The Physical Conditions of Emission-line Galaxies at Cosmic Dawn from JWST/NIRSpec Spectroscopy in the SMACS 0723 Early Release Observations

Trump, Jonathan R.; Haro, Pablo Arrabal; Simons, Raymond C.; Backhaus, Bren E.; Amorin, Ricardo O.; Dickinson, Mark; Fernandez, Vital; Papovich, Casey; Nicholls, David C.; Kewley, Lisa J.; Brunker, Samantha W.; Salzer, John J.; Wilkins, Stephen M.; Almaini, Omar; Bagley, Micaela B.; Berg, Danielle A.; Bhatawdekar, Rachana; Bisigello, Laura; Buat, Veronique; Burgarella, Denis; Calabro, Antonello; Casey, Caitlin M.; Ciesla, Laure; Cleri, Nikko J.; Cole, Justin W.; Cooper, M. C.; Cooray, Asantha R.; Costantin, Luca; Croton, Darren; Ferguson, Henry C.; Finkelstein, Steven L.; Fujimoto, Seiji; Gardner, Jonathan P.; Gawiser, Eric; Giavalisco, Mauro; Grazian, Andrea; Grogin, Norman A.; Hathi, Nimish P.; Hirschmann, Michaela; Holwerda, Benne W.; Huertas-Company, Marc; Hutchison, Taylor A.; Jogee, Shardha; Juneau, Stephanie; Jung, Intae; Kartaltepe, Jeyhan S.; Kirkpatrick, Allison; Kocevski, Dale D.; Koekemoer, Anton M.; Lotz, Jennifer M.; Lucas, Ray A.; Magnelli, Benjamin; Matharu, Jasleen; Perez-Gonzalez, Pablo G.; Pirzkal, Nor; Rafelski, Marc; Rose, Caitlin; Seille, Lise-Marie; Somerville, Rachel S.; Straughn, Amber N.; Tacchella, Sandro; Vanderhoof, Brittany N.; Weiner, Benjamin J.; Wuyts, Stijn; Aaron Yung, L. Y.; Zavala, Jorge A.

Published in:
Astrophysical Journal

DOI:
10.3847/1538-4357/acba8a

Publication date:
2023

Document version
Publisher's PDF, also known as Version of record

Document license:
CC BY

Citation for published version (APA):
Trump, J. R., Haro, P. A., Simons, R. C., Backhaus, B. E., Amorin, R. O., Dickinson, M., Fernandez, V., Papovich, C., Nicholls, D. C., Kewley, L. J., Brunker, S. W., Salzer, J. J., Wilkins, S. M., Almaini, O., Bagley, M. B., Berg, D. A., Bhatawdekar, R., Bisigello, L., Buat, V., ... Zavala, J. A. (2023). The Physical Conditions of Emission-line Galaxies at Cosmic Dawn from JWST/NIRSpec Spectroscopy in the SMACS 0723 Early Release Observations. Astrophysical Journal, 945(1), [35]. https://doi.org/10.3847/1538-4357/acba8a
The Physical Conditions of Emission-line Galaxies at Cosmic Dawn from JWST/NIRSpec Spectroscopy in the SMACS 0723 Early Release Observations

Jonathan R. Trump, Pablo Arrabal Haro, Raymond C. Simons, Bren E. Backhaus, Ricardo O. Amorín, Mark Dickinson, Vital Fernández, Casey Papovich, David C. Nicholls, Lisa J. Kewley, Samantha W. Brukner, John J. Salzer, Stephen M. Wilkins, Omar Almaini, Micaela B. Bagley, Danielle A. Berg, Rachana Bhatawdekar, Omar Almaini, Caitlin M. Casey, Laura Bisigello, Véronique Buit, Denis Burgarella, Antonello Calabrò, Laure Ciesla, Nikko J. Cleri, Justin W. Cole, M. C. Cooper, Asantha R. Cooray, Luca Costantin, Darren Croton, Henry C. Ferguson, Steven L. Finkelstein, Seiji Fujimoto, Jonathan P. Gardner, Eric Gawiser, Mauro Giavalisco, Raymond C. Simons, John J. Salzer, Sandro Tacchella, Jennifer M. Lotz, Nikko J. Cleri, Andrea Grazian, L. Y. Aaron Yung, Casey Papovich, Jasleen Matharu, Stephen M. Wilkins, Nor Pirzkal, and Jorge A. Zavala

