

Coma Physics of an Interstellar Object: JWST Spatial-Spectral Mapping of 3I/ATLAS

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ABSTRACT

We report a survey of molecular emission from cometary volatiles using the James Webb Space Telescope (JWST) toward interstellar object 3I/ATLAS carried out on UT 2025 December 22 and 23 at a heliocentric distance (r_H) of 2.37 – 2.41 au. These measurements of CO, CO₂, H₂O, CH₃OH, and CH₄ sampled molecular chemistry in 3I/ATLAS as it receded from its encounter with our Sun and entered the vicinity of the H₂O ice line — the region between $r_H = 2 - 3$ au where the temperature becomes too low for H₂O to vigorously sublime and CO and CO₂ begin to control the overall activity. CO was the most abundant molecule, followed by H₂O and CO₂, whose molecular abundances with respect to CO were $(40.5 \pm 3.1)\%$ and $(41.6 \pm 0.3)\%$, respectively. This work presents spatial-spectral maps of column density and rotational temperature as a function of distance from the nucleus for all detected species. The spatial distributions of both quantities were highly anisotropic for the apolar species in the coma of 3I/ATLAS, yet were more nearly symmetric for the polar molecules. These results demonstrate how volatiles were segregated in the nucleus ices of 3I/ATLAS and reveal heating and cooling mechanisms in its coma. Derived maps of the ortho-to-para ratio (OPR) for H₂O were flat with increasing distance from the nucleus and consistent with a coma-averaged value $\text{OPR} = 2.7 \pm 0.2$, slightly less than the expected equilibrium value of three.

Keywords: Interstellar Objects (52) — Molecular spectroscopy (2095) — Near infrared astronomy (1093) — Comae (271) — Comets (280)

1. INTRODUCTION

Comets provide a window into the early solar system. They formed in the cold disk midplane of the protosolar disk during the era of planet formation and were subsequently scattered to the Kuiper disk or the Oort cloud. Studying the volatile composition of their nuclei gives clues to the chemistry and prevailing conditions present where and when they formed in the disk (M. J. Mumma & S. B. Charnley 2011; N. Biver et al. 2024b). Alongside studies of overall composition, near-infrared spectroscopy of comets can provide insights into the physics of their comae, or expanding atmospheres of gas and dust, by sampling ro-vibrational transitions of a suite of volatiles. Such works, both observational and theoretical, have traditionally focused on solar system comets which were measured at $r_H < 2$ au, where H_2O is the most abundant coma molecule and drives outgassing and overall thermal physics (e.g., V. Tenishev et al. 2008; N. Fougere et al. 2012; B. P. Bonev et al. 2013, 2014).

Here we report a study of the coma physics and chemistry of an altogether different subject, the interstellar object 3I/ATLAS, measured at $r_H \sim 2.4$ au post-perihelion using the JWST NIRSpec integral field unit (IFU) covering $\lambda = 1.06 - 5.14 \mu\text{m}$. The third interstellar object discovered to date (and the second with a comet-like coma; D. Z. Seligman et al. 2025), the coma composition of 3I/ATLAS throughout its perihelion passage has been reported with spectroscopy conducted across the electromagnetic spectrum (e.g., N. Biver et al. 2026; I. M. Coulson et al. 2026; D. Hutsemékers et al. 2026; N. X. Roth et al. 2026a; M. A. Cordiner et al. 2025b; Z. Xing et al. 2025; W. B. Hoogendam et al. 2025; A. Alvarez-Candal et al. 2025). Our post-perihelion JWST observations afforded the opportunity to leverage the spatial-spectral mapping capabilities of the NIRSpec IFU to conduct high-resolution spaxel-by-spaxel studies of the column density and rotational temperature distributions of multiple species in its coma (each spaxel subtends $0''.1$, corresponding to ~ 130 km projected distance per spaxel at the distance of 3I/ATLAS from JWST). These species were CO, CO_2 , and H_2O , which are often the most abundant molecules in cometary nuclei and take turns driving activity depending on r_H (e.g., O. Harrington Pinto et al. 2022), as well as the trace species CH_3OH and CH_4 . Section 2 provides details of the observations and data analysis procedures. Section 3 presents our results, and Section 4 discusses our results in the context of solar system comets studied to date.

2. OBSERVATIONS AND DATA REDUCTION

Interstellar object 3I/ATLAS reached perihelion ($q = 1.35$ au) on 2025 October 29. We conducted post-perihelion observations of 3I/ATLAS using the JWST NIRSpec IFU. The object's r_H ranged from $2.37 - 2.41$ au, its distance from the telescope (Δ_{JWST}) from $1.79 - 1.80$ au, and the solar phase angle (ϕ) ranged from $22.7^\circ - 21.6^\circ$. Observations used a representative resolving power $\lambda/\Delta\lambda \sim 2700$. A single 642 s exposure of the G235H/F170LP grating starting on UT 2025 December 22 03:36 sampled emission from $\lambda = 1.06 - 3.05 \mu\text{m}$ and captured the H_2O $\nu_1 + \nu_3$ vibrational bands near $2.68 \mu\text{m}$. Five 700 s exposures of the G395H/F290LP grating beginning on UT 2025 December 23 08:07 characterized emission from $\lambda = 2.87 - 5.14 \mu\text{m}$. This setting measured molecular emission from CO ($v = 1 - 0$), CO_2 (ν_3), CH_3OH (ν_2, ν_3, ν_9), CH_4 (ν_3), and H_2O hot bands near $4.5 \mu\text{m}$.

Background exposures with identical circumstances (exposure time, grating settings) were planned offset from the comet position by $300''$; however, two of the five background exposures for the G395H grating failed owing to background star issues, with follow-up attempts scheduled for later in 2026. Careful examination of the available background exposures did not reveal emission from any known interstellar infrared sources or zodiacal light, so analysis proceeded without background subtraction to maximize the signal-to-noise ratio (SNR). Exposures were processed using the JWST Pipeline version 1.20.2 with CRDS `jwst_1464.pmap` context files and aligned onto a common spatial-spectral axis using the Drizzle algorithm (D. R. Law et al. 2023). An observing log is provided in Appendix A.

We generated spatial-spectral maps of molecular column density (N , m^{-2}) and rotational temperature (T_{rot} , K) by performing a spaxel-by-spaxel analysis of the NIRSpec IFU data cubes. Each modeled quantity was retrieved using molecular emission models in the NASA Planetary Spectrum Generator (PSG; G. L. Villanueva et al. 2018). We extracted and modeled spectra from each $0''.1$ spaxel using the `jwstComet` package (N. X. Roth 2026b), which provides for flexible spectral extraction from JWST IFU data cubes using functions from the `astropy` and `photutils` libraries, followed by automated interfacing with the NASA PSG API. The data cubes were converted from units of MJy sr^{-1} to Jy pixel^{-1} , then spectra were extracted from the data cubes using the `photutils` `RectangularAperture` function in combination with the `aperture_photometry` function (method = 'center'). Fluxes and 1σ instrumental noise on a per-spaxel basis were derived from the `SCI` and `ERR` extensions of the FITS files.

Contributions from gaseous and continuum emission were identified by comparing the spectra with expected spectral line positions for each species from quantum mechanical models of fluorescent emission generated with the PSG.

Each spectrum was baseline subtracted using second- or third-order polynomial baselines. This baseline accounts for continuum emission from the dust and nucleus, as well as scattered sunlight and instrumental artifacts. We chose the lowest possible polynomial order that could account for the spectral shape while avoiding higher order polynomials to avoid introducing spurious features into the spectra. The baselines were fit simultaneously with the molecular emission models using the Optimal Estimation Method implemented in the PSG. Techniques employing simultaneous fitting of the continuum baseline and molecular emission models have been applied to decades of cometary infrared spectroscopy studies (e.g., M. A. DiSanti et al. 2003; G. L. Villanueva et al. 2011; B. P. Bonev et al. 2014; M. A. DiSanti et al. 2017; N. X. Roth et al. 2018; S. Faggi et al. 2019; C. Ejeta et al. 2024). Fitting the baselines and emission models simultaneously ensured that uncertainties on the baseline fit were propagated into uncertainties on each retrieved quantity (i.e., N or T_{rot}). These fits included a correction for opacity effects on a spaxel-by-spaxel basis (see G. Villanueva et al. 2025; N. X. Roth et al. 2023, for further details).

We used a fixed resolution element, $\Delta\lambda$, that was determined based on the central wavelength of each spectral extract. For $1.80 \mu\text{m} \leq \lambda \leq 3.2 \mu\text{m}$, we set $\Delta\lambda = 0.79 \text{ nm}$, and for $3.2 \mu\text{m} < \lambda \leq 5.10 \mu\text{m}$, we set $\Delta\lambda = 1.32 \text{ nm}$. These values are in good agreement with those from curves for dispersion as a function of wavelength provided by the Space Telescope Science Institute¹⁴. We assumed a gas expansion speed, v_{exp} , of 0.345 km s^{-1} for CO and 0.310 km s^{-1} for all other species based on velocity resolved ALMA measurements of CO and HCN on 2025 December 22 (M. Cordiner et al. 2026). Uncertainties on the derived parameters were retrieved from the diagonal elements of the covariance matrix, scaled by the square root of the reduced χ^2 statistic of the fit.

