positive emission in the 1400 Å to 1600 Å region mixed with emission from dissociative electron impact excitation of CO\(_2\), discussed further in Section 3.5. Note the non-Gaussian shape of Lyman-\(\alpha\) due to gain sag of the Alice detector, rendering it inadequate for diagnostic purposes. Other notable features not analyzed in this chapter are labeled with a smaller font.

3.4 Difference spectra resulting from the subtraction of the 15:04 UTC spectrum from the 19:18 and 21:27 UTC spectra on November 7. Notice the substantial difference in O I] 1356/O II]304 Å emission, as well as the minimal contribution from the CO Fourth Positive group despite an increase in C I emission.

3.5 Light curves for dominant atomic emission features during all observing blocks listed in Table 3.1, plotted by rows over which the brightness is calculated. Only emissions in rows 18 through 23 are co-added to maximize coma signal. The displayed errorbars are largely the result of brightness variations between rows, in addition to the odd-even detector effect. The dotted and dashed vertical line marks the quiescent spectrum, the blue vertical lines mark two outbursts discussed in Noonan et al. (2021c), and the red dashed vertical line marks the nearLyman-aligned jet observation that is referenced here and discussed further in Noonan et al. (2021c).

3.6 Emission maps created from Alice observations taken between 21:16 and 22:07 UTC on November 7 (observing block 2). The sunward direction is to the right. The weighted intensity barycenter of off-nucleus emission is marked with a white star in each map. The color bar marks 0 to 75 Rayleighs. Contours on the plot mark 10 Rayleigh isophotes. The overlaid NAVCAM image was taken at 21:18 UTC November 7. Error on brightnesses is at most ∼5 Rayleighs for displayed brightnesses, error on pixel position is ±1.2 km, approximately the size of an Alice pixel subtended at the nucleus.
3.7 Emission maps created from Alice observations taken between 22:13 and 22:59 UTC on November 7 (observing block 3). The sunward direction is to the right. The weighted intensity barycenter of off-nucleus emission is marked with a white star in each map. The color bar marks 0 to 75 Rayleighs. Contours on the plot mark 10 Rayleigh isophotes. The overlaid NAVCAM image was taken at 23:40 UTC November 7. Error on brightnesses is at most ∼5 Rayleighs for displayed brightnesses, error on pixel position is ±1.2 km, approximately the size of an Alice pixel subtended at the nucleus. 

3.8 Emission maps created from Alice observations taken between 23:04 and 23:56 UTC on November 7 (observing block 4). The sunward direction is to the right. The weighted intensity barycenter of off-nucleus emission is marked with a white star in each map. The color bar marks 0 to 75 Rayleighs. Contours on the plot mark 10 Rayleigh isophotes. The overlaid NAVCAM image was taken at 23:40 UTC November 7. Error on brightnesses is at most ∼5 Rayleighs for displayed brightnesses, error on pixel position is ±1.2 km, approximately the size of an Alice pixel subtended at the nucleus. 

3.9 Emission maps created from Alice observations taken between 02:04 and 02:55 UTC on November 8 (observing block 7). The sunward direction is to the right. The weighted intensity barycenter of off-nucleus emission is marked with a white star in each map. The color bar marks 0 to 75 Rayleighs. Contours on the plot mark 10 Rayleigh isophotes. The overlaid NAVCAM image was taken at 01:20 UTC November 7. Error on brightnesses is at most ∼5 Rayleighs for displayed brightnesses, error on pixel position is ±1.2 km, approximately the size of an Alice pixel subtended at the nucleus. 

3.10 VIRTIS-H - $H_2O$ 2.7 $\mu$m band maps. Data on nucleus acquisitions are shown as white dots to outline the nucleus shape and are used in map generation. The colorbar shows the intensity of the water emission feature. The white line extends the rotation axis from the south pole. The sunward direction is to the right (see yellow sun). Note the difference in field of view (FOV) compared to Alice maps in Figures 3.6-3.9. 

3.11 VIRTIS-H - $CO_2$ 4.27 $\mu$m band maps. Data on nucleus are not included to minimize signal from the nucleus and are shown as white dots. The colorbar shows the intensity of the emission feature. The white line extends the rotation axis from the south pole. The sunward direction is to the right (see yellow sun).
LIST OF FIGURES – Continued

3.12 Maps derived from MIRO line areas of the (110-101) transition of H$_2^{18}$O for November 7 20:55 UTC to November 8 10:24 UTC. An outline of the nucleus is shown in white at the correct position and scale for the midpoint of the scan. The line is mostly in absorption against the nucleus; black regions correspond to negative line areas where water appears in absorption. Discrepancy between the white outline and black region is the result of the long duration for the raster scan to acquire the full frame, during which the nucleus will rotate. The sunward direction is to the right in each panel. . . . . . . 154

3.13 Spatial profiles of an earlier jet (a) and of map 1 (b). The spatial profile derived from map 1 is the X=0.5 km row of the emission map, shown in Fig. 3.6. The sunward direction is in the +X direction. Each detector row subtends approximately 1.2 km. Of particular interest is the extension of enhanced O I 1356 Å emission to approximately 10 km in the activity maps, with brightnesses approaching 60 Rayleighs, and the slope similarity of the three emission features which indicates they share the same emission process, dissociative electron impact emission. Compare to Figure 4 of Feldman et al. (2016). Note that 1σ errors on each brightness are less than 5%. . . . . . . . . . . . . . 155

3.14 Alice quiescent-subtracted spectra showing the post-activity onset near-nucleus coma. The spectrum from 15:04 UTC shown in Figure 3.3 is used as the quiescent spectrum. The relative abundances of CO$_2$ and O$_2$ are listed in Table 3.2. Note that Lyman-α emission is omitted from fitting due to gain sag of the detector. . . . . . . . . . . . . . 156

4.1 A Rosetta NavCam image taken on 2015 October 5 at 23:45:02, just prior to the CME impact, with the Alice slit overlaid. The Sun is toward the top, illuminating portions of both the head and body of 67P. The flattest “underside” portion of the body is facing Rosetta. At this time the full length of the Alice slit subtends 76 km at the nucleus distance, approximately 4.2 km per pixel. (Image Credit: NAVCAM) . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . 170

4.2 Top: Alice spectrum before CME impact taken at 00:38:59 UTC 5 October with similar, though not identical, pointing to the CME impact period. Reflected sunlight from the nucleus can be seen in the 1700–2100 Å area of rows 17 and 18. Bottom: Alice spectrum during CME impact taken at 00:17:38 UTC 6 October. . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . 172
LIST OF FIGURES – Continued

4.3 Top: Three spectra taken by the Alice instrument during similar pointing instances but with three distinct emission signatures. All spectra are made using rows 13-17, representing the rows closest to the nucleus. Integration time for each image is stated in the legend. Statistical uncertainties are plotted but are smaller than the line thickness. Bottom: The first and second emission spikes with the quiescent spectrum subtracted are plotted. Notice the increase in Lyman-β emission between the first and second emission spikes. . . . 173

4.4 Brightness vs. Time for October 5–6. All times displayed are in UTC. Gaps in data indicate periods where the Alice slit was more than 1 degree off of nadir or was not taking data. The nucleus is closest to rows 13–17 for this period, with rows 18–22 capturing sunward coma and rows 8–12 capturing anti-sunward coma. Rows closest to the nucleus see the strongest emission, followed by the sunward and anti-sunward coma. The solid angle differences for rows 12 and 18 are corrected for in the brightness calculation. The largest relative increase in emission occurs for O I 1356 Å. 1-σ error bars are not plotted but are between 1–7 Rayleighs. . . . . . . . . . . . . . . . . . . . 179

4.5 The quiescent and background-subtracted spectrum from the second spike with dissociative electron impact of H₂O and CO₂ (e+H₂O and e+CO₂) model spectra. The expected emission from O I 1304 Å and O I 1356 Å from these two sources is then subtracted from the total, as shown in Equations 4.1 and 4.2. . . . . . . . . . . . . . . . . . . . . . . . . . 180

4.6 Comparison of Alice O I 1356 Å emission from rows 13–17 (blue stars) with the warm (5–100 eV) electron density (red triangles) as defined by Broiles et al. (2016b) and Broiles et al. (2016a) from the IES instrument. The x axis begins at the start of the CME as reported by the RPC magnetometer in Edberg et al. (2016b). O II1356 Å measurements that may indicate a possible outburst are marked. This possible outburst time coincides with slightly elevated electron fluxes that may be indicative of an outburst as well. Labels 1 and 2 denote the two electron spikes that coincide with spikes in O I 1356 Å emission. Spectra with an off nadir angle less than 1° are used to create the plot. . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . 182
LIST OF FIGURES – Continued

4.7 Emission line ratios as a function of time from rows 13-17. Labels 1 and 2 mark the same boundaries for electron spikes as in Figure 4.6. The x-axis starts at the time of the first RPC detection of the CME arrival at 20:15 UTC. Of particular interest is the O I 1304/1356 Å ratio near 1 during the impact, the drop in C II 1657/Lyman-β Å, and the increase to Lyman-β/O I 1304 Å and O I 1304/1356 Å ratios during the secondary outburst.

5.1 Diagram showing approximate points of the COS aperture for each of the settings described in Table 5.1 relative to the coma of 46P. Each white circle represents the field-view-of the COS aperture subtended at Δ=0.22 au and the radius of the full image is 12", approximately 1910 km. The background image is a simple Haser model for H₂O at rₜ = 1.18 au, which was not observed in the COS bandpass, to provide context for the type of flux decrease that was expected if dissociative electron impact emission were present. The image is independent of production rate and thus has units of s cm⁻². The offset direction is not necessarily representative of the as-executed offset angle.

5.2 Co-added spectra with 39 pixel binning to improve signal in emission features with low flux, specifically Lyman-β near 1026 Å. Note that only Lyman-α at 1215.7 Å, is easily identifiable. An enlarged high resolution profile of Lyman-α is presented in Figure 5.4.

5.3 Co-added spectra with 13 pixel binning to improve signal in emission features with low flux. In addition to Lyman-α emissions at 1215.7 Å the O I 1302 Å multiplet is easily identified and presented in Figure 5.6. With the exception of S I 1425 Å, shown enlarged in Figure 5.7, no other significant atomic or molecular emissions were identified.

5.4 Profile of the Lyman-α emission for each co-added pointing and central wavelength setting with no binning applied. The contribution of geocoronal and interplanetary hydrogen emission to the cometary spectrum is relatively constant for each offset and is minimal, if not negligible.

5.5 Profile of the Lyman-α emission for the two comet-centered co-added spectra and central wavelength setting with no binning applied. A gaussian fit to the data is plotted and the residuals resulting from subtracting the model from the data are plotted below.

5.6 Enlarged section of Figure 5.3 to show O I triplet emission between 1302 and 1306 Å. This spectrum has only been binned by a factor of 3 to show line profiles and relative shapes.
5.7 Enlarged section of Figure 5.3 to show S II 1425 Å emission. . . . . . . 211
5.8 Enlarged section of Figure 5.3 with 13-pixel binning to show lack of CO Fourth Positive Group emissions between 1350 and 1420 Å. CO emission features at 1368, 1384, 1392, and 1420 Å are absent. . . . . . 211
5.9 Normalized ratio of O I triplet emission at 1302, 1304, and 1306 Å for co-added spectra at each pointing offset in arcseconds. In general the O $^3S^0$ J=2 to the O $^3P$ J=1 transition at 1302 Å becomes more populated as the offset increases, but the line ratios are never in good agreement with the ratios defined by the known $A$ values (Kramida et al., 2019). The expected ratios for $A_I/\sum A_n$ are shown with a solid black line for O I 1302 Å, a dot-dash line for O I 1305 Å, and a dotted line for O I 1306 Å. Errorbars are smaller than the markers. . . . . . . 223
## LIST OF TABLES

<table>
<thead>
<tr>
<th>Table</th>
<th>Title</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.1</td>
<td>VIRTIS-M observations contemporary with Alice observations</td>
<td>84</td>
</tr>
<tr>
<td>2.2</td>
<td>Dust outburst properties in the VIRTIS-M VIS channel</td>
<td>99</td>
</tr>
<tr>
<td>2.3</td>
<td>OSIRIS Narrow Angle Camera observations used in this work</td>
<td>104</td>
</tr>
<tr>
<td>2.4</td>
<td>Modelled relative abundances for $\text{H}_2\text{O}$, $\text{CO}_2$, and $\text{O}_2$ for the quiescent-subtracted spectra shown in Figures 2.14, 2.14, and 2.14. The error-bars on these modelled relative abundances are between 30 and 35%, the result of uncertainties in emission brightness, emission cross section ratio measurements in the literature, and to a lesser degree, the model fitting error. Errors are higher for lower Lyman-$\beta$ brightnesses, as this increases the brightness measurement uncertainty for the determination of the baseline $\text{H}_2\text{O}$, by definition set to 1 to find the relative abundances of $\text{CO}_2$ and $\text{O}_2$.</td>
<td>114</td>
</tr>
<tr>
<td>3.1</td>
<td>Dust outburst properties in the VIRTIS-M VIS channel</td>
<td>137</td>
</tr>
<tr>
<td>3.2</td>
<td>Modelled abundances for $\text{CO}_2$ and $\text{O}_2$ relative to $\text{H}_2\text{O}$ derived from quiescent-subtracted spectra shown in Figure 3.14. Errors for $\text{CO}_2$/H$_2$O are approximately 30% for observing blocks 2, 3, and 4 and closer to 45% for observing block 6 due to the decreased signal in Lyman-$\beta$. Errors for $\text{O}_2$/H$_2$O are higher due to errors induced by residual subtraction and are near 40-45% for observing blocks 2, 3, and 4 and closer to 55% for observing block 6. We conservatively adopt the error to be 50% for observing blocks 2, 3 and 4, accordingly. The errors on the ratios are calculated from the root mean square of the error in the data, fitting error, and error in laboratory measurements of the emission line used for relative intensity calibration. These are added in quadrature with the deviation in line ratios as a function of impacting electron energy. The last two sources of error are the same for each observation.</td>
<td>161</td>
</tr>
<tr>
<td>4.1</td>
<td>Electron impact emission line ratios for various gases and qualitative compositions relevant to cometary activity derived from Ajello (1971a), Ajello (1971c), Makarov et al. (2004), Kanik et al. (2003), and Mumma et al. (1972)</td>
<td>174</td>
</tr>
<tr>
<td>4.2</td>
<td>Observed emission line ratios for periods described in Sections 3 and 4</td>
<td>4185</td>
</tr>
<tr>
<td>4.3</td>
<td>Calculated $\text{O}_2$/H$_2$O abundances from the emission spikes described in Sections 4.3/4.4 and plotted in Figure 4.3.</td>
<td>191</td>
</tr>
</tbody>
</table>
### LIST OF TABLES – Continued

<table>
<thead>
<tr>
<th>Table</th>
<th>Description</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>5.1</td>
<td>46P/Wirtanen HST COS Observation Log</td>
<td>202</td>
</tr>
<tr>
<td>5.2</td>
<td>Derived column densities for H, O, and S in the near-nucleus coma of 46P/Wirtanen from COS data taken between January 8 and 20, 2019.</td>
<td>214</td>
</tr>
<tr>
<td>5.3</td>
<td>Measured production rates of common volatiles for 46P/Wirtanen during previous apparitions. References are 1) Fink et al. (1998), 2) Schulz et al. (1998), 3) Farnham and Schleicher (1998), 4) Altwegg et al. (1999), and 5) Stern et al. (1998).</td>
<td>216</td>
</tr>
</tbody>
</table>
The study of cometary activity as a strategy to probe the icy planetesimals from early solar system formation is a relatively new endeavor. The effort began in earnest after observational confirmation in the late 1960’s that the vast amounts of hydrogen and hydroxyl (OH) molecules in cometary comae are evidence of an icy object sublimating water into space. In the decades since, a key goal of solar system science has been to observe more comets with a wider array of techniques in order to constrain the initial molecular building blocks of our solar system, characterize composition patterns between comet types, and identify any peculiarities that may make our solar system more suitable for life than any other. However, cometary activity is an uncooperative partner in this investigation; at times the activity can be sporadic and weak, at other times explosive, and at far fewer times predictable. Understanding what processes can influence observations of cometary activity, specifically in the ultraviolet (UV) wavelengths of light, is the motivation for this Dissertation. Four projects are described in this work that probe how the UV emissions from two comets, 67P/Churyumov-Gerasimenko and 46P/Wirtanen, reflect the outgassing molecules from their surface and the processes that govern their emissions. Following an introduction about comet formation, dynamics, and observations, three chapters are dedicated to observations from the Alice UV spectrograph to investigate emission processes near (within 100s of km) the nucleus of 67P. The processes can range from outbursts of material from the cometary surface to outbursts of energetic plasma ejected from the Sun, revealing new science about the relevant scales for photon and collisional excitation mechanisms. The lessons learned from near-nucleus coma observations at 67P are then applied to 46P with a remote observing campaign using the Hubble Space Telescope to search for similar traces of the emission mechanism. Ultimately this Dissertation reflects on the
implications of the work on the larger astrophysical community and lays out future directions for UV comet research.
CHAPTER 1

Introduction

1.1 The Comet Cipher

Comets have always occupied a large part of the human interest in the skies, offering distinct rungs to climb for improving our understanding of the physical processes in our universe. This rather lofty statement may seem a touch poetic, but despite the prose it is grounded in science history. The theory of gravity was refined thanks to the passage of the Comet of 1680 (C/1680 V1), providing Isaac Newton with an eccentric orbit to characterize (Newton, 1848), the fluorescence of molecules like $\text{C}_2$ was first detected in cometary comae (Donati, 1864; Huggins, 1868), and the formulation of radiation pressure from the solar wind inferred from the morphology of comet dust tails (Bredichin, 1880; Bobrovnikoff, 1927). There is little doubt that some of the most substantial areas of progress in physics and spectroscopy are heavily influenced by comet observations.

Perhaps the close relationship between comets and refinements to physics are to be expected; with the notable exception of the planets, comets are some of the largest objects in the solar system thanks to their enormous tenuous gas atmospheres, or comae. These comae glow, or fluoresce, when exposed to the light from the Sun. The combination of reflected sunlight from dust and this fluorescence make them not only bright but extended objects easily tracked by the naked eye when bright enough. This last component is of key importance; it is the brightest comets that have always been the best measured, characterized, and (Zhou et al., 1996). When observing comets and their comae there is always an observational bias that needs to be acknowledged so that the observational results can be placed in the proper context. For nearly the entirety of human history comets have been used to understand physics at large. Since the advent of ultraviolet comet observations, in the last 50
years the challenge has been applying these physical frameworks to comets to more completely understand their composition, activity, and evolution. The motivation to accomplish this is driven by the hypothesis that comets are some of the best preserved building blocks of the early solar system that are readily available to study, ideally containing volatile compounds and thermally isolated materials that would unlock the process of planetary formation.

These two goals, obtaining a better understanding of the physics and chemistry that govern what is detected from comets in the modern day and using the measured compositions of comets to uncover the earliest days of our solar system’s formation, are intimately linked. Ideally comets would be thoroughly mixed, with the bulk composition of the whole object represented on the every smaller constituent size scale, and would evenly sublimate their contents to space as they warmed. The composition of the coma would be directly representative of the whole nucleus, and the nucleus directly representative of a specific region of the protoplanetary disk where it formed. Then with forward dynamical models of the early solar system, chemical maps of the protoplanetary disk could be generated based on an inventory of comet compositions, thanks to their well-behaved and consistently studied properties on a range of brightness scales. With such a map on hand to inform planetary formation models, we could begin to significantly constrain the formation of the Earth based on its own chemical abundance and the delivery of water to the Earth, both of which have proved critical to the generation of life. Alas, comets are decidedly not homogeneous, do not have any sort of consistent activity, and have defied expectations whenever a closer look has been taken by spacecraft during flyby or rendezvous missions. Comets are geological bodies shaped by evolutionary processes, each with their own individual history. To link observations of gas in the coma to the primitive history, an understanding of the storage and release of ices and volatiles, as well as the physical processes that form and excite the atoms and molecules in the coma.

This reality drives the majority of the work in this dissertation. In an attempt to prepare the reader for (and in many ways, remind myself) what the problem of
comet emissions and activity entails. I have brought together what I consider the most important elements driving this research in the introduction. Both sets of boundary conditions on the comet problem, the formation and the observed state, need to be described in detail to understand how one could influence the other. The next section of this introduction describes the formation and evolution of comets as described in the current literature, providing the reader with the essential facts and theories that govern the properties comets should have formed with. This subsection describes general stellar and protostellar disk formation theories, planetary and planetesimal formation, and the orbital evolution and processing of comets after their formation. Following this description of the early boundary conditions the next section then describes the necessary physics and chemistry that govern how comets are observed in their current orbits in this modern era. In the context of this particular dissertation I largely focus on the storage, release, and dissociation of volatile gases within comets as well as the emission mechanisms that produce the photons we observe. Previous observations of comets in the ultraviolet (UV) are described in the section after that, and the introduction is concluded with an overview of this Dissertation’s structure and motivation.

1.2 Comets in Context

As tempting as it is to dive headlong into the structure and physics of comets themselves, the abundance and variation of comets must be discussed first to sufficiently mitigate the deep-seated desire to solve the history of the solar system by observing and “solving” a single type of object. This dissertation focuses closely on two comets in particular, 46P/Wirtanen and 67P/Churyumov-Gerasimenko, both of which are some of the best characterized comets in the observational catalog. However, they are just two comets of the currently predicted billions in the solar system so it is necessary to place them in the context of the full comet population to correctly understand two issues; what information from these individual comets can be extrapolated to the broader comet population and what information provides a unique
insight into the formation of that particular comet.

To accomplish this contextualization, there are five questions that this introduction will seek to provide the background to. The questions are broad and intended to serve as anchor points for the reader to refer back to throughout the dissertation just as they served to guide the studies themselves.

1. Where do comets sit in the hierarchy of the solar system formation?

2. Why do we study them?

3. What properties do we hope to measure from them?

4. How do we study them?

5. What assumptions do we rely on?

Losing sight of these questions while studying comets leads to what has been referred to as “stamp collecting;" observing comets because we can but forgetting to tie the observed properties back to the larger picture of comet evolution, planetary formation, and solar system chemistry. With this in mind we can begin our brief review of the current state of cometary formation and evolution science and lay the foundation for this dissertation’ novel research.

1.2.1 Early Solar System Formation

The careful handling of cometary compositions as well as the inferences and connections that can be made to the solar system’s formation invites a brief overview of the current theories of early solar system formation; in order to fully understand the challenge presented, the rules and guidelines must be clearly outlined. In this case the rules and guidelines are informed by observations of the many interstellar clouds and protoplanetary disks that can be observed from Earth-based observatories. Studying the properties and evolution of nurseries for other solar systems ideally would yield clues about the initial formation of our own, but the extent to
which some of the same chemical abundances can be inferred is still not entirely known.

Planetary systems are formed as a result of the collapse of cloud cores within larger molecular clouds, which can be millions of solar masses in size and span hundreds of thousands of astronomical units ($\sim 1.49 \times 10^{13}$ km). These molecular clouds have compositions that are dominated by H$_2$, He, and CO, but have approximately 1% of their mass accounted for in small dust grains (Boss, 2004). These dust grains are critical for the collapse of smaller cloud cores, as they are efficient at cooling the surrounding gas and thereby decreasing the thermal pressure. This decrease of thermal pressure can no longer overcome the gravitational force of the cloud core’s mass, and the core begins to contract in a process defined by James Jeans, now known as “Jeans Collapse” (Jeans, 1902).

For a cloud core of a given temperature, $T_{\text{core}}$, the mass at which the core will begin to be collapse, or the Jeans mass, can be derived if the number density, $n$, of the core is known or assumed:

$$M_J = \sqrt{\frac{T_{\text{core}}^3}{n}}$$

(1.1)

The impact of larger densities of dust on protosolar, and perhaps protoplanetary, development can be seen in Equation 1.1; if dust acts as a radiator in molecular clouds and protoplanetary disks and decreases $T_{\text{core}}$, it effectively reduces the required mass for gravitational collapse proportional to $T_{\text{core}}^{3/2}$. As individual cloud cores reach Jeans masses proportional to their temperature and number density within the larger molecular cloud, protostellar cores with a wide range of initial masses will begin to take shape.

At the center of each of these young protostellar cores is an H$_2$ core, approximately 10 au in radius. On a timescale of approximately 1 million years (Larson, 1969) a protoplanetary disk forms around the protostellar core, conserving the initial angular momentum of the larger collapsing core. Infalling gas and dust moves to the midplane of this protoplanetary disk, damped by the gravitational attraction of the disk and interactions with other particles and molecules. The protoplanetary disk
also transfers mass to the protostellar core. As more gas and dust accretes onto this core and deposits energy, the temperature of the core is raised to the point where the molecular hydrogen making up the bulk of the protostellar core dissociates. The energy devoted to dissociating the molecular hydrogen lowers the temperature of the core, leading the core to contract until it is approximately 3 solar radii in size. At this stage the protostar is dominated by atomic H, and once its interior reaches 10 million K proton-proton fusion effectively begins. As mentioned previously, these protostellar cores are unlikely to happen in isolation within a molecular cloud, and a wide range of initial masses are seeded by thermal and magnetic instabilities. The formation of many stars in a nearby environment at a range of different sizes can have drastic effects on protoplanetary disk chemistry and lifetimes, even if the initial chemical compositions of protostellar clumps are essentially identical, due to the variability introduced by differing stellar radiation fields (Shu et al., 1993). These initial conditions set the stage for the development of the solar system.

The resulting protoplanetary disk has three distinguishable chemical zones, differentiated by their temperatures and density (Dutrey et al., 2014, Fig. 1.1). Working from the uppermost layer shown in Figure 1.1, we have the hot and diffuse photon dominated region (PDR). UV light from other stars in the birth cluster as well as cosmic rays heat this relatively thin region, preventing significant molecular growth and limiting the dominant species to those that can survive in such harsh radiation: atoms, ions, and the durable polycyclic hydrocarbons (PAHs). This region contains little dust, which settles nearer to the midplane of the disk, and thus very few gas-grain chemical interactions take place in this region. However, the strong ionization in the disk atmosphere helps drive a rich gas phase and gas-grain chemistry in the warm, but shielded, molecular layer of the disk. The combination of a small amount of UV/X-ray radiation penetrating the disk atmosphere as well as some turbulent mixing can begin to process the chemical abundances derived from the original cloud core; as the initial CO, CO$_2$, H$_2$O ices are liberated from grains, they can interact with newly produced ions capable of promoting rapid proton transfer and ion-molecule processions, spurring chemical evolution (Herbst
and Klemperer, 1973; Watson, 1974; Woodall et al., 2007; Wakelam et al., 2012).

Further shielded from outside radiation at the center of the disk, where the light from the central star cannot penetrate and cosmic rays and UV radiation from the surrounding stellar environment are absorbed in the outer zones, lies the cold midplane. Temperatures in this region are below 20 K, with only UV photons produced via local electron-neutral reactions and cosmic rays heating the environment. In this way the midplane chemistry mimics that of a dense molecular cloud core; most volatiles are frozen out onto dust grains, with some of the more volatile compounds like CO, N₂, and CH₄ capable of thermal desorption due to their low sublimation temperatures. This 5-7 orders of magnitude difference in density between the disk atmosphere and the central midplane, as well as the temperature difference, seed the early protoplanetary disk with a variety of chemical abundances that, ideally, would be reflected in the planetesimals formed from them.

As pointed out in Lunine and Gautier (2004), tracing three particular elements in protoplanetary disks is useful for cometary science: O, N, and S. Each of these elements is closely tied to a volatile species well known in both protoplanetary disks and comets and yield clues about the evolution of the protostellar disk chemistry. Oxygen is largely contained within H₂O, which is can be clearly seen as an important source of planetary construction in not only comets but their source populations like the Kuiper Belt as well. However, it is also important to note that several comets have been shown to have O sources dominated by other volatiles; McKay et al. (2019) showed that the activity of Oort Cloud comet C/2016 R2 (PanSTARRS) was dominated by CO₂ and CO gases rather than H₂O, while Bodewits et al. (2020) and Cordiner et al. (2020) showed that the production rates of CO from interstellar comet 2I/Borisov rivaled the water production rates. Given the expected abundance of H₂O relative to both CO₂ and CO in the disk, these observations show the complexity, and perhaps untapped nature, of the protoplanetary disk model. Mousis et al. (2021) showed the effect of “cold traps” near the CO ice line could supercharge the CO/H₂O ratio of individual objects with respect to the bulk disk, and Cleeves (2016) has shown that multiple CO ice lines are possible within a protoplanetary disk. Both
scenarios would facilitate formation of planetesimals with a large range of CO/H$_2$O ratios. Nitrogen presents an additional tether to the molecular cloud abundances, as it can be present in both an extremely volatile molecular form N$_2$ or in the more stable NH$_3$ and HCN, which are only slightly more volatile than water. This makes N a unique probe of temperature within the disk; abundant N$_2$ in a comet would suggest an extremely cold and shielded formation as well as residency in a cold region of the solar system, while its absence suggests a consistent period spent above $\sim$18 K, the sublimation temperature of N$_2$ at protoplanetary disk pressures (Qi et al., 2019). Measurements of NH$_3$ can be used to discern NH$_3$/H$_2$O ratios, which in turn offer clues about both a comet’s formation location and thermal history. Lastly, sulfur is a key tracer due to the range of volatilities that its compounds span, allowing significant presence in the refractory components of the inner solar system within chondrites as well as trapped in cometary water ice in the form of H$_2$S and even S$_2$ (Biver and Bockelée-Morvan, 2019). The chemistry of sulfur compounds is linked closely to H$_2$O abundance at the temperatures modeled for the inner protoplanetary disk, and therefore the relative abundance of the two should be an excellent indicator for the formation locations and conditions for comets. Keeping these three elements and their dominant compounds as guideposts for understanding cometary formation is an essential tool; as the numerous relative abundances and ratios associated with comet observations can quickly lose meaning if this direct call-back to protoplanetary disk chemistry is lost.

With the basics of protoplanetary disk formation described here the stage is now set for cometary formation. All that is required to set the cascading accretion of particles in motion is a gentle nudge.

1.2.2 Forming the Modern Solar System

Once the collapsed molecular cloud core has created a star and protoplanetary disk rich with refractories and volatiles, the assembly of the larger scale planetesimals, the precursor to all of our planets, dwarf planets, and small bodies, can efficiently begin.
Figure 1.1: Diagram detailing the components of a typical $1\,M_\odot$ T Tauri disk as a function of radius from star and height above the disk midplane adapted from Dutrey et al. (2014). The photon dominated region, where the volume density is approximately $200-300\,\text{cm}^{-3}$ is labeled. Two solid black lines represent isotherms at 17 and 20 K, respectively. Note in particular the high temperatures and low densities where cosmic ray and UV radiation is dominant along the hot “atmosphere” of the disk that is exposed, while the cooler molecular layer and midplane of the disk have densities between 5 and 7 orders of magnitude higher, depending on the radius, respectively.
The growth of icy particles in the midplane of the disk relies on the different orbital velocities of the gas and dust particles. The particles in the disk settle to the midplane as inclined orbits are damped by both the gravity of the disk and drag force from the gas. Once in the midplane, particles dominated by their Keplerian orbital velocity, dictated by the gravitational force of the mass interior to their orbit, but the gas particles move somewhat slower, as the thermal pressure gradient of the disk acts against the gravitational force (Whipple, 1972; Weidenschilling, 2004). This causes the gas to enact a drag force on the dust particles that is dependent on the density of the gas disk, causing the particles to decrease in velocity and drift inwards to maintain angular momentum. The decay in semi-major axis associated with this effect lessens for larger particle sizes until they effectively decouple from the gas in the disk at sizes that are dependent on the gas density of the disk.

Determining which types of planetesimals form in the disk, and where, has been a persistent question in planetary science. Modeling icy particles in the disk and the energy involved in the formation of the larger planetesimals is still one of the more poorly understood problems in astrophysics. Icy particles can coagulate into larger agglomerations while drifting radially inwards in the disk if the relative velocities are low, but such a process is heavily reliant on the strength and porosity of the particles (Weidenschilling, 1997; Sirono and Greenberg, 2000; Weidenschilling, 2004). For icy particles to grow to the sizes of typical cometary components, \( \sim 100 \) meters in size, particles must be able to collide and coagulate efficiently, something that is difficult to do in a dense disk when particles are larger than a centimeter in size at 1 au (Blum and Wurm, 2000; Birnstiel et al., 2012). Overcoming this centimeter barrier has brought about several additional accretion theories, each with specific requirements and implications for the resulting bodies:

1. gravitational instability, (i.e. Jeans collapse)
2. streaming instability, (i.e. aerodynamic clumping)

A brief review of each mechanism is useful to highlight what sort of evidence could be observed in the remnant planetesimals.
Formation via gravitational instability: In the same manner that an over-dense core in a molecular cloud will begin to collapse as the gravitational force overcomes the outward force from thermal and magnetic pressures, gravitational instabilities within the disk derive from turbulence in a settled disk of critical density (Safronov and Zvjagina, 1969; Goldreich and Ward, 1973). Once enough particles settle into the midplane and the critical density is reached, parts of the disk can collapse into large planetesimals (∼100 m in diameter) (Goldreich and Ward, 1973). These relatively large planetesimals then quickly begin to gather remaining dust/icy grains in the vicinity, kicking off more classical hierarchical planetary accretion. If gravitational instability dominated planetesimal formation the composition of comets would be unique samples of the disk’s icy grains that had reached the maximum allowable growth before they are unaffected by gas drag and can no longer drift inwards. This would suggest all planetesimal components are of similar sizes, with little macroscale inherited structure. The size of these “pebbles” would be dictated by the gas density of the disk at the radial location of the instability: approximately 10 cm at 1 au, but as small as 3 mm at 100 au (Birnstiel et al., 2012). Particles of this size could then be detectable either in the coma of a comet or, more conclusively, identified in surface images (Kretke and Levison, 2015). This would also imply that the range of comet sizes that we see, from 100 meters to ∼30 km in radius (Bauer et al., 2013), are either the direct result of gravitational instability or a planetesimal that swept up more icy pebbles after its formation. Due to the increase in relative velocities of planetesimals as they increase in size, it is difficult to reconcile any efficient collisional accretion between planetesimals that formed from gravitational instability (Weidenschilling, 1997), as the process would be destructive rather than constructive. Summarily, the formed cometary planetesimals would be collisionally pristine reservoirs of specific disk locations and timestamps.

Formation via streaming instability: Gravitational instabilities can be localized and accelerated when turbulence is added to disk models. The process is driven by the aerodynamics of the disk, wherein the different pressure gradients and velocities for dust and gas create conditions that can trap pebbles, creating clumps near the
critical density (Youdin and Goodman, 2005; Raettig et al., 2015). In order for this to occur efficiently, the solid-to-gas ratio of the disk must be elevated compared to the solar abundance (Johansen et al., 2009), a property that can be accomplished in disk models that take photoevaporation and stratified turbulence into account (Carrera et al., 2017). Planetesimals formed via streaming instability should also show microstructures indicative of pebbles, as the collisional velocities of particles in the clump are between 0.5 and 5 m/s (Johansen et al., 2009). An added benefit of the the streaming instability method is its swiftness; all dust grains in an initial disk can be fully incorporated into planetesimals within 3 Myrs (Carrera et al., 2017) when the disk conditions are right. This is much faster than the expected 10 Myr lifetime of the protoplanetary disk and allows ample time for the gas giants to accrete gas from the disk. However, it would seem that the process is most efficient at planetesimal formation outside the giant planet zone. Carrera et al. (2017) note that in their models few planetesimals were produced between 3 and 30 au. As discussed in the next section, the 5-30 au region is thought to be the original source region for what are now Jupiter family comets.

The streaming instability takes place over the first few million years of the disk’s lifetime, finishing well before the stellar wind dissipates the remaining gas. Gravitational instability doesn’t have the same time constraint, but is aided by the presence of gas in the disk. This period, from when the icy particles settle into the midplane to their accretion into larger planetesimals, is likely the last opportunity for any thermal processing prior to cometary formation (Lunine and Gautier, 2004). However, just how much thermal processing these particles underwent before incorporation into the larger icy planetesimals is still poorly constrained. The pristine nature of icy grains originating from the initial molecular cloud is reliant on the luminosity of the protoplanetary disk and protostar in the infrared and sub-millimeter wavelengths, which is sensitive to changes in accretion rates of material (Chick and Cassen, 1997). Additionally, the presence of crystalline silicate grains in the Stardust sample from 81P/Wild 2 would suggest that dust grains exposed to high temperatures in the inner disk were efficiently transported out to the outer midplane (Brownlee et al.,
2006; McKeegan et al., 2006; Nakamura et al., 2008; Brownlee, 2014). However, the overall bulk elemental chemistry of the protoplanetary disk should still be representative of the molecular cloud, and any sublimated volatiles from icy grains accreting onto the disk will still be incorporated into the disk chemistry.

1.2.3 The Planetesimals

The last, and perhaps most poorly understood part, of our solar system’s formation rests with the distribution of the planetesimals formed from the accretion processes described above. Forming the exact structure of the solar system as we observe it today using dynamical models has proven to be a monumental task, with entire careers dedicated to that pursuit. The component of orbital evolution for the planetesimals is also intimately linked to comets, as they have likely experienced some of the largest changes to orbital properties of any remaining small body population in the solar system. We pick the thread up following the formation of the giant planets, which are responsible for the scattering interactions that tossed the remaining icy planetesimals into the proverbial freezers that are the relatively constrained classical Kuiper Belt (a $\sim$35-50 au), associated scattered disk (a $\sim$35 - 100’s of au), and isotropic Oort Cloud (a $\geq$ 1000 au).

The Oort Cloud and the Kuiper Belt are the cometary reservoirs from which our solar system’s current comets derive, having been emplaced in the epoch of giant planet migration. In fact, the initial evidence for the Oort Cloud, an isotropically distributed comet reservoir, was derived from long period comets’ orbital energies and inclinations (van Woerkom, 1948; Oort, 1950), which were inconsistent with the interstellar origin hypodissertation at the time. As Dones et al. (2004) points out, Halley (1705) speculates on the existence of a comet group with extremely long orbital periods, which could be interpreted as what we now refer to as the Oort Cloud. In a similar fashion, the low inclination distribution of short period Jupiter Family comets (JFCs) provided both Kenneth Edgewort and Gerard Kuiper with the constraints that the comets must originate from a similarly inclined population beyond Neptune (Edgeworth, 1949; Kuiper, 1951), a theory that was fully charac-
terized by Fernández (1980). The Kuiper Belt was first sampled with the detection of 1992 QB 1 by Jewitt and Luu (1993), with thousands of Kuiper Belt Objects (KBOs) discovered since. These reservoirs and the chemical properties of the planetesimals that they contain strongly depend on the orbital evolution of the early solar system, especially of the giant planets responsible for sculpting their currently observed orbital properties.

The exact formation locations of the giant planets (Jupiter, Saturn, Uranus, and Neptune) in the protoplanetary disk is still a subject of debate. In order for these planets to efficiently accrete large amounts of gas from the disk they must have formed swiftly in the disk, prior to the initiation of stellar winds from the young Sun. Identifying the initial formation locations of the gas giants is complicated by this; since they form while the protoplanetary disk is still present, the gravitational interaction between the gas in the disk and the giant planets will transfer angular momentum between them (Dones et al., 2015, and references therein). The same can also be said of gravitational interactions between planets and planetesimals. Planetesimals in the giant planet region have dynamical lifetimes limited to $\sim 10$ million years of planet formation (Holman and Wisdom, 1993; Levison and Duncan, 1993; Dones et al., 2004, 2015). The formation of the scattered disk is a natural consequence of planetesimals forming in the giant planet region. As the initially very massive disk of planetesimals interior to Jupiter’s orbit interacts with Jupiter and are scattered outward, Jupiter accordingly moves to a lower semi-major axis. For Saturn, Uranus, and Neptune, the opposite happens, and they move outwards (Fernandez and Ip, 1984). This process simultaneously efficiently scatters the planetesimals thought to have formed near Jupiter and Saturn out to form the distant and spherically distributed Oort Cloud and the Kuiper Belt’s scattered disk (the “hot population”) and provides a mechanism for planetary migration. Remnant Kuiper Belt Objects, thought to have formed in place and remained stable, are often called “cold classicals” due to their primordial narrow inclination distribution that indicates they were not scattered outward. The presence

These periods of planetary migration have been broken into two recent popular
models; the “Nice” and the “Grand Tack” models (Dones et al., 2015). Both of these models have implications for broad population characteristics of comets, and no single comet observation will verify or reject either theory, but it is important to describe each theory and the populations that they predict are emplaced both in the Oort Cloud and Kuiper Belt. The current distribution of Kuiper Belt indicates that smooth planet migration alone is not the only mechanism for populating the scattered disk, and interactions between the giant planets are necessary to explain our solar system’s architecture.

The Nice model was motivated from the promising results for explaining the orbit of Pluto and other trans-Neptunian objects trapped in mean motion resonances with Neptune with the smooth migration model presented in Malhotra (1993, 1995). However, those models resulted in the giant planets having eccentricities much lower than their current values. The first attempt to solve this dilemma was executed in Thommes et al. (1999), with Uranus and Neptune forming nearer to Jupiter and Saturn than they currently reside to form them at higher surface densities in the protoplanetary disk and thus shorter timescales then if they formed at their current orbits. Rather than the smooth migration to produce the outer solar system shown by Fernandez and Ip (1984); Malhotra (1993, 1995), Thommes et al. (1999) showed that it was possible to scatter Uranus and Neptune out to their current orbits via interactions with Jupiter and Saturn. Following this revelation a new model was developed, termed the Nice Model after the city in France where it was first proposed by dynamicists (Tsiganis et al., 2005; Morbidelli et al., 2005; Gomes et al., 2005) to investigate how resonance crossing could influence the eccentricities of the giant planets. The initial iteration of the Nice model had Saturn form just inside the 1:2 MMR with Jupiter, which allows the two planets to interact quite quickly once Jupiter begins to migrate inwards. This resonance crossing event rapidly pumps the eccentricities of the outer planets, clearing planetesimals via scattering interactions, and results in Uranus and Neptune scattering out to their current orbits. Like in the Thommes et al. (1999) model their orbits are damped via interactions with the remaining planetesimal disk, leaving the giant planets in a configuration consistent
with their current orbits. However, the physical mechanism to cause the initial migration was still assumed and not understood. The second iteration of the Nice model, aptly nicknamed “Nice II”, focused more closely on the interactions between the giant planets and a gas disk thanks to new modeling done by Morbidelli et al. (2007). The Nice II model was able create the instability necessary to drive the planetary migration by relatively tightly packing the outer solar system: Jupiter would start at 5.4 au, Saturn in a 2:3 resonance with Jupiter, “Ice I” at a 2:3 with Saturn, and “Ice II” in a 3:4 resonance with Ice I. This would stack all of the gas giants between 5.4 and 11.7 au in a configuration that was relatively stable until the planetesimal disk, with massive particles, would produce enough interactions to more closely pack the outer planets and force a dramatic instability late in the early solar system (∼300 to 1000 million years after formation). The suite of Nice models favors that objects formed beyond 15 au became the P- and D-type asteroids that dominate the Jupiter Trojan regions. This same region would also be the source for many Oort Cloud and scattered disk objects that had their orbits raised and circularized following interactions with the migrating planets (Levison et al., 2011). Each of these iterations has proved useful for investigating the implications of giant planet interactions, but ultimately the specific resonance crossings tested fail to maintain the secular architecture of the giant planets.

The Grand Tack model, developed by Walsh et al. (2011), starts with Jupiter forming just outside the water ice snow line at 4 au, then migrating inward via planetesimal interactions with the primitive asteroid belt until reaching approximately the current orbit of Mars at 1.5 au. Provided Saturn forms just inside 5 au, the giant planet begins to accrete mass very quickly around 100,000 years, and quickly “catches” Jupiter by becoming locked into a 3:2 mean motion resonance after a quick period of inward migration. At this time Jupiter has a semi-major axis of ∼1.5 au, roughly where Mars sits in the current configuration of the solar system. At this point both Jupiter and Saturn interact with this resonance, as well as the slowly depleting gas disk, and begin an outward migration that in turn captures Uranus and Neptune approximately 200,000 years after the initial migration begins. Over
the course of 600,000 years the giant planets grow to their current masses, requiring
the presence of the gas disk, and orbits consistent with their current orbital ar-
angement. For the remnant planetesimals the model works well for explaining the
observed stony and carbonaceous dichotomy in the inner and outer asteroid belt, but
would imply that many of the planetesimals scattered into the Oort Cloud should
be of similar composition to both the carbonaceous asteroids observed in the main
belt as well as the icy satellites of Saturn. There are three notable caveats to the
Grand Tack model identified by Raymond and Morbidelli (2014) and summarized in
Dones et al. (2015). The first is that it is unclear exactly how Saturn, which needs
to migrate inwards quickly to reach the 3:2 MMR, can do so provided that Jupiter
has very recently migrated through the same region, sweeping it of the dust and gas
necessary to drive Saturn’s migration. Bitsch et al. (2014) showed that it is possible
for the gas conditions of the disk to substantially change if Jupiter formed prior
to Saturn, opening an avenue for Saturn’s speedy migration. Second, the outward
migration instigated by Saturn’s arrival into the 3:2 MMR is only produced if the
mass ratio between Jupiter and Saturn is between 2 and 4. Whether or not this
ratio can be kept constant as they migrate outwards, presumably accreting mass,
is not yet fully understood. Lastly, given the expectation from the model that the
Oort Cloud comets, C-types, and Saturnian satellites likely formed in the same disk
region, one would also expect that their isotopic ratios were also similar. This is
not the case, suggesting that the populations are not sourced from the same distinct
chemical region of the disk (Alexander et al., 2012; Davis et al., 2014).

An additional theory worth mentioning for completeness is the constraint im-
posed by the stability of the inner terrestrial planet orbits. The relatively smooth
movement of the secular resonances during Jupiter’s migration works excellently for
sculpting the outer solar system, but the giant planet wreaks havoc on the inner
solar system through substantial eccentricity forcing via secular resonances (Brasser
et al., 2009; Agnor and Lin, 2012) thanks to the long duration of the resonance cross-
ing events. To address this, the “Jumping Jupiter” theory was proposed by Brasser
et al. (2009), wherein Jupiter’s semi-major axis was rapidly reduced by scattering a
single ice giant outwards rather than millions of smaller planetesimal size objects. By substantially decreasing the resonance crossing time for the inner terrestrial planets the stability of Mercury, Venus, Earth, and Mars can be preserved. The rapid movement of Jupiter in the Jumping Jupiter theory would produce a similar scattering of planetesimals as well, populating both the Oort Cloud and scattered disk of the Kuiper Belt.