Department of Physics, 196 Auditorium Road, Unit 3046, University of Connecticut, Storrs, CT 06269, USA
2 NSF’s National Optical-Infrared Astronomy Research Laboratory, 950 N. Cherry Avenue, Tucson, AZ 85719, USA
3 Space Telescope Science Institute, 3700 San Martin Drive, Baltimore, MD, 21218 USA
4 Instituto de Investigación Multidisciplinar en Ciencia y Tecnología, Universidad de La Serena, Raul Bittún 1305, La Serena 2204000, Chile
5 Departamento de Astronomía, Universidad de La Serena, Av. Juan Cisternas 1200 Norte, La Serena 1720236, Chile
6 Department of Physics and Astronomy, Texas A&M University, College Station, TX, 77843-4242, USA
7 George P. and Cynthia Woods Mitchell Institute for Fundamental Physics and Astronomy, Texas A&M University, College Station, TX, 77843-4242, USA
8 Research School of Astronomy and Astrophysics, Australian National University, Canberra, ACT 2600, Australia
9 ARC Centre of Excellence for All Sky Astrophysics in 3 Dimensions (ASTRO 3D), Australia
10 Department of Astronomy, Indiana University, 727 East Third Street, Bloomington, IN 47405, USA
11 Astronomy Centre, University of Sussex, Falmer, Brighton BN1 9QH, UK
12 Institute of Space Sciences and Astronomy, University of Malta, Msida MSD 2080, Malta
13 School of Physics and Astronomy, University of Nottingham, University Park, Nottingham NG7 2RD, UK
14 Department of Astronomy, The University of Texas at Austin, 2515 Speedway, Stop C1400, Austin, TX 78712, USA
15 European Space Agency, ESA/ESTEC, Keplerlaan 1, 2201 AZ Noordwijk, The Netherlands
16 Dipartimento di Fisica e Astronomia “G.Galilei,” Università di Padova, Via Marzolo 8, 35131 Padova, Italy
17 INAF—Osservatorio Astronomico di Padova, Vicolo dell'Osservatorio 5, I-35122, Padova, Italy
18 Aix Marseille Univ, CNRS, CNES, LAM Marseille, France
19 INAF Osservatorio Astronomico di Roma, Via Frascati 33, I-00078 Monteporzio Catone, Rome, Italy
20 Department of Physics & Astronomy, University of California, Irvine, 4129 Reines Hall, Irvine, CA 92697, USA
21 Centro de Astrobiología (CAB/CSIC-INTA), Ctra. de Ajalvir km 4, Torrejón de Ardoz, E-28850, Madrid, Spain
22 Centre for Astrophysics & Supercomputing, Swinburne University of Technology, Hawthorn, VIC 3122, Australia
23 ARC Centre of Excellence for All Sky Astrophysics in 3 Dimensions (ASTRO 3D), Australia
24 Cosmic Dawn Center (DAWN), Jagtvej 128, DK-2200 Copenhagen N, Denmark
25 Astrophysics Science Division, NASA Goddard Space Flight Center, 8800 Greenbelt Road, Greenbelt, MD 20771, USA
26 Physics and Astronomy Department, Rutgers, The State University of New Jersey, Piscataway, NJ 08854, USA
27 Physics Department, University of Massachusetts Amherst, 710 North Pleasant Street, Amherst, MA 01003-9305, USA
28 Institute of Physics, Laboratory of Galaxy Evolution, EPFL, Observatoire de Sauverny, 1290 Versoix, Switzerland
29 Physics & Astronomy Department, University of Louisville, 40292 KY, Louisville, USA
30 Instituto de Astrofísica de Canarias, La Laguna, Tenerife, Spain
31 Universidad de la Laguna, La Laguna, Tenerife, Spain
32 Universidad de la Laguna, La Laguna, Tenerife, Spain
33 Université Paris-Cité, LERMA—Observatoire de Paris, PSL, Paris, France
34 Department of Physics, The Catholic University of America, Washington, DC 20064, USA
35 Center for Research and Exploration in Space Science and Technology, NASA/GSFC, Greenbelt, MD 20771, USA
36 Laboratory for Multiwavelength Astrophysics, School of Physics and Astronomy, Rochester Institute of Technology, 84 Lomb Memorial Drive, Rochester, NY 14623, USA
37 Department of Physics and Astronomy, University of Kansas, Lawrence, KS 66045, USA
38 Department of Physics and Astronomy, Colby College, Waterville, ME 04901, USA
39 Gemini Observatory/NSF’s National Optical-Infrared Astronomy Research Laboratory, 950 N. Cherry Avenue, Tucson, AZ 85719, USA
40 Université Paris-Saclay, Université Paris Cité, CEA, CNRS, AIM, F-91191, Gif-sur-Yvette, France
41 ESA/AURA, Space Telescope Science Institute, 3700 San Martin Drive, Baltimore, MD, 21218 USA
42 Department of Physics and Astronomy, Johns Hopkins University, Baltimore, MD 21218, USA
43 Center for Computational Astrophysics, Flatiron Institute, 162 5th Avenue, New York, NY 10010, USA
44 Kavli Institute for Cosmology, University of Cambridge, Madingley Road, Cambridge, CB3 0HA, UK
45 Cavendish Laboratory, University of Cambridge, 19 JJ Thomson Avenue, Cambridge, CB3 0HE, UK
46 MMT/Steward Observatory, University of Arizona, 933 N. Cherry Street, Tucson, AZ 85721, USA
47 Department of Physics, University of Bath, Claverton Down, Bath BA2 7AY, UK
48 Department of Physics, University of Bath, Claverton Down, Bath BA2 7AY, UK
The Astrophysical Journal, 945:35 (11pp), 2023 March 1

Received 2022 July 22; revised 2022 November 30; accepted 2022 December 18; published 2023 March 6

Abstract

We present rest-frame optical emission-line flux ratio measurements for five $z > 5$ galaxies observed by the James Webb Space Telescope Near-Infrared Spectrograph (NIRSpec) in the SMACS 0723 Early Release Observations. We add several quality-control and post-processing steps to the NIRSpec pipeline reduction products in order to ensure reliable relative flux calibration of emission lines that are closely separated in wavelength, despite the uncertain absolute spectrophotometry of the current version of the reductions. Compared to $z \sim 3$ galaxies in the literature, the $z > 5$ galaxies have similar [O III] $\lambda$5008/H$\beta$ ratios, similar [O III] $\lambda$3464/H$\gamma$ ratios, and higher ($\sim$0.5 dex) [Ne III]$\lambda$3870/[O II]$\lambda$3728 ratios. We compare the observations to MAPPINGS V photoionization models and find that the measured [Ne III]$\lambda$3870/[O II]$\lambda$3728, [O III]$\lambda$3464/H$\gamma$, and [O III]$\lambda$5008/H$\beta$ emission-line ratios are consistent with an interstellar medium (ISM) that has very high ionization ($Q(\gamma) \sim 8 - 9$, units of cm$^{-3}$), low metallicity ($Z/Z_\odot \lesssim 0.2$), and very high pressure ($log(P/k)$ $\sim 8 - 9$, units of cm$^{-3}$). The combination of [O III]$\lambda$3464/H$\gamma$ and [O III]$\lambda$(4960 + 5008)/H$\beta$ line ratios indicate very high electron temperatures of $4.1 < log(T_e/K) < 4.4$, further implying metallicities of $Z/Z_\odot \lesssim 0.2$ with the application of low-redshift calibrations for “T-based” metallicities. These observations represent a tantalizing new view of the physical conditions of the ISM in galaxies at cosmic dawn.