We generated our maps using spectra extracted from relatively unblended molecular bands of each species. This included the CO ($v = 1 - 0$) band centered near $4.66 \mu\text{m}$, the CO₂ ν_3 band centered near $4.25 \mu\text{m}$, the H₂O $\nu_1 + \nu_3$ band near $2.68 \mu\text{m}$, the CH₃OH ν_3 band near $3.51 \mu\text{m}$, and the CH₄ ν_3 band centered near $3.30 \mu\text{m}$. Although we did not detect spectrally unblended lines of OH* (prompt emission, the vibrationally excited photodissociation product of H₂O which traces the spatial distribution of the latter; B. P. Bonev et al. 2006), we conservatively included it in our models by setting $N(\text{OH}^*) = N(\text{H}_2\text{O})$ when retrieving $N(\text{CH}_3\text{OH})$. We then fixed the assumed $N(\text{OH}^*)$ and derived $N(\text{CH}_3\text{OH})$ at each spaxel when retrieving $N(\text{CH}_4)$ and $T_{\text{rot}}(\text{CH}_4)$. We constrained our maps to within ± 15 spaxels of the nucleus position (corresponding to $\pm \sim 1800 \text{ km}$ projected distance) owing to insufficient SNR at larger distances, especially for CH₄ and CH₃OH.

In addition to providing the overall H₂O column density, the H₂O $2.68 \mu\text{m}$ band includes multiple strong, unblended lines of its nuclear spin isomers, ortho- and para-H₂O, enabling us to generate maps of $N(o - \text{H}_2\text{O})$ and $N(p - \text{H}_2\text{O})$. We used these to create a map of the ortho-to-para ratio (OPR) for H₂O. The NASA PSG generates g -factors for ortho- and para-H₂O assuming the statistical equilibrium value of 3 regardless of T_{rot} (G. Villanueva et al. 2025). Thus, $\text{OPR} = 3 \times N(o - \text{H}_2\text{O})/N(p - \text{H}_2\text{O})$ as modeled with the PSG.

Although the H₂O hot bands near $4.5 \mu\text{m}$ measured on December 23 were detected with a sufficient signal-to-noise ratio (SNR) to derive N , we could not determine a well-constrained OPR or T_{rot} . We instead assumed the OPR and radial dependence of $T_{\text{rot}}(\text{H}_2\text{O})$ determined from the $2.68 \mu\text{m}$ bands on December 22 and fixed that when retrieving $N(\text{H}_2\text{O})$ on December 23. To account for several H₂O hot band lines which blend with CO, we then fixed $N(\text{H}_2\text{O})$ at each spaxel while retrieving $N(\text{CO})$ and $T_{\text{rot}}(\text{CO})$.

3. RESULTS

A representative JWST spectrum of 3I/ATLAS extracted from a nucleus-centered $1''.5$ diameter aperture is shown in Figure 1. Our resulting spaxel-by-spaxel maps for CO, CO₂, H₂O, CH₃OH, and CH₄ are shown in Figure 2. Maps of o-H₂O, p-H₂O, and OPR are shown in Figure 3. The difference in spatial coverage between the $2.68 \mu\text{m}$ H₂O maps and those of the remaining species is owing to the single G235H exposure for the former vs. five stacked G395H exposures for the latter. A comparison of H₂O maps derived on December 22 and December 23 is given in Appendix B. Here we analyze the higher S/N H₂O emission from the $2.7 \mu\text{m}$ band measured on December 22.

Expansion dilution of the coma leaves trends in gas distribution difficult to discern in plots of N . Plotting $N \times \rho$, where ρ (m) is the radial distance from the nucleus, corrects for this effect and more readily reveals coma anisotropies: isotropic outgassing in the absence of photolysis and coma acceleration would produce a flat $N \times \rho$ dependence with nucleocentric distance. Differences are dramatically evident among the major constituents of 3I/ATLAS's coma as

¹⁴ <https://jwst-docs.stsci.edu/jwst-near-infrared-spectrograph/nirspec-instrumentation/nirspec-dispersers-and-filters#gsc.tab=0>

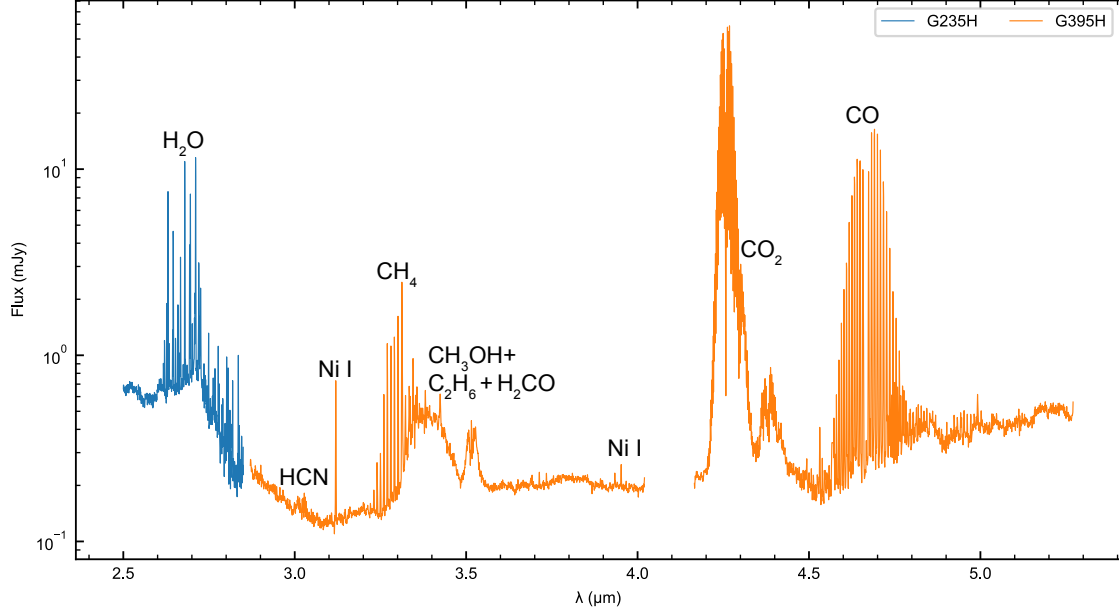


Figure 1. JWST spectrum of 3I/ATLAS extracted in a $1''.5$ diameter aperture centered on the nucleus position. Major species are labeled.

shown in Figure 2. Continuum maps are provided in Appendix C for comparison with the gas. A comparison of maps produced with and without the PSG correction for opacity is given in Appendix D.

As $N \propto Q/v_{\text{exp}}$, is important to keep in mind that asymmetries in v_{exp} will manifest as asymmetries in the $N \times \rho$ maps. The strong asymmetries in T_{rot} for CO and CO_2 mean such an asymmetry in v_{exp} is expected, but the JWST data do not have sufficient spectral resolution to test this. CO, the most abundant molecule by at least a factor of two, shows an apparent dual jet structure, with one oriented in the projected sunward direction and another perpendicular to it. The sunward jet is physically consistent with the lower T_{rot} projected in the same direction, yet the absence of a corresponding trend in T_{rot} along the perpendicular jet is puzzling.

CO_2 and CH_4 display a simpler morphology with apparent excess in the projected anti-sunward direction. The anti-sunward excess of CO_2 may be an effect of an asymmetry in v_{exp} if the asymmetry were not sufficiently strong to be reflected in the CO map. Alternatively, the contrasting distributions of CO and CO_2 may be due to the effects of rotation of differing active sites into and out of the field of view along the line of sight, as our observations covered $\sim 1/3$ of 3I/ATLAS’s 16.16 hr. rotational period (T. Santana-Ros et al. 2025). Analysis of time-series spectra is beyond the scope of this manuscript and the subject of a future publication.

In contrast, H_2O and CH_3OH (although at lower SNR for the latter) show $N \times \rho$ maps which are much more symmetric. Although there is an appearance of increasing $N \times \rho$ with ρ for these species, which may be consistent with production from extended sources such as icy grain sublimation, it is important to note that the innermost spaxels are affected by significant flux losses due to the finite PSF, and the significance of the trend is unclear. However, M. Cordiner et al. (2026) found evidence for an H_2O extended source based on “Q-curve” analysis of the less optically thick $4.5 \mu\text{m}$ hot bands.

The spatial variations in T_{rot} are similarly striking and vary from molecule to molecule. CO, CO_2 , and CH_4 show a common temperature morphology, having distinctly higher values in the projected anti-sunward direction. On the whole, these molecules have higher T_{rot} (and maintain it to greater nucleocentric distances) than CH_3OH or H_2O . In contrast, the H_2O temperature peaks at the nucleus position and drops quickly and nearly isotropically. CH_3OH appears to follow a similar spatial morphology to H_2O , but SNR limitations preclude a detailed inter-comparison between these species.