The edge of the Kuiper Belt may also provide a clue about the dynamical conditions of the early solar system. There is a dearth of low-eccentricity Kuiper Belt objects with semi-major axes greater than 50 au, even though protoplanetary disk models still predict planetesimal formation in the region (see Figure 1.2). Gladman and Volk (2021) review several possibilities that could explain this edge, including observational biases, gaps in the initial protoplanetary disk, as well as a stellar passage. For the purposes of this dissertation a stellar passage would have the largest effect on the cometary population. Although a stellar passage is unlikely to be the source of the KB edge due to its disruption of the cold classicals, it is nonetheless intriguing to discuss some previous investigations. Melita et al. (2002) showed that this truncation to the planetesimal disk could be reproduced if there was a close stellar passage. There is a relatively narrow window for such a passage to occur, however; Levison and Morbidelli (2003) concluded that any such approach needs to happen soon after Uranus and Neptune form in order to preserve the later formation and stability of Oort Cloud, which is tenuously bound to the solar system due to its distance from the Sun. Additionally, they also conclude that the mass of scattered disk planetesimals would be similar to the total mass of the Oort Cloud, which is in turn inconsistent with the current number of detections of extended scattered disk objects. Such close stellar encounters ($r_{hel} \sim 200$ au) are estimated to be rare (García-Sánchez et al., 2001) but nonetheless more likely if our Sun formed in a dense stellar cluster (Bate et al., 2003).

From these models there are two distinct hypotheses regarding relative compositions of the two current cometary reservoirs, the Oort Cloud and the scattered disk, and planetesimal populations they are populated from. In the first, and ear-
liest, the Oort Cloud is populated with objects that formed among the gas giants between 5 and 30 au and were scattered outwards via interactions with those planets, in turn causing migrations that forced Neptune outward, sweeping up the outer disk into the scattered disk hot population as well as trapping some planetesimals into the MMRs. For this case we would then expect that Oort Cloud comets would be sampling the region just beyond the water ice line, while objects in the classical and scattered disk of the Kuiper Belt should be core samples of the planetesimal disk beyond Neptune (Mumma et al., 2003; Mumma and Charnley, 2011; Mandt et al., 2015). For the second hypodissertation, and our modern understanding, the Oort Cloud and scattered disk are derived from the same population of planetesimals between 5 to 35 au, and at their implantation into either reservoir should have similar variations in compositions (Tsiganis et al., 2005; Mandt et al., 2015). However, the far colder residency in the Oort Cloud may help to preserve the hypervolatile ices like CO and CO$_2$ for the lifetime of the solar system compared to objects in the nearer and somewhat warmer scattered disk (A’Hearn, 2011).

Another mechanism worth mentioning that is capable of populating the Oort Cloud is interstellar planetesimal capture from the stellar birth cluster. First proposed by Zheng et al. (1990) and elaborated on in Levison et al. (2010), this theory shows that in a moderately dense stellar birth cluster it is possible that up to $\sim$90% of Oort Cloud comets formed in other systems. Such a large fraction of interstellar interlopers in the Oort Cloud could serve to substantially bias the bulk composition of Oort Cloud comets, complicating the goal of identifying chemical properties of different locations in our solar system’s protoplanetary disk. Given the simulation’s reliance on assumed properties like average comet mass, the protoplanetary disk mass, as well as orbital configuration and sizes of the planets it remains uncertain just how likely this particular theory is. Nonetheless, it is important to keep in mind when trying to contextualize the exotic abundances of comets like C/2016 R2 (PanSTARRS), Comet Morehouse, and 96P/Macholz, which were all found to have an incredibly high CO to H$_2$O ratios (McKay et al., 2019; Biver et al., 2018; Schleicher, 2008).
Comets are removed from the Oort Cloud and Kuiper Belt via gravitational perturbations. In the case of the Oort Cloud, these perturbations come from the galactic tide (Heisler and Tremaine, 1986; Levison et al., 2001) and nearby passing stars (Weissman, 1980; Hills, 1981), while for the Kuiper Belt interactions with Neptune serve to inject objects into the solar system (Holman and Wisdom, 1993; Duncan et al., 2004; Volk and Malhotra, 2008; Dones et al., 2015). The Oort Cloud is relatively simple to perturb; because the objects are so far from the Sun, even a slight gravitational attraction from an external source can be enough to decrease the comet’s perihelion to send it plunging into the inner solar system and further interactions with the giant planets. Kuiper Belt objects have a much more chaotic journey that involves time spent beyond Neptune, in the transitional Centaur population that orbits between Jupiter and Saturn, and the Jupiter Family comets, with pathways that flow both in and out of the inner solar system (Tiscareno and Malhotra, 2003; Volk and Malhotra, 2008; Sarid et al., 2019).

While a member of the Centaur population, the remnant planetesimal has its last opportunity for processing prior to its arrival in the inner solar system as a Jupiter Family comet. For the purposes of this introduction, a Centaur can be considered any minor planet with a semi-major axis or perihelion that is between the orbits of Jupiter and Neptune. Fernández (1980) postulated that the active Centaur Chiron could be evidence of a diffusive process for producing comets from a (then-theoretical) trans-Neptunian belt, a theory that has been bolstered with both dynamical and observational evidence since. The fact that objects like Chiron, 29P/Schwassmann-Wachmann 1 (Trigo-Rodríguez et al., 2010; Miles et al., 2016; Wierzchos and Womack, 2020; Schambeau et al., 2019), and the recently discovered P/2019 LD2 (ATLAS) (Steckloff et al., 2020; Kareta et al., 2021; Bolin et al., 2021) all display varying levels of activity implies that devolatilization is an important process for the Centaurs. As the Centaurs’ orbits never bring them within the region where water ice sublimation can become prevalent (∼3.5 au from the Sun) this activity is likely the result of hypervolatiles like CO or CO\textsubscript{2}, although more exotic sources have been proposed (Miles et al., 2016). Regardless of the driving
volatile, the activity of the Centaur population and their position as a dynamic intermediate between the Kuiper Belt and JFC population suggests that some JFCs will have sublimating comae that may not be directly related to the protoplanetary disk composition.

The orbits of the currently known comets, Centaurs, and KBOs are shown in Figure 1.2 to illustrate the distribution of semi-major axes and perihelia that are currently known. The most frequent calculation that can be made to discern between the JFCs, Centaurs, Halley-type comets, and long period comets is with the orbital relation to Jupiter known as the Tisserand parameter, suggested by Carusi and Valsecchi 1987; Duncan et al. 2004. The Tisserand parameter, $T_J$, with respect to Jupiter can be calculated as:

$$T_J = \frac{a_J}{a} + 2 \sqrt{(1 - e^2) + \frac{a_J}{a} \cos(i)}$$  (1.2)

where $a_J$ is Jupiter’s semi-major axis, and $a, e,$ and $i$ are the semi-major axis, eccentricity, and inclination of the comet, respectively. When $T_J$ for a comet is equal to or less than 3, the comet will experience strong influence from Jupiter during close approaches. This is illustrated in Figures 1.2 and 1.3. The JFCs host both comets investigated within this dissertation, and this holding pond of comets lives at a peculiar dynamical crossroads. Once Centaurs become JFCs, their dynamical lifetimes are just a few tens to hundreds of thousands of years before either scattering back into the Centaur population, disintegrating, or impacting the Sun, inner, or outer planets (Levison and Duncan, 1994; Sarid et al., 2019). The number of active comets was thought to be 5-20 times less than the number of faded, or dormant, nuclei (Levison and Duncan, 1994), although recent efforts have shown than the current observed population could be explained with JFC activity persisting for 4000 years (Nesvorný et al., 2017). This leaves a relatively narrow window where comets are actively sublimating the bulk ice matrix of the nucleus within the water ice sublimation zone, releasing the remaining volatiles as well as dust into the broader coma. The abundance of the hypervolatiles that sublimate at temperatures far colder than water like CO, CO$_2$, and N$_2$, our ideal thermal sensors for constrain-
Figure 1.2: Semi-major axis and perihelion distribution of known comets, Centaurs, and KBOs as queried from the Minor Planet Center in November of 2021. The intensity color bar shows the Tisserand parameter for each object, as calculated in Equation 1.2. Note the clustering of $T_J \leq 3$ at low semi-major axes and moderate perihelion.

The formation and dynamical evolution of Jupiter family comets provides several mechanisms to alter the observed cometary compositions from the initial molecular cloud composition. The thermal structure of the protoplanetary disk, the vertical mixing between the warm molecular layer and the icy midplane, and gas turbulence can all serve to alter the chemistry of the forming icy grains. Following planet formation the scattered disk, the likely original source of the JFCs, populated from a variety of locations in the giant planet region, with potentially chemically different...

...ing the formation location in the disk, are thus tied to the total residence time in the scattered disk as well as the Centaur region.

The formation and dynamical evolution of Jupiter family comets provides several mechanisms to alter the observed cometary compositions from the initial molecular cloud composition. The thermal structure of the protoplanetary disk, the vertical mixing between the warm molecular layer and the icy midplane, and gas turbulence can all serve to alter the chemistry of the forming icy grains. Following planet formation the scattered disk, the likely original source of the JFCs, populated from a variety of locations in the giant planet region, with potentially chemically different...
Figure 1.3: Semi-major axis and inclination distribution of known comets, Centaurs, and KBOs as queried from the Minor Planet Center in November of 2021. The intensity color bar shows the Tisserand parameter for each object, as calculated in Equation 1.2. Note the clustering of $T_J \leq 3$ at low semi-major axes and low inclinations.
planetesimal populations. Finally, after their residence in the cold storage of the scattered disk and injection into the Centaur and ultimately JFC populations, the comets are subjected to substantial thermal changes. All of these influence the interpretation of the observed JFC composition, and demand a holistic dynamical, chemical, and physical investigation for each comet to properly understand the data. So far many of the chemical and dynamical constraints have been discussed; now it’s time to discuss the physics that govern cometary activity and our measurements thereof.

1.3 The Physics of Comet Activity

At the time of writing this dissertation we do not yet have a way to transport the mass spectroscopy instrumentation, or anything for that matter, back 4.5 billion years to the formation of the solar system to obtain the ground truth of its chemical composition. The best option that we have is to observe the "sweet spot" objects; too big to be cleared away via radiation pressure but too small to be effected by differentiation. Ideally these small and least processed objects in the solar system would allow us to see what the initial conditions of planetary formation were like. Larger objects, like the traditional planets and larger asteroids as well as some Kuiper Belt objects, have undergone thermal, hydrological, and chemical processing that makes it difficult to interpret the molecules that they formed from. In theory asteroids and comets, on the other hand, never experienced enough pressure or heat to obfuscate these clues about the solar system’s past, provided a perfectly frozen physical sample can spontaneously manifest itself in a Earth-based lab for study. Obtaining these samples is incredibly hard to do; the Stardust flyby mission to 81P/Wild-2 only sampled dust grains in the extended coma (Brownlee, 2014), and the extensive difficulties and trials of both the JAXA Hayabusa-2 and NASA OSIRIS-REx missions for asteroid sample return are well documented (Tsuda et al., 2019; Kikuchi et al., 2020; Lauretta et al., 2017; Hergenrother et al., 2019; Lauretta et al., 2019). Cometary sample return missions will have the added challenge of
substantial activity and debris to maneuver in and around, not to mention the difficulty in either a) preserving the refractory component of a cometary sample as volatiles are sublimated from it, or b) cyrogenically preserving a pristine cometary sample of both volatiles and refractories for the journey back to Earth but they are high on the wishlist as viable targets in NASA’s New Horizons call for proposals. As such, three comet sample return mission proposals were submitted to the previous call, with the CAESAR mission reaching the final round (Milam et al., 2020). With this improved method of characterizing the chemical and physical components of comets and asteroids still out of reach, we must lean on spacecraft and Earth-based observatory observations. Remote characterization of asteroid and comet compositions requires spectroscopy across a wide range of wavelengths and a vast catalog of atomic, molecular, and mineralogical data to compare to, often from laboratory sources in conditions that may or may not be similar to those encountered in astrophysical environments.

The previous section covers how comets form and are introduced to the inner solar system, giving them the properties they posses at the time of observation. In this section we will now discuss the physics that govern how these properties can be measured remotely. Broadly speaking this is encompassed by the term “activity”. In the last 400 years this has been the box into which comet relative intensity, magnitude, photometric, spectrophotometric, and spectral measurements have all been placed. Because cometary activity is the very thing that makes these objects so interesting as astrophysical targets, for the purpose of this dissertation, it is not only useful but necessary to review the physics that enable their observation. To that end there are three broad physical processes that need to be reviewed: orbital evolution of JFCs, the sublimation of volatiles, and the emission mechanisms that enable their detection.

1.3.1 Orbital Evolution and Thermal Processing of Jupiter Family Comets

The most substantial drivers of cometary activity are the vast swings in temperature that comets’ eccentric orbits enable. The amount of energy available for the
sublimation of ices from a comet’s surface scales as the inverse square of the comet’s
distance from the Sun, so even small changes to a comets semi-major axis and ec-
centricity can have large implications for the thermal budget of a comet nucleus.
There are many excellent reviews on this particular matter (e.g. Delsemme, 1982;
Meech and Svoren, 2004, for the curious reader), and the next few paragraphs will
attempt to summarize the most critical components of those articles.

During a future Jupiter Family comet’s long tenure in the Kuiper Belt, there
is a mechanism that can affect their activity levels once in the inner solar system.
Cosmic rays, which are highly accelerated particles from high energy astrophysical
events, irradiate the KBOs at a relatively constant rate. This irradiation can do
two things to the cometary ices. The bombardment of the initial icy planetesimal
surface with keV to GeV energy ions produces a non-volatile crust as the bonds
of the ices (H$_2$O, CO$_2$, CO) are broken and rebonded into C-C, C-S, C-N, and C-O
bonds as hydrogen is removed from the molecules (Strazzulla et al., 1991). The
upper few meters of the KBO/future comet will also form radicals, like OH and
CN, from the irradiation (Strazzulla, 1999). The combination of the crust and
radical formation alter both the albedo of the comet’s surface and the chemical
composition of the upper layers (Strazzulla, 1999). The formation of a darker crust
on the comets surface increases the energy absorbed from the Sun, and in turn heats
the interior materials, accelerating sublimation of subsurface volatiles. Experiments
have also shown that the strength of these crust surface layers can be significant,
allowing volatiles to sublimate from under them without the destruction of the
crust (Strazzulla et al., 1991; Meech and Svoren, 2004). This suggests that the
accumulated crust likely remains important during first steps of the KBO to Centaur
to JFC pathway, where solar fluxes are still relatively weak compared to the inner
solar system, but may ultimately fracture once a significant fraction of the nucleus
becomes active.

The formation of a dark crust has substantial implications for the activity of a
JFC once dynamically introduced to the inner solar system. Most simply, balancing
the incoming solar radiation with the energy radiated by the nucleus and contained
within the sublimating molecules showcases the role albedo plays in the steady state activity of a comet. The energy balance equation, as stated in Meech and Svoren (2004), is:

$$\frac{(1 - A_B L_{\odot})}{4\pi r^2} = \epsilon \sigma T^4 + \mathcal{P}_\mu \sqrt{\frac{m_\mu}{2\pi k T}} \mathcal{H}_\mu$$

(1.3)

where $A_B$ is the Bond albedo, $L_{\odot}$ is the solar luminosity, $r$ is the heliocentric distance, $\epsilon$ is the surface emissivity, $\sigma$ is the Stefan-Boltzmann constant, $\mathcal{P}_\mu$ is the saturation vapor pressure for a given molecule $\mu$, $m_\mu$ is the mass of the molecule, $T$ is the temperature, $k$ is the Boltzmann constant, and $\mathcal{H}_\mu$ is the latent heat of sublimation. Note that this assumes only one molecule is sublimating, and that a sum of all volatile molecules is needed to correctly account for the expected sublimation rates. Note that this is essentially only true for the sub-solar point on the nucleus; to correctly compensate for solar incidence angle, $\cos(\phi)$, should be factored into the solar insolation energy equation on the left of Equation 1.3.

This sublimation not only serves to deplete the upper layers of the very volatile CO and CO$_2$ molecules in the Centaur region, but may also be responsible for reorganizing the structure of JFCs. Safrit et al. (2021) explored the effect of what was described as a “sublimative YORP” force, $10^{4-5}$ times stronger than the typical photon-driven YORP force derived for asteroids (Bottke et al., 2006). They found that for the typical size of JFCs (1-8 km in radius) nearly all would be expected to experience a sublimative torque that would accelerate their rotation rate beyond the critical limit, allowing them break up and reaccrete into bilobate nuclei. The slow relative velocities of the reaccretion would preserve volatile abundance, but could also create new heterogeneous structures that further drive cometary activity. Hirabayashi et al. (2016) showed that the bilobate shape is then somewhat resilient against future sublimative torques; as the rotation rate increased, the two lobes simply move apart and then reaccrete slowly, returning to a similar shape. While this does imply that the JFC population is broadly reshaped while transitioning through the Centaur formation, it is unclear just how much CO and CO$_2$ is readily available to supply the sublimative torque.
As the upper layers of the comet are devolatilized via both cosmic ray irradiation and solar heating, a new structure will begin to develop. Below the cohesive crust devolatilization will continue, tracking the thermal wave where the temperature is high enough to sublimate volatile ices. This leads to a depleted layer of cometary ice, where some of the volatiles have been released to the surface via micro- or macroporosities and some have recondensed below the thermal wave. For JFCs we would expect that the upper few meters of cometary material should be depleted of CO and CO$_2$ after a few million years spent at semi-major axes less than 13 au, the heliocentric distance at which CO$_2$ efficiently sublimes (Figure 1.4, (Meech and Svoren, 2004, Table 1)). Crystalline water ice and other less volatile materials will remain intact, effectively insulating the interior nucleus. Given the low formation temperatures expected for the KBO source population ($\sim$30-50 K) it is expected that the bulk of water ice accretes into the amorphous form, and does not crystallize until reaching a temperature of between 90-160 K (Laufer et al., 1987). The porous structure of amorphous ice leaves cavities that can be filled with other volatile materials, which would be released upon the annealing process, by which the amorphous ice transitions to a crystalline structure. During this transition the trapped volatiles are released and likely escape the ice matrix. Such a process would explain the simultaneous increase in compounds in the coma of comet Hale-Bopp at 7 au, all that had a wide range of volatilities (Biver et al., 2002). For comet 9P/Tempel 1, which was the target of the Deep Impact mission and was observed to have consistent outbursts, this depletion layer, devoid of volatiles like CO and CO$_2$, was hypothesized to extend 30-100 meters below the surface (Belton and Melosh, 2009).

The relationship between orbital properties and the sublimative activity of a comet is perhaps best demonstrated by comparing the expected mass loss for various volatiles as a function of orbital parameters. Centaurs and JFCs occupy a wide range of orbital semi-major axes and eccentricities and a relatively modest range of inclinations inherited from their source region, the scattered disk of the Kuiper Belt. This means that JFCs can undergo a similarly large range of sublimation
Figure 1.4: Plots detailing the sublimation rate of $\text{H}_2\text{O}, \text{CO}_2, \text{CO}$ for an idealized comet with Bond albedo of 0.04 and emissivity of 0.9. Parameters are taken from Prialnik et al. (2004), plot styled after Delsemme (1982) and Meech and Svoren (2004).

Even just a brief few thousand year stay in the Centaur region should provide evolution pathways, as their orbits change on relatively short timescales (c.f. Figure 1.5). By convolving the sublimation rates of several different volatiles with these orbital pathways we can show how the production rate changes as a function of time for objects in the JFC-Centaur conveyor belt (Fig. 1.6). These production rates should be considered maximum values, as they assume that there is always volatile ice available to sublimate at the surface and ignore the effect of sublimation through a porous medium (Prialnik et al., 2004).
Figure 1.5: Results of a simple Rebound simulation (Rein and Liu, 2012) showing the semi-major axis (black), perihelion (magenta), and eccentricity of a sample of 100 comets placed into near circular orbits just beyond Jupiter (i.e. Centaurs) allowed to evolve dynamically with the Sun, Jupiter, Saturn, Uranus, and Neptune perturbing their orbits for 10,000 years. Comets are scattered both inward and outward from these orbits, evolving into JFCs and back into Centaurs. Note in particular that the perihelion of this population is never raised beyond the initial value on this timescale.
Figure 1.6: Idealized production rates for four Centaurs from the Rebound simulation shown in Figure 1.5 transitioning between the Centaur and JFC populations. A radius of 5000 meters, a Bond albedo of 0.04, an emissivity of 0.9, and an active area that is 5% of the total surface area for H\textsubscript{2}O, CO, CO\textsubscript{2} is assumed. The semi-major axis is plotted with a faint blue line for context. Rotation rate and solar incidence angle effects are ignored for simplicity.
ample time to deplete the upper layers of a comet of the volatiles CO and CO$_2$, possibly creating some of the geologic features like scarps and pits observed at 67P (El-Maarry et al., 2016). Sarid et al. (2019) show that the typical residency is nearer to 1-10 Myrs. Therefore, comets arriving onto JFC-like orbits for the first time may exhibit a depletion in CO and CO$_2$ that is indicative of the abundances in the upper layers, but not of the bulk comet abundance. This discrepancy is one of several motivations for obtaining observations of JFC production rates not only over the course of a perihelion passage but over multiple apparitions. Explosive outburst or significant mass wasting events can expose colder, more thermally shielded material that will sublimate rapidly, and successive perihelion approaches can reveal changes to dust production and volatile outgassing rates that could indicate more pristine material is being removed. However, remote observations require physical models of two additional components: the distribution of cometary neutrals in the extended coma and the emissions mechanisms that enable their detection. We now turn our attention to the former.

1.3.2 Tools for Characterizing Cometary Activity

Observations of the extended nature of comets, especially in the advent of atomic spectroscopy, motivated attempts in the early 1900’s to quantify the distribution of observed emissions. Eddington (1910) first attempted to derive a model that could characterize the apparent distribution of comet Morehouse (1910), described as the “Fountain model”, which was later improved by independent efforts from Mocknatsche (1938) and Fokker (1953). As reviewed in Wallace et al. (1958), those authors were able to derive an equation for the column density of molecules at some distance from the nucleus $R$ as viewed from the observed position:

$$N = \frac{Q}{4\pi vR}$$

(1.4)

where $Q$ is the production rate of the molecule in mol s$^{-1}$, $v$ is the molecular outflow velocity, and $R$ is the impact parameter from the surface of the comet
nucleus. Applying this model to comet observations quickly showed that there was a discrepancy between the observed and expected distributions, as the Fountain model overpredicted the density at larger distances from the nucleus. Upon this realization, as well as the one that most emissions from comets in the visible were not from neutral molecules but rather from the products of neutrals dissociated by sunlight, Haser (1957); Haser et al. (2020) considered a photodestructive process and derived two equations that have become two of the most frequently used empirical models for coma distribution (Combi et al., 2004). The first describes the number density distribution of the parent molecule at some distance \( r \) from the nucleus (\( \text{H}_2\text{O}, \text{CO}_2, \text{HCN}, \text{etc} \)):

\[
n_p = \frac{Q}{4\pi r^2 v} (e^{-\frac{r}{\gamma_p}})(1.5)
\]

while the second describes the number density of the derived, or “daughter”, species:

\[
n_d = \frac{Q}{4\pi r^2 v} \frac{\gamma_d}{\gamma_p - \gamma_d} (e^{-\frac{r}{\gamma_p}} - e^{-\frac{r}{\gamma_d}})(1.6)
\]

both of these equations \( Q \) and \( v \) represent the parent production rate and velocity, and \( \gamma \) represents a value termed the scale length, which is itself characterized by:

\[
\gamma = \tau v (1.7)
\]

where \( \tau \) is the lifetime of either the parent or daughter at the desired heliocentric distance. Because the velocity and lifetime are have opposite relationships to heliocentric distance (\( \tau \alpha r_h^2 \), \( \nu \alpha r_h^{-2} \)), the scale length is therefore typically assumed to be constant. Somewhat paradoxically, observations of radicals in cometary comae are often the best way to measure the lifetimes (Randall et al., 1992), by using a Haser model and fitting the lifetime. This is due to the accessibility to many species in the optical wavelengths and the relatively high fluorescence rates.

These three equations make it trivial to calculate the number density of a species at a specific distance from the nucleus, but for a remote observer the more important quantity is the total number of molecules within a visible column. To determine this
column density, it’s necessary to either use Haser’s analytical equations for column density or integrate the Haser function for density for the line of sight. The distance that the observer is looking from the nucleus is typically called the impact parameter and given the designation $\rho$, and the column density can be written as:

$$N_d(\rho) = \frac{Q}{2\pi rv} \frac{\gamma_d}{\gamma_p - \gamma_d} \left( \int_0^{\rho/\gamma_p} K_0(y) dy - \int_0^{\rho/\gamma_d} K_0(y) dy \right)$$

(1.8)

where $K_0(y)$ represents the modified Bessel function of the first kind (Boas, 2006). The development of the Small Body Python repository (Mommert et al., 2019) makes incorporation of the Haser model into data analysis trivial. There are also constituents in the cometary atmosphere that require another step to the Haser model dissociation, as explored by O’dell et al. (1988) to explain the spatial distribution of $C_2$. However, these models have limited use for the species of interest for this dissertation (H,O,C,S) due to the velocity kicks imparted to those atomic components from the dissociation of their parents ($H_2O, OH, CO_2, H_2S, CS_2, etc$).

Several authors noticed that the Haser model scalelength were inconsistent with physical photodissociation rates. To better understand the observations more physical models were developed in the 1980’s. Characterizing the distribution of these atomic species, specifically $H$, has led to two different methods that Combi et al. (2004) describes in detail. The first, commonly referred as the vectorial model due to its vector math approach to determining the resulting atomic $H$ velocity vector from dissociation of $H_2O$, was developed by Festou (1981) to numerically calculate the number density and thus the column density for atomic $H$ and OH. The second, developed near simultaneously, is the Monte Carlo outflow model that creates a statistically significant number of the molecules and can determine the distribution directly. We focus now on the vectorial model, which has been most frequently used to characterize the distribution of radicals in the near nucleus coma.

A major result of Festou (1981) was that a key component of determining the density distribution was evaluating the collision sphere for the molecules in question. The distance within which a molecule can have on average one collision is defined
in Equation 4 of Festou (1981) as:

\[ r_c = \frac{\sigma_M^2 Q_T \bar{v}_r}{u} \]

(1.9)

where \( \sigma_M \) is the molecular radius, \( u \) is the molecular velocity, \( Q_T \) is the molecular production rate in mol/s, and \( \bar{v}_r \) is the module of the mean relative velocity between molecules, typically derived as \( \bar{v}_r = \sqrt{2} \bar{v} \). Once this collisional radius has been determined two sets of equations are defined for determining the densities depending on if the molecular source is considered a point source (i.e. \( r_c \approx r_n \)) or the collision sphere is much larger than the molecular source (\( r_c \gg r_n \)), as well as whether the molecules of interest are produced inside or outside of the collision sphere (see Table 1 of Festou (1981)). Most importantly, the vectorial model takes into account the contribution of molecules produced outside of the collision sphere and provides an accurate representation of the density of products that receive a velocity kick from the dissociation of their parent molecules. While the works in this dissertation do not make use of the vectorial model, it presents one of the most obvious next steps to take in addressing some of the atomic S distributions for 46P/Wirtanen in Chapter 5.

A comparison of the Haser and vectorial models is useful to illustrate the limits of both (Fig. 1.7). Both models are tuned to the dissociation of H\(_2\)O forming OH for this test case, with the lifetimes and exothermic velocities detailed in Table 1 of Combi et al. (2004) and the heliocentric distance of 0.87 au used in Festou (1981). In particular it is useful to note that the vectorial model predicts a much flatter distribution near the nucleus than the Haser model, which reaches its shallowest slope when the scale lengths of the parent and daughter molecules are identical. The ability to characterize these slope differences in the density distribution becomes even more critical when the parent molecule is not obvious and several different Haser and/or vectorial models need to be compared (ex. CS\(_2\) vs H\(_2\)S for S distributions, or C\(_3\) and C\(_2\)H\(_4\) for C\(_2\)).
Figure 1.7: Comparison of a 2-component Haser model and a vectorial model for the distribution of OH from a \( \text{H}_2\text{O} \) parent for a comet with a \( Q_{\text{H}_2\text{O}} \) of \( 10^{28} \) mol s\(^{-1}\) at 0.87 au, as is the test case described in Festou (1981).
1.3.3 Emission Physics in Cometary Atmospheres

In order to compare a modeled density distribution to comet data, whether an image or a spectrum, knowledge of the contributing atoms and molecules as well as the efficiency of the electronic, vibrational, and rotational transitions that create emission features is required. The strength of these transitions are measured as an efficiency for fluorescence processes, typically referred to as a “g-factor”, while for collisional processes it is referred to as a cross section. For the different excitation mechanisms referred to in this section, it is important to note that the final expression should always obtain units of photons s$^{-1}$ and when multiplied by a column density produce a flux in photons per area per second. In theory, the entire cometary UV emission spectrum should be reproducible from a combination of these emission mechanisms and a reflected solar spectrum.

There are two emission mechanisms to discuss that are relevant for cometary comae in the ultraviolet: resonance scattering of sunlight, or fluorescence, and dissociative electron impact excitation. The first process relies on the incoming flux of solar light to excite electrons between electronic levels in atoms and molecules and therefore obeys a strict $r^{-2}$ dependence with the heliocentric distance. Dissociative electron impact excitation is a more complex mechanism; it relies on the availability of energetic electrons. These free electrons can be the result of excited photoelectrons freed from the photodissociation of molecules that create ions, or from the availability of free electrons in the solar wind.

**Photon-driven Emissions**

Resonance scattering emissions (also called resonance fluorescence) are directly proportional to the amount of light received by atoms and molecules in the cometary coma. Resonance scattering is the absorption and re-emission of a photon at the same wavelength by an atom or molecule. A clear example of this would be the emissions from atomic hydrogen in the cometary coma, which are the result of electrons that have been excited by solar Lyman-α photons to the n=2 electronic level.
returning to the ground state of the hydrogen atom. The “scattering” component
of the term comes from the fact that the photon is emitted in a random direction
relative to the original velocity vector of the inbound photon, effectively “scatter-
ing” the photon. In the far ultraviolet (FUV) this particular mechanism is quite
powerful due to the strength of many atomic solar features relative to the contin-
uum. Because the Sun has a temperature of \(\sim 5780 \) K, the FUV emission from the
blackbody equation is quite weak when compared to an O or A type star.

If the wavelength of light that is emitted to relax the electron from the excited
state is not the same wavelength as the absorbed photon the process is termed fluo-
rescence; it is also sometimes specifically called “pumping” when a specific emission
feature is responsible for the UV photon that was absorbed (i.e. solar Lyman-\(\alpha\)
pumping of Cr II NIR emissions in Eta Carinae (Zethson et al., 2001)). The upper
energy state is populated by the absorption of the UV photon, but the strongest
transitions from that upper energy state are to intermediate energy levels. Like
resonance fluorescence emissions, fluorescence emissions are linearly dependent on
the solar flux.

This linear dependence on the stellar radiation environment makes these photon
driven processes susceptible to changes in the solar spectrum. The solar cycle is ap-
proximately 11 years long, and during solar maximum substantially more ionizing
FUV radiation is produced then at solar minimum. This decreases the lifetime of
species at the same heliocentric distance (Huebner and Mukherjee, 2015), changing
the inputs to the Haser and vectorial models described in the previous section. How-
ever, the fluorescence efficiencies can also vary substantially with these solar spectral
variations. For this reason it is imperative to use the solar spectrum taken nearest
in time to the relevant observations to directly calculate the fluorescence efficiencies
for transitions of interest. Additionally, at longer wavelengths the solar continuum
is dotted with atomic absorption features that can drastically change the available
continuum flux for NUV and visible wavelengths. These absorptions features, called
the Fraunhofer lines (von Fraunhofer, 1817; Kirchhoff, 1860), can drop the solar flux
to just 1/1000th of the flux in adjacent wavelengths. This facilitates rapid changes
in g-factors for objects, like comets, that can have large heliocentric velocities that cause the observed solar spectrum from the comet reference frame to be blue shifted (negative heliocentric velocities) or red shifted (positive heliocentric velocities).

These reference frame shifts to the solar spectrum have been observed to occur from two comet traits. The first, termed the Swings effect after its discoverer, is the change to the fluorescence efficiency that occurs due to the comet’s heliocentric radial velocity (Swings, 1941). Because comets have eccentric orbits, by definition their velocity relative to the Sun changes rapidly. For objects in circular orbits, which maintain a constant distance from the Sun and therefore have a heliocentric radial velocity of 0 km/s, the Swings effect can be ignored. For some species, like C\(_2\), there isn’t much of a change, while for some atomic features, like Ni and Fe, it is very strong, while in others it can lead to unique spectral signatures, as is the case with NH\(_3\) (Kawakita and Watanabe, 2002). As described earlier, large heliocentric velocities on the order of 20 km s\(^{-1}\) will shift the observed solar spectrum at the comet by a significant \(\Delta \lambda \sim 1/\AA\) so as to drastically change the solar flux for an atomic or molecular transition. Swings (1941) discovered the effect while observing CN, which fluoresces strongly in the visible wavelengths where the solar spectrum is riddled with narrow Fraunhofer absorption lines. For UV observations, a significant heliocentric velocity can shift the comet-observed solar spectrum so that resonance fluorescence becomes quite weak; without a strong solar continuum in the FUV the solar atomic lines are the dominant excitation source. Shifting the observed solar spectrum even just a few tenths of an Å relative to an atomic resonance line will produce a radically different spectrum in the FUV due to the narrow line widths of atomic FUV features.

The Greenstein effect was discovered to be a second order effect noticeable in high-resolution CN spectra of comet Mrkos (1957d) (Greenstein, 1958). Like the Swings effect, it relies on a radial heliocentric velocity, but rather than deriving from the orbital parameters, the Doppler shift in the Greenstein effect comes from the expansion velocity of the gas coma. Atoms and/or molecules expanding towards the Sun from the nucleus will experience a more blueshifted solar spectrum than
the atom/molecule moving expanding away from the Sun, leading to an asymmetric distribution of flux despite a isometric distribution of fluorescing molecules in an unprocessed image. Due to the comparatively low velocities for the gas expansion rate of the coma (1-8 km s\(^{-1}\)), depending on the species and the heliocentric distance (Combi et al., 2004), this effect is only significant for high spectral resolution observations and narrowband imaging of the full coma that can reveal asymmetries.

In both cases it is important to take into account the shift of the entire solar spectrum as well as the absorption features for the relevant atoms and molecules, as it’s possible for higher energy transitions to experience a higher flux and populate lower energy state transitions via a cascade. This effect was originally discovered by (Bowen, 1947) in observations of planetary nebulae and identified as the likely source of excess O I 1302 multiplet emission in comets Kohoutek and West, both of which had heliocentric velocities over 45 km s\(^{-1}\) (Feldman and Brune, 1976; Feldman et al., 2004). The excited O I \(^3\)P state was populated via cascade of electrons excited to the O I \(^3\)D state via coincidence excitation from solar Lyman-\(\beta\) emission at 1025.72 Å due to the large heliocentric velocity induced blueshift of the solar spectrum. These heliocentric velocities are only expected for LPC’s, and therefore these effects are not expected to contribute significantly to FUV JFC emission spectra, but are key to keep in mind when analyzing cometary emissions.

We now turn our attention to applying the resonance fluorescence efficiency to our model column densities from a Haser or vectorial model. Following Feldman et al. (2004), the total number of emitted photons m\(^{-2}\) s\(^{-1}\) for a column density of \(N_M\) species can be calculated as:

\[
F(r_h, \lambda) = N_M g(r_h, v_h, \lambda)\Omega(4\pi)^{-1}
\]

where \(g(r_h, v_h, \lambda)\) is the heliocentric distance and velocity dependent g-factor for the species transition at wavelength \(\lambda\) and \(\Omega\) is the solid angle that is covered by the area of interest in the slit or aperture of the observation. For cometary observations a more typical unit of measure is the surface brightness unit of Rayleighs. One Rayleigh is 10\(^{10}\) photons per meter square second steradian (m\(^{-2}\) s\(^{-1}\) steradian\(^{-1}\)),

\[
(1.10)
\]
converting Equation 1.10 to:

\[ B(\lambda) = 10^{-10} g(r_h, v_h, \lambda) \bar{N}_M \]  

(1.11)

where \( \bar{N}_M \) is the average column density of molecules (in m\(^{-2}\) over the field of view subtended by solid angle \( \Omega \)). One critical thing to note is that the FUV atomic emissions that this dissertation is mostly concerned with are the result of atoms that have been dissociated from parent molecules and have moved quite some distance away from their dissociation location. This discrepancy in dissociation position and fluorescence position means that the observed distribution informs us about the daughter product and not the parent molecule. The explicit equations for deriving the fluorescence efficiency g-factors from atomic properties are in Appendix A for completeness.

**Plasma Driven Excitation**

Some atoms and molecules can be excited to higher energy states as well as classically forbidden spin states from processes other than photon absorption. Energetic electrons, that is to say electrons with energies over \( \sim 10 \) eV, the typical threshold energy for these reactions, are capable of producing atomic and molecular emissions when they impact a molecule, dissociating it into components that are typically excited. The process, though not the mechanism, is similar to the prompt emission of OH from the photodissociation of H\(_2\)O or classically forbidden O I \(^1\)D emission produced by the photodissociation of CO\(_2\) and CO. The energies of electrons in the plasma are not quantized, and this allows them to populate the classically forbidden states while still obeying angular momentum conservation laws. This last fact is what makes unambiguously identifying these emissions in the FUV possible; the fluorescence efficiency for populating the O I \(^5\)S\(_o\) - \(^3\)P intercombination multiplet is incredibly small, while it is one of the stronger features in electron impact spectra of e+H\(_2\)O, e+CO\(_2\), e+CO, and e+O\(_2\) (Makarov et al., 2004; Ajello, 1971a,c; Kanik et al., 2003; Ajello et al., 2019).
There are two likely sources of these energetic electrons in a comet coma: photoelectrons that are produced, and therefore excited, in the coma by the photodissociation of neutrals (Feldman et al., 2015b; Chaufray et al., 2017) and accelerated solar wind electrons (Galand et al., 2020). Given the two different sources of the electrons, it is important to note a technicality with regards to what to call the resulting emission. When the dissociative electron impact emissions are produced by the excited photoelectrons, the analogous term would be “nightglow” for planetary bodies, though Chaufray et al. (2017) use the term “electroglow”. Conversely, when the dissociative electron impact emissions are the result of solar wind derived electrons accelerated along the comets ambipolar electric field into the coma, that is explicitly an “auroral” feature (Galand et al., 2020). This is a level of pedantry few will ever truly need to wield, but nonetheless important to note.

Deriving the brightness due to dissociative electron impact emissions is identical to Equation 1.11 with the exception that the excitation rate must be explicitly calculated based on two new components: the plasma energy distribution and the equivalent cross sections (typically in m\(^{-2}\) or cm\(^{-2}\)) as measured in a laboratory. These cross sections, which measure the efficiency of the e+neutral reaction resulting in a photon at the transition of interest, are a function of the electron energy and must be convolved with the plasma energy distribution and integrated across the range of relevant energies. To this end, the brightness, in Rayleighs, of emission X from e+M takes on the form:

\[
B_X = 10^{-10} \int_{E=E_{Th}}^{\infty} n_M v_E J(E) \sigma_{X_M}^X(E) \, dE
\]

where \(E_{Th}\) is the threshold energy of the transition in question, \(n_M\) is the number density of neutral molecule M, \(v_E\) is the electron velocity, \(J(E)\) is the energy distribution of the plasma, and \(\sigma_{X_M}^X(E)\) is the cross section for transition X from e+M as a function of energy. However, this equation makes the assumption that the number density of neutral molecule M and the plasma energy distribution are both constant across the line of sight captured in the observations. There are also \(L\) molecules contributing to emission X that need to be taken into account, so
the equation needs to take on a more generalized form:

\[
B_X = 10^{-10} \sum_l \int_{S} \int_{E=\infty}^{E_{Th,L}} n_t(s) v_E J(E,s) \sigma_X^t(E) \, dE \, ds
\]  

(1.13)

There is a difficulty presented with this generalized format, deriving from the line of sight. Ideally, the plasma density and energy distribution would be characterized as a function of the line of sight, with full energy distributions available to be convolved with the number density distribution. In practice, the plasma energy distribution is measured from the nearest location and assumed to be constant along the line of sight. This in turn also mitigates the need to know the neutral number density distribution as a function of \(S\), and the equation can be simplified to use a column density:

\[
B_X = 10^{-10} \sum_L \int_{E=E_{Th,L}}^{\infty} N_L J(E) \sigma_X^L(E) \, dE
\]  

(1.14)

Unlike the FUV fluorescence emissions, the neutral column densities responsible for these emissions are the parent molecules from the nucleus: \(\text{H}_2\text{O}, \text{CO}_2, \text{CO}, \text{and O}_2\). This means that the distribution of dissociative electron impact emissions in the coma traces the parent molecules and not the daughter products, even though the observed emissions are largely from atomic species. They are produced into the excited state at the location of the electron impact dissociation event, and can therefore be used as accurate tracers of parent molecule distributions. This is explored further in Chapter 3.

There are three components of this equation that govern the strength of dissociative electron impact emissions, two of which are contained within the energy distribution function \(J(E)\). The first, and most obvious, is an increase to the affected neutral column density just as would be expected for photon derived emissions. The other two derive from two ways to maximize \(J(E)\), which is the product of an electron density, in \(\text{cm}^{-3}\) or \(\text{m}^{-3}\), and a probability distribution function that when integrated from \(E_{Th,\infty}\) yields one. One simple way to increase emissions from dissociative electron impact is to increase the number density of electrons impacting the
neutral column of interest; this produces a simple linear increase. The second possibility, increasing the electron distribution at energies with higher cross-sections, is not as direct, and requires a well characterized cross-section for the particular molecule and transition of interest. Most, but not all, of the relevant UV dissociative electron impact emissions have peak cross sections for photon emission at $\sim 100$ eV, while a typical cometary electron distribution can be described by Boltzmann or sum of kappa functions (Broiles et al., 2016a), both of which have maximum probabilities at lower energy levels. Introducing a population of more energetic electrons over the threshold energy to the neutral column where measurements are being made will then increase the value of $\int_{E=\text{Th,L}}^{\infty} N_L J(E) \sigma_L^{X}(E) \, dE$, and increase the contribution from dissociative electron impact emission without an increase to the electron density.

**Spectral Fingerprints**

In a pure fluorescence spectrum it’s rather trivial to derive properties of the coma directly from the coma emissions, as long as the basic properties about the comet’s heliocentric distance, velocity, as well as distance from the Earth are known to properly calculate the fluorescence efficiency for Equation 1.11. However, the FUV emissions from atomic species in a cometary coma that result from photon- and electron-driven processes need to be used to check forward models of each mechanism to characterize the column densities and attempt to constraint the plasma environment. Due to the variations in the the electron density and energy distribution that are likely to occur across the length scales of a cometary coma, these forward models will only be able to characterize a column-averaged set of plasma properties. Iterative modeling of the plasma density and energy distribution to fit these spectra can yield fractionally more information about the plasma environment, but leaves degeneracies in the neutral column density, electron number density, and electron probability distribution function.

For comparison, the photon flux across the expanse of the coma can largely be considered identical except very near to the nucleus, where the coma may be op-
tically thick for some neutrals provided a large enough production rate. Because the g-factor is then assumed to not vary significantly across the coma, the average column density can be easily derived from the intensity of observed emissions. With dissociative electron impact, there are now three unknowns rather than just one that all vary along the line of sight. This makes deriving the exact column density of neutrals affected by dissociative electron impact a difficult task requiring substantial Markov Chain Monte Carlo modeling from synthetic or measured electron energy distributions convolved with laboratory measurements of the desired e+neutral transitions.

However, there is an assumption that can be made to allow an accurate derivation of relative abundances of affected neutrals in the coma. If one assumes that the incoming electron distribution, no matter how varied, is impacting a thoroughly mixed coma with no large scale spatial variation in composition, then only the relative efficiencies of each emission process need to be compared to characterize the neutral coma. An example spectrum is displayed in Figure 1.8. This method is used in both Chapters 2 and 3, while a simplified version is employed in Chapter 4.

Resonant and fluorescent scattering in cometary comae have been observed in the UV for just over 50 years, while true confirmation of of dissociative electron impact emissions has only happened in the last five. We now turn to the next section to discuss how these emissions have been previously characterized in the literature and describe how those observations have shaped the scope and structure of this work.

1.4 UV Comet Observations

Observing the UV emissions from comets at wavelengths shorter than the atmospheric cutoff near 3000 Å only became accessible once telescopes could be placed into low Earth orbit, above the majority of the Earth's UV absorbing atmosphere. Beginning with comets Tago-Sato-Kosaka 1969 IX and Bennet 1970 II, which were observed by the Orbiting Astronomical Observatory-2 (OAO-2) and Orbiting Geophysical Observatory-5 (OGO-5), vacuum ultraviolet observations of comets de-
Figure 1.8: An example set of modeled resonance fluorescence and dissociative electron impact spectra overlaid on a typical FUV comet coma spectrum from 67P/Churyumov-Gerasimenko by the R-Alice spectrograph. The plot on the left shows modeled contributions from individual sources (dissociative electron impact and resonance fluorescence), and the plot on the right shows only the model added to a solar continuum spectrum vs. the observed cometary spectrum. Note that the line shape of the hydrogen Lyman-α feature at 1216 Å is substantially lower than predicted. This is due to gain sag of the R-Alice detector, and renders that area of the detector less sensitive to incoming Lyman-α photons.
livered images showing an enormous (∼ millions of km) atomic hydrogen coma. Subsequent rocket and satellite observations identified the A-X band of OH, a key argument for significant water ice in support of the Whipple “icy conglomerate” comet model (Whipple, 1950). However, the difficulty in observing in the FUV (700-1900 Å ), due to the opacity of the Earth’s atmosphere in the UV and the need for rocket, satellite, or spacecraft observations, has not changed substantially in the last 50 years; the Hubble Space Telescope is currently the only FUV capable telescope with a guest observer program. With a rather limited number of papers investigating the FUV emissions of comets it is not only reasonable, but possible to describe many of the seminal papers of UV comet science prior to the work described in this dissertation. There are certainly several observational and laboratory astrophysicists that stand out among these works, without which it is entirely unclear what the state of the subfield would be today. In no particular order those scientists are Paul Feldman, Michael F. A’Hearn, George R. Carruthers, Jean-Loup Bertaux, Harold Weaver, Michel Festou, William Jackson, Hörst Uwe Keller, Michael Combi, and Chet Opal.