Unified Astronomy Thesaurus concepts: Emission line galaxies (459); Galaxies (573); High-redshift galaxies (734)

Supporting material: figure sets

1. Introduction

Emission lines provide a wealth of information about the physical conditions of galaxies. In particular, rest-frame optical lines can reveal the star formation rate (Kennicutt & Evans 2012), nebular dust attenuation (Buat et al. 2002; Groves et al. 2012), active galactic nucleus (AGN) content (Baldwin et al. 1981; Veilleux & Osterbrock 1987), and the metallicity (Lequeux et al. 1979; Tremonti et al. 2004), ionization (Kewley et al. 2019b), and density (Dopita et al. 2000) of the interstellar medium (ISM). Pairs of high-ionization and low-ionization lines that are closely separated in wavelength—for example, [N II] $\lambda$6584/H$\alpha$, [O III]$\lambda$5008/H$\beta$, [O III]$\lambda$3464/H$\gamma$, and [Ne III] $\lambda$3870/[O II] $\lambda$3728—are relatively insensitive to dust attenuation and so are especially useful as probes of ISM conditions.

The advent of efficient, multiobject optical and near-infrared spectroscopic surveys has expanded our knowledge of galaxy physical conditions from the local universe to the peak of cosmic star formation at $z \sim 2$ (Madau & Dickinson 2014). Galaxies at $1 < z < 3.5$ have lower metallicity than $z \sim 0$ galaxies of the same stellar mass (Henry et al. 2013; Steidel et al. 2014; Maiolino & Mannucci 2019; Sanders et al. 2021), as expected from enrichment by star formation. But beyond the metallicity evolution they also have higher ionization (Liu et al. 2008; Kewley et al. 2015; Shapley et al. 2015; Strom et al. 2018; Backhaus et al. 2022; Papovich et al. 2022). Compared to the current epoch, galaxies at $1 < z < 2$ have higher AGN content (Trump et al. 2011; Juneau et al. 2014; Coil et al. 2015), higher-density H II regions (Brinchmann et al. 2008; Liu et al. 2008; Davies et al. 2021), and more $\alpha$-enrichment from Wolf-Rayet stars and/or massive binaries (Masters et al. 2014; Strom et al. 2017; Sanders et al. 2020).

About a quarter of the stars in our universe assemble at $z \gtrsim 2$ (Madau & Dickinson 2014). Galaxies at these early times are expected to have even more extreme ISM conditions, with lower metallicity and higher ionization observed in their rest-frame UV emission (Smit et al. 2014; Stark et al. 2015; Amorín et al. 2017; Stark et al. 2017; Hutchison et al. 2019). The observed mid-infrared colors of high-redshift galaxies also suggest contribution from rest-frame optical emission lines with very high equivalent widths (van der Wel et al. 2011; González et al. 2012; Smit et al. 2014; Endsley et al. 2021), implying high star formation rates and a highly ionized ISM. But directly measuring rest-frame optical emission lines of galaxies at $2 < z < 5$ has been enormously challenging due to high sky background from the ground, and has been entirely impossible at $z > 5$... until now.

The launch of the James Webb Space Telescope (JWST; Gardner et al. 2006) opens an entirely new window on the high-redshift universe. JWST Near-Infrared Spectrograph (NIRSpec) spectroscopy spans observed-frame 1–5 $\mu$m, enabling detection of rest-frame optical emission lines to $z \lesssim 9$. Figure 1 highlights the coverage of the JWST/NIRSpec medium-resolution gratings for various rest-frame optical emission lines as a function of redshift. The advent of JWST observations finally allows for a direct comparison of physical conditions over 13 Gyr of cosmic time, using the same set of rest-frame optical emission-line diagnostics from cosmic dawn to the current epoch.

In this paper we investigate the emission-line properties of five $z > 5$ galaxies with JWST/NIRSpec spectroscopy from Early Release Observations of the galaxy cluster SMACS J0723.3-7327 (henceforth SMACS 0723). Section 2 describes the observations and data reduction, which includes some post-processing to ensure reliable relative flux calibration. Section 3 describes our spectral fitting and measurements of emission-line flux ratios. In Section 4 we compare our new $z > 5$ line-ratio measurements with previous observations at lower redshift and with theoretical photoionization models, finding that the high-redshift galaxies have very high ionization ($log(Q/\text{cm s}^{-3}) \sim 8 - 9$) and low (but nonzero) metallicities ($Z/Z_\odot \sim 0.1$). We summarize the results in Section 5.
In this work we use SMACS 0723 Early Release Observations with G235M and G395M to show its wavelength coverage in a lighter shade for illustrative purposes only.

The Astrophysical Journal, 945:35 (11pp), 2023 March 1

2. Observations

SMACS 0723 was observed by program No. 2736 as part of the JWST Early Release Observations⁴⁹ (Pontoppidan et al. 2022). In this work we focus on the NIRSpec observations of the five galaxies at \( z \geq 5 \) that were presented by Carnall et al. (2023). All five of these galaxies are gravitationally lensed by the foreground cluster; ID 4590 (\( z = 8.5 \)) has a magnification factor of 8, while the other four galaxies have more modest magnification factors of 1.5–2 (using the parametric model of Pascale et al. 2022). SMACS 0723 was also observed with NIRISS spectroscopy and with NIRCam and MIRI imaging, although we do not use those data in this work.

The JWST data used in this paper can be found in MAST at DOI:10.17909/67ft-nb86.

2.1. NIRSpec Observational Setup

The details of the NIRSpec instrument and the microshutter array (MSA) are described by Jakobsen et al. (2022) and Ferruit et al. (2022), respectively.

SMACS 0723 was observed with the G235M/F170LP (1.75–3.15 µm) and G395M/F290LP (2.9–5.2 µm) grating/filter pairs, each of which has spectral resolution of \( R \approx 1000 \). Each grating was observed with two NIRSpec visits, with each visit using a three-nod pattern and two integrations of 20 groups (2918 s) per nod. The coadded spectra from each visit (combining from the three nods) have a total exposure time of 8754 s in each grating. Targets for the MSA configuration were selected using the NIRCam imaging in the field, especially prioritizing targets with photometric redshifts of \( z > 6 \). Each target was observed using a “slitlet” aperture of three microshutters, and the design also included empty shutters for background subtraction.