An average column density, $\langle N \rangle$, was calculated by averaging individual column densities derived for each spaxel within a $0''.2$ wide annulus centered on the nucleus, which was defined as the continuum photocenter, with $r_{\text{in}} = 1''.6$

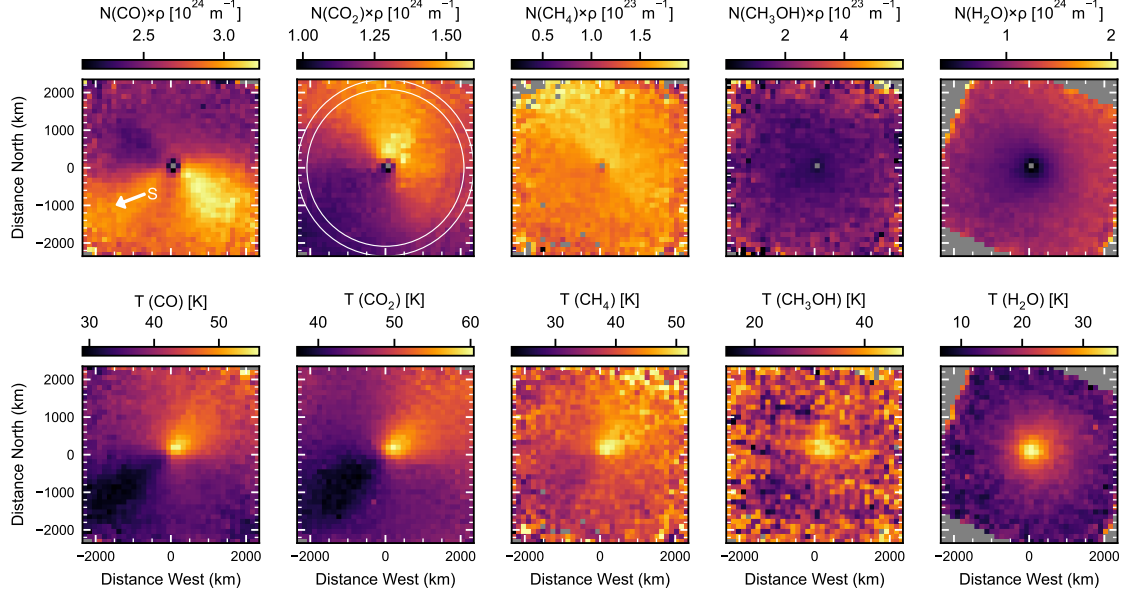


Figure 2. Upper Panels. Maps of $N \times \rho$ for CO, CO₂, CH₄, CH₃OH, and H₂O. The white arrow shows the projected direction of the Sun. The white annulus shows the region used to calculate representative Q . Note that the H₂O map was derived from the 2.68 μ m bands measured on December 22, whereas the remaining maps were constructed from the December 23 observations. **Lower Panels.** Maps of molecular rotational temperatures.

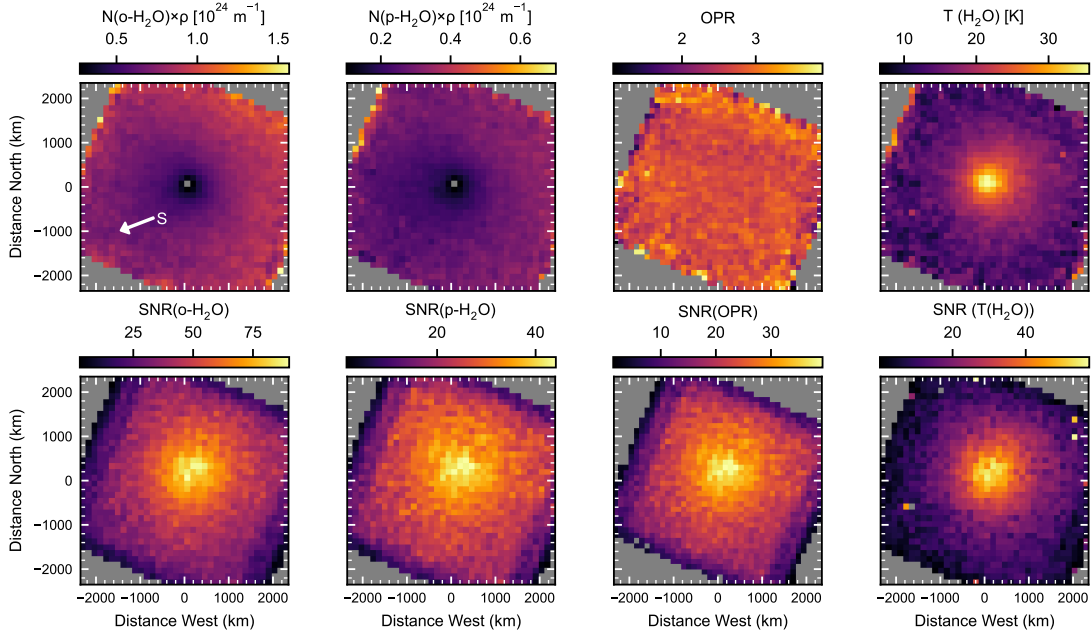


Figure 3. Upper Panels. Maps of $N \times \rho$ for ortho-H₂O and para-H₂O, the derived OPR, and $T_{\text{rot}}(\text{H}_2\text{O})$ for the 2.68 μ m band measured on December 22. Note that N for each species has been corrected for the derived OPR. **Lower Panels.** Signal-to-noise ratio (SNR) for each of the respective quantities in the upper panels.

Table 1. Molecular Production Rates in 3I/ATLAS and Comets Measured

Molecule	Q (10^{26} s^{-1})	$Q_x/Q(\text{CO})$ (%)	$Q_x/Q(\text{H}_2\text{O})$ (%)	$\langle Q_x/Q(\text{H}_2\text{O}) \rangle$ (%)
2025 December 22, G235H/F170LP				
H ₂ O	15.7 ± 0.1	...	100	100
2025 December 23, G395H/F290LP				
CO	38.2 ± 0.1	100	246 ± 19	5.2 ± 1.3
CO ₂	15.9 ± 0.1	41.6 ± 0.3	103 ± 8	12 ± 2
H ₂ O	15.5 ± 1.2	40.6 ± 3.1	100	100
CH ₃ OH	2.65 ± 0.03	6.94 ± 0.09	17.1 ± 1.3	2.06 ± 0.20
CH ₄	2.06 ± 0.01	5.39 ± 0.03	13.3 ± 1.0	0.78 ± 0.09

NOTE— $\langle Q_x/Q(\text{H}_2\text{O}) \rangle$ are average molecular abundances with respect to water in comets reported in [O. Harrington Pinto et al. \(2022\)](#); [N. Dello Russo et al. \(2016\)](#).

and $r_{\text{out}} = 1''8$. These $\langle N \rangle$ were converted to representative molecular production rates (Q , s^{-1}) following [B. P. Bonev et al. \(2017\)](#) as:

$$Q = \frac{\langle N \rangle A_{\text{FOV}}}{\tau(r_H) f(x)} \quad (1)$$

where A_{FOV} is the area of the aperture (m^2), $\tau(r_H)$ is the molecular photolysis lifetime at r_H ([W. F. Huebner & J. Mukherjee 2015](#)), and $f(x)$ is the Haser filling factor (the fraction of coma molecules expected within the aperture after correcting for adiabatic expansion and solar photolysis). The resulting production rates are given in Table 1.

Our map of the OPR for H₂O demonstrates an essentially flat value with nucleocentric distance, independent of changes in the total column density, T_{rot} , or SNR. We derived a coma-averaged value of OPR = 2.7 ± 0.2 by calculating statistics for values retrieved within a 10-spaxel radius of the comet photocenter (Appendix E).

4. DISCUSSION AND INTERPRETATION

4.1. Evolving Heterogeneous Outgassing

Our measurements reveal a CO-driven coma in 3I/ATLAS ($\text{CO}_2/\text{CO} = (42.4 \pm 0.9)\%$ and $\text{H}_2\text{O}/\text{CO} = (44.4 \pm 0.7)\%$) with a complex outgassing geometry which varies from species to species. The volatile composition of 3I/ATLAS during our observations is in general super-enriched compared to water with respect to values found in solar system comets ([N. Dello Russo et al. 2016](#); [O. Harrington Pinto et al. 2022](#); [N. Biver et al. 2024b](#)). Our measurements provide a rare characterization of the interplay between N and T_{rot} for a comet at $r_H \sim 2.4$ au post-perihelion, and thus traversing the H₂O ice line.

At these distances, H₂O sublimation becomes less vigorous as solar insolation attenuates, leaving CO and CO₂ to gradually overtake H₂O as the primary activity drivers. The analysis of these three species in [M. Cordiner et al. \(2026\)](#) is consistent with 3I/ATLAS's transition from H₂O- to CO-dominated outgassing as it receded from the Sun. Since the majority of comet composition studies are undertaken interior to $r_H \sim 3$ au in H₂O-dominated comae (e.g., [N. Dello Russo et al. 2016](#); [M. Lippi et al. 2021](#), and references therein), this caveat must be kept in mind, as $Q(x)/Q(\text{H}_2\text{O})$ in 3I/ATLAS during our observations may no longer be strictly indicative of bulk nucleus ice abundances. On the other hand, serial pre-perihelion ALMA measurements and near-perihelion IRAM 30-m measurements of CH₃OH found that it was significantly enriched compared to solar system comets ([N. X. Roth et al. 2026a](#); [N. Biver et al. 2026](#)), consistent with the interpretation that 3I/ATLAS was generally enriched in trace volatiles regardless of activity driver.

Our representative $Q(\text{CO})$ and $Q(\text{CO}_2)$ are each slightly lower than reported in [M. Cordiner et al. \(2026\)](#), whereas our $Q(\text{H}_2\text{O})$ on December 22 is higher, but the value on December 23 agrees with theirs within 1σ . Both studies are consistent with a CO-dominated coma where H₂O/CO and CO₂/CO were on the order of 40%. These differences may

be explained by differing methodologies for each study: whereas [M. Cordiner et al. \(2026\)](#) constructed a “Q-curve” and calculated terminal production rates based on the averages of several annuli, we report Q calculated from a single outer annulus. Similarly, our $Q(\text{CH}_4)$ and $Q(\text{CO}_2)$ are lower than reported in [M. Belyakov et al. \(2026\)](#) based on JWST MIRI observations taken five days before and four days after our observations, although they hypothesized that $Q(\text{CH}_4)$ was quite variable during mid-late December. The differences in $Q(\text{CO}_2)$ may be attributed to additional uncertainties in modeling the $15\ \mu\text{m}$ CO_2 band measured with MIRI, which is superimposed on strong thermal emission, compared to the $4.25\ \mu\text{m}$ band measured with NIRSpec in this study. Future JWST observations of cometary CO_2 with significantly smaller temporal separation between MIRI and NIRSpec measurements may help to reconcile potential uncertainties when modeling the emission bands sampled by each instrument.