1.4.1 UV Comet Observations in History

As previously mentioned FUV comet observations were first attempted with the OAO-2 and OGO-5 satellites, which were cable of obtaining FUV images of the hydrogen Lyman-α feature (Code et al., 1972; Bertaux and Blamont, 1973). These large field of view images covered over 20 million kilometers to an axis and were used to observe “bright” comets, (e.g. comets Tago-Sato-Kosaka and Bennet, $Q_{H2O} \sim 1 \times 10^{29}$ s$^{-1}$). By the time the next bright comet had arrived, Comet Kohoutek 1973 XII, a suite of UV observations were executed, ranging from spectroscopy via rocketborne instrumentation (Feldman et al., 1974; Opal and Carruthers, 1977) to Lyman-α images from a UV camera on Skylab (Carruthers et al., 1974) and a rocket (Opal et al., 1974). Just three years later comet West 1976 VI also proved to be bright enough for UV rocket spectroscopy, which in turn produced the first complete UV spectrum for a comet (Feldman and Brune, 1976; Smith et al., 1980).
By 1980 Comets Seargent 1978 XV (Jackson et al., 1979) and Bradfield 1979 X (Feldman et al., 1980) had also been observed with the newly launched International Ultraviolet Explorer (IUE) satellite, commissioned in 1978. This geosynchronous observatory offered unparalleled UV capability, and its large rectangular slit (10" by 20") provided excellent sensitivity to the extended cometary comae of these first two comets. Each of these early comets appeared quite similar in FUV spectra; strong H, O, and OH emissions indicative of photodissociation of water, strong emissions from atomic C and S, and trace emissions from other radicals like CS, C_2, and CO_2^+ (Feldman et al., 1980; Weaver et al., 1981; Jackson et al., 1979). CO emission from the Fourth Positive group was detected in comets West and Bradfield, but appeared to be far lower than necessary to explain the atomic C I emissions (Weaver et al., 1981).

At this point all UV comet observations had been of particularly bright long period comets, which introduces the first bias of UV comet science. Due to the low FUV fluorescing efficiencies compared to the visible wavelengths, the extended nature of the coma and the complications with surface brightness that follow, and the low efficiencies of the UV capable detectors at the time, only these bright comets were guaranteed to be detected, and thus targeted for observations. Weaver et al. (1981) sought to change this by adding UV observations of six “faint” comets, including four short period comets, to the mix: Comet Meier, Comet Panther, 2P/Encke, 8P/Tuttle, 19P/Borely, and 38P/Stephan-Oterma. However, three of these comets are unique in their own right when compared to the broader JFC population. 2P/Encke, one of the most evolved comets, has a short orbital period of just 3.3 years and the lowest perihelion of any periodic comet with the exception of 96P/Machholz. 8P/Tuttle has a low Tisserand parameter of 1.6 thanks to its relatively high inclination of ∼54° that places it outside the normal range for a JFC (2 ≤ T_J ≤ 3). 38P/Stephan-Oterma lies in an orbital period of 38 years, classifying it as a Halley-type comet, rather than a short-period or Jupiter family comet. As noted earlier, the source regions for both Encke-type and Halley-type comets is still ambiguous. Weaver et al. (1981) were able to measure the spectrum for these comets.
at approximately the same helio- and geocentric distances and showed that they all produced very similar spectra. However, these “faint” comets still displayed water production rates \( \geq 10^{28} \text{ s}^{-1} \), rendering them quite bright by the current standards for detections of cometary activity.

IUE’s geosynchronous orbit and large FOV enabled FUV observations of over 50 comets prior to 1996 (Feldman et al., 2004), but the relatively low sensitivity of the detector electronics limited observations to the brightest, and thus most active. By 1987 the cometary sample observed by IUE contained 26 comets, 11 of which were JFCs, four Halley-types, seven LPCs, and four dynamically new or young comets. The identification of \( \text{S}_2 \) for the first time in any astrophysical object was made via IUE observations of comet IRAS-Araki-Alcock, a dynamically new or young Oort Cloud comet, providing a new benchmark for measuring previous thermal limits due to its high volatility (A’Hearn et al., 1983, 1999). Only one comet has been confirmed to possess the same emission feature since, C/1996 B2 (Hyakutake), via observations with HST thirteen years later (Weaver et al., 1996; A’Hearn et al., 1999; Kim et al., 2003), though a tentative detection was made in with an IUE spectrum (Laffont et al., 1998). Given the relationship between sulfur compounds and \( \text{H}_2\text{O} \) abundances in the inner protoplanetary disk (Lunine and Gautier, 2004), follow up detections of the volatile in more comets are eagerly sought after. The difficulty lies in the fact that \( \text{S}_2 \) has a lifetime of just 500 seconds at 1 au (A’Hearn et al., 1983), rendering it necessary to observe the near-nucleus coma (\( \sim 100\text{’s km scale} \)) to capture the \( \text{S}_2 \) emission before it dissociates.

With the successful launch of the Hubble Space Telescope in 1990 and two new UV sensitive instruments, the Faint Object Spectrograph (FOS) and the Goddard High Resolution Spectrograph (GHRS), a new era of FUV comet observations began. With a narrower field of view than IUE and improved sensitivity, the near-nucleus coma of comets became spectroscopically resolvable (Weaver and Feldman, 1992; Feldman, 1996; Weaver, 1998). Between 1990 and the decommissioning of the FOS and GHRS instruments in 1997, an additional thirteen comets were added to the FUV comet observations observation, bringing the number to over 60. These ob-
servations included characterization of the then anticipated target for the European Space Agency *Rosetta* mission, 46P/Wirtanen (Stern et al., 1998), captured S_2 emissions from C/1996 Hyakutake (Weaver et al., 1996; A’Hearn et al., 1999; Kim et al., 2003), detected the CO Fourth Positive and Cameron bands in comets Hartley 2 and Hyakutake (Weaver et al., 1994; McPhate et al., 1996), and detailed investigation of the C_2 Mulliken system to constrain the source of the common cometary radical (Sorkhabi et al., 1997).

In 1997 FOS and GHRS were replaced with the Space Telescope Imaging Spectrograph (STIS), which boasted improved angular resolution and a range of narrower slit options for higher spectral resolution investigations. In 2009 STIS was joined by the Cosmic Origins Spectrograph (COS), boasting even better FUV sensitivity and resolutions for a 2.5'' circular aperture. Both instruments have been used to great effect; observations have been used to constrain CO production rates more effectively via modeling of the Fourth Positive group (Lupu et al., 2007) as well as monitor the activity of 103P/Hartley 2 during the EPOXI mission flyby (Weaver et al., 2011; Feaga et al., 2013) and to identify H_2 Lyman system emissions in C/2001 A2 (LINEAR). The detection of H_2 was shown to be not from primordial H_2, which as a hypervolatile would indicate an extremely low bulk temperature for the last 4.5 billion years, but rather produced from the photodissociation of H_2CO (Feldman et al., 2002; Feldman, 2015). In total, prior to the work presented in this dissertation, four comets have been observed with COS, and an additional 14 observed in STIS at UV wavelengths.

For completeness it is worth noting that the FUSE mission launched in 1999, providing unrivaled access to FUV wavelengths between 900 and 1200 Å. Feldman et al. (2002) were able to use the high resolution spectrum of C/2001 A2 (LINEAR) from FUSE to identify the fluorescence of the (6-v”) band of the H_2 Lyman system, as mentioned in the previous paragraph. FUSE observations of four comets, C/2000 MW1 (LINEAR), McNaught-Hartley, C/2001 A2 (LINEAR), and C/2004 Q4 (NEAT), were ultimately acquired. The first three comets in the list were used to search for the elusive Ar emission at 1134 Å that would be able to provide a di-
rect indication of the thermal history of the comets and reveal their primordiality, without success.

In some senses, IUE provided the “golden era” of UV comet observations, with large-FOV coma observations that allowed characterizations of the bulk coma composition in long (60-120 minute) exposures only possible in geosynchronous orbit. FOS and GHRS, as well as the current STIS and COS instruments, have improved sensitivity and narrower fields of view but are subject to newer scheduling constraints required by low Earth orbit, including terminator considerations, the South Atlantic Anomaly, and increased slewing rates. In addition, there is currently no large FOV UV instrument available to take broader bulk measurements of the cometary comae, limiting the comparisons of current day FUV comet observations to IUE spectra due to the large difference in spatial scales measured.

All of these observations pre-date the arrival of the European Space Agency Rosetta spacecraft, and the Alice ultraviolet spectrograph (UVS) (Stern et al., 2007), to comet 67P/Churyumov-Gerasimenko in 2014. During the escort mission, the FUV instrument was able to probe just hundreds of meters from the cometary surface at times, and within tens of kilometers nearly constantly. This large difference in relevant scales in the cometary coma compared to previous UV observations, over four orders of magnitude, places the 67P UV observations in a league of their own, unlikely to be rivaled within the next thirty years. Given this unique observational set it’s important to take the space to underscore why the Alice instrument was selected for the first comet escort mission.

1.4.2 UV Comet Observations At Large and Small Scales: Goals of the Alice UVS

The Alice UVS on board the ESA Rosetta spacecraft was the first, and only, FUV spectrograph to make comet observations of the near-nucleus coma with spatial resolutions of less than 100 km. Given the enormous length scales of typical cometary volatiles and the models used to characterize their distribution over thousands, if not tens of thousands, of kilometers a brief review of the scientific goals of the Alice instrument are useful.
The scientific objectives for the Alice UVS are given in full detail in Stern et al. (2007); given that the Alice instrument was selected for flight on the Rosetta spacecraft in 1998, just after the decommissioning of IUE it’s intriguing to compare the goals to what was being done with IUE. The scientific objectives, as stated in Stern et al. (2007), are as follows:

1. Search for and determine the evolved rare gas content of the nucleus to provide information on the temperature of formation and thermal history of the comet since its formation. (Specifically Ar and Kr, detected in Hale-Bopp by Stern et al. 2000)

2. Determine the production rates of the parent molecule species, H$_2$O, CO, and CO$_2$, and their spatial distributions near the nucleus, thereby allowing the nucleus/coma coupling to be directly observed and measured on many timescales.


4. Study the onset of nuclear activity in ways Rosetta otherwise cannot.

5. Spectral mapping of the entire nucleus of 67P/C-G at FUV wavelengths in order to both characterize the distribution of UV absorbers on the surface, and to map the FUV photometric properties of the nucleus.

6. Study the photometric and spectrophotometric properties of small grains in the coma as an aid to understanding their size distribution and how they vary in time.

7. Map the spatial and temporal variability of O$^+$, N$^+$, S$^+$, and C$^+$ emissions in the coma and ion tail in order to connect nuclear activity to changes in tail morphology and structure near perihelion.

Several of these components, namely items 2, 3, and 6, can be seen as easily derived from the ensemble of UV comet observations that had taken place prior to the
instrument’s selection with rocket-borne instruments, IUE, HST’s FOS and GHRS, as well as excitement of the then upcoming FUSE observations. Item 1 is derived from the discovery of Ar in the spectrum of comet Hale-Bopp (Stern et al., 2000), which also prompted a sensitive upper limit study in three comets with FUSE observations (Weaver et al., 2002). Items 4 and 5 represent the surface and dust studies that were possible thanks to the suite of instruments on board for context imaging and mapping, allowing a spatially resolved map of nucleus reflectance properties in the FUV to be produced (Feaga et al., 2015; Feaga et al., 2017).

A key component to these objectives is indicative of the difficulty in obtaining UV observations: varying timescales for activity and composition. Earth-based comet observations must be planned, at a minimum, weeks in advance, and often months to years, as the UV observatory time must be proposed for, accepted, and observations planned. With Alice, the coma and nucleus of 67P was observed nearly continuously for over two years, providing the largest ever FUV dataset of a comet. However, nearly all of these observations are taken at comet-centric distances less than the typical resolvable spatial scale of Earth-based observations, so a critical part of the Alice dataset analysis becomes, “how can this rich dataset that covers unprecedented temporal and spatial resolution in the FUV be applied to future large scale FUV observations?”

1.5 Motivation and Organization of this dissertation

Compared to the long baseline of comet observations extending thousands of years back in human history, FUV observations of comet observations are a relatively recent invention. Sensitive computational models have been developed to track the chaotic evolution of scattered disk objects as they become Centaurs and JFCs, but we can only understand their behavior statistically, describing their potential evolution in terms of probabilities. Thanks to FUV, as well as IR (Ootsubo et al., 2012), observations, we know now that comets are composed largely of a mixture of H$_2$O, CO$_2$, and CO ices, but we are still unsure of how they are mixed within
the nucleus to and how that constrains the comet formation process. Simple and more complicated models for the distribution of neutral and radical components of the coma were developed to explain the distribution of molecular and atomic emissions, all reliant on the emission efficiencies of the observed transitions governed by incident solar radiation, heliocentric velocity, and the plasma environment. The unprecedented coverage of the Alice observations at 67P/Churyumov-Gerasimenko enabled a wide range of activity states and emission environments to be sampled, all of which leave a unique spectral fingerprint, yielding critical information about the comet’s composition, structure, formation, and evolution. The hardest part is determining which processes are at work in a given observation and removing degeneracies that can explain the increase or decrease in emissions: nucleus rotation, changes to the phase angle, shadowed regions of the nucleus becoming illuminated, illuminated regions becoming shadowed, arrival of energetic plasma from solar transients, outbursting of the nucleus. For the first time in FUV observations, all of these components not only mattered, but could actually be characterized. This dissertation is the culmination of research carried out to understand how the small spatial scale, high frequency observations of the Alice instrument could be applied to the large spatial scale, low frequency observations in the FUV by Earth-based observatories like HST. The dissertation is structured as follows.

In Chapter 2, the unique properties of a series of outbursts observed by the Alice UVS on November 7-8 of 2015 are described, probing the evidence that different outburst types can produce distinctive spectra that could be detected remotely. Chapter 3 follows the aftermath of those outbursts, using maps of atomic emission features in the near-nucleus coma to investigate the similarities in distribution between dissociative electron impact emissions and molecular neutral densities. To explore the effect of the solar transients on the cometary FUV emissions Chapter 4 examines a case study where a coronal mass ejection (CME), a large eruption of high energy solar plasma, impacted the coma of 67P. Observations of comet 46P/Wirtanen made with the COS instrument on HST are presented in Chapter 5 that search for evidence of the dissociative electron impact emission seen at 67P by
the Alice and OSIRIS instruments and apply the lessons learned from the Rosetta mission. Chapter 6 synthesizes the results into a comprehensive summary of the relevance and importance of FUV comet observations at large and small scales. The chapter also explores several of the remaining questions to be scrutinized with future FUV observations and archival FUV observation analysis and provides a few concluding remarks about the complexities of de-biasing comet emissions. This is followed by two appendices that provide detailed derivations and background on resonance scattering and fluorescence as well as plasma derived emissions, respectively. All references for the dissertation can be found after the appendices.
CHAPTER 2

Analysis of Hybrid Gas-Dust Outbursts Observed at 67P/Churyumov-Gerasimenko

The contents of this chapter were originally published as “Analysis of Hybrid Gas-Dust Outbursts Observed at 67P/Churyumov-Gerasimenko” in The Astronomical Journal, volume 162 (Noonan et al., 2021c).

2.1 Introduction

The European Space Agency’s Rosetta spacecraft escorted the comet 67P/Churyumov-Gerasimenko from August 2014 until September 2016. For a broad range of comet and heliocentric distances the spacecraft observed changes to the comet’s coma, nucleus, and plasma environment. One particularly frequent form of these changes comes from cometary outbursts. Characterizing outbursts and their impact on the near-nucleus coma is critical to understanding the relationship between outburst traits, chemical composition, and level of dissociative electron impact. So far both gas and dust outbursts have been identified by the Alice instrument, with several outbursts even having overlapping traits (Feldman et al., 2016; Steffl et al., 2015, 2018). This dichotomy is difficult to disentangle with any single instrument’s dataset; a multi-instrument approach is required to make meaningful progress in proper outburst characterization (Grün et al., 2016; Pajola et al., 2017; Agarwal et al., 2017). The initiation of outbursts, gas or dust, may leave unique clues in the coma signature that could be traced with a multi-instrument technique. Reviewing the library of Rosetta data, identifying outbursts in the data, and correlating different instrument datasets represents the next crucial step in understanding the chaotic nature and source of cometary outbursts.
Alice observations of outbursts have revealed a range of compositions and emission processes within these periods of increased activity. H$_2$O, CO$_2$, CO, and O$_2$ were all indirectly observed within outbursts via emission from the daughter products H$_2$C, and O (Feldman et al., 2016). The supervolatile species O$_2$ is thought to be the outburst initiator based on the outburst model put forward by Skorov et al. (2016), which modeled the similarly volatile CO, due to the abundance of O$_2$ in outbursts (Feldman et al., 2016). The increased emission strength of the semi-forbidden O I] 1356 Å feature during outbursts with respect to other atomic emissions also indicates changes to the dissociative electron impact emission environment, but whether that increase is caused by an increase in the neutral density, electron density, electron energy, or a combination of the three remains to be determined (Feldman et al., 2016). This correlation has been among the most intriguing results from Rosetta; the discovery of the prevalence of dissociative electron impact emission, the result of collisions between energetic electrons and neutral molecules like H$_2$O, CO$_2$, and O$_2$, both at large heliocentric distances when it was correlated with solar wind interaction (Feldman et al., 2015b; Bodewits et al., 2016; Galand et al., 2020) and nearer perihelion when it was more sporadic and linked to transient events (Feldman et al., 2016; Noonan et al., 2018). This emission mechanism is tied to the near-nucleus coma, typically within 10 kilometers of the nucleus, and had remained undetected in any comet prior to the Rosetta mission.

During the perihelion passage, several outbursts were observed with the Optical, Spectroscopic and Infrared Remote Imaging System (OSIRIS) and Visible InfraRed Thermal Imaging Spectrometer (VIRTIS) onboard Rosetta (Coradini et al., 2007), in both VIRTIS-H and VIRTIS-M channels. The outbursts have very different morphologies, with narrow and collimated plumes (August 10, September 13) and broad blobs (September 14) (Vincent et al., 2016; Lin et al., 2017; Rinaldi et al., 2018; Bockelée-Morvan et al., 2017). The outbursts have been characterized by sudden increases in dust scattered solar light over a period of 5-30 minutes, without a corresponding enhancement of CO$_2$ or H$_2$O vibrational bands characteristic of the comet dust activity. This rapid onset is correlated with a change of the visible and
infrared dust color from red to less red implying the presence of very small grains (∼100 nm) in the outburst material. The sudden increase is also correlated with a large increase of the color temperature (from 300 K to up to 630 K) and large bolometric albedos (∼0.7) indicate bright grains in the ejecta, which could either be silicatic grains, implying the thermal degradation of the carbonaceous material, or icy grains. The 3 µm absorption band from water ice is not detected in the spectra, whereas signatures of organic compounds near 3.4 µm are observed in emission. However, for the same outburst, Alice has observed a strong absorption feature around 170 nm, characteristic of water ice (Steffl et al., 2015, 2018). Because the UV wavelengths are more sensitive to the small particles with respect to the IR wavelengths, the presence of the absorption feature around 170 nm and the absence at 3 µm would be consistent with the presence of very small ice particles, less than 100 nm.

At the moment cometary outbursts are well-known but poorly understood phenomena. The aim of this work is to take advantage of the capabilities of three instruments to analyze the dust and gas coma behaviour during these transient events in the post-perihelion period when the comet was at a heliocentric distance of 1.61 au. The comparison allows us to infer possible time evolution properties of the gas and dust activity. this chapter reviews data taken between 12:00 UTC and 19:18 UTC on 2015 November 7 and is intended to serve as a companion paper to an additional multi-instrument analysis undertaken by Noonan et al. (2021a), which describes data taken between 21:26 UTC November 7 and 10:30 UTC November 8, 2015.

In Section 2.2, we describe the ALICE and VIRTIS-M instruments and datasets. In Sections 2.3, 2.4, and 2.5 the results from each instrument, including OSIRIS and NAVCAM, are discussed individually. Finally, in Section 2.6 we combine the three separate analyzes to show the inverse relationship in these outbursts between gas and dust production, the implication for different outburst mechanisms, and provide an argument for further investigation of the Alice data for small outbursts. A brief summary of our findings is outlined in Section 2.7.
### Table 2.1. VIRTIS-M observations contemporary with Alice observations

<table>
<thead>
<tr>
<th>ID</th>
<th>VIS File name</th>
<th>$r_{\text{sub}}$</th>
<th>$t_{\text{start}}$</th>
<th>$t_{\text{exp}}$</th>
<th>$\Delta t$</th>
<th>$\Phi$</th>
<th>Subsolar long.</th>
<th>Subsolar lat.</th>
<th>Heliocentric distance</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>V1.00405529400</td>
<td>256 126 432 45.07 16 15:04:40 2592 230 62.77 -16.62 50.93 1.61</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>2</td>
<td>V1.00405532100</td>
<td>256 126 432 45.07 16 15:49:41 2592 230 62.77 -14.05 28.41 1.61</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>3</td>
<td>V1.00405534800</td>
<td>256 126 432 45.07 16 16:34:40 2592 230 62.77 +14.05 357.43 1.61</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>4</td>
<td>V1.00405537500</td>
<td>256 126 432 45.07 16 17:19:41 2592 230 62.77 +13.67 324.61 1.61</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>5</td>
<td>V1.00405540200</td>
<td>256 126 432 45.07 16 18:04:40 2592 230 62.77 +13.53 324.61 1.61</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>6</td>
<td>V1.00405542900</td>
<td>256 126 432 45.07 16 18:49:40 2592 230 62.77 +13.53 324.61 1.61</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

**Note:**

- **Column 1:** Assigned letter for each image cube containing an outburst. **Column 2:** Observation file name.
- **Column 3:** Cube size in number of samples, number of scan lines and spectral bands (432 for each channel). **Column 4:** Pixel size at the distance of the observation. **Column 5:** Exposure time for each line. **Column 6:** Start time of the image cube (UTC). **Column 7:** Total duration time for the image cube from acquisition start to stop. **Column 8:** Distance of spacecraft from the comet center. **Column 9:** Observation phase angle. **Column 10:** Subsolar longitude. **Column 11:** Subsolar latitude. **Column 12:** Heliocentric distance.
2.2 Observations

The outbursts in this chapter were identified while examining the atomic emission light curves from the Alice instrument for the companion paper. In Alice data outbursts are best characterized as sharp increases to atomic emissions relative to prior observations. To correctly identify an outburst items such as geometry changes must be ruled out.

2.2.1 Geometry and Spacecraft Pointing

On 2015 November 7, Rosetta and 67P were moving away from the Sun after perihelion in August 2015 and had a heliocentric distance of 1.61 au. At 12:00 UTC on November 7, when the first observations used in this analysis were taken, Rosetta was 237 km from the nucleus of 67P. Between 12:00 UTC and 19:18 UTC, when the final observations were taken prior to an observing gap, the spacecraft had decreased its comet-centric distance to 228 km. Over that same time period the phase angle decreased from 64° to 61.5°.

2.2.2 Alice Instrument Description

The Alice instrument was a low-power and light-weight imaging spectrograph onboard the Rosetta spacecraft with the goals of constraining the comet’s UV surface properties, identifying atomic emissions from the coma, and understanding nucleus-coma interactions. The Alice instrument had a bandpass of 700 Å-2050 Å with a spectral resolution characterized in flight to be 11 Å at the center of the “dog bone” shaped slit, which had a narrow central section and wide top and bottom sections. The upper and lower portions were both 0.10° (210 µm) wide, while the narrow center was 0.05° (100 µm) wide in the middle 2.0° of the slit. The lower and middle sections were 2.0° long, while the upper section was 1.53°. In total the slit was 5.53° long. The detector in the Alice instrument was a microchannel plate with 32 rows in the spatial dimension and 1024 columns in the spectral dimension. Only rows 5 through 23 (zero indexed) of the 32 spatial rows were exposed to incoming light from
the aperture. Each detector row subtended 0.30° on the sky. One notable detector effect that was present in the data is identified as the odd/even effect, where the Alice detector tended to push counts to odd rows over even rows (Feldman et al., 2011; Chaufray et al., 2017). The full details of the instrument are available in Stern et al. (2007).

2.2.3 Alice Dataset

From 12:00 UTC until 19:18 UTC on November 7 the Alice instrument was in a stable pointing scheme, where there was minimal motion to the instrument’s line of sight. At this time the Alice slit was centered on the nucleus of 67P, with the upper rows in the sunward direction and the lower rows in the anti-sunward direction (Figure 2.1). A total of 38 exposures were taken in this period. In this period of time the distance from the spacecraft to the comet decreased from 237.0 to 228.8 km, the subspacecraft latitude was between -3.20° and -0.99°, and the sub-spacecraft longitude ranged from 103.6° to -109.0°. The end of the “stare” scheme observations occurred at 19:18 UTC and Alice observations ceased until the ride-along observations described in detail by Noonan et al. (2021a). Additional information on Alice observing schemes and planning can be found in Pineau et al. (2018).

2.2.4 VIRTIS-M Instrument Description

The Visual Infrared and Thermal Imaging Spectrometer (VIRTIS; Coradini et al. (2007)) was composed of two spectral instruments: VIRTIS-M and VIRTIS-H. VIRTIS-M was the visible (230 – 1000 nm, 432 bands) and infrared (1000 – 5000 nm, 432 bands) imaging spectrometer with a field of view of 3.6° (along the slit axis) and an instantaneous field of view (IFOV) of 250 μrad. The instrument acquired hyperspectral cubes by scanning in time the target scene line by line. The duration of the acquisition (Δt in Table 2.1) is given by the number of lines (including periodic dark current frames) times the internal repetition time, where the repetition time is the time between two consecutive steps necessary to move the internal scan
Figure 2.1: NAVCAM images from November 7 at 15:11, 17:15, and 19:18 UTC with nucleus pixels masked to highlight faint activity. The Alice slit is overlaid in white. The Sun is to the right in all three images. With the exception of faint jets emanating from the neck in image c) there is no evidence of significant background activity.
Figure 2.2: The figure shows the configuration of the nucleus of the comet and outburst with respect to the VIRTIS-M slit (horizontal red line) and its scan direction (red arrow). The VIRTIS-M data cubes are acquired with a scan in which each line corresponds to a given time (white arrows). The orange thick line shows the Sun direction. The spacecraft is approximately in a terminator orbit with a phase angle of 90°, so that one side of the comet is illuminated by the Sun and the other side is in darkness.
Figure 2.3: VIRTIS-M images taken between 15:04 and 18:49 UTC on November 7. The maps are composite images where the comet nucleus image (taken as an average in the wavelength range between 0.45 and 0.55 µm) is superimposed on the maps of the dust continuum at 0.55 µm to highlight activity and the Sun is always at the top of each image. The images on the top of each VIRTIS-M image show the configuration of the nucleus with respect to the VIRTIS-M frames (green rectangles) and the Alice slit in red from the Rosetta 3D tool. Frames 2 and 4 correspond to outbursts A and B, respectively, with both notable extensions and intensities of dust relative to the other frames. The radiance has units of W m$^{-2}$ sr$^{-1}$ µm$^{-1}$. The cube details are listed in Table 2.1.
mirror by one IFOV (Fig. 2.2). The integration time ($t_{\text{exp}}$ in Table 2.1) is lower than the internal repetition time. The maximum $3.6^\circ \times 3.6^\circ$ FOV was imaged by repeating acquisition on successive 256 scan mirror steps (lines). From a distance of 100 km this corresponds to a 6.4 km $\times$ 6.4 km swath with a resolution of 25 m pix$^{-1}$. As an example, we show in Fig. 2.3 the VIRTIS-M hyperspectral cubes with the line and time axes.

**VIRTIS-M dataset**

Because of the failure in early May 2015 of the cryocooler, which is necessary to operate the IR channel, our analysis is restricted to VIS hyperspectral images. The spectra and images used for the analysis were reduced using the VIRTIS calibration pipeline (Ammannito et al., 2006; Filacchione, 2006), with additional corrections derived from in-flight data. We removed defective pixels and cosmic-ray strikes using a median filter despiking algorithm, which was employed only in the spatial dimensions of the data and therefore left the spectral data intact.

On November 7, from 6:29 to 19:26 UTC, VIRTIS-M (VM) acquired 17 images that lasted about 40 min each. Six of these observations are contemporary with Alice observations, between 15:03 and 16:53 UTC, and provide useful context. As shown in Fig. 2.3, in this range of time VM observed two outbursts (image cubes A and B) and small and strong jets in the other observations. The hyperspectral cubes are obtained from a target distance of 230 km with the FOV covering an area of $14.5 \times 7.2$ km$^2$. The spacecraft was approximately on a terminator orbit so that the Sun illuminated one side and the other side was in darkness (Fig. 2.2). Figure 2.3 displays the intensity maps of the dust continuum in units of W m$^{-2}$ sr$^{-1}$ $\mu$m$^{-1}$. The maps are a composite image where the comet nucleus (as an average in the wavelength range 0.45 - 0.55 $\mu$m) is superimposed on the image of the dust continuum averaged in a bandpass of 0.10 $\mu$m centered on 0.55 $\mu$m. The Sun is at the top of the image, and on the day side, the dust activity shows a predictable behavior that is correlated with the illumination conditions. Table 2.1 provides the
geometry information for the hyperspectral cube calculated by a routine (Acton, 1996) that uses the spacecraft trajectory and orientation stored in SPICE kernels, and the 67P SHAP5 shape model for the comet nucleus (Jorda et al., 2016). The image was acquired line by line by means of a scanning mirror, taking 20 seconds per line with the final image composed of a sequence of consecutive lines in the vertical direction (Fig. 2.2). The analysis of the VM continuum can be limited by in field straylight when the instrument slit is partially filled by the bright nucleus, and a sizable portion of the incoming photons is spread into the adjacent coma pixels. For the outburst events studied here, there is no stray light because they are out of these regions.

2.3 ALICE Results: Gas properties

Here we discuss Alice UV observations of the period between 12:00 and 19:18 UTC on November 7 and describe properties of several useful Alice data products; spectra, light curves, and spatial profiles.

2.3.1 Spectra

Alice observations from 12:00 to 19:18 UTC were taken during a stable pointing scheme with little to no motion in the Alice slit relative to the nucleus for the duration. The exposure taken at 15:04 UTC on November 7, which is the quiescent background spectrum, contains the hydrogen emission features Lyman-α and -β, though Lyman-α has a non-standard line shape due to detector gain sag in that area (Fig. 2.4, blue spectrum). The same spectrum shows the O I $\lambda$ 1356/1304 Å ratio is $<1$, evidence that both dissociative electron impact and resonance scattering emission are within the Alice slit for relatively quiet periods of cometary activity (Kanik et al., 2003; Feldman et al., 2016), though resonance fluorescence along the Alice line of sight is dominant. O I $\lambda$ 1356 Å is the result of a spin-forbidden transition and is only present as as a result of dissociative electron impact, and its strength relative to the O I $\lambda$ 1304 Å triplet can be used to infer compositions. In cases where
dissociative electron impact excitation on O\textsubscript{2} or CO\textsubscript{2} is dominant we would expect the O I\textsuperscript{[1]} 1356/O I 1304 Å ratio to approach 2 while if e+H\textsubscript{2}O dominates the value is closer to 0.3 (Hall et al., 1998; Feldman et al., 2016, 2018a; Noonan et al., 2018). A O I\textsuperscript{[1]} 1356/O I 1304 Å ratio greater than 1 can be seen in the spectra taken at 16:07, 17:32, and 19:18 UTC on November 7, both in Figure 2.4 and after quiescent subtraction to remove background coma emissions and interplanetary medium contribution to the Lyman series in Figure 2.5. The carbon emission features for this period are dominated by C I 1561 and 1657 Å, both capable of being produced by photodissociation and dissociative electron impact of CO\textsubscript{2} and CO, though the line ratios suggest a mixture of resonance fluorescence and e+CO\textsubscript{2} as the main contributor (Ajello, 1971a,c; Ajello et al., 2019). CO Fourth Positive emission appears blended with atomic carbon and sulfur features between 1400 and 1600 Å specifically the 4-0, 5-1, 3-0, 4-1, 2-0, 1-0 and 0-0 bands, but far below the levels seen in spectra presented in Feldman et al. (2018a) and are not characterized in this work.

To highlight spectral characteristics we have chosen three spectra that correspond to two VIRTIS-M outbursts and one jet; the first corresponds to outburst A at 16:07 UTC on November 7, the second to outburst B at 17:32 UTC, and the third to a jet at 19:18 UTC (Fig. 2.4). These three spectra allow spectral comparison of two prominent types of cometary activity: outbursts and jets. Quiescent-subtracted spectra are displayed in Figure 2.5 to properly convey the spectral signature of each activity. Lyman-β and the C I 1561 and 1657 Å features have no strong changes for the first VIRTIS-M outburst, but show much larger increases for both the second VIRTIS-M outburst and jet (Fig. 2.5). Additionally, the O I 1304 and 1356 Å emissions for each spectrum show different characteristics; the first VIRTIS-M outburst shows an O I\textsuperscript{[1]} 1356/O I 1304 ratio of <1, the second a ratio >1, and the jet a ratio of ~1.

The UV spectra contained in this analysis all share some weaker features that we will discuss here. First, the Lyman-β emission feature is blended with O I 1025.72 Å emission at the resolution of the Alice instrument. However, the O I contribution to the Lyman-β + O I 1025.72 Å blend can be determined from e+O\textsubscript{2} modelling
Figure 2.4: Spectra derived from rows 15-18 taken during a quiescent period, the VIRTIS-M outburst detections, and near-alignment of a cometary jet with the Alice slit on November 7. Of particular interest is the O I \( \lambda 1356 \) and O I \( \lambda 1304 \) ratio, indicative of dissociative electron impact. Spectra are offset by 2.5 photons cm\(^{-2}\) s\(^{-1}\) Å\(^{-1}\). There is also faint CO Fourth Positive emission in the 1400 Å to 1600 Å region mixed with emission from dissociative electron impact excitation of CO\(_2\), discussed further in Section 2.6. Errorbars are plotted but are largely smaller than the line-width at wavelengths less than 1800 Å.

Figure 2.5: Difference spectra resulting from the subtraction of the 15:04 UTC spectrum from the 16:07 and 17:32 UTC spectra on November 7. Spectra are offset by 2.5 photons cm\(^{-2}\) s\(^{-1}\) Å\(^{-1}\). Notice the substantial difference in O I \( \lambda 1356 \)/O I \( \lambda 1304 \) Å emission between VIRTIS-M outbursts A and B.
done at 200 eV by Ajello and Franklin (1985) if the O\textsubscript{2} column density is known, though we note that this energy is significantly above the expected mean energy for electrons in the near-nucleus environment (Clark et al., 2015). Because the O\textsubscript{2} column density is typically not known a priori, we instead implement the line ratio for the O I 1356/1025.72 Å features from dissociative electron impact of O\textsubscript{2}, which is approximately 35, and is therefore negligible compared to the typical strength of Lyman-\(\beta\). Given the low \(g\)-factor for fluorescence of the O I 1025.72 Å transition we assume this ratio is accurate for our data. Second, there is evidence of S I emission in Figure 2.4 as a weak triplet at 1807, 1820, and 1826 Å but these contributions are no longer clear in the quiescent-subtracted spectra in Figure 2.5 except in the aligned jet spectrum. This implies that there is weak S I emission at 1425 and 1473 Å blending with CO Fourth Positive group emissions. However, given that the S I and CO emissions are negligible in the quiescent subtracted spectra and are therefore not large components of either the outbursts or jet we will not focus on them.

2.3.2 Light Curves

By integrating Lyman-\(\beta\), O I 1304, O I] 1356, and C I 1657 Å emission features in rows 17-22 of the Alice slit for observations taken during the period between 12:00 and 19:18 UTC on November 7 light curves detailing changes to cometary activity can be made, allowing confirmation of outbursts and other transient events. In Figure 2.6 we clearly see stable atomic emissions from 12:00 until \(\sim\)16:00 UTC. At 16:07 UTC there is a sharp increase in O I emissions that quickly subsides back to the quiescent levels. A much stronger increase in emissions then occurred at 17:32 UTC, had a 5-20 Rayleigh decrease by 18:00 UTC, which was then sustained until 19:18 UTC.

From the Alice light curves several key pieces of information become clear. The first outburst identified by VIRTIS-M has a small CO\textsubscript{2} component, indicated by the small change in C I 1657 Å emission relative to the normal comet activity between 12:00 and 16:00 UTC. Second, the first outburst is smaller not just in
Figure 2.6: Light curves for dominant atomic emission features between 12:00 and 20:00 UTC on November 7, integrated over rows 15-18 on the Alice detector. Error-bars on each point are driven by variation between rows, which is amplified by the odd-even detector effect. The observation used for quiescent subtraction is marked with a black dot-and-dashed line, observations coinciding with VIRTIS-M outburst detections are marked with blue lines for outbursts A and B at 16:07 and 17:32 UTC, respectively. The observation of the nearly in-slit jet is marked with a red dashed line.
emission strength but also in duration compared to the second outburst. For the first outburst quiescent emission levels were reached in the Alice spectrum at 16:13 UTC, while for the second it appears substantial cometary activity followed the outburst and persisted until the end of Alice observations at 19:18 UTC. This may be an indication that the second outburst may have increased more typical cometary activity like jets, which are sustained longer than outbursts. Third, the O I] 1356/O I 1304 ratio for the period shows that outburst A has a substantially lower value than either outburst B or the aligned jet (Fig. 2.6). O I] 1356/O I 1304 ratios at or above 1 have previously been indicative of significant dissociative electron impact of CO$_2$ and O$_2$ in the inner coma (Feldman et al., 2018a). The high O I] 1356/O I 1304 ratio persists well past 19:18 UTC into the period covered by Noonan et al. (2021a), until 12 November 2015. This consistent and elevated ratio indicates that the dissociative electron impact emissions were elevated for days, regardless of comet rotation, which could be tied to increased cometary activity, plasma density, plasma energy, or a combination of all three. This chapter will focus only on the outbursts that appear to initiate this extend period of elevated electron impact emissions.

2.3.3 Spatial Profiles

During the stable pointing scheme on November 7 both the sunward and anti-sunward portions of the near-nucleus coma were observed in the same observations, an ideal geometry for developing one-dimensional spatial profiles of the near-nucleus coma. Several of these profiles are shown in Figure 2.7.

The earliest spatial profile is taken from the quiescent observation at 15:04 UTC and shows the inner coma as typically observed by Alice; strong emission on the sunward side, with weak emission on the anti-sunward side (Feldman et al., 2015b, 2018a). This dichotomy is exhibited by all four emission features shown in the profiles in Figure 2.7. Emission strengths gathered from spectra taken at 16:07 and 17:32 UTC show the impact of outbursts A and B, while the emissions from 19:18 UTC are of the activity resulting from outburst B. All three emission features without substantial solar continuum contribution from the nucleus see an increase
at the 0 km mark; Lyman $\beta$ increases from $\sim$22 to 30 Rayleighs at 17:32 UTC, O I 1304 Å rises from 19 to 25 Rayleighs, O I [1356 Å from 0 to 10 Rayleighs. Additionally, O I [1356 Å shows a factor of 5 increase in emission near the nucleus, from a maximum of 8 Rayleighs at 15:04 UTC to 40 Rayleighs at 17:32 UTC. The slope for the O I 1356 Å spatial profile at 17:32 UTC is also steeper than in the quiescent period, approximately $-1.86 \pm 0.90$ Rayleighs/km compared with the $-0.45 \pm 0.03$ Rayleighs/km at 15:04 UTC. This slope increases between the 17:32 UTC and 19:18 UTC datasets to $-2.07 \pm 0.31$ Rayleighs/km, possibly indicating a relaxation of the near-nucleus coma to the quiescent state at the end of the stable Alice observations on November 7 and possibly a weakening of the jet.

The profiles for both Lyman-$\beta$ and O I 1304 Å appear flat between 3 and 7 km for the observations taken at 17:32 and 19:18 UTC, something that is not captured in the linear fit to the slope. This feature is missing in both the O I [1356 and C I 1657 Å spatial profiles. There are two factors that make determining the significance of these changes difficult with the limited number of observations: the low spatial resolution and the odd-even effect experienced by Alice. The 1.2 km/pixel size combined with the tendency of the Alice detector to push counts to odd rows over even rows complicates peak determination, so all positions stated above have a pixel size uncertainty associated with them of $\pm 1.2$ km for these stable pointing spatial profiles.

2.4 VIRTIS Results: Dust properties

In this section, we analyze the physical properties of the dusty outbursts observed by VIRTIS-M in terms of lightcurve, color, filling factor and dust mass loss. In Table 2.4, we list all the relevant information obtained from the analysis of our data set as time, duration, longitude, and latitude of the estimated source region of the outburst, radiance level, and color at the maximum of the light curves. The duration is computed using the time at which the radiance returned to the pre-outburst value or when the coma observation starts and ends.
Figure 2.7: Spatial profiles of dominant emission features in Alice spectra at 15:04, 16:07, 17:32, and 19:18 UTC. The sunward direction is in the +X direction. Each detector row subtends approximately 1.2 km. Of particular note is the change in slope for O I] 1356 Å between quiescent, initial activity at 17:32 UTC, and the parallel jet observation at 19:18 UTC between 0 and 12 km.
Table 2.2. Dust outburst properties in the VIRTIS-M VIS channel

<table>
<thead>
<tr>
<th>ID</th>
<th>VIS filename</th>
<th>Detection time</th>
<th>Duration</th>
<th>Local time range</th>
<th>Long range</th>
<th>Lat range</th>
<th>Max radiance</th>
<th>color %/ 100 nm</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td>V100405532100</td>
<td>[16:13, 16:18]</td>
<td>4.8</td>
<td>[17:00, 17:06]</td>
<td>[70.37, 73.40]</td>
<td>[-58.73, -38.56]</td>
<td>0.08</td>
<td>13.1 ± 1.3</td>
</tr>
<tr>
<td>B</td>
<td>V100405537500</td>
<td>[17:33, 17:48]</td>
<td>15</td>
<td>[13:16, 17:01]</td>
<td>[25.18, 354.98]</td>
<td>[-57.09, -18.73]</td>
<td>0.06</td>
<td>12.4 ± 2.4</td>
</tr>
</tbody>
</table>

**Note:** *Column 1:* Assigned letter for each image cube. *Column 2:* Observation file name. *Column 3:* Start and stop detection time for the dust plume. *Column 4:* Observed outburst life time. *Column 5:* Local time range of outburst source on surface (see Section 2.6.3). *Column 6:* Longitude range of dust plume source on surface (see Section 2.6.3). *Column 7:* Latitude range of outburst source on surface (see Section 2.6.3). *Column 8:* Radiance at 0.55 µm at the maximum of the outburst emission in W m$^{-2}$ sr$^{-1}$ µm$^{-1}$. *Column 9:* color at the maximum of the outburst radiance (see Section 2.4.2).
2.4.1 Outburst morphology and light curves

In this section, we analyze the evolution of the given outbursts and we characterize the spatial distribution of both the dust background and the ejected dust. As shown in Rinaldi et al. (2018) to distinguish, in the VM data, between transient events and long-lasting features such as jets, which are stable for more than one comet rotation as shown by Vincent et al. (2016), we adopted the following criteria: the transient events observed by VM were identified by their light curve (radiance at a given wavelength versus time) characterized by a sudden brightness increase in the coma that is associated with a release of gas and dust over a very short timescale, that is 5-30 min (Farnham et al., 2007; Miles et al., 2016; Bockelée-Morvan et al., 2017; Rinaldi et al., 2018). The light curve of a transient event can only be derived when the scan occurs along the radial direction of the plume. The VM data are acquired with a temporal scan, as shown in Fig. 2.2, in which each line corresponds to a given time. This allows us to reconstruct the temporal evolution of the event. The two outbursts were captured in two consecutive VM data cubes, acquired 42 min apart. In Fig. 2.3 A, the dust distribution shows a wide structure whose behaviour is correlated with the illumination conditions, with an outburst of dust blobs in the direction of the Sun. The wide shape can be the result of a complex event, with more ejecta sources on different active regions of the surface. The wide and well-defined internal structures have a maximum intensity of 0.08 W m$^{-2}$ sr$^{-1}$. In Fig. 2.3 B, we see the onset of another less-intense event, manifested as a collimated structure with a maximum intensity of 0.06 W m$^{-2}$ sr$^{-1}$ (Table. 2.4).

In Fig. 2.3, the temporal profiles (multicolor curves) in the bottom plots have been extracted along the yellow lines sown in the upper images. The colors used for the VM data points correspond to the distance from the comet center. According to the description of the shape model by Preusker et al. (2017), this center is defined as the center of mass. Fig. 2.8 shows outburst light curves where the radiance has been multiplied by the distance as a means for better visualising changes in the coma. Before the outburst event both profiles have an approximately constant value in time.
Figure 2.8: Light curves of the outbursts A (left) and B (right) acquired on November 7. The multicolor curves are the VM radiance at 0.55 µm multiplied by the distance from the comet center. The images on the top show the VM image frame for the observations A and B, and the yellow lines show where the lightcurve profiles have been extracted. The colorbar used for the VM light curves refer to the distance from the comet center and not the intensity displayed in the upper plots. For reference, a flatter curve represents a more linear relationship between radiance and distance from comet center. The deviations present at 16:13 UTC and 17:33 UTC are interpreted as the start of the outbursts.
Figure 2.9: Images of the outburst of November 7 in the VIS at 0.55 \( \mu m \) (upper plots) and the VIS spatial distribution of the color (lower plots) calculated in the yellow square of the dust image. The colorbar used for the VM color maps refer to \% (100 nm)\(^{-1} \) for the cometary dust in the lower plots and not the intensity displayed in the upper plots. The location of maximum radiance, assumed to be the outburst source, has been marked with a red star. Ejecta from outburst A or B do not display any evident color gradient, unlike other outbursts observed by VM (Rinaldi et al., 2018).

between 0.05 and 0.09. This is consistent with a cometary coma in a steady state, with constant dust production and outflow speed together with the conservation of dust grains. Each outburst in Fig. 2.8 is identifiable by a sharp increase in the light curve that deviates from the radiance and distance product, which should be linear in nature for a steady state dust environment. Outburst A started at 16:13 h UTC and ended at 16:18 UTC. Outburst B is a less intense outburst starting at 17:33 UTC and ending at 17:48 UTC. Unfortunately, both curves do not cover the complete evolution of the outburst because the data do not show when the radiance returned to the pre-outburst value after the maximum. Both light curves show the typical behaviour of outburst evolution; a sudden increase of the dust radiance, reaching maximum intensity a few minutes later followed by a return to a typical dust environment by the next scan (Belton et al., 2008; Knollenberg et al., 2016; Bockelée-Morvan et al., 2019; Rinaldi et al., 2018).
2.4.2 Color

Previously in the literature it has been shown by Miles et al. (2016), Bockelée-Morvan et al. (2017), and Rinaldi et al. (2018) that cometary outbursts have been associated with possible compositional and particle size changes. These changes would be evidenced by spatial and temporal evolution of the color, normalized reflectivity gradient, or reddening, measured in % (100 nm)$^{-1}$ (Jewitt and Meech, 1986). The color can be calculated using the values of the reflectance at two or more wavelengths. The reflectance, $R$, is a dimensionless quantity calculated by dividing the measured scattered light intensity $I$ by the solar incident flux. Taking the wavelength dependent solar flux from Kurucz (1994), the mean reflectance gradient % (100 nm)$^{-1}$, $r$, for a particular wavelength interval becomes:

$$r = \frac{R_{\lambda_2} - R_{\lambda_1}}{\lambda_2 - \lambda_1} \times \frac{200}{R_{\lambda_2} + R_{\lambda_1}}.$$  \hspace{1cm} (2.1)

The reflectances used are averages over a narrow bandpass of 10 nm in width centered on 550 nm ($\lambda_1$) and 750 nm ($\lambda_2$), chosen to optimise the Signal-to-Noise Ratio (SNR) and so minimise the internal error in the color determination. We obtained a two-dimensional color map using the spectrum for each pixel in the image (Fig. 2.3). The color uncertainties are evaluated with the method used by Rinaldi et al. (2018), by propagating the formal error that is inversely proportional to the SNR. Outside the outburst the uncertainty is higher because the radiance and the SNR are both very low (Fig. 2.3). For this reason, the color fluctuations outside the dust plume region delimited by the contour lines in Fig. 2.3 are not realistic. Inside the outburst the radiance and the SNR give us an uncertainty of about 15-20%. In Fig. 2.3, the two-dimensional color maps, for outbursts A and B, do not show evidence of different reddening values in the outburst dust continuum with respect to the surrounding coma, which implies that we do not observe dust with different physical characteristics (Bockelée-Morvan et al., 2017; Rinaldi et al., 2018). The color maps of both outbursts show a VIS color gradient at the maximum of the outburst ejecta with a value of $13.1 \pm 1.3 \%$ (100 nm)$^{-1}$ for outburst A and
Table 2.3: OSIRIS Narrow Angle Camera observations used in this work.