2.2. Data Reduction and Quality Checks

We perform a complete reduction from Level 0 raw uncalibrated data (“_uncal.fits” files) available on the Mikulski Archive for Space Telescopes server (MAST)⃣⃣ processed using version 1.8.2 of the JWST Science Calibration Pipeline with the “jwst-1015.pmap” calibration context. This reduction includes updates to the instrument models, gain response, flats and detector-level calibration files released in the months following the observations of the ERO programs. The reduced 2D spectra (“s2d”) have a rectified trace with a flat slope, drizzled from the significantly curved (by 14–24 pixels over the spectral range) trace observed on the detector. The pipeline-reduced 1D spectra (“s1d”) are extracted from the 2D spectra using an “extended” aperture with a width of 8 pixels. We instead extract spectra using a narrower “point-source” aperture, as described below.

We confirmed that the reduced 1D spectra have excellent wavelength calibration, with differences of \( \Delta z / z \lesssim 10^{-4} \) in best-fit line centers for different emission lines across the observed spectral range. We also confirmed that the reduced 2D spectra have a flat trace, with consistent spatial profiles of

---

⁴⁹ https://www.stsci.edu/jwst/science-execution/approved-programs/webb-first-image-observations

⃣⃣ https://mast.stsci.edu/
emission lines over the spectral range of each grating. The 2D line profiles for the galaxies are shown in Figure 2.

The current (version 1.8.2) data reduction pipeline uses a flux calibration that relies on knowledge of the instrument before launch. The pre-launch instrument throughput is known to differ from the post-launch performance (see Figure 20 of Rigby et al. 2022). We also find that synthetic photometry from the spectra have a median difference of ~30% from the NIRCam photometry in the F200W, F356W, and F444W filters (and a smaller median difference of 14% in the F277W filter). For these reasons we avoid analysis and interpretation that require absolute spectrophotometric calibration, like using individual emission-line fluxes or widely separated line ratios (e.g., [O III]/[O II]). We confirm below that the spectra have reliable relative spectrophotometry for pairs of emission lines that are closely separated in wavelength.

The default 8-pixel “extended” extraction width used by the current (version 1.8.2) pipeline is generally too large for the compact high-redshift sources that are the focus of this paper: Figure 2 shows that all of our sources have their spectral trace confined to 4–5 pixels. We also found that the “extended” extraction apertures were often not well-centered on the target, such that the 1D spectrum included a significant amount of the “negative-nod” flux above and below the coadded 2D spectrum. The 1D spectra produced by these wide-extraction apertures often include emission from serendipitous sources and detector artifacts that lie outside the trace of the main source. The wide-extraction spectra generally have inconsistent emission-line flux measurements between the two visits that differ by up to a factor of ~2, with even worse (factor of ~10) differences in the continuum emission. In addition, the wide-extraction spectra often have unphysical Balmer line ratios: e.g., Hβ/Hγ ~ 1 compared to atomic calculations of Hβ/Hγ ≈ 2.1 for a broad range of temperature and density (Osterbrock 1989). Other work on this same data set (Brinchmann 2022; Curti et al. 2022; Schaerer et al. 2022; Taylor et al. 2022) noted some of the same issues with the pipeline-reduced data and took independent approaches to mitigating them.

Rather than using the wide-extraction 1D spectra from the pipeline, we produce new 1D spectra from a narrower “point-source” extraction width individually optimized for each source (typically ~4 pixels wide). This required significant customization of the (version 1.8.2) NIRSpec reduction pipeline in order to accurately align the extraction window with the position of the source. These narrow-extraction 1D spectra represent a dramatic improvement over the wide-extraction versions: they avoid much of the contamination from serendipitous sources and detector artifacts and have emission-line fluxes that are two to four times larger due to avoiding the negative-nod emission present in the “extended” apertures. Most importantly, they have consistent emission-flux measurements between visits (with one exception noted in Section 3). We also visually inspect the 1D and 2D spectra and mask obvious defects in the spectra, generally caused by chip gaps or bad pixels on the CCD.

The flux uncertainties of our reduced 1D spectra appear to be underestimated by a factor of ~2 (and by a factor of ~1.3 in the wide-extraction spectra), as measured from a comparison of the normalized median absolute deviation (NMAD) of the flux with the median of the flux uncertainty for each source, calculated in wavelength regions without emission lines and avoiding chip gaps and bad pixels. We increase the flux uncertainty of the spectra using the ratio of the NMAD of the flux to the median flux uncertainty, i.e., an error rescaling factor of NMAD(f)/median(σf). We note that this error rescaling may still remain an underestimate of the true noise if the pixels of the spectrum are correlated.

Our post-processing improvements in flux calibration and 1D extraction represent a significant improvement over the (version 1.8.2) pipeline-reduced 1D spectra. However, our flux calibration additionally relies on pre-launch knowledge of the instrument that differs from the measured post-launch performance (Figure 20 of Rigby et al. 2022). In addition, the wavelength-dependent spatial resolution of NIRSpec will cause wavelength-dependent effects from aperture losses when using a fixed-width 2D spectral extraction. Despite these potential problems in the absolute flux calibration, we find that the relative flux calibration is consistent for pairs of emission lines that are near one another in wavelength. The line ratios of near-pair lines are also consistent between visits, as discussed in Section 3. Thus we are confident in using ratios of emission lines that are closely separated in wavelength, but we caution against the use of emission-line fluxes and equivalent widths, and against the direct comparison of lines that are widely separated in wavelength (like [O III]λ4364/[O III]λ5008).