The molecule-dependent coma morphology observed in 3I/ATLAS resembles the heterogeneous jet structures identified in the Centaur 29P/Schwassmann–Wachmann 1 ([S. Faggi et al. 2024](#)). However, unlike 29P, whose activity is driven primarily by hypervolatiles at a heliocentric distance of ≈ 5 au, the JWST observations of 3I/ATLAS were obtained following intense perihelion activity, during which water production reached $\sim 2 \times 10^{29}\ \text{s}^{-1}$ ([M. R. Combi et al. 2026](#)). The observed volatile segregation may therefore reflect the exposure of chemically heterogeneous subsurface reservoirs following substantial perihelion mass loss rather than purely primordial compositional heterogeneity, similar to the evolution of comets C/2009 P1 (Garradd) and 2I/Borisov ([D. Bodewits et al. 2014](#); [D. Bodewits et al. 2020](#)).

4.2. Coma Physics of an Interstellar Object

The coma physics in 3I/ATLAS revealed by our maps are just as remarkable as its molecular abundances. It is important to note that these maps are inherently biased to emission perpendicular to the line of sight owing to the low spectral resolution of JWST. Velocity-resolved measurements from radio facilities (e.g., [N. Biver et al. 2026](#); [M. Cordiner et al. 2026](#)) are required to incorporate a detailed treatment of emission along the line of sight. Such an integration and analysis is the subject of a future publication. Nevertheless, the CO, CO_2 , and CH_4 rotational temperatures show a clear dichotomy along an axis similar to the sky-projected Sun-comet radius vector, with the anti-sunward direction providing considerably higher values. Similar behavior has been observed in other comets, namely joint JWST and ALMA studies of comet C/2022 E3 (ZTF; [K. D. Foster et al. 2026](#)) and ALMA and IRAM 30-m studies of comet 46P/Wirtanen ([M. A. Cordiner et al. 2023](#); [N. Biver et al. 2021](#)). This was explained by a combination of more efficient adiabatic cooling in the sunward-facing hemisphere of the coma, along with the heating effects of icy grain sublimation in the anti-sunward direction.

Most comets are characterized via remote sensing when they are within ~ 3 au from the Sun (e.g., [M. Lippi et al. 2021](#); [N. Dello Russo et al. 2016](#)). For these studies, H_2O is the most abundant coma molecule and dominates excitation in the inner coma ($r < 1000$ km; [V. Tenishev et al. 2008](#); [N. Fougere et al. 2012](#); [R. Marschall et al. 2024](#)), where collisions thermalize the rotational temperature to the kinetic temperature of the gas. Yet H_2O was a trace species during our observations of 3I/ATLAS, and the spatial distributions of its column density and rotational temperature stand apart from all other molecules (except CH_3OH) in this study. These differences in coma temperature distributions can be understood in terms of the overall abundances and radiative cooling efficiencies of each species. CO is the most abundant molecule and plays an outsized role in setting the temperature structure of the coma. However, CO_2 and H_2O are both $\sim 40\%$ of CO and must contribute as well. The apolar species are likely the best tracers of the kinetic temperature profile of the inner, collisional coma given their small dipole moments (and thus lower radiative cooling efficiency), whereas the rotational temperature profiles for the polar species H_2O and CH_3OH depart from the kinetic temperature more quickly ([D. Bodewits et al. 2024](#)).

We calculated azimuthally averaged radial T_{rot} profiles for CO, CH_3OH , and H_2O in 3I/ATLAS and compared them against predictions from the three-dimensional SUBLIME radiative transfer and excitation model for cometary atmospheres ([M. A. Cordiner et al. 2022](#)). Our methods for generating the SUBLIME models are detailed in Appendix F. It is important to note that our spherically symmetric SUBLIME models do not attempt to reproduce the complex, anisotropic, and species-dependent outgassing geometry evident in Figure 2 and are only intended to test whether the general trends observed in the coma of 3I/ATLAS can be reproduced with state-of-the-art radiative transfer models. Figure 4 shows a progression for each species that indeed qualitatively matches our observations. The CO model drops by only ~ 8 K within 1750 km from the nucleus, yet remains ~ 2 K warmer than the observations. In contrast, the H_2O model falls out of collisional equilibrium quickly and dramatically owing to its higher dipole moment and radiative cooling efficiency, whereas CH_3OH follows an intermediate trend in cooling. The observed CH_3OH T_{rot} cools significantly more quickly than the models close to the nucleus. Similarly, the observed H_2O T_{rot} profile is cooler than

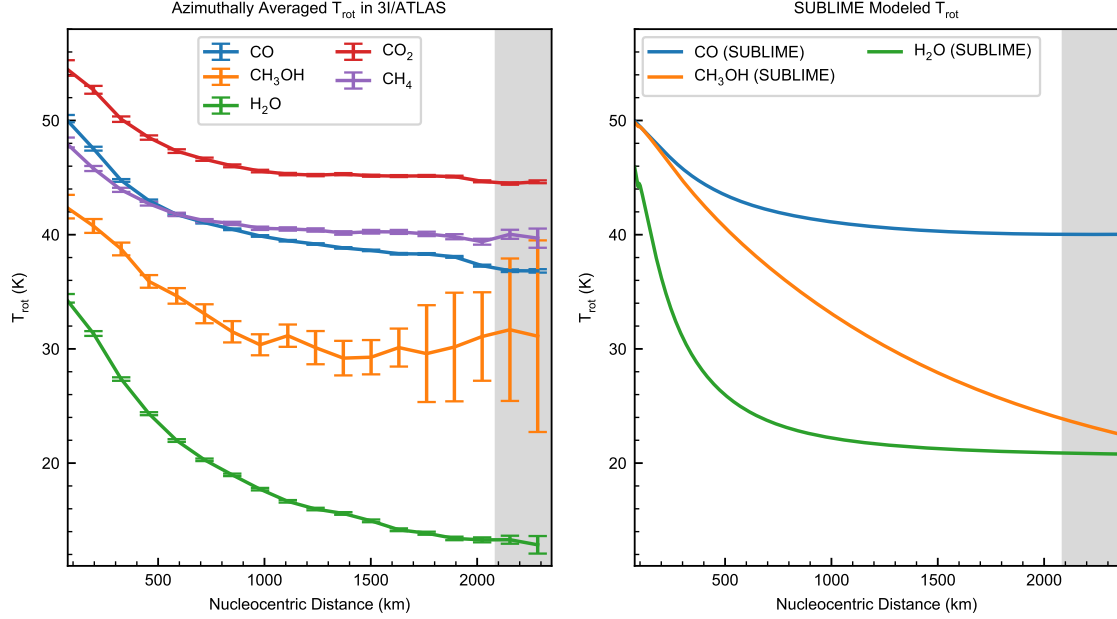


Figure 4. **Left.** Observed azimuthally averaged T_{rot} for CO, CO₂, CH₄, CH₃OH, and H₂O. **Right.** Modeled T_{rot} as a function of nucleocentric distance for CO, CH₃OH, and H₂O using the SUBLIME radiative transfer code. The gray shaded region shows the projected radial extent of the annulus from which representative Q 's were extracted for each molecule (Table 1). The x -axis extends to approximately the field of view of our spatial-spectral maps.

the model close to the nucleus, yet the model's steep initial cooling levels off at ~ 1000 km from the nucleus whereas the observed profile continues to drop. The slower drop in the observed temperature compared to the model may be a signature of sublimative gas heating from icy grains in the coma, consistent with the results of M. Cordiner et al. (2026). Additional cooling through mechanisms such as coma gas acceleration may explain these trends, but these effects are not considered in our models. These observational and model results in 3I/ATLAS for polar vs. apolar species as a function of increasing nucleocentric distance are consistent with predictions for comets in general (D. Bodewits et al. 2024).

The rotational temperature distributions are remarkably similar to results found by JWST for comet C/2017 K2 (PanSTARRS), where the temperature distributions of H₂O and CH₃OH were closely matched, yet CH₄ and (to a lesser extent) CO followed that of CO₂, despite CO and CH₄ having considerably different column density distributions from CO₂ (C. E. Woodward et al. 2025). The trends in the overall magnitude of the CO, CO₂, and CH₄ temperatures compared to H₂O and CH₃OH in 3I/ATLAS were also very similar to C/2017 K2, with the former apolar species being higher (and staying so) out to considerably larger nucleocentric distances than the latter polar species. This was explained in terms of the increased rotational cooling efficiency for polar H₂O and CH₃OH compared to apolar CO, CO₂, and CH₄ (C. E. Woodward et al. 2025). It is interesting to note that observations of C/2017 K2 were conducted when H₂O was the dominant volatile, whereas our observations of 3I/ATLAS were of a CO-driven coma.