<table>
<thead>
<tr>
<th>Observation Time</th>
<th>Exposure Time (s)</th>
<th>Phase Angle (°)</th>
</tr>
</thead>
<tbody>
<tr>
<td>15:04:56</td>
<td>0.675</td>
<td>63.3</td>
</tr>
<tr>
<td>16:04:56</td>
<td>0.675</td>
<td>63.2</td>
</tr>
<tr>
<td>16:14:56</td>
<td>0.675</td>
<td>63.2</td>
</tr>
</tbody>
</table>

a value of $12.4 \pm 2.4 \% \ (100 \text{ nm})^{-1}$ for outburst B.

2.5 Additional Datasets

2.5.1 OSIRIS Images

During the relevant time period there are 24 images taken by the Optical, Spectroscopic, and Infrared Remote Imaging System (OSIRIS) that are useful for comparing the observed outbursts to those described in Vincent et al. (2016). The Narrow Angle Camera (NAC) has a field of view of $2.20 \times 2.22$ degrees, which subtends approximately $9.0 \times 9.0$ km at 67P’s distance at 15:03 UTC and $8.8 \times 8.8$ km for 19:18 UTC (Keller et al., 2007). Between 15:03 and 16:53 UTC on November 7 the OSIRIS NAC took 12 observations with exposure times of 0.675 seconds, long enough to capture cometary activity off of the comet’s limb. There are no OSIRIS observations taken until November 9 after the 16:53 UTC observation on November 7.

Three of these observations are contemporary with key observations by Alice and VIRTIS-M and provide useful context (Fig. 2.10). The 15:05 UTC OSIRIS image taken within one minute of the Alice exposure at 15:05 UTC confirms that cometary activity is indeed quiescent at that period. This relatively quiet activity continued until at least 16:05 UTC (Fig. 2.10b). The first outburst detected in the Alice and VIRTIS-M data occurred at some point in the next 3 minutes, because in the 16:15 UTC OSIRIS exposure a substantial amount of activity is detected (Fig. 2.10c). This is in agreement with Alice data that shows a sharp increase in atomic emission at 16:07 UTC (Fig. 2.6).

The high resolution of the OSIRIS images allows us to examine the limb of the
comet and the fine structure of the outburst. By first subtracting the 16:05 UTC image to create an irradiance difference image (Fig. 2.11) and then enlarging the sunward limb of the nucleus (Fig. 2.12) we can identify four new active sites on the limb of the nucleus that were not active ten minutes prior, at most. This suggests that outburst A is new activity and not the extension of existing active sites.

For comparison of outburst A to outbursts previously studied by OSIRIS we completed the same calculations for relative intensity as described in Vincent et al. (2016). The integrated irradiance \( (W \text{ m}^{-2} \text{ sr}^{-1} \text{ nm}^{-1}) \) was found by summing the individual pixel irradiances in a trapezoidal area extending between 50-500 meters from the comet limb. The total irradiance is then multiplied by \( 4\pi r_c^2 \), where \( r_c \) is the spacecraft-comet distance, to calculate the luminosity of the outburst. For outburst A we find that the luminosity was \( 1.12 \times 10^{12} \text{ W} \), an order of magnitude weaker than the strongest outburst recorded in Vincent et al. (2016) but consistent with the other 33 outbursts described in Table 3 of that same paper. Without OSIRIS data for outburst B we can’t calculate the relative intensity, but a simple scaling of the maximum radiance observed by VIRTIS-M for each outburst provides a reasonable estimate of the relative luminosity. In effect,

\[
\frac{R_{B,VM}}{R_{A,VM}} = \frac{L_{B,O}}{L_{A,O}} \rightarrow \frac{R_{B,VM}}{R_{A,VM}} \times (L_{A,O}) = L_{B,O}
\]  

(2.2)

, where \( R \) indicates the max radiance of outbursts A and B from VIRTIS in W m\(^{-2} \) sr\(^{-1} \) \( \mu \text{m}^{-1} \) and \( L \) indicates the luminosity of the outbursts in the OSIRIS images in W. From this we find \((0.06/0.08) \times 1.12 \times 10^{12} \text{ W} = 8.4 \times 10^{11} \text{ W} \), or 8% of the maximum radiance of \( 1.18 \times 10^{13} \text{ W} \). This is still greater than almost half of the outbursts reported in Vincent et al. (2016). These OSIRIS context observations show that the outbursts observed by Alice, VIRTIS-M, and OSIRIS on November 7 are not unique compared to previously observed outbursts except in two ways: the instrument datasets available over the relevant time period and the distinct differences between the two outbursts themselves despite their close temporal proximity.
Figure 2.10: Three OSIRIS NAC images with 0.675 s exposure times taken between 15:05 and 16:15 UTC on November 7. The overexposed nucleus has been masked in the images to highlight activity and the Sun is to the right in these images. Both the top and middle image are taken during periods of typical cometary activity. The top corresponds with the Alice spectrum taken at 15:04 UTC in Figure 2.4, which is used for Alice quiescent subtraction. The image in the middle was taken 15 minutes prior to the Alice outburst detected in the 16:07 UTC Alice spectrum and the outburst imaged at 16:15 by OSIRIS, which is displayed in the bottom image. The Alice slit is overlaid in white with the approximate location of row 15 identified.
Figure 2.11: Image displaying the change in irradiance between OSIRIS NAC observations at 16:04 and 16:13 UTC on November 7. The Sun is to the right in the image. The exposure taken at 16:04 UTC has been subtracted from the 16:14 UTC exposure to show the change in activity levels. Between the two images the comet nucleus rotated approximately 5°, leading to some artifacts in the difference image on the masked surface.
Figure 2.12: Image showing a close-up of the change in limb activity in Figure 2.11 with a shifted color scheme to highlight the outburst’s fine structure. Note that four distinct areas are all active at 16:14 that were not at 16:04 UTC. The area integrated for outburst brightness as described in Vincent et al. (2016) is shown by a white trapezoid.
2.5.2 NAVCAM Images

Of the three available NAVCAM images taken during the period in question only one shows increased cometary activity coincident with Alice observations of an emissions increase. These three NAVCAM images are shown in Figure 2.1. In the NAVCAM image at 19:18 UTC, a jet can be seen extending along the Alice slit (Figure 2.13). This particular NAVCAM image was taken at the same time as an Alice exposure, displayed in red in Figure 2.4, and informs us that the spectrum is not taken during a period of strong outbursting but jet activity. The morphology of the 19:18 NAVCAM image is unlike the outbursts detected by VIRTIS-M and observed in the OSIRIS images, and appears to be more collimated than the other activities. This is particularly useful for identifying differences in composition and excitation processes between outbursts and more common cometary jets.

In addition, the alignment of the first jet with the Alice slit means that the spatial profiles shown in Figure 2.4 can provide insight into dominant emission mechanisms within the jet itself and how they compare to small and large outbursts, as discussed in the next section.

2.6 Discussion

The observations from Alice and VIRTIS-M data show two outbursts of different magnitudes, both in gas and dust emissions, occurring within a short period followed by approximately 1.5 hours of elevated activity before Alice observations cease. Such an overlap presents the opportunity for dust and gas analysis and a discussion about the implications for cometary outburst mechanisms.

2.6.1 Excitation Mechanisms

The substantial presence of O I 1356 Å emission and the spectral fit of dissociative electron impact emission of H₂O and CO₂ makes it clear that the dominant atomic emission mechanism relevant for near-nucleus cometary activity is driven by electron-neutral interactions, whether jets or outbursts. The substantial increase of
Figure 2.13: NAVCAM image from November 7 at 19:18 UTC, with Alice slit overlay in red. Subfigures b) and c) have been stretched to show cometary activity in the southern hemisphere. The slit was aligned with the activity at that time. The spectrum is shown in Figure 2.4. This geometry is representative of the stable pointing scheme. For this period the Alice slit subtends 22 km at the nucleus distance, approximately 1.2 km per pixel. The white vector in the image denotes the rotational axis of 67P. The Sun is to the right in all three images.
Figure 2.14: Alice quiescent-subtracted spectra showing the spectrum near outburst A (a), outburst B (b), and the outburst and/or jet (c). The spectrum from 15:04 UTC shown in Figure 2.4 is used as the quiescent spectrum. The modeled relative molecular abundances are reported in Table 2.4.
the extent of the spatial profile for the semi-forbidden emission of O I] 1356 Å in Figure 2.7 for the outbursts and jet shows that the near-nucleus plasma environment is critically important for understanding the UV emissions. Without simultaneous plasma measurements taken within the outbursts it is difficult to know how much of this change in dissociative electron impact emission is due to increases in the neutral density, electron density, or electron energy. Improved modeling of the plasma effects on the UV emissions from 67P has been executed for periods where Rosetta was much closer to the nucleus, and electron distribution information from RPC-IES could be combined with ROSINA molecular abundances and VIRTIS or MIRO column densities to calculate emission rates (Galand et al., 2020; Stephenson et al., 2021). For this set of observations we are without those datasets, and must fall back to models that can only fit the relative abundances of CO₂ and O₂ to H₂O. Such models rely on the emission line ratios derived from laboratory work with dissociative electron impact and are insensitive to the plasma properties near the nucleus.

Given the concurrent observations from VIRTIS-M indicating the substantial presence of dust it is useful to compare the activity in question to the dusty outburst of 2016 February 19 discussed in Grün et al. (2016) and Hajra et al. (2017). Hajra et al. (2017) showed that the near-nucleus plasma environment experienced a 3-fold increase in total electron density while simultaneously experiencing a 2-9 fold decrease in electrons greater than 10 eV. If a dusty outburst released little new volatile material and neutral density remained constant while the average electron energy decreased and the "cold" electron density increased, this would result in the calculation of a lower limit for column density assuming the 100 eV cross sections from the literature are implemented. Such a decrease to two of the three components for determining dissociative electron impact excitation rates would produce a significant decrease in dissociative electron impact excitation in Alice data. Put simply, comet dust outbursts should produce less dissociative electron impact excitation emissions than gas outbursts, most easily identifiable by the O I] 1356 Å emission feature.
If dusty outburst A possessed similar plasma properties as that discussed in Hajra et al. (2017), Alice spectra appear consistent with the decrease in electron energy, and thus lower emissions than would be typically expected from an outburst. In contrast, the presence of high-threshold energy C II 1335 Å emission at 17:32 UTC in outburst B (Figure 2.14) is interesting given the VIRTIS-M result that outburst B was a weaker dust outburst than outburst A, despite Alice measurements showing increased gas emissions. The weaker dust outburst B may not have damped the electron energies to nearly the same level as the stronger dust outburst A, made evident in the appearance of atomic emission features with larger threshold energies like C I 1279 and C II 1335 Å, at 26 and 40 eV respectively (Ajello, 1971a; Ajello et al., 2019). This suggests that gas and dust outbursts do experience different levels of dissociative electron impact emission and present unique spectral signatures in the UV, specifically of high-threshold energy atomic emission features. However, to be sure of the correlation more outbursts with similar gas/dust properties observed by both Alice and the plasma instruments on board Rosetta must be analyzed.

2.6.2 Gas Composition

Given the progression from weak outgassing at 12:00 UTC to elevated activity levels with a substantial jet at 19:18 UTC here we analyze the composition of three key spectra. To identify the unique composition of the activity these spectra have been quiescent subtracted using the 15:04 UTC spectrum, leaving emissions produced by the newly introduced neutrals from the respective outbursts or jet. These emissions can be fit with a relative abundance model for dissociative electron impact emission of H₂O, CO₂, CO, and O₂ at 100 eV (Makarov et al., 2004; Ajello et al., 2019; Mumma et al., 1972; Ajello, 1971a,c; Kanik et al., 2003). The model first determines the relative abundance of CO₂/H₂O by taking the line ratios of the Lyman-β and C I emission features. The relative abundances were then used to model the contribution from e+H₂O and e+CO₂ to O I emission features, using published line ratios from the aforementioned literature. These model spectra were then subtracted from the Alice data and the residual O I emission features were fit with an O₂ dissociative
Table 2.4: Modelled relative abundances for H$_2$O, CO$_2$, and O$_2$ for the quiescent-subtracted spectra shown in Figures 2.14, 2.14, and 2.14. The errorbars on these modelled relative abundances are between 30 and 35%, the result of uncertainties in emission brightness, emission cross section ratio measurements in the literature, and to a lesser degree, the model fitting error. Errors are higher for lower Lyman-β brightnesses, as this increases the brightness measurement uncertainty for the determination of the baseline H$_2$O, by definition set to 1 to find the relative abundances of CO$_2$ and O$_2$.

<table>
<thead>
<tr>
<th>Observation ID</th>
<th>UTC Time</th>
<th>CO$_2$/H$_2$O</th>
<th>O$_2$/H$_2$O</th>
</tr>
</thead>
<tbody>
<tr>
<td>ra_151107160746_hisa_lin</td>
<td>16:07</td>
<td>0.6</td>
<td>0.21</td>
</tr>
<tr>
<td>ra_151107173215_hisa_lin</td>
<td>17:32</td>
<td>1.0</td>
<td>0.14</td>
</tr>
<tr>
<td>ra_151107191814_hisa_lin</td>
<td>19:18</td>
<td>1.2</td>
<td>(\lesssim)0.10</td>
</tr>
</tbody>
</table>

electron impact model. The calculated abundances for CO$_2$ and O$_2$ relative to H$_2$O for 16:07, 17:32, and 19:18 UTC are shown in Table 2.4.

This model is not without caveat. We make the assumption that atomic cross section ratios measured at 100 eV are accurate for the range of electron energies above each transition’s threshold energies. This holds true for the main atomic emissions (Lyman-β, O I 1304, O I] 1356, and C I 1657), but not all observed Alice features. An extension of this assumption requires that atomic transitions that have higher threshold energies (e.g. C II 1335 Å) need to be properly addressed. This is done via a scaling factor implemented in the fitting algorithm. Physically this is an attempt to capture the plasma environment’s difference from the modeled Maxwellian distribution and the depletion of electrons with energies higher than threshold energy of certain atomic emissions. This model parameter is unitless and allowed to vary between 0 and 1, and in the fits shown in Figure 2.14 this parameter ranges between 0.1 and 0.25.

The calculated relative abundances for outburst A, outburst B, and the jet yield unique insight into the progression of cometary activity. At the peak of outburst A the CO$_2$/H$_2$O ratio was 0.6±0.2, while outburst B exhibits a different composition of CO$_2$/H$_2$O=1.0±0.3. These relative abundances are particularly interesting because the values, when paired with the brightness of the emission features, suggest that
outburst B had a much stronger gas component than outburst A, despite the larger dust irradiances measured by VIRTIS-M for outburst A, and that there was a much stronger CO$_2$ component for outburst B, indicating more volatile rich material. The elevated emission from CO$_2$ continues after the outburst appears to be over; the jet has a CO$_2$/H$_2$O ratio of approximately 1.2±0.4 before Alice observations cease. This implies that the sublimation of H$_2$O is largely responsible for lifting the dust in the outbursts, not CO$_2$. This result requires confirmation through separate events, which in turn will require analysis of more outburst events in the Alice and VIRTIS-M catalog, as the implications for the interpretation of cometary activity are significant.

We point out that there is excess C I 1657 Å in the 19:18 UTC spectrum that is being fit with the e+CO$_2$ spectra with a strength of about 2-3 Rayleighs, contributing to an over-subtraction of the O I 1304 Å emission feature when subtracting the model from the observations. This 2-3 Rayleigh emission can partially be explained as the result of photodissociation and excitation of C I from the newly introduced CO$_2$ column, which has an excitation rate of $\sim$1.1×10$^{-8}$ photons s$^{-1}$ molecule$^{-1}$ at 1 au (Wu et al., 1978). This produces a predicted integrated brightness of $\sim$3 Rayleighs for a column density of $\sim$3±0.7×10$^{15}$. Without concurrent water column measurements from VIRTIS or MIRO to compare to, we must compare to the closest date available, when the MIRO instrument measured a total water column of 2×10$^{16}$ cm$^{-2}$ just a few days later on 11 November 2015 (Biver et al., 2019). Using a direct comparison of the derived CO$_2$ column density from the excess C I 1657 Å emission and the later water column measurement would lead to a CO$_2$/H$_2$O ratio of 0.15, but this would be comparing a quiescent-subtracted derived value to a total coma value, and is therefore misleading. To order of magnitude the required CO$_2$ column density to explain the excess C I 1657 Å emission is near the measured water column density, and therefore any weak additional C I 1657 Å is likely from photodissociation of CO$_2$. All other C I and C II emission features experience a negligible amount of solar resonance scattering and are fit well with the e+CO$_2$ synthetic spectrum for those two spectra. The final jet observation at 19:18 UTC
shows residual emission of C I 1657, 1561, and what may be weak CO Fourth Positive Group emission, specifically the (0-1), (0-0), and (1-0) bands between 1400 and 1600 Å. We also note that these features may also represent low-energy electron impact on CO$_2$, described in Ajello et al. (2019) but these are not implemented in our models owing to their low contribution to the overall emission. The calculated CO$_2$/H$_2$O ratios of 0.57-1.5 fall within the range expected for the regional composition of the southern hemisphere of 67P from both Alice and ROSINA observations (Feldman et al., 2018a; Mall et al., 2016).

The O$_2$ column density is more difficult to calculate. Both outburst A and outburst B show excess O I] 1356 Å emission in the $e^+$(H$_2$O + CO$_2$) subtracted spectra that could be an indication of $e^+$O$_2$, but the residuals are poorly fit by the electron impact model owing to lack of corresponding O I 1304 Å emission. However, given the lack of CO Fourth Positive Group emissions there is not another likely neutral molecule that could be the source of the emissions, so we can cautiously treat this excess as an indicator of $e^+$O$_2$. We can constrain the O$_2$/H$_2$O to be approximately 0.21±0.07 and 0.14±0.05 for outbursts A and B. By contrast there is little excess O I] 1356 Å emission detected in the model subtracted jet spectrum (Figure 2.14). These O$_2$/H$_2$O abundances are consistent with previous Alice observations of outbursts and transient events (Feldman et al., 2016; Noonan et al., 2018), but substantially lower than values taken later on November 7 2015 (Noonan et al., 2021a). There are no atomic or molecular emissions present in the spectra that would suggest dissociative excitation of additional neutrals plays a significant role at this time, and therefore we can treat these particular outbursts as representative of a typical small scale cometary outburst.

The post-outburst period for outbursts A and B are very different, offering insight into the different areas exposed during the course of each. Quiescent atomic emission levels are reached quickly after outburst A but following outburst B there is an increased brightness of atomic C and O features in Fig. 2.6 that lasts at least until 19:18 UTC. While the compositions are relatively similar, this suggests that outburst B exposed fresh material with substantial H$_2$O and CO$_2$, which began to sublimate
Figure 2.15: Source regions of the outbursts detected by VIRTIS-M. The red and yellow rectangles correspond to the outbursts A and B, respectively. The map is centered on the small lobe, the big lobe covers the left-hand and right-hand side of the map, and the contact area between the two lobes covers mainly the top of the map (regions Hapi and Seth). The boundary regions, shown in the map, have been defined by El-Maarry et al. (2015); El-Maarry et al. (2016)

...immediately. This may explain the lack of excess O I] 1356 Å in the 19:18 UTC jet observation; the more volatile O₂ has been depleted, leaving a spectrum well fit by e+(H₂O+CO₂) (Fig. 2.14). Therefore outburst A, which was substantially weaker in atomic emission, must have occurred in an area depleted in volatiles and was unable to sustain activity. Outburst B on the other hand, saw a sharp appearance of O I] 1356 Å possibly indicating O₂, followed by sustained sublimation of CO₂ and H₂O. This would suggest O₂ as the initiating volatile for a rapid outflow outburst model like that of Skorov et al. (2016).

2.6.3 Outburst Location

Fig. 2.15 shows the outburst source regions projected on a morphological map of 67P/CG displaying the region boundaries defined by El-Maarry et al. (2015) and El-Maarry et al. (2016). In the VIRTIS-M images analyzed in this work, the dust
ejecta are seen only in one image, and the source location of the outbursts is not visible. Hence, we can only roughly identify the source location. We selected the pixels inside the outburst ejecta and determined the projected latitude and longitude on the surface at the intersection with the vector passing through the center of the target (tangent point). Both outburst sources are located in the Southern hemisphere, approximately at the latitude range from -20° to -80°. The location of outburst A is in the boundary region, between Anhur and Bes. Such boundary areas are characterised by discontinuities in the local terrain, either textural or topographic as observed in Vincent et al. (2016) and Fornasier et al. (2019b). The location of outburst B is in the boundary region, between Anhur, Neith, Wosret and Sobek. These regions are located in the southern part of the neck. This region is considerably more complex texturally than in the north. Neith is bounded by Wosret on one side and Sobek on the other. It forms the major steep cliff from an edge (the Neith-Wosret boundary) down into the neck itself. The surface is very rough on intermediate scales. There do not appear to be any large scale structures (Thomas et al., 2018). Neither of these projected source regions has a previously detected outburst from Vincent et al. (2016) within their bounds, but the Anhur region has been classified as very active and volatile-rich (Fornasier et al., 2019b,a).

2.6.4 Comparing Alice and VIRTIS-M

Alice and VIRTIS-M observations are largely divided into gas and dust characterization, but close inspection of the overlapping characteristics of the dust components are warranted with this dataset. Here we discuss three different methods to compare dust reflected solar continuum between the UV and visible observations. If we assume that the reflected UV light is directly proportional to the reflected visible light (VIRTIS-M 5500 Å) (Table 2.1), referencing the SORCE solar continuum for November 7 from the the LISIRD database¹, and that the visible and UV albedos are similar, we find that the total dust contribution to the continuum between 1850-1950 Å should be approximately ∼93 and 70 Rayleighs for outbursts A and

¹http://lasp.colorado.edu/lisird/data/sorce_ssi_l3/
B, respectively. These are consistent with the changes in brightness observed in the nearest row to the nucleus limb of 100 and 80 Rayleighs for outbursts A and B (Figure 2.16). These zeroth order estimates could be further refined by addressing albedo and phase function variations as the UV albedo of 67P has been measured to have a strong blue slope, leading to a lower albedo at wavelengths between 1850 and 1950 Å (Feaga et al., 2015). The UV albedo of the comet surface red-ward of 1830 Å is not well characterized, so we can try the other edge case and assume that the albedo between 1800 and 1830 Å, 0.03 at zero-degree phase, is a good proxy for the UV dust reflectance. The ratio of UV to visible albedo then needs to be accounted for in the expected dust contribution to the continuum. Using the VIRTIS-M albedo at 5500 Å, 0.06 (Capaccioni et al., 2015), we get a ratio of 0.5 and an expected Alice continuum brightnesses of 47 and 35 Rayleighs for outbursts A and B, respectively. These values both underpredict the observed brightness, so a more representative albedo must be found via a different method.

As an alternative we can derive the albedo from the measured Alice and VIRTIS-M brightnesses and the VIRTIS-M albedo to find UV/visible albedos ratios of 1.07 and 1.14, corresponding to UV albedos of 0.065 and 0.069 when scaling the albedo of 0.06 at 5500 Å from Capaccioni et al. (2015). These slightly increased FUV albedos for outbursts A and B may represent the increased presence of water ice grains, which have higher UV albedos than carbonaceous material redward of 1700 Å (Hendrix et al., 2010; Steffl et al., 2015). However, a strong decrease in color slope was not observed in the VIRTIS-M dust data, which would be expected if a large number of large water ice grains (∼mm-size) were incorporated into the outburst plume (Calvin et al., 1995). For smaller grains this effect is much less pronounced, as the albedo is nearly constant between 5000 and 8000 Å for 20 µm size ice grains. Outbursts characterized from OSIRIS data by Fornasier et al. (2019a) exhibited a blue slope, albeit in the visible wavelength range, and were inferred to contain icy grains.
Figure 2.16: Brightness in Rayleighs for row 16 of the Alice detector, integrated between 1850 and 1950 Å. Vertical lines represent quiescent (black dot-dash), outburst (blue solid), and jet (red dashed) observations. For this period of stable pointing row 16 was just off of the nucleus limb and only contains solar continuum emission reflected off dust. Of particular note are the $\sim 36\%$ and $\sim 22\%$ increases in brightnesses over the previous continuum measurements for outbursts A and B, respectively. Error bars on each measurement are smaller than the size of the points.
Hybrid Gas-Dust Outbursts

The early division of Alice outbursts into gas and dust types was observationally driven, with gas outbursts lacking dust components and dust outbursts lacking a gas component (Feldman et al., 2016; Steffl et al., 2015). Hybrid outbursts have been identified with Alice observations (Steffl et al., 2018), and here we build on the concept. What the combined VIRTIS-M and Alice observations here portray is a range of outburst types bracketed by gas outbursts at one end and dust outbursts at the other. Previously characterized Alice gas outbursts may have had a weak FUV solar continuum reflectance that was not initially recognized owing to its limited brightness and distribution from the nucleus limb, which would then lead to a new classification in this combined gas/dust outburst type.

Feldman et al. (2016) interpreted the gas outbursts observed by Alice as evidence of an outburst mechanism relying on a deepening fracture exposing volatile gases, likely driven by O$_2$, rather than CO as described by Skorov et al. (2016). Conversely, other outbursts were linked to cliff collapses and geological failure (Steckloff et al., 2016; Vincent et al., 2016; Pajola et al., 2017). The outbursts studied in this work do not fit neatly into either classification with the lack of direct observations of the landscape during the outburst due to the large cometocentric distance, making it difficult to directly identify the mechanical process that caused either outburst. However, there are several key components of the outbursts that provide clues.

1. Alice measurements of atomic emissions indicative of dissociating neutrals and VIRTIS-M VIS maps of reflected solar continuum from dust, are inversely correlated for outbursts A and B.

2. UV spectra for outburst A are depleted in high-threshold energy atomic emissions from e+CO$_2$, a sign that the local plasma environment is depleted in electrons above 25 eV.

3. Following outburst B there is sustained sublimation observed by Alice, indicating exposure of fresh volatiles.
4. Analysis of the FUV continuum shows that there is good agreement with the expected brightness from VIRTIS-M measurements of the max radiance for outburst A with the measured UV comet albedo of 0.041, but outburst B is unexpectedly bright in the FUV and is better matched with an albedo of 0.069, possibly indicative of the presence of water ice grains in the outburst plume. However, substantial color differences were not detected between the plumes and surrounding coma in the VIRTIS data.

5. The source regions for each outburst lie in the Anhur region, a known outburst region with consolidated material and large discontinuities.

These results point to possible mechanisms for each outburst. Outburst A requires a smaller gas contribution, a large dust contribution, and cannot spur further sublimation from the exposed region. This suggests that structural failure of a largely volatile-depleted cliff is a likely mechanism for outburst A; the crumbling cliff face produces a large quantity of dust but has already been largely depleted of volatiles and did not expose substantial new material. The lack of high-threshold energy emissions also corroborates previous plasma observations of a cliff collapse outburst (Hajra et al., 2017), which show an overall increase in total electron density but a depletion of electrons greater than 40 eV. The Anhur region has had substantial activity, both jets and outbursts, and has substantial volatile content (Fornasier et al., 2019b,a).

Outburst B requires a smaller dust contribution that is higher in UV albedo, implying the presence of water ice grains, and a larger gas contribution without damping the near-nucleus plasma environment to preserve high-threshold energy atomic emissions from e+CO$_2$. These conditions are more closely aligned with the outbursts described in Feldman et al. (2016) and by the fracture propagation model of Skorov et al. (2016) than outburst A. However, we have two other conditions that need to be addressed: the sustained activity following the outburst and the presence of water ice grains. Sustained activity, especially with the substantial amount of CO$_2$ observed, requires a volatile-rich region to be exposed. The water ice grains could
be the result of CO$_2$ gas sublimating deep in the fracture dragging icy grains from the interior out with the flow before the grains begin to sublimate as well. This mechanism could also explain the relatively flat extension of the Lyman-β and O I 1304 Å spatial profile in Figure 2.7 for 17:32 and 19:38 UTC; an extended source of H$_2$O has become available, one that was not present in outburst A at 16:07 UTC.

Without direct observations of the source regions during the outbursts a multi-instrument approach contains a wealth of information that can be used to constrain the outburst mechanisms. Further cross-analysis of as of yet unidentified outbursts in the Alice and VIRTIS datasets should yield improved spectral criteria to identify outburst mechanisms remotely.

2.7 Summary

In this chapter we analyzed three distinct activity types observed within five hours on 2015 November 7: a small outburst, a large outburst, and a cometary jet. The following results were shown from the Alice, OSIRIS, and VIRTIS-M datasets regarding the outbursts on November 7:

1. Alice, OSIRIS, and VIRTIS-M observations of outbursts indicated that these are not uniquely strong or compositionally distinct and are therefore likely representative of other outbursts at 67P.

2. Outbursts A and B display both gas and dust components and are therefore not entirely “gas” nor “dust” outbursts as previously described in Alice literature (Feldman et al., 2016; Steffl et al., 2015) but are better classified as “hybrid” outbursts (Steffl et al., 2018).

3. The dust color as measured by VIRTIS-M is 13.1% (100 nm)$^{-1}$ and 12.4% (100 nm)$^{-1}$ for outbursts A and B respectively.

4. Outburst A likely originated in the far east Anhur region, outburst B likely originated in the boundary regions of the southern neck, between Worset, Neith, Sobek and Anhur.
5. Alice observations of the gas components show that outburst B was approximately twice as strong based on atomic emissions, which is inverse of the VIRTIS-M measured dust irradiiances. VIRTIS-M observations of the dust component show that outburst A had a maximum radiance approximately 2.5× that of outburst B.

6. Alice spectra taken during outburst A show a lower CO$_2$/H$_2$O ratio (0.6) than in outburst B (1.0). Outburst A also has a higher O$_2$/H$_2$O, 0.21±0.07 compared to 0.14±0.05 for outburst B.

7. Comparison of the Alice FUV continuum between 1850 and 1950 Å to VIRTIS-M dust irradiances shows that each outburst produced enough FUV reflectance to be detected in the Alice data, once investigated closely.

8. Outburst A is likely the result of structural surface feature failure (i.e. mass wasting). Outburst B contains elevated CO$_2$, indicating a more pristine surface origin (i.e. fracture deepening) and sustains increased activity for over two hours.

9. The jet resulting from outburst B has a moderate CO$_2$/H$_2$O ratio (1.2) and appears depleted of O$_2$ compared to earlier activity, evidence that O$_2$ may have initiated the outburst and exposed new volatile-rich material that sublimated CO$_2$ and H$_2$O at least until 19:18 UTC.

Analysis of these outbursts shows that mixed gas and dust outbursts have features within their FUV and visible spectra that can help constrain the initiating outburst mechanisms. Obtaining spectra of the relevant near-nucleus coma in the future will be difficult without improved space-based UV-capable observatories or spacecraft, to say nothing of the temporal resolution required to properly identify outbursts. Even identifying outbursts in the optical wavelength ranges with imaging, where sensitivities are significantly higher, is difficult and requires both high-cadence and high-sensitivity observations (Boehnhardt et al., 2016; Knight et al., 2017; Farnham et al., 2019; Farnham et al., 2021, Kelley et al. in press). However, the Rosetta
mission dataset contains many more events to analyze. The outbursts discussed in this article are just two out of the dozens still requiring analysis in the *Rosetta* datasets awaiting further interrogation. The large dataset from the Alice spectrograph on *Rosetta* is unique, with nearly constant observation of a near-nucleus coma in the UV for two and a half years, providing a cometary UV dataset unlikely to be equaled for years to come. Multi-instrument analysis of cometary outbursts has already proven to be of critical importance for understanding outburst mechanics and there is much more to be done with the data available. Cometary outbursts require further investigations to verify spectroscopic characteristics, both within the *Rosetta* datasets and in theoretical work.

2.8 Acknowledgements

This work was made possible thanks to the ESA/NASA *Rosetta* mission with contributions from ESA member states and NASA. The Alice team would like to acknowledge the support of NASA’s Jet Propulsion Laboratory, specifically through contract 1336850 to the Southwest Research Institute. JWN and JWP would also like to acknowledge funding from NASA’s *Rosetta* Data Analysis Program through grant number 80NSSC19K1304. JWN would also like to acknowledge Peter Stephenson for insightful discussion regarding dissociative electron impact environments and modeling. The team also acknowledges the useful comments from the reviewer, which improved this manuscript.

We thank the following institutions and agencies for support of this work: Italian Space Agency (ASI, Italy) contract number I/024/12/1, center National d’Études Spatiales (CNES, France), DLR (Germany), NASA (USA) Rosetta Program, and Science and Technology Facilities Council (UK). VIRTIS was built by a consortium, which includes Italy, France, and Germany, under the scientific responsibility of the Istituto di Astrofisica e Planetologia Spaziali of INAF, Italy, which also guides the scientific operations. The VIRTIS instrument development, led by the prime contractor Leonardo-Finmeccanica (Florence, Italy), has been
funded and managed by ASI, with contributions from Observatoire de Meudon financed by CNES, and from DLR. We thank the Rosetta Science Ground Segment and the Rosetta Mission Operations center for their support throughout all the phases of the mission. The VIRTIS calibrated data will be available through the ESA’s Planetary Science Archive Website (www.rssd.esa.int) and is available upon request until posted to the archive.
CHAPTER 3

Spatial Distribution of Ultraviolet Emission from Cometary Activity at 67P/Churyumov-Gerasimenko

The contents of this chapter were originally published in as “Spatial Distribution of Ultraviolet Emission from Cometary Activity at 67P/Churyumov-Gerasimenko” in The Astronomical Journal, volume 162 (Noonan et al., 2021a)

3.1 Introduction

From August of 2014 through September of 2016 the European Space Agency’s Rosetta spacecraft performed escort operations around the comet 67P/Churyumov-Gerasimenko, observing changes to the comet’s nucleus, coma, and plasma environment at a range of heliocentric and comet-centric distances. The comprehensive survey carried out by Rosetta instruments has provided valuable insight into comet outgassing and outbursts. In particular, observations by the Alice ultraviolet (UV) spectrograph (Stern et al., 2007) revealed the prevalence of dissociative electron impact emission at heliocentric distances greater than 2 au (Feldman et al., 2016; Galand et al., 2020; Stephenson et al., 2021) that was also observed by the OSIRIS instrument (Bodewits et al., 2016), and that observations of outbursts with different local origins, observing geometries, outgassing rates, and compositions displayed substantial increases in dissociative electron impact emission (Feldman et al., 2016; Noonan et al., 2021c).

These transient events highlight the variable nature of comets and provide insight into how the near-nucleus coma is affected by injections of gas within a short period of time. Given the consistent presence of dissociative electron impact emission near the nucleus at the larger heliocentric distances observed by Rosetta and during outburst (Feldman et al., 2016, 2018a; Noonan et al., 2021c), it is criti-
cal to understand how perturbations to the near-nucleus coma affect the electron impact emission features and overall UV spectrum. Previous studies have shown a one dimensional spatial profile along the Alice slit, detailing the sunward and anti-sunward asymmetry of emission features and the radial extent for dissociative electron impact emission during outbursts (Feldman et al., 2016). Due to the typical stare-type observations of Alice these one dimensional spatial profiles were the best representation of the spatial behavior of coma emission features.

However, inner coma mapping has been implemented with both the Visible InfraRed Thermal Imaging Spectrometer (VIRTIS) (Coradini et al., 2007) and Microwave Instrument on the Rosetta Orbiter (MIRO) (Gulkis et al., 2007). Migliorini et al. (2016) used VIRTIS to simultaneously map the $\text{H}_2\text{O}$ and $\text{CO}_2$ column densities in April of 2015, while Fink et al. (2016) obtained $\text{H}_2\text{O}$ and $\text{CO}_2$ production rates for a period in February 28 as well as April 27 of 2015. Outbursts that occurred around the comet’s perihelion in August 2015 were mapped by Rinaldi et al. (2018) using VIRTIS high resolution data, showing an increase in dust production and change of dust color. The MIRO instrument implemented a raster technique to measure the distribution of abundant cometary molecules, including $\text{H}^{18}_2\text{O}$ at 3.4 au (Biver et al., 2015), when activity levels were low due to the relatively large heliocentric distance. The same technique was extended to other isotopologues of water, $\text{CH}_3\text{OH}$, $\text{NH}_3$, and CO in over 100 maps to determine production rates and radial dependencies (Biver et al., 2019).

Using coordinated pointings we have created atomic emission maps and compare Alice UV maps to calibrated maps from VIRTIS and MIRO. The additional spatial dimension from this technique provides detail on the influence of outbursts on the near-nucleus coma and plasma environment, and in particular how the spatial distribution of dissociative electron impact changes during the period. Given the expected gap in time between the Rosetta mission and the next UV-enabled comet spacecraft, it is of critical importance to understand what processes could be observed from Earth-based observatories under optimal conditions, especially if a spectroscopic identifier for small outbursts can be determined in Alice data. The
relationship between UV emissions and the cometary plasma environment is better characterized now thanks to Rosetta (Galand et al., 2020; Stephenson et al., 2021), but is still far from completely understood. The work of Galand et al. (2020) and Stephenson et al. (2021) showed that for comet/spacecraft distances less than 100 km the observed Alice UV brightness near the nucleus could be well modeled with in-situ electron population measurements from the Rosetta Plasma Consortium Ion and Electron Spectrograph (RPC-IES) (Burch et al., 2007), water column density measurements from MIRO or VIRTIS, and abundances of CO$_2$, O$_2$, and CO relative to water from the ROSINA mass spectrometer (Balsiger et al., 2007). Critically, Galand et al. (2020) found that solar wind electrons accelerated along the ambipolar electric field of the nucleus were responsible for generating these FUV emissions observed by Alice at large heliocentric distances, making them auroral in nature. If electron impact is detected in future UV comet observations then it may be possible to not only continue compositional characterization via atomic emission lines but expand into remote plasma characterization of excitation regions of the inner coma with improved modeling of dissociative electron impact excitation (Galand et al., 2020; Stephenson et al., 2021).

This chapter discusses a unique period of activity that occurred while the Alice instrument made “ride-along” observations during VIRTIS-led pointings. The VIRTIS and MIRO instruments mapped the distribution of H$_2$O and CO$_2$ in the coma using raster scans at this time, providing context maps to compare to the new Alice maps. Furthermore, analysis of these maps shows evidence of an expanding zone of influence where electron impact dominates over fluorescence for short time scales, even at a relatively low heliocentric distance. This chapter reviews data taken between 21:16 UTC on 2015 November 7 and 02:55 UTC on November 8 and is intended to be a companion paper to Noonan et al. (2021c) which reviews data taken on November 7 between 12:00 UTC and 19:18 UTC. Section 2 will discuss the instrument, the relevant observations, and their geometry. Section 3 details the method used to map the Alice data. Section 4 describes the three data products that can be derived from Alice data for this time period: spectra, spatial profiles,
and 2-D maps. Maps from the VIRTIS-H and MIRO instruments are presented for comparison. Section 5 then discusses the morphology, composition, and excitation processes of the activity and their implications. A summary is presented in Section 6.

3.2 Observations

3.2.1 Instrument Description

The Alice instrument was a light-weight and low-power imaging spectrograph onboard the Rosetta spacecraft tasked with characterizing the surface properties, coma composition, and coupling of the coma and nucleus. To fulfill these goals, the instrument was designed to be sensitive from 700 - 2050 Å with a filled-slit spectral resolution determined in flight to be 11 Å in the center of the “dog bone” shaped slit, which was narrower in the middle than on the bottom or top. The narrow center is 0.05° (100 µm) wide in the middle 2.0° of the slit, while the upper and lower portions are both 0.10° (210 µm) wide. The lower and middle sections of the slit measure 2.0° long, with the upper section measuring 1.53°. The Alice detector was a microchannel plate with 1024 columns in the spectral dimension and 32 rows in the spatial dimension. Of the 32 spatial rows, only rows 5 through 23 (zero indexed) were exposed to light from the slit. Each row subtended 0.30° on the sky. One detector effect that can affect results is the odd/even effect, which was the tendency of the Alice detector to push counts to odd rows over even rows (Feldman et al., 2011; Chaufray et al., 2017). The instrument is described in detail in Stern et al. (2007).

3.2.2 Geometry and Spacecraft Pointing

On 2015 November 7-8, Rosetta and 67P were 1.61 au away from the Sun, outbound in their orbit after passing through perihelion in August 2015. The first observations used in this analysis were taken when Rosetta was 240 km from the nucleus of 67P on 15:04 UTC November 7. The spacecraft then slowly approached 67P, reaching
as close as 215 km by the end of the VIRTIS raster observations at 10:30 UTC on November 8. The phase angle decreased from 64° to 61.5° over the same time period. More information on the pointing geometry of each block is presented in Table 3.1, and further information on Alice observation modes can be found in Pineau et al. (2018).

Stable Pointing

From 15:04 UTC until 19:18 UTC on November 7 the Alice instrument was in a stable pointing mode, where there was minimal motion of the instrument’s line of sight for a long period of time. At this time the Alice slit was centered on the nucleus of 67P, with the upper rows in the sunward direction and the lower rows in the anti-sunward direction (Figure 3.1). From this pointing geometry Alice observed an increase in activity starting at 16:00 UTC that was recorded until the end of scheduled observations at 19:18 UTC. At this time Alice observations ceased until the ride-along observations. A more complete analysis of this period of interest is presented in Noonan et al. (2021c) but several individual observations from this period are referenced here.

Raster Pointing

Following an approximately 1.5 hour gap in observations, the Alice instrument resumed exposures during a VIRTIS-driven pointing mode designed to map the inner coma of 67P. The raster scans began at approximately 20:45 UTC November 7 and continued until 10:30 UTC on November 8, with Alice observations starting at 21:16 UTC November 7. The scan rate of the Alice slit during the raster varies throughout the period, so for the 300 s exposures the area scanned by the slit varies from 0.1 to 1.4 degrees (0.38-5.32 km) with an average of 0.6 degrees (2.28 km). This limits the spatial resolution of the Alice data, which is affected by “smearing”, which can spread the signal from one area of the coma over 2-3 spatial pixels depending on the individual observations scan rate. These inner coma raster scans for this particular
Figure 3.1: NAVCAM image from November 7 at 19:18 UTC with nucleus pixels masked to highlight faint activity. The rotation axis of 67P is marked with a white arrow. The Alice slit is overlaid in red and the Sun is to the right. With the exception of faint jets emanating from the neck there is no evidence of background activity.
time period moved the Alice boresight, centered in row 15 of the detector, within 5 km of the nucleus center in both the X and Y spacecraft directions.

3.3 Mapping Methods

We developed processing software to create emission maps from the Alice spectral images taken during raster ride-along observations driven by VIRTIS and MIRO. Observations from the period between 20:45 UTC on November 7 and 05:18 UTC November 8 were split into groups of ten where possible, further detailed in Table 3.1. Groups of roughly ten are chosen where possible to balance temporal resolution (∼50 minutes) with spatial coverage of the inner coma (Figure 3.2). For each individual observation within a block, a Python routine is used to iterate through each row of each observation, to filter for the presence of any stellar continuum or presence of the anomalous “Chameleon” feature that may contaminate the measurements (Noonan et al., 2016). Following this check the brightnesses of four strong diagnostic atomic emission features at 67P are determined: Lyman-β, the O I 1304 triplet, O I] 1356 Å and C I 1657 Å. This is done by integrating the flux in the 3-σ range of each emission feature’s center wavelength, assuming FWHM of 11 Å for each feature. We note that for C I 1657 Å emission this would lead to a blending with the CO Fourth Positive Band emission at 1653 Å (Figure 3.3). However the abundance of CO at this time is not significant enough to contaminate the atomic carbon substantially; based on the strength of the CO Fourth Positive (0-1) emission feature at 1600 Å which is approximately equivalent to the strength of the CO Fourth Positive (0-2) emission at 1653 Å we would expect less than 5% of the integrated flux for C I 1657 Å to be attributable to CO Fourth Positive Group emissions. Each row of the Alice spectral image, which corresponds to a different spatial coordinate relative to the nucleus at the start and end of each observation, is tagged with the X/Y pointing of the row in spacecraft coordinates from mid-exposure taken from the FITS headers, and the brightness is calculated in Rayleighs. Based on the SPICE kernels of the reconstructed spacecraft trajectory, pointing, and scan rate the size that an Alice
pixel subtends at the nucleus is calculated for the middle of each exposure. This allows a dataset of coordinates, brightnesses, and the observation’s pixel height and width at the nucleus to be generated for each observing block.