3. Emission-line Flux Ratio Measurements

We fit for the following emission lines in each spectrum (noted by vacuum wavelengths in angstroms):

1. [O II]λ3728.48 (the 3727+3729 doublet is blended in the R ≈ 1000 medium-resolution NIRSpec grating)
2. [Ne III]λ3870.86
3. Hγλ4341.69
4. [O III]λ4364.44
5. Hβλ4862.72
6. [O III]λ4960.30
7. [O III]λ5008.24

We find the best-fit Gaussian function (and associated uncertainties) for each emission line using a Levenberg–Marquardt least-squares method implemented by the mpfit-t1D code.51 We subtract a continuum that is determined by smoothing (by a boxcar of 100 pixels) and interpolating the flux from all regions that are <5σ above the median flux of the spectrum (i.e., over line-free regions). We fit the spectra from each of the two visits independently. Examples of the emission-line fits are shown in Figure 3. In a few cases, a line flux cannot be measured due to contaminating emission that extends beyond the main spectral trace (likely from a detector artifact or serendipitous source):

1. ID 4590, second visit; [O III]λ4960
2. ID 8140, first visit; [O III]λ4364
3. ID 10612, second visit; [O II]λ3728

Table 1 presents the source IDs, spectroscopic redshifts, and signal-to-noise ratios (S/Ns) of each emission-line measurement for each visit of the observations. Table 2 presents the measured line ratios, generally computed from the average line measurements of the two visits. The line ratio is measured from only one visit if a line of the ratio cannot be measured in the other visit, i.e., [O III]λ5008/[O III]λ4960 for ID 4590 and

51 https://pages.physics.wisc.edu/~craigm/idl/fitting.html
[Ne III]/[O II] for ID 10612. Neither [O III]λ4364 nor Hγ are robustly (>3σ) detected in ID 8140 and so the [O III]λ4364/Hγ line ratio is unconstrained for this galaxy.

We determined the spectroscopic redshift for each source using the best-fit line center for [O III]λ5008, which was the brightest emission line in each spectrum. As noted in Section 2.2, the reduced NIRSpec 1D spectra have excellent wavelength calibration, and we found differences of only Δz/z ≲ 10⁻⁴ when measuring the redshift from the line centers of other emission lines.

Most of the emission lines are measured from the G395M spectrum, with bluer lines measured in the G235M spectrum for the lower-redshift sources. Because comparison with NIRCam photometry of the same galaxies indicates that the absolute flux calibration is suspect by a factor of ∼0.3, we use only ratios of near-pair emission lines rather than individual emission-line fluxes. In cases where an emission line is measured in the wavelength range 2.9 < λ(μm) < 3.2 that is covered by both gratings, we take care to measure both lines in a given ratio from the same grating, given the differences in line flux measured from each grating (noted in Section 2.2).

The measured line strengths are generally consistent within their uncertainties between the two visits. ID 4590 is an exception, with a factor of ∼2 difference in the measured line fluxes between the two visits. This is caused by a shutter that failed to open in one of the nod positions of the first (007) visit, as identified by Curti et al. (2022). Excluding ID 4590, the ratio of emission-line strengths measured in each visit is 0.99 ± 0.14 (mean and standard deviation of the sample) for lines that are >5σ detected. Note that despite the difference in line fluxes, the emission-line ratios of ID 4590 are consistent between the two visits. Table 2 also demonstrates that the measured [O III] λ5008/[O II]λ4960 = 2.98 ± 0.12 (mean and standard deviation of the sample), matching the atomic physics calculation (Storey & Zeippen 2000) and establishing the reliability of the relative flux calibration for near-wavelength line pairs.

4. Line-ratio Diagnostics

We infer galaxy properties from emission-line pairs that are closely separated in wavelength: namely [O III]λ5008/Hβ, [O III]λ4364/Hγ, and [Ne III]λ3870/[O II]λ3728. The use of ratios of emission lines that are closely separated in wavelength avoids the issues with the absolute flux calibration described in Section 2.2, and is also largely insensitive to dust attenuation.

In each subsection below, we compare the observations with model spectra from Kewley et al. (2019a), produced using the MAPPINGS V photoionization code (Sutherland et al. 2018). These models use input stellar ionizing spectra from Starburst99 (Leitherer et al. 1999), which use a Salpeter (1955) initial mass function and include stellar mass loss. MAPPINGS V uses atomic data from the CHIANTI 8 database (Dere et al. 1997; Del Zanna et al. 2015) and applies photoionization, recombination, excitation, and dust depletion of model H II regions in a plane-parallel geometry for the ionizing spectra. We use the “pressure
models” of Kewley et al. (2019a) for a grid of pressure log(P/k), ionization52 log(Q), and metallicity Z/Z_⊙:

1. Pressure log(P/k) = [7, 8, 9], units of cm^{-3}
2. Ionization log(Q) = [7, 8, 9], units of cm s^{-1}
3. Metallicity Z/Z_⊙ = [0.05, 0.2, 0.4, 1.0]

The MAPPINGS V models are characterized in terms of the total metallicity Z with respect to solar, but relative abundances of each element are not simply scaled from the solar abundances. At low metallicities, the models use α-enhanced abundances as described in Nicholls et al. (2017); for example, the relative [O/Fe] abundance is 0.5 dex higher than solar for Z/Z_⊙ < 0.1. The alpha-enhancement at low metallicity in the MAPPINGS V models is motivated by studies of stellar abundances (e.g., Amarsi et al. 2019) and is also similar to the alpha-enhancement observed in nebular emission from both low-metallicity galaxies at z ≳ 2 (e.g., Steidel et al. 2016; Topping et al. 2020; Cullen et al. 2021) and from a more detailed study of relative abundances in our z > 5 galaxies (Arellano-Córtoia et al. 2022).

The ionizing spectra of low-metallicity stars are not well constrained by observations, and at Z/Z_⊙ = 0.05 the spectrum is essentially extrapolated from the Starburst99 inputs. That means the model spectra are most uncertain at the lowest metallicities, although they generally appear to be smooth continuations of the better-constrained models with higher metallicity. The MAPPINGS V models also use a single plane-parallel geometry for the ionization and may not effectively model H II regions with multiphase pressure and ionization and/or more complex geometries (Xiao et al. 2018; Kewley et al. 2019b).