4.3. Ortho-to-Para Ratio and Spin Temperatures in Comets

Despite its relegation to a trace species during our observations of 3I/ATLAS, H₂O provides insights into the nature of the OPR in comets. Water, like many hydrogen-bearing molecules, exists in distinct nuclear spin symmetry forms known as ortho and para species. These forms arise from the fundamental quantum mechanical requirement that the total molecular wavefunction obey specific symmetry constraints under exchange of identical nuclei. In H₂O, the two equivalent protons give rise to ortho and para states with statistical weights in a 3:1 ratio. Under thermodynamic equilibrium, the OPR depends on temperature. At high temperatures, the OPR approaches the statistical value of three, whereas at low temperatures the population shifts toward the lowest-energy symmetry species. The temperature that reproduces a measured OPR under equilibrium conditions is referred to as the spin temperature.

A key property of ortho and para species is their radiative independence. Electric dipole transitions conserve nuclear spin symmetry; consequently, ortho levels are connected only to other ortho levels, and para levels only to para levels. Radiative processes therefore cannot inter-convert the two species. Conversion requires specific non-radiative mechanisms, such as proton exchange reactions, interactions with paramagnetic species, catalytic processes on surfaces, or magnetic interactions. In low-density astrophysical environments and cometary comae, these processes may proceed slowly, allowing the OPR to become effectively “frozen”.

This radiative isolation historically motivated the interpretation that the measured spin temperature may reflect the temperature at which the molecule formed or last achieved nuclear spin equilibrium (e.g., M. J. Mumma et al. 1987; B. P. Bonev et al. 2007; D. Bockelée-Morvan et al. 2009; G. L. Villanueva et al. 2011). However, recent laboratory studies suggest a more complex picture, indicating that the OPR may be reset upon desorption (e.g., T. Hama et al. 2018) and that spin symmetry properties can be partially altered during phase transitions between ice and gas (e.g., K. M. Yocum et al. 2023).

In the case of 3I/ATLAS, we find that the OPR remains equilibrated and notably constant throughout the coma, even as the rotational temperature falls below 30 K. This represents a significant new observational result in the study of cometary OPRs. Although previous works (B. P. Bonev et al. 2007; D. Bockelée-Morvan et al. 2009) have found similar results at higher temperatures, none have demonstrated these trends at such cold temperatures. The constancy of the ratio indicates that it is not being reset within the coma and instead reflects conditions associated with the release of water from the nucleus. The coma-averaged OPR = 2.7 ± 0.2 corresponds to $T_{\text{spin}} = 34^{+11}_{-5}$ K, yet whether the measured OPR directly traces the formation conditions or origin of the object remains uncertain. Nevertheless, the 3I/ATLAS observations show that rapid physical processes in the expanding coma, including substantial adiabatic cooling, are insufficient to alter the statistical spin symmetry distribution of the molecule once it has been established.

5. CONCLUSION

The sensitivity and spatial-spectral mapping capabilities of JWST have revealed the coma physics of an interstellar object as it receded from its encounter with our Sun. Our spaxel-by-spaxel maps show stark dichotomies in the column density and rotational temperature distributions of the apolar vs. polar species in 3I/ATLAS’ coma. CO was the most abundant molecule and set the overall temperature structure of the coma, yet the increased radiative cooling efficiency of the polar molecules caused them to fall out of thermal equilibrium much more quickly than their apolar counterparts, resulting in significantly different T_{rot} distributions for CH₃OH and H₂O compared to CO, CO₂, and CH₄. Our high-resolution mapping of the OPR in H₂O measured a flat dependence with nucleocentric distance even at low (< 20 K) temperatures, confirming that the OPR is not altered in the coma. Reproducing the complexity of coma excitation revealed in 3I/ATLAS will require new detailed kinetic modeling as JWST measurements of H₂O and CO₂ in comets challenge our understanding of coma physics.

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Table 2. Observing Log

Date	UT Time	T_{int}	r_{H}	Δ_{JWST}	ϕ_{STO}	λ
(2025)		(s)	(au)	(au)	($^{\circ}$)	(μm)
22 Dec	03:36	642	2.37	1.79	22.7	1.06 – 3.05
23 Dec	08:07	700	2.40	1.80	21.8	2.87 – 5.14
	09:57	700	2.41	1.80	21.8	2.87 – 5.14
	11:43	700	2.41	1.80	21.7	2.87 – 5.14
	12:56	700	2.41	1.80	21.7	2.87 – 5.14
	13:58	700	2.41	1.80	21.7	2.87 – 5.14

NOTE—UT times are given at the start of each exposure. T_{int} is the total on-source integration time. r_{H} , Δ_{JWST} , and ϕ_{STO} , and $\psi_{\odot}$ are the heliocentric distance, JWST-centric distance, and phase angle (Sun–Comet–Earth), respectively, of 3I/ATLAS at the time of observations.

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Software: Astropy ([Astropy Collaboration et al. 2013, 2018, 2022](#)), Astroquery ([A. Ginsburg et al. 2019](#)), photutils ([L. Bradley et al. 2025](#)), jwstComet ([N. X. Roth 2026b](#))

APPENDIX

A. OBSERVING LOG

Table 2 provides an observing log for our JWST observations of 3I/ATLAS.

B. COMPARISON OF H₂O MAPS ON DECEMBER 22 AND DECEMBER 23

Figure 5 shows a comparison of H₂O maps in 3I/ATLAS on December 22 (2.7 μm band measured with G235H) and December 23 (4.5 μm band measured with G395H).

C. CONTINUUM MAPS IN 3I/ATLAS

Figure 6 shows continuum maps in 3I/ATLAS (multiple by ρ) for the G235H (December 22) and G395H (December 23) settings.

D. OPACITY CORRECTIONS TO COLUMN DENSITY IN THE PSG

We refer to [G. Villanueva et al. \(2025\)](#); [N. X. Roth et al. \(2023\)](#) for a detailed discussion of the opacity corrections performed by the PSG. Here we give a brief overview of the formalism and document how the corrections affected our calculated N for the major species in 3I/ATLAS’ coma during our observations: CO, CO₂, and H₂O.

For a low solar phase angle, the integrated column density measured by an observer is approximately the column density of the incident solar flux. The average linewidth of the pump (w_p , cm^{−1}) can be computed as $w_p = (2v_p f_{ul}/c)$,

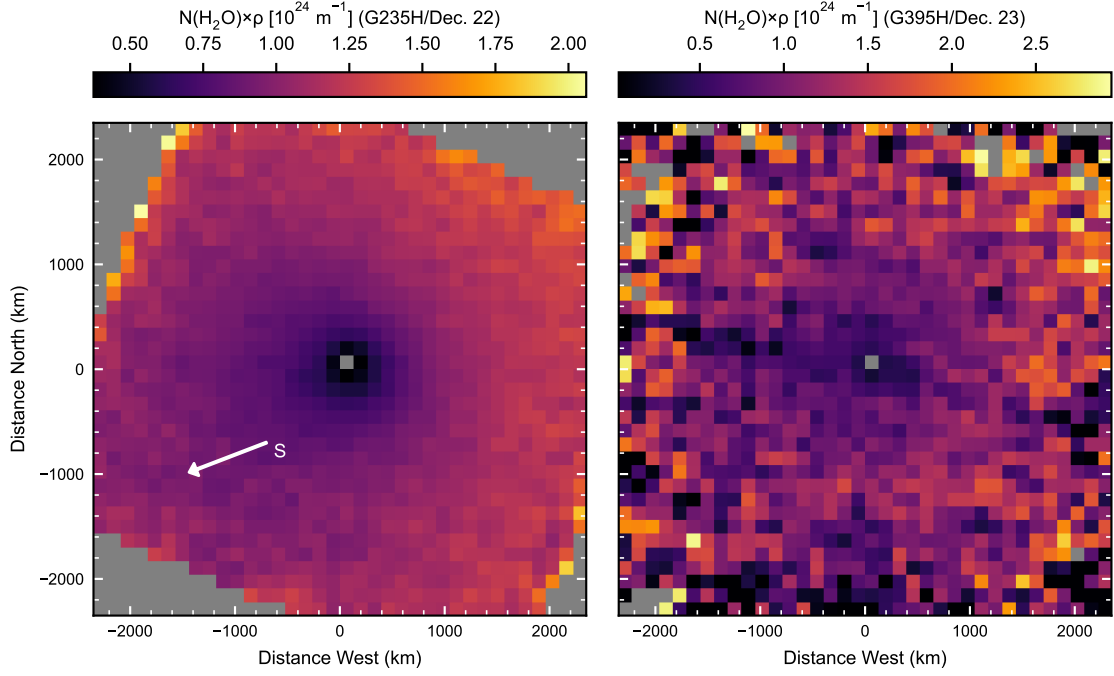


Figure 5. **Left.** H_2O map in 3I/ATLAS on December 22. **Right.** H_2O map in 3I/ATLAS on December 23.