Due to the scan motion care must be taken to correctly account for the true location of the nucleus in the maps compared to the average position of the Alice rows. To accomplish this the weighted intensity barycenter of reflected solar continuum emissions between 1850 and 1950 Å is computed to find the center of the nucleus in the Alice data in X,Y space. The barycenter is then shifted until it aligns with the center of the illuminated nucleus in the nearest NAVCAM image, which may or may not have been taken within the set of Alice observations that the map is derived from and thus have a slightly different geometry. This process is shown in Figure 3.2. The FUV continuum also includes reflected sunlight off of dust near the nucleus, but manual inspection of each produced map reduces any effects of systematic nucleus offset between observing block maps. The large pixel size of the resulting images allows general activity to be distinguished but prevents fine structures from being resolved.

After the brightnesses for each row of every observation in an observing block are obtained, the individual row brightnesses are mapped to their X/Y locations relative to the comet nucleus. This array of points is then interpolated to generate a map of each emission feature, with pixel sizes no smaller than the Alice detector pixel subtended at the largest cometocentric distance within the observing block plus the distance covered by the slit while scanning during the observation, assuming a constant scan rate for the five minute exposure.

3.3.1 NAVCAM Correlation

Of the three available NAVCAM images taken during the period in question only one has meaningful activity context information for the Alice data and is shown in Figure 3.1. In the NAVCAM image at 19:18 UTC, a series of jets can be clearly seen extending across the Alice slit. Comparing the activity, captured in projection, to the geomorphological areas presented in El-Maarry et al. (2016), it seems likely
Figure 3.2: Series of plots depicting the mapping method described in Section 3.3. The top figure depicts the average location of each row of the Alice detector for each observation in block 1 from Table 3.1, with the color scheme detailing the row number (row 5 is dark purple, on the left, row 23 is yellow, on the right). The figure second from the top shows the interpolation of the rows to a grid with a pixel size defined by the pixel size of each row and the scan rate of the Alice detector. The figure third from the top details the initial map that is generated by the program before any correction is applied to shift the measured reflected solar signal to center on the nucleus. The bottom figure shows the solar reflectance map for block 1 after the weighted barycenter shift has been applied. The Sun is to the right (+X) in this and all maps presented.
that the activity can be linked to solar illumination of the Geb, Neith, or Sobek regions, which are experiencing the highest intensity sunlight around this time. The NAVCAM image allows us to place the nearest spectrum taken by Alice, the 19:18 UTC spectrum plotted in Figure 3.3, into the context of southern hemisphere jet activity. The increase in overall emission that occurs between the last stable pointing spectrum at 19:18 UTC and the first raster observations at 21:16 UTC would suggest that a new jet or jets became active or an outburst occurred in the 87 minutes between the observations, altering both the observed direction and intensity of emission. Due to the uncertainty of the source of the newly introduced emissions, we will refer to this as an activity increase.
### Table 3.1. Dust outburst properties in the VIRTIS-M VIS channel

<table>
<thead>
<tr>
<th>Observing Block</th>
<th>Number of Observations</th>
<th>Time Range (UTC)</th>
<th>Comet Distance (km)</th>
<th>Sub-Spacecraft Latitude (°)</th>
<th>Sub-Spacecraft Longitude (°)</th>
<th>Pointing Scheme</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>25</td>
<td>15:04-19:18</td>
<td>+233.5 – +228.8</td>
<td>-2.29 – -0.99</td>
<td>15.1 – -109.0</td>
<td>Stare</td>
</tr>
<tr>
<td>2</td>
<td>10</td>
<td>21:16-22:07</td>
<td>+226.7 – +225.8</td>
<td>-0.36 – -0.08</td>
<td>-166.8 – +168.2</td>
<td>Raster</td>
</tr>
<tr>
<td>3</td>
<td>9</td>
<td>22:13-22:59</td>
<td>+225.7 – +225.0</td>
<td>-0.05 – +0.20</td>
<td>+165.4 – +142.9</td>
<td>Raster</td>
</tr>
<tr>
<td>4</td>
<td>10</td>
<td>23:04-23:56</td>
<td>+224.9 – +224.0</td>
<td>+0.23 – +0.51</td>
<td>+140.1 – +114.9</td>
<td>Raster</td>
</tr>
<tr>
<td>5</td>
<td>5</td>
<td>00:02-00:32</td>
<td>+223.9 – +223.6</td>
<td>+0.54 – +0.71</td>
<td>+112.1 – +97.0</td>
<td>Raster</td>
</tr>
<tr>
<td>6</td>
<td>10</td>
<td>01:13-01:58</td>
<td>+222.9 – +222.1</td>
<td>+0.94 – +1.19</td>
<td>+77.4 – +55.2</td>
<td>Raster</td>
</tr>
<tr>
<td>7</td>
<td>10</td>
<td>02:04-02:55</td>
<td>+222.0 – +221.1</td>
<td>+1.22 – +1.51</td>
<td>+52.4 – +27.1</td>
<td>Raster</td>
</tr>
<tr>
<td>8</td>
<td>25</td>
<td>03:01-05:18</td>
<td>+221.0 – +218.9</td>
<td>+1.55 – +2.33</td>
<td>+24.5 – -42.8</td>
<td>Raster</td>
</tr>
</tbody>
</table>
3.4 Results

Due to the nature of the observing schemes, several different data products can be made to better understand the near-nucleus coma and the effects of the strengthened activity. The two observing schemes of November 7-8 provide spectra, spatial profiles, and maps to draw comparisons between activity periods and instrument maps.

3.4.1 Spectra

Alice observations taken immediately prior to the mapping scheme, between 15:04 and 19:18 UTC (Table 3.1), are stationary relative to the nucleus and provide a higher signal-to-noise ratio and little uncertainty in the pointing of the Alice boresight. These initial spectra yield no unique features compared to other previously published outbursts or activity (Feldman et al., 2016, 2018a) but spectra taken during this period display contribution from dissociative electron impact of the common volatiles H$_2$O and CO$_2$, as well as two outbursts containing O$_2$, evident from a O I] 1356/O I 1304 Å ratio that is above 1. Analysis of these spectra is presented in Noonan et al. (2021c), and it is recommended that the reader begin with that article to familiarize themselves with the events prior to the raster observations.

A quiescent spectrum is shown from an Alice observation taken at 15:04 UTC, the last time on November 7 prior to the activity detailed in Noonan et al. (2021c) (see Fig. 3.3, 15:04 UTC spectrum). Atomic emissions from H, O, C and S are all clearly visible, evidence for photodissociation and dissociative electron impact on H$_2$O and CO$_2$. The O I] 1356/O I 1304 Å ratio is less than 1, indicating a presence of e+H$_2$O/CO$_2$, but below the ratio $\geq 1$ that would indicate substantial dissociative electron impact of O$_2$. There also appears to be weak emission of the CO Fourth Positive group between 1400 and 1600 Å which is likely the result of resonance fluorescence and e+CO$_2$ (Ajello, 1971a,c; Ajello et al., 2019).

For comparison to this early quiescent period, we have chosen two times that correspond to two unique points in the activity; the first corresponds to emissions
Figure 3.3: Stable pointing spectra from rows 18-23 taken during a quiescent period (black), a jet observation (magenta), and just following a large activity increase on November 7 (cyan). Flux error is plotted but is smaller than the plotted line width. Of particular interest is the O I] 1356 and O I 1304 ratio, indicative of dissociative electron impact. Spectra are offset by 3 photons cm$^{-2}$ s$^{-1}$ Å$^{-1}$. Rows 18-23 are between 5 and 11 km in the sunward direction from the nucleus center for these times. There is also faint CO Fourth Positive emission in the 1400 Å to 1600 Å region mixed with emission from dissociative electron impact excitation of CO$_2$, discussed further in Section 3.5. Note the non-Gaussian shape of Lyman-α due to gain sag of the Alice detector, rendering it inadequate for diagnostic purposes. Other notable features not analyzed in this chapter are labeled with a smaller font.
Figure 3.4: Difference spectra resulting from the subtraction of the 15:04 UTC spectrum from the 19:18 and 21:27 UTC spectra on November 7. Notice the substantial difference in O I 1356/O I 1304 Å emission, as well as the minimal contribution from the CO Fourth Positive group despite an increase in C I emission.

seen at 19:18 UTC on November 7, the second taken at 21:27 UTC, right after the start of Alice raster observations (See Figure 3.3). These spectra detail two unique activity types, allowing a spectral comparison of both cometary jets following outbursts and a later activity increase. To better compare the changes between the activity and quiescent observations a difference spectrum is produced for each exposure, seen in Figure 3.4. Lyman-β and the C I 1561 and 1657 Å features appear to show little change between the jets and activity increase observations, possibly indicating that the H$_2$O and carbon-bearing species maintained an elevated production rate for the hour and a half duration between the observations. The O I 1304 and 1356 Å emissions do not exhibit the same characteristics; the jet shows an O I 1356/O I 1304 ratio of $\sim$1 while at the start of raster observations this ratio is greater than 1. This latter ratio is expected from electron impact dissociation of O$_2$ (Kanik et al., 2003) which we will discuss further in Section 3.5, and suggests that the jet active at 19:18 UTC is depleted of the super-volatile O$_2$.

There are several additional points to be made about these UV spectra that can complicate their analysis, which we outline here. Evidence of S I emission in
Figure 3.3 is present in each spectrum as a weak triplet at 1807, 1820, and 1826 Å but not evident in the quiescent-subtracted spectra in Figure 3.4. The presence of S I emission in the 1800 Å region suggests that there are weaker S I multiplets in the 1473 and 1425 Å regions as well (approximately in 1:2 and 2:5 ratios relative to the S I 1807 Å feature; see Kaufman (1982); Roettger et al. (1989a); Meier and A’Hearn (1997)), though likely blended with weak CO Fourth Positive emission that appears to be present at a low level (<2 Rayleighs) in Figure 3.3 and does not appear strongly in a difference spectrum (Figure 3.4). The line ratios between the strong C I multiplets at 1657 and 1561 Å, and to an extent the weaker 1597 Å CO Fourth Positive Group feature, are in disagreement with that expected from pure dissociative electron impact on CO or CO$_2$ (Ajello, 1971a,c; Ajello et al., 2019).

We also note that Lyman-β is contaminated with O I 1025.72 Å emission, which is not resolved. The O I contribution to the Lyman-β + O I 1025.72 Å blend can be estimated from e+O$_2$ cross sections at 200 eV of Ajello and Franklin (1985) provided the O$_2$ column density is known, though this electron energy is significantly above the expected mean in the near-nucleus environment (Clark et al., 2015). As shown in Ajello and Franklin (1985) the line ratio for the O I 1356/1025.72 Å features resulting from dissociative electron impact of O$_2$ is approximately 35, so the e+O$_2$ contribution to Lyman-β is assumed to be negligible and ignored.

3.4.2 Light Curves

By integrating each emission feature in a spectrum over a set number of rows and plotting these integrated emission strengths as a function of time a light curve can be made, detailing the rise and fall of atomic emissions from photodissociation or dissociative electron impact excitation of H$_2$O, CO$_2$, CO, and O$_2$. Light curves for Lyman-β, O I 1304, O I] 1356, and C I 1657 Å, the four strongest emission features except for Lyman-α, are shown for the relevant time period in Figure 3.5. The general trend is the same for all emission features. An initial increase in activity commences around 16:00 UTC, with two outbursts spiking the emissions up to 4× that of the quiescent emission. These outbursts finished by 17:32 UTC, and
Figure 3.5: Light curves for dominant atomic emission features during all observing blocks listed in Table 3.1, plotted by rows over which the brightness is calculated. Only emissions in rows 18 through 23 are co-added to maximize coma signal. The displayed errorbars are largely the result of brightness variations between rows, in addition to the odd-even detector effect. The dotted and dashed vertical line marks the quiescent spectrum, the blue vertical lines mark two outbursts discussed in Noonan et al. (2021c), and the red dashed vertical line marks the nearLyman-aligned jet observation that is referenced here and discussed further in Noonan et al. (2021c).
emissions are elevated relative to the quiescent activity until the end of Alice observations. When Alice observations resume at 21:18 UTC, emissions are almost a factor of two stronger than at the peak of the previous activity for O I emissions, while Lyman-$\beta$ and C I 1657 Å emissions remain in a similar elevated state as they were at 19:18 UTC. Over the next two hours a decrease in emissions is seen. This indicates that at some point during the observing gap there was a substantial increase in activity. In one possible case, the activity began to occur immediately before the 21:18 UTC observation and produced a maximum emission immediately after. On the other extreme, the increase in activity could have occurred immediately after observations ceased at 19:18 UTC and decreased to the values measured at 21:18 UTC. In this case the maximum emissions can be estimated by approximating the slope of the light curves and working backwards. For slopes of $-10$ Rayleighs $\text{hr}^{-1}$ this would imply that the upper limit activity case would have peaked at between 60 and 80 Rayleighs for the atomic emissions. However, without additional information to support either option we will avoid further speculation.

These light curves are complicated by the change in observing modes. Prior to 19:18 UTC the pointing is stable and centered on the nucleus with no change. After 21:18 UTC the raster scans had begun, changing the previously consistent relative location of each row relative to the nucleus. This effect manifests in the light curves taken after 21:18 UTC as scatter in the data points, as the rows capture different areas of the near-nucleus coma with each raster observation, keeping the center of the Alice slit within 3 km off of the nucleus in any direction. We note that the atomic emission is best characterized from rows 18-23 on the detector, which are not contaminated by reflected sunlight from the nucleus of the solar emission features in this stable pointing.

3.4.3 Emission Mapping

For the period described in Section 3.2.2, four sets of four maps were made to illustrate near-nucleus emission following the initial activity that occurred in observing block 1 (Table 3.1). These emission maps are generated from the observations con-
tained in blocks 2, 3, 4, and 7 described in Table 3.1 in an attempt to discern the morphology of the initial activity observed in block 1. The varied spatial coverage due to the change in location of the Alice slit helps to mitigate the contribution from the instrumental odd/even effect, though the effect is still visible at the edges of some maps. The maps produced from Blocks 5 and 6 are omitted owing to limited spatial coverage. The intensity barycenter of each emission map is calculated by weighting each pixel by intensity, multiplying each grid of X and Y locations by the intensity of pixels over 30 Rayleighs, summing the X and Y weighted averages and dividing by the sum of the intensity weights. For C I 1657 Å the additional masking of pixels brighter than 90 Rayleighs prevents the solar reflectance off the nucleus from dominating the barycenter. This produces an intensity barycenter in the cometocentric coordinates that can be used to calculate an angle relative to the nucleus.

The first map (Figure 3.6) is derived from the first 10 observations taken after observations resumed at 21:18 UTC on November 7 and shows the strongest presence of the four emission features, with the highest intensities located between $-45^\circ$ and $-60^\circ$, or clockwise, relative to the Sun-comet line exhibiting strengths up to 70-80 Rayleighs, notably higher than the brightnesses reported in the spectra at 19:18 UTC (Figure 3.3). Each emission feature shows substantial strength on the sunward side of the nucleus (on the right of the nucleus in the overlaid NAVCAM images). The resolution of the Alice instrument for this period is unable to discern a jet from more general increased activity, but the difference between the opposite sides of the near-nucleus coma is greater than 50 Rayleighs on average. The distance between the intensity barycenter and the nucleus is largest in Figure 3.6 for all emission features and is between $35^\circ$ and $39^\circ$ clockwise of the Sun-comet line that extends along the X-axis.

Maps made from observing block 3 showcase the behavior of the emissions as the nucleus rotates beneath Rosetta. (Compare Figure 3.6 to Figures 3.7 and 3.8). In this period, Alice spectra have better coverage in the $+90^\circ$ sector ($X \geq 0, Y \geq 0$), leading to a sharp cutoff at the 0.0 km mark in Y. One hour after the observations
used in Figure 3.6, there is already a substantial decrease in the brightness of the emission features, specifically hydrogen and oxygen features that are less susceptible to reflected sunlight. The rotation of the nucleus, the scanning motion of the Alice spectrograph, and the near-nucleus dust reflecting solar emission during these observations may produce the noticeable “smear” in the maps like Figure 3.8. This extension appears in both the C I 1657 Å and FUV continuum integrated channel used to correct the position of data, and is treated as a maximum positional uncertainty in the data when comparing to the VIRTIS-H and MIRO maps. For Lyman-β, O I 1304 and 1356 Å the intensity barycenter has moved much closer to the nucleus but remains at a similar angle relative to the Sun-comet line, varying between 38-39° for the emission features. However, for C I 1657 Å the intensity barycenter falls upon the nucleus. This trend continues in Figure 3.8, where each intensity barycenter is calculated to be within one map pixel of the nucleus location.

By observing block 7 the emission strength had continued to drop, approaching a nearly uniform, though still elevated, level in Figure 3.9, the last full coverage map available from Alice data. Almost ten hours after the first increase in activity at approximately 16:07 UTC on November 7, the UV maps no longer exhibit spatial heterogeneity in the coma, suggesting a decrease or cease to the activity/process that elevated the emissions initially, and a gradual return to a steady state near-nucleus coma. The intensity barycenters remain clustered close between 35-38° clockwise of the Sun-comet line, but very near the limb of the nucleus.

3.4.4 Correlation to VIRTIS and MIRO

Comparing the morphology of the Alice maps to those of VIRTIS-H and MIRO, instruments that were designed to map molecular emission and absorption at 67P, we can determine the validity of the UV mapping method. Each instrument is sensitive to different wavelengths of light, so each map will have slightly different relevant scales and morphologies but in general for a period experiencing a significant increase of activity we would expect all remote instruments that were observing to observe emission increases (Grün et al., 2016). Using this simple assumption we can
Figure 3.6: Emission maps created from Alice observations taken between 21:16 and 22:07 UTC on November 7 (observing block 2). The sunward direction is to the right. The weighted intensity barycenter of off-nucleus emission is marked with a white star in each map. The color bar marks 0 to 75 Rayleighs. Contours on the plot mark 10 Rayleigh isophotes. The overlaid NAVCAM image was taken at 21:18 UTC November 7. Error on brightnesses is at most ∼5 Rayleighs for displayed brightnesses, error on pixel position is ± 1.2 km, approximately the size of an Alice pixel subtended at the nucleus.
Figure 3.7: Emission maps created from Alice observations taken between 22:13 and 22:59 UTC on November 7 (observing block 3). The sunward direction is to the right. The weighted intensity barycenter of off-nucleus emission is marked with a white star in each map. The color bar marks 0 to 75 Rayleighs. Contours on the plot mark 10 Rayleigh isophotes. The overlaid NAVCAM image was taken at 23:40 UTC November 7. Error on brightnesses is at most $\sim$5 Rayleighs for displayed brightnesses, error on pixel position is $\pm$ 1.2 km, approximately the size of an Alice pixel subtended at the nucleus.
Figure 3.8: Emission maps created from Alice observations taken between 23:04 and 23:56 UTC on November 7 (observing block 4). The sunward direction is to the right. The weighted intensity barycenter of off-nucleus emission is marked with a white star in each map. The color bar marks 0 to 75 Rayleighs. Contours on the plot mark 10 Rayleigh isophotes. The overlaid NAVCAM image was taken at 23:40 UTC November 7. Error on brightnesses is at most ∼5 Rayleighs for displayed brightnesses, error on pixel position is ±1.2 km, approximately the size of an Alice pixel subtended at the nucleus.
Figure 3.9: Emission maps created from Alice observations taken between 02:04 and 02:55 UTC on November 8 (observing block 7). The sunward direction is to the right. The weighted intensity barycenter of off-nucleus emission is marked with a white star in each map. The color bar marks 0 to 75 Rayleighs. Contours on the plot mark 10 Rayleigh isophotes. The overlaid NAVCAM image was taken at 01:20 UTC November 7. Error on brightnesses is at most $\sim 5$ Rayleighs for displayed brightnesses, error on pixel position is $\pm 1.2$ km, approximately the size of an Alice pixel subtended at the nucleus.
qualitatively and quantitatively compare activity maps between Alice, VIRTIS-H, and MIRO, which were all observing during the same raster observations.

**VIRTIS-H Maps**

Data gathered from the VIRTIS-H instrument enables mapping of both the H$_2$O and CO$_2$ near-nucleus environment via the 2.7 $\mu$m and 4.27 $\mu$m emission bands, respectively. Owing to an excess of scattered light during these observations, the processing of VIRTIS-H data to convert from intensity to column density is difficult. Additionally, deriving total column densities from Alice for direct comparison becomes difficult owing to the number of emission processes that become relevant along the Alice line of sight when not centered on the nucleus (Feldman et al., 2018a; Chaufray et al., 2017). However, for the purposes of determining the viability of the Alice maps a relative comparison from VIRTIS-H is quite useful.

Maps made by the VIRTIS-H team from observations during the raster scan have a similar time resolution to that of the Alice maps, with a $\Delta t$ between maps of approximately one hour. Spatial resolution is improved relative to the Alice maps, providing context for the morphology seen in the Alice maps. Both the H$_2$O (Figure 3.10) and CO$_2$ maps (Figure 3.11) exhibit an intensity $2.5 \times$ stronger at an angle of approximately $-45^\circ$ relative to the Sun-comet line, near the south pole direction displayed with a white solid line, than at $+60^\circ$ for the same time period as Alice observing block 2 (Figure 3.10,3.11 upper left map; Figure 3.6; respectively). However, the molecular emission does not display the same extension as the Alice atomic emission. As the comet proceeds to rotate in the next maps, covering from 22:36:06 UTC November 7 to 09:48:22 UTC November 8, the intensity remains large within 5 km of the nucleus (all panels) and occasionally begins to approach $30^\circ$ to $45^\circ$ relative to the Sun-comet line (panels b, c, d, and e). Panel b) of Figures 3.10 and 3.11 coincides with observing block 3 (Figure 3.7, which lacks coverage in the same area where the relative intensity is highest in the VIRTIS-H maps.

The VIRTIS-H CO$_2$ intensity has the greatest variability between maps. The strongest periods of relative emission are seen at 21:26 UTC of November 7 and 04:16
UTC on November 8 (Fig. 3.11). The earlier instance shows the most extension from the nucleus along the south pole axis, while the latter is rotated approximately 30° anti-sunward from the south pole axis. Only for the 21:26 UTC map is there a matching Alice component map that can be correlated to the VIRTIS-H CO$_2$ intensity measurements. Both the Alice C I 1657 Å and VIRTIS-H CO$_2$ maps from 21:00-22:00 UTC show a significant extension from the southern hemisphere.

**MIRO Maps**

The data available from MIRO for this period are more sparsely sampled in terms of spatial resolution compared to VIRTIS-H, but allow for useful comparison to both the Alice and VIRTIS-H data. MIRO maps display line area in K km s$^{-1}$, derived from the H$_2^{18}$O emission feature at 547.676 GHz, which was optically thin at the time of observation (Figure 3.12), yielding a qualitative idea of the relative water column density. Due to the short integration times and regions with mixed absorption and emission of H$_2$O it is difficult to create precise water column density maps as described in Gulkis et al. (2015), Biver et al. (2015), and Biver et al. (2019), with the model detailed in Zakharov et al. (2007) and Lee et al. (2011). In all MIRO maps there is an increased line area in the south pole direction in agreement with the VIRTIS-H maps of the same time period. In the first three maps the integrated intensity is as high as 80 K km/s. This elevated line area is a factor of 2-3 higher than areas of the coma perpendicular to the south pole at the time of the activity increase, but the low resolution makes interpretation from these maps alone difficult. To an order of magnitude this upper value is consistent with VIRTIS-H post-perihelion water column densities of $\sim 2.7 \times 10^{16}$ cm$^{-2}$ (Bockelée-Morvan et al., 2016; Biver et al., 2019). All three instrument maps show evidence of large scale activity increase on the southern hemisphere that begins to decrease substantially after 1:15 UTC on November 8.
Figure 3.10: VIRTIS-H - H$_2$O 2.7 $\mu$m band maps. Data on nucleus acquisitions are shown as white dots to outline the nucleus shape and are used in map generation. The colorbar shows the intensity of the water emission feature. The white line extends the rotation axis from the south pole. The sunward direction is to the right (see yellow sun). Note the difference in field of view (FOV) compared to Alice maps in Figures 3.6-3.9.

3.5 Discussion

The addition of two-dimensional spectral maps for this period of activity provides a new analysis tool for understanding cometary activity in the UV. The alignment of the initial jet seen in the NAVCAM images with the Alice slit, the additional activity that takes place just before the raster pointing scheme, and the availability of the MIRO and VIRTIS-H datasets for context invite us to address the morphology, composition, and emission mechanisms of the cometary activity.
Figure 3.11: VIRTIS-H - CO$_2$ 4.27 μm band maps. Data on nucleus are not included to minimize signal from the nucleus and are shown as white dots. The colorbar shows the intensity of the emission feature. The white line extends the rotation axis from the south pole. The sunward direction is to the right (see yellow sun).
Figure 3.12: Maps derived from MIRO line areas of the (110-101) transition of $\text{H}_2^{18}\text{O}$ for November 7 20:55 UTC to November 8 10:24 UTC. An outline of the nucleus is shown in white at the correct position and scale for the midpoint of the scan. The line is mostly in absorption against the nucleus; black regions correspond to negative line areas where water appears in absorption. Discrepancy between the white outline and black region is the result of the long duration for the raster scan to acquire the full frame, during which the nucleus will rotate. The sunward direction is to the right in each panel.
Figure 3.13: Spatial profiles of an earlier jet (a) and of map 1 (b). The spatial profile derived from map 1 is the X=0.5 km row of the emission map, shown in Fig. 3.6. The sunward direction is in the +X direction. Each detector row subtends approximately 1.2 km. Of particular interest is the extension of enhanced O I 1356 Å emission to approximately 10 km in the activity maps, with brightnesses approaching 60 Rayleighs, and the slope similarity of the three emission features which indicates they share the same emission process, dissociative electron impact emission. Compare to Figure 4 of Feldman et al. (2016). Note that 1σ errors on each brightness are less than 5%.
Figure 3.14: Alice quiescent-subtracted spectra showing the post-activity onset near-nucleus coma. The spectrum from 15:04 UTC shown in Figure 3.3 is used as the quiescent spectrum. The relative abundances of CO$_2$ and O$_2$ are listed in Table 3.2. Note that Lyman-α emission is omitted from fitting due to gain sag of the detector.
3.5.1 Morphology

Information from the NAVCAM images suggests that there was a jet active prior to the activity onset and before the raster pointing started. The Alice slit was aligned with this jet during the stare pointing, but subsequent rotation of the comet would have prevented the jet from producing the consistent morphology shown in the four instrument maps. The NAVCAM activity shown in Figure 2.1 is seen along the Sun/comet line (taken to be 0°) as opposed to the ~−40 to −45° angle seen in the later Alice, MIRO, and VIRTIS-H maps. Further, the emission strengths change between the stable Alice spectra and the raster maps, from ~30 Rayleighs to ~50 Rayleighs, implying a change in production rate of the active area as well as location as the nucleus rotated approximately 60° between 19:18 UTC and 21:18 UTC (Figure 3.5).

The projection of a jet perpendicular to the Wosret region is unable to explain the emission that is seen extending along the south pole, as the region is nearly antipodal to the the instrument line-of-sight at the time of mapping (21:00 UTC and on). Barring an outburst at the south pole of 67P, which was the site of only one recorded outburst prior to November 7 (Vincent et al., 2016), the source of the outburst would be on the southern portion of the neck or small lobe, with a normal vector that when seen in profile from Rosetta appears to be parallel to the south pole of 67P. Given these constraints we can discuss several candidate areas that have been identified as possible outburst locations and the major clues favoring them.

The decline in elevated emissions after Alice observations restarted at 21:16 UTC suggests that a sharp increase in activity had occurred during the Alice observation gap. During this observing gap (19:18-21:16 UTC) a small area, previously in shadow owing to an overhang in the Neith region (El-Maarry et al., 2016), is fully illuminated. This overhang area previously had an outburst identified in Vincent et al. (2016) (outburst 28 in Table 1) that saw a relative increase in brightness of 10% on 2015 September 10, just under two months before the activity increase discussed in this chapter. However, five outbursts were identified with similar timestamps on...
that date in Sobek and Anukhet as well, making it difficult to attribute any observed ultraviolet emission in Alice observations on that day to a specific region (Fornasier et al., 2019a). There are two outburst sites located farther south in the Geb region that produce outburst vectors that do not have a south pole parallel component and will be eliminated as a possibility. The cluster of possible outburst sites is contained between 270° and 315° longitude and −15° to −45° in latitude and experienced local noon at the time of the activity increase. We note that the possible outburst sites are between 60° and 120° west of the likely outburst sites identified by VIRTIS-M in Noonan et al. (2021c).

We cannot rule out that the activity that occurred during the gap period may be due to rapid sublimation driven by the quick change in illumination of Neith region, which was shielded by an overhang on Wosret prior to the Alice observing gap. The vector normal to this region would extend at an angle approximately 35-40° clockwise from the Sun-comet line as seen from Rosetta. However, the direct comparison between the jets and the later activity shown in Figure 3.6 is a strong indicator that the activity drove the electron impact emission dominated region surrounding the nucleus three times farther from its boundaries at 15:04 UTC, which is difficult to explain with insolation-driven sublimation alone.

We can isolate spatial profiles from the activity emission maps (Figure 3.13), which we can then compare to the earlier observations from 19:18 UTC (See Noonan et al. (2021c)). The spatial profile from the X=0.5 km row of the observing block 2 emission map shows significant emission of Lyman-β, O I 1304, and O I] 1356 Å between 0 and 13 km in the sunward direction from the nucleus. All three emission features show a similar slope with respect to distance from the nucleus, and the presence of O I] 1356 Å at or above a 1:1 ratio with O I 1304 Å suggests dissociative electron impact as a dominant mechanism out to 13 km from the nucleus, distinctly farther than in the earlier profiles (Figure 3.13a).
3.5.2 Composition

Ideally we would be able to derive the composition using a method similar to Galand et al. (2020) and Stephenson et al. (2021); combining IES electron data with measured water column densities from MIRO or VIRTIS and relative coma abundances of CO$_2$, O$_2$, and CO from ROSINA. However, this same method is unfortunately not applicable for the set of observations considered in this chapter for numerous reasons: the nucleus is slightly more active, outbursts (and therefore rapid changes to the near-nucleus coma composition) are prevalent, the spacecraft was over twice as far away from the nucleus, precise water column measurements are unavailable from VIRTIS and MIRO, and it’s unclear if the accelerated solar wind electrons are still the dominant source for the inner coma during outburst emissions. The change in atomic line ratios is a clear indicator that the the composition of the near-nucleus coma has changed, as this is not possible through changes in plasma energy or density alone. This leaves us with two options: assume the plasma density and distribution along the Alice line of sight and use the absolute dissociative electron impact cross sections from the literature to derive column densities of neutrals, or fit the relative intensity spectra from dissociative electron impact excitation of H$_2$O, CO$_2$, and O$_2$ to the observations and derive relative abundances of the neutrals. Due to the large distance from the nucleus during this period, and the possibility that the spacecraft was looking through different plasma environments on different sides of the diamagnetic cavity (Madanian et al., 2016), we will use the latter method.

Compositional analysis of several key times during observing blocks 1 and 2 was completed to determine the dominant components of the initial jet and activity increase using spectra that had been background and quiescent-subtracted using the quiescent average spectrum from earlier on November 7 shown in Fig. 3.3. The remaining emission lines show significant dissociative electron impact emission that can be fit with relative intensity spectra using laboratory electron impact emission data for H$_2$O, CO$_2$, CO, and O$_2$ (Makarov et al., 2004; Ajello et al., 2019; Mumma et al., 1972; Ajello, 1971a,c; Kanik et al., 2003). As described in detail by Stephenson
et al. (2021) the excitation cross sections for each emission feature as a function of energy are limited, but every emission feature in our data is characterized at electron impact energies of 100 eV. By fitting the 100 eV electron impact H$_2$O and CO$_2$ models to Lyman-$\beta$ and C I 1657, 1561, and 1278 Å as well as C II 1335 Å emissions first and subtracting off both molecules’ contributions to the O I 1304 and 1356 Å emission features, the 100 eV O$_2$ electron impact spectrum can be fit to the residual (Figures 3.14). In the absence of in-plume plasma energy distribution data the assumption that the atomic cross section ratios taken at 100 eV prevail at the range of electron energies above their threshold energies must be made in order to compute these relative abundances. This assumption was used by Feldman et al. (2015b), but comes with the errors on those measurements in addition to the uncertainties introduced by any deviation from the assumed constant ratio in the experimental data. Based on the dissociative electron impact excitation rates as a function of energy for H$_2$O, CO$_2$, CO, and O$_2$ (Makarov et al., 2004; Ajello et al., 2019; Mumma et al., 1972; Ajello, 1971a,c; Kanik et al., 2003) we find this value to be between 5 and 20%, depending on which transitions are compared. As noted in Table 1 of Stephenson et al. (2021) many of these features are assumed to have the same shape as other measurements in the source literature (ex. O I 1304 and O I 1356 Å in Makarov et al. (2004)), which would render our assumed constant ratio, somewhat optimistically, perfect. We will thus taken the upper limit error of 20%, and sum in quadrature with the known error in the excitation measurements at 100 eV to find that our relative abundance calculations should be within ±30-36 % of the actual relative abundance. For transitions with significantly higher threshold energies, like C II 1335 Å, a scaling factor has been added to the fitting algorithm. Physically this represents the depletion of electrons with energies over 44 eV from the population of electrons over the lower threshold energies of the other transitions, which are between ~15 and 25 eV. For example, if all electrons in the environment were ≥44 eV, this factor would be 1, and no depletion of the C II 1335 Å feature relative a ratio with C I 1657 Å expected at 100 eV would be present. The scaling factors are allowed to vary between 0 and 1, with the model finding
Table 3.2: Modelled abundances for CO$_2$ and O$_2$ relative to H$_2$O derived from quiescent-subtracted spectra shown in Figure 3.14. Errors for CO$_2$/H$_2$O are approximately 30% for observing blocks 2, 3, and 4 and closer to 45% for observing block 6 due to the decreased signal in Lyman-β. Errors for O$_2$/H$_2$O are higher due to errors induced by residual subtraction and are near 40-45% for observing blocks 2, 3, and 4 and closer to 55% for observing block 6. We conservatively adopt the error to be 50% for observing blocks 2, 3 and 4, accordingly. The errors on the ratios are calculated from the root mean square of the error in the data, fitting error, and error in laboratory measurements of the emission line used for relative intensity calibration. These are added in quadrature with the deviation in line ratios as a function of impacting electron energy. The last two sources of error are the same for each observation.

fits between 0.1 and 0.25 to produce the observed emission, indicating that the near-nucleus environment has a significantly lower number of electrons over 44 eV than the number of electrons over 15 eV. This parameter does not steer the relative abundance model, which is driven by the C I 1657 Å: Lyman-β ratio to determine CO$_2$/H$_2$O, but is interesting to note.

The observations at 21:44 UTC, in observing block 2, yield a spectrum in rows 18-23 with a small change in CO$_2$/H$_2$O composition relative to the earlier spectrum at 19:18 UTC, resulting in CO$_2$/H$_2$O = 0.6±0.2, a 1.2-σ difference from the value of 1.2±0.4 measured earlier during jet activity at 19:18 UTC (Noonan et al. (2021c)). These values are somewhat higher than the typical coma values between 0.3-0.5 observed by the VIRTIS instrument (Bockelée-Morvan et al., 2016).

The strengths of C I 1561 and 1657 Å are slightly inconsistent with e+CO$_2$ as the sole source of the atomic carbon emissions. For e+CO$_2$ the expected line ratio would be 2:1 for C I 1657:1561 Å (Ajello et al., 2019), but the value in these data is often near 3 following quiescent spectrum subtraction (Fig. 3.14). This excess is
most clearly seen in Figure 3.14 a) and b), where the electron impact fit has difficulty matching both emission features with the e+CO₂ model. Given that e+CO is not a significant source of either C I 1657 or 1561 Å in this particular dataset, this discrepancy is likely associated with a significant column of C atoms. We can quantify the necessary atomic carbon column by multiplying the C I 1561 Å emissions by 2, subtracting the resulting value from the measured C I 1657 Å emission, and using the g-factor, or fluorescence efficiency, for the C I 1657 Å feature to calculate the requisite atomic carbon column. For the spectra displayed in Figure 3.14 a) and b) we find residual emissions of ∼5 Rayleighs, and an atomic carbon column density of approximately 5×10¹¹ cm⁻² is required to explain the observed line ratios. The source of this atomic carbon column is likely caused by photodissociation of CO₂.

To explain the residual atomic C I 1657 Å emission with a combined photodissociation and excitation rate for C I 1657 Å from CO₂ at 1.6 au of 5.3×10⁻⁹ s⁻¹ (Wu et al., 1978) requires a CO₂ column of ∼1×10¹⁵ cm⁻², approximately 10% the water column measured by the VIRTIS instrument three days later on 8 November 2015 (Biver et al., 2019). This comparison is not robust, as our determination is from quiescent subtracted spectra in an actively outbursting coma, while the later VIRTIS measurements are not. However, this comparison does show that the derived CO₂ column to explain excess atomic carbon emissions is on the same order of what would be expected.

By fitting an e+O₂ spectrum to the quiescent- and e+(H₂O+CO₂)-subtracted spectra from the secondary activity from observing block 2, we are able to calculate a relative abundance of O₂/H₂O of 0.3 (±50%). This is elevated with respect to the early mission relative abundance for O₂/H₂O of ∼0.05 described by the ROSINA team (Bieler et al., 2015), but falls within the range of 0.05-0.3 reported in other Alice observations (Feldman et al., 2016; Noonan et al., 2018; Keeney et al., 2017, 2019). The appearance of strong O I emission has previously been attributed to gaseous outbursts, and we cannot rule out an outburst occurring during the gap in observations as the cause of the activity change as discussed in Section 3.4.2. Notably, the residual spectrum at 19:18 UTC of the jet does not show similar O I
emission, and is poorly fit by $\text{O}_2/\text{H}_2\text{O} \sim 0.1$ (Noonan et al., 2021c), the detection limit for the routine. This is determined by adding a synthetic e+$\text{O}_2$ spectrum to Alice data and attempting to retrieve that signal, with a $\text{O}_2/\text{H}_2\text{O}$ ratio of 0.1 being the lowest for the data in question. This suggests that the period captured in the Alice, VIRTIS, and MIRO is new onset activity, compositionally distinct from earlier sustained activity.

If the outgassing velocity of neutrals is assumed to be $\sim 600-800 \text{ m s}^{-1}$, as modeled in Fougere et al. (2016a) and Lai et al. (2017), neutrals would have crossed the slit in approximately 15 seconds, much less than the duration of an Alice exposure at this time. This implies that there was continuous outgassing of $\text{O}_2$ and other volatiles for this period. However, it is important to note that this slit-crossing timescale may vary by as much as a factor of two during the observations due to the scanning motion of the slit. This same scanning behavior makes it difficult to co-add spectra reliably to lower the upper limit of detection.

3.5.3 Excitation Processes

The extension of the electron impact environment out to distances of 13 km from the nucleus during the raster despite the lack of large changes in measured molecular emissions from MIRO and VIRTIS-H, and the lack of similar extension during the earlier Alice jet observations, is intriguing. Electron impact is important in the near-nucleus coma, but the changes in spatial profiles for $\text{O I} \lambda 1356 \text{ Å}$ between Figures 3.13a) and 3.13b), which can be interpreted as an indicator of the dissociative electron impact dominated region, then suggest an increase to dissociative electron impact emission without substantial changes to molecular column density. However, it is difficult to explain the changes in relative molecular abundances if only the near-nucleus plasma has experienced increases in average energy and/or density, as this does not drastically change the expected emission line ratios. In short, dissociative electron impact emission in the jet only appears to be dominant out to $5 \pm 1.2 \text{ km}$ while in the spatial profile taken from the raster maps it extends all the way out to $13 \pm 1.3 \text{ km}$. All 3 emission features shown in Figure 3.13b) show the
same sharp decrease at this point, similar to the 15 Rayleigh drop for O I] 1356 Å shown in Figure 3.13a). Further interpretation is difficult owing to the odd/even effect of the Alice detector, but it is clear that the profile of the cometary jet does not match that of the later activity. Spectroscopically and compositionally the activity appears to be more similar to outburst B identified earlier on November 7 (Noonan et al., 2021c), while the extension out to 13 km also suggests changes to the near-nucleus plasma environment that extended the typical region for dissociative electron impact. Without plasma data from that region of the coma it is difficult to disentangle these combined effects.

Further, it is useful to compare the activity in question to the dusty outburst of 2016 February 19 discussed in Grün et al. (2016) and Hajra et al. (2017). Hajra et al. (2017) found that the plasma environment experienced a 3-fold increase in electron density while simultaneously experiencing a 2-9 fold decrease in electrons with energies over 10 eV. In the case where neutral density remains constant while the average energy decreases and the “cold” electron density increases would result in the calculation of a lower limit for column density if the 100 eV cross sections from the literature are implemented. These changes to the plasma environment would produce a dramatic decrease in dissociative electron impact excitation in Alice data, providing a qualitative case study to compare with data taken on November 7-8. Referring back to Figure 3.5, we see that the semi-forbidden O I] 1356 Å emission remains elevated by a factor of five relative to quiescent values until 02:00 UTC on November 8. The observed activity may have a higher energy and/or density electron distribution than the earlier quiescent period. When compared to the dusty outburst discussed in Hajra et al. (2017) the observed activity spectra is inconsistent with an order of magnitude decrease in electron energy, especially given the presence of high-threshold energy C II 1335 Å emission at 21:44 UTC. This, in tandem with the dust outburst observations in Noonan et al. (2021c), suggests that gas and dust outbursts experience different levels of dissociative electron impact emission and may have unique spectral signatures in the UV. Even without direct observations of the dust contribution during this period of high activity Alice observations are not
consistent with a dusty outburst or outbursts as the driver of activity.

3.6 Summary

Cometary activity in 67P/Churyumov-Gerasimenko was observed by Alice, VIRTIS-H, and MIRO instruments on November 2015 7-8. Over the course of 12 hours Alice observations were taken in a ride-along scheme during a series of VIRTIS raster observations. In this chapter we discussed the following results:

1. Alice spectra acquired during the stable observations show an elevated level of dissociative electron impact emission relative to quiescent activity levels, evident from an O I] 1356/O I 1304 Å brightness ratio of $\sim 1$, and have different spectral signatures than cometary activity measured just prior to the start of the raster observations.

2. Observations taken during the raster scan show a similar composition to those taken during the earlier outbursts of the stare scheme, with a moderate CO$_2$/H$_2$O ratio of $\sim$0.6-1.2 and significant presence of O I] 1356 Å emission out to 13 km, indicative of an extended dissociative electron impact dominated emission region. Due to the large spacecraft - comet distance ($\sim$230 km) we are unable to determine if the extension of this region is due to enhanced neutral column density, electron density, electron energies, or a combination of the three.

3. A spectrum taken at the peak emission period at 21:44 UTC on November 7 shows a relative abundance for O$_2$/H$_2$O of $\sim$0.3 ($\pm$50%), which is increased relative to both earlier outbursts at 16:07 and 17:32 UTC and the cometary activity at 19:18 UTC. The O$_2$/H$_2$O ratio remains elevated until 01:47 UTC on November 8, at which point a decreased Lyman-$\beta$ signal makes it difficult to determine the relative abundance.

4. Alice, MIRO, and VIRTIS-H maps all show significant atomic and molecular emissions from the southern hemisphere of 67P between 21:00 UTC on
November 7 and 02:00 UTC on 2105 November 8. The direction of activity observed in the Alice maps, between 35-40° clockwise from the Sun-comet line, is consistent with that observed in the MIRO and VIRTIS-H maps.

5. Alice C I 1657 Å and VIRTIS-H CO₂ maps between 21:00 and 23:00 UTC on November 7 show similar morphology, and given the reasonable, though not perfect, fit of e+CO₂ to Alice spectra we find that CO₂ is likely the dominant contributor to carbon emission features at this time.

The addition of two-dimensional emission maps to the Alice dataset provides a useful tool for understanding the near-nucleus coma environment and the regions where emission mechanisms dominate, and future work will apply this same mapping method to other similar raster observations in the Alice dataset. Future UV comet observations capable of detecting the inner coma region may produce similar observations and allow comparisons to a wider range of comets and activity, ultimately improving interpretation of observations with larger spatial scales.

3.7 Acknowledgements

This work was made possible thanks to the ESA/NASA Rosetta mission with contributions from ESA member states and NASA. The Alice team would like to acknowledge the support of NASA’s Jet Propulsion Laboratory, specifically through contract 1336850 to the Southwest Research Institute. Parts of this research were completed by LESIA, Observatoire de Paris, with financial support from CNRS/Institut des sciences de l’univers. A component of this research was carried out at the Jet Propulsion Laboratory, California Institute of Technology, under a contract with the National Aeronautics and Space Administration. JWN would like to acknowledge Peter Stephenson for his helpful discussions regarding dissociative electron impact modeling. The team would also like to acknowledge the anonymous reviewer for initiating insightful discussions within the team that strengthened the paper.
CHAPTER 4

Ultraviolet observations of Coronal Mass Ejection impact on comet 67P/Churyumov-Gerasimenko by Rosetta Alice

The contents of this chapter were originally published as “Ultraviolet observations of Coronal Mass Ejection impact on comet 67P/Churyumov-Gerasimenko by Rosetta Alice” in The Astronomical Journal, volume 156 (Noonan et al., 2018).

4.1 Introduction

The European Space Agency (ESA) Rosetta spacecraft was launched in 2004 to perform an orbital study of the comet 67P/Churyumov-Gerasimenko, the first mission of its kind. Following rendezvous with the comet on 2014 August 6, the Rosetta spacecraft was able to observe the surface and activity of the comet from close distances. The Alice ultraviolet spectrograph on board the spacecraft measured the atomic and molecular far ultraviolet (FUV) emissions. These observations help to characterize the atomic and molecular composition, reflectance properties of the comet’s surface and the composition and time variation of the comet’s coma (Stern et al., 2007).

Previous papers analyzing Alice data have explored the near nucleus coma ($d_{\text{comet}} \leq 100$ km) environment, the dominant emission from electron impact dissociation of water, and the spectral signature of outbursts from the nucleus (Stern et al., 2015; Feldman et al., 2015b, 2016; Chaufray et al., 2017; Keeney et al., 2017; Feldman et al., 2018a). These studies have shown that the contribution of dissociative electron impact excitation to coma emission is significant and observable, as well as that molecular oxygen ($O_2$) appears to be abundant, even more so than pre-perihelion in-situ mass spectrometer data have shown (Bieler et al., 2015; Fougere et al., 2016b).