4.1. OHNO: O III/Hβ and Ne III/O II

Figure 4 presents the “OHNO” line-ratio diagnostic of [O III]/Hβ versus [Ne III]/[O II], with the line-ratio measurements of the z > 5 galaxies shown by large red stars. We use the samples of Backhaus et al. (2022) as a low-redshift comparison, with line ratios for z ~ 2 in galaxies in the CLEAR survey (Simons et al. 2023, in preparation) measured from Hubble Space Telescope (HST)/WFC3 grism spectroscopy. A sample of ~28,000 z ~ 0 galaxies with detected OHNO

52 We quantify ionization using Q = e^{47.9 + 4.4 log(Z)} / 4.4 log(M_H), noting that many papers also use U = Q/c (or log U = log(Q/(cm s^{-1})) ~ 10.48 for ionization.

emission lines from the Sloan Digital Sky Survey (SDSS; York et al. 2000) is shown by gray contours. Figure 4 also shows stacked line-ratio measurements from MOSDEF observations (Sanders et al. 2021) as pink and maroon points. The high- and low-redshift samples have different line-luminosity selection limits and so inter-comparison is nontrivial. The lack of robust absolute flux calibration means that we cannot construct samples of low-redshift galaxies that are matched to our z > 5 galaxies (following, e.g., Juneau et al. 2014; Backhaus et al. 2022). Instead, we generally focus our discussion below on comparing the z > 5 galaxies to the most extreme (highest ionization and lowest metallicity) galaxies present in the low-redshift samples.

Compared to the lower-redshift comparison samples, the z > 5 galaxies in SMACS 0723 have similar [O III]/Hβ ratios but have [Ne III]/[O II] ratios that are higher by ~0.5 dex. The redshift evolution of [Ne III]/[O II] at fixed [O III]/Hβ appears to be broadly consistent from z ~ 0 to z ~ 2 to z ~ 3 to z > 5, with z ~ 3 MOSDEF and z ~ 2 CLEAR [Ne III]/[O II] ratios that are higher than the “evolution-matched” z ~ 0 sample and z > 5 [Ne III]/[O II] ratios that are even higher than the z ~ 2 and z ~ 3 ratios. The redshift evolution of [Ne III]/[O II] from z ~ 0 to z ~ 2 and z ~ 3 has been discussed in previous work (e.g., Zeimann et al. 2015; Strom et al. 2017; Kewley et al. 2019; Jeong et al. 2020; Sanders et al. 2021; Backhaus et al. 2022) and requires a harder ionizing spectrum, likely caused by some combination of massive α-enhanced low-metallicity stars, higher-density (and higher-pressure) H II regions, and increased AGN content at higher redshift.

Here we demonstrate the same trend of increasing [Ne III]/[O II] with redshift in galaxies at z > 5. The redshift evolution cannot be explained by the observed anticorrelation of [Ne III]/[O II] with stellar mass (e.g., Sanders et al. 2021; Backhaus et al. 2022) since the lowest-mass SDSS, CLEAR, and MOSDEF galaxies have lower (by ~0.5 dex) [Ne III]/[O II] than the low-metal z > 5 galaxies. We note that there is not an obvious trend of [Ne III]/[O II] with redshift among the z > 5 galaxies: for example a z ~ 7.7 (ID 6355) galaxy has the lowest [Ne III]/[O II] and a z = 6.4 (ID 5144) galaxy has the highest [Ne III]/[O II], with ratios that are >3σ inconsistent given their observational uncertainties. This likely indicates a diversity of [Ne III]/[O II] ratios in individual z > 5 galaxies, perhaps associated with the diversity of stellar mass, star formation rate, abundances, and/or age among this sample.

| ID | Redshift | Visit | [O II] | [Ne III] | Hγ | [O III]4364 | Hβ | [O III]4960 | [O III]5008 |
|----|----------|-------|-------|---------|-----|-------------|----|------------|------------|
| 4590 | 8.4957   | 7     | 2.1   | 3.9     | 11.9| 3.8         | 14.1| 11.2       | 24.2       |
| 4590 | 8.4957   | 8     | 2.5   | 5.6     | 8.8 | 3.5         | 14.9| 11.1       | 29.8       |
| 5144 | 6.3792   | 7     | 5.2   | 8.0     | 11.0| 2.8         | 20.5| 31.9       | 62.9       |
| 5144 | 6.3792   | 8     | 5.3   | 7.3     | 10.7| 5.1         | 18.4| 32.9       | 59.3       |
| 6355 | 7.6651   | 7     | 17.2  | 11.1    | 11.5| 3.1         | 19.0| 36.0       | 70.6       |
| 6355 | 7.6651   | 8     | 16.2  | 10.8    | 8.8 | 2.1         | 18.2| 33.7       | 66.2       |
| 8140 | 5.2753   | 7     | 9.0   | 2.4     | 0.8 | ***         | 6.1 | 11.5       | 21.0       |
| 8140 | 5.2753   | 8     | 10.4  | 4.0     | 1.0 | 1.3         | 4.3 | 9.5        | 19.4       |
| 10612| 7.6597   | 7     | 4.2   | 9.5     | 9.5 | 5.1         | 17.5| 29.9       | 57.4       |
| 10612| 7.6597   | 8     | ***   | 9.1     | 9.4 | 4.2         | 15.8| 27.6       | 52.5       |