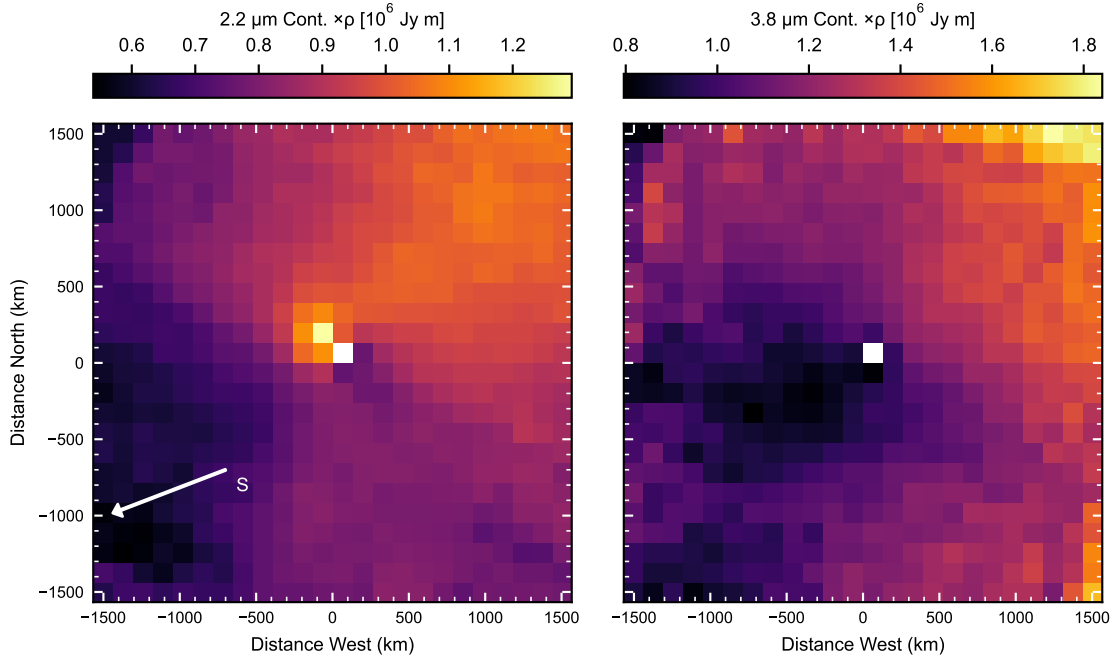


Figure 6. **Left.** Map of the $2.2 \mu\text{m}$ continuum intensity, measured on December 22, multiplied by ρ . **Right.** Map of the $3.8 \mu\text{m}$ continuum intensity, measured on December 23, multiplied by ρ .

where v_p is the gas expansion velocity (m s^{-1}), f_{ul} is the emission frequency (cm^{-1}), and c is the speed of light. The integrated opacity across the pump is then $\tau_p = N_{\text{col}} S_p / v_p$, where N_{col} is the integrated column density (molecules cm^{-2}) along the line of sight and S_p is a weighted “representative” line intensity ($\text{cm}^{-1} \text{ molecule cm}^{-2}$). This weighted line intensity is calculated after keeping track of the associated line intensities that result in the specific emission for every g -factor ($\text{photon s}^{-1} \text{ molecule}^{-1}$) and calculating a corresponding weighted pump intensity.

The transmittance at the end of the column is $e^{-\tau_p}$ at the frequency of the pump. For low opacities, the pumps are optically thin given the small number of molecules attenuating the solar pump at the pump frequency. As the opacity increases along the column for the solar pump, the observer only receives radiation up to $\tau_p < 1$, so the expected fluorescence efficiency can be approximated as

$$g_{\text{thick}} = \frac{1 - e^{-\tau_p}}{\tau_p} g_{\text{thin}} \quad (\text{D1})$$

We note that this is a first-order correction to a complex problem. Applying the correction, the optically thin column density is related to the optically thin column density and optically thin g -factors (g_i) as

$$N_{\text{thick}} = \frac{\sum_i \frac{(1 - e^{-\tau_i})}{\tau_i} g_i}{\sum_i g_i} N_{\text{thin}} \quad (\text{D2})$$

We applied these corrections to all retrievals in this study when generating our maps. We also generated maps forcing the use of optically thin g -factors for comparison. Figure 7 shows the differences in retrieved quantities for our maps for CO, CO₂, and H₂O. As expected, the most significant differences occur in the central spaxels (where PSF losses are also at play) and for CO and CO₂. Differences for H₂O are much smaller, consistent with its lower opacity throughout the NIRSpc field of view. We note that the annulus used to calculate representative Q ’s is located in the outer regions of the field of view, where agreement between the optically thick and optically thin quantities is good for all species.

E. COMA AVERAGED H₂O OPR

Figure 8 shows our coma-averaged OPR generated by considering statistics within a 10-spaxel radius of the photo-center.

F. SUBLIME RADIATIVE TRANSFER MODELS

The SUBLIME radiative transfer model includes a full non-LTE treatment of coma gases, collisions with molecules and electrons, and pumping by solar radiation, along with a time-dependent integration of the energy level population equations. We calculated collisional rates for each species with CO (the dominant coma molecule during our observations) using the thermalization approximation (J. Crovisier 1987; N. Biver et al. 1999; D. Bockelée-Morvan et al. 2012), using an average collisional cross-section with CO of $5 \times 10^{-14} \text{ cm}^2$ and an electron collisional scaling factor $x_{\text{ne}} = 0.2$ (M. A. Cordiner et al. 2025a). We used a spherically symmetric outgassing model and set the gas expansion velocity to constant values of 0.345 km s^{-1} for CO and 0.310 km s^{-1} for CH₃OH and H₂O (M. Cordiner et al. 2026). We set molecular production rates for each species to their values in Table 1. We generated a radial kinetic temperature profile matching the observed azimuthally averaged T_{rot} profile for CO. We then calculated the model T_{rot} as a function of radius for each species using molecular linelists from the LAMDA database (F. L. Schöier et al. 2005; D. Rabli & D. R. Flower 2010). We included rotational energy levels up to $E_u \leq 4500 \text{ K}$ for CO, $E_u \leq 1400 \text{ K}$ for H₂O, and $E_u \leq 400 \text{ K}$ for CH₃OH. These cutoffs minimize computational complexity while still adequately sampling the rotational energy manifold at the $\sim 20 - 50 \text{ K}$ rotational temperatures in the coma of 3I/ATLAS.

G. HCN AND NI IN 3I/ATLAS

We additionally detected HCN and Ni I in 3I/ATLAS; however, the SNR of the former at off-nucleus positions was insufficient for spaxel-by-spaxel mapping. We instead extracted a single spectrum from a $1''.5$ diameter nucleus-centered aperture (Figure 9) and retrieved $Q(\text{HCN})$ and $T_{\text{rot}}(\text{HCN})$ with the PSG. We obtain $Q(\text{HCN}) = (8.22 \pm 0.67) \times 10^{24} \text{ s}^{-1}$ and $T_{\text{rot}}(\text{HCN}) = 27 \pm 3 \text{ K}$. The resulting molecular abundance ratios are $\text{HCN}/\text{CO} = (0.22 \pm 0.02)\%$ and $\text{HCN}/\text{H}_2\text{O} = (0.53 \pm 0.06)\%$. This T_{rot} for polar HCN is consistent with the trends measured for CH₃OH and H₂O compared to the apolar species.

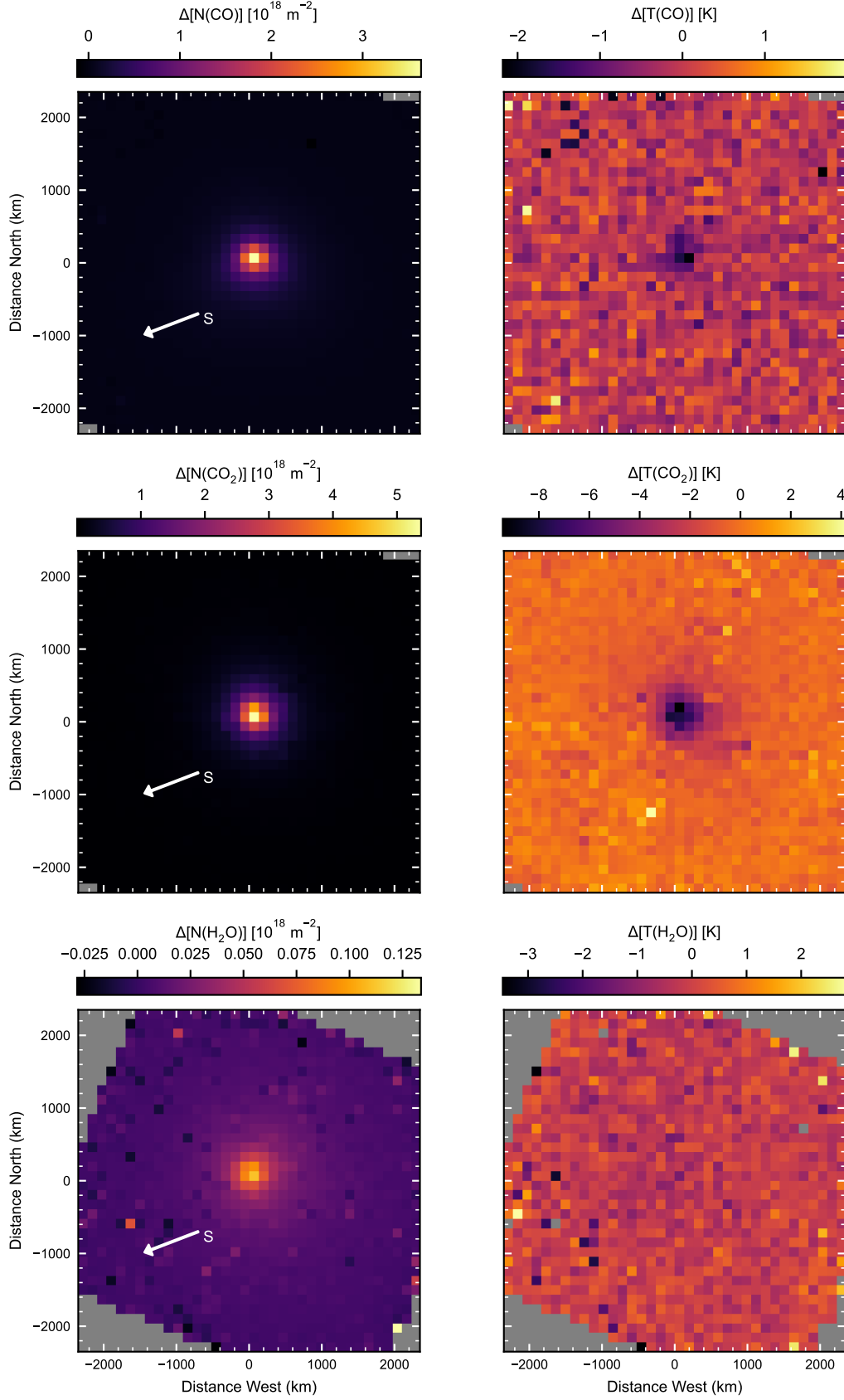


Figure 7. From top. Maps of differences between N and T_{rot} for optically thick and optically thin PSG retrievals for CO, CO₂, and H₂O, where $\Delta N = N_{\text{thick}} - N_{\text{thin}}$ and $\Delta T = T_{\text{thick}} - T_{\text{thin}}$.