The interaction between solar system objects and powerful solar events like coro-
nal mass ejections (CMEs) has long been a subject of interest for space physicists and planetary scientists alike. Emission spikes in conjunction with the arrival of solar events have been observed on other solar system objects as well, though none as small as a comet. For example, observations of Venus’ atmosphere during solar events showed a substantial increase to the O I 5577 Å emission line following interactions with CMEs, co-rotating interaction regions (CIRs), or the solar wind (Gray et al., 2014). Substantial data have been gathered on both Earth’s and Mars’ ionospheric reactions to CME impacts indicating that a CME arrival is accompanied by a compression of the planetary magnetosphere, precipitation of energetic particles into the atmosphere, and an increase in electron density, as well as aurora and nightglow emission (Haider et al., 2009). Additionally, modeling of the Martian atmosphere has shown that during a solar energetic particle event the electron density could reach as high as $10^4$ cm$^{-3}$ within 100 km of the surface (Sheel et al., 2012). A combined CME/CIR impact occurring 2014 October 22 on 67P was observed and described in Edberg et al. (2016a) and Witasse et al. (2017) and witnessed by Alice. The resulting emissions are described in Feldman et al. (2015b) but were only recognized as the result of the CME impact following that paper’s publication. Visible observations of the 2007 CME impact on comet 2P/Encke by STEREO were from too great a distance to directly observe the behavior of the inner coma in response to the increased flux of energetic particles (Vourlidas et al., 2007).

Here we describe a substantial increase in atomic UV emission lines coincident with the arrival of a coronal mass ejection (CME) at 67P. A brief overview of the Alice instrument is given in Section 2. Section 3 discusses observations of the observed emission spike that was seen on 2015 October 5-6, the same date and time that Edberg et al. (2016b) reported that a CME impacted the coma of 67P. Section 4 reviews the Alice spectra and Ion and Electron Spectrometer (IES) data gathered during this CME, and compares Alice and Rosetta Plasma Consortium (RPC) results to establish that there is a relationship between the impact of the CME and the UV emissions observed by Alice. In Section 5 we discuss the possible sources of electrons that could contribute to the observed emission and discuss the O$_2$/H$_2$O
ratio calculated during the emission spikes. Section 6 provides a summary.

4.2 The Alice Spectrograph

The Alice Spectrograph was designed to characterize the surface, coma, and nucleus/coma coupling of comet 67P. It is a low-power, lightweight, imaging far-ultraviolet (FUV) spectrograph designed to gather spatially resolved spectra from 700–2050 Å with a spectral resolution of 8–12 Å for sources that extend the length of the slit (Stern et al., 2007). The rectangular slit is 5.5° long and has a shape reminiscent of a “dog bone”, wider on the bottom and top than the middle. The slit is 0.05° (100 µm) wide in the middle 2.0° section of the slit, and 0.10° (210 µm) wide in the top and bottom sections for a spectral resolution of 8 Å and 12 Å respectively. The microchannel plate (MCP) detector active area is 35×20 mm with a pixel size 34×620 µm for the 1032 spectral columns and 32 spatial rows. Rows 6-24 are illuminated by the slit, the other rows only see dark counts. Detector rows 12 and 18 are transition rows with intermediate solid angles between the narrow and wide sections. Each detector row subtends 0.30° on the sky. The detector has two solar blind photocathodes (CsI and KBr) and a two-dimensional double delay-line readout enabling spectral and spatial information to be logged for every detected photon. The system uses an off-axis telescope feeding into a 0.15-m normal incidence Rowland circle spectrograph with a concave holographic reflection grating, all in an open environment. At the comet, the system experienced an unexpected time-variable feature blue-ward of Lyman β between columns 700 and 900 on the detector, most likely due to cometary dust and ions impacting the detector (Noonan et al., 2016). The feature did not affect the analyses presented in this chapter.

4.3 Observations and Analysis

The emission spikes we discuss in this chapter were observed during 23:30–03:30 UTC 2015 October 5–6 and were captured by the Alice instrument during observing schemes that were not designed for optimal characterization of such activity. The
Figure 4.1: A *Rosetta* NavCam image taken on 2015 October 5 at 23:45:02, just prior to the CME impact, with the Alice slit overlaid. The Sun is toward the top, illuminating portions of both the head and body of 67P. The flattest “underside” portion of the body is facing *Rosetta*. At this time the full length of the Alice slit subtends 76 km at the nucleus distance, approximately 4.2 km per pixel. (Image Credit: NAVCAM)
large cometocentric distance of *Rosetta* means that the UV emission is sampled from an area much closer to the nucleus than the spacecraft. Due to the less than optimal pointing of Alice for this period, it is useful to review the observation design and pointing scenario.

### 4.3.1 Alice Observations

The Alice instrument has multiple observation modes, the most common being a five or ten-minute “histogram” that uses the double delay-line detector to integrate a 2-D wavelength and spatial position image, where each pixel is a sum of the events detected at that spatial-spectral location (Stern et al., 2007). This observing mode is optimal when Alice’s slit is stationary relative to its target. Any scanning motion of the slit in the along-slit direction at a rate greater than one spatial pixel per exposure time will smear the image. The Alice data files contain SPICE-based pointing and geometry information at the start of the exposure, but no information about how the pointing changes during the exposure.

Resonance fluorescence and dissociative electron impact on gases are expected sources of emission multiplets measured by Alice during this post-perihelion observation. Electron impact is believed to be the more significant source of emission for the period analyzed in this chapter due to the dominance of the semi-forbidden O I 1356 Å multiplet (discussed further below). Experimentally determined electron impact emission efficiencies, or cross sections, as a function of energy for Lyman-β, O I 1304 Å, O I 1356 Å, and C I 1657 Å emission multiplets are used to constrain the composition of the coma. This is done by comparing observed line ratios to the ratios of the 100 eV cross sections for emission features for qualitative gas compositions displayed in Table 4.1. There is some tolerance to the values given in Table 4.1 due to the variation in the average electron energy at the comet, but in general the cross section ratios taken at 100 eV are best characterized in the literature. The ratios of the energy integrated cross sections provided in section 4.3.4 are similar to the ratios of the cross sections at 100 eV. Table 4.1 and other multiplet emissions are used to analyze the UV spectra gathered during the CME in Section 4.4. While
Figure 4.2: Top: Alice spectrum before CME impact taken at 00:38:59 UTC 5 October with similar, though not identical, pointing to the CME impact period. Reflected sunlight from the nucleus can be seen in the 1700–2100 Å area of rows 17 and 18. Bottom: Alice spectrum during CME impact taken at 00:17:38 UTC 6 October.
Figure 4.3: Top: Three spectra taken by the Alice instrument during similar pointing instances but with three distinct emission signatures. All spectra are made using rows 13-17, representing the rows closest to the nucleus. Integration time for each image is stated in the legend. Statistical uncertainties are plotted but are smaller than the line thickness. Bottom: The first and second emission spikes with the quiescent spectrum subtracted are plotted. Notice the increase in Lyman-β emission between the first and second emission spikes.
Table 4.1: Electron impact emission line ratios for various gases and qualitative compositions relevant to cometary activity derived from Ajello (1971a), Ajello (1971c), Makarov et al. (2004), Kanik et al. (2003), and Mumma et al. (1972)

<table>
<thead>
<tr>
<th>Gas</th>
<th>$O_1$ 1304</th>
<th>$O_1$ 1356</th>
<th>$H_1 \text{Lyman-}\beta$</th>
<th>$H_1 \text{Lyman-}\beta$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$H_2O$</td>
<td>$\sim$3</td>
<td>0</td>
<td>$\sim$3</td>
<td></td>
</tr>
<tr>
<td>$CO_2$</td>
<td>$\sim$2</td>
<td>$\sim$1</td>
<td>0</td>
<td></td>
</tr>
<tr>
<td>$CO_2$ and $O_2$</td>
<td>$\sim$1</td>
<td>$\sim$3</td>
<td>0</td>
<td></td>
</tr>
<tr>
<td>$O_2$</td>
<td>0.5</td>
<td>0</td>
<td>0</td>
<td></td>
</tr>
</tbody>
</table>

not ideal, mixed gas electron impact UV emission studies have yet to be attempted.

4.3.2 Geometry and Spacecraft Pointing

Starting at 23:30 UTC 2015 October 5 and continuing to 06:00 October 6, the Rosetta remote sensing instruments were performing a steady off-nadir angle scan. The Rosetta spacecraft was in an approximately terminator orbit at 40° latitude on the nucleus. The comet orientation for this period of time is captured in the NavCam image in Figure 4.1. At this time Rosetta was at a heliocentric distance of 1.4 AU, having reached perihelion on 2015 August 13. The spacecraft was on its way back to the near-nucleus coma from a day-side excursion that took place in late 2015 September. During this excursion Rosetta reached 1500 km from the nucleus in the Sun-ward direction. The CME impact occurred when Rosetta was traveling towards the nucleus, from distances between 800 and 750 km (Edberg et al., 2016b).

Observations from VIRTIS (Coradini et al., 2007) post perihelion place $H_2O$ column densities around $2-4 \times 10^{20}$ m$^{-2}$ at this time (Bockelée-Morvan et al., 2016). Alice observations of the water column density in the months leading up to perihelion support the observations made by VIRTIS (Chaufray et al., 2017).

The scanning motion of the Alice instrument was along the Sun/comet line, parallel to the direction of the slit. Over the course of the impact observations the scanning motion of the slit ranged from 0.00006 to 0.03 degrees per second, reducing the effectiveness of plotting the emission as a function of row/distance from nucleus. For the observations closest in time to the occurrence of the emission spikes discussed
in this chapter, the scanning rate averaged 0.001 degrees per second, or about one detector row per 300 second observation. These observations took place with an off nadir angle less than one degree from the nucleus, allowing a line of sight that captures emission from the near-nucleus environment, under 10 km from the nucleus.

Just after 00:00 UTC on October 6, the brightness of all measured emission lines began to increase (Figure 4.2). $\text{O I}$ 1304 and 1356 Å has a relatively uniform brightness across the slit, while $\text{C I}$ 1657 Å and weak $\text{C I}$ 1561 Å are present in the upper rows as well. Note the appearance of weak sulfur and carbon multiplets at 1429 and $\sim$1470 Å, respectively, and a stronger sulfur multiplet at 1807, 1820, and 1826 Å. The presence of sulfur and sulfur-bearing species in the coma has been reported by Calmonte et al. (2016). Several spatially summed spectra from detector rows 13-17 for this time are shown in Fig. 4.3 to display the unique emission observed during this period. The first observation, taken on October 5 at 00:49 and plotted in blue, shows the coma two rotations ($\sim$24 hrs) prior to the CME impact from a similar off-nadir angle and Sun/comet orientation at a cometocentric distance of 860 km. The nucleus is captured as well in these early observations, producing the continuum at the red-ward side of the detector. The second observation, taken on October 6 at 00:52 and plotted in orange, shows a spectrum taken during the first spike of emission in Alice data. The third observation, taken on October 6 at 02:29 and plotted in green, is from the second emission spike. The second and third spectra are from the two spikes of the distinct increases in emission. The emission values of $\text{O I}$ 1304 Å are nearly identical for the two spikes. In contrast, the second spike of the Lyman-β emission line is significantly stronger than the first and both $\text{O I}$ 1356 Å and $\text{C I}$ 1657 Å are weaker. All observations have a similar pointing scheme and $\leq 1^\circ$ off-nadir angle for the center of the slit. The oxygen, carbon, and hydrogen emissions for the first period have similar relative increases, but only the hydrogen emission increases further in the second emission spike. When the quiescent coma spectrum is subtracted from the emission spike spectra to produce a difference spectrum, this relative change is more pronounced (Fig. 4.3).

By integrating the emission multiplets for spectra taken between the 5th and
6th of October where the slit center, which coincides with detector row 15, is within 1 degree of the nucleus a plot of their brightness as a function of time can be used to look for the key moments and areas of emission. This is shown in Figure 4.4. Each observed multiplet experiences two emission spikes; the secondary spike for Lyman-β is stronger than the primary. This is in contrast to the other multiplets where the secondary emission peaks are weaker than the primary. Each multiplet experiences a relatively smooth decrease back to quiescent levels starting on October 6th at 03:15. It should be noted that the line of sight for the Alice instrument did not intersect the nucleus of 67P during the CME impact period, except for the set of observations made October 5 between 21:11 and 21:39 UTC and one observation on October 6 at 02:48 UTC. This means, as with all limb or coma observations, that the interplanetary medium Lyman-α and β emissions are included in the observations at a constant background level that are subtracted in the the quiescent-subtracted spectra for compositional analysis. Compared to the observations taken 24 hours (i.e. approximately two comet rotations) earlier from a distance of 860 km, we see that line brightnesses increased 5–8 times for Lyman-β and O I 1304 Å, and approximately 15 times their quiescent value for O I 1356 Å (Figure 4.4).

4.3.3 Complementary Observations

To correlate Alice observations to the CME passage we use in situ data gathered by the Rosetta Plasma Consortium instruments, specifically the Ion and Electron Spectrometer (RPC-IES) (Burch et al., 2007). During the CME impact RPC-IES collected data on the electron energy distribution at Rosetta at regular intervals (Edberg et al., 2016b), and these data that have been fit with kappa functions described in Broiles et al. (2016b). RPC-IES measures electrons above 4.3 eV, which allows measurement of the lowest energy electrons responsible for dissociative electron impact emission. Threshold energies for dissociative electron impact are unique to each molecule, but the lowest threshold energies are \( \sim 15 \) eV for relevant UV emission features. RPC-IES measurements can characterize all electrons that can contribute to the electron impact emission features with minimal effect from
the spacecraft’s potential, which is typically negative, and therefore repels a portion of the low energy electrons from IES below the threshold energies. Suprathermal electrons (10–200 eV) may have energies linearly shifted, but this effect is small (Clark et al., 2015). Observations from the other four RPC instruments are not discussed in detail but are mentioned in this chapter.

4.3.4 Dissociative Electron Impact Analysis

Laboratory experiments have measured the cross sections for the O I 1304 Å, O I 1356 Å, C I 1657 Å, and Lyman-β transitions for electron impact on each of the expected major components of the coma: H₂O, CO₂, O₂, and CO (Ajello, 1971a,c; Makarov et al., 2004; Mumma et al., 1972; Kanik et al., 2003; Ajello and Franklin, 1985; Ajello, 1971b). The four dominant molecules in the coma can dissociate into O fragments and be excited into OI, allowing for O I 1304 Å and O I 1356 Å from all four sources. The molecule- and transition-specific cross sections for Lyman-β and C I 1657 Å are used as indicators for H₂O and CO₂, respectively. Lyman-α is not used for this analysis due to instrument gain sag in that portion of the detector, though relative changes are still apparent.

Mathematically, the ratio of the O₂ and H₂O column densities can be written as a function of the observed brightnesses of the O I 1304 Å, O I 1356 Å, and Lyman-β in the coma and their energy integrated cross sections:

\[
\frac{N_{O_2}}{N_{H_2O}} = 0.068 \left( \frac{B_{\text{OI1304,Total}}}{B_{\text{OI1304,H}_2O}} - \frac{B_{\text{OI1304,CO}_2} + B_{\text{OI1304,H}_2O}}{B_{\text{OI1304,H}_2O}} \right) \tag{4.1}
\]

\[
\frac{N_{O_2}}{N_{H_2O}} = 0.104 \left( \frac{B_{\text{OI1356,Total}}}{B_{\text{Lyman-β,H}_2O}} - \frac{B_{\text{OI1356,CO}_2} + B_{\text{OI1356,H}_2O}}{B_{\text{Lyman-β,H}_2O}} \right) \tag{4.2}
\]

where \(N\) is the column density, \(B\) is the brightness of the emission feature in Rayleighs, and the numerical constant represents the ratio of energy integrated g-factors for the O I 1304 Å and O I 1356 Å features between O₂ and H₂O. Each individual integrated g-factor can be calculated using:

\[
G_{\lambda,y} = \int_{E_y^{300eV}} \sigma_\lambda^y(E) f_{pde}(E) dE, \tag{4.3}
\]
where $\sigma$ is the analytically derived cross section efficiency of dissociative electron impact for molecule $y$ and emission feature $\lambda$ as a function of electron energy as described in Shirai et al. (2001) and Kanik et al. (2003). The lower limit of integration $E_T$ is defined as the threshold energy below which the emission feature will not appear. $f_{pe}(E)$ is the electron population distribution as measured at the spacecraft.

This method loses effectiveness during periods with small amounts of electron impact activity, which are associated with a O I 1304/1356 Å ratio near 1. CO$_2$ and CO have O I 1304 Å and O I 1356 Å cross sections similar to O$_2$, but have dissociative cross sections for unique carbon emission features, producing a “fingerprint” in spectra at the C II 1335 Å, C I 1561 Å, and C I 1657 Å multiplets; if seen, these would indicate that CO$_2$ and/or CO are present rather than O$_2$. The low CO/CO$_2$ ratio observed at 67P around perihelion (Mall et al., 2016) and similarity of the carbon features to dissociative electron impact of CO$_2$ makes CO unlikely to contribute significantly to these carbon multiplets for the CME impact period. For this reason CO is excluded from subtraction in Equations 4.1 and 4.2.

An electron impact model for H$_2$O and CO$_2$ derived from Makarov et al. (2004); Ajello (1971c) and Shirai et al. (2001) is fit to quiescent, background-subtracted data to determine contribution to the O I 1304 Å and O I 1356 Å emission features. The expected contribution is subtracted in Equation 4.1 to prevent an overestimation of the O$_2$ abundance relative to H$_2$O. An example of this model fit is displayed in Figure 4.5. The model assumes a H$_2$O column density of $10^{20}$ m$^{-2}$ from VIRTIS measurements (Bockelée-Morvan et al., 2016), 30% CO$_2$/H$_2$O relative abundance, 100 eV electron energy, and a Gaussian distribution of photons about the emission feature wavelength, and multiplies the spectrum by a constant until the modeled spectrum resembles the observed. Emission features with threshold energies higher than the average of 15 eV, like the C II 1335 Å feature, have an additional constant to lower their values. This correction is used to scale for the electron energy distribution at 67P having a significant number of electrons at energies lower than the threshold of these features, but high enough to create C I 1657 Å or Lyman-\(\beta\) emission. All
Figure 4.4: Brightness vs. Time for October 5–6. All times displayed are in UTC. Gaps in data indicate periods where the Alice slit was more than 1 degree off of nadir or was not taking data. The nucleus is closest to rows 13–17 for this period, with rows 18–22 capturing sunward coma and rows 8–12 capturing anti-sunward coma. Rows closest to the nucleus see the strongest emission, followed by the sunward and anti-sunward coma. The solid angle differences for rows 12 and 18 are corrected for in the brightness calculation. The largest relative increase in emission occurs for O I 1356 Å. 1-σ error bars are not plotted but are between 1–7 Rayleighs.
Figure 4.5: The quiescent and background-subtracted spectrum from the second spike with dissociative electron impact of H$_2$O and CO$_2$ (e+H$_2$O and e+CO$_2$) model spectra. The expected emission from O I 1304 Å and O I 1356 Å from these two sources is then subtracted from the total, as shown in Equations 4.1 and 4.2.

electron impact cross sections available from the literature to synthesize the model spectra are taken at 100 eV.

We use the same method as Feldman et al. (2016), which takes advantage of the small O I 1356 Å cross section for H$_2$O. This method requires the assumption that electron impact on O$_2$ contributing to O I 1027 Å emission is minimal relative to Lyman-β emission. The cross section of O I 1027 Å for O$_2$ is about an order of magnitude lower than that of Lyman-β for H$_2$O, so this is a reasonable approximation (Ajello and Franklin, 1985; Makarov et al., 2004).

Using the relative cross sections for analysis works under the assumption that
the same electron population affects each of the four gases. The model describes the measurements well with minimal adjustment, so this is reasonable assumption to make. This method only yields information on relative abundance, not column density.

4.4 Results

The large increase in emission that occurs after 00:00 UTC on October 6 yields the opportunity to explore the composition of the near-nucleus coma, provided there are no simultaneous outbursts of gas from the nucleus. The period during and following the CME impact is of interest due to the correlation of electron density and semi-forbidden O I 1356 emission multiplet. The increased signal-to-noise ratio for this period allows a qualitative determination of the coma composition during the CME impact for the Alice line of sight.

4.4.1 Concurrent Electron Density Measurements

Using the O I 1356 Å emission multiplet as a proxy for the electron density near the nucleus, we compare the O I 1356 Å emission to the measured electron density from the RPC-IES instrument on board the Rosetta spacecraft in Figure 4.6. The electron impact emission of O I 1356 Å and the electron density both experience an increase starting at 00:00 UTC on October 6. The O I 1356 Å emission peaks nearly simultaneously with the electron density during the CME arrival and decreases smoothly back to quiescent levels, contrasting the fast drop in electron density measured at the spacecraft after 04:00 UTC (Figure 4.6).

The energy distribution of these IES-measured electrons also shows a shift in the energy spectrum. Figure 5 of Edberg et al. (2016b) shows that during the CME impact there is a larger number of electrons with energies ≥50 eV than measured in previous days. These observed energies have larger lab-measured dissociative impact cross sections for the relevant molecules, which could explain the increase in emission (Makarov et al., 2004; Ajello, 1971a; Kanik et al., 2003; Ajello and Franklin, 1985;
Figure 4.6: Comparison of Alice O I 1356 Å emission from rows 13–17 (blue stars) with the warm (5–100 eV) electron density (red triangles) as defined by Broiles et al. (2016b) and Broiles et al. (2016a) from the IES instrument. The x axis begins at the start of the CME as reported by the RPC magnetometer in Edberg et al. (2016b). O I 1356 Å measurements that may indicate a possible outburst are marked. This possible outburst time coincides with slightly elevated electron fluxes that may be indicative of an outburst as well. Labels 1 and 2 denote the two electron spikes that coincide with spikes in O I 1356 Å emission. Spectra with an off nadir angle less than 1° are used to create the plot.
Ajello, 1971b). However, the electrons detected by RPC-IES are at the spacecraft, whereas the emission of O I 1356 Å may come from anywhere along the line of sight within Alice’s field of view. This becomes critical during the impact of a coronal mass ejection because, as Edberg et al. (2016b) report, the plasma environment was compressed, allowing solar wind ions to be detected directly by Rosetta for the first time since April 2015. This compression would cause a very different plasma environment at the spacecraft than along the Alice line of sight passing near the nucleus.

The arrival of the CME is characterized by an increase in the electron density and energy, appearance of solar wind ions, and an increase in the magnetic field strength (Edberg et al., 2016b), first occurring at 20:15 UTC October 5. All of these factors were measured by the RPC instruments at Rosetta, so the same characteristics may not be applicable across Alice’s line of sight. Figure 4.6 shows that the warm electron population (electrons with energies between 5–100 eV) correlates with O I 1356 Å emission, with both emission spikes corresponding to maxima of the IES warm electron population. It also appears that the decay in O I 1356 Å emission with time correlates to the decreasing electron density after the CME passes, around 02:45–03:00 on October 6. The correlation of these two measurements indicates that the CME directly or indirectly increased the electron impact emission of the near-nucleus coma.

The likelihood of an outburst occurring at the same time as the CME arrival is small, though it cannot be ruled out. The four O I 1356 Å brightnesses measured an hour after the RPC magnetometer detected the arrival of the CME, but 3 hours before the first steep increases in electron density at the spacecraft, may indicate a gas outburst (Figure 4.6). If so, this would be an outburst similar to the one detailed in Feldman et al. (2016) happening just after the CME arrival. A first order calculation of the probability of an outburst overlapping with the CME using the outburst frequency of 0.78 outbursts/day from Vincent et al. (2016) suggests a 2% chance of this particular case. These observations may also be an indication of a more rapid change in the near-nucleus electron environment following the CME.
impact, but without simultaneous electron measurements at both locations there is unfortunately no way to disentangle the two possibilities.
Table 4.2. Observed emission line ratios for periods described in Sections 3 and 4

<table>
<thead>
<tr>
<th>Observation</th>
<th>Time (UTC)</th>
<th>$d_{\text{comet}}$ (km)</th>
<th>Scan Rate ($^\circ$/s)</th>
<th>Off-Nadir Angle ($^\circ$)</th>
<th>$\text{OI } 1304$</th>
<th>$\text{OI } 1356$</th>
<th>$\text{CI } 1657$</th>
<th>$\text{HI Lyman} - \beta$</th>
<th>$\text{HI Lyman} - \beta$</th>
</tr>
</thead>
<tbody>
<tr>
<td>October 5 Pre-CME</td>
<td>00:08–00:38</td>
<td>875</td>
<td>6.36E-5</td>
<td>0.54</td>
<td>2.8±0.6</td>
<td>0.64±0.05</td>
<td>0.96±0.03</td>
<td></td>
<td></td>
</tr>
<tr>
<td>October 6 CME Spike 1</td>
<td>00:46–00:57</td>
<td>763</td>
<td>8.29E-5</td>
<td>0.45</td>
<td>0.96±0.7</td>
<td>0.73±0.1</td>
<td>0.86±0.01</td>
<td></td>
<td></td>
</tr>
<tr>
<td>October 6 CME Spike 2</td>
<td>02:29–02:48</td>
<td>756</td>
<td>8.64E-5</td>
<td>0.44</td>
<td>1.2±0.1</td>
<td>0.47±0.08</td>
<td>1.20±0.07</td>
<td></td>
<td></td>
</tr>
<tr>
<td>October 6 Post-CME</td>
<td>06:42–06:52</td>
<td>737</td>
<td>1.38E-4</td>
<td>0.52</td>
<td>4.3±1.4</td>
<td>0.33±0.2</td>
<td>1.7±0.6</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

**Note**—Observed emission line ratios for four distinct periods described in Sections 3 and 4. Pre-CME values are taken from three exposures made two comet rotations earlier with similar, though not identical, pointing to the spectra plotted in Figure 4.2a. All values are taken from rows 13-17. CME spike values correspond to the three exposures closest to the maximum spectrum for each spike, both shown in Figure 4.3. The post-CME values are calculated from three exposures gathered just before the final gap in data at 07:37 UTC on October 6. This period is used as the quiescent subtraction due to the identical pointing.
4.4.2 Spectra

The most likely cause of the spikes in emission is the CME, whether through direct impact of CME electrons or higher order interactions, such as magnetic reconnection events or ionization of neutrals by CME energetic particles. In either case the significant presence of the semi-forbidden O I 1356 Å line is an indication that the emission spike has a large electron impact component; as a spin-forbidden transition it can only occur from electron impact and not resonance fluorescence. Providing there was not a gas outburst from the comet at a coinciding time this data would provide a sampling of the near-nucleus coma. If this is the case, a brief comparison of the line ratios during the CME to Table 4.1 shows that the portion of the coma observed would be in reasonable agreement with a mixture of H₂O and O₂ plus a small component of CO₂. This mixture would produce spectral features similar to the outburst composition of O₂/H₂O ≥ 0.5 and a C I 1657 Å emission with an unclear origin found by Feldman et al. (2016). Though sulfur and sulfur-bearing compounds have been observed at 67P, the observed sulfur multiplet emission does not correspond to electron impact on SO₂ (Calmonte et al., 2016; Vatti Palle et al., 2004). By subtracting the quiescent period spectra from the spectra taken during the CME we can attempt to identify the composition in the coma at the time of the CME and examine the effect the solar event had on the coma. The line ratios of four periods of specific interest are summarized in Table 4.2 and analyzed here.

**Pre CME Emission**

The first period of interest covers four observations made between 00:08 and 00:38 UTC, during which the Alice slit intersects the nucleus of 67P. The emission is consistent with the October 5 00:49 UTC spectrum plotted in Figure 4.3. This time period is characterized by low levels of emission of the Lyman-β, O I 1304 Å, O I 1356 Å, and C I 1657 Å multiplets, most likely indicative of the pre-CME coma environment. The emission multiplet ratios from Table 4.2 for the rows closest to the nucleus, and thus most affected by electron impact excitation due to the line of
sight integration and higher column density, indicate a H$_2$O-dominant coma with carbon compounds contributing to the C I 1657 Å multiplet, but with no obvious O$_2$ signature. There is a nearly 24-hour time difference between this period of interest and the first emission spike during the CME impact. This time difference opens the possibility that the composition of the coma seen by Alice two comet rotations prior to the CME impact was different from the coma composition observed during the CME impact.

**First Emission Spike**

Emission from the coma reaches the first spike on October 6th at 00:52 UTC, just over an hour after the initial CME impact (Edberg et al., 2016b). Spectra taken between 00:46 and 00:57 on October 6 are used to characterize this spike. This period corresponds to the maximum density of solar wind ions measured by the ICA instrument during the CME (see figure 4b of Edberg et al. 2016b). Table 4.2 and Figure 4.7 show that the line ratios that occur during the CME are not similar to what was observed during two cometary rotations earlier; the O I 1304/1356 Å ratio has dropped to $\approx 1$, indicating the presence of O$_2$ (Feldman et al., 2016; Kanik et al., 2003). The C I 1657 Å/Lyman-β ratio for this period increases from 0.64 to 0.73, and the Lyman-β/O I 1304 Å ratio decreases from 0.96 to 0.86. Following this spike all emission lines experience a decline until the second spike occurs. Additionally, this period is missing CO emission from electron impact on CO$_2$, which has maximum cross sections between 20-40 eV (Ajello, 1971c). This suggests that the dominant electrons are in the 100 eV range, where cross sections are maximized for O$_2$, H$_2$O, and CO$_2$ carbon and oxygen emission.

**Second Emission Spike**

The second spike occurs approximately 1.5 hours after the first, with the maximum reached at 02:34 UTC during a short 46-second exposure. Due to the short exposure time the signal-to-noise ratio is lower than the surrounding exposures at 02:29 and
02:48 UTC. Measurements from the IES instrument show the highest density and energy of electrons occur during this time period (Figure 4.6 of this chapter and Figure 4c of Edberg et al. 2016b). Again, we see that the emission increases for all of the largest multiplets, but unlike the first spike Lyman-β experiences the largest relative increase. The C I 1657 Å/Lyman-β ratio dropped further from the first spike, down to 0.47. Similarly, the Lyman-β/O I 1304 Å ratio increases up to 1.2, the result of a stronger Lyman-β presence in the second spike and a decreased presence of O I 1304 Å and O I 1356 Å emission (see Figure 4.4). The O I 1304/1356 Å ratio rose slightly to 1.2, indicating a lower abundance of O₂ in the coma. The increases seen with Lyman-β also suggest a change to the O₂/H₂O relative abundance. Individual spectra near this spike show some evidence of electron impact on CO₂ producing CO emission (Fig 4.3) in the 1400 to 1500 Å region. The CO emission suggests that the incident electron population has a cooler population with energies nearer to the CO emission from dissociative electron impact on CO₂ (Ajello, 1971c). Alice observations cease before a decrease in the emission spike is observed, leaving the possibility that the increase in emissions continued.

Post CME Emission

As observations resumed again at 03:15 UTC all emissions experienced a steep decrease down to a background level (Figure 4.4). This smooth decline stands in contrast to the sharp drop seen in the electron density by IES at the spacecraft (Figure 4.6), suggesting a difference between the near-nucleus and spacecraft-measured electron populations. Using the O I 1356 Å multiplet as a proxy for electron impact emission shows that the contribution of electron impact to the emissions almost entirely disappears. The O I 1304/1356 ratio rose to 5.3 due to the decrease in the electron impact emission, and continued to rise after this time period (Figure 4.7). The changes in Lyman-β and the C I 1657 Å multiplet seen in the second emission spike continue, with the C I 1657 Å/Lyman-β ratio measured near 0.4–0.8 from the resumption of observations at 03:15 UTC onward. For the post-CME time period described here the value was 0.35. Compare this trend to the period just prior to
the second emission spike in Figure 4.7, which shows a steady increase to the ratio prior to the end of observations. The lack of electron impact emission for this time period prevents the accurate use of Table 4.1 for analyzing composition.

4.5 Discussion

The emissions spikes observed on October 6 present several problems for decisive analysis. Due to the timing of the emission compared to the CME impact it seems most likely that the emission is driven by changes to the electron environment, though we cannot rule out that an outburst occurred at the same time. The four significant detections of O I 1356 Å around October 5 21:25 UTC, approximately 3 hours before the substantial increase to the RPC-IES measured electron density (Figure 4.6), may be a sign of an outburst similar to that reported in Feldman et al. (2016). Here we attempt to distinguish between possible scenarios that could have increased electron energy and/or density and how they compare to observations.

4.5.1 Electron Impact Emission

The detection of the semi-forbidden O I 1356 Å emission line for the duration of the CME as measured by IES supports the hypothesis that the change in emissions during this period was the result of increased electron impact on the coma of 67P (Figure 4.6). The 1:1 ratio of O I 1304 Å and O I 1356 Å in Figure 4.7 is a prime indicator of the electron environment’s effect on the coma, since the only way for these to reach equal levels is as a result of electron impact (Kanik et al., 2003; Ajello, 1971a,c). Due to the unique circumstances surrounding these observations we would like to address several hypotheses for how the electron environment could have become more favorable for electron impact emission during the CME impact.

**Introduction of CME Electrons**

The simplest case is that the increase in electron impact could result from the introduction of CME electrons to the near-nucleus environment. The RPC instruments
Figure 4.7: Emission line ratios as a function of time from rows 13-17. Labels 1 and 2 mark the same boundaries for electron spikes as in Figure 4.6. The x-axis starts at the time of the first RPC detection of the CME arrival at 20:15 UTC. Of particular interest is the O I $\lambda 1304/1356$ Å ratio near 1 during the impact, the drop in C I $\lambda 1657$/Lyman-$\beta$ Å, and the increase to Lyman-$\beta$/O I $\lambda 1304$ Å and O I $\lambda 1304/1356$ Å ratios during the secondary outburst.
Observation $\frac{O_2}{H_2O}$ from Equation 1 $\frac{O_2}{H_2O}$ from Equation 2
Rows 13-17 Rows 18-22 Rows 13-17 Rows 18-22
October 6 CME Spike 1 0.14±0.01 0.13±0.02 0.14±0.01 0.15±0.01
October 6 CME Spike 2 0.10±0.01 0.06±0.01 0.08±0.01 0.05±0.02

Table 4.3: Calculated O$_2$/H$_2$O abundances from the emission spikes described in Sections 4.3/4.4 and plotted in Figure 4.3.

on board Rosetta observed and reported on this electron population in Edberg et al. (2016b), which was rich with electrons in the 10–200 eV energy range. If this population of electrons penetrated into the near-nucleus environment, the energies would be ideal for maximizing emission from electron impact based on lab-determined cross sections. Because the RPC measurements are taken in situ and Alice results represent a line-of-sight integration, assumptions must be made about the electron and gas density along the line of sight in order to properly determine this effect’s contribution. However, this hypothesis does not explain the difference in slope between the observed O I 1356 Å emission and the in situ electron measurements, which would be expected to match exactly if the CME electrons were the main contributor due to the short lifetime of the excited state, and under the assumption of uniformity for the CME electron density on the scale of the Rosetta-comet distance. This mismatch between slopes, especially in the period following 04:00 UTC, is clearly seen in Figure 4.6.

Compression of the Diamagnetic Cavity

The CME impact onto the comet likely compressed the plasma environment of the coma, allowing solar wind ions to penetrate closer to the nucleus for the first time since March 2015 (Edberg et al., 2016b). The most important aspect of the CME’s effect on the environment for dissociative electron impact emission is the compression of the diamagnetic cavity, within which there is no magnetic field. At 67P the region inside the diamagnetic cavity was determined to be somewhat depleted of electrons between 150-200 eV and substantially depleted of electrons
around 100 eV (Nemeth et al., 2016), making the cavity less favorable for electron impact emission. Furthermore, the electron gyroradius is small compared to other length scales in the plasma of the coma environment, preventing electrons from the extended coma and solar wind from passing into the cavity. This would imply that the electron population best suited for dissociative electron impact excitation exists just outside the cavity, where electrons have the highest density and energy distribution and the neutral number density is highest.

The diamagnetic cavity radius was first calculated using a balance of the Lorentz and neutral friction force (Cravens, 1987; Ip and Axford, 1987), but we can now bolster this with observational constraints from RPC measurements. At 67P the diamagnetic cavity was found to extend farther from the nucleus then expected (Goetz et al., 2016b,a), and can be calculated using:

\[ r_c = \left( \frac{B(r)^2}{c^2 Q^{3/2}} + \frac{1}{r^2} \right)^{-1/2}, \]  

(4.4)

where \( B(r) \) is the magnetic field measured at radius \( r \), \( c \) is the constant \( 7.08 \times 10^{-18} \) km nT s\(^{3/4} \), and \( Q \) is the production rate of the comet (Timar et al., 2017).

If the production rate of the comet is assumed to be constant during the passage of the CME the radius of the diamagnetic cavity can be calculated using the magnetometer measurements stated in Edberg et al. (2016b) and spacecraft-comet radius. In the initial conditions, with a measured magnetic field magnitude of 40 nT, a water production rate of \( 7 \times 10^{27} \) s\(^{-1} \) from Hansen et al. (2016), and a spacecraft-comet distance radius of 876 km this corresponds to a cavity extending 134 km from the nucleus. For magnetic field magnitudes of 60 and 100 nT and spacecraft-comet radii of 766 and 756 km for emission spikes 1 and 2 this corresponds to radii of 85 and 54 km, respectively.

These two different cavity radii probe regions of the coma with approximately 2.5 and 6 times the number density of neutrals at the original cavity radii, if a Hasić model of neutral distribution is assumed. When the higher density and energy electron population of the CME are coupled with the higher neutral density of the inner coma regions, the area most favored for dissociative electron impact emission
is a shell just outside of the diamagnetic cavity boundary. Taking into account the factor of 2.5-6 increase in neutral density, the factor of 6-10 higher electron flux from the CME, and the factor of 2-3 higher average electron energy we see the electron impact emission could be expected to increase between a factor of 10-20 over the quiescent values, depending on the emission spike and time of RPC observations (Edberg et al., 2016a). This increase is similar in magnitude to the spikes show in Figure 4.4.

The orientation of the Alice slit during this time period, parallel to the Sun-comet line and within a degree of the nucleus in the middle of the slit, means that even when the diamagnetic cavity was most compressed in emission spike 2 the line of sight for all rows still passed through the outer coma, through the diamagnetic cavity, and back into the outer coma on the other side. Throughout the CME impact the middle and upper rows of the detector would have captured these two boundary regions of the cavity, providing additional continuity to the observation pointing and geometry. This should allow the first order comparison done above to hold for these situations, but there are some caveats. The structure of the diamagnetic cavity has been shown to have sinusoidal heterogeneities in the structure (Goetz et al., 2016a; Henri et al., 2017), and it is possible that there were changes to the structure and radius of the diamagnetic cavity due to the CME.

The subsequent expansion of the diamagnetic cavity following the passage of the CME and a subsequent decrease in magnetic field magnitude could explain the smooth decline in O I 1356 Å emission. More simulation work is required to further explore this possibility, specifically with magnetohydrodynamic and hybrid modeling to properly constrain the behavior of the magnetic field lines near the nucleus in these direct CME impact cases.

**Lower Hybrid Waves**

Additional plasma physics could also contribute to the increase in dissociative electron impact emission. The lower hybrid waves observed in the plasma environment of 67P by the RPC instruments may have played a role. These waves, which are
the result of lower hybrid drift instabilities in the plasma, were observed by the Langmuir probe (LAP) on board *Rosetta* in October and November of 2015, approximately the same time post-perihelion as the CME impact (Karlsson et al., 2017). The ion and electron gradients that drive the instabilities creating lower hybrid waves are heavily influenced by interactions with the solar wind, so an energetic event like the CME could have drastically amplified the waves observed just a few weeks later by LAP. Lower hybrid waves are capable of heating the thermal electron population (5–10 eV) to energies above the threshold energy for electron impact emission (15–20 eV) (Karlsson et al., 2017; André et al., 2017). A boost to this super-threshold population from increased lower hybrid waves during the CME impact could explain the decoupling between the electron density and dissociative electron impact emission after the second emission spike shown in Figure 4.6, where it is clear that there is a divergence between the electrons measured by RPC and the impacting electron population along the Alice line of site.

4.5.2 *O*₂ in the Coma

The strong appearance of O I 1304 Å and O I 1356 Å emission in the spectra taken by Alice indicates that there is a substantial amount of O₂ present in the coma of 67P at the time of the CME impact, or introduced to the near-nucleus coma from an outburst. O₂/H₂O abundances calculated using Equations 4.1 and 4.2 on a sample of three spectra centered on the maxima of emission spikes 1 and 2 are shown in Table 4.3. The lower rows of the slit are not used in analysis due to the decreased dissociative electron impact emission observed there. The first emission spike has an average O₂/H₂O ratio of 0.14. The second emission spike has an average value of 0.08, just over half that of the first.

These calculated values show an O₂/H₂O relative abundance that ranges from two to five times that of the O₂/H₂O ratio of 0.038 found by Bieler et al. (2015) and below that of the O₂/H₂O ratio of ~ 0.22 found by Feldman et al. (2016) for several outbursts in 2015. This level of O₂ in the coma is not unique, however. Stellar appulse observations taken with Alice in 2015 show a range of 0.1 to 0.6 for
The drop in the relative abundance between the first and second emission spikes suggests a change to the coma composition in the hour and half between them, which may or may not be related to the CME. All cases suggest that the presence of O$_2$ at 67P is substantial, which requires mechanisms for trapping the highly volatile O$_2$ into ice and/or for forming O$_2$ through chemical pathways (Mousis et al., 2016; Taquet et al., 2016; Dulieu et al., 2017).

4.6 Summary

Based on the comparison between the IES measured electron densities, cross sections of water, carbon dioxide, and molecular oxygen and the observed line ratios for FUV spectra taken during the CME impact on 2015 October 5–6, we believe that substantial electron impact dissociation took place. Although the exact source of the increased emission cannot be specifically stated, the timing of the emission spikes matches the arrival of the electrons attributed to the CME. The unique electron environment allowed Alice to observe the near-nucleus coma environment in a way that had previously only affected a region within tens of km of the surface (Feldman et al., 2015b). Two emission spikes correlate to IES measurements of increased electron density, magnetometer measurements of increased magnetic field magnitudes, and have two different O$_2$/H$_2$O ratios, indicating change to the region affected by electron impact emission in the 90 minutes separating the spikes. The emission along the Alice line of sight decays over the next several hours back to the quiescent level following a steep drop in the warm electron density as measured by IES at the Rosetta spacecraft. The near nucleus environment experienced profound changes during the CME impact that resulted in the dominance of electron impact emission for the duration. This period of increased emission was used to calculate the O$_2$/H$_2$O abundance ratio, ranging from 0.06–0.16. This research supports the results of Bieler et al. (2015), who found that the levels of molecular oxygen are high enough to no longer fit current cometary formation models, and that the process that creates these reservoirs of molecular oxygen in the comet is still unknown.
However, the O$_2$/H$_2$O ratio in this event was several times higher than the result of Bieler et al. (2015). The O$_2$/H$_2$O ratio values found by this work are lower than the ratio found by Feldman et al. (2016) and agree with low impact parameter values from stellar appulse observations (Keeney et al., 2017).

4.7 Acknowledgements

The research presented here was made possible by the ESA/NASA Rosetta mission with contributions from ESA member states and NASA. The Alice team would like to acknowledge the support of NASA’s Jet Propulsion Laboratory, specifically through contract 1336850 to the Southwest Research Institute. Work at University of Oslo was supported by the Research Council of Norway grant No. 240000. We also want to thank our reviewer for their insightful feedback and edits. We would like to acknowledge ISSI for offering us the opportunity to have very valuable discussions on this topic as part of the International Team 'Plasma Environment of comet 67P after Rosetta (402)'.

CHAPTER 5

FUV Observations of the Inner Coma of 46P/Wirtanen

The contents of this chapter were originally published as “FUV Observations of the Inner Coma of 46P/Wirtanen” in The Planetary Science Journal, volume 2 Noonan et al. (2021b).

5.1 Introduction

Comets are frequently described as the well-preserved primitive remnants of our solar system’s formation, offering insight into the chemical abundances of their formation location in the protoplanetary disk. This assumption is based on the source regions for comets: the Kuiper-Edgeworth Belt for Jupiter-family comets (JFCs) and the Oort Cloud for long-period comets (LPCs), both of which have temperatures well below the sublimation point of common volatiles and should preserve the primordial ice abundances over billion year timescales (A’Hearn, 2011). Directly measuring the ice compositions of comet nuclei is nearly impossible, unless icy grains are lifted from the surface and can be studied (e.g. Protopapa et al. (2018)), and we are limited to investigating the emissions from gas in the coma produced by sublimating cometary ices. These emissions require modeling of the distribution of molecules and emission mechanisms in the coma to properly derive abundance of the parent molecules and tie them to nucleus properties (Combi et al., 2004). Far Ultraviolet (FUV) observations of cometary comae have been instrumental in characterizing the atomic budget of comets (Feldman et al., 2017; Bodewits et al., 2020), and provide a directly comparable metric to protoplanetary disks. However, our understanding of the physical processes that drive cometary emissions, and that are subsequently used to derive these primordial properties, is not yet complete. The European Space Agency’s Rosetta mission revealed the prevalence of dissociative electron impact in
the coma of 67P/Churyumov-Gerasimenko at heliocentric distances beyond 2.8 au in the near nucleus coma (≤ 100 km), which can produce different spectral signatures than the more commonly detected resonance fluorescence and photodissociation mechanisms, and thus affects interpretation of those observations (Feldman et al., 2015a; Bodewits et al., 2016). The presence of dissociative electron impact could allow detection of molecules which do not have emission features, like O₂, in the extreme inner coma, as it produces direct emission from dissociation of parent molecules with unique emission line ratios. However, the process was most consistent at large heliocentric distances, and was more related to transient events nearer perihelion. Such a process helped reveal the presence of faint water emissions from Europa attributed to a plume (Roth et al., 2017) and the presence of species that are difficult to detect via traditional photodissociation and fluorescence, as with O₂ on both Ganymede and Callisto (Hall et al., 1998; Cunningham et al., 2015). This discovery brought forth two particular questions: Is dissociative electron impact present in other comet comae? What local conditions need to be met to produce significant dissociative electron impact emissions?

The unique combination of extensive prior observation, substantial contemporaneous observation during the 2018-2019 close approach, and the ability to plan observations implementing the lessons learned from the Rosetta mission provided an unprecedented opportunity to characterize the atomic and molecular emissions of 46P in the FUV.