Note. Emission lines are measured independently for each of the two NIRSpec visits for each source. Asterisks (***)) indicate a problem in the spectrum (a detector artifact or other emission beyond the main spectral trace) that prevents a measurement of the emission line.
Table 2
Emission-line Ratios

| ID   | Redshift | [Ne III]/[O II] | [O III]4364/Hγ | [O III]5008/Hβ | [O III]5008/[O III]4960 |
|------|----------|----------------|----------------|----------------|------------------------|
| 4590 | 8.4957   | 1.82 ± 0.63    | 0.28 ± 0.06    | 3.05 ± 0.17    | 2.85 ± 0.28            |
| 5144 | 6.3792   | 1.32 ± 0.22    | 0.27 ± 0.05    | 6.45 ± 0.25    | 3.04 ± 0.08            |
| 6355 | 7.6651   | 0.48 ± 0.04    | 0.21 ± 0.06    | 8.23 ± 0.32    | 3.10 ± 0.07            |
| 8140 | 5.2753   | 0.39 ± 0.09    | **           | 6.82 ± 0.98    | 2.85 ± 0.22            |
| 10612| 7.6597   | 1.84 ± 0.48    | 0.37 ± 0.06    | 6.97 ± 0.31    | 2.99 ± 0.08            |

Note. Line ratios are measured from the average of the two visits (excepting the cases where a line cannot be measured in one visit). Error bars indicate 1σ uncertainties. The [O III]4364/Hγ ratio cannot be measured for ID 8140 and is marked by asterisks (**).
shown. The [O III]λ5008/Hβ and [O III]λ4364/Hγ line ratios are largely insensitive to ISM pressure, and so the three curves of different pressures (log(P/k) = [7, 8, 9]) have very similar line ratios. As in the OHNO diagram in Figure 4, the observed line ratios in Figure 5 are consistent with the MAPPINGS models for a highly ionized and low-metallicity ISM, with log(Q) ≈ 8 − 9 and Z/Z⊙ ≤ 0.2.

4.3. Electron Temperature and Metallicity

The ratio of the [O III]λ4364 and the [O III]λ4960 + 5008 doublet can be used to measure the electron temperature of the ISM. These lines are all collisionally excited, and the [O III] λ4364 line de-excites from a higher energy orbital, such that higher [O III]λ4364 emission relative to [O III]λ4960 + 5008 implies higher-energy electrons are responsible for the collisional excitation. The electron temperature can be used with the [O III]λ4960 + 5008, [O II]λ3728, and Balmer lines for a “direct” metallicity estimate (e.g., Izotov et al. 2006; Pérez-Montero 2017; Nicholls et al. 2020), although this requires good flux calibration between the widely separated [O II] and [O III] lines. In this work we use empirical correlations that have been found between electron temperature and the “direct” metallicity (Amorín et al. 2015; Pérez-Montero et al. 2021) to measure “Te-based” metallicities.

We cannot directly compare our measured [O III]λ4364 and [O III]λ4960 + 5008 line fluxes because of the uncertain absolute flux calibration of the NIRSpec spectra (see Section 2.2 for details). Instead, we rely on the reliable relative flux calibration and use the measured ratios of [O III]λ4364/Hγ and [O III]λ(4960 + 5008)/Hβ, along with the intrinsic (relatively insensitive to temperature) Balmer ratio H/β/Hγ = 2.1 (Osterbrock 1989). In other words, we measure the [O III] ratio as follows, abbreviating the [O III] lines by their wavelengths:

\[
\frac{\lambda4364}{\lambda(4960 + 5008)} = \frac{\lambda4364}{H\gamma} \left( \frac{\lambda4960 + 5008}{H\beta} \right)^{-1} \times (2.1)^{-1}. \tag{1}
\]

Note that this method also implicitly corrects the [O III]λ4364/[O III]λ4960 + 5008 ratio for dust attenuation.

We use Equation (4) of Nicholls et al. (2020) to estimate Te and Equation (1) of Pérez-Montero et al. (2021) to estimate metallicity from the electron temperature.33 We use a Te-based metallicity because it can be calculated solely from near-pair line ratios (Equation (1)), as opposed to the “direct” metallicity that additionally requires use of the [O II] line and, by extension, robust absolute flux calibration. Uncertainties are calculated for both Te and metallicity using Monte Carlo resampling of the line ratios, including the calibration uncertainties for Te-based metallicity reported in Equation (1) of Pérez-Montero et al. (2021).

The inferred electron temperatures and Te-based metallicities, and their 1σ uncertainties, are shown in Table 3. Electron temperature and metallicity cannot be calculated for ID 8140 (z = 5.3) because its [O III]λ4364/Hγ line ratio is unconstrained. Our electron temperature measurements agree very well with other studies of these galaxies (Arellano-Córdova et al. 2022; Brinchmann 2022; Curti et al. 2022; Schaerer et al. 2022; Taylor et al. 2022; Katz et al. 2023), despite the independent approaches to flux calibration and spectral extraction used in each work. ID 4590 has an estimated electron temperature that exceeds the maximum value (log(Te/K) ≈ 4.3) used in the calibration of Pérez-Montero et al. (2021), and so its low metallicity represents a (modest) extrapolation of the relation. The sample of metal-poor z ≈ 0 galaxies compiled by Nakajima et al. (2022) similarly lacks analogs to the high Te (and high-ionization line ratios) measured for the z > 5 galaxies.

It is important to note that the electron temperature measured in this fashion is associated with the portion of the ISM emitting the [O III] lines and may not be representative of the broader gas conditions. Significant gradients in density and/or ionization in the ISM may lead to a mix of high- and low-ionization regions, and the [O III] electron temperature probes only the former. Our use of the Pérez-Montero et al. (2021) metallicity relationship also implicitly assumes that the high-redshift galaxies have the same relationship between metallicity and [O III] electron temperature as the calibration sample of high-ionization galaxies at low redshift. Nonetheless, the Te-based metallicity estimates presented in Table 3 have excellent agreement with the low metallicities implied from the comparison to the MAPPINGS models in Figures 4 and 5.

Table 3

| ID   | Redshift | log(M*/M⊙) | log(Te/K) | log(O/He)+12 |
|------|----------|------------|-----------|--------------|
| 4590 | 8.4957   | 7.10 ± 0.12 | 4.37 ± 0.07 | 7.49 ± 0.26  |
| 5144 | 6.3792   | 7.39 ± 0.04 | 4.18 ± 0.04 | 7.87 ± 0.17  |
| 6355 | 7.6651   | 8.23 ± 0.09 | 4.09 ± 0.05 | 8.10 ± 0.17  |
| 10612| 7.6597   | 7.72 ± 0.05 | 4.23 ± 0.04 | 7.75 ± 0.19  |

Note. Stellar masses are from Carnall et al. (2023). Error bars indicate 1σ uncertainties, and for metallicity include the calibration uncertainty associated with the Te-based relationship.