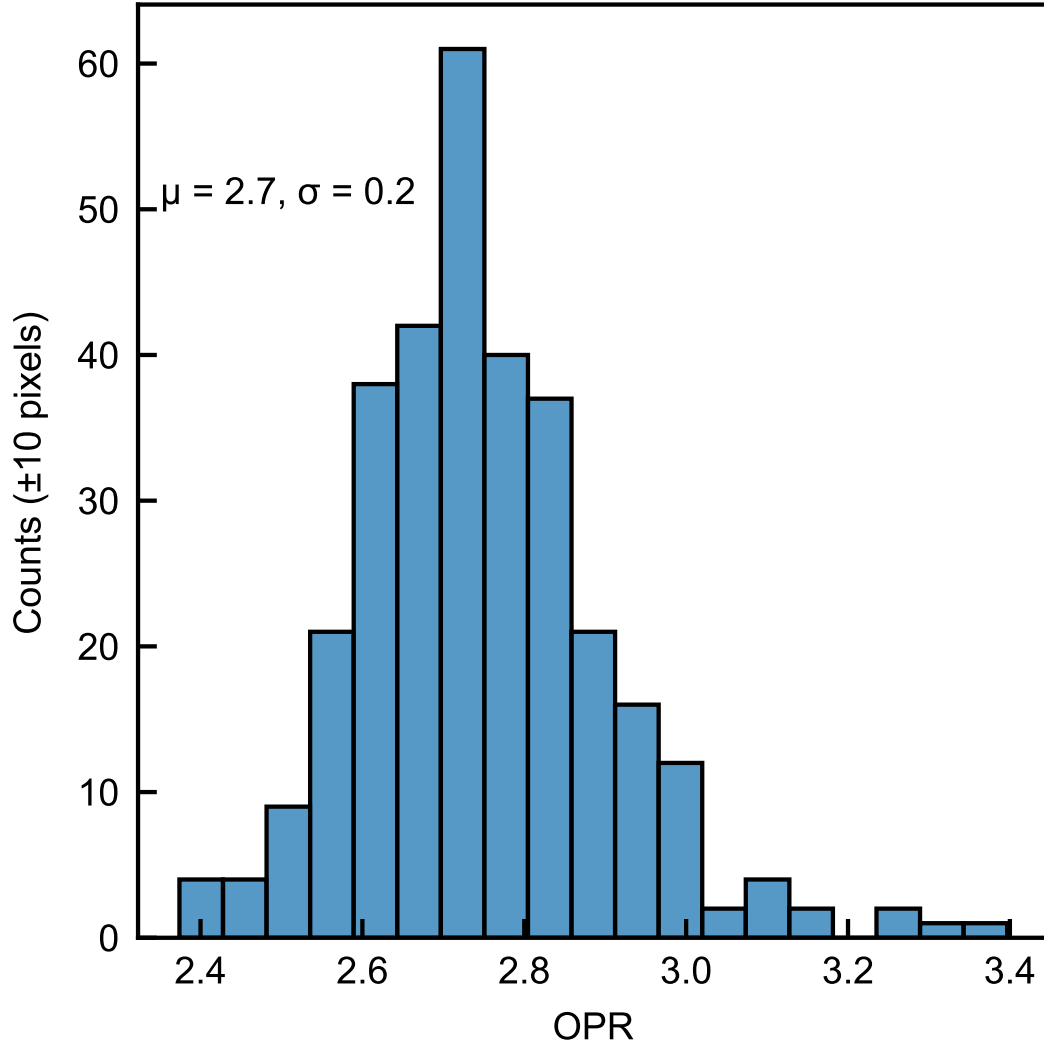


Figure 8. Histogram of spaxel-by-spaxel OPR values for H₂O drawn within a 10-spaxel radius of the comet photocenter.

Table 3. Detected Ni I Lines in 3I/ATLAS

λ (μm)	$\int F_{\lambda} d\lambda$ ($10^{-19} \text{ W m}^{-2}$)	g ($10^{-24} \text{ J s}^{-1} \text{ mol}^{-1}$)	A (10^{-3} s^{-1})	Lower Level	Upper Level	Confidence
3.119	17.3 ± 0.1	112 ± 34	78	$3d^9(^2D)4s(^3D_3)$	$3d^9(^2D)4s(^1D_2)$	D
3.915	1.21 ± 0.06	7.0 ± 2.1	6.2	$3d^9(^2D)4s(^3D_2)$	$3d^9(^2D)4s(^1D_2)$	D

NOTE— λ is the lab-measured wavelength of each transition. $\int F_{\lambda} d\lambda$ is the integrated intensity of each transition in 3I/ATLAS extracted from a nucleus-centered $1''.5$ diameter aperture. g is the calculated g-factor and A is the Einstein-A coefficient. The lower and upper state configurations for each transition are given. Einstein-A coefficients for both lines are rated with “D” confidence level in the NIST ASD (A. Kramida et al. 2024) indicating 50% confidence in the calculated coefficient.

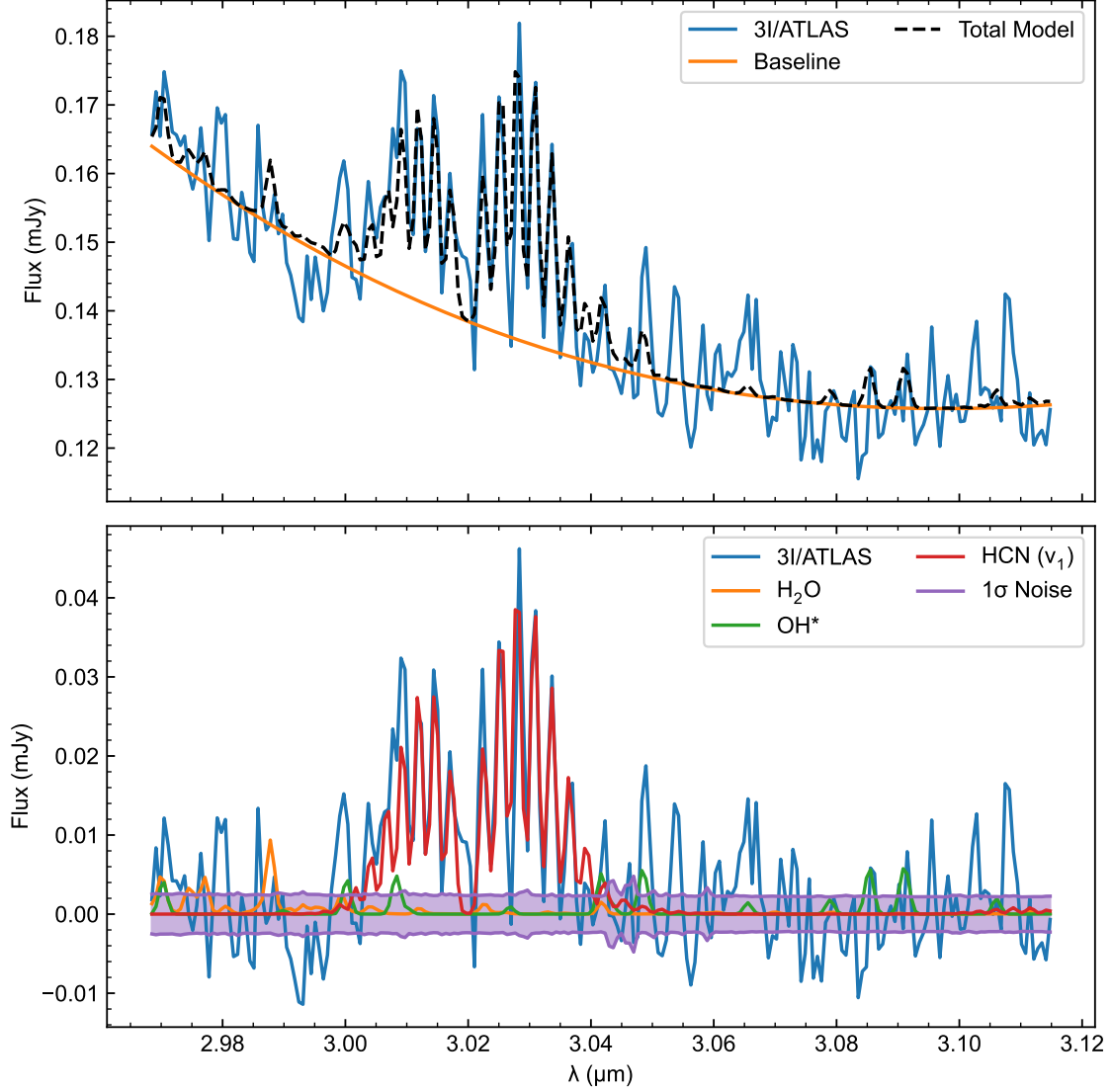


Figure 9. **Upper.** 3I/ATLAS 3 μm spectrum with total molecular emission model and spectral baseline shown. **Lower.** Baseline-subtracted spectrum with individual molecular models and the 1σ noise envelope overplotted.