In this chapter we discuss observations of 46P/Wirtanen obtained January 9-20, 2019 with the Cosmic Origins Spectrograph (COS) on the Hubble Space Telescope (HST) between wavelengths of 900 and 1430 Å. In Section 5.2 we review the observing strategy, as well as the COS instrument and COS data reduction. The reduced spectra, derived column densities, and calculated production rates for assumed parent species are discussed in Section 5.3. Section 5.4 compares these results to previous apparitions of 46P as well as studies from the 2018-2019 apparition. Our conclusions are presented in Section 5.5.
Figure 5.1: Diagram showing approximate points of the COS aperture for each of the settings described in Table 5.1 relative to the coma of 46P. Each white circle represents the field-view-of the COS aperture subtended at $\Delta=0.22$ au and the radius of the full image is $12''$, approximately 1910 km. The background image is a simple Haser model for H$_2$O at $r_h = 1.18$ au, which was not observed in the COS bandpass, to provide context for the type of flux decrease that was expected if dissociative electron impact emission were present. The image is independent of production rate and thus has units of $s\, cm^{-2}$. The offset direction is not necessarily representative of the as-executed offset angle.
5.2 Observations

To access the same region of the FUV probed by the Rosetta Alice ultraviolet spectrograph (Stern et al., 2007) that escorted comet 67P/Churyumov-Gerasimenko for over two years we executed observations with the Cosmic Origins Spectrograph on the Hubble Space Telescope with the G130M grating (Green et al., 2012). For these FUV observations two separate cross delay line detector arrays are used, each with 16384 spectral and 1024 spatial pixels. Not all pixels are exposed to incoming light. The G130M grating provides a resolving power between $1.75-2.25 \times 10^4$ over the bandpass between 900 to 1430 Å. The narrow aperture of the COS instrument, 2.5” in diameter, allowed a discrete probing of the inner 1350 kilometers of 46P’s coma, as shown in Figure 5.1. Two instrument settings were used, one centered at 1096 Å and the other at 1291 Å for three pointings (centered, 2.5”, and 8” offsets) chosen to search for near-nucleus coma emissions and dissociative electron impact like those observed at 67P (Feldman et al., 2015a, 2016; Bodewits et al., 2016; Chaufray et al., 2017; Feldman et al., 2017), a transition zone near the collisionopause (Mandt et al., 2016), and a radius beyond the expected collisional zone where only photodissociation and prompt emission were expected. Spectra taken with a central wavelength of 1096 Å were able to capture wavelength ranges between 900 and 1230 Å in hopes to detect the strongest transitions of the Lyman series of hydrogen atoms in the coma: Lyman-α and -β, at 1215.72 and 1025.7 Å, respectively. Properties of each COS exposure from Guest Observer (GO) program 15625 (PI: D. Bodewits) are presented in Table 5.1.

For this set of observations it is important to note the low heliocentric velocity of 46P, varying between 7.70 and 9.9 km s$^{-1}$ (Table 5.1). This low velocity decreases the strength of the Swings effect (Swings, 1941), by which the redshift or blueshift of the solar spectrum relative to the comet can enhance or decrease atomic and molecular fluorescence efficiencies, and therefore limits variation of our calculated efficiencies from typical values at 1 au. For the wavelength range covered by the G130M spectral element (900 - 1430 Å), the feature that benefits the most from this effect is cometary
sulfur emission at 1425 Å, which is produced by resonance scattering of the solar S I feature by S atoms (Roettger et al., 1989a; Feldman et al., 2017), and thus increases the fluorescence efficiency, making it easier to detect. However, the low geocentric velocity makes it difficult to resolve any extended geocoronal emission contribution to the Lyman-α emission at 1215.6 Å (McCoy et al., 1992). We discuss our method of geocoronal emission subtraction in Section 5.2.1 and analysis of the line shape of Lyman-α in Section 5.3.

Observations were scheduled after the comet’s close approach between January 9 and 20 of 2019 to mitigate two factors. The first, and most pressing, was that HST would have difficulty tracking 46P with the accuracy required to keep the inner coma within the narrow aperture at close approach due to the high relative motion across the sky. By scheduling observations for a period when 46P was at a larger geocentric distance the on sky motion of the comet was within the HST maximum slew rate capability. The second issue lies with the characteristics of observing cometary comae; comets appear brightest when their coma are distant and therefore more concentrated on the sky. By observing the inner coma when the comet was just \( \sim 0.20 \) au away, much of the light from the extended coma is excluded, rendering the object relatively faint by typical spectroscopic standards, but significantly brighter than if observations had been conducted at 0.07 au at closest approach. This improved the acquisition likelihood as well as spectroscopic data.

We note that there are contemporaneous observations taken with the Space Telescope Imaging Spectrograph (STIS) in the same observing campaign (GO-15625 PI: D. Bodewits). These will be discussed in a separate publication (Venkataramani et al, in prep). All observations used in this publication are available in the Mikulksi Archive for Space Telescopes\(^1\).

\(^1\)https://archive.stsci.edu/
<table>
<thead>
<tr>
<th>Observation ID</th>
<th>Date (UTC)</th>
<th>Center Wavelength (Å)</th>
<th>Exposure Time (s)</th>
<th>Offset Angle (&quot;)</th>
<th>∆(^a,b) (AU)</th>
<th>Heliocentric Distance(^c) (AU)</th>
<th>Heliocentric Range-rate(^d) (km/s)</th>
<th>Offset Distance(^d) at 46P (km)</th>
</tr>
</thead>
<tbody>
<tr>
<td>ldx60901</td>
<td>2019-01-15 17:19:49</td>
<td>1096.0</td>
<td>1630.18</td>
<td>0</td>
<td>0.2</td>
<td>13.15</td>
<td>1.15</td>
<td>8.99</td>
</tr>
<tr>
<td>ldx61001</td>
<td>2019-01-16 13:57:17</td>
<td>1096.0</td>
<td>1630.21</td>
<td>0</td>
<td>0.21</td>
<td>13.07</td>
<td>1.15</td>
<td>9.17</td>
</tr>
<tr>
<td>ldx61101</td>
<td>2019-01-16 17:07:58</td>
<td>1096.0</td>
<td>1630.18</td>
<td>0</td>
<td>0.21</td>
<td>13.13</td>
<td>1.15</td>
<td>9.19</td>
</tr>
<tr>
<td>ldx61201</td>
<td>2019-01-17 13:48:50</td>
<td>1096.0</td>
<td>1630.18</td>
<td>0</td>
<td>0.22</td>
<td>13.9</td>
<td>1.16</td>
<td>9.36</td>
</tr>
<tr>
<td>ldx61010</td>
<td>2019-01-09 18:12:10</td>
<td>1291.0</td>
<td>1700.16</td>
<td>0</td>
<td>0.17</td>
<td>9.91</td>
<td>1.12</td>
<td>7.7</td>
</tr>
<tr>
<td>ldx62000</td>
<td>2019-01-10 21:24:45</td>
<td>1291.0</td>
<td>1660.19</td>
<td>0</td>
<td>0.18</td>
<td>11.64</td>
<td>1.13</td>
<td>7.96</td>
</tr>
<tr>
<td>ldx61301</td>
<td>2019-01-18 15:13:47</td>
<td>1096.0</td>
<td>1630.18</td>
<td>2.5</td>
<td>0.22</td>
<td>14.27</td>
<td>1.16</td>
<td>9.57</td>
</tr>
<tr>
<td>ldx61401</td>
<td>2019-01-13 11:14:44</td>
<td>1096.0</td>
<td>1630.21</td>
<td>2.5</td>
<td>0.19</td>
<td>11.37</td>
<td>1.14</td>
<td>8.52</td>
</tr>
<tr>
<td>ldx61501</td>
<td>2019-01-14 11:05:31</td>
<td>1096.0</td>
<td>1630.14</td>
<td>2.5</td>
<td>0.2</td>
<td>11.92</td>
<td>1.14</td>
<td>8.73</td>
</tr>
<tr>
<td>ldx61601</td>
<td>2019-01-14 07:54:47</td>
<td>1096.0</td>
<td>1630.18</td>
<td>2.5</td>
<td>0.2</td>
<td>11.85</td>
<td>1.14</td>
<td>8.71</td>
</tr>
<tr>
<td>ldx60301</td>
<td>2019-01-12 17:40:49</td>
<td>1291.0</td>
<td>1700.13</td>
<td>2.5</td>
<td>0.19</td>
<td>11.39</td>
<td>1.13</td>
<td>8.37</td>
</tr>
<tr>
<td>ldx60401</td>
<td>2019-01-16 10:45:23</td>
<td>1291.0</td>
<td>1700.16</td>
<td>2.5</td>
<td>0.21</td>
<td>12.84</td>
<td>1.15</td>
<td>9.14</td>
</tr>
<tr>
<td>ldx62901</td>
<td>2019-01-18 07:15:50</td>
<td>1096.0</td>
<td>1630.14</td>
<td>8</td>
<td>0.22</td>
<td>13.77</td>
<td>1.16</td>
<td>9.5</td>
</tr>
<tr>
<td>ldx63001</td>
<td>2019-01-18 16:49:10</td>
<td>1096.0</td>
<td>1630.18</td>
<td>8</td>
<td>0.23</td>
<td>14.49</td>
<td>1.17</td>
<td>9.87</td>
</tr>
<tr>
<td>ldx63101</td>
<td>2019-01-19 18:13:50</td>
<td>1096.0</td>
<td>1630.11</td>
<td>8</td>
<td>0.23</td>
<td>14.31</td>
<td>1.16</td>
<td>9.58</td>
</tr>
<tr>
<td>ldx63201</td>
<td>2019-01-20 08:30:41</td>
<td>1096.0</td>
<td>1630.11</td>
<td>8</td>
<td>0.23</td>
<td>14.31</td>
<td>1.16</td>
<td>9.89</td>
</tr>
<tr>
<td>ldx62501</td>
<td>2019-01-13 16:00:16</td>
<td>1291.0</td>
<td>1750.21</td>
<td>8</td>
<td>0.19</td>
<td>11.56</td>
<td>1.14</td>
<td>8.57</td>
</tr>
<tr>
<td>ldx62601</td>
<td>2019-01-15 07:44:32</td>
<td>1291.0</td>
<td>1750.14</td>
<td>8</td>
<td>0.2</td>
<td>12.43</td>
<td>1.15</td>
<td>8.91</td>
</tr>
</tbody>
</table>

Table 5.1: 46P/Wirtanen HST COS Observation Log

\(^a\) Queried from JPL Horizons

\(^b\) Geocentric Distance

\(^c\) Geocentric Range-rate

\(^d\) Observations with both identical instrument settings and offsets are co-added to create spectra presented in Figures 5.2 and 5.3
5.2.1 Data Reduction

All COS data were processed with the CALCOS pipeline before any further reduction (Rafelski, 2018). The CALCOS pipeline accounts for flatfield correction, pulse height filtering, geometric correction, thermal corrections, and flux calibrations of raw COS spectra. Following the CALCOS reduction each individual spectrum had a scaled airglow spectrum subtracted. Attempts were made to scale this spectrum by average angle to Earth-horizon, but ultimately given the non-detection of N I 1200 Å, which was the benchmark for the importance of airglow and geocorona features, the integrated flux between 1198 and 1202 Å was used to scale an averaged airglow spectrum which was then subtracted from each x1dsum spectrum before any coaddition. Airglow spectra were obtained from the HST COS deliberate airglow observation page\(^2\).

For emission features with such large signal-to-noise ratios in individual spectra we can extract integrated line brightnesses from those calibrated spectra. To search for emission features that may have emissions too faint to observe in the original COS data we can both bin the spectrum and co-add spectra with the same location relative to the nucleus. Binned and co-added spectra are shown in Figures 5.2 and 5.3, while the high signal-to-noise co-added but unbinned Lyman-\(\alpha\) and O I 1302 Å triplet emissions are shown in Figures 5.4, 5.5, and 5.6.

All spectral fluxes recorded by the CALCOS pipeline are in units of ergs cm\(^{-2}\) Å\(^{-1}\) s\(^{-1}\) and are converted to units of Rayleighs, a surface brightness unit useful for extended objects. One Rayleigh corresponds to 10\(^6\) photons cm\(^{-2}\) s\(^{-1}\) sr\(^{-1}\), so a conversion function is used to convert the COS spectral data first from an energy flux in ergs to a photon flux based on photon energy, then to a surface brightness. This is done via the equation

\[
B(R) = \left(\frac{4\pi}{10^6}\right)\Omega F \tag{5.1}
\]

where \(\Omega\) is the solid angle of the COS aperture in steradians, 1.84×10\(^{-9}\) sr, and \(F\) is the flux from the object in photons cm\(^{-2}\) s\(^{-1}\) Å\(^{-1}\).

\(^2\)https://www.stsci.edu/hst/instrumentation/cos/calibration/airglow
5.3 Results

5.3.1 Spectra

Co-added spectra for each pointing offset and wavelength setting are presented in Figures 5.2 and 5.3. We strongly detect the emission features of three atomic species in these data: H (1215.7 and 1025.7 Å), O (1302 Å triplet), and S (1425 Å).

Lyman-α has been used frequently to measure the hydrogen coma from observations with much larger fields of view than HST COS (degrees as opposed to arcseconds) and is a powerful diagnostic for determining the water production rates of comets (McCoy et al., 1992; Combi and Feldman, 1992; Combi et al., 1998, 2019; Mayyasi et al., 2020; Combi et al., 2020). While the Lyman-β transition was detected in our coadded spectra, it was at a much lower significance due to increased detector noise blueward of 1100 Å. Lyman-α is very strong but proper interpretation of the brightness requires modeling the distribution and radiative transfer of H atoms in the inner coma. The minimal geocoronal contribution is due to the fortunate observing geometry for 46P’s apparition, which required nightside observations for HST, and the narrow Field of View (FOV) of the COS instrument. Similarly, the ecliptic longitude and latitude of 46P placed it in the ”downwind” interstellar direction, which has a low IPM contribution to the Lyman-α emission of between 300 and 400 Rayleighs (Pryor et al., 2013). A high resolution profile of the Lyman-α emission is shown in Figure 5.4 for each co-added pointing offset, and shows the dominance of cometary hydrogen emissions for the COS observations, with only minor contributions from both the Earth’s geocorona and the interplanetary medium in this particular dataset relative to the brightness of the coma. Emission from the 2-1 transition of deuterium at 1215.33 Å is not clearly present when subtracting off a best fit gaussian (Fig. 5.5). We note that the Lyman-α profile of both the airglow and cometary emissions is poorly fit by both Cauchy-Lorentzian and Voigt profiles, and is instead best characterized with a Gaussian profile with a σ between 0.36-0.38 Å, corresponding to a velocity of 83-87.5 km/s. This is much larger than the expected velocities of H atoms in the inner coma (8-26 km/s) (Combi et al., 2004),
and is therefore the limiting resolution of our observations and not indicative of the actual emission profile. The Gaussian fit overpredicts flux at the peak of the emission feature by a small amount and underpredicts flux on the wings but the effect is nearly symmetric, making it difficult to detect deuterium emissions or the IPM contribution directly. We note that this is larger than the expected line spread function of the COS instrument, due to the aperture filling observations of the comet. The $3\sigma$ resolution of the filled COS aperture is measured to be $\sim 1\,\text{Å}$ in our spectra, similar to previous cometary COS observations and airglow measurements.

The atomic oxygen triplet emission at 1302, 1304, and 1306 Å has an excellent signal-to-noise ratio for all pointings. The spectral resolution provided by the G130M element from COS allows this triplet to be completely resolved (Fig. 5.6). With no clear evidence of self absorption in the O I triplet via inversion at the emission peaks nor redistribution of flux from the stronger O I 1302 Å feature to other features that would indicate significant optical thickness in the atomic oxygen coma, it is reasonable to allow discussion of the diagnostic potential of the O I triplet in Section 5.4.

The last strongly detected atomic emission feature is the triplet of atomic sulfur around 1425 Å in our data, shown in Figure 5.7. As described in Section 5.2 the strength of this feature is enhanced by the low heliocentric velocity of 46P, increasing the fluorescence efficiency of the cometary sulfur from the solar sulfur emission feature.

We note that several atomic and molecular features often observed in cometary FUV spectra (Weaver et al., 1981; Feldman et al., 2018b, 2017) were not detected; we do not see any evidence of the C I 1277 or C II 1335 Å emission that could indicate either dissociative electron impact emission of CO$_2$ or CO, or from reflected sunlight from the near-nucleus dust or the nucleus itself. This non-detection is supported by the lack of CO Fourth Positive Group emissions between 1350 - 1430 Å which produces a number of features that would be identifiable in our wavelength range (Fig. 5.8) (Lupu et al., 2007; Bodewits et al., 2020). Another notable absentee in particular is N I 1200 Å emission, which would have implied significant contribution
Figure 5.2: Co-added spectra with 39 pixel binning to improve signal in emission features with low flux, specifically Lyman-β near 1026 Å. Note that only Lyman-α at 1215.7 Å, is easily identifiable. An enlarged high resolution profile of Lyman-α is presented in Figure 5.4.

of airglow emissions to the spectrum.

5.3.2 Coma Emission Modeling

For each observed atomic emission feature we calculate the heliocentric velocity dependent fluorescence efficiency, or g-factor, from the Einstein coefficients, oscillator strengths, and energy levels available through the National Institutes of Standards and Technology Atomic Spectra Database\(^3\) (Kramida et al., 2019). To properly account for the solar emission feature shapes we implement the high-resolution SUMER spectrum from Curdt et al. (2001), available through the BASS200 archive\(^4\). The high resolution spectrum is in relative flux units, normalized to solar emission at 680 Å. The solar spectrum from each day is then determined by multiplying the

\(^3\)https://www.nist.gov/pml/atomic-spectra-database
Figure 5.3: Co-added spectra with 13 pixel binning to improve signal in emission features with low flux. In addition to Lyman-α emissions at 1215.7 Å the O I 1302 Å multiplet is easily identified and presented in Figure 5.6. With the exception of S I 1425 Å, shown enlarged in Figure 5.7, no other significant atomic or molecular emissions were identified.
Figure 5.4: Profile of the Lyman-α emission for each co-added pointing and central wavelength setting with no binning applied. The contribution of geocoronal and interplanetary hydrogen emission to the cometary spectrum is relatively constant for each offset and is minimal, if not negligible.

daily averaged flux from the TIMED-SEE instrument (Woods et al., 1998, 2000)\(^5\) for a given day of observations at 680 Å by the SUMER-averaged relative spectrum to produce a high resolution (~0.01 Å) solar spectrum for calculating g-factors. Solar flux is integrated over a bin ±0.7 Å of the red/blueshifted transition wavelength and the g-factor calculated in accordance with Equation 3 in Feldman et al. (2004).

Once g-factors have been calculated for the detected atomic emission features, average column densities can be retrieved from the measured brightnesses. This is done via the equation:

\[
\bar{N}_a = \frac{(10^6 B_i)}{g_i} \quad (5.2)
\]

where \(\bar{N}_a\) is the atomic column density in molecules cm\(^{-2}\), \(B_i\) is the integrated brightness of feature in Rayleighs, and \(g_i\) is the g-factor of the atomic transition in phs s\(^{-1}\) molecule\(^{-1}\). Once a column density has been found for the COS aperture, we can attempt to find the production rates of the likely parent molecules for

\(^5\)Available at [https://www.lasp.colorado.edu/lisird/data/timed_see_ssi_l3/](https://www.lasp.colorado.edu/lisird/data/timed_see_ssi_l3/)
Figure 5.5: Profile of the Lyman-α emission for the two comet-centered co-added spectra and central wavelength setting with no binning applied. A gaussian fit to the data is plotted and the residuals resulting from subtracting the model from the data are plotted below.
Figure 5.6: Enlarged section of Figure 5.3 to show O I triplet emission between 1302 and 1306 Å. This spectrum has only been binned by a factor of 3 to show line profiles and relative shapes.
Figure 5.7: Enlarged section of Figure 5.3 to show S I 1425 Å emission.

Figure 5.8: Enlarged section of Figure 5.3 with 13-pixel binning to show lack of CO Fourth Positive Group emissions between 1350 and 1420 Å. CO emission features at 1368, 1384, 1392, and 1420 Å are absent.
each atomic species by running the two- or three component Haser model for each observation’s timestamp heliocentric and geocentric distance.

\[ Q_n = \frac{\bar{N}_a(\pi \rho^2)}{H(r_h, \Delta)} \]  

(5.3)

where \( Q_n \) is the neutral production rate, \( \rho \) is the radius that the COS aperture subtends at the comet in cm, and \( H(r_h, r_\delta) \) is the two- or three-component Haser model result integrated as a function of heliocentric and geocentric distance of 46P for the subtended size of the COS aperture at 46P. By multiplying the average column density by the aperture area the total number of molecules in the field can be found for the numerator. The Haser model is numerically integrated along the line of sight for a range of aperture radii, which are then summed to produce a result with units of s, as it has not been multiplied by a production rate. Production rates for likely parent molecules were calculated using two- and three-component Haser models (Haser, 1957; Festou, 1981). Given the small area subtended by the COS aperture at the distance of 46P/Wirtanen, which is only slightly larger than the collisional radius for the outflowing neutrals (~300 km, Eq. 5 of Festou (1981)), we only used these models for the 0” pointing observations. Lifetimes for \( \text{H}_2\text{O}, \text{H}_2\text{S}, \text{CS}_2, \text{and S}_2 \) were taken from Huebner and Mukherjee (2015), Meier and A’Hearn (1997), and A’Hearn et al. (1983) for solar minimum. The velocity for water was assumed to follow the 0.85\( r_h^{-2} \) km s\(^{-1} \) relation from Combi et al. (2004), while the sulfur bearing molecules and atoms were given initial velocities of 0.59\( r_h^{-2} \) km s\(^{-1} \) from Jackson et al. (1986). We note that for the velocity of \( \text{OH} \) resulting from dissociation of \( \text{H}_2\text{O} \) we use the velocity of 1.33 km s\(^{-1} \) found by Fink and Combi (2004) specifically for 46P/Wirtanen. Velocities of atomic H were set to 18 km s\(^{-1} \), atomic O 1.33 km s\(^{-1} \), and atomic S to 1 km s\(^{-1} \).

None of our model runs were able to produce reasonable production rates for parent molecules, often reaching values 10-20\( \times \) that of Combi et al. (2020). A well known issue with the Haser model is its difficulty in reaching high enough column densities near the nucleus (Festou, 1981), so this is rather unsurprising. Similar attempts were made with a vectorial model for H using the publicly available Web
Vectorial Model\(^6\), and a similar over estimation of the water production rates found. However, the web vectorial model accurately describes the OH column densities observed in the STIS data, so this issue is likely limited to the narrow COS aperture. For this reason we are unable to accurately produce parent molecule abundances from this dataset at this time, and further work is necessary. Therefore, we will limit our analysis to the atomic column densities and production rates.

\(^6\)https://www.boulder.swri.edu/wvm//
<table>
<thead>
<tr>
<th>Observation ID</th>
<th>Geocentric Distance (au)</th>
<th>Offset Angle (&quot;')</th>
<th>$N_H$ (mol cm$^{-2}$)$^a$</th>
<th>$N_O$ (mol cm$^{-2}$)$^b$</th>
<th>$N_S$ (mol cm$^{-2}$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>ldx60101</td>
<td>0.1691</td>
<td>0.0</td>
<td>1.62e+13</td>
<td>4.62e+13</td>
<td>1.27e+14</td>
</tr>
<tr>
<td>ldx60201</td>
<td>0.1756</td>
<td>0.0</td>
<td>3.74e+13</td>
<td>1.47e+14</td>
<td>2.23e+14</td>
</tr>
<tr>
<td>ldx60301</td>
<td>0.1865</td>
<td>2.5</td>
<td>1.94e+13</td>
<td>5.73e+13</td>
<td>1.12e+14</td>
</tr>
<tr>
<td>ldx60401</td>
<td>0.2089</td>
<td>2.5</td>
<td>2.04e+13</td>
<td>3.79e+13</td>
<td>2.16e+14</td>
</tr>
<tr>
<td>ldx60901</td>
<td>0.2159</td>
<td>0.0</td>
<td>3.61e+13</td>
<td>N/A</td>
<td>N/A</td>
</tr>
<tr>
<td>ldx61001</td>
<td>0.2106</td>
<td>0.0</td>
<td>3.66e+13</td>
<td>N/A</td>
<td>N/A</td>
</tr>
<tr>
<td>ldx61101</td>
<td>0.2097</td>
<td>0.0</td>
<td>3.56e+13</td>
<td>N/A</td>
<td>N/A</td>
</tr>
<tr>
<td>ldx61201</td>
<td>0.2205</td>
<td>8.0</td>
<td>2.94e+13</td>
<td>N/A</td>
<td>N/A</td>
</tr>
<tr>
<td>ldx61301</td>
<td>0.192</td>
<td>8.0</td>
<td>1.38e+13</td>
<td>2.63e+13</td>
<td>1.39e+13</td>
</tr>
<tr>
<td>ldx61401</td>
<td>0.1908</td>
<td>2.5</td>
<td>3.11e+13</td>
<td>N/A</td>
<td>N/A</td>
</tr>
<tr>
<td>ldx61501</td>
<td>0.196</td>
<td>2.5</td>
<td>3.31e+13</td>
<td>N/A</td>
<td>N/A</td>
</tr>
<tr>
<td>ldx61601</td>
<td>0.1968</td>
<td>2.5</td>
<td>3.20e+13</td>
<td>N/A</td>
<td>N/A</td>
</tr>
<tr>
<td>ldx62501</td>
<td>0.202</td>
<td>8.0</td>
<td>1.95e+13</td>
<td>3.84e+13</td>
<td>8.18e+13</td>
</tr>
<tr>
<td>ldx62601</td>
<td>0.2226</td>
<td>2.5</td>
<td>3.53e+13</td>
<td>N/A</td>
<td>N/A</td>
</tr>
<tr>
<td>ldx62901</td>
<td>0.2045</td>
<td>0.0</td>
<td>4.10e+13</td>
<td>N/A</td>
<td>N/A</td>
</tr>
<tr>
<td>ldx63001</td>
<td>0.223</td>
<td>8.0</td>
<td>3.16e+13</td>
<td>N/A</td>
<td>N/A</td>
</tr>
<tr>
<td>ldx63101</td>
<td>0.2297</td>
<td>8.0</td>
<td>2.72e+13</td>
<td>N/A</td>
<td>N/A</td>
</tr>
<tr>
<td>ldx63201</td>
<td>0.2336</td>
<td>8.0</td>
<td>2.86e+13</td>
<td>N/A</td>
<td>N/A</td>
</tr>
</tbody>
</table>

Table 5.2: Derived column densities for H, O, and S in the near-nucleus coma of 46P/Wirtanen from COS data taken between January 8 and 20, 2019.

$^a$ 1-$\sigma$ error bars on the column densities are dominated by variability in the solar flux and are placed at 30% of each value.

$^b$ Values for $N_O$ and $N_S$ are listed as N/A when the O I and S I emissions were not captured in the CENWAVE 1096 spectra.
5.4 Discussion

Due to the higher than expected activity of 46P in past apparitions, it may be suggested that 46P could be analogous to 103P/Hartley 2, where CO$_2$ gas drove out large amounts of water ice grains which resulted in water production rates that exceeded what was expected if water was released by the surface of the comet alone (Bertaux et al., 1999; Fink and Combi, 2004; A’Hearn et al., 2011; Kelley et al., 2013; Protopapa et al., 2014; Combi et al., 2019; Lis et al., 2019). These icy grains are short lived ($\sim 10^4$ s at 1 au) and therefore likely to sublimate throughout the COS aperture for each of the pointings if present in the coma of 46P (Yang et al., 2009, 2014; Protopapa et al., 2018). The close approach to Earth of 46P/Wirtanen in December 2018 just over two years after the end of the Rosetta mission offered a timely opportunity to investigate this question, as well as probe the electron impact plasma environment. Comet 46P/Wirtanen was the primary target of the Rosetta mission before a launch delay necessitated changing the target to comet 67P/Churyumov-Gerasimenko. As such, there is a substantial amount of literature dedicated to 46P published between 1996 and 2004 regarding the activity and volatile abundances in previous apparitions. In contrast to 67P, which had a relatively low water production rate for its size ($3 \times 4 \times 5$ km (Sierks et al., 2015)) of 5-7 $\times 10^{27}$ s$^{-1}$ (Hansen et al., 2016), 46P has been more active than expected for its relatively small size ($r=0.63$ km$^7$), (Lamy et al., 1998; Lis et al., 2019), with peak water production rates between 0.7-5 $\times 10^{28}$ s$^{-1}$ (Groussin and Lamy, 2003; Groussin et al., 2007; Kobayashi and Kawakita, 2010; Combi et al., 2020). The chemical compositions of the two comae are exceedingly different as well; while the coma of 67P was shown to contain significant levels of CO$_2$ and CO (Bockelée-Morvan et al., 2016; Feldman et al., 2017), neither molecule has been directly detected in 46P’s coma despite detections of CO$_2^+$ in UV spectra from 1998 (Stern et al., 1998; Altwegg et al., 1999) and observations of the same mid-UV bandpass in Venkataramani et al. (in prep). A summary of production rates for common cometary species previously measured in

https://news.arizona.edu/story/ua-researcher-captures-rare-radar-images-comet-46pwirtanen
Table 5.3: Measured production rates of common volatiles for 46P/Wirtanen during previous apparitions. References are 1) Fink et al. (1998), 2) Schulz et al. (1998), 3) Farnham and Schleicher (1998), 4) Altwegg et al. (1999), and 5) Stern et al. (1998).

<table>
<thead>
<tr>
<th>Species</th>
<th>Production Rate(s) (10^{27}) mol s(^{-1})</th>
<th>Dates</th>
<th>Refs</th>
</tr>
</thead>
<tbody>
<tr>
<td>H(_2)O</td>
<td>3-50</td>
<td>1998,2008</td>
<td>1,2,3,4,5</td>
</tr>
<tr>
<td>CN</td>
<td>0.00069 - 0.039</td>
<td>1998</td>
<td>1,2,3,4</td>
</tr>
<tr>
<td>C(_2)</td>
<td>0.0005 - 0.065</td>
<td>1998</td>
<td>1,2,3,4</td>
</tr>
<tr>
<td>CS(_2)</td>
<td>0.02</td>
<td>1998</td>
<td>5</td>
</tr>
</tbody>
</table>

the coma of 46P/Wirtanen is given in Table 5.3. Given the previously known differences between the two comets it’s intriguing to find that close examination of our FUV spectra yield even more discrepancies between them. The measured spectra of 46P are noticeably devoid of many of the emission features observed by the Alice ultraviolet spectrograph in the inner coma of 67P/Churyumov-Gerasimenko (Feldman et al., 2016, 2017) or those reported in the review of COS comet observations by Feldman et al. (2018b). We focus the discussion here on the Lyman \(\alpha\), O I triplet, and S I 1425 Å emissions and what they indicate about our models of the near-nucleus emissions as well as the implications for future observations. We note that our observations only overlap with the four comets reported in Feldman et al. (2018b) between 1400 and 1430 Å in this particular paper, limiting comparison to atomic sulfur and CO abundances.

5.4.1 Upper limits on CO Abundance

The non-detection of the CO Fourth Positive group emissions between 1350 and 1420 Å allows us to place an upper limit on both the column density and production rate of carbon monoxide (Fig. 5.8). Using wavelengths, Einstein coefficients, and oscillator strengths for the first seven vibrational transitions from Morton and Noreau (1994) and Beegle et al. (1999) we calculate a total fluorescence efficiency for the (4-0) band of \(1.44\times10^{-7}\) phs s\(^{-1}\) for the average heliocentric distances and velocities for the comet-centered pointings (Table 5.1). Given observational sensi-
tivities down to 1 Rayleigh for the integrated band wavelength range between 1419 and 1421 Å, we can then calculate an upper limit for the average column density of CO within the COS aperture using Equation 5.2. We find that our observations were sensitive to $\bar{N}_{CO}$ of $6.9 \times 10^{12}$ cm$^2$. Due to the high spatial resolution of the observations we follow the same model for production of CO as Weaver et al. (2011). This model argues that the long lifetime of CO at 1 AU of $1.5 \times 10^6$ s can be ignored and the production rate derived from $Q = N_{CO}vd$, where $v$ is the velocity of CO molecules and $d$ is the diameter of the COS aperture in cm at 46P. Using the same $v$ of $7.8 \times 10^4$ cm s$^{-1}$ as Weaver et al. (2011) and a $d$ of $3.37 \times 10^7$ cm we place an upper limit on the total production rate of CO at $1.8 \times 10^{25}$ mol s$^{-1}$. This upper limit is near the production rate measured for 103P/Hartley 2 by Weaver et al. (2011). Taking into account the 30% error on these g-factors, this would put the 3-σ upper limit for the CO/H$_2$O ratio for the period of our observations at $<8 \times 10^{-2}$. This upper limit would place 46P/Wirtanen in the middle of the range of CO/H$_2$O values in Biver and Bockelée-Morvan (2019).

5.4.2 Upper limits on dissociative electron impact emission

The lack of any O I 1356 Å is a robust indicator that dissociative electron impact is not a significant source of emissions for the inner coma of 46P. Sampling the noise in the co-added spectra near the expected O I 1356 Å feature shows that we were sensitive to approximately 1 Rayleigh integrated over the 1352-1358 Å region. Our calculations for the emission rate of O$_2$ and H$_2$O, from Kanik et al. (2003) and Makarov et al. (2004), respectively, show that for an expected Maxwellian electron distribution characterized by a temperature of 25 eV and an electron density of 50 electrons cm$^{-3}$ the COS co-added spectrum brightness upper limit translates to a column density of $\sim4 \times 10^{14}$ cm$^{-2}$ for O$_2$ and $\sim4 \times 10^{16}$ cm$^{-2}$ for H$_2$O. If dissociative electron impact occurs in the near nucleus coma the total affected column of either molecule must be less than either of these stated values. We note that this upper limit for the O$_2$ column density is of similar magnitude to the column densities of O$_2$ detected by the Alice ultraviolet spectrograph onboard the Rosetta mission, but
was acquired over a much larger FOV subtended at the comet (Noonan et al, in prep.). With observations sensitive down to 0.1 R/Å, this means that the portion of the inner coma of 46P susceptible to large scale dissociative electron impact (d_c < \sim 50 \text{ km}) could not have had a total integrated brightness greater than 1 R. This strongly implies that dissociative electron impact in the inner coma is unobservable from HST even with an extremely favorable apparition. The relevant scale is simply too small to be captured adequately, even with a 2.5” FOV and a low geocentric distance.

5.4.3 Atomic emission

Given the robust detections of three atomic emission features we investigate the properties available from each.

Lyman-α emissions

Emission from the 2-1 transition of the hydrogen atom is easy to detect but often difficult to analyze, especially on small spatial scales. Line profiles of the Lyman-α emission from each of the co-added spectra show deviation from standard Voigt profiles, indicating the presence of effects from optically thick column densities near the nucleus convolved with the line spread function of the COS instrument at 1215 Å. We do not detect the deuterium 2-1 electron transition (rest wavelength 1215.33 Å) due to the \sim 1 Å resolution of the COS data from which a direct D/H ratio could be calculated. However, we can place an upper limit on the abundance of deuterium by subtracting a best fit gaussian profile from the Lyman-α emission and summing the remaining emission between 1215.0 and 1215.7 Å to find integrated brightnesses between 68 and 330 R for the co-added spectra. Given the similar g-factors for the D (1-0) transition and the H (1-0) transition, this corresponds to an upper limit on deuterium column density abundance between 0.29 and 1.43 \times 10^{11} \text{ cm}^2, for a conservative upper limit on the D/H ratio of 46P/Wirtanen of 0.005, approximately an order of magnitude larger than is typical for Jupiter family comets and measured
for 46P/Wirtanen (Altwegg et al., 2015; Lis et al., 2019). A more involved effort to model the emission profile of Lyman-\(\alpha\) emission will be attempted in future work.

Deriving a water production rate from the Lyman-\(\beta\) emission is useful to compare with the near daily water production rates calculated by Combi et al. (2020) for the 2018-2019 apparition of 46P/Wirtanen. Finding integrated brightnesses of the Lyman-\(\beta\) feature in coadded spectra, between 65 and 170 Rayleighs, and the associated calculated g-factor between \(5.0-5.33 \times 10^{-6} \text{ s}^{-1}\), allows us to calculate aperture averaged hydrogen column densities between 1.2 and 3.2 \(\times 10^{13} \text{ cm}^2\). These column densities are in agreement with those derived from Lyman-\(\alpha\), but our two- and three-component Haser models have difficulty matching these column densities. Combi et al. (2020) use the Solor Wind ANisotropies (SWAN) instrument and a more involved physical model of the H atom distribution, in addition to large coma images within 8 degrees of the nucleus; here we are specifically focusing on the coma within 2.5” of the nucleus, a radius that is approximately 23,000 times smaller. We recognize that the two-component Haser model will not accurately represent the environment within the \(\sim\)340 km diameter aperture of COS at 46P/Wirtanen, and a simple model was unable to produce production rates within the uncertainty range of the values reported in Combi et al. (2020). This discrepancy discourages us from using the Haser model for the offset pointings; a hybrid model is required to properly analyze both the emission feature profile and spatial profiles and will be described in a future publication.

O I 1302 Å triplet emissions

The O I resonance triplet is resolved here for the first time in a cometary coma, offering insight into the interplay between collisional- and photo-excitation of fragment species. As illustrated in Fig. 5.6 each individual transition from \(^3S^0\) to the \(^3P_{J=2,1,0}\) states is resolved at wavelengths of 1302.2, 1304.9, and 1306.0 Å. One expects the contribution of each transition to the total triplet emission (e.g. \(\frac{F_{1302}}{F_{1302}+F_{1304}+F_{1306}}\)) to follow the ratios between known Einstein \(A\)-values of the three transitions. However, this does not seem to be the case for the O I \(^3S_1\) triplet emission observed.
in the inner coma of 46P. For co-added spectra at each of the three pointing angle offsets the normalized ratio of each transition feature was determined and is shown in Figure 5.9. Both the contribution of the $^3S_1$ to $^3P_2$ (1302 Å) and $^3S_1$ to $^3P_0$ (1306 Å) transitions increase at offset 2.5”, with the 1302 Å line further increasing at 8” offset. Interestingly, the largest deviation from the expected triplet contribution is for the 1302 Å transition to ground. Both 1304 and 1306 Å transitions decay to the metastable $^3P_1$ and $^3P_0$ levels, with the largest deviations seen between the 0” and 8” offsets. All three transitions have $A$ values in order $10^7 - 10^8$ s$^{-1}$ (Kramida et al., 2019), leading to a lifetime around 1.6 ns, indicating that travel and de-excitation of O I outside the FOV contributes negligibly to the observed ratios. Additionally, uncertainty in the $A$ values cannot be the cause; the $A$ values for the O I triplet lines are known to within $\sim$3% (Kramida et al., 2019). In all cases, the uncertainty in the intensity changes is considerably less than the observed change in contribution.

We investigated the possibility that the O I triplet features may contain contributions from the increasing density of S atoms, which have electronic transitions from the $^3P^o$ to the $^3P$ state and have a series of emissions present between 1302 and 1308 Å. We find the g-factor for the strongest S I transitions between 1302 and 1305 Å to be $\sim$1.1×10$^{-8}$ s$^{-1}$ for the dates in question, and using the atomic sulfur column density calculated from the S I 1425 Å emission of $\sim$1.7×10$^{13}$ cm$^{-2}$ we find that less than 0.1 Rayleighs can be attributed to S I emission in the 1302-1306 Å region.

We note that the line shape of the O I triplets is well fit by Gaussian rather than Voigt profiles, with $\sigma = 0.33 - 0.35$ Å, in the co-added spectra in Figure 5.6. The goodness of fit with Gaussian profiles is not unexpected given that the O coma is an extended source. There is no clear evidence that would indicate that the O I transitions are optically thick.

Assuming a water production rate of $\sim$ 7×10$^{27}$ mol. s$^{-1}$, the density of molecules in our FOV (100s km from the nucleus) is in order 7×10$^{17}$ m$^{-3}$. Assuming a collisional cross section in order 10$^{-15}$ cm$^{-2}$, the mean free path $\lambda_{MFP} = 1/\sigma \rho$ between collisions is $\sim$3 mm. The collisional frequency, $\nu = v_{rms}/\lambda_{MFP}$, is then found from
the root-mean-square velocity of the gas and the local mean free path. Assuming an O I gas temperature of 100 K yields \( v_{\text{rms}} \sim 220 \, \text{m/s} \), from which the collisional rate in the near coma follows as \( \sim 7.6 \times 10^4 \, \text{s}^{-1} \). Thus, following population of the \( ^3S_0 \) state, the collisional frequency is too small by 5 - 6 orders of magnitude to begin contributing via collisional de-excitation, indicating that collisional effects are insufficient for explaining the triplet ratios.

An alternative explanation for the triplet emission contributions may be the incident solar radiation, with stimulated emission enhancing the observed line intensities. The assumed incident solar flux from SUMER (see Sec. 5.3.2) at the O I triplet wavelengths is approximately 1:1:1 between the 3 triplet lines, which suggests negligible contributions of heterogenous stimulated emission from \( ^3S_1 \). However, there is extensive literature on understanding O I triplet emission in the solar spectrum, including detailed radiative transfer models of O I resonance line excitation (Bhatia and Kastner, 1995) and (Carlsson and Judge, 1993) (who also found non-Voigt line profiles), polarization (Anusha et al., 2014), and frequency cross redistribution effects (Miller-Ricci and Uitenbroek, 2002). Our co-added spectra were observed over a period of 9 days, during which it may be possible that changes in the solar spectrum preferentially enhanced the 1302 Å emission, though this proposition conflicts with the SUMER solar spectra. Given the negligible contribution from collisional effects, the most likely cause of the deviations in relative triplet emission intensities (Fig. 5.9) is the incident solar flux. As these lines are also sensitive diagnostics at the source of the O I solar flux, one can expect similar diagnostic potential when observed in an O-rich environment such as cometary comae. In particular, these lines may offer an additional way to distinguish between photon- and electron-dominated environments in future observations.

Understanding atomic oxygen emissions and its implications for high resolution spectroscopy of the near-nucleus coma are a critical component for improving the scientific return from comet spectroscopy. Given the observed differences in O I triplet emission with offset angle, these transitions may prove to be useful diagnostics of the conditions in the inner coma. At present, developing a time-dependent atomic
model of the incident solar radiation producing $^3S_1 \rightarrow ^3P_J=0,1,2$ emission is beyond the scope of this work. Further studies of the O I transitions in the near- and extended-comae of comets is required to fully understand the diagnostic potential of these lines.

**S I 1425 Å emissions**

The detection of S I 1425 Å emission was unexpected given the narrow FOV (Figure 5.7). Such a detection was possible because of the relatively low heliocentric velocity of 46P/Wirtanen during the observations, enabling efficient resonance scattering of the solar S I feature (Roettger et al., 1989b; Feldman et al., 2018b). Our derived column densities for atomic sulfur in 46P in Table 5.2 are similar to those derived by Feldman et al. (2018b) for both C/2014 Q2 (Lovejoy) and 153P/Ikeya-Zhang, which were measured to have $N_S$ of 1.2 and $2.0 \times 10^{14}$ cm$^{-2}$, respectively. Given the high abundance of S in the inner nucleus it is necessary to identify potential parent molecules from the nucleus.

A favorite parent molecule for cometary atomic sulfur is S$_2$, due to both its short lifetime and single atomic components (A’Hearn et al., 1983; Meier and A’Hearn, 1997). For production rates on the order of $10^{25}$ mol s$^{-1}$ the S$_2$ band emission between 2800-3100 Å should be easily detectable (A’Hearn et al., 1983). Therefore, the lack of S$_2$ band emission in STIS observations taken as part of the same campaign (Venkataramani et al., 2020, in prep) suggests that consideration of CS$_2$ is a reasonable source of S I 1425 Å emission, via photodissociation into CS and S, is necessary. CS$_2$ has a relatively short lifetime of 590 s (Jackson et al., 1986) compared to the 82000 s lifetime of H$_2$O (Combi et al., 2004), and is just approximately 150 s longer than that of S$_2$ (Meier and A’Hearn, 1997). However, the previously measured CS$_2$ production rates between $2-5 \times 10^{-2}$ that of H$_2$O (Stern et al., 1998), and a similar measurement of CS production rates $1-2 \times 10^{-2}$ that of H$_2$O from the concurrent STIS observations (Venkataramani et al., in prep) are insufficient to explain the observed abundance of atomic sulfur in the observations. Other molecules identified in Feldman et al. (2018b) like H$_2$S and SO$_2$ could also contribute to the atomic sulfur
Figure 5.9: Normalized ratio of O I triplet emission at 1302, 1304, and 1306 Å for co-added spectra at each pointing offset in arcseconds. In general the O $^3S^0$ J=2 to the O $^3P$ J=1 transition at 1302 Å becomes more populated as the offset increases, but the line ratios are never in good agreement with the ratios defined by the known $A$ values (Kramida et al., 2019). The expected ratios for $A_I/\Sigma A_n$ are shown with a solid black line for O I 1302 Å, a dot-dash line for O I 1305 Å, and a dotted line for O I 1306 Å. Errorbars are smaller than the markers.
column density, but require two dissociations to produce a sulfur atom. This makes them rather unfavorable as dominant sources for the inner coma, but necessary to consider in future modeling. As stated in other sections it is difficult to derive reasonable production rates of the likely parent molecules from these extreme inner coma column densities with empirical Haser and physical vectorial models, and a more robust modeling approach is required.

**Atomic Production Rates of the near-nucleus coma**

With detections of H, O, and S we can place some constraints on the atomic production rates of the inner coma of 46P from UV observations. However, we note that these values are representative of the near-nucleus coma, not of the overall cometary abundance, and are therefore difficult to directly compare with other comets. For this reason, we derive the atomic production rates for the near-nucleus coma from the comet-centered observations. From the column densities in Table 5.2 we derive $Q_H$, $Q_O$, and $Q_S$ with a simple Haser model for column densities, with lifetimes of $1.5 \times 10^6$, $1.8 \times 10^6$, and $9.1 \times 10^6$ s for H, O, and S (Huebner and Mukherjee, 2015; Meier and A’Hearn, 1997). We use a velocity of 18 km/s for H and for O and S a velocity more reflective of the OH velocity for 46P/Wirtanen as found by Fink and Combi (2004), 1.33 km/s. We can then use the equation for column density from a simple Haser model:

$$Q = \bar{N}2\pi \rho v e^{\beta^3}$$  \hspace{1cm} (5.4)

where $N$ is the average column density across the aperture, $\rho$ is the distance from the nucleus, and $\beta = (\nu \tau)^{-1}$, where $\nu$ is the velocity of the atoms and $\tau$ is the lifetime.

We find that the average atomic production rates for H and O are $3.4 \pm 0.3 \times 10^{27}$ and $1.3 \pm 0.7 \times 10^{27}$, respectively. The similarity between $Q_H$ and the water production rates of Combi et al. (2020) suggest that the dominant source of H in the inner coma is indeed the first dissociation of H$_2$O, and that both Haser and vectorial models are unable to accurately represent the densities observed. The production rate
of O is approximately two times lower than that of H. Given that two dissociations of \( \text{H}_2\text{O} \) are needed to produce a single O atom the discrepancy between \( Q_H \) and \( Q_O \) is not unexpected. \( \text{H}_2\text{O} \) is therefore capable of producing all observed O and no other abundant oxygen-bearing molecules are needed to explain the observed column densities. This is in agreement with our non-detection of CO and \( \text{CO}_2^+ \) in Venkataramani et al., in prep.