53 Nicholls et al. (2020) and Pérez-Montero et al. (2021) use different atomic data sets, those of Lennon & Burke (1994) and Storey et al. (2014), respectively, but the two data sets are very similar, with only minor differences that are much smaller than the observational uncertainties for the lines used in this work.
metallicity predictions of galaxies at $z = 7$ in the FLARES simulations (Lovell et al. 2021).

At fixed stellar mass, the metallicities of our $z > 6$ galaxies are generally consistent with the metallicities of auranor-[O III]-selected galaxies of similar (log($M_*/M_\odot$) < 9) stellar mass at $z \approx 2.5$. The $z > 6$ galaxies are also consistent with the stacked $z \approx 2$ strong-line metallicity measurements of Henry et al. (2021) and with a low-mass extrapolation of the $z \approx 1.9$ mass–metallicity relationship of Papovich et al. (2022). However the large stellar mass uncertainties of our $z > 6$ galaxies mean that they are also broadly consistent with slightly lower metallicities at fixed stellar mass compared to the lower-redshift samples.

The broad distribution of mass and metallicity among the $z > 6$ sample is also notable. The galaxy with the highest metallicity (12 + log(O/H) = 8.1 for ID 6355) has very bright emission lines, implying a very high star formation rate. This galaxy also has a clumpy and extended morphology that is suggestive of a merger (Carnall et al. 2023). The other three $z > 6$ galaxies all have lower metallicities and lower stellar masses, with ID 4590 at $z = 8.5$ having the lowest metallicity and lowest stellar mass of the sample. It is interesting to measure such diversity in chemical enrichment and mass assembly in the early universe among our limited sample of $z > 6$ galaxies.

5. Conclusions

We use JWST/NIRSpec spectroscopy from the SMACS 0723 Early Release Observations to study the physical conditions of the ISM in five galaxies at $z > 5$. We identify several caveats in the current (v1.8.2) reduction pipeline, including uncertain absolute flux calibration, too-wide spectral extractions, and underestimated uncertainties. We mitigate these issues using a custom spectral extraction, as described in detail in Section 2.2. We caution against use of NIRSpec observations that require absolute spectrophotometry or accurate continuum detection, such as equivalent widths and comparisons of lines widely separated in wavelength, especially if using the standard (v1.8.2) pipeline products. However, we find that the relative flux calibration is reliable, as determined by the stability of measured line ratios in different visits and by a measured [O III]λ5008/[O III]λ4960 = 3 for all galaxies.

We measure the ratios of rest-frame optical emission lines that are closely separated in wavelength, including [Ne III]λ3870/[O III]λ3728, [O III]λ4364/Hγ, and [O III]λ5008/Hβ. Compared to lower-redshift ($z \approx 3$) galaxies, the $z > 5$ galaxies have similar [O III]λ5008/Hβ, similar [O III]λ4364/Hγ, and $\sim 0.5$ dex higher [Ne III]λ3870/[O III]λ3728. The $z > 5$ emission-line ratios are generally well described by MAPPING V photoionization models for an ISM that has very high ionization (log($Q_z$) ≳ 8.9), very high pressure (log($P/k$) ≳ 8.9), and low metallicity ($Z/Z_\odot \lesssim 0.2$).

The [O III]λ4364/Hγ and [O III]λ5008/Hβ emission-line ratios indicate very high electron temperatures of 4.1 < log($T_e/K$) < 4.4 in the four $z > 6$ galaxies. We use these electron temperatures to estimate $T_e$-based nebular metallicities of 7.5 < 12 + log(O/H) < 8.1 ($Z/Z_\odot \lesssim 0.2$) in the 4 $z > 6$ galaxies. Using stellar masses published in other work, we present a mass–metallicity diagram that compares the $z > 6$ galaxies with lower-redshift samples and with theoretical simulations. The $z > 6$ metallicities are broadly consistent with $z \approx 2$ galaxies of similar stellar mass, although our interpretation is limited by highly uncertain stellar masses.

These measurements demonstrate the impressive capability of JWST spectroscopy for understanding the physical conditions of the gas in galaxies at cosmic dawn. We look forward to upcoming JWST observations of larger samples of galaxies that will further probe the assembly and chemical enrichment of the first galaxies in the universe.

The authors are enormously grateful to all of the people who designed, built, launched, deployed, and commissioned the James Webb Space Telescope. The observations from this spacecraft are truly incredible and awe-inspiring.

This work is based on observations made with the NASA/ESA/CSA James Webb Space Telescope. The data were obtained from the Mikulski Archive for Space Telescopes at the Space Telescope Science Institute, which is operated by the Association of Universities for Research in Astronomy, Inc., under NASA contract NAS 5-03127 for JWST. These observations are associated with program No. 2736. The authors acknowledge the ERO team for developing their observing program with a zero-exclusive-access period.

The CEERS team thanks Pierre Ferruit and the NIRSpec GTO team for providing NIRSpec IPS simulated data and for general good counsel, and the STScI NIRSpec instrument team for extensive assistance regarding the JWST Pipeline and data simulations.

This work is supported by NASA grants JWST-ERS-01345 and JWST-AR-01721. J.R.T. and B.E.B. additionally acknowledge support from NSF grant CAREER-1945546. R.C.S. acknowledges support from Fondecy Regular 1202007. P.G.P.-G. acknowledges support from grant PGC2018-093499-B-I00 funded by MCI/DEI/10.13039/501100011033. A.Y. is supported by an appointment to the NASA Postdoctoral Program (NPP) at NASA Goddard Space Flight Center, administered by Oak Ridge Associated Universities under contract with NASA.