For Ni I, we detected the 3.119 μm and 3.915 μm transitions, with the former sufficiently bright for spaxel-by-spaxel mapping. 3I/ATLAS has been noted as an Ni- and Fe-rich object based on studies at optical wavelengths (D. Hutsemékers et al. 2026). We first analyzed spectra of both transitions extracted from a nucleus-centered $1''.5$ diameter aperture (Figure 10). We calculated g -factors and $\langle N \rangle$ for each transition following S. Bromley et al. (2021), then calculated $Q(\text{Ni})$ using Equation 1. We obtained $\langle N \rangle = (3.66 \pm 0.02) \times 10^{15} \text{ m}^{-2}$ and $\langle N \rangle = (4.1 \pm 0.2) \times 10^{15} \text{ m}^{-2}$ for the 3.119 μm and 3.951 μm transitions, respectively. We calculated $f(x)$ using active sun photodissociation rates for Ni (W. F. Huebner & J. Mukherjee 2015) along with our assumed $v_{\text{exp}} = 0.310 \text{ km s}^{-1}$ and assuming a range of parent scale lengths from 0 km to 2000 km, giving values ranging from $Q(\text{Ni}) = (2.2 - 6.8) \times 10^{24} \text{ s}^{-1}$.

Next we considered spaxel-by-spaxel mapping of the (baseline-subtracted) 3.119 μm transition (Figure 11). We calculated $\langle N \rangle = (4.95 \pm 0.03) \times 10^{15} \text{ m}^{-2}$ from averaging all spaxels within a $1''.5$ diameter aperture, providing a range of $Q = (3.0 - 8.3) \times 10^{24} \text{ s}^{-1}$ depending on the parent scale length. Our $Q(\text{Ni})$ for both methods lie in the range reported by M. Belyakov et al. (2026) based on MIRI observations of 3I/ATLAS conducted on nearby dates to the NIRS spec observations reported here.

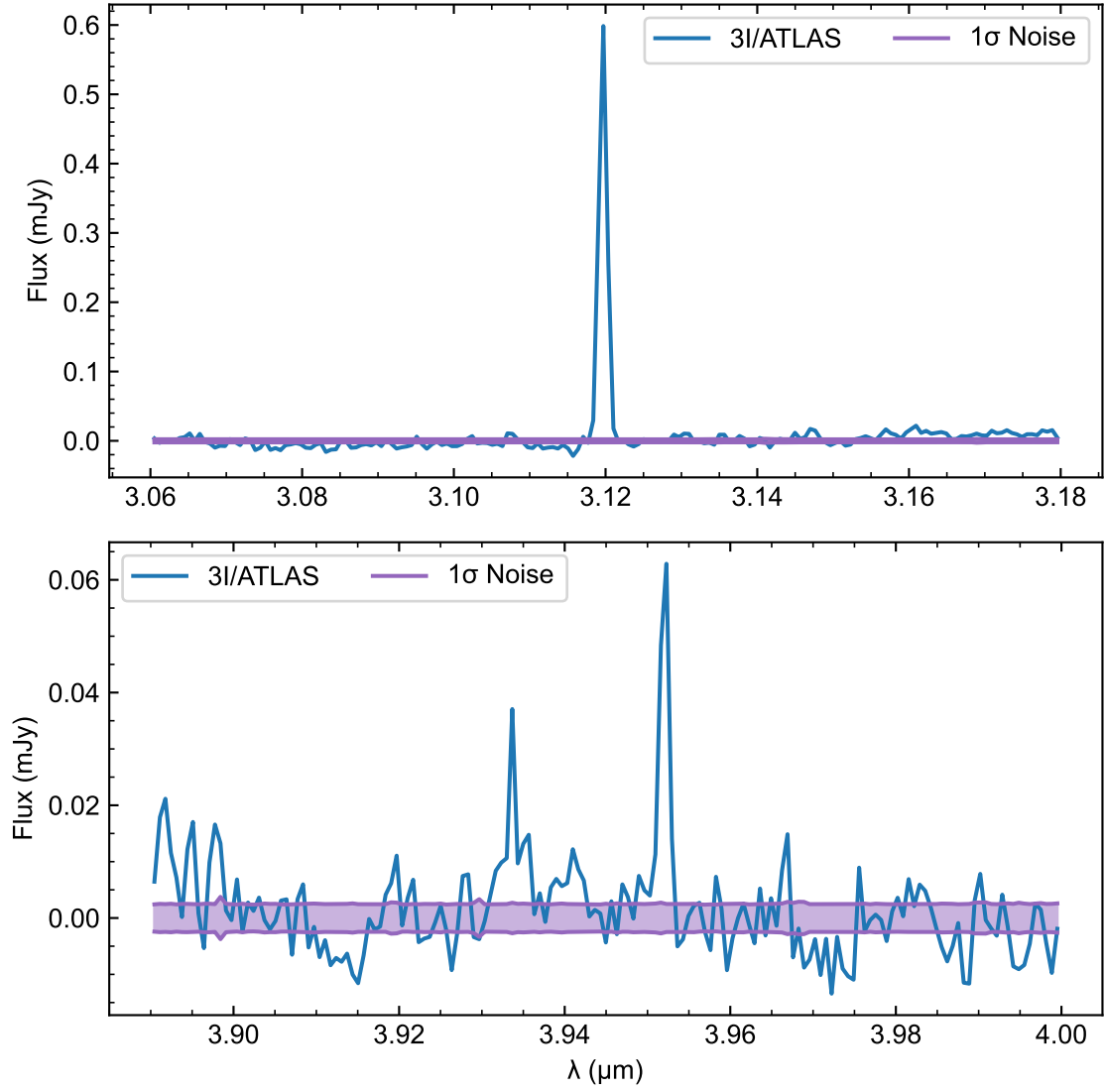


Figure 10. Baseline-subtracted Ni I 3.119 μm and 3.951 μm spectra in 3I/ATLAS extracted from a nucleus-centered $1''.5$ diameter aperture.

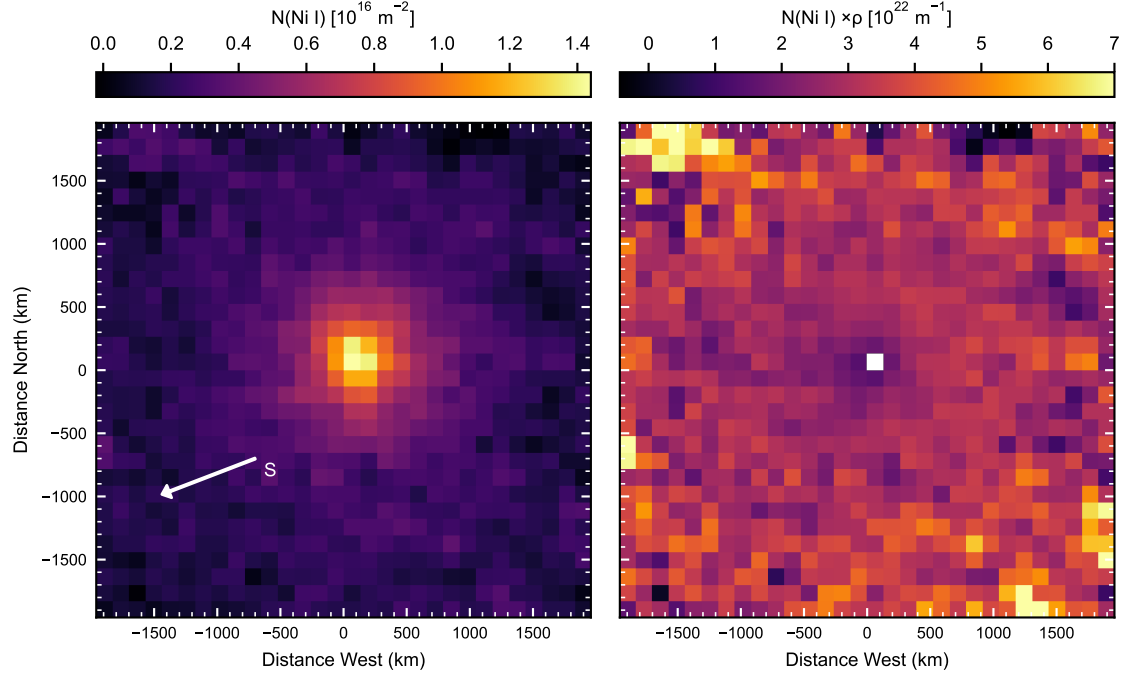


Figure 11. Left. $N(\text{Ni I})$ map of the $3.119 \mu\text{m}$ transition in 3I/ATLAS. **Right.** $N(\text{Ni I}) \times \rho$ for the $3.119 \mu\text{m}$ transition in 3I/ATLAS.

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