The production rate of sulfur is less easily explained. The inner coma of 46P/Wirtanen has \( Q_S \) of \( 2.3 \pm 0.5 \times 10^{27} \text{ s}^{-1} \), rivaling the production of hydrogen atoms. As described in the previous section this number is difficult to obtain with the known production rates of sulfur-bearing \( \text{CS}_2 \), and the preferred parent \( \text{S}_2 \) does not have the corroborating emission in the 2600-2900 Å range in STIS data for the needed production rates. Calmonte et al. (2016) provide a variety of sulfur-bearing molecules detected in the near-nucleus environment of 67P/Churyumov-Gerasimenko, but to match the COS observations there are two clear constraints. Whatever the unknown sulfur parent, it must have a lifetime on the order of 100’s of seconds and be produced directly either from the nucleus itself or from sublimating grains within the first 10’s of km from the nucleus. In addition, the non-sulfur daughter products of the dissociation cannot contribute substantially to either the H or O columns. This is similar to one particular finding of Calmonte et al. (2016); 27% of atomic S in the inner coma of 67P/Churyumov-Gerasimenko could not be linked to a parent molecule. The Alice UVS also reported significant amounts of atomic sulfur in the coma, with no clearly identifiable parent molecule (Feaga et al., 2015; Feldman et al., 2017). A similar situation may be present in the inner coma of 46P/Wirtanen, where a large component of S atoms has no clearly identifiable parent molecule, and may be sublimating off of the cometary surface or from grains in the inner coma. This conclusion also warrants a closer look at the production of sulfur in the inner coma of other comets observed with COS, especially C/2014 Q2 (Lovejoy) and 153P/Ikeya-Zhang (Feldman et al., 2018b).
5.5 Summary

In this chapter we have presented spectra of 46P/Wirtanen from 900 - 1430 Å taken when the comet was between 0.16 and 0.23 au from Earth and 1.12 and 1.17 au from the Sun. During this period the 2.5” diameter aperture of HST COS subtends between 337 and 402 km at the comet, allowing portions of the near-nucleus coma to be observed. Our results can be summarized as follows:

1. We found no evidence of CO Fourth Positive Group emission between 1350 and 1430 Å, and use the (4-0) band at 1420 Å to place a $3\sigma$ upper limit on the production rate of CO at $3.6 \times 10^{25}$ mol s$^{-1}$, approximately 8% that measured for H$_2$O.

2. No evidence of dissociative electron impact was detected via the semi-forbidden O I 1356 Å emission feature. We place upper limits on the aperture averaged column densities of H$_2$O and O$_2$ susceptible to dissociative electron impact at $\sim 4 \times 10^{14}$ cm$^{-2}$ for O$_2$ and $\sim 4 \times 10^{16}$ cm$^{-2}$ for H$_2$O.

3. The O I 1302 - 1306 Å triplet was resolved for the first time in a cometary coma, yielding relative line ratios which change with offset and are inconsistent with known $A$ values. Future observations will be required to uncover the diagnostic potential of these lines.

4. Derived atomic production rates of H and O imply that the only substantial source of H and O in the coma is H$_2$O. This suggests that CO$_2$ and O$_2$ are not abundant in the coma of 46P/Wirtanen for the 2018-2019 apparition.

5. The derived production rates of atomic sulfur are only slightly less than that of H. This production rate is difficult to explain with the known sulfur-bearing molecules on 46P and suggests that atomic sulfur may be entering the near-nucleus coma directly from the nucleus or grains very near the surface, similar to 67P/Churyumov-Gerasimenko (Calmonte et al., 2016).
Attempts to derive parent molecule production rates using Hase and vectorial modeling were unable to produce values within reasonable agreement of water production rates from Combi et al. (2020). Monte Carlo modeling of the inner coma is required to properly interpret observations taken at offsets and perform full analysis of the information contained within the Lyman-α and O I 1302 Å emission profiles. Given the continued observed abundance of sulfur in the inner nucleus of comets (Feldman et al., 2018b) we recommend a re-examination of past comets observed with COS and STIS with improved modeling as well as further study of possible pathways for atomic sulfur to be introduced into the inner coma.

Acknowledgements

Based on observations with the NASA/ESA/CSA Hubble Space Telescope obtained at the Space Telescope Science Institute, which is operated by the Association of Universities for Research in Astronomy. All authors extend their sincere thanks to Alison Vick, Tom Brown, Tony Sohn, and William Fischer for helping schedule and execute these challenging observations. Incorporated, under NASA contract NAS5-26555. All authors acknowledge support by HST program number GO-15625 (PI D. Bodewits), which was provided through a grant from the STScI under NASA contract NAS5-26555. Part of the research was carried out at the Jet Propulsion Laboratory, California Institute of Technology, under a contract with the National Aeronautics and Space Administration (80NM0018D0004).
6.1 Connecting Emissions to Cometary Compositions and Formation

There’s an excellent quote from Delsemme (1982) that rings especially true in the context of this dissertation.

Observed atoms, radicals, or ions are visible mostly by accident because they happen to have large cross sections to absorb solar photons; they scatter these photons back at the same wavelength (resonance) or at a different wavelength (fluorescence).

We did not get to choose which atomic species fluoresced strongly in solar light. No doubt if we had, it’s all but certain that something like sodium would not be the choice for one of the most easily detectable atomic features. Studies of $\text{C}_2$, $\text{C}_3$, and CN, all radicals with uncertain parents and dissociation pathways, are the norm because they, as Festou says, are visible by coincidence. The fluorescing UV comet spectrum that has been studied for decades is a result of the convolution of molecular cloud chemistry, shock heating and processing during protoplanetary disk formation, planetesimal formation processes, orbital evolution, and sublimation history, all constrained by the g-factors of the components of the coma. Of all the fluorescence emissions in the UV, only the CO Fourth Positive group emissions observed in several comets appear to be a parent distribution (Lupu et al., 2007).

This dissertation explored two methods that attempt to break the reliance on fluorescence, to varying degrees of success: high resolution characterization of comet outbursts in the UV and fortuitous solar transient impact on the cometary coma. Both methods rely on the dissociative electron impact emissions that result from energetic electrons breaking apart neutral atoms into excited components which then
emit photons very near the parent dissociation location (e.g. Ajello et al. (2019)). The confirmation of dissociative electron impact emission in the cometary coma by Feldman et al. (2015a) meant that it was now possible, with a few well justified assumptions about the plasma density and energy, to measure the relative abundance of several parent molecules. Despite originating from a different mechanism than Festou describes, these observed emissions, ripe for studying thanks to the coincidental happenstances of quantum mechanics, yield several distinct conclusions from this body of work that can be used to improve scientific return from comets, Centaurs, and protoplanetary disk observations.

6.1.1 Outburst Influences on FUV Cometary Spectra

As discussed in Chapters 2 and 3, there were several improvements to the initial first order calculations made in Feldman et al. (2015a) with comprehensive spectral modeling that enabled constraints to be placed on the relative abundance of H$_2$O, CO$_2$, and O$_2$ for several outbursts. From those studies there are two critical conclusions that motivate future FUV comet observations. The first, described in Chapter 2, revealed that two outbursts within just a few hours of each other showed substantially different relative compositions of H$_2$O, CO$_2$, and O$_2$, as well as content of dust. When combined with the visible wavelength context observations from the Rosetta VIRTIS instrument and NAVCAM it is clear that the outbursts likely represented two different initiation mechanisms. The dust-poor, CO$_2$- and O$_2$-rich outburst represents something more akin to a fracture reaching a volatile reservoir (Skorov et al., 2016), while the dust-enhanced and CO$_2$- and O$_2$-depleted outburst is what would be expected from the collapse of a weakened cliff (Steckloff et al., 2016). These characterizations of the parent molecules in the outburst outflow from dissociative electron impact modeling represent the first time that, to this author's knowledge, that the cometary spectrum has yielded direct evidence about the type of outburst on the comet surface. The frequency, strength, and composition of these outbursts is indicative of heterogeneity in the comet's structure and potential asymmetry in the sublimation front. Obtaining abundant measurements of these properties for
a multitude of comets, cross-referencing with visible and near-infrared data, and comparing with protoplanetary disk observations and models will prove critical for improving our understanding of cometary evolution, especially as we become more sensitive to the activity of distant objects.

Spatial distribution maps of the outburst displayed in Chapter 3 showed that the dissociative electron impact emission measured from the outbursts does indeed trace the parent distribution. The additional observations made by the MIRO and VIRTIS instruments to map the distribution of H$_2$O and CO$_2$ in the coma in the microwave and infrared wavelengths, respectively, yielded excellent agreement with the atomic H, C, and O emissions due to dissociative electron impact emissions by the Alice UVS. This combination of results is promising in the face of a new generation of FUV-capable detectors with higher spatial and spectral resolution than the current generation (France et al., 2016, 2017). Observations of the distinct spectral signatures of dissociative electron impact emissions from parent molecules would be a powerful tool for characterizing activity on scales currently out of reach for HST, as shown in Chapter 5. If a large aperture, large FOV, and FUV capable instrument is selected as part of the next flagship observatory mission, as requested in the 2020 Astronomy and Astrophysics Decadal survey (National Academies of Sciences and Medicine, 2021), there is the possibility for quick remote outburst characterization via the spectroscopic identifiers presented in this work. However, without additional FUV observatories to relieve proposal pressure from HST, it will be difficult to obtain both the observational cadence and duration that an outburst monitoring campaign requires; outbursts are stochastic events with no obligation to be governed by telescope proposals. If FUV monitoring campaigns of comets can be accomplished with a dedicated Cubesat or smallsat observatory, remote identification of these outbursts would be possible and further exploration of the comet outburst spectral signature enabled.
6.1.2 O$_2$ in the Cometary Coma

The discovery of abundant O$_2$ in the coma of 67P/Churyumov-Gerasimenko was unexpected (Bieler et al., 2015), and the pursuit of different explanations for its prolific appearance has left a trail of papers that fall into roughly two categories: the abundance is primordial (e.g. Mousis et al. 2016; Taquet et al. 2016; Heritier et al. 2018) and the abundance is due to photochemical pathways (Yao and Giapis 2017, see full review of the current literature by Luspay-Kuti et al. 2018). The bulk of the evidence from photochemical models shows that the production of O$_2$ cannot be explained from photochemistry alone, and that the majority of O$_2$ is likely pristine (Heritier et al., 2018), but until data for the full mission has been analyzed and published, it is difficult to fully rule out one or the other (Luspay-Kuti et al., 2018). The detection at 67P prompted a closer look at data from the Giotto mass spectrometer data from the flyby of comet 1P/Halley, which revealed molecular oxygen levels at a similar abundance relative to water ($\sim$4%) (Rubin et al., 2015). Future detections of O$_2$ must be carried out with space based observatories for three reasons: the similar volatility between O$_2$ and CO, the comparatively low abundance expected from solar system formation models (Zheng et al., 2006), and the difficulty in observing the molecule. This last point is due to the fact it is a homonuclear, and thus non-polar, molecule as well as that it is a major component of the Earth’s atmosphere, rendering the emissions of the $^{16}$O-$^{16}$O molecule optically thick from any ground based mm/sub-mm observatory capable of observing the rotational transitions. The isotopologue $^{18}$O-$^{16}$O has been used as a proxy for the bulk O$_2$ content in previous searches with ALMA (Taquet et al., 2018) in order to avoid the saturated telluric lines. In fact, to date, molecular oxygen has been detected in just one more astrophysical object outside our solar system then in comets, with only three confirmed detections in molecular clouds (Larsson et al., 2007; Goldsmith et al., 2011; Liseau et al., 2012; Chen et al., 2014; Wang et al., 2020).

Given the elusive nature of the molecule, the unique spectrum produced by e+O$_2$
in the FUV makes the addition of FUV instrumentation to future comet missions a key strategy for measuring the chemical composition of the near-nucleus coma. Trapping O$_2$ early in the planetesimal formation process also gives key insights into the thermal environment of the disk and gives credence to a cold outer disk formation location of 67P prior to scattering by the outward migration of Neptune. Constraining the abundance of molecular oxygen in molecular clouds and protoplanetary disks represents a difficult task, but it is a necessary one in order to understand the amount of chemical processing that could happen between the protoplanetary disk formation and planetesimal accretion.

6.1.3 The HST Bottleneck

The enticing results from Chapters 2 through 4, detailing the ways that dissociative electron impact can be used to constrain the parent molecule abundances and distribution, directly motivated the study of 46P/Wirtanen described in Chapter 5. In order to observe the small scales that Rosetta and Alice UVS captured at 67P, the close flyby distance of 46P was the last possibility to carry out the remote search for dissociative electron impact emission in the near-nucleus coma for at least the next 50 years with the current suite of Earth-based observatories; there simply are no known comets with close approaches like that in the near term. To achieve similar scales, the comet had to be within ~0.17 au of the Earth. The hope of the experiment was that the observations with the aperture centered on the nucleus would capture evidence of dissociative electron impact in the form of substantial O I 1356 Å emissions, evident in so many of the spectra obtained by Alice. However, the high spatial resolution enabled by such a close approach also brings the comet within ~1.2 au of the Sun, increasing the production rates of H$_2$O and CO$_2$ and decreasing the intensity of dissociative electron impact emissions (Schindhelm et al., 2016). Even with the lower than expected water production rates for 46P during the 2018-2019 close approach, there was still no evidence of dissociative electron impact within ~200 km of the nucleus.

The extended nature of the cometary coma and the necessity of a low helio-
centric distance to achieve the proper spatial resolution place a limit on detecting dissocia
tive electron impact emissions from comets with HST. In order to probe the small spatial scales with the COS 2.5” diameter aperture, which doesn’t encode spatial information, the comet must be close enough that the inner ∼100’s of km of the coma fill the aperture. However, at those close distances the surface brightness of the coma is quite low, as the vast majority of the coma is now outside of the aperture. Furthermore, the fluorescence of the photodissociation products that fill the aperture is far more substantial due to the increased g-factor at 1 au vs. the 3 au where dissociative electron impact was first discovered at 67P.

Unlike comet observations with the large FOV and geosynchronous IUE observatory, FUV comet observations with HST remain somewhat of a rare opportunity, with only 14 solar system comets and one interstellar comet being targeted to date. The small apertures of the COS and STIS instruments, while excellent for nearly all other forms of astrophysical observations, make it difficult to measure the extended coma of comets in an accurate manner compared to IUE. Where IUE was able to truly measure the atomic budget of a comet coma, HST observations are limited to studies of just the inner part of the coma with COS. Theoretically the 0.2” × 52” slit for STIS would be an excellent tool to characterize the atomic budget, but the FUV MAMA detector that it uses for FUV observations has far lower efficiency than the COS FUV microchannel plate detector and is thus only really useful for UV-bright targets, like Europa (Feldman et al., 2000). Because there has only been a single full FUV capable observatory (as FUSE was a narrow range of FUV wavelengths) for almost the last 25 years, there is now a observation bias to FUV comet observation quite similar to the early bias imposed in the 1970s.

In order for a comet to warrant study with HST it must be a) extremely bright and unique (e.g. isotropic comets 2004/QW4 LINEAR), b) previously characterized and needs additional context (eg. 46P, 67P), or c) completely unique in its own right (e.g. 2I/Borisov). Low activity comets, which are likely the best comets to identify dissociative electron impact emissions and thus directly measure relative abundances and distributions of parent molecules, are inherently difficult to observe
due to their low surface brightness and even more difficult to observe with the narrow FOV of COS. Without a large FOV FUV-capable telescope with a high resolution spectrograph, à la IUE, these faint comets will simply never be observed in the FUV; in the current FUV observing environment it must be feasible with HST.

This HST bottleneck, ignoring the Director’s Discretionary proposal route for the time being, comes in the structure of the current HST proposal process as well. Targets must be identified at least 6 months prior to the observations taking place, and the 12:1 oversubscription of HST in general makes the possibility of any routine characterization to identify evolution of cometary emissions with a high temporal cadence program extremely unlikely for selection. Neither of these constraints is particularly unique to HST, but because the FUV community at large is entirely constrained to the operations of COS and STIS, there are limited options for creativity with observations.

These options are limited, but not zero.

6.2 Future Studies with New and Existing FUV Comet Data

There is no comet mission with a FUV spectrograph either being studied or in the planning stages as of the writing of this dissertation. Given this paucity, it is doubtful that the unique capability of near-nucleus FUV observations from a spectrograph to constrain emission mechanisms and coma composition on small spatial and temporal scales can be capitalized on for at least two decades. However, any future comet mission, whether escort or rendezvous, should strongly consider the addition of a high resolution FUV spectrograph to the mission payload. The low data transmission requirements, relatively simply command and data handling, and low power consumption compared to the ability to observe nearly constantly allows enormous scientific opportunities and a wealth of data. However, given that the Alice instrument is now resting on the surface of 67P/Churyumov-Gerasimenko, additional science questions must be investigated either with existing FUV observations or with the single telescope that currently operates with FUV spectroscopic
capability, HST. Given the three key elements identified in the previous section, there are three future projects that warrant pursuit.

6.2.1 Comparison to UV Protoplanetary Disk Observations

The enticing nature of comets derives from their status as a probe of the early solar system environment and as chemical time capsules preserved in the Oort Cloud or Kuiper Belt. By wearing their composition on their proverbial sleeve as they sublimate away during their inner solar system foray, they are ripe for direct comparison to the protoplanetary disks we want to be able to model from cometary compositions. Protoplanetary disk observations in the FUV have benefited greatly from the addition of the COS instrument to HST’s suite (France et al., 2012; Hoadley et al., 2015; Arulanantham et al., 2021), especially for identifying atomic emissions from H, C, and O as well as molecular emissions and/or absorptions from H$_2$ and CO. These molecules are viewed as excellent tracers for the disk gas at large, and the high resolution line profiles from COS observations can provide key details about the radial distribution of the gas within the disk (Hoadley et al., 2015). These observations also have the additional benefit of capturing all of the FUV emissions from these protoplanetary disks, thanks to their point-source like appearance in the COS aperture, allowing calculations of the H/O, C/O, and S/O ratios of the gas to be made provided adequate detections of the atomic and expected abundant molecular emission features (H$_2$ and CO) are present in the spectrum. Even though the FUV emissions from the protoplanetary disk are not sourced from within the midplane where planetesimals are forming, it is still of astrophysical interest to characterize the atomic ratios to understand how they compare to the more frequently observed molecular emissions of carbon monoxide in the sub-mm wavelengths. The sub-mm rotational transitions of CO characterize colder parts of the disk nearer to the midplane where planetesimals form, while the UV emissions will originate nearer to the disk’s surface where UV light from the central star can still penetrate.

The frequent observations of dissociative electron impact emissions at 67P may also be applied to protoplanetary disk observations. France et al. (2011) report
emissions in two T Tauri stars indicative of dissociative electron impact on H$_2$. Given the high stellar activity of these stars, the observations of the inner cometary comae with Alice, and the tools developed to characterize the convolution of fluorescence and collisionally excited spectra, may be applied to observations of T Tauri stars to search for evidence of additional abundant components in the protoplanetary disk. Such an effort will no doubt require a high level of collaboration between protoplanetary disk observers, modelers, and FUV cometary spectroscopists, but offers the opportunity for a direct comparison between the comet and protoplanetary disk atomic species in a way that is unique to the FUV wavelengths.

The strange multiplet ratios observed in the O I 1302, 1304, and 1306 Å emission in the coma of 46P/Wirtanen also warrant further investigation in the COS archives. As described in Chapter 5, the expected contribution to the integrated brightness of the multiplet from each of the emissions changed as a function of distance from the center of the nucleus. Given that this was the first time the O I 1302 Å has been completely resolved in a comet’s coma, searching for similar deviations from the expected line ratio may be a second order indicator of collisional excitation processes. However, with only a single comet observation resolving the multiplet, it is hard to make any reasonable conclusions. Studying the emission feature both with future HST COS proposals for comets and revisiting protoplanetary disk observations can provide additional thermal, density, and plasma environment constraints to this intriguing development.

There is a relatively small database of FUV protoplanetary disks observed with COS since its installation in 2009 that is ripe for comparison to the comet spectra gathered with IUE, as that instrument’s FOV captures the largest amount of the atomic cometary coma. While an initial comparison can be done with archival retrieval of protoplanetary disks observed with COS and of comets observed with IUE, until large FOV observations of comets can be obtained again in FUV wavelengths, it is unlikely that much progress can be made in characterizing the atomic ratios in the broader comae of comets. For protoplanetary disk observations with COS, a higher spectral resolution can be achieved because they are closer approximations to
point sources in the COS aperture then the extended coma of solar system comets, which fill the COS FOV even at large geocentric distances thanks to the 2.5” diameter aperture. That observations of comets and protoplanetary disks taken with the same telescope, the same instrument, the same grating setting, and the same detector can still have substantially different spectral resolutions speaks to the some of frustrations of comet observations. Even our “apples to apples” comparisons can still have a worm in them here and there.

6.2.2 The Cometary Sulfur Question

The sources and distribution of cometary sulfur are still poorly understood, and S abundance in isotropic comets even less so (Meier and A’Hearn, 1997; Feaga et al., 2015; Calmonte et al., 2016; Noonan et al., 2021b). High spectral resolution observations of comets help to bridge the gap not only between isotropic cometary atomic abundances and typical Jupiter Family Comets but between comets and protoplanetary disk abundances, which also show peculiar properties of sulfur/sulfur bearing molecules (Kama et al., 2019). Comets occupy a unique space where a significant portion of their sulfur reservoir is trapped in icy grains, rather than refractories, allowing bulk characterization with spectroscopy of the broader fluorescing coma where the trapped sulfur-bearing molecules dissociate. This property reflects comets as a key piece of understanding protoplanetary disk chemistry; investigations of protoplanetary disks have shown that SO, CS, and H$_2$S account for less than 1% of sulfur (Dutrey et al., 1997; Ruffle et al., 1999; Wakelam et al., 2004; Fuente et al., 2016; Dutrey et al., 2011; Martín-Doménech et al., 2016; Semenov et al., 2018; Hily-Blant et al., 2021). Given the importance of sulfur compounds in the astrobiological context, both as a critical component for sulfur-based metabolism (Schulze-Makuch et al., 2004) and as a potential biosignature (Domagal-Goldman et al., 2011), understanding the properties of sulfur abundances in comets marks a crucial next step for the astrophysics community at large.

Thanks to the efforts of many comet scientists, there are a significant number of IUE, Hubble Faint Object Spectrograph (FOS), COS, and STIS observations of
comets with abundant sulfur that have not been fully investigated. UV Comet observations with FOS and COS allow sensitive limits to be placed on atomic sulfur emissions via the SI emissions at 1425, 1479, and 1667 Å, while NUV observations with STIS allow sensitive limits for CS, and thus CS$_2$, via the (0-0) and at 2576 Å and S$_2$ via vibrational bands between 2828 and 3055 Å. From these detections or upper limits ratios of carbon and sulfur can be derived for comparison to protoplanetary disks, production rates of CS$_2$ can be calculated and compared to the water production rates, and the overall sulfur budget of the comets characterized and contrasted to previously observed comets. One difficulty that has prevented much of this analysis from being completed is an accurate and robust model for the distribution of atomic S in the coma; much of the observations of S indicate that there is an extended source. Only IUE and HST have had the capability to measure this combination of sulfur multiplets and parent molecules; there is no other publicly available telescope with sensitivity between 1600 and 3000 Å. The topic is ripe for an archival proposal to the STScI to revisit the ~60 comet FUV spectra for a second look and investigate the sulfur abundances of dynamically new, long, and short period comets, model the distribution of the atomic S, and better understand how they compare to protoplanetary disk abundances.

6.2.3 The Solar Flashlight

The discovery of abundant dissociative electron impact emissions in the near-nucleus coma of 67P and the difficulty in observing the process on the same spatial scales with Earth-based observatories calls for a different approach. Taking the results from Chapter 4, where the impact of a coronal mass ejection produced some of the brightest emissions observed in the FUV for the entire Rosetta mission, an observational campaign can be formulated. The concept is simple: take advantage of the well characterized solar transient observations that are executed by solar observatories like SOHO and STEREO, cross-reference the solar longitude of the events with the locations of active comets and Centaurs, and then either a) retroactively search for any observations of those objects that would be contemporaneous with
the impact of the events, or b) set up a cut-and-dry target of opportunity campaign with HST to capture the impact.

While the concept of these observations is simple, the execution is exceeding difficult due to the aforementioned “HST Bottleneck”. However, the concept may ultimately be most useful for studying activity on low-activity main belt comets and active Centaurs like 29P/Schwassmann-Wachmann 1. With an orbital semi-major axis of 6 au and negligible heliocentric velocity thanks to a nearly circular orbit, the g-factors for fluorescence emissions are approximately 36 times lower for 29P than for near Earth comet approaches, like 67P. The large geocentric distance also serves to concentrate more of the near-nucleus coma into the COS aperture, increasing the surface brightness of the emissions. There is also mounting evidence that previous detections of CO$^+$ in the coma of 29P can be explained by the energetic particle flux from the solar wind (Werbowy and Pranszke, 2013; Ivanova et al., 2019; Wierzchos and Womack, 2020) at baseline, which would make any increased particle flux and energy from solar transient events more efficient at stimulating ionization and excitation of the neutral CO likely sublimating from the surface.

Observations of CO$^+$ in conjunction with long-exposure time FUV observations to characterize electron impact on H$_2$O, CO$_2$, CO, and O$_2$ can provide conclusive evidence of the particle dissociative environment around active Centaurs and shed light on the what drives these objects’ strange activity patterns. CO$^+$ fluoresces strongly even at 6 au thanks to a relatively large g-factor, and there are CO$^+$ emission bands accessible in the NUV and visible wavelengths. In fact, it is likely that several of the standard HST Wide Field Camera 3 (WFC3) filters used in previous observations of 29P and other Centaurs are actually contaminated with the CO$^+$ emissions and may not be as indicative of the dust distribution. If this is indeed the case, much of the visible data on Centaurs at wavelengths lower than 5000 Å needs to be reviewed in the context of the abundant CO$^+$ emissions as well.

A combined HST COS and STIS observing campaign of active Centaurs during solar maximum, when solar wind particle fluxes are highest, over the course of several years would prove extremely valuable to our understanding of how the solar wind can
influence emissions at heliocentric distances where fluorescence processes are much more inefficient than in the inner solar system. Observations of active Centaurs and JFCs near aphelion in the UV and visible wavelengths, making use of the solar activity to measure the faint coma, will provide a useful benchmark for the level of persistent activity these objects maintain, and connecting these sublimation rates to the dynamical evolution of the object will be beneficial for understanding how the coma composition can evolve with time. While the current observing situation and “HST Bottleneck” prohibits the more ambitious Target of Opportunity triggering on solar transient events with vectors that would see them impact active Centaurs, it should by no means be discounted as dedicated small-sats become more feasible for such specific missions and goals.

6.3 More Questions than Answers

There is something inherently fascinating in the tricky nature of cometary activity observations; the activity that simultaneously defines them obfuscates their surface and limits characterization of the nucleus. The characterizations of the volatile abundances in their comae are only as good as our understanding of the emission mechanisms, which in turn are biased towards low heliocentric distances. Just how indicative are the coma abundances of volatiles like CO, CO$_2$, and H$_2$O of the primordial formation environment? Is a Jupiter Family Comet, freshly injected from the Kuiper Belt, a better indicator of the initial volatile abundances of the original molecular cloud, or is the Oort Cloud comet? Would a dead comet, if confirmed to truly be a dead comet, be the best example of the early solar system refractory compositions in the cold outer disk, or the most processed? Does a brand new comet, not yet fully illuminated by the Sun, have a pristine surface from the early solar system or an irradiated frost layer, with the most chemically altered surface possible? Only a few of these are even touched on in this dissertation as they cover such a broad scope of comet science, but all of those questions are relevant and necessary to consider thoroughly.
There are no answers to these questions in this dissertation, but the work explored within it has given one critical piece of information in the pursuit of their solution. Comet spectra can be strongly influenced by the plasma environment that they exist in, yielding UV emissions that give clues about key parent molecule abundances and distributions. Exploiting this new tool in a variety of projects will help to monitor comet and Centaur activity at a large range of heliocentric distances, improve our knowledge of how outbursts can vary in frequency, size, and strength, provide clues about what that means for the comet’s structure and evolution, and probe new physical regimes with plasma-neutral interactions. At first glance it seems that the golden age of FUV comet observations may be drawing to a close, with the end of the Rosetta mission and Alice UVS and a replacement for HST’s FUV capability only existing on paper. At times while writing different portions of this dissertation, it was easy to get discouraged, fretting about what this work will actually mean to comet science if there are no FUV-capable facilities to carry on investigations in the next twenty years. The reality of the problem is that the act of studying comets in the FUV is a cipher of its own, a puzzle in how to take in observations of different wavelengths and molecules, weaving them with different models of solar system dynamics, cometary outflows, and planetary migration. The nature of these UV observations taking place in a unique regime of energies and densities at the intersection of geology and plasma physics requires all assumptions to be interrogated and foundational aspects to be rederived to identify which components truly affect the whole. In an analogous manner, ultimately this work became a unique contribution to the body of comet literature, a key piece of the larger picture, whether there is an FUV observatory next year or next century. The last part, the most crucial part, in all of the work covered in this dissertation was not the comet cipher; it was proving to myself that I am capable of contributing to the solution.
APPENDIX A

Calculating Photo-fluorescence Efficiencies

In order to calculate the fluorescence efficiency of a single transition within an atom or molecule several components are required. The first is the solar flux at the wavelength of the transition as measured at 1 au from the Sun after applying the proper redshift/blueshift to a solar reference spectrum:

\[ F_\odot(\lambda) = F_\odot(\lambda) \left( \sqrt{\frac{(1 + \dot{r}_h/c)}{(1 - \dot{r}_h/c)}} \right) \]  

(A.1)

where \( \dot{r}_h \) is the heliocentric velocity of the object in cm s\(^{-1} \), \( c \) is the speed of light measured in cm s\(^{-1} \), and the solar flux is measured in photons cm\(^{-2} \) s\(^{-1} \) Å\(^{-1} \). This flux then needs to be scaled to the appropriate heliocentric distance of the object via the inverse square law:

\[ \pi F_\odot(\lambda, r_h) = \frac{\pi F_\odot(\lambda)}{r_h^2} \]  

(A.2)

, where \( r_h \) is the heliocentric distance of the nucleus. With the solar flux adjust for the heliocentric distance and velocity we can now begin to calculate the transition properties.

The solar flux also needs to be adjusted for the light that can be absorbed and scattered from the particles between the area of interest and the illumination source, in this case the Sun. This is accomplished with the form:

\[ \pi F_\odot(\lambda, r_h, \dot{r}_h) = \pi \frac{F_\odot(\lambda)}{r_h^2} (1 + \dot{r}_h/c)/(1 - \dot{r}_h/c) \]  

\( \tau_\lambda(z)/\mu_0 \)

Where \( \tau_\lambda(z)/\mu_0 \) is the slant optical thickness at the wavelength of interest \( \lambda \). As detailed in Chamberlain and Hunten (1990) the intensity of photons scattered by a unit volume in a given vector \((\mu, \phi)\) at an angle \( \Theta \) relative to the Sun vector at \((\mu_0, 0)\) for the transition from some excited state \( J' \) to a lower energy state \( J \) can
be written as
\[ E(z|\mu, \phi) = n(z)\pi \frac{pe^2}{mc^2} \lambda^2 \mathcal{F}(\lambda, z) f(J_0J') \bar{\omega}(J'J_i) \frac{p(\Theta)}{4\pi} \] (A.3)

which reflects the generalized case where atmospheric where \( z \) represents the height above some surface, \( n(z) \) is the number density of the particle of interest, \( e \) is the electron charge in coulombs, \( m \) is the particle mass in grams, and \( f(J_0J') \) and \( \bar{\omega}(J'J_i) \) reflect the transition specific oscillator strength and single scattering albedo, respectively. \( p(\Theta) \) is the phase function that is applied to the single scattering albedo. The final units of \( E(z|\mu, \phi) \) are photons cm\(^{-3}\) s\(^{-1}\) steradian\(^{-1}\).

Now for the case of cometary atmospheres on large scales, absorption and scattering by particles is typically ignored due to the low densities, and the equation loses its dependence on \( z \). However, observations taken in the near-nucleus coma of highly active comets should carefully consider optical thickness effects on the incident solar flux and resulting fluorescence.

The oscillator strength, \( f(J_0J') \), can be calculated from the the transition probability Einstein Coefficient \( A \) via:
\[ f(J_0J') = \frac{mc}{8\pi^2 e^2} \lambda^2 \bar{\omega}(J') A(J'J_i) \] (A.4)

The transition probabilities and oscillator strengths can for atomic transitions can be retrieved directly from the National Institute of Standards Atomic Spectral Database (https://physics.nist.gov/PhysRefData/ASD/lines_form.html), while molecular transitions are often the subject of single publications.

The single scattering albedo, \( \bar{\omega} \), is described by:
\[ \bar{\omega}(J'J_i) = \frac{A(J'J_i)}{\sum_i A(J'J_i) + \eta(J'J_i)[M]} \] (A.5)

where \( A(J'J_i) \) is the transition probability for transition \( J' \rightarrow J_i \) and \( \eta(J'J_i)[M] \) reflects the rate coefficient for collisional deexcitation for the transition, which is often considered negligible in cometary comae.
Combining these together we can calculate the fluorescence efficiency, \( g \) of the \( J' \) to \( J_i \): transition:

\[
g(J'J_i) = \pi \mathcal{F} \frac{\pi e^2}{mc^2} (\lambda)^2 f(J_0J') \sum_i A(J_iJ_i) + \eta(J_iJ_i)[M] \tag{A.6}
\]

For the abundance of cometary cases the anisotropy of scattering, \( p(\Omega) \) in Equation A.3 can be ignored, as effects from magnetic field strength are negligible. Additionally, as stated in Feldman et al. (2004), when the spectroscopic measurements are of moderate to low resolution and the individual components of an atomic multiplet are not resolvable the single scattering component can be set to 1, If the multiplet is resolvable, then the single scattering albedo for each transition needs to be solved explicitly:

\[
\tilde{\omega}(J'J_i) = \frac{(2J' + 1)e^{\frac{-E'}{kT}}}{\sum_i (2J_i + 1)e^{\frac{-E_i}{kT}}} \tag{A.7}
\]

where for a given momentum value \( J' \) the single scattering albedo is the numerator divided by the sum of all transitions that have the same starting and ending electronic states, with different values of \( J \). The energy of the transition is \( E \), which can easily be found via \( E = h\nu = hc/\lambda \). Note that the population of each state is dependent on the temperature of the gas, \( T \), which is in Kelvin.

The total intensity of emissions from a unit volume of \( n(z) \) particles cm\(^{-3} \) along vector \((\mu, \phi)\) can then be written as:

\[
\mathcal{E}(z|\mu, \phi) = g(J'J_i)n(z)4\pi \tag{A.8}
\]

and integration along \( z \) yields a column density emission rate in the isotropic case yields:

\[
\mathcal{J}(J'J_i) = \frac{g(J'J_i)N_{eq}}{4\pi} \tag{A.9}
\]

For remote observations the distance to the column must be taken into account when determining the observable flux:

\[
\mathcal{J}(r, J'J_i) = \frac{g(J'J_i)N_{eq}}{4\pi r^2} \tag{A.10}
\]

with units of photons sec\(^{-1} \) for the transition \( J' \) to \( J_i \).
APPENDIX B

Calculating Plasma Dependent Emission Efficiencies

B.1 Dissociative Electron Impact Emissions

The brightness of some emission feature from transition \( X \) stimulated by electron impact, characterized as \( B_X \) is dependent on the particle flux of energetic electrons along the line of sight \( s \), \( J(E, s) \) [cm\(^{-2}\)s\(^{-1}\)eV\(^{-1}\)], and the number density of the neutral species \( l \) that emission feature \( X \) derives from, \( n_l(s) \) [cm\(^{-3}\)], along the observed line of sight. If the excited states creating the emission have brief lifetimes, the emission brightness is given by

\[
B_X = 10^{-6} \sum_l \int_S \int_{E=E_{Th,l}}^\infty n_l(s) J(E, s) \sigma^X_l(E) \, dE \, ds \text{ [Rayleigh] (B.1)}
\]

where the integral is over the line of sight, yielding an equivalent column density. Each major neutral species in the coma contributing to \( X \) are summed over to give the total brightness from dissociative excitation. The energies of the impacting electrons are not quantized this process, which renders it capable of producing atoms in classically forbidden states, which quickly release a “forbidden” photon.

Electron impact emission brightness is not dependent on the total electron density, but rather the density of electrons which exceed the emission threshold energy, \( E_{Th} \). Electrons that have energies below this threshold will not dissociate and excite molecules and atoms, as the emission cross section \( \sigma^X_l(E) = 0 \) in this energy range.

Provided a constant energetic electron flux along the line of sight, Eq. (B.1) can be reduced to

\[
B_X = 10^{-6} \sum_l N_l \nu^X_l \quad (B.2)
\]

where \( N_l \) represents the neutral species column density, \( l \), and \( \nu^X_l \) is the emission frequency of the species for the relevant emission feature. When presented in this
manner $\nu_I^X$ is comparable to the $g$-factor derived in Appendix A. This assumption is valid at large heliocentric distances where electron-neutral collisions are infrequent and significant energy degradation of electrons along the line of sight is unlikely. Chaufray et al. (2017) found that emissions are consistent with a constant suprathermal flux throughout the neutral column when the cometary outgassing rate was low ($Q < 10^{26}$ s$^{-1}$).

**B.2 Recombination Emission**

For completeness it is useful to describe how emissions from recombination, where an electron becomes bound to an atom or molecule, can be derived. To calculate the brightness of emission feature $Y$ of a column of ion species $J$ in Rayleighs using the same notation as described in Sect. B.1:

$$B^Y = 10^{-6} \int L.O.S. \alpha^Y_J(T_e) n_J(z) n_e(z) \, ds$$  \hspace{1cm} (B.3)

where $\alpha^Y_J$ is the partial rate coefficient in cm$^3$s$^{-1}$, $n_J$ is the ion number density in cm$^{-3}$, $n_e$ is the electron number density in cm$^{-3}$, integrated over the line of sight of the column. We note that this notation is consistent for both radiative and dissociative recombination. In the same manner as with dissociative excitation, if the electron flux and temperature is assumed to be constant for the column and the column density of the ion species is known, this simplifies to:

$$B^Y = 10^{-6} N_J \nu^Y_J(T_e)$$  \hspace{1cm} (B.4)

where $N_J$ is the column density of ion species $j$ in cm$^{-2}$, and $\nu^Y_J$ is the emission rate. Note that $\nu^Y_J$ has units of s$^{-1}$ and is the product of $\alpha^Y_J$, the partial rate coefficient, and $N_e$, the column density of electrons. We refer the curious reader to Tinsley et al. (1973) and Rybicki and Lightman (1979) for a broader treatment of these emission mechanisms.

Recombination, like dissociative electron impact, is able to populate classically forbidden states of atoms that are capable of producing emissions like OI] 1356 Å
For this reason it would be difficult to disentangle recombination emissions from the dissociative electron impact emissions among the spectra taken by the Alice UVS if both were of similar magnitude, but the current estimates of recombination contribution to the UV emission features are negligible and Alice spectra are fit well by dissociative electron impact alone.

Ion-ion recombination emission involves the mutual neutralization of two ions, one positively charged and one negatively charged, that results in two excited atoms capable of transitioning to the ground state and releasing photons. The column emission rate of feature Y for ion-ion recombination of atom X can be determined by:

$$B_Y = \int_{L.O.S} \frac{\beta_Y K_1 K_2 n_X(s) n_{X^+}(s) n_e(s)}{K_2 n_{X^+}(s) + K_3 n_X(s)} ds$$  \hspace{1cm} (B.5)

where $\beta_Y$ is the total recombination fraction that yields transition Y and $K_1$, $K_2$, and $K_3$ are the reaction rate coefficients for the radiative attachment reaction:

$$X + e^- \rightarrow X^- + h\nu',$$  \hspace{1cm} (B.6)

the mutual neutralization reaction:

$$X^- + X^+ \rightarrow X^* + X^* + KE,$$  \hspace{1cm} (B.7)

and the loss process:

$$X^- + X \rightarrow X_2 + e^-,$$  \hspace{1cm} (B.8)

respectively. All reaction rate coefficients given here, both $\alpha$ and $K_{1,2,3}$, have units of cm$^3$s$^{-1}$.

B.3 Determining Relative Neutral Abundances for Noonan et al. (2018)

The analysis described in Noonan et al. (2018) to derive the relative neutral abundance of CO$_2$ and O$_2$ to H$_2$O uses a different method than Noonan et al. (2021c) and Noonan et al. (2021a). For clarity and preservation, the methodology used is described here.
In general to calculate the brightness \( B \) in Rayleighs of an emission feature emitted from column density of molecule Y and atom x with both electron impact and resonance scattering:

\[
B_\lambda = 10^{-6} g^y_\lambda \int_0^\infty n_x dz + 10^{-6} n_e g^y_\lambda \int_{d_s/c-nucleus+50km}^{d_s/c-nucleus-50km} n_y dz, \tag{B.9}
\]

where

\[
g^y_\lambda = \int_{E_{threshold}}^{\infty} \sigma^y_\lambda(E)f_{pde}(E)dE, \tag{B.10}
\]

Where \( E_{threshold} \) is the threshold energy of electron impact emission for that molecule and emission feature. In the quiescent subtracted CME impact spectra we would expect the contribution from resonance scattering to be near zero, allowing us to assume the brightness of an emission feature is due entirely to electron impact on one of our three main coma components: \( \text{H}_2\text{O}, \text{CO}_2 \), and \( \text{O}_2 \). If there is evidence an outburst occurred in the observation period this assumption no longer holds.

\[
N_y = \int_{d_s/c-nucleus+50km}^{d_s/c-nucleus-50km} n_y dz \tag{B.11}
\]

\[
B_\lambda = 10^{-6} n_e [g^{\text{O}_2}_\lambda N_{\text{O}_2} + g^{\text{CO}_2}_\lambda N_{\text{CO}_2} + g^{\text{H}_2\text{O}}_\lambda N_{\text{H}_2\text{O}}], \tag{B.12}
\]

Taking ratios of the total brightness of emission feature \( \lambda \) and the expected contribution from \( \text{H}_2\text{O} \):

\[
\frac{B_{Total}}{B_{\text{H}_2\text{O}}} = \frac{10^{-6} n_e [g^{\text{O}_2}_\lambda N_{\text{O}_2} + g^{\text{CO}_2}_\lambda N_{\text{CO}_2} + g^{\text{H}_2\text{O}}_\lambda N_{\text{H}_2\text{O}}]}{10^{-6} n_e [g^{\text{H}_2\text{O}}_\lambda N_{\text{H}_2\text{O}}]}, \tag{B.13}
\]

canceling out the Rayleigh conversion factor and electron density \( n_e \) and expanding \( g^y_\lambda \):

\[
\frac{B_{Total}}{B_{\text{H}_2\text{O}}} = \int_{E_{\text{threshold}}}^{300eV} \frac{\sigma^{\text{H}_2\text{O}}_\lambda(E)f_{pde}(E)dE}{N_{\text{H}_2\text{O}}} \left( \int_{E_{\text{threshold}}}^{300eV} \sigma^{\text{O}_2}_\lambda(E)f_{pde}(E)dE N_{\text{O}_2} \right) + \int_{E_{\text{threshold}}}^{300eV} \sigma^{\text{CO}_2}_\lambda(E)f_{pde}(E)dE N_{\text{CO}_2} + \int_{E_{\text{threshold}}}^{300eV} \sigma^{\text{H}_2\text{O}}_\lambda(E)f_{pde}(E)dE N_{\text{H}_2\text{O}} \right) \tag{B.14}
\]
and we can define a new variable $G_{\lambda, y}$:

$$G_{\lambda, y} = \int_{E_{Ty}}^{300eV} \sigma_{\lambda}^{y}(E) f_{pde}(E) dE,$$

(B.15)

where $f_{pde}(E)$, the probability distribution of the electrons, is characterized by IES data at the spacecraft. If we assume this distribution is the same along our observation line of sight an integral to be taken for our electron impact g-factor described in Equation 2. We can solve for $G$ using laboratory data and the known distribution at the spacecraft.

$$\frac{B_{Total}}{B_{H_2O}} = \frac{G_{\lambda}^{O_2} N_{O_2} + G_{\lambda}^{CO_2} N_{CO_2} + G_{\lambda}^{H_2O} N_{H_2O}}{G_{\lambda}^{H_2O} N_{H_2O}},$$

(B.16)

This equation then has taken into account the different energy thresholds, unlike my previous Equation 1. These expected contributions to emission features can also be modeled to a first order using the 100 eV cross sections for CO$_2$ and H$_2$O molecules at a transition, and create a synthetic electron impact spectra that matches the observed carbon and hydrogen emission features, respectively. The expected contribution of those molecules to the O I 1304 Å and O I 1356 Å emission features can then be placed into Equation 8. Rearranging Equation 8 we find:

$$\frac{B_{Total}}{B_{H_2O}} = \frac{G_{\lambda}^{O_2} N_{O_2} + B_{\lambda,CO_2} + B_{\lambda,H_2O}}{B_{\lambda,H_2O}}$$

(B.17)

$$\frac{N_{O_2}}{N_{H_2O}} = \frac{B_{Total}}{B_{H_2O}} - \frac{B_{\lambda,CO_2} + B_{\lambda,H_2O}}{B_{\lambda,H_2O}} \left( \frac{G_{\lambda}^{H_2O}}{G_{\lambda}^{O_2}} \right)$$

(B.18)

$$\frac{N_{O_2}}{N_{H_2O}} = \left( \frac{B_{Total}}{B_{H_2O}} - \frac{B_{O11304,CO_2} + B_{O11304,H_2O}}{B_{O11304,H_2O}} \right) (0.0679)$$

(B.19)

$$\frac{N_{O_2}}{N_{H_2O}} = \left( \frac{B_{Total}}{B_{H_2O}} - \frac{B_{O11356,CO_2} + B_{O11356,H_2O}}{B_{Ly-\beta,H_2O}} \right) (0.104)$$

(B.20)
REFERENCES


Huggins, W. (1868). XXI. Further observations on the spectra of some the stars and nebulae, with an attempt to determine therefrom whether these bodies are moving towards or from the earth, also observations on the spectra of the sun and of comet II., 1868. *Philosophical Transactions of the Royal Society of London*, (158), pp. 529–564.